

Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study

Yamina Bouzidi, Lotfi Belkhiri, Michel Ephritikhine, Jean-François Halet, Abdou Boucekkine

▶ To cite this version:

Yamina Bouzidi, Lotfi Belkhiri, Michel Ephritikhine, Jean-François Halet, Abdou Boucekkine. Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study. Journal of Organometallic Chemistry, 2017, 847, pp.82-89. 10.1016/j.jorganchem.2017.03.002 . cea-01487700

HAL Id: cea-01487700 https://cea.hal.science/cea-01487700

Submitted on 2 Oct 2017

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés. ED MAN



Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study

Yamina Bouzidi ^{a,b}, Lotfi Belkhiri ^{b,*}, Michel Ephritikhine ^c, Jean-François Halet ^{d,*}, and Abdou Boucekkine ^{d,*}

 ^a Département de Chimie, Université de Batna 1, 05000 Batna, Algeria
 ^b URCHEMS, Département de Chimie, Université des Frères Mentouri Constantine 1, 25017 Constantine, Algeria
 ^c NIMBE, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France
 ^d Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - Université de Rennes 1, 35042 Rennes Cedex, France

ABSTRACT

The chemistry of cyanide complexes of the *f*-elements has witnessed significant recent advances, showing in particular the remarkable ability of the cyanide ligand to stabilize uranium compounds in their +3 to +6 oxidation states and its capacity to adopt two distinct ligation modes, namely cyanide M–CN or isocyanide M–NC, towards trivalent f-ions. Here, we have theoretically investigated the tris(cyanide) complexes $[ML_2X_3]^{2-}(M = Ce^{3+}, U^{3+}; L =$ C_5H_4Me , N(SiMe₃)₂; X = CN, NC), using relativistic DFT computations, focusing on cvanide (CN⁻) and isocyanide (NC⁻) coordination competition and differences between their electronic structures. X-ray crystal data reveal distinct coordination modes of the CN ligand towards uranium and cerium metal centers. Interestingly, in the case of the cerium complexes, and contrarily to the uranium ones, the coordination mode of the cyanide ligand depends on the co-ligand L attached to the metal. The observed coordination in these tris(cyanide) complexes is driven by the binding energies of the CN⁻/NC⁻ ligands to the metals. The solvent is shown to play a determining role for the chosen coordination. The developed methodology can help to confirm the cyanide or isocyanide coordination mode when X-ray crystal data are not conclusive or to predict the configuration of a complex to be synthesized. Another application is in the field of lanthanide(III)/actinide(III) differentiation.

Keywords: Cyanide, *f*-complexes, Ln(III)/An(III) differentiation, CN-coordination isomerism, DFT calculations, solvation effects

* Corresponding authors. E-mail address: lotfi.belkhiri@umc.edu.dz (L. Belkhiri), halet@univ-rennes1.fr (J.-F. Halet), abdou.boucekkine@univ-rennes1.fr (A. Boucekkine)

Dedicated to our good friend and colleague John Gladysz on the occasion of his 65th Birthday.

1. Introduction

Since the first synthesis of *f*-element cyanide complexes in the early seventies [1], the cyanide CN^{-} ligand has gained a prominent position in both *d*- and *f*-coordination chemistry mainly because of its strong coordinating ability, its capacity to stabilize a wide range of oxidation states and to adopt different ligation modes, thus giving a rich variety of homo and heteropolynuclear compounds with interesting stereochemistry and properties [2]. This is attributed to the strong σ -donor character of the cyanide and isocyanide ligands, *via* donation from either the C-localized orbital of CN^{-} (carbon lone pair) or the N-localized one of NC⁻ with nitrogen major character [2b]. Therefore, this field is currently attracting attention in various domains, especially in *d*-metal coordination chemistry, with applications in biology and materials science, exemplified with the discovery of molecular-based assemblies with cyanide bridges, giving magnetic materials and providing significant insights into magneto-structural correlations [3].

However, *f*-element cyanide complexes have received much less attention, while the lanthanide and actinide chemistry experienced a spectacular development during the last decades [4,5]. Indeed, the different binding modes of cyanide or isocyanide CN^-/NC^- anions towards trivalent *f*-ions was reported recently, revealing a potential application in lanthanide(III)/actinide(III) differentiation [5a,6,7]. Thus, a number of mono and polycyanide complexes of cerium and uranium have been isolated and crystallographically characterized, starting from the metallocene complexes $[M(Cp^*)_2(CN)_3]^{2-}$ (M = Ce, U; Cp* = C₅Me₅) which were the first trivalent molecular polycyanide compounds of an *f*-element to have been structurally characterized [2b], followed by the successive syntheses of the mononuclear $[MN^*_3(CN)]^-$, $[MN^*_3(CN)_2]^{2-}$, $[MN^*_2(CN)_3]^{2-}$ and cyanido-bridged dinuclear $[(MN^*_3)_2(\mu-CN)]^-$ (M = Ce, U; N* = N(SiMe_3)_2) anionic compounds [2a]. It is worth noting that the bis(silylamide) ligand N* seems to play a crucial role in stabilizing these polycyanide complexes. It was observed in these latter species that the cerium(III) complexes are

isomorphous but not isostructural to their uranium(III) counterparts because of the distinct cyanide or isocyanide M–CN/NC linkage in the crystal. This striking difference between the cyanide and isocyanide ligation modes in the uranium and cerium compounds was tentatively explained by the fact that the U(III) ion is softer than the Ce(III) ion in the *hard and soft* (*Lewis*) acids and bases (HSAB) classification and will have a greater affinity for the softer carbon end of the CN ligand [2b].

Synergetic studies at both experimental and theoretical levels were carried out investigating the fundamental chemical differences between the 4*f* elements, lanthanides (Ln), and the 5*f* elements, actinides (An), in this field [8-10]. In particular, the coordination competition between cyanide (CN⁻) and isocyanide (NC⁻) has been studied theoretically in the case of uranyl derivatives [2b, 8, 9], and also for pentacyanide and isocyanide complexes of (IV), U(V) and U(VI) of general formula $[X_2U(CN)_5]^{q-}$ (X = O, Cp = C₅H₅) [2b,8]. Indeed, it has been shown that cyanide coordination is preferred, although the isocyanide form is also a stable configuration [8]. Two structurally stable structures have been predicted with cyanide linkage mode for the $[UO_2(CN)_5]^{4-}$ and $[Cp_2U(CN)_5]^{-}$ uranyl and Cp-type systems.

In this context, we reported recently a theoretical study on the preferential ligation modes of the cyanide and isocyanide ligands in the Ce(III)/U(III) bis(cyanide) $[MN*_3(CN)_2]^{2-}$ complexes [10a]. Based on X-ray data and computational DFT analysis, the preference in M–CN/NC ligation modes has been rationalized by considering the electronic structures and the ligand-to-metal binding energies. Specifically, it has been found that the stronger σ donating ability of the cyanide ligand toward uranium and not cerium is related to the better energy matching between 6d/5f uranium metal and ligand orbitals [11]. The same observation has been made in the case of U(III) and U(IV) bis(silylamide) mono and bis(cyanide) complexes $[UN*_3X]^{q-}$ and $[UN*_3X_2]^{q-}$ (q = 2, 1; X = CN, NC), the covalency contribution to the bonding being also at work (orbital mixing) [10b].

Although the cyanide M–CN ligation mode is ubiquitous for various uranium complexes in different oxidation states (III-VI) [12], the preference for cyanide or isocyanide coordination could remain controversial for some systems. Indeed, as noted by previous theoretical studies [8,9], controversy still exists about the preference for the C or N coordination in the case of uranyl ion derivatives, where the cyanide complexes might be more stable than their isocyanide congeners, noting that the energy difference is only 3.3 kcal.mol⁻¹ [9c].

In the present study, we have investigated using relativistic density functional theory (DFT), the electronic structures of several analogous tris(cyanide) complexes of cerium(III) and uranium(III), with different cyanide and isocyanide ligation modes. The target systems are the bis(cyclopentadienyl) and bis(silylamide) tris(cyanide) compounds $[M(Cp^*)_2(CN)_3]^{2^-}$ and $[MN^*_2(CN)_3]^{2^-}$ (M = Ce, U), which have been synthesized recently and crystallographically characterized [10a]. Unexpected coordination modes have been observed. For the bis(cyclopentadienyl) complexes, the X-ray crystal structures show the unambiguous M–C bonding mode of the CN ion. On the contrary, the observed structures of the bis(silylamide) Ce(III) and U(III) complexes exhibit distinct coordination modes of the cyanide CN ligand, through the N or C atom to the Ce(III) or U(III) ions, respectively. Our aim is to rationalize these particular coordinations, especially in the context of Ln(III)/An(III) differentiation.

2. Results and discussion

"The determining factor (*vide infra*) leading to the M-CN or M-NC coordination mode is the binding energy between the metal fragment and the CN or NC ligand [10a,b]. As shown below, these binding energies differences between isomers range from *ca*. 4 to 14 kcal/mol, except for the $[UN*_2X_3]^{2-}$ case for which these binding energies differences are much smaller.

2.1. DFT molecular geometry optimization of the tris(cyanide) complexes

We consider the actual complexes of general formula $[ML_2X_3]^{2-}$ (M = Ce³⁺/U³⁺; L = Cp*/N* and X = CN/NC) and their hypothetical isomers. All structures were fully optimized using the BP86 functional coupled to the polarized double- ζ Slater basis set (DZP) in the framework of the relativistic zeroth-order regular approximation (ZORA). The solvent (THF) was treated using the COSMO solvation model, implemented in the ADF program (see Computational details). As previously stated [13,14], ZORA/BP86/DZP computed geometries of *f*-elements complexes are generally in good agreement with X-ray crystal structures. Computed bond lengths M–X, M–L (L = Cp* and N*) and C–N/N–C of the optimized structures (Fig. 1 and 2) are reported in Table 1 for the actual complexes [MCp*₂(CN)₃]^{q-} (M = Ce³⁺, U^{3+/4+}; q = 2, 1) (**1a**) and (**1b**) (complexes **6** and **5** in ref. 2b) , and their hypothetical isomers [MCp*₂(NC)₃]^{q-} (**2a**) and cyanide uranium(III) [UN*₂(CN)₃]²⁻ (**2b**) complexes (respectively

complexes **4a** and **4b** in reference 10a) and their hypothetical isomers, are also given in Table 1.



Fig. 1. ZORA/BP86/DZP optimized geometry of the bis(cyclopentadienyl) tris(cyanide) $[MCp*_2X_3]^{2-}$ complexes (M = Ce³⁺, U³⁺; X = CN) **1a** (left) and **1b** (right). The blue, black, and white spheres are nitrogen, carbon, and hydrogen atoms, respectively.



Fig. 2. ZORA/BP86/DZP optimized structures of the bis(silylamide) tris(cyanide/isocyanide) complexes $[MN*_2X_3]^{2-}$ complexes (M = Ce³⁺, U³⁺; X = CN, NC), **2a** (left) and **2b** (right). The orange, blue, black, and white spheres are silicon, nitrogen, carbon, and hydrogen atoms, respectively.

The computed geometries of the actual $[MCp*_2(CN)_3]^{2-}$ Ce^{III}–CN and U^{III/IV}–CN compounds are in good agreement with the available X-ray data, noting however a slight discrepancy of *ca*. 0.06 Å for the metal-ligand bond distance in the case of the bis(silylamide) Ce^{III}–NC derivtive (Table 1). This good agreement shows once again the reliability of the ZORA/BP86/DZP method in computing molecular *f*-complex geometries. Notably, the

shortening of the metal-ligand bond distances when going from U(III) to U(IV), in line with uranium ionic radii variation [15], is well predicted by computation.

Table 1

Relevant optimized averaged metal-ligand bond distances (Å) at the ZORA/BP86/DZP level and X-Ray data where available (in bold) for the $[ML_2X_3]^{q-}$ complexes (M = Ce³⁺, U³⁺ and U⁴⁺; X = CN/NC; L = Cp*/N*; q = 2, 1) in the gas phase and in solution (in italics).

Complex	<m-c n=""></m-c>	Δ (Å) ^a	<c-n n-c=""></c-n>	<m-l></m-l>
$[\mathbf{MCp}^*_2\mathbf{X}_3]^{\mathbf{q}}$				Q
Ce ³⁺	2.665/2.535 2.655/2.546 2.666/-		1.178/1.182 <i>1.176/1.177</i> 1.158/ -	2.621/2.638 2.586/2.583 2.562/ -
U ³⁺	2.612/2.492 2.585/2.489 2.640/ -	0.053/0.043 0.070/0.057	1.178/1.183 <i>1.177/1.180</i> 1.156/ -	2.571/2.560 2.509/2.534 2.534/ -
U^{4+}	2.501/2.389 2.520/2.424 2.520/ -		1.175/1.185 1.176/1.180 1.158/ -	2.482/2.507 2.476/2.493 2.446 / -
$[MN_{2}^{*}X_{3}]^{q}$			Y	
Ce ³⁺	2.666/2.511 2.657/2.523 - /2.580	Ar	1.176/1.183 <i>1.175/1.179</i> - /1.164	2.413/2.427 2.379/2.387 - /2.390
U ³⁺	2.605/2.462 2.593/2.472 2.600/ -	0.061/0.049 0.064/0.051	1.178/1.185 <i>1.176/1.181</i> 1.148/ -	2.377/2.394/ 2.348/2.358 2.334/ -
U^{4+}	2.512/2.374 2.543/2.416		1.175/1.186 <i>1.175/1.182</i> -	2.239/2.253 2.198/2.220 -

^a Metric difference between Ce–C/N and U–C/N bond distances.

It is worth noting that the comparison between the two Ce(III) and U(III) analogous complexes $[MCp*_2(CN)_3]^{2^-}$ in Table 1 reveals a significant shortening of the computed metalligand bond distances when going from the cerium to the uranium species. Indeed, the M–CN bond distances in the $[MCp*_2(CN)_3]^{2^-}$ gas phase species are equal to 2.665 for Ce *vs.* 2.612 Å for U, and 2.535 *vs.* 2.492 Å for the corresponding M–NC ones in $[MCp*_2(NC)_3]^{2^-}$. This bond length shortening is also observed for the solvated species with a greater contraction of the U(III)–CN/NC bond distances comparatively to the Ce(III) species. The metric difference Δ between the Ce–C/N and U–C/N bond distances computed at the ZORA/BP86/DZP level is predicted to be larger for the cyanide CN than for the isocyanide NC ligand (0.053 *vs.* 0.043)

Å), which is slightly amplified by solvation (0.070 *vs.* 0.057 Å), suggesting that the former, *i.e.*, the cyanide form, leads to a more covalent bonding than the isocyanide one. These features illustrate the distinct coordination modes of these two ligands towards the Ce(III) and U(III) ions, as experimentally observed.

The U–CN/NC bond length shortening relatively to Ce–CN/NC is also observed for the U– L (L = Cp* and N*) coordination. Moreover, no significant difference is computed for C– N/N–C distances when moving from Ce(III) to U(III) complexes, suggesting that no M \rightarrow X π back-donation occurs, and that the M–X bond is essentially σ in character. The electronic structure analysis will shed light on these points.

2.2. Electronic structures of the tris(cyanide) complexes

As reported previously for the bis(cyanide) compounds $[MN*_3X_2]^{2-}$ (M = Ce^{III} and U^{III}, X = C–N/N–C) [10a], the better energy matching of the C-localized σ lone pair orbital of the cyanide ligand with the U^{III}(5 f^2) metal-based orbitals makes it a much more effective donor than the N-localized σ orbital, which is much lower in energy [9]. This feature was also reported to explain the cyanide U(III)–CN and isocyanide U(IV)–NC coordination mode in the [UN*₃X₂]^{2-/1-} complexes [10b]. To investigate further the electronic structure and metal-ligand bonding, natural bond order/natural population analyses (NBO/NPA) [16a] (see Appendix A, computational details) were performed on the optimized geometries of the cyanide and isocyanide systems at the ZORA/BP86/DZP level. The NPA approach proved to probe the covalency in *f*-element complexes with results in better agreement with experimental trends [16b,c,d] than the Mulliken population analysis (MPA) [16e], especially in the context of lanthanide(III)/actinide(III) differentiation [10,11,16f].

NPA results for the complexes $[ML_2X_3]^{2-}$ (M = Ce³⁺, U³⁺; L = Cp*/N*; X = CN/NC) under consideration are given in Table 2. Natural metal (q_M), carbon and nitrogen atomic net charges as well as the metallic spin population ρ_M are reported. ρ_M is computed to be the difference between the total α and β spin electronic populations. In the case of the bis(cyclopentadienyl) MCp*₂(CN)₃ complexes, examination of the NPA results (Table 2) indicates a small difference between the metal natural charges (q_M) for the cyanide M–CN and isocyanide M–NC complexes (+1.53/+1.74) for Ce³⁺ and (+0.73/+1.03 for U³⁺) which are consistent with the slightly stronger σ -donation of the cyanide ligand to the U(III) ion, since

the ligand-to-metal donation is stronger when the positive metallic net charge becomes smaller, in agreement with previous findings [10a]. This difference becomes more pronounced when the two Ce(III)/U(III)–X systems are compared (namely +1.53 for cerium vs. +0.73 for uranium, in the case of a CN coordination), which could account for Ce(III)/U(III) differentiation. In the case of the bis(silylamide) MN_2^* complexes, the metal natural charge (q_M) for the cyanide U–CN is lower than for the isocyanide U–NC (namely +1.30 vs. +1.54) indicating a stronger ligand-to-metal donation, and it is also lower than for the cyanide Ce–CN ones (*i.e.*, +1.71) consistent with the U–CN/NC bond length shortening relatively to Ce–CN/NC. It is noteworthy that solvation effects do not modify the trends observed for the isolated complexes.

Table 2

ZORA/BP86/DZP NPA results for the $[MCp*_2X_3]^2$	$(M^{*}_{2}X_{3})^{2}$ (M = Ce ³⁺ , U ³⁺ , X =
CN/NC) complexes in the gas phase and in solution	n (in italics).

M–(CN/NC)	NPA spin populati	on	NPA net charge				
Structure	$ ho_{ m M}$	$q_{\rm M}$	<c-n></c-n>	<n-c></n-c>			
_		$[MCp*_{2}X_{3}]^{2-}$	-				
Ce(III)	0.989/0.993	+1.53/+1.74	-0.12: -0.57	-0.81: +0.04			
	0.985/0.981	+1.49/+1.72	-0.28: -0.63	-0.76: -0.01			
U(III)	2.913/2.898	+0.73/+1.03	-0.23: -0.56	-0.71: +0.05			
	2.874/2.873	+0.56/+1.01	+0.05: -0.63	-0.66: -0.04			
		$[MN_{2}X_{3}]^{2-}$					
Ce(III)	1.019/1.018	+1.71/+1.88	-0.17: -0.54	-0.85: +0.09			
	1.003/1.016	+1.66/+1.86	-0.11: -0.61	-0.80: +0.02			
U(III)	2.949/2.921	+1.30/+1.54	-0.11: -0.53	-0.85: +0.10			
	2.929/2.901	+1.23/+1.50	-0.04: -0.59	-0.70: +0.03			

Comparison of the charge distribution on the C–N coordination reveals a slightly but significantly lower C cyanide natural charge in U(III) than in Ce(III) species, especially for the bis(silylamide) MN₂* complexes (e.g., -0.11 vs. -0.17), which sustains its stronger σ -donation for the actinide system (in vacuum). These trends seem to be amplified by solvation, since the negative net charge borne by the C cyanide in the U(III) system decreases significantly (-0.11 vs. -0.04), sustaining its stronger σ -donation towards the actinide ion. Interestingly, the total charges of the C–N moiety in the case of Ce(III) and U(III) cyanide coordination are equal to -0.69 vs. -0.79 for the MCp*₂ complexes and -0.71 vs. -0.64 for

the MN₂* ones, respectively. Similarly, the total charges of the N–C isocyanide for the Ce(III) and U(III) systems, equal to -0.77 vs. -0.66 and -0.76 vs. -0.75 for the two MCp*₂ and MN₂* systems, respectively, show that the isocyanide donation ability is similar in the bis(silylamide) complexes. Thus, it seems that the stronger C cyanide covalent bonding towards UN₂* moieties contributes to the chosen coordination mode of this species. The covalent factors, presumably slight, likely to originate mainly from the cyanide and/or isocyanide σ -donation abilities and the better energy matching between metallic orbitals d/f and ligand orbitals, are responsible for the Ce(III)/U(III) differentiation, this point being supported by bond order (BO) calculations. To further assess these electronic factors, *i.e.*, the ionic and/or covalent contribution to the cyanide/isocyanide coordination preference, the Nalewajski-Mrozek (NM) bond indices [17a,b] and Mayer bond orders [17c] for the M–CN/NC and C–N/N–C bonds were computed and are reported in Table 3.

Table 3

ZORA/BP86/DZP Mayer bond orders and Nalewajski–Mrozek (NM) bond indices for the $[ML_2X_3]^{2-}$ (M = Ce³⁺, U³⁺; L = Cp*, N*; X = CN/NC) complexes in the gas phase and in solution (in italics).

Compound		M–(CN/NC)	Mayer b	ond order	NM bo	NM bond index		
		(Å)	<m–c n=""></m–c>	<c-n n-c=""></c-n>	<mc n=""></mc>	<cn nc=""></cn>		
$[MCp*_{2}X_{3}]^{2-}$	Ce(III)	2.665/2.535	0.447/0.387	2.814/2.665	0.695/0.642	3.165/3.114		
		2.655/2.546	0.431/0.361	2.835/2.755	0.687/0.612	3.168/3.156		
	U(III)	2.612/2.492	0.529/0.466	2.759/2.624	0.837/0.801	3.117/3.059		
		2.585/2.489	0.530/0.445	2.780/2.712	0.859/0.785	3.100/3.054		
$[MN*_2X_3]^{2-}$	Ce(III)	2.666/2.511	0.440/0.396	2.829/2.633	0.838/0.952	3.192/3.109		
		2.657/2.523	0.426/0.364	2.841/2.723	0.796/0.894	3.190/3.152		
	U(III)	2.605/2.462	0.540/0.491	2.777/2.585	0.885/0.868	3.130/3.043		
		2.593/2.472	0.532/0.467	2.790/2.670	0.882/0.830	3.123/3.078		

As expected, the NM approach, which accounts for both ionic and covalent contributions, gives greater metal-ligand bond orders, up to two times, than Mayer ones which essentially takes into account covalent contributions. It is noteworthy that NM and Mayer analyses give larger M–CN/NC BOs for uranium complexes than for their cerium congeners, correlating well with structural features and NPA results. For the C–N/N–C bonds, the covalent character is high, so that the NM and Mayer indices get closer. It is worth noting that for all systems, Mayer analysis, consistently gives M–C cyanide bond orders higher than M–N isocyanide ones, *e.g.* 0.447 *vs.* 0.387 and 0.529 *vs.* 0.446 for CeCp*₂ and UCp*₂ systems, respectively.

These trends, namely higher BOs for M–C cyanide than for isocyanide M–N coordination, are corroborated by the NM results for the bis(cyclopentadienyl) MCp*₂ systems. On the other hand, this is the opposite is computed for the bis(silylamide) MN*₂ species. Indeed, the isocyanide Ce–N NM is predicted to be higher than the Ce–C cyanide one (0.952 *vs.* 0. 838) in the CeN*₂ system, whereas the opposite is computed for the UN*₂ congeners, the U–C NM being slightly but significantly higher than the U–N one (0.885 *vs.* 0.868), in accordance with the experimental observation. The NM approach correlates well with the experimental structural data and as stated recently by other works, [10,17d] appears to be more reliable because it both accounts for ionic and covalent contribution. Notably, the slight difference between the cyanide M–C and isocyanide M–N Nalewajski-Mrozek BOs reflects the subtle balance between the ionic/covalent contributions in their coordination preference. It is noteworthy that the computed COSMO/THF results performed to take account of the solvation species in solution are in line with the gas phase ones and confirm the crucial role of the bis(silylamide) MN*₂ co-ligand in the Ln(III)/An(III) differentiation.

2.3. Molecular orbital (MO) analysis of the tris(cyanide) complexes

MO frontier diagrams of the trivalent complexes $[ML_2X_3]^{2-}$ (M = Ce³⁺ or U³⁺; L = Cp* or N*; X = CN/NC) are given in Fig. 3 and 4. For the sake of simplicity, only α spin-MOs are shown. Different sets of MOs appear. For all cyanide and isocyanide complexes, the diagrams show that the highest occupied α spin-orbitals, *i.e.*, the SOMO, SOMO-1 and SOMO-2 in U(III) (f^3) complexes and the SOMO in the Ce(III) (f^4) counterpart are essentially metallic in character, with a strong f orbital contribution. In the case of the U(III) systems, a weak cyanide or isocyanide ligand contribution of *ca*. 4% is observed in the SOMOs. However, neither presence of metal-to-ligand π back-donation nor π interaction appears between the metal center and the cyanide or isocyanide ligands, since the participation of the C-localized orbital of CN⁻ or N-localized orbital of NC⁻ is null. This confirms the fact that these ligands remain mainly σ donors in character in these species.



Fig. 3. ZORA/BP86/DZP α spin-MO diagram for M–CN (left) and M–NC (right) $[MCp*_2X_3]^{2-}$ (X = CN/NC) complexes (C_2 symmetry). From the left to the right, the M *d*, M *f*, ML₂, and X₃ percentage contributions are given in brackets. Contour values are ±0.03 (e/bohr³)^{1/2}.

More interestingly, the sets of occupied M–CN/NC MOs, deeper in energy, exhibit mainly the σ donation character of the CN or NC ligand. First of all, the comparison of the electronic structure of the cyanide U–CN and Ce–CN compounds with that of their isocyanide congeners in the [MCp*₂X₃]^{2–} complexes (Fig. 3), reveals that the metal *d/f* orbitals weight is slightly larger for the cyanide M–CN complexes than for their M–NC analogues, as it can be seen in the σ -donating 62a, 63a, 57b and 70a, 71a, 65b MOs, namely 7.2–18.4 *vs.* 11.1– 14.4 % for Ce–CN and U–CN, respectively. This weight is reduced to 3.0–7.4 *vs.* 4.8–8.4 % for Ce–NC and U–NC, respectively, for the same MO bonding sets. It is worth noting that the 6*d*/5*f* actinide orbitals both contribute more significantly to the U–CN bonding. This is in agreement with the coordination preference of uranium.

Moving back to the bis(silylamide) MN*₂ systems, the MO diagram of Fig. 4 shows that the metal d/f orbitals contributions within the bonding σ -donating pair U–CN/NC, *i.e.*, 151a, 152a MOs are in the range 9.8–21.5 vs. 1.7–9.0% for U–CN and U–NC, respectively, in line with NM bond orders and NPA analyses discussed above, and correlating well with the observed cyanide UN*₂–CN coordination. Furthermore, these bonding σ -donating pairs, *i.e.*, 151a, 152a MOs, are slightly lower in energy for the U–CN coordination than for the hypothetical U–NC one, namely –0.90 and –1.12 vs. –0.61 and –0.80 eV, respectively, sustaining the stronger interaction between the 6d/5f U(III) orbitals and C-cyanide ones due to a better energy matching [11].



Fig. 4. ZORA/BP86/DZP α spin-MO diagram for M–CN (left) and M–NC (right) $[MN*_2X_3]^{2-}$ (X = CN/NC) complexes (C_1 symmetry). From the left to the right, the M d, M f, ML₂, and X₃ percentage contributions are given in brackets. Contour values are ±0.03 $(e/bohr^3)^{1/2}$.

Considering the bis(silylamide) Ce–CN/NC pair, as shown by the MO analysis (Fig. 4), the 135a and 136a MOs exhibit metal contributions of 19.0 and 7.5 % *vs*. 7.4 and 1.8 % mainly 5*d* orbitals, for Ce–CN and Ce–NC bonding, respectively. Moreover, the Ce–CN bonding levels are slightly lower in energy than the Ce–NC congeners (*i.e.*, –0.87 and –1.09 *vs*. –0.62 and –0.70 eV, respectively) and the small gap between the SOMO and the Ce–CN/NC pair σ -donating MOs (3.33 *vs*. 3.11 eV) suggest that the preferred CN/NC coordination is, in this case, under ionic or/and covalent subtle control, as noted by NPA and NM bond orders analysis (see above Tables 2 and 3).

As shown by the MO analysis (Fig. 3 and 4), the isocyanide M–NC interaction seems to be weaker than the cyanide M–CN interaction, as corroborated by metallic percentages in bonding M–CN/NC MOs, which are greater in the latter. This could explain the energy stability difference between the cyanide and isocyanide systems and the coordination mode preference to the uranium(III) and cerium(III) centers.

As indicated by the electronic structure and MO analysis, the variations in structural and bonding parameters of the considered complexes could be explained by the σ -donating abilities of the cyanide and isocyanide ligands and the occurrence of a higher covalent character of the bonding in the case of the U(III) complexes. However, even though structural parameters and electronic factors can account for the latter effects [18], they cannot always

permit to differentiate the CN/NC coordination mode preference for actinide(III) and lanthanide(III) systems in terms of their relative stabilities, as recently noted [10a].

The chosen coordination mode is mainly driven by a good match between the energies of the metal AOs within the MCp*₂ and MN*₂ fragments, and the carbon or nitrogen lone pair energies of the cyanide ligand. The energies of the metal orbitals involved in bonding with the cyanide ligand are lower by *ca.* 1 eV for the CeN*₂ fragment relatively to CeCp*₂. Let us remind that the nitrogen lone pair of the cyanide ligand is lower in energy than the carbon lone pair. This result would explain why in the cerium compounds the cyanide coordination is observed with the Cp*₂ co-ligands and the isocyanide with the N*₂ ones. On the contrary, the cyanide coordination in the case of the uranium complexes is not uniquely driven by this sole factor, since it is observed for the two complexes under consideration. The investigation of the bonding energies is required to clarify this issue.

2.4. Energy decomposition analysis

In order to get some additional information on the energy factors driving the preferred coordination of the cyanide or isocyanide ligands to the cerium or uranium atoms in the actual $[ML_2X_3]^{2-}$ complexes (M = Ce³⁺ or U³⁺; L = Cp* or N*; X = CN/NC) and their hypothetical isomers, an energy decomposition analysis was carried out (see Appendix A, computational details). The bonding energies of the ligands to the metal centers were calculated according to the following fragmentation scheme:

$$[ML_2]^+ + 3 X^- \rightarrow [ML_2X_3]^{2-} (L = Cp^* \text{ or } N^*; X = CN \text{ or } NC)$$

These total bonding energies (TBE_{frag}) computed at the spin unrestricted ZORA/BP86/DZP level (see Appendix) are given in Table 4.

Table 4

Energy decomposition analysis at the ZORA/BP86/DZP level for the complexes $[ML_2X_3]^{2-}$ (M = Ce³⁺ or U³⁺; L = Cp* or N*; X = CN(left)/NC(right)) in the gas phase and in solution (in italics).

ion	$E_{\text{Pauli}} (\text{eV})$	$E_{\rm elstat}({\rm eV})$	$E_{\rm st}({\rm eV})$	$E_{\rm orb}({\rm eV})$	$E_{\rm solvat}({ m eV})$	TBE _{frag} (eV)	ΔE (kcal/mol)
Ce ³⁺	6.001/6.314	-16.928/-16.225	-10.927/-9.910	-6.700/-7.257	-	-17.628/-17.186	0.0/10.1

	5.856/6.011	-16.265/-16.286	-10.409/-10.275	-6.852/-6.713	-4.651/-4.629	-21.885/-21.589	0.0/6.8
U ³⁺	7.788/8.383	-17.873/-17.869	-10.084/-9.485	-7.945/-8.209	-	-18.030/-17.695	0.0/7.7
U	8.209/8.369	-18.001/-17.868	-9.791/-9.498	-8.276/-8.099	-4.637/-4.572	-22.677/-22.142	0.0/12.3
			[MN*2	${}_{2}X_{3}]^{2}$			
Ce ³⁺	5.703/6.297	-16.935/-17.821	-11.231/-11.523	-7.143/-7.458	-	-18.375/-18.981	13.9/0.0
Ct.	5.599/5.865	-17.319/-17.635	-11.719/-11.769	-6.719/-6.943	-4.506/-4.405	-22.915/-23.087	4.0/0.0
T1 ³⁺	8.247/8.874	-18.634/-18.916	-10.387/-10.041	-8.439/-8.849	-	-18.826/-18.891	1.5/0.0
U	7.943/8.369	-18.619/-18.851	-10.676/-10.489	-8.107/-8.300	-4.458/-4.381	-23.212/-23.132	0.0/1.8

Considering first the computed energy for isolated complexes (namely in vacuum), it can be seen that the TBE_{frag} for the cyanide M–CN coordination of the MCp*₂ complexes are significantly higher (in absolute value) than the isocyanide M–NC ones, as shown by their relative stability ΔE , in agreement with the experimental observation, *i.e.*, the actual structures. We note that for the MN*₂ complexes, the most stable species is correctly predicted for the isocyanide Ce–NC species but not for the cyanide U–CN species. Indeed, the relative stability given by ΔE clearly highlights the difference in M–CN/NC coordination between the Ce(III) and U(III) ions, in agreement with the experimental findings, except for the UN*₂ complex, where ΔE in vacuum indicates a U–NC coordination, noting that the energy difference is small, 1.50 kcal/mol only.

As expected, considering the different energy terms (Table 4), the steric term (E_{st}) is slightly more destabilizing for the U(III) than for the Ce(III) species, especially in the bis(silylamide) MN*₂, due to the shorter metal–ligand distances in the former. Notably, in the bis(cyclopentadienyl) MCp*₂ series, the steric term, which is the sum of the Pauli repulsion (repulsion between electron pairs) and the stabilizing electrostatic interactions, reveals that the isocyanide binding mode for the two Ce(III) and U(III) ions is less sterically favored than the cyanide binding mode. This is due to a higher Pauli repulsion related to smaller M–N bond lengths than M–C ones.

More interestingly, the steric term in the bis(silylamide) $MN*_2$ species reveals that the isocyanide Ce–NC binding mode is slightly more sterically favored than the cyanide Ce–CN one (*i.e.*, -11.52 vs. -11.23 eV) whereas the opposite is observed for the U–CN/NC

coordination (*i.e.*, -10.38 vs. -10.04 eV), confirming the preference for the cyanide coordination mode.

The orbital term E_{orb} (stabilizing energy due to orbital mixing) is slightly larger in the M–NC case than in the M–CN one. However, the difference is small and is due to the competitive contribution of the covalent (orbital mixing) and the polarization factors, these latter being larger for the smaller M–NC bond distances [10]. Indeed, we must keep in mind that the orbital E_{orb} part includes both a polarization term due to the rearrangement of the metal and ligand charge distribution with complexation, and covalency if their orbitals overlap [19]. Unfortunately, these two terms cannot be evaluated separately [19b]. Moreover, the polarization component is likely not the same for the C or N coordination modes, so that difference in E_{orb} cannot be directly related to difference in covalency. Furthermore, as stated by others authors [9,11], the best energy matching between the d/f orbitals and the upper C-cyanide or the lower N-isocyanide σ -donating MO is likely to play a crucial role in this coordination preference.

In addition to the gas phase analysis we have also computed the complexation energies incorporating the effect of the solvent (THF) using the COSMO solvation approach (Table 4). Indeed, the main trends observed for isolated complexes are maintained in solution. Interestingly, in the case of the uranium $[UN*_2X_3]^{2-}$ species, the U–CN coordination appears now to be favored relatively to the U–NC one, by 1.8 kcal/mol, in agreement with experimental data [10a]. This theoretical result is in line with the fact that the synthesis of this complex was made in solution. It is noteworthy that using the most extended basis set available in the ADF program for all atoms, i.e. the ZORA/TZ2P one, the coordination preference of the cyanide towards U(III) is confirmed for the bis(silylamide) complex. Indeed, the same trend is obtained, i.e. the cyano isomer is more stable than the isocyano one (by 1.2 kcal/mol at the TZ2P level *vs*. 1.8 kcal/mol at the DZP one) when the solvent effect is taken into account, the opposite being obtained in the gas phase.

3. Conclusion

The observed distinct coordination modes of cyanide and isocyanide ligands towards cerium(III) and uranium(III) in the tris(cyanide) complexes $[ML_2X_3]^{2-}$ (M = Ce³⁺/U³⁺; L = Cp*/N*; X = CN/NC) were investigated using relativistic DFT/ZORA/BP86 computations both in the gas phase and solution. The coordination modes, M–CN or M–NC, were well

rationalized by the consideration of the binding energies of the cyanide and isocyanide ligands to the metal ions and by the confrontation of the DFT optimized geometries to the X-ray crystal data. The effects of cyanide and isocyanide coordination on structural properties of the complexes, especially in the bis(silylamide) compounds $[MN*_2X_3]^{2-}$, have been rationalized considering electronic indices like NPA charges and bond orders. Furthermore, the variations in structural and bonding parameters of the considered complexes could be explained by an MO analysis. The coordination preference of the cyanide and isocyanide ligands towards the $[MCp*_2]$ and $[MN*_2]$ moieties results mainly from the best energy matching between the d/fmetallic orbitals and the upper energy C-cyanide or the lower N-isocyanide σ -donating MOs. More generally, MO analysis shows that the stronger σ -donating ability of the cyanide ligand towards actinide bis(silylamide) systems over their cerium congeners is related to the higher covalent bonding character which plays a significant role in metal-ligand coordination preference.

The calculated total bonding energies between the $[MCp_2^*]$ and $[MN_2^*]$ (M = Ce, U) metallic fragments and the CN/NC ligands could permit prediction of the M-CN/NC coordination preference towards the Ce(III)/U(III) pair. Indeed, considering the experimental and hypothetical structures in their gas and solvated phases, it was found that the TBE_{frag} bonding energies for the cyanide M-CN coordination in the MCp*₂ complexes are significantly higher (in absolute value) than the isocyanide M-NC ones, as shown by their relative stability ΔE , agreeing well with the experimental structures. In the MN^{*}₂ series, the isocyanide Ce-NC coordination was clearly predicted more stable than the Ce-CN one, whereas the correct cyanide coordination of the uranium complex is found only if solvent effects are taken into account. This result is rather rewarding since the latter uranium complex has been synthesized in solution. The developed methodology seems able to predict the correct isomer with confidence in all cases. Nevertheless, the preferred cyanide or isocyanide coordination mode is driven by a subtle balance between steric, ionic or/and covalent factors, as well as solvent effects, so that it could be difficult to predict with certainty, on the basis of the theoretical computation alone, the preferred coordination mode, especially when the binding energies are not very different [10].

Appendix A. Computational details

All molecular geometries of the tris(cyanide) complexes $[ML_2X_3]^{2-}$ (M = Ce³⁺/U³⁺; X = CN/NC ; L = Cp*/N*) were fully optimized, starting from crystal structures where available, at the scalar relativistic DFT level of theory using the Amsterdam Density Functional (ADF2014.07) program package [20].

Scalar relativistic effects were taken into account via the Zeroth Order Regular Approximation (ZORA) [20e-g]. The Vosko–Wilk–Nusair functional (VWN) [21a] for the Local Density Approximation (LDA) and gradient corrections for exchange and correlation of Becke and Perdew (BP86 functional) [21b,c] were used for geometry optimization and analytical computation of the frequencies of the normal modes of vibration. Double- ζ Slater-type valence orbitals (STO) augmented by one set of polarization functions were used for all atoms. For all elements, the basis sets were taken from the ADF/ZORA/DZP database. Several theoretical studies have shown that such a ZORA/BP86/DZP approach reproduces the experimental geometries and ground state properties of *f*-element compounds with a satisfying accuracy [14]. Finally, for all complexes, we considered the highest (2S+1) spin state as the ground state configuration, *i.e.*, doublet (f^4) spin states for the Ce(III) and quartet (f^3) for U(III) systems.

In order to provide a better understanding of the metal-ligand bonding, a Natural Population Analysis (NPA) [16a] was carried out. It has been shown that such an approach provides reliable results for *f*-element complexes [16b,c,d,f].

As the ADF program supplies an energy decomposition of the metal-ligand bonding into chemically useful terms, spin-unrestricted fragment calculations were carried out considering the two molecular moieties in interaction, *i.e.*, ML₂ and X₃ (X = CN/NC) for the $[ML_2X_3]^{2-}$ complexes (M = Ce or U; L = N* or Cp*). This energy decomposition, which is based on the transition-state method developed by Morokuma [22a,b] and Ziegler *et al.* [22c], provides insights into the balance of the different bonding electronic or electrostatic factors at work between the isolated cation or metallic moiety and the ligands in a complex. Thus, within this scheme, the resulting total bonding energy TBE_{frag} between two fragments can be decomposed into two terms as TBE_{frag} = E_{steric} + E_{orb} , where E_{steric} is, in our case, the steric interaction energy between the MCp*₂ or MN*₂ (Cp* = C₅Me₅ and N* = N(SiMe₃)₂) metallic fragment and the CN or NC ligand and E_{orb} is the orbital (covalent) contribution to the metal–CN/NC bond. The steric energy term (E_{steric}) is itself decomposed into a destabilizing term

 E_{Pauli} , the electronic repulsion due to the Pauli principle, and E_{elstat} , the stabilizing electrostatic energy between the two fragments $E_{\text{steric}} = E_{\text{Pauli}} + E_{\text{elstat}}$. The bonding energies have been computed at the ZORA/BP86/DZP level. ΔE in Table 4 is the energy difference between the two M-CN and M-NC isomers (differences of their TBE_{frag}).

Appendix B. Supplementary material

Cartesian coordinates of DFT optimized geometries.

Acknowledgments

The authors are grateful to Algerian CNEPRU (project 2015-2018: E00920140093), for financial support. GENCI-IDRIS and GENCI-CINES for an allocation of computing time (Grant No. 2015-2016-080649). The COST CM-1006 action is also acknowledged.

References

- (1) (a) B.L. Kalsotra, B.D. Jain, R.K. Multani, J. Inorg. Nucl. Chem. 34 (1972) 2265–2269. (b) B. Kanellakopulos, E. Dornberger, H. Billich, J. Organomet. Chem. 76 (1974) C42–C44.
- (2) (a) J.C. Berthet, P. Thuéry, M. Ephritikhine, Dalton Trans. 44 (2015) 7727-7742 and references therein. (b) J. Maynadié, J.C. Berthet, P. Thuéry, M. Ephritikhine, Organometallics 26 (2007) 2623–2629.
- (3) (a) M. Verdaguer, A. Bleuzen, V. Marvaud, J. Vaissermann, M. Seuleiman, C. Desplanches, A. Scuiller, C. Train, R. Garde, G. Gelly, C. Lomenech, I. Rosenman, P. Veillet, C. Cartier, F. Villain, Coord. Chem. Rev. 1023 (1999) 190–192. (b) M. Ohba, H. Ōkawa, Coord. Chem. Rev. 198 (2000) 313–328. (c) P. Przychodzen, T. Korzeniak, R. Podgajny, B. Sieklucka, Coord. Chem. Rev. 250 (2006) 2234–2260. (d) S. Tanase, J. Reedijk, Coord. Chem. Rev. 250 (2006) 2501–2510. (e) S. Wang, X.H. Ding, Y.H. Li, W. Huang, Coord. Chem. Rev. 256 (2012) 439–464.
- (4) (a) A. Boucekkine, L. Belkhiri, *f-Element Complexes*. In Comprehensive Inorganic Chemistry II, J. Reedijk, K. Poeppelmeier, Eds. Elsevier: Oxford. 9 (2013) 277–319.
 W.J. Evans, Organometallics 35 (2016) 3088–3100. (b) F.T. Edelmann, Coord. Chem.

Rev. 318 (2016) 29–130. F.T. Edelmann, Coord. Chem. Rev. 284 (2015) 124–205. (c) T.J. Marks, Organometallics 32 (2013) 1133–1136.

- (5) (a) M. Ephritikhine, Dalton Trans. 21 (2006), 2501–2516. (b) S.T. Liddle, D.P. Mills, Dalton Trans. (2009) 5592–5605. (c) O.P. Lam, K. Meyer, Polyhedron, 32 (2012) 1–9.
 (d) R.J. Baker, Coord. Chem. Rev. 256 (2012) 2843–2871. (e) T.W. Hayton, Chem. Commun. 49 (2013) 2956–2973. (f) M.B. Jones, A.J. Gaunt, Chem. Rev. 113 (2013) 1137–1198.
- (6) (a) K.L. Nash, In Handbook on the Chemistry and Physics of Rare Earths, K.A. Jr. Gschneidner, L. Eyring, G.R. Choppin, G.H. Lander, Eds. Elsevier Science: Amsterdam, The Netherlands, (1994), Vol. 18, Chapter 121. (b) *The Chemistry of the Actinide and Trans-actinide Elements*, 3rd ed., L.R. Morss, N.M. Edelstein, F. Fuger, Eds. Springer: Dordrecht, The Netherlands, (2006).
- (7) A.E.V. Gorden, M.A. DeVore, II, B.A. Maynard, Inorg. Chem. 52 (2013) 3445–3458.
- (8) N. Iché-Tarrat, N. Barros, C.J. Marsden, L. Maron, Chem. Eur. J. 14 (2008) 2093–2099.
- (9) (a) C. Clavaguera-Sarrio, S. Hoyau, N. Ismail, C.J.J. Marsden, Phys. Chem. A. 107 (2003) 4515–4525. (b) J.L. Sonnenberg, P.J. Hay, R.L. Martin, B.E. Bursten, Inorg. Chem. 44 (2005) 2255–2262. (c) D.P. Hernández, R. Ramírez-Tagle, E. Codorniu-Hernández, L.A. Montero-Cabrera, R. Arratia-Pérez, Polyhedron 29 (2010) 975–984.
- (10) (a) A. Hervé, Y. Bouzidi, J.C. Berthet, L. Belkhiri, P. Thuéry, A. Boucekkine, M. Ephritikhine, Inorg. Chem. 53 (2014) 6995–7013. (b) A. Hervé, Y. Bouzidi, J. C. Berthet, L. Belkhiri, P. Thuéry, A. Boucekkine, M. Ephritikhine, Inorg. Chem. 54 (2015) 2474–2490.
- P.L. Arnold, Z.R. Turner, N. Kaltsoyannis, P. Pelekanaki, R.M. Bellabarba, R.P. Tooze, Chem. Eur. J. 16. 16 (2010) 9623–9629.
- (12) M. Straka, M. Patzschke, P. Pyykkö, Theor. Chem. Acc. 109 (2003) 332–340.
- (13) (a) Q.Y. Wu, C.Z. Wang, J.H. Lan, C.L. Xiao, X.K. Wang, Y.L. Zhao, Z.F. Chai, W. Q. Shi, Inorg. Chem. 53 (2014) 9607–9614. (b) B. Averkiev, M. Mantina, R. Valero, I. Infante, A. Kovacs, D. Truhlar, L. Gagliardi, Theor. Chem. Acc. 129 (2011) 657–666.
- (14) (a) M. Roger, L. Belkhiri, T. Arliguie, P. Thuery, A. Boucekkine, M. Ephritikhine, Organometallics 27 (2008) 33–42. (b) A.J. Gaunt, S.D. Reilly, A.E. Enriquez, B.J. Scott, J.A. Ibers, P. Sekar, K.I. M. Ingram, N. Kaltsoyannis, M. P. Neu, Inorg. Chem. 47 (2008) 29–41. (c) M. Roger, L. Belkhiri, P. Thuery, S. E. Bouaoud, A. Boucekkine, M. Ephritikhine, Inorg. Chem. 48 (2009) 221–230. (d) S. Meskaldji, L. Belkhiri,; T.

Arliguie, M. Fourmigue, M. Ephritikhine, A. Boucekkine, Inorg. Chem. 49 (2010)
3192–3200. (e) S. Meskaldji, A. Zaiter, L. Belkhiri, A. Boucekkine, Theor.Chem. Acc.
131 (2012) 1151–1159. (f) B. Teyar, L. Belkhiri, K. Costuas, A. Boucekkine, K. Meyer, Inorg. Chem. 55 (2016) 2870–2881.

- (15) R.D. Shannon, Acta Crystallogr, Sect. A. 32 (1976) 751–767.
- (16) (a) A.E. Reed, L.A. Curtiss, F. Weinhold, Chem. Rev. 88 (1988) 899–926. (b) A.E. Clark, J.L. Sonnenberg, P.J. Hay, R.L. Martin, J. Chem. Phys.121 (2004) 2563–2570.
 (c) M. Straka, P. Hrobarik, M. Kaupp, J. Am. Chem. Soc. 127 (2005) 2591–2599. (d) H. Wu, Q.-Y. Wu, C-Z. Wang, J-H. Lan, Zi-R. Liu, Z-F. Chai, W-Q. Shi, Dalton Trans. 45 (2016) 8107–8117. (e) R.S. Mulliken, J. Chem. Phys. 23 (1955) 1833–1840. (f) P. Yang, I. Warnke, R.L. Martin, P.J. Hay, Organometallics 27 (2008) 1384–1392.
- (17) (a) R.F. Nalewajski, J. Mrozek, Int. J. Quant. Chem. 51 (1994) 187–200. (b) R.F. Nalewajski, J. Mrozek, A. Michalak, Int. J. Quant. Chem. 6 (1997) 589–601. (c) I. Mayer, Chem. Phys. Lett. 7 (1983) 270–274. (d) B. Sadhu, M. Sundararajan, T. Bandyopadhyay, Inorg. Chem. 55 (2016) 598–609.
- (18) M.L. Neidig, D.L. Clark, R.L. Martin, Coord. Chem. Rev. 257 (2013) 394–406.
- (19) (a) B. Vlaisavljevich, P. Miro, C.J. Cramer, L. Gagliardi, I. Infante, S.T. Liddle, Chem.Eur. J. 17 (2011) 8424–8433. (b) L. Petit, C. Adamo, P. Maldivi, Inorg. Chem. 45(2006) 8517–8522. (c) D. Manna, S. Mula, A. Bhattacharyy, S. Chattopadhyay, T. K. Ghanty, Dalton Trans. 44 (2015) 1332–1340.
- (20) (a) G. te Velde, F.M. Bickelhaupt, S.J.A.V. Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders, T. Ziegler, Chemistry with ADF, J. Comput. Chem. 22 (2001) 931–967. (b) C. Fonseca Guerra, J.G. Snijders, G. te Velde, E.J. Baerends, Theor. Chem. Acc. 99 (1998) 391–403. (c) ADF2014, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com. (d) A.D. Becke, J. Chem. Phys. 88 (1988) 2547–2553. (e) E.V. Lenthe, E.J. Baerends, J.G. Snijders, J. Chem. Phys. 99 (1993) 4597–4610. (f) E.V. Lenthe, E.J. Baerends, J.G. Snijders, J. Chem. Phys. 101 (1994) 9783–9792. (g) E.V. Lenthe, A.E. Ehlers, E. J. Baerends, J. Chem. Phys. 110 (1999) 8943–8953.
- (21) (a) S.D. Vosko, L. Wilk, M. Nusair, Can. J. Chem. 58 (1980) 1200–1211. (b) A.D. Becke, Phys. Rev. A. 38 (1988) 3098–3100. (c) J.P. Perdew, Phys. Rev. B 34 (1986) 7406. J.P. Perdew, in *Electronic Structure of Solids* '91, Ed. P. Ziesche, H. Eschrig, Akademie Verlag, Berlin, 11 (1991). (d) J.P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244–13249. (e) J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77

(1996) 3865–3868. (f) J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 78 (1997) 1396.

(22) (a) K. Morokuma, J. Chem. Phys. 55 (1971) 1236–1244. (b) K. Kitaura, K. Morokuma, Int. J. Quant.Chem. 10 (1976) 325–340. (c) T. Ziegler, A. Rauk, Theor. Chim. Acta. 46 (1977) 1–10.

Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study

Yamina Bouzidi ^{a,b}, Lotfi Belkhiri ^{b,*}, Michel Ephritikhine ^c, Jean-François Halet ^{d,*}, and Abdou Boucekkine ^{d,*}

^a Département de Chimie, Université de Batna 1, 05000 Batna, Algeria
^b URCHEMS, Département de Chimie, Université des Frères Mentouri Constantine 1, 25017 Constantine, Algeria
^c NIMBE, CEA, CNRS, Université Paris-Saclay,CEA Saclay, 91191 Gif-sur-Yvette, France
^d Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - Université de Rennes 1, 35042 Rennes Cedex, France

Highlights

- Different ligation modes of cyanide/isocyanide ligands towards trivalent Ce(III)/U(III) ions.
- Relativistic DFT/ZORA investigation accounting solvation effects.
- Dependence of the M–CN/NC coordination preference on the steric, ionic, covalent factors, co-ligand, and solvation effects.

CEP (CE)

Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study

Yamina Bouzidi ^{a,b}, Lotfi Belkhiri ^{b,*}, Michel Ephritikhine ^c, Jean-François Halet ^{d,*}, and Abdou Boucekkine ^{d,*}

^a Département de Chimie, Université de Batna 1, 05000 Batna, Algeria
 ^b URCHEMS, Département de Chimie, Université des Frères Mentouri Constantine 1, 25017 Constantine, Algeria
 ^c NIMBE, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette,

France

^d Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - Université de Rennes 1, 35042 Rennes Cedex, France

Supplementary Information

Cartesian coordinates of DFT optimized geometries.

	[MCp* ₂ X ₃] ^q / q=2- ,1- /X=CN ,NC/ GAZ								
[Ce	e(III)Cp*₂CN₃]	2-			[Ce	e(III)Cp*2NC3]	2-		
1 Ce	0.000000000000	0.00000000000	0.662157345200		1 Ce	0.00000000000	0.000000000000	0.768988710600	
2 N	0.0000000000000	2 726049970000	4.473082654000		20	0.00000000000000000	2.662852600000	4.446721466000	
4.0	0.0003420930800	0.0000000000000000000000000000000000000	2 205422151000		4 N	0.00000000000	0.0000000000000000000000000000000000000	2 264090124000	
4C	-0.417392077300	2 585003675000	1 241293223000		5 N	-0.253396091900	2 503149597000	1 223800742000	
6 C	2.047694898000	0.343201361900	-1.382503998000		6 C	2.039385842000	0.200771171200	-1.376836986000	
7 C	2.130878989000	1.521198489000	-0.581825116900		7 C	2.187950419000	1.379417240000	-0.590108161000	
8 C	2.628106787000	1.141088081000	0.701578806600		8 C	2.669558318000	0.987747457600	0.695479695500	
9 C	2.853257207000	-0.265610856700	0.690675451800		9 C	2.817518516000	-0.430856334500	0.698246513500	
10 C	2.493862205000	-0.762946573500	-0.598896747200		10 C	2.430028796000	-0.918002202200	-0.586246219300	
11 C	1.763758775000	0.309156840900	-2.856446193000		11 C	1.754127382000	0.169934613600	-2.849472099000	
12 H	2.680382217000	0.494954075400	-3.449472830000		12 H	2.684186600000	0.271383501500	-3.441961765000	
13 H	1.030792118000	1.071770170000	-3.158556435000		13 H	1.088167717000	0.987568192300	-3.159991866000	
14 H	1.369676232000	-0.665466803000	-3.178561441000		14 H	1.279571213000	-0.771541507400	-3.160577215000	
15 C	1.916794684000	2.926203279000	-1.065870868000		15 C	2.046311331000	2.788255056000	-1.085146770000	
10 H	1.514268595000	3.573179139000	-0.274856437100		10 H	1.095030545000	3.462182308000	-0.292950408300	
18 H	2.861825480000	3.371929563000	-1.433355235000		18 H	3.008713897000	3.177968823000	-1.470937402000	
19 C	2.930879266000	2.072843034000	1.839840410000		19 C	3.046120978000	1.915449612000	1.814296221000	
20 H	2.782777209000	1.582003551000	2.812127215000		20 H	2.919127271000	1.436812229000	2.795402331000	
21 H	2.269486591000	2.949340862000	1.825595948000		21 H	2.416256343000	2.815095989000	1.817348475000	
22 H	3.977936681000	2.430004259000	1.800274464000		22 H	4.102987391000	2.234978837000	1.734084785000	
23 C	3.439587092000	-1.069484386000	1.815420425000		23 C	3.375816230000	-1.258270554000	1.820024837000	
24 H	4.545724150000	-1.073911782000	1.771362271000		24 H	4.478192557000	-1.335862379000	1.754326657000	
25 H	3.091512981000	-2.110833485000	1.787791054000		25 H	2.961021238000	-2.275037557000	1.810327466000	
26 H	3.147052070000	-0.665089863100	2.794494635000		26 H	3.132332912000	-0.827100924000	2.801233902000	
27 C	2.720429876000	-2.159634770000	-1.100494159000		27 C	2.585843711000	-2.327725755000	-1.074191927000	
28 H	2.020262807000	-2.423856496000	-1.907678999000		28 H	1.913818845000	-2.543422017000	-1.917979387000	
29 H	2.575483748000	-2.904209797000	-0.306837864500		29 H	2.348655216000	-3.057660065000	-0.288874733400	
30 H	3.743248668000	-2.2/894/694000	-1.508034534000		30 H	3.618698961000	-2.518689391000	-1.4243/06/8000	
32 0	0.003420950800	-3.730948879000	1.406185150000		32 N	0.369424743800	-2 503149597000	1.420515226000	
33 C	-2.047694898000	-0.343201361900	-1.382503998000		33 C	-2.039385842000	-0.200771171200	-1.376836986000	
34 C	-2.130878989000	-1.521198489000	-0.581825116900		34 C	-2.187950419000	-1.379417240000	-0.590108161000	
35 C	-2.628106787000	-1.141088081000	0.701578806600		35 C	-2.669558318000	-0.987747457600	0.695479695500	
36 C	-2.853257207000	0.265610856700	0.690675451800		36 C	-2.817518516000	0.430856334500	0.698246513500	
37 C	-2.493862205000	0.762946573500	-0.598896747200		37 C	-2.430028796000	0.918002202200	-0.586246219300	
38 C	-1.763758775000	-0.309156840900	-2.856446193000		38 C	-1.754127382000	-0.169934613600	-2.849472099000	
39 H	-2.680382217000	-0.494954075400	-3.449472830000		39 H	-2.684186600000	-0.271383501500	-3.441961765000	
40 H	-1.030792118000	-1.071770170000	-3.158556435000		40 H	-1.088167717000	-0.987568192300	-3.159991866000	
41 H	-1.369676232000	0.665466803000	-3.178561441000	Y	41 H	-1.279571213000	0.771541507400	-3.160577215000	
42 C	-1.916794684000	-2.926203279000	-1.065870868000		42 C	-2.046311331000	-2.788255056000	-1.085146770000	
43 H	-1.514268595000	-3.573179139000	-0.274856437100		43 H	-1.695030545000	-3.462182308000	-0.292950408300	
44 H	-2.861825480000	-2.963436791000	-1.898383732000	/	44 H	-1.510559507000	-3.177968823000	-1.470937402000	
46 C	-2.930879266000	-2.072843034000	1.839840410000		46 C	-3.046120978000	-1.915449612000	1.814296221000	
47 H	-2.782777209000	-1.582003551000	2.812127215000		47 H	-2.919127271000	-1.436812229000	2.795402331000	
48 H	-2.269486591000	-2.949340862000	1.825595948000		48 H	-2.416256343000	-2.815095989000	1.817348475000	
49 H	-3.977936681000	-2.430004259000	1.800274464000		49 H	-4.102987391000	-2.234978837000	1.734084785000	
50 C	-3.439587092000	1.069484386000	1.815420425000		50 C	-3.375816230000	1.258270554000	1.820024837000	
51 H	-4.545724150000	1.073911782000	1.771362271000		51 H	-4.478192557000	1.335862379000	1.754326657000	
52 H	-3.091512981000	2.110833485000	1.787791054000		52 H	-2.961021238000	2.275037557000	1.810327466000	
53 H	-3.147052070000	0.665089863100	2.794494635000		53 H	-3.132332912000	0.827100924000	2.801233902000	
54 C	-2.720429876000	2.159634770000	-1.100494159000		54 C	-2.585843711000	2.327725755000	-1.074191927000	
55 H	-2.020262807000	2.423856496000	-1.90/678999000		55 H	-1.913818845000	2.543422017000	-1.91/9/938/000	
50 H	-2.3/3463/48000	2.904209797000	-0.500637864500		57 H	-2.346035210000	2 518680301000	-0.2008/4/33400	
[U	(III)Cp* ₂ CN ₃] ²	-	1.550034334000		[U(III)Cp* ₂ NC ₃] ²	-		
1 U	0.000000000000	0.00000000000	0.693105122500		1 U	0.000000000000	0.000000000000	0.664625353000	
2 N	0.00000000000	0.00000000000	4.456691964000		2 C	0.00000000000	0.00000000000	4.319730655000	
3 N	-U.397896091000	3.690327760000	1.515900192000		3 C	-U.387448409300	3.590307312000	1.404297020000	
40	0.000000000000000	2 53650/0/1000	5.278930557000		4 N	0.00000000000000000	2 439791999000	3.137208501000	
60	2.368842994000	-0.921176233800	-0.605739074300		60	2.369944770000	-0.891760090600	-0.606668924500	
70	1.976424121000	0.212236714200	-1.381308185000		7 C	1.980304733000	0.258166036900	-1.361038308000	
8 C	2.148022431000	1.379076393000	-0.576063082800		8 C	2.164071410000	1.409075622000	-0.534932961900	
1						'			

9.0	2.646523899000	0.965499386700	0.696375330900	9 C	2.651100472000	0.971260239100	0.731526509300	
10.0	2 783486533000	-0.452699697700	0.678056838400	10.0	2 783244111000	-0.448290372900	0.687293182600	
11 C	2.493121756000	-2.327449838000	-1.116241867000	11 C	2.512063446000	-2.282511665000	-1.151083997000	
12 H	1.756929473000	-2.537286360000	-1.906811341000	12 H	1.772090349000	-2.487573038000	-1.939912690000	
13 H	2.318651656000	-3.064254534000	-0.320989344100	13 H	2.356988820000	-3.038797109000	-0.370709183000	
14 H	3 496228466000	-2 512212720000	-1 548513178000	14 H	3 514094643000	-2 441693440000	-1 596054335000	
15.0	1 727054677000	0.210613090100	-2 860127156000	15.0	1 737864494000	0 285648155000	-2 8/1716736000	
15 C	1.079352277000	1.042645681000	-3 170092250000	16 H	1 100223011000	1 130819928000	-3 138835065000	
10 H	1.247166951000	-0 718308643000	-3 199123445000	17 H	1 249391645000	-0.631/89810800	-3 199481124000	
10 11	2.674228226000	-0.718308043000	-3.135123445000	10 11	2.00772000000	-0.031485810800	-3.135481124000	
18 H	2.674238336000	0.310463056600	-3.428608545000	18 H	2.68//28868000	0.386424910100	-3.405919230000	
190	2.003768574000	2.793448818000	-1.050808285000	190	2.030996262000	2.832018480000	-0.991324179400	
20 H	2.938308883000	3.138107331000	-1.526229732000	20 H	2.961360847000	3.1/3/12/19000	-1.498278133000	
21 H	1.749241946000	3.473785938000	-0.226398547800	21 H	1.829416700000	3.508129872000	-0.152/0192/000	
22 H	1.199337394000	2.895438300000	-1.795439488000	22 H	1.208775025000	2.961707716000	-1.704665955000	
23 C	3.039607845000	1.867050548000	1.830940262000	23 C	3.029797979000	1.856227814000	1.883017532000	
24 H	2.890782213000	1.376174611000	2.802861891000	24 H	2.910141544000	1.335949993000	2.843519408000	
25 H	2.433863666000	2.782933925000	1.843928191000	25 H	2.392715090000	2.749966842000	1.924544408000	
26 H	4.105523584000	2.158486432000	1.762000830000	26 H	4.083743004000	2.187142527000	1.809446979000	
27 C	3.351280454000	-1.290282041000	1.787255845000	27 C	3.346869970000	-1.310371413000	1.779111497000	
28 H	4.457413109000	-1.313605179000	1.745736130000	28 H	4.448766930000	-1.387721653000	1.701942406000	
29 H	2.983213090000	-2.322979698000	1.737479598000	29 H	2.927882378000	-2.324668596000	1.743591448000	
30 H	3.063722520000	-0.901022300500	2.774549461000	30 H	3.110855741000	-0.905355151300	2.773161912000	
31 N	0.397896091000	-3.690327760000	1.515900192000	31 C	0.387448409300	-3.590307312000	1.404297020000	
32 C	0.254902033200	-2.536504041000	1.323045130000	32 N	0.280052445400	-2.439791998000	1.149287192000	
33 C	-2.368842994000	0.921176233800	-0.605739074300	33 C	-2.369944770000	0.891760090600	-0.606668924500	
34 C	-1.976424121000	-0.212236714200	-1.381308185000	34 C	-1.980304733000	-0.258166036900	-1.361038308000	
35 C	-2.148022431000	-1.379076393000	-0.576063082800	35 C	-2.164071410000	-1.409075622000	-0.534932961900	
36 C	-2.646523899000	-0.965499386700	0.696375330900	36 C	-2.651100472000	-0.971260239100	0.731526509300	
37 C	-2.783486533000	0.452699697700	0.678056838400	37 C	-2.783244111000	0.448290372900	0.687293182600	
38 C	-2.493121756000	2.327449838000	-1.116241867000	38 C	-2.512063446000	2.282511665000	-1.151083997000	
39 H	-1.756929473000	2.537286360000	-1.906811341000	39 H	-1.772090349000	2.487573038000	-1.939912690000	
40 H	-2.318651656000	3.064254534000	-0.320989344100	40 H	-2.356988820000	3.038797109000	-0.370709183000	
41 H	-3.496228466000	2.512212720000	-1.548513178000	41 H	-3.514094643000	2.441693440000	-1.596054335000	
42 C	-1.727054677000	-0.210613090100	-2.860127156000	42 C	-1.737864494000	-0.285648155000	-2.841716736000	
43 H	-1.079352277000	-1.042645681000	-3.170092250000	43 H	-1.100223011000	-1.130819928000	-3.138835065000	
44 H	-1.247166951000	0.718308643000	-3.199123445000	44 H	-1.249391645000	0.631489810800	-3.199481124000	
45 H	-2.674238336000	-0.310463056600	-3.428608545000	45 H	-2.687728868000	-0.386424910100	-3.405919230000	
46 C	-2.003768574000	-2.795448616000	-1.050808283000	46 C	-2.036996262000	-2.832018480000	-0.991524179400	
47 H	-2.936306663000	-3.158107351000	-1.526229732000	47 H	-2.961560847000	-3.173712719000	-1.496276135000	
48 H	-1.749241946000	-3.473785938000	-0.226398547800	48 H	-1.829416700000	-3.508129872000	-0.152701927000	
49 H	-1.199337394000	-2.895438300000	-1.795439488000	49 H	-1.208775025000	-2.961707716000	-1.704665955000	
50 C	-3.039607845000	-1.867050548000	1.830940262000	50 C	-3.029797979000	-1.856227814000	1.883017532000	
51 H	-2.890782213000	-1.376174611000	2.802861891000	51 H	-2.910141544000	-1.335949993000	2.843519408000	
52 H	-2.433863666000	-2.782933925000	1.843928191000	52 H	-2.392715090000	-2.749966842000	1.924544408000	
53 H	-4.105523584000	-2.158486432000	1.762000830000	53 H	-4.083743004000	-2.187142527000	1.809446979000	
54 C	-3.351280454000	1.290282041000	1.787255845000	54 C	-3.346869970000	1.310371413000	1.779111497000	
55 H	-4.457413109000	1.313605179000	1.745736130000	55 H	-4.448766930000	1.387721653000	1.701942406000	
56 H	-2.983213090000	2.322979698000	1.737479598000	56 H	-2.927882378000	2.324668596000	1.743591448000	
57 H	-3.063722520000	0.901022300500	2.774549461000	57 H	-3.110855741000	0.905355151300	2.773161912000	
ſ. I	11/)Cp* CN 11	-		E 11/		L-		
10	0.0000000000000000000000000000000000000	0.000000000000	0.498247659300	101				
2 N	-0.006121805906	-3.596980631000	1.269106245000	10	0.0000000000000	0.000000000000	0.530890778500	
3 N	0.0000000000000	0.000000000000	4.171972244000	2 C	0.012301319410	-3.545588480000	1.061853406000	
4 N	0.006121805906	3.596980631000	1.269106245000	3 C	0.000000000000	0.000000000000	4.081818081000	
5 C	-0.009639042411	-2.439685628000	1.059658680000	4 C	-0.012301319410	3.545588480000	1.061853406000	
6 C	0.000000000000	0.000000000000	2.997217064000	5 N	0.003140854492	-2.383955272000	0.828748276200	
7 C	0.009639042411	2.439685628000	1.059658680000	6 N	0.000000000000	0.000000000000	2.896467294000	
8 C	-2.667769700000	0.712457745500	0.745934941600	7 N	-0.003140854492	2.383955272000	0.828748276200	
9 C	-2.668050356000	-0.714247608400	0.730830216300	8 C	-2.657116844000	0.719974661500	0.770092334400	
10 C	-2.275947090000	-1.143844297000	-0.573170776300	9 C	-2.658319790000	-0.708038772100	0.777365803700	
11 C	-2.019662334000	0.021287448080	-1.361539616000	10 C	-2.316890683000	-1.154846233000	-0.537087348300	
12 C	-2.276253382000	1.169769389000	-0.548906811300	11 C	-2.077947405000	-0.005562485418	-1.347685065000	
13 C	-3.109315756000	1.567249268000	1.896421385000	12 C	-2.314772174000	1.152357206000	-0.549290486600	
14 H	-4.207119027000	1.682650979000	1.890345956000	13 C	-3.077674098000	1.600039448000	1.908817966000	
15 H	-2.658040153000	2.565864142000	1.855182271000	14 H	-4.171481773000	1.749516208000	1.901360640000	
16 H	-2.826465783000	1.124382182000	2.860664679000	15 H	-2.596923398000	2.584762020000	1.856004983000	
17 C	-3.110530665000	-1.592779751000	1.862876005000	16 H	-2.807602339000	1.160744176000	2.877877024000	
18 H	-2.817501567000	-1.176304580000	2.835698150000	17 C	-3.080251472000	-1.576936010000	1.923845886000	
19 H	-2.669213834000	-2.594263470000	1.794874757000	18 H	-2.846473903000	-1.109629338000	2.889053509000	
20 H	-4.209326609000	-1.697590965000	1.861140125000	19 H	-2.570447974000	-2.548297252000	1.902850304000	
21 C	-2.324782642000	-2,547916531000	-1.097389569000	20 H	-4.168670305000	-1.758999353000	1.893938093000	
				21 C	-2.407735286000	-2.559213812000	-1.050313443000	

22 H	-3.296189704000	-2.737472924000	-1.587310447000	1			
22 11	2 100027746000	2 285727271000	0 20875 2672200	22 H	-3.366636630000	-2.704123019000	-1.578714393000
2511	2.100037740000	5.205727271000	0.250752075500	23 H	-2.346689957000	-3.293110021000	-0.239695619500
24 H	-1.541846946000	-2.739980285000	-1.844823252000	24 H	-1.602857477000	-2.800192006000	-1.758591963000
25 C	-1.795823978000	0.038190528340	-2.845315079000	25.6	4 053 40304 7000	0.010000.100750	2 020045272000
26 H	-1.246112610000	-0.847171464300	-3.192166812000	25 C	-1.853483917000	-0.013989423750	-2.830915273000
27.11	1 226040011000	0.025774226600	2 170476217000	26 H	-1.290312087000	-0.898607150200	-3.158042188000
2/ П	-1.236040911000	0.925774350000	-3.170478317000	27 H	-1.304583077000	0.875102772200	-3.169780338000
28 H	-2.759127166000	0.050792277940	-3.386303545000	20 LL	2 914050476000	0.025472970720	2 277141667000
29 C	-2.332184466000	2.583892064000	-1.044242142000	20 П	-2.814059476000	-0.025472879750	-3.377141007000
20 11	1 545072091000	2 700171002000	1 780260176000	29 C	-2.398653819000	2.551669350000	-1.077650250000
3011	-1.343072981000	2.755171558000	-1.780205170000	30 H	-1.589873781000	2.782296804000	-1.784893325000
31 H	-2.208236675000	3.305334660000	-0.228740314500	21 Ц	2 228065400000	2 204014041000	0 274711522100
32 H	-3.301726522000	2.775655072000	-1.537050363000	5111	-2.338003400000	3.294014941000	-0.274711333100
33 C	2.667769700000	-0.712457745500	0.745934941600	32 H	-3.354547996000	2.694731973000	-1.611881410000
				33 C	2.657116844000	-0.719974661500	0.770092334400
34 C	2.276253382000	-1.169769389000	-0.548906811300	34 C	2.314772174000	-1.152357206000	-0.549290486600
35 C	2.019662334000	-0.021287448080	-1.361539616000	340	2.514772174000	1.152557200000	0.545250480000
36 C	2 275947090000	1 143844297000	-0 573170776300	35 C	2.077947405000	0.005562485418	-1.347685065000
50 0	2.275547656666	11115011257000	0.575170770500	36 C	2.316890683000	1.154846233000	-0.537087348300
37 C	2.668050356000	0.714247608400	0.730830216300	37 C	2 658319790000	0 708038772100	0 777365803700
38 C	3.109315756000	-1.567249268000	1.896421385000	57 0	2.050515750000	0.7000000772100	
39 H	4 207119027000	-1 682650979000	1 890345956000	38 C	3.077674098000	-1.600039448000	1.908817966000
3511	4.207115027000	1.002050575000	1.050545550000	39 H	4.171481773000	-1.749516208000	1.901360640000
40 H	2.658040153000	-2.565864142000	1.855182271000	40 H	2 596923398000	-2 584762020000	1 856004983000
41 H	2.826465783000	-1.124382182000	2.860664679000	-10 11	2.550525550000	2.504702020000	1030001303000
42 C	2 332184466000	-2 583892064000	-1 044242142000	41 H	2.807602339000	-1.160744176000	2.877877024000
72 0		2.555552004000		42 C	2.398653819000	-2.551669350000	-1.077650250000
43 H	3.301726522000	-2.775655072000	-1.537050363000	43 H	3,354547996000	-2.694731973000	-1.611881410000
44 H	1.545072981000	-2.799171998000	-1.780269176000		4 5000707070	2.2020000	4 7040000000
45 H	2.208236675000	-3,305334660000	-0.228740314500	44 H	1.589873781000	-2.782296804000	-1.784893325000
				45 H	2.338065400000	-3.294014941000	-0.274711533100
46 C	1.795823978000	-0.038190528340	-2.845315079000	46 C	1.853483917000	0.013989423750	-2.830915273000
47 H	2.759127166000	-0.050792277940	-3.386303545000		1.000-0000000000	5.015505425750	
48 H	1.246112610000	0.847171464300	-3.192166812000	47 H	2.814059476000	0.025472879730	-3.377141667000
+0 11	1.240112010000	5.047171404500	5.152100012000	48 H	1.290312087000	0.898607150200	-3.158042188000
49 H	1.236040911000	-0.925774336600	-3.170476317000	40 H	1 304583077000	-0.875102772200	-3 169780338000
50 C	2.324782642000	2.547916531000	-1.097389569000	4511	1.504565077000	0.075102772200	-3.109780338000
51 H	3 29618970/000	2 737472924000	-1 587310447000	50 C	2.407735286000	2.559213812000	-1.050313443000
5111	5.250105704000	2.757472524000	1.50/51511/000	51 H	3.366636630000	2.704123019000	-1.578714393000
52 H	2.188837746000	3.285727271000	-0.298752673300	52 H	2 346689957000	3 203110021000	-0.239695619500
53 H	1.541846946000	2.739980285000	-1.844823252000	52.11	2.510005557000	5.235110021000	
54 C	3.110530665000	1.592779751000	1.862876005000	53 H	1.602857477000	2.800192006000	-1.758591963000
540	5.110550005000	1.552775751000	1.002070000000	54 C	3.080251472000	1.576936010000	1.923845886000
55 H	2.817501567000	1.176304580000	2.835698150000	55 H	2 846473903000	1 109629338000	2 889053509000
56 H	2.669213834000	2.594263470000	1.794874757000	5511	2.010113505000	1.105025550000	2.005055505000
				56 H	2.570447974000	2.548297252000	1.902850304000
57 H	4 209326609000	1 697590965000	1 861140125000				
57 H	4.209326609000	1.697590965000	1.861140125000	57 H	4.168670305000	1.758999353000	1.893938093000
57 H	4.209326609000	1.697590965000	1.861140125000	57 H	4.168670305000	1.758999353000	1.893938093000
57 H	4.209326609000	1.697590965000	1.861140125000	57 H	4.168670305000	1.758999353000 7	1.893938093000
57 H	4.209326609000	1.697590965000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1.	57 H	4.168670305000	1.758999353000 Z	1.893938093000
57 H	4.209326609000	1.697590965000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1	57 H	4.168670305000 CN ,NC /GA ((III)N*2NC3] ²⁻	1.758999353000 Z	1.893938093000
57 H [Ce 1 Ce	4.209326609000 (III)N* ₂ CN ₃] ²⁻ 13.490106620000	1.697590965000 22.521990030000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000	57 H /X=0 1 Ce	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000	1.758999353000 Z 22.519003230000	1.893938093000 0.156744398900
57 H [Ce 1 Ce 2 Si	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.183970060000	1.697590965000 22.521990030000 24.031669560000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1- 0.130086868000 1.867627026000	57 H /X=0 1 Ce 2 Si	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000	1.758999353000 Z 22.519003230000 24.024249040000	1.893938093000 0.156744398900 1.862358691000
57 H [Ce 1 Ce 2 Si 3 Si	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000	1.697590965000 22.521990030000 24.031669560000 24.858052630000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1. 0.130086868000 1.867627026000 -1.036970627000	57 H - /X=0 1 Ce 2 Si 3 Si	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000	1.758999353000 Z 22.519003230000 24.024249040000 24.865717960000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000
57 H [Ce 2 Si 3 Si 4 Si	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.18397006000 11.569644710000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.037376.660000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1. 0.130086868000 1.867627026000 -1.036970627000 2.409244487000	57 H /X=0 [Ce 1 Ce 2 Si 3 Si 4 Si	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 11.5597065980000	1.758999353000 Z 22.519003230000 24.024249040000 24.865717960000 20.916762370000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 2.11370432000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000	1.758999353000 Z 22.519003230000 24.024249040000 24.865717960000 20.974560370000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.009631850000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1- 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000	1.758999353000 Z 22.519003230000 24.024249040000 24.865717960000 20.974560370000 20.007919270000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.09631850000 20.486856770000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000	57 H - /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000	1.758999353000 Z 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.007919270000 20.5592630810000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.608299590000 11.65865530000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.09631850000 20.48685670000 22.60118438000	1.861140125000 [MN* ₂ X ₃] ^q /q=2-,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.76633320000	1.758993353000 Z 22.519003230000 24.024249040000 24.865717960000 20.974560370000 20.07919270000 22.631010720000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.668862530000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.0246656552000 2.0246656552000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁷ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.76333320000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.974560370000 20.007919270000 20.592630810000 22.631010720000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C	4.209326609000 (III)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 12.180530040000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.09631850000 20.486856770000 22.601184380000 24.589817230000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.0246656552000 -0.990801766500	57 H - /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.746333320000 12.289375080000	1.758999353000 Z 22.519003230000 24.024249040000 24.865717960000 20.974560370000 20.07919270000 20.592630810000 22.631010720000 24.459234590000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 12.180530040000 15.442192240000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.979705460000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.76633320000 12.289375080000 15.445746030000	1.758993353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.592630810000 22.631010720000 24.459234590000 23.919774630000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 12.180530040000 15.442192240000 13.166854510000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.0979705460000 20.09631850000 20.48685677000 22.601184380000 24.589817230000 23.927297210000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.74084474000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.957065980000 11.553493270000 14.409736670000 14.5242357400000 12.289375080000 15.445746030000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 23.91974630000 23.91974630000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000
57 H [Cee 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.60829590000 11.685862530000 12.180530040000 13.166854510000 13.166854510000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.0246656552000 -0.990801766500 0.307092500100 -1.744084474000 1.0174084474000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁷ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.5242357400000 11.746333320000 15.445746030000 13.140988870000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.007919270000 22.631010720000 22.631010720000 23.919774630000 21.030997440000	1.893938093000 0.156744398900 1.86235869100 -1.02468278000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 12.180530040000 15.42192240000 13.166854510000 15.120157300000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.09931850000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.746333320000 12.289375080000 13.140988870000 13.140988870000 14.958356150000	1.758999353000 2.519003230000 24.024249040000 24.865717960000 20.974560370000 20.07919270000 20.592630810000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 19.654137750000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.608299590000 12.180530040000 13.46854510000 15.42192240000 13.166854510000 15.120157300000 10.870267570000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.099631850000 20.086856770000 22.601184380000 23.927297210000 21.035876060000 19.575999270000 22.629245990000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 11.74633320000 15.248375080000 15.445746030000 13.140988870000 14.958356150000 10.921811340000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.592630810000 22.631010720000 24.459234590000 23.91774630000 21.030997440000 19.654137750000 22.684377160000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.97011551800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000
57 H [Cee 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.6829590000 13.166854510000 15.120157300000 10.870267570000 11.654547110000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.09931850000 20.486856770000 22.60184380000 24.589817230000 23.927297210000 23.927297210000 19.57599270000 22.629245990000 25.505325190000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000	57 H /X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.524235740000 11.746333320000 12.289375080000 13.14098870000 14.958356150000 10.921811340000 11.751158850000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.0974560370000 20.0974560370000 20.592630810000 22.4459234590000 23.919774630000 21.030997440000 19.654137750000 22.684377160000 25.400367520000	1.893938093000 0.156744398900 1.86235869100 -1.02468278000 -2.412704224000 -2.4037078100 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.60829590000 11.685862530000 12.180530040000 15.442192240000 13.166854510000 13.166854510000 11.654547110000 11.654547110000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.09631850000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000 22.629245990000 25.505325190000 25.505325190000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710190000 2.871789423000 -1.510362883000 -3.23200940000	57 H C C C C C C C C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁷ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.746333320000 12.289375080000 13.40988870000 13.40988870000 14.95356150000 10.921811340000 11.751158850000 15.01970520202	1.758999353000 2.519003230000 24.024249040000 24.865717960000 20.007919270000 20.592630810000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 22.684377160000 22.684377160000 23.40367520000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.60829590000 11.685862530000 12.180530040000 13.166854510000 13.166854510000 13.166854510000 14.69277980000 14.968927980000	1.697590965000 24.031669560000 24.858052630000 20.09931850000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 21.035876060000 19.575999270000 22.629245990000 25.505325190000 23.564149590000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000	57 H (Cec 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 14 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.74633320000 12.289375080000 15.445746030000 13.140988870000 14.958356150000 10.921811340000 11.751158850000 15.018705030000	1.758993353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.592630810000 22.63101720000 24.459234590000 23.919774630000 21.03097440000 19.654137750000 25.40367520000 23.525188870000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.4329590000 13.166854510000 15.422192240000 13.166854510000 15.120157300000 10.870267570000 11.654547110000 14.968927980000 14.075454980000	1.697590965000 24.031669560000 24.4858052630000 20.0979705460000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 21.035876060000 19.57599270000 22.629245990000 25.505325190000 23.564149590000 24.205785870000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 14 C 15 Si 6 N 10 N	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.5242357400000 15.445746030000 13.14098870000 14.958356150000 10.921811340000 11.751158850000 15.018705030000 14.108578690000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 23.919774630000 21.030997440000 19.654137750000 22.684377160000 23.525188870000 24.142866800000	1.893938093000 0.156744398900 1.862358691000 -1.02468278000 -2.412704224000 -2.300370781000 1.420146387000 0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.278353814000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 13.1668545100000 15.42015730000 10.870267570000 11.654547110000 14.968927980000 15.473633220000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 23.927297210000 23.927297210000 23.957599270000 23.564149590000 23.56785870000 23.67285870000 23.67285870000	1.861140125000 [MN* ₂ X ₃] ^q /q=2- ,1: 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.0246656552000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 1.510362883000 3.257827189000 4.217356126000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 12 C 12 Si 3 Si 4 Si 5 Si 6 N 7 N 10 Si 10	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 14.597365980000 14.524235740000 11.74633320000 15.445746030000 13.14098870000 14.958356150000 10.921811340000 11.751158850000 15.018705030000 14.108578690000 15.532077720000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.007919270000 20.592630810000 22.613010720000 23.919774630000 21.030997440000 22.64377160000 23.525188870000 23.525188870000 23.52518860000 23.52518870000 23.52518870000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.278353814000 4.222054591000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 16 H 16 H	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 12.180530040000 15.42192240000 13.166854510000 15.120157300000 10.870267570000 11.654547110000 14.968927980000 14.075454980000 15.473633220000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.09931850000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000 22.629245990000 23.505325190000 23.505325190000 23.672297340000 23.672297340000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.51052883000 3.242300904000 3.257827189000 4.217356126000 4.31756626000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 16 H 17 H	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 11.74633320000 12.289375080000 13.140988870000 13.140988870000 14.958356150000 10.921811340000 11.751158850000 14.108578690000 15.532077720000 14.108578090000	1.758999353000 1.758999353000 2 22.519003230000 24.024249040000 24.865717960000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 25.400367520000 23.525188870000 24.4286880000 23.652253430000 23.652253430000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 4.222054591000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 12.180530040000 13.46854510000 15.42122240000 13.166854510000 15.427370000 11.654547110000 14.968927980000 14.075454980000 15.473633220000 14.632029430000	1.697590965000 22.521990030000 24.031669560000 24.858052630000 20.0979705460000 20.09631850000 22.601184380000 22.601184380000 23.927297210000 21.033876060000 19.575999270000 22.629245990000 22.52935190000 23.564149590000 23.564149590000 23.564149590000 23.567297340000 23.672297340000 23.672297340000 22.518055830000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.30709250100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960965000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 14 C 16 H 17 H	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 12.289375080000 13.14098870000 13.14098870000 14.958356150000 10.921811340000 11.751158850000 15.018705030000 14.108578690000 15.532077720000 14.710751330000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 23.919774630000 21.030997440000 19.654137750000 25.400367520000 23.525188870000 24.142866800000 23.652253430000 22.470967180000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.278353814000 4.222054591000 3.191098854000
57 H [Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.68299590000 13.166854510000 15.422192240000 15.422192240000 16.54547110000 14.968927980000 14.075454980000 15.473633220000 14.632029430000 16.799336890000	1.697590965000 24.031669560000 24.458052630000 20.09931850000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 22.632245990000 23.564149590000 23.55325190000 23.564149590000 23.5784694750000 25.784694750000	1.861140125000 [MN*2X3] ⁹ /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 16 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.4224357400000 13.14098870000 13.14098870000 13.14098870000 14.958356150000 10.921811340000 11.751158850000 15.018705030000 14.108578690000 15.532077720000 14.710751330000 16.792925900000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.0974560370000 20.0974560370000 20.592630810000 22.631010720000 23.919774630000 22.634377160000 25.40367520000 23.525188870000 24.142866800000 23.652253430000 22.470967180000 25.783871150000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.40370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.278353814000 4.222054591000 3.191098854000 2.341035436000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 15.442192240000 15.442192240000 15.42192240000 10.870267570000 11.654547110000 14.958927980000 14.075454980000 16.379336890000 16.799336890000 17.575395600000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.09631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000 22.629245990000 23.56325190000 23.56325190000 23.57858870000 23.672297340000 22.518055830000 25.784694750000 26.163449470000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710190000 2.871789423000 1.510362883000 3.257827189000 4.217356126000 3.17660965000 2.334174613000 1.652083936000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 14 C 15 H 16 H 17 H 16 H 17 H 16 H 17 H	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 14.597365980000 14.524235740000 14.5242357400000 15.445746030000 13.140988870000 14.98356150000 14.98356150000 14.01875650000 14.108578690000 14.515380000 16.592925900000 17.547954600000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.6300072000 22.439234590000 23.919774630000 21.030997440000 25.400367520000 23.525188870000 23.65253430000 22.47967180000 25.783871150000 26.188210970000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.27835814000 4.222054591000 3.191098854000 2.341035436000 1.650208060000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 16 H 17 H	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 15.120157300000 15.120157300000 15.120157300000 14.968927980000 14.075454980000 14.075454980000 14.075454980000 15.473633220000 14.679336890000 17.575395600000 17.2575395600000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000 22.629245990000 23.564149590000 23.564149590000 23.57805830000 23.57805830000 25.784694750000 25.784694750000 25.6163449470000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.510362883000 3.242300904000 3.275827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000	57H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 14 C 15 H 16 H 17 H 18 C 19 H 19 H 10 H	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 15.445746030000 15.445746030000 13.14098870000 14.958356150000 10.921811340000 11.751158850000 15.532077720000 14.710751330000 16.79292590000 17.547954600000 17.547954600000	1.758993353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.592630810000 22.63101720000 24.439234590000 23.919774630000 21.030997440000 19.654137750000 25.400367520000 23.52518870000 24.142866800000 23.652253430000 22.470967180000 25.488210970000 26.88210970000 26.88210970000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.92067239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.27833814000 4.222054591000 3.3191098854000 2.341035436000 1.650208060000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.431817110000 14.608299590000 15.422192240000 15.422192240000 15.422192240000 15.426545710000 15.426545710000 14.968927980000 14.075454980000 14.632029430000 16.799336890000 17.575395600000 17.229854790000	1.697590965000 24.031669560000 24.858052630000 20.0979705460000 20.09631850000 20.485856770000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 22.6292459902000 25.505325190000 23.564149590000 23.564149590000 23.5784694750000 25.784694750000 25.784694750000 25.6633000000	1.861140125000 [[MN*2X3] ⁹ /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 15.445746030000 15.445746030000 13.14098870000 14.958356150000 10.921811340000 15.51158850000 15.513705030000 14.108578690000 15.532077720000 14.710751330000 16.792925900000 17.547954600000 17.547954600000 17.241844080000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 23.919774630000 21.030997440000 19.654137750000 25.400367520000 23.525188870000 24.142866800000 23.652253430000 22.470967180000 25.783871150000 25.78531200000	1.893938093000 0.156744398900 1.862358691000 -1.02468278000 -2.412704224000 -2.300370781000 1.420146387000 0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.278353814000 4.222054591000 3.191098854000 2.341035436000 1.650208060000 3.348446402000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.000453060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 13.166854510000 15.422192240000 16.54547110000 11.654547110000 11.654547110000 14.968927980000 14.9582780000 14.075454980000 15.473633220000 14.575395600000 17.575395600000 17.229854790000 15.969138580000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 23.927297210000 23.575999270000 23.56149590000 23.57285870000 23.57285870000 23.57285870000 23.57285870000 25.784694750000 25.762303000000 25.762303000000 26.506817850000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 1.510362883000 3.257827189000 4.217356126000 3.176560995000 2.334174613000 1.652083936000 3.349581831000 2.336243794000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 10 N 11 C 12 C 13 C 13 C 14 C 13 C 14 C 14 C 14 C 15 H 16 H 17 H 16 H 17 H 18 C 19 H 10 H	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.5242357400000 11.746333320000 13.140988870000 15.445746030000 13.140988870000 14.958356150000 10.921811340000 15.532077720000 14.710751330000 16.792925900000 17.547954600000 17.241844080000 15.947557770000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.974560370000 20.007919270000 20.592630810000 23.59234590000 23.919774630000 24.459234590000 23.919774630000 25.40367520000 23.525188870000 23.525188870000 23.5253430000 25.783871150000 25.783871150000 25.78531200000 25.78531200000 26.48979150000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.278353814000 4.222054591000 3.191098854000 2.341035436000 1.650208060000 3.348446402000 2.366539423000
57 H CCe 1 Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 16 C 19 H 20 H	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.431817110000 11.685862530000 13.166854510000 15.120157300000 15.120157300000 14.698227880000 14.654547110000 14.968927880000 14.67545480000 15.473633220000 16.799336890000 17.259854790000 15.969138580000 15.969138580000 15.969138580000 15.969138580000 15.969138580000	1.697590965000 24.031669560000 24.858052630000 20.099631850000 20.099631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876060000 19.575999270000 22.629245990000 23.564149590000 23.5785870000 23.57858870000 23.578694750000 25.784694750000 25.784694750000 25.784694750000 25.784694750000	1.861140125000 [[MN*2X3] ⁹ /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 3.257827189000 3.257827189000 3.349581831000 2.336243794000 2.36243794000 2.048232925000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 14 C 16 C 17 C 18 C 19 C 19 C 19 C 19 C 10 C	4.168670305000 CN,NC /GA CN,NC /GA (III)N*2NC3] ²⁻ 13.466098780000 15.997065980000 15.997065980000 11.553493270000 14.409736670000 14.524235740000 15.445746030000 15.445746030000 13.140988870000 14.958356150000 14.958356150000 14.08578690000 15.532077720000 17.541844080000 15.94755770000 15.975390820000	1.758993353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.592630810000 22.63101720000 24.459234590000 23.919774630000 21.03097440000 19.654137750000 25.400367520000 23.52518870000 24.142866800000 23.652253430000 24.142867180000 25.788371150000 26.818210970000 25.75853120000 26.48797150000 25.47935012000 25.75853120000 26.48797150000 26.48797150000 26.48797150000 27.906155160000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.278353814000 4.222054591000 3.348446402000 2.366539423000 2.01779919000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 H 23 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.431817110000 13.46825950000 13.166854510000 15.422192240000 13.166854510000 14.968927980000 14.075454980000 14.968927980000 14.632029430000 16.799336890000 17.575395600000 17.575395600000 17.229854790000 15.969138580000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 13.96852500000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.692250120000 17.575395600000 17.69225012000 17.69225012000 17.692250120000 17.69225012000 17.69225012000 17.69225012000 17.6925012000 17.6925012000 17.6925012000 17.2985470000 17.6925012000 17.6925012000 17.6925012000 17.59550000 17.59550000 17.59550000 17.59550000 17.59550000 17.69225012000 17.59550000 17.59550000 17.59550000 17.59550000 17.69225012000 17.59550000 17.5955	1.697590965000 24.031669560000 24.888052630000 20.0979705460000 20.09631850000 20.488856770000 22.601184380000 23.927297210000 23.927297210000 23.927297210000 23.525325190000 23.55325190000 23.564149590000 23.5728970000 23.57297340000 23.57284694750000 25.762303000000 26.506817850000 22.887038500000 22.887038500000 22.887038500000 23.8844072000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 0.30709250100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.33427474000 2.048232925000	57 H CCe 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 10 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.99705980000 15.99705980000 14.409736670000 14.524235740000 14.5242357400000 13.14098870000 13.14098870000 13.14098870000 14.958356150000 14.958356150000 14.08578690000 15.532077720000 14.710751330000 15.732925900000 17.547954600000 17.241844080000 17.735930820000 17.43330050000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 25.400367520000 23.525188870000 24.142866800000 23.652253430000 22.470967180000 25.78531200000 26.48797150000 22.618210970000 25.78531200000 24.6155160000 23.9197450000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.348446402000 2.341035436000 1.650208060000 3.348446402000 2.341935436000 1.65020806000 1.650208060000 1.650208060000 1.6502080600000000000000000000000000000000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.000453060000 11.569644710000 14.43187110000 14.43187110000 14.60829590000 13.166854510000 15.422192240000 15.422192240000 15.42657570000 11.654547110000 14.968927980000 14.632029430000 14.632029430000 15.473633220000 14.575395600000 17.575395600000 17.229854790000 15.969138580000 17.692250120000 17.377856760000	1.697590965000 24.031669560000 24.458052630000 20.0979705460000 20.09631850000 20.486856770000 21.63817230000 23.927297210000 23.927297210000 23.927297210000 23.564149590000 23.564149590000 23.572297340000 23.672297340000 25.784694750000 25.784694750000 25.784694750000 25.762303000000 25.66317850000 22.887038500000 21.838449770000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.048232925000 1.935614470000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 13 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 14 C 16 17 C 16 17 C 17	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.4224357400000 13.14098870000 13.14098870000 14.958356150000 10.921811340000 15.5135856150000 15.5137770000 15.532077720000 15.445746030000 15.532077720000 17.241844080000 15.947557770000 17.735930820000 17.443309590000	1.758999353000 2.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.309974630000 21.30997440000 19.654137750000 22.684377160000 23.525188870000 24.142866800000 23.5251887150000 24.428046800000 25.783871150000 26.183210970000 25.78531200000 26.487979150000 22.906155160000 21.854857540000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.412704224000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.72964804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.278353814000 4.222054591000 3.348446402000 2.366539423000 2.017799619000 1.877097928000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H	4.209326609000 (IIII)N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.431817110000 14.608299590000 11.685862530000 13.166854510000 15.442192240000 16.479633220000 14.95892780000 15.473633220000 16.799336890000 17.575395600000 17.229854790000 15.969138580000 17.692250120000 17.377856760000 18.159969350000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 23.575999270000 24.205785870000 23.564149590000 23.5784694750000 23.5784694750000 25.78630300000 25.784694750000 25.762303000000 25.762303000000 26.1634494770000 25.763817850000 22.887038500000 21.838449770000 22.997066110000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 1.510362883000 3.257827189000 4.217356126000 3.17660965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.362232925000 1.935614470000 3.040931610000	57 H (Ce 1 Ce 2 Si 3 Si 5 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 14 C 14 C 14 C 14 C 15 C 14 C 16 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 14.597065980000 14.524235740000 14.5242357400000 15.445746030000 15.445746030000 14.988356150000 14.988356150000 15.91158850000 15.53207720000 14.710751330000 16.792925900000 17.241844080000 15.947557770000 17.43309590000 17.443309590000 18.201022110000	1.758999353000 2.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.3101720000 24.459234590000 23.919774630000 21.030997440000 25.40367520000 23.52518870000 24.4286680000 23.52518870000 24.42456820000 25.783871150000 26.188210970000 25.78531200000 26.487979150000 21.854857540000 22.99565750000	1.893938093000 1.802358691000 -1.024682780000 -2.412704224000 -2.30037781000 1.420146387000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836182000 3.253836182000 1.650208060000 3.348446402000 2.36539423000 2.017799619000 1.877097928000 3.013428973000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 24 H 25 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.63299590000 13.166854510000 13.166854510000 15.42192240000 13.166854510000 15.42192240000 14.958927980000 14.954547110000 14.968927980000 14.95454980000 15.473633220000 14.632029430000 15.757395600000 17.575395600000 17.229854790000 15.969138580000 17.692250120000 18.15999350000 18.15999350000 18.15999350000 18.15999350000 18.5978903000 13.136764920000 13.136764920000 13.144768220000 13.14476820000 13.14476820000 14.5250120000 14.54768920000 15.575355600000 15.575355600000 15.599138580000 15.599138580000 15.47454768920000 15.47454768920000 15.4745475700000 15.474547570000 15.474547570000 15.474547570000 15.474547570000 15.474547570000 15.474547570000 15.474547570000 15.474547570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.474557570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.474557570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.4745475570000 15.47454755700000 15.47454755700000 15.47454757700000000000000000000000000000	1.697590965000 24.03166956000 24.48805263000 20.979705460000 20.09931850000 20.485856770000 22.601184380000 24.589817230000 21.031876600000 19.575999270000 22.629245990000 22.6325190000 23.564149590000 23.5672297340000 23.572497340000 25.5784694750000 26.163449470000 25.76230300000 26.506817850000 21.838449770000 22.99706110000 23.1092156000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960955000 2.334174613000 1.65083936000 3.349581831000 2.336243794000 2.048232925000 1.935614470000 3.040931610000 1.284058291000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 4 Si 5 Si 6 N 7 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 14 C 19 N 10 N 11 C 12 C 14 C 19 H 12 C 14 C	4.168670305000 CN ,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.997065980000 15.997065980000 14.409736670000 14.524235740000 14.524235740000 15.445746030000 15.445746030000 13.140988870000 14.958356150000 14.958356150000 14.08578690000 15.532077720000 14.710751330000 16.792925900000 17.547954600000 17.547954600000 17.443309590000 18.494340460000 18.494340460000	1.758993353000 2 22.519003230000 24.024249040000 24.852717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 19.654137750000 22.684377160000 23.525188870000 24.142866800000 23.52518870000 24.142867180000 25.788371150000 26.48797150000 25.7883710000 25.7883710000 26.487979150000 21.85487540000 21.854857540000 23.154423600000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.92067239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.278353814000 4.22204591000 3.348446402000 2.366539423000 1.877097928000 3.013428973000 1.26103933000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 C	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.18397006000 11.569644710000 14.431817110000 14.431817110000 14.430829590000 15.422192240000 15.422192240000 15.422192240000 15.4261730000 10.870267570000 11.654547110000 14.968927980000 14.95454980000 15.473633220000 14.632029430000 15.757395600000 17.575395600000 17.575395600000 17.579385600000 17.229854790000 15.969138580000 17.377856760000 18.459478920000 18.454788920000 18.559693260000 19.558934680000 11.59969350000 11.559693450000 13.55693360000 13.55969350000 13.55969350000 13.5569350000 13.5569350000 13.55969350000 13.5569350000 13.55969350000 13.5589530000 13.5589530000 13.5589530000 13.5589530000 13.55895350000 13.55895350000 13.55895350000 13.55855550000 13.558555555 13.55855555555555555 14.5555555555555555555555	1.697590965000 24.031669560000 24.858052630000 20.0979705460000 20.09631850000 20.485805770000 22.601184380000 24.589817230000 21.035876060000 19.57599270000 22.629245990000 23.564149590000 23.5643950000 23.572297340000 25.784694750000 25.784694750000 25.762300000 25.762300000 25.762300000 21.838449770000 22.887038500000 21.838449770000 23.100921560000 23.100921560000	1.861140125000 [MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.40934487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.30709250100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.24320904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.346232925000 1.935614470000 3.040931610000 1.284058291000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 17 N 10 C 10 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.99705980000 11.553493270000 14.409736670000 14.524235740000 11.746333320000 13.14098870000 13.14098870000 13.14098870000 13.14098870000 14.5215855010000 15.532077720000 14.710751330000 15.532077720000 17.547954600000 17.547954600000 17.241844080000 15.947557770000 17.443309590000 18.494340460000 18.49430460000 18.49430460000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.63101720000 22.631010720000 23.919774630000 21.03097440000 19.654137750000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.78531200000 26.48379150000 22.906155160000 21.854857540000 23.154423600000 23.154423600000 23.5253440000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.3191098854000 2.341035436000 1.650208060000 3.348446402000 2.365539423000 2.017799619000 1.877097928000 3.01428973000 1.260103933000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 C	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.00045306000 11.569644710000 14.431817110000 14.63299590000 13.166854510000 15.422192240000 15.422192240000 16.654547110000 14.958927980000 16.679336890000 17.575395600000 17.575395600000 17.599316850000 17.59953500000 17.377856760000 18.159969350000 18.45476892000 18.5568923480000	1.697590965000 24.031669560000 24.858052630000 20.09931850000 20.09931850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 23.927297210000 23.524149590000 23.56149590000 23.5785870000 23.5785870000 25.784694750000 25.76230300000 25.76230300000 25.76230300000 22.887038500000 21.838449770000 22.997066110000 23.10921560000 26.70762375000	1.861140125000 [MN*2X3] ^q /q=2,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 1.510362883000 3.257827189000 4.217355126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.36223925000 1.935614470000 3.040931610000 1.284058291000 -0.922181641900	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 13 C 14 C 12 C 13 C 14 C 12 C 13 C 14 C 12 C 13 C 14 C 12 C 13 C 14 C	4.168670305000 4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.997065980000 15.997065980000 14.597065980000 14.5242357400000 14.5242357400000 13.140988700000 13.140988700000 14.958356150000 14.958356150000 15.5132077720000 14.710751330000 15.532077720000 17.241844080000 15.947557770000 17.4139598020000 17.413309590000 18.201022110000 18.494340460000 15.513286660000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.592630810000 22.5130000 23.919774630000 24.459234590000 23.919774630000 25.40367520000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.783871150000 26.487979150000 22.906155160000 21.854857540000 22.99565750000 23.154423600000 26.703524490000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.348446402000 2.341035436000 1.650208060000 3.348446402000 2.366539423000 2.017799619000 1.877097928000 3.013428973000 1.260103933000 -0.912934310300
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 C 27 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.431817110000 13.166854530000 15.422192240000 15.424192240000 15.424192240000 15.42454510000 14.968927980000 14.075454980000 14.075454980000 15.473633220000 14.679336890000 17.57539560000 17.5739560000 17.692250120000 17.37856760000 18.159969350000 18.454768920000 15.568923480000 14.47556370000	1.697590965000 24.031669560000 24.858052630000 20.979705460000 20.009631850000 20.486856770000 22.601184380000 24.589817230000 23.927297210000 21.035876660000 23.927297210000 22.629245990000 23.564149590000 23.5632519000 23.57858870000 23.578684750000 25.786230300000 25.786349470000 25.78230300000 26.163449470000 22.518058850000 21.838449770000 22.97066110000 23.100921560000 26.707623750000 26.672752000	1.861140125000 [[MN*2X3] ⁹ /q=2-,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.510362883000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.364232925000 1.935614470000 3.040931610000 1.284058291000 -0.922181641900 -0.853927899600	57 H (X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 14 C 14 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H	4.168670305000 CN,NC /GA CN,NC /GA CN,NC /GA 13.466098780000 15.997065980000 15.997065980000 14.409736670000 14.524235740000 14.524235740000 15.445746030000 15.445746030000 13.140988870000 14.958356150000 14.958356150000 14.08578690000 15.532077720000 14.710751330000 15.532077720000 17.241844080000 15.947557770000 17.41844080000 17.43395930000 17.443309590000 18.201022110000 18.494340460000 15.513286660000 14.417308250000	1.758993353000 21.5519003230000 24.024249040000 24.02429040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.592630810000 22.63101720000 24.45923459000 23.919774630000 21.03097440000 19.654137750000 22.64377160000 23.52518870000 23.652253430000 23.652253430000 25.788371150000 26.482797150000 22.906155160000 23.85487540000 23.85487540000 23.99555750000 23.154423600000 26.703524490000 26.70354490000 26.703576680000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.34844602000 2.366539423000 2.017799619000 1.877097928000 3.013428973000 1.260103933000 -0.912934310300 -0.912934310300
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 C 27 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 11.569644710000 14.431817110000 14.431817110000 13.4682530000 13.166854510000 15.42192240000 13.166854510000 15.42192240000 14.968927980000 14.954547110000 14.968927980000 14.95454980000 14.7575395600000 17.575395600000 17.575395600000 17.229854790000 15.969138580000 17.377856760000 18.159693000 18.45476892000 15.568923480000 15.568923480000 15.568923480000 15.4769390000 15.568923480000 15.568923480000 14.476536370000 15.911769390000	1.697590965000 24.031669560000 24.4858052630000 20.0979705460000 20.09631850000 20.48585670000 22.601184380000 24.589817230000 23.927297210000 23.927297210000 22.639245990000 25.505325190000 23.564149590000 23.572397340000 23.572397340000 23.672297340000 25.76230300000 25.76230300000 25.76230300000 22.69817850000 22.69817850000 22.897066110000 23.100921560000 23.100921560000 26.822435220000 26.82245220000 26.82245220000 26.82245220000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.990801766500 0.30709250100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.24230904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.048232925000 1.935614470000 3.0409316110000 0.083327899600 -1.822140483000	57 H 7 X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 19 H 12 C 14 C 14 C 14 C 14 C 19 H 12 C 14 H 12 C 14	4.168670305000 4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.99705980000 11.553493270000 14.409736670000 14.524235740000 13.14098870000 13.14098870000 13.14098870000 13.14098870000 14.958356150000 14.108578690000 15.532077720000 14.710751330000 15.532077720000 17.241844080000 15.735930820000 17.241844080000 15.735930820000 18.49340460000 18.49340460000 15.513286660000 14.417308250000 14.417308250000 15.855975610000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 22.631010720000 24.459234590000 23.919774630000 21.030997440000 25.40367520000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.78531200000 26.487979150000 21.854857540000 23.9525440000 23.5254430000 24.4542600000 25.70837640000 25.906587680000 27.54388950000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.241035436000 1.65028060000 3.348446402000 2.366539423000 1.670797928000 3.013428973000 1.260103933000 -0.91293410300 0.889569545900 -1.805026826000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 H 26 H 26 H 26 H 26 H 27 H 28 H 26 H 26 H 27 H 28 H 26 H 26 H 27 H 28 H 26 H 27 H 28 H 26 H 27 H 28 H 26 H 27 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.569644710000 14.43187110000 14.630299590000 15.422192240000 15.422192240000 15.422192240000 15.12015730000 10.870267570000 11.654547110000 14.968927980000 14.95454980000 15.473633220000 16.799336890000 17.575395600000 17.575395600000 17.229854790000 15.969138580000 17.692250120000 17.377856760000 18.159969350000 18.45476892000 15.96138580000 14.476536370000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91176930000 15.91769 15.91769000 15.91767 15.9176 15.9176 15.9176 15.9176 15.917 15.9176	1.697590965000 24.031669560000 24.458052630000 20.979705460000 20.979705460000 20.486856770000 21.63817230000 23.927297210000 23.927297210000 23.927297210000 23.524149590000 23.564149590000 23.57245870000 23.672297340000 25.784694750000 25.784694750000 25.784694750000 25.78230300000 25.7824694750000 25.782300000 25.78245920000 25.78245920000 25.78245920000 25.782300000 25.78245920000 22.88703850000 21.838449770000 23.100921560000 26.622455220000 26.77623750000 26.822455220000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.245173160000 27.2451731600000 27.2451731600000 27.2451731600000 27.2451731600000 27.2451731600000 27.2451731600000 27.245173160000000000 27.245173160000000000000 27.2451731600000000000000000000000000000000000	1.861140125000 [[MN*2X3] ⁹ /q=2,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.307092500100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.48232925000 1.93561447000 3.040931610000 1.284058291000 -0.922181641900 -0.85392789600 -1.822140483000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.4224357400000 15.445746030000 15.445746030000 13.14098870000 14.958356150000 10.921811340000 15.513277720000 14.710751330000 16.792925900000 17.547954600000 17.547954600000 17.241844080000 15.947557770000 17.443309590000 18.201022110000 18.494340460000 15.432850000 14.417308250000 14.417308250000 15.4330300000	1.758999353000 2 22.519003230000 24.024249040000 24.85717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.30997460000 23.919774630000 21.03097440000 19.654137750000 25.400367520000 23.525188870000 24.142866800000 23.5251887150000 25.783871150000 26.48210970000 25.7838710000 26.48377150000 26.48377150000 26.48377150000 27.57838710000 26.48377150000 26.48377150000 26.48379150000 27.906155160000 21.854857540000 22.99565750000 23.154423600000 26.790587680000 27.254388950000 27.254388950000 27.254388950000 27.254388950000 27.254388950000 27.254388950000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.412704224000 -2.412704224000 1.920673239000 0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.3191098854000 2.341035436000 1.650208060000 3.348446402000 2.36539423000 2.017799619000 1.877097928000 3.01428973000 1.260103933000 -0.912934310300 -0.859569545900
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 H 27 H 28 H 29 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.00045306000 11.569644710000 14.431817110000 14.68299590000 13.16854510000 15.442192240000 15.442192240000 16.54347110000 14.958927880000 16.54347110000 14.958927880000 16.799336890000 17.575395600000 17.575395600000 17.599386890000 17.595395600000 17.596938580000 17.692250120000 17.377856760000 18.159969350000 18.159969350000 18.5568923480000 14.476536370000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.90000 15.911769390000 15.90000 15.900000 15.90000000 15.9000000 15.9000000000000000000000000000000000000	1.697590965000 24.031669560000 24.858052630000 20.09931850000 20.09931850000 20.486856770000 22.601184380000 24.58817230000 23.927297210000 23.927297210000 23.927297210000 23.5245990000 25.50325190000 23.564149590000 23.57285870000 23.57285870000 23.57285870000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.76230300000 25.7623750000 26.60817850000 22.8870850000 22.8870850000 22.8870850000 22.997066110000 23.10921560000 26.707623750000 26.822435220000 27.245173160000 27.245173160000	1.861140125000 [MN*2X3] ^q /q=2,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 1.510362883000 3.257827189000 4.217356126000 3.3175660965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.336243794000 2.36223925000 1.935614470000 3.040931610000 1.284058291000 -0.922181641900 0.853927899600 -1.822140483000 -0.44317531080	57 H 7 X=0 1 Ce 2 Si 3 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 14 C 13 C 14	4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 16.202908360000 15.997065980000 11.553493270000 14.409736670000 14.5242357400000 13.140988700000 15.445746030000 14.958356150000 14.958356150000 14.10751330000 14.01751330000 15.532077720000 14.710751330000 15.947557770000 17.241844080000 15.947557770000 17.4134095900000 18.201022110000 18.494340460000 15.513286660000 14.417308250000 15.855975610000 15.855975610000 15.943039300000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 21.3010720000 24.459234590000 23.919774630000 25.40367520000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.783871150000 26.487979150000 22.996155160000 23.15442560000 23.15442360000 26.703524490000 26.70357680000 27.191018610000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.412704224000 -2.30037781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.348446402000 2.365539423000 1.65028066000 3.34844602000 2.365539423000 1.65028066000 3.013428973000 1.6502806000 3.013428973000 1.260103933000 -0.912934310300 -0.859569545900 -1.805026826000 -0.02534835790
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 H 22 H 24 H 25 H 26 H 29 H 30 C	4.209326609000 ((III))N*2CN3) ²⁻ 13.490106620000 16.00045306000 11.569644710000 14.431817110000 14.63299590000 13.166854510000 15.42192240000 15.42192240000 15.42192240000 15.42192240000 15.42192240000 14.968927980000 14.954547110000 14.968927980000 14.95454710000 15.47363320000 14.632029430000 15.57395600000 17.29854790000 15.969138580000 17.37856760000 18.15999350000 18.454768920000 15.568923480000 15.568923480000 15.568923480000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.911769390000 15.98015150000 17.898015150000	1.697590965000 24.031669560000 24.488052630000 20.097705460000 20.099705460000 20.09931850000 20.486856770000 21.63887670000 21.033876060000 19.575999270000 22.629245990000 23.527297210000 23.524149590000 23.564149590000 23.572497340000 23.572497340000 25.576230300000 26.634494750000 26.63474970000 21.8378010000 22.97066110000 23.10921560000 22.9716610000 22.9716610000 22.97245173160000 27.245173160000 27.245173160000 27.188378010000 24.76023380000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 2.030757126000 1.490309387000 2.024665652000 -0.990801766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.510362883000 3.242300904000 3.257827189000 4.217356126000 3.176960955000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.36243794000 3.40931610000 1.284058291000 -0.922181641900 -0.853927899600 -1.822140483000 -0.44317531080 -0.279242689000	57 H (X=0 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 9 N 10 N 11 C 12 C 13 C 14 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 20 H 21 H 22 H 23 H 24 H 25 H 26 H 27 H 26 H 27	4.168670305000 4.168670305000 CN,NC /GA (III)N*2NC3] ² 13.466098780000 15.997065980000 15.997065980000 14.409736670000 14.524235740000 14.524235740000 15.445746030000 15.445746030000 13.14098870000 14.958356150000 14.08578690000 14.710751330000 15.532077720000 17.24184408000 15.94755770000 17.44309590000 18.20102110000 18.494340460000 15.513286660000 14.417308250000 18.494340460000 15.513286660000 14.417308250000 15.94309300000 15.94309300000 15.94309300000 15.9445220000	1.758993353000 24.0249040000 24.0249040000 24.65717960000 20.97456037000 20.97456037000 20.97456037000 20.97456037000 20.97456037000 20.97456037000 22.63101720000 24.43923459000 23.919774630000 21.030997440000 19.654137750000 22.540367520000 23.525188870000 24.14286800000 23.5253430000 24.14286800000 25.788371150000 26.48210970000 25.788371200000 26.48797150000 22.906155160000 23.154423600000 24.8437540000 23.9055750000 23.154423600000 24.7935488950000 27.254388950000 27.191018610000 24.827309250000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.92067239000 -0.970115351800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.348446402000 2.366539423000 2.017799619000 1.87007928000 3.01342897300 1.260103933000 -0.912934310300 -0.859569545900 -1.805026826000 -0.025534835790 -1.242809859000
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 G 23 H 24 H 25 H 24 H 25 H 24 H 25 H 26 H 27 H 28 H 29 H 20 H 21 H 20 H 21 H 22 H 23 H 24 H 25 H 26 H 27 H 27 H 28 H 29 H 20 H 21 H 26 H 27 H 27 H 28 H 29 H 20 H 21 H 20 H 21 H 20 H 21 H 20 H 21 H 22 H 23 H 24 H 25 H 26 H 27 H 27 H 27 H 28 H 29 H 20 H 20 H 21 H 20 H 21 H 25 H 26 H 27 H 27 H 27 H 28 H 29 H 20 H 21 H 20 H 21 H 22 H 25 H 26 H 27 H 27 H 26 H 27 H 27 H 27 H 26 H 27 H 27 H 26 H 27 H 27 H 26 H 27 H 27 H 26 H 27 H	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 11.569644710000 14.431817110000 14.431817110000 14.4308299590000 15.422192240000 15.422192240000 15.422192240000 15.42192240000 15.12015730000 10.870267570000 11.654547110000 14.968927980000 14.968927980000 15.473633220000 14.632029430000 15.757395600000 17.575395600000 17.575395600000 17.575395600000 17.575395600000 17.575395600000 17.575395600000 15.969138580000 17.69220120000 15.568923480000 15.568923480000 15.91769330000 16.023880640000 17.898015150000 18.449094280000	1.697590965000 24.031669560000 24.4858052630000 20.0979705460000 20.09631850000 20.485805770000 22.601184380000 21.4589817230000 21.035876060000 19.57599270000 22.629245990000 22.505325190000 23.564149590000 23.572297340000 23.572297340000 25.76230300000 25.76230300000 25.76230300000 21.838449770000 22.887038500000 21.838449770000 23.30092156000 23.30092156000 26.822435220000 26.822435220000 27.245173160000 27.245173160000 27.245173160000 27.245173160000	1.861140125000 [[MN*2X3] ^q /q=2-,1 0.130086868000 1.867627026000 -1.036970627000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 0.30709250100 -1.744084474000 2.031710199000 2.871789423000 -1.510362883000 3.24230094000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.336243794000 2.336243794000 1.935614470000 3.040931610000 1.284058291000 -0.853927899600 -1.822140483000 -0.853927899600 -1.822140483001 -0.853927899600 -1.822140483001 -0.4124817531080 -1.279242689000 -0.412481745200	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C	4.168670305000 4.168670305000 CN,NC /GA (III)N*2NC3] ²⁻⁵ 13.466098780000 15.99705980000 15.99705980000 14.52435740000 14.524235740000 14.524235740000 15.445746030000 15.445746030000 15.445746030000 15.51158850000 15.513755030000 14.710751330000 15.947557770000 17.241844080000 15.947557770000 17.443309590000 18.49430460000 15.513286660000 18.49430450000 15.513286660000 15.513286660000 15.513286660000 15.513286660000 15.513286000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.513286000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.5132860000 15.515757 15.515757 15.515757 15.51575757 15.5157575757575757575757575757	1.758999353000 22.519003230000 24.024249040000 24.855717960000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.974560370000 20.592630810000 22.631010720000 23.919774630000 21.030997440000 19.654137750000 25.400367520000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.783871150000 26.487979150000 22.99565750000 23.15442360000 23.99565750000 23.15442360000 26.703524490000 26.703524490000 27.254388950000 27.254388950000 27.191018610000 24.827309250000 25.39416950000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.300370781000 1.420146387000 1.920673239000 -0.97011551800 0.311563038000 -1.729664804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.348446402000 2.341035436000 1.650208060000 3.348446402000 2.365539423000 2.017799619000 1.870709728000 3.013428973000 1.260103933000 -0.85956545900 -1.805026826000 -0.025534835790 -1.242809859000 -0.372316266100
57 H [Ce 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 C 27 H 28 H 29 H 30 C 31 C 32 H 29 H 30 C 31 C 32 H 32 C 32 C 33 C 35	4.209326609000 ((III))N*2CN3] ²⁻ 13.490106620000 16.183970060000 16.000453060000 11.56944710000 14.431817110000 14.431817110000 14.6829590000 13.166854510000 15.42192240000 15.42192240000 15.420157300000 10.870267570000 11.654547110000 14.968927980000 14.075454980000 15.473633220000 15.473633220000 17.575395600000 17.575395600000 17.29854790000 15.969138580000 17.692250120000 17.377856760000 18.15999350000 18.454768920000 15.568923480000 14.476536370000 15.47693670000 15.47453467000 15.47453470000 15.474534768920000 15.568923480000 14.476536370000 15.449094280000 18.205144820000 18.	1.697590965000 24.031669560000 24.858052630000 20.09931850000 20.09931850000 20.486856770000 22.601184380000 24.589817230000 23.9272972100000 23.9272972100000 23.9272972100000 25.05325190000 25.50325190000 25.5784694750000 25.784694750000 25.784694750000 25.76230300000 25.784694750000 25.76230300000 25.784694750000 25.76230300000 21.83844970000 22.88703850000 21.8384970000 22.877623750000 26.707623750000 27.18837810000 24.76023380000 25.5156375750000 25.5156375750000	1.861140125000 [[MN*2X3] ⁹ /q=2,1 0.130086868000 1.867627026000 -2.409344487000 -2.320757126000 1.490309387000 2.024665652000 -0.99081766500 0.307092500100 -1.744084474000 2.031710109000 2.871789423000 -1.510362883000 3.257827189000 4.217356126000 3.176960965000 2.334174613000 1.652083936000 3.349581831000 2.336243794000 2.048232925000 1.935614470000 3.40931610000 1.284058291000 -0.922181641900 -0.922181641900 -0.922181641900 -0.823102700 -1.822140483000 -0.424317531080 -1.279242689000 -1.279242689000 -0.412481745200 -2.164931301000	57 H (Ce 1 Ce 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 13 C 13 C 14 C 14 C 13 C 14 C 14 C 13 C 14 C 13 C 14 C 14 C 14 C 15 H 16 H 12 C 14 C 13 C 14 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 13 C 14 C 15 H 12 C 14 C 13 C 14 C 15 H 12 C 14 C 13 C 14 C 13 C 14 C 15 H 12 C 12 C 14 C 15 H 12 C 12 C 12 C 14 C 15 H 12 C 12 C	4.168670305000 4.168670305000 CN,NC /GA (III)N*2NC3) ²⁻⁵ 13.466098780000 15.997065980000 15.997065980000 14.597065980000 14.42235740000 14.524235740000 13.14098870000 13.14098870000 13.14098870000 14.958356150000 14.958356150000 14.958356150000 15.513277720000 14.710751330000 15.532077720000 17.241844080000 15.947557770000 17.241844080000 15.947557770000 17.443309590000 18.49430460000 15.513286660000 14.417308250000 15.943039300000 15.943039300000 15.94450870000 18.494450870000 18.494450870000 18.494450870000 18.49480810000	1.758999353000 2 22.519003230000 24.024249040000 24.855717960000 20.0974560370000 20.0974560370000 20.0974560370000 20.592630810000 22.631010720000 24.459234590000 23.919774630000 26.4377160000 25.400367520000 23.525188870000 24.142866800000 23.652253430000 24.70967180000 25.758531200000 26.487979150000 22.906155160000 23.154423600000 23.154423600000 26.703524490000 26.70352490000 27.7191018610000 25.239416950000 25.239416950000 25.239416950000 25.239416950000 25.239416950000 25.239416950000 25.239416950000 25.239416950000 25.239416950000	1.893938093000 0.156744398900 1.862358691000 -1.024682780000 -2.412704224000 -2.430370781000 1.420146387000 1.920673239000 -0.970115351800 0.311563038000 -1.72964804000 1.994709667000 2.767911719000 -1.443529654000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.253836382000 3.241035436000 1.650208060000 3.348446402000 2.366539423000 2.31652639423000 1.870037928000 3.013428973000 1.260103933000 -0.912934310300 -0.85554835790 -1.805026826000 -0.372316266100 -2.312600465000

33 H 18.219074290000 23.717954720000 -1.429129147000	33 H 18.255316770000 23.795447110000 -1.392609522000
54 C 15.251289010000 24.281975000000 -2.081458957000	54 C 15.507524020000 24.270009050000 -2.088550971000
35 H 15.443209750000 23.223961320000 -2.904976551000	35 H 15.586655690000 23.235182310000 -2.927748454000
36 H 15.691449430000 24.877996950000 -3.498520421000	36 H 15.709507300000 24.915739200000 -3.487993117000
37 H 14.164089590000 24.446437410000 -2.702862778000	37 H 14.211202090000 24.348730390000 -2.719686415000
38 C 10.980229670000 19.227371550000 -2.910378424000	38 C 10.970202050000 19.220150180000 -2.917387932000
	20 4 11 60255550000 18 762612280000 2 602052566000
59 H 11.00506/1/0000 18.//249/4/0000 -5.095258966000	59 H 11.005555590000 18.705015280000 -5.092902500000
40 H 9.948231816000 19.285955500000 -3.295703389000	40 H 9.943170421000 19.276427640000 -3.316280682000
41 H 10.978096200000 18.548577370000 -2.044403772000	41 H 10.957942490000 18.543380920000 -2.049731922000
42 C 11.380122100000 22.056429070000 -3.966069510000	42 C 11.375593310000 22.044936090000 -3.976063569000
43 H 11.568247570000 23.110722810000 -3.712900569000	43 H 11.570123310000 23.099069150000 -3.727570095000
44 H 10 260610780000 21 082652150000 4 280267658000	44 H 10 257225700000 21 075916070000 4 202602540000
4411 10.500010760000 21.585052150000 -4.580207058000	4411 10.337220700000 21.573810070000 -4.3550553540000
45 H 12.091361990000 21.759734290000 -4.751553127000	45 H 12.088069450000 21.740050180000 -4.757274189000
46 C 10.280286310000 21.585665330000 -1.162540074000	46 C 10.245259660000 21.579576030000 -1.183834044000
47 H 10.274730200000 20.998053400000 -0.232573943400	47 H 10.235996410000 20.994015890000 -0.252533786800
48 H 9.278347138000 21.498952650000 -1.616228020000	48 H 9.248533407000 21.483904120000 -1.647089275000
40 H 10 411602000000 22 644717150000 0 801712024200	40 H 10 271705700000 22 628906240000 0 014561002600
49 H 10.411092990000 22.044/17150000 -0.891/15054500	49 H 10.371793790000 22.038806240000 -0.914301003600
50 C 14.579848920000 20.001362430000 -4.230931745000	50 C 14.570017850000 20.003926100000 -4.210492384000
51 H 13.668076340000 19.623558200000 -4.718578077000	51 H 13.665574120000 19.618818320000 -4.706088416000
52 H 15.419373820000 19.360957240000 -4.550053266000	52 H 15.418016520000 19.372364380000 -4.524793764000
53 H 14.764213880000 21.017315990000 -4.612512126000	53 H 14.747775610000 21.022748950000 -4.587833060000
E4 C 14 242497060000 18 101602660000 1 7016E7411000	E4 C 14 222260100000 18 19E171260000 1 781208926000
54 C 14.245467900000 18.191002000000 -1.791057411000	54 C 14.222200100000 18.1851/1500000 -1.781508820000
55 H 14.230596640000 18.131635670000 -0.692832765500	55 H 14.203222490000 18.117780970000 -0.683015324000
56 H 15.092898840000 17.589368350000 -2.155180181000	56 H 15.074038610000 17.585940270000 -2.144626239000
57 H 13.317118320000 17.739883880000 -2.174374335000	57 H 13.297954170000 17.734544500000 -2.170831618000
58 C 16.140837760000 20.532277690000 -1.686343719000	58 C 16.117992670000 20.525028540000 -1.659497078000
59 H 16 415280920000 21 558511860000 -1 965910912000	59 H 16 393378620000 21 552855750000 -1 032562820000
3511 10.413280320000 21.338311800000 -1.303510813000	3311 10.3333/8020000 21.322333/30000 -1.352302825000
60 H 16.899544910000 19.857423320000 -2.117169797000	60 H 16.876538500000 19.851873880000 -2.093538856000
61 H 16.205180490000 20.443959840000 -0.592038388900	61 H 16.178334010000 20.433524310000 -0.565709433600
[11/11]NI* CN 1 ²⁻	[1](11)NI* NC 1 ²⁻
[U(III)IN '2CIN3] 1 U 9 870916846000 7 217636646000 4 891487284000	1 U 9 861076137000 7 194637680000 4 882952268000
2 51 10.886976370000 9.675800247000 2.439903953000	2 51 10.864918380000 9.655939107000 2.443029080000
3 Si 7.988545376000 9.718245472000 3.321013915000	3 Si 7.978844037000 9.768608085000 3.332980513000
4 Si 12.295229180000 8.288082051000 7.336557932000	4 (1) 42 270(200000 0 200040400000 7 200704404000
· · · · · · · · · · · · · · · · · · ·	4 51 12.278679690000 8.260311010000 7.335784161000
5 Si 12.469356030000 5.409775118000 6.411824719000	4 51 12.470135410000 5.384883170000 6.426952779000
5 si 12.469356030000 5.409775118000 6.411824719000 6 N 11 60268170000 5.417510807000 2.017356773000	4 si 12.27867990000 8.2003101000 7.335784161000 5 si 12.490135410000 5.384883170000 6.426952779000 6 c 11.449734590000 5.421042793000 2.110827884000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000	4 si 12.27867990000 8.26031010000 7.335784161000 5 si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000	4 Si 12.278679690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000	4 Si 12.278679690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000
5si 12.469356030000 5.409775118000 6.411824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.563263773000 5.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000	4 Si 12.278679690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000
5 si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000	4 Si 12.278679890000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000
5 Si 12.46935603000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 5.96150420000 6.318865332000	4 Si 12.278679690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.83655220000 5.999356907000 3.034945521000
5 Si 12.46935603000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 5.99158200000 6.318685332000 11 C 11.058883660000 5.9915620942000 2.909270893000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.99356907000 4.362432652000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.058883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000	4 Si 12.27867/890000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.983655200000 5.99356907000 3.034945521000 12 N 8.162999523000 5.432470024000 4.863120685000
5 si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.058883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000	4 Si 12.27867/s90000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710303000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.983655200000 5.993356907000 3.034945521000 12 N 8.16299523300 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000
5si 12.469356030000 5.409775118000 6.411824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.553263773000 5.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 6.991958200000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 1.74628510000 6.948854107000 6.333936215000 11 N 10.98365520000 5.99356907000 3.034945521000 12 N 8.16299523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.66162094200 2.909270893000 12 C 8.05685108000 5.40126886200 5.000409349000 13 C 8.550806667000 8.350282651000 6.855958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907000 3.034945521000 12 N 8.16299952300 5.432470024004 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.56788549000 2.42744965000 15 H 11.156651270000 11.95695990000 3.440115077000
5 Si 12.46935603000 5.409775118000 6.411824719000 6 N 11.602668170000 5.41975118000 6.411824719000 7 N 7.239924675000 4.563263773000 5.05136733000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.058883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 12.088020720000 2.01408414000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.993356907000 3.034945521000 12 N 8.162999523000 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.95695990000 2.422744965000 15 H 11.156651270000 11.95695990000 3.440115077000 16 H 10.091886100000 12.90299364150000 2.422749655000
5 si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.89510660000 2.419840142000 15 H 11.12156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084144000	4 Si 12.27867/980000 8.26031101000 7.335744151000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 1.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.4932470024000 4.863120685000 12 N 8.16299523300 5.432470024000 4.86312068000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.44011507700 16 H 10.091886100000 12.050094150000 2.02099364000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.96162094200 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.5895106600000 2.419840142000 15 H 11.121156060000 12.048602790000 2.01408414000 16 H 10.059612840000 12.248602790000 2.01408414000 17 H 11.821582660000 11.927125010000 1.79969753300	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.61991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907003 3.034945521000 12 N 8.162999523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.050094150000 2.02099364000 17 H 11.849776850000 11.883973380000 1.799798166000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.87748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 12.048602790000 2.01408414000 16 H 10.059612840000 12.227653000 1.799697953000 18 C 10.762649740000 9.120227653000 0.625053507100	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 1.744628510000 6.948854107000 6.333396215000 11 N 10.983655200000 5.999355907000 3.034945521000 12 N 8.162390638000 8.266425377000 6.725793201000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.050094150000 2.02009364000 17 H 11.849776850000 11.88397338000 1.799378166000 18 C 10.731178910000 9.105100283000 0.62747629866
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952950000 3.431636829000 10 N 11.756021680000 5.9919820000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126886200 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084414000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.120227653000 0.625053507100 19 H 11.616577250000 9.503774500000 0.041739893470	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 1.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907000 3.034945521000 12 N 8.16299952300 5.432470024000 4.863126685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.05094150000 2.020099364000 17 H 11.849776850000 11.8397338000 1.79978166000 18 C 10.731178910000 9.10510028300 0.627476298600
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.419775118000 6.411824719000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.05668518000 5.40126886200 5.000409349000 13 C 8.5509806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589516660000 2.419840142000 15 H 11.121156060000 11.927125010000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084414000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.12022765300 0.625053507100 19 H 11.616577250000 9.50374500000 0.04179389347	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 3.034945521000 11 N 10.98365520000 5.99356907000 3.034945521000 12 N 8.162999523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.56789549000 2.422744965000 15 H 11.56651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.050094150000 2.020099364000 17 H 11.84977685000 11.88397338000 1.799798166000 18 C 10.73117891000 9.10510283000 0.627476288600
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.60268170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799659753000 18 C 10.762649740000 9.120227653000 0.041793893470 20 H 9.837230063000 9.467069318000 0.143111957300 21 H 10.7872040790000 8.027638890070	4 Si 12.27867980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.38488317000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.99335690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 1.156651270000 11.95690599000 3.4011507700 16 H 10.91886100000 12.0509415000 2.02099364000 17 H 11.849776850000 11.8397338000 1.79978166000 18 C 10.73117891000 9.47551820600 0.4627476298600 19 H 11.58871757000 9.45751826000 0.150672302
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.058883660000 5.96162094200 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.01408414000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.12022765300 0.625053507100 19 H 11.616577250000 9.50377450000 0.041793893470 20 H 9.837230063000 9.467069318000	4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907003 3.034945521000 12 N 8.16299523000 5.432470024000 4.863120685000 13 N 8.612356638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.050094150000 2.02099364000 17 H 11.849776850000 11.883973380000 1.799798166000 18 C 10.73117891000 9.10510283000 0.627476298600 19 H 11.58871757000 9.475518206000
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.87748319000 7.773417753000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.90270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084414000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.102227653000 0.62553507100 19 H 11.616577250000 9.50374550000 0.41733893470 20 H 9.837230063000 9.467069318000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999355907000 3.04945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.05009415000 2.020099364000 17 H 11.849776850000 11.88397338000 1.79978166000 18 C 10.73117891000 9.10510028300 0.627476298600
55 12.469356030000 5.409775118000 6.411824719000 6N 11.602668170000 5.417610807000 2.017356773000 7N 7.239924675000 4.563263773000 5.051036423000 8N 8.031916513000 8.87748319000 7.773417763000 9N 9.598507450000 9.075952960000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.40126886200 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.589510660000 2.419840142000 15H 11.121156060000 11.982636800000 3.437404900000 16H 10.059612840000 12.048602790000 2.014084414000 17H 11.821582660000 11.927125010000 1.799697953000 18C 10.762649740000 9.120227653000 0.625053507100 19H 11.616577250000 9.503774500000 0.41793893470 20H 9.837230063000 9.467069318000 0.143111957300 21H 10.7872040900000 8.020548999000 0.58082046	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907000 3.034945521000 12 N 8.16299952300 5.432470024000 4.863126685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.0509415000 2.020099364000 17 H 11.849776850000 11.88397338000 0.627476298600 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.588717570000 9.46783764700 <td< th=""></td<>
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.60268170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.073417763000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.82158660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.120227653000 0.041793893470 20 H 9.837230063000 9.4670693180000 0.14179389347	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 3.034945521000 11 N 10.98365520000 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.56789549000 2.422744965000 15 H 10.56651270000 11.95690599000 3.440115077000 16 H 10.091866100000 12.050094150000 2.02009364000 17 H 11.849776850000 11.88397338000 1.799798166000 18 C 10.73117891000 9.10510283000 0.627476298600 19 H 11.588717570000 8.05469083000 0.58077930500
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 3.437404900000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.100227653000 0.041793893470 20 H 9.83723006300 9.467069318000 0.14311195730	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.38488317000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710303000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907000 3.034945521000 12 N 8.16299523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.400115077000 16 H 10.091886100000 12.050094150000 2.02099364000 17 H 11.84976850000 11.88397338000 1.799798166000 18 C 10.73117891000 9.10510283000 0.627476298600 19 H 1.588717570000 9.475518206000
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.058883660000 5.96162094200 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.407063118000 0.41311957300 21 H 10.1787204090000 8.002548999000 0.580820469	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.94885410700 6.33939521500 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235663800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.42274965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.050094150000 2.02009364000 17 H 11.84977685000 11.88397338000 1.79978166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.58871757000 9.47518266600 0.04099
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.87748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.889510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.01408414000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.102227653000 0.625053507100 19 H 11.616577250000 9.6037450000 0.414311957300 21 H 0.782040900000 8.02054899000	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.33336215000 11 N 10.98365520000 5.99935590700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.42274965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.05009415000 2.020099364000 17 H 11.84977685000 11.88397338000 0.797938166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.58871757000 9.46783764700 0.15
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.60268170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.073417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.85695820800 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.98263680000 3.43740490000 16 H 10.059612840000 12.048602790000 2.01408414000 17 H 11.821582660000 11.927125010000 1.79969795300 18 C 10.762649740000 9.102227653000 0.625053507100 19 H 11.616577250000 9.5037453000 0.413111957300 21 H 10.787204090000 8.02048899000 0.580820469800	4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.493956907000 3.034945521000 12 N 8.162390532000 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.0509415000 2.020099364000 17 H 18.84977685000 11.88397338000 0.627476298600 19 H 11.58871757000 9.46783764700 0.150672302400 21 H 10.736465550000 8.005469083000 <
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.073417763000 9 N 9.59850745000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.00409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.92227653000 0.625053507100 16 H 10.059612840000 1.20227653000 0.625053507100 17 H 11.821582660000 1.1927125010000 0.143111957300 21 H 10.7872040900000 8.020548999000 0.580820469800 22 C 12.604479730000 9.4007398004 0.4045927490000 23 H 12.83493819000 9.40100739800 0.4050827490000 </th <th>4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710303000 3.432693486000 10 N 11.74462851000 6.948854107000 6.339396215000 11 N 10.98365520000 5.99335690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.0509415000 2.02099364000 17 H 11.84977685000 11.88397338000 0.627476298600 19 H 11.588715750000 9.457837647000 0.15672302400</th>	4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710303000 3.432693486000 10 N 11.74462851000 6.948854107000 6.339396215000 11 N 10.98365520000 5.99335690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.0509415000 2.02099364000 17 H 11.84977685000 11.88397338000 0.627476298600 19 H 11.588715750000 9.457837647000 0.15672302400
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.073417763000 9 N 9.59850745000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.102227653000 0.625053507100 19 H 11.616577250000 9.503774500000 0.143111957300 21 H 10.7872040900000 8.02964899000 0.580820469	4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235663800 8.26642537700 6.725793201000 14 C 10.99561685000 11.56789549000 2.422744965000 15 H 11.15665127000 11.95690599000 3.44011507700 16 H 10.091886100000 12.0509415000 2.02099364000 17 H 184977685000 11.8397338000 1.799798166000 18 C 10.73117891000 9.10510283000 0.627476298600
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.073417763000 9 N 9.59850745000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 3.437404900000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799697953000 18 C 10.762649740000 9.620548999000 0.64350327100 19 H 11.616577250000 9.50377450000 0.413111957300 21 H 0.7826497400009 9.401007398000 4.0459927490	4 Si 12.7867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.38488317000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.94885410700 6.333396215000 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.42274965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.05009415000 2.020099364000 17 H 11.84977685000 11.88397338000 1.79978166000 18 C 10.73117891000 9.4578174700 0.150672302400 21 H 10.3646575000 8.00546908300 0.580779930
55 12.469356030000 5.409775118000 6.411824719000 6N 11.602668170000 5.417610807000 2.017356773000 7N 7.239924675000 4.563263773000 7.73417763000 8N 8.031916513000 8.87748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 5.991958200000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.401268862000 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.982636800000 2.419840142000 15H 11.121156060000 11.982636800000 2.01408414000 17H 11.821582660000 11.927125010000 1.799697953000 18C 10.762649740000 9.102227653000 0.625053507100 19H 11.616577250000 9.50374550000 0.41733893470 20H 9.837230063000 9.467069318000 0.141311957300 21H 10.787204090000 8.020548999000 5.80820469800<	4 Si 12.27867/980000 8.26031101000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.999356907000 3.04945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235663800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.42274965000 15 H 11.156651270000 11.956905990000 3.440115077000 16 H 10.091886100000 12.05009415000 2.020099364000 17 H 11.84977685000 11.8397338000 1.79978166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.58871757000 9.46783764700 0.150
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.589510660000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.92227653000 0.625053507100 18 C 10.762649740000 9.10224759000 0.141793893470 20 H 9.837230063000 9.467069318000 0.480206469800<	4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.34269348600 10 N 11.744628510000 6.948854107000 6.339396215000 11 N 10.98365520000 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 1.156651270000 11.95690599000 3.44011507700 16 H 10.9188610000 12.05099415000 2.02099364000 17 H 11.84977685000 11.8397338000 0.62747629860 18 C 10.73117891000 9.475518206000 0.104096553100 20 H 9.809261594000 9.46783747000 0.150672302400 21 H 10.7364655760000 9.472542732000 4.0243
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.40126882000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.92712501000 1.799697953000 18 C 10.762649740000 9.102227653000 0.625053507100 19 H 11.61657725000 9.5037450000 0.143111957400 21 H 10.787204090000 8.020548999000	4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 5.99356907000 3.034945521000 10 N 11.744628510000 5.99356907000 3.034945521000 12 N 8.16239053300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.09188610000 12.0509415000 2.02099364000 17 H 11.8497685000 11.88397338000 1.79978166000 18 C 10.73117891000 9.4751820600 0.04099653100 20 H 9.80926159400 9.467837647000 0.150672302400
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 3.437404900000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.01408414000 17 H 11.821582660000 1.927125010000 1.799697953000 18 C 10.762649740000 9.10222765300 0.625053507100 19 H 11.61657752000 9.50377450000 0.143111957300 21 H 10.787204090000 8.020548999000	4 Si 12.7867/980000 8.26031101000 7.335744151000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.74628510000 6.94885410700 6.33339521500 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.6123568800 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 11.15665127000 11.95690599000 3.44011507700 16 H 10.09188610000 12.05009415000 2.02009364000 17 H 11.84977685000 11.88397338000 1.79978166000 18 C 10.73117891000 9.4583742700 0.150672302400 21 H 10.73646575000 8.005469083000 0.58079930500 </th
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.563263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.96162094200 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 3.437404900000 15 H 11.121156060000 11.9827125010000 1.799697853000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.799697553000 18 C 10.762649740000 9.10227653000 0.41793893470 20 H 9.337230063009 9.467069318000 0.414311957300 21 H 10.787204090000 8.02054899900	4 Si 12.27867/980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 8 C 8.009716864000 8.707257677000 7.64661541000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 1.744628510000 6.948854107000 6.333396215000 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.16235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.56789549000 2.42274965000 15 H 11.15665127000 11.95690599000 3.440115077000 16 H 10.091886100000 12.05009415000 2.02099364000 17 H 11.84977685000 11.88397338000 1.799798166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.5871757000 9.46783764700 0.150672302400 21 H 10.332455780000 9.422425732004 4.024390106000 <
55 12.469356030000 5.409775118000 6.41824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.563263773000 7.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 6.991958200000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.401268862000 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.589510660000 2.419840142000 15H 11.12115606000 11.98263680000 3.43740490000 16H 10.059612840000 12.048602790000 2.01408414000 17H 11.821582660000 11.927125010000 1.79969795300 18C 10.762649740000 9.10222765300 0.62505307100 19H 11.616577250000 9.58072649800 0.548029469800 22C 12.604479730009 9.110591153000 3.011435499000 </th <th>4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 5.999355690700 3.034945521000 12 N 8.1629952300 5.43247002400 4.861310685000 13 N 8.61235063800 8.26642537700 6.725793201000 14 C 10.995616850000 11.56789549000 2.42274965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.0509415000 2.020099364000 17 H 11.84977685000 11.8397338000 1.79978166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.58871757000 9.46783764700 0.150672302400 </th>	4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 8.661991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 5.999355690700 3.034945521000 12 N 8.1629952300 5.43247002400 4.861310685000 13 N 8.61235063800 8.26642537700 6.725793201000 14 C 10.995616850000 11.56789549000 2.42274965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.0509415000 2.020099364000 17 H 11.84977685000 11.8397338000 1.79978166000 18 C 10.73117891000 9.10510028300 0.627476298600 19 H 11.58871757000 9.46783764700 0.150672302400
55 12.469356030000 5.409775118000 6.41824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.563263773000 7.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 5.901958200000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.40126882000 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.589510660000 2.419840142000 15H 11.121156060000 11.927125010000 1.79969793000 18C 10.762649740000 9.120227653000 0.625053507100 19H 11.61657725000 9.50377450000 0.141793893470 20H 9.837230063000 9.467069318000 0.445092749000 21H 10.365847550000 9.507327928000 2.357606895000 22C 12.604479730000 9.4100739800 2.357606895000 <th>4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 5.99356907000 3.034945521000 10 N 11.744628510000 5.993356907000 3.034945521000 12 N 8.16299523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.91886100000 12.0509415000 2.02009364000 17 H 11.84977685000 11.8397338000 0.627476298600 19 H 11.588715750000 9.4578518206000 0.040996553100 20 H 9.809261594000 9.467837647000 0.156672302400 21 H 10.7364655760000 9.45824327002 <td< th=""></td<></th>	4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 5.99356907000 3.034945521000 10 N 11.744628510000 5.993356907000 3.034945521000 12 N 8.16299523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.91886100000 12.0509415000 2.02009364000 17 H 11.84977685000 11.8397338000 0.627476298600 19 H 11.588715750000 9.4578518206000 0.040996553100 20 H 9.809261594000 9.467837647000 0.156672302400 21 H 10.7364655760000 9.45824327002 <td< th=""></td<>
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.563263773000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 6.991958200000 6.318685332000 11 C 11.05883660000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.00409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084414000 17 H 11.821582660000 11.92712501000 1.799697953000 18 C 10.762649740000 9.10022765300 0.625053507100 19 H 11.616577250000 9.50377450000 0.143111957300 21 H 10.787204090000 8.02548999000 5.86820469800 22 H 12.64479730000 9.401007398004	4 Si 12.27867/690000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.94885410700 6.339396215000 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235663800 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 11.15665127000 11.95690599000 3.44011507700 16 H 10.99188610000 12.05099415000 2.02099364000 17 H 11.84977685000 11.83897338000 1.799798166000 18 C 10.73117891000 9.1051028300 0.62747628860 19 H 11.58871757000 9.4751820600 0.40996553100 20 H 9.8926159400 9.467837647000 0.15672302400<
5 Si 12.469356030000 5.409775118000 6.41824719000 6 N 11.602668170000 5.417510807000 2.017356773000 7 N 7.239924675000 4.562263773000 5.051036423000 8 N 8.031916513000 8.877748319000 7.773417763000 9 N 9.598507450000 9.075952960000 3.431636829000 10 N 11.756021680000 5.961620942000 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 3.437404900000 15 H 11.121156060000 11.927125010000 1.799597953000 16 H 10.059612840000 9.407069318000 0.4143911957300 17 H 11.821582660000 9.467069318000 0.4143111957300 18 C 10.762649740000 9.0202765300 0.58022068800 21 H 10.78720409000 8.019806302000 2.357606895000 22 C 12.604479730000 9.1002738000 4.045092749000 24 H 13.363847550000 9.573027928000	4 Si 12.7867/980000 8.260311010000 7.335744151000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566583336000 9.07710308300 3.432693486000 10 N 11.744628510000 6.94885410700 6.33339521500 11 N 10.98365520000 5.99935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.6123568300 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.09188610000 12.05009415000 2.02009364000 17 H 11.84977685000 11.88397338000 1.79978166000 18 C 10.73117891000 9.457851820600 0.40996553100 20 H 9.80926159400 9.4678374700 0.150672302400 21 H 10.73646575000 8.005469083000 0.5807799305
5 Si 12.469356030000 5.409775118000 6.411824719000 6 N 11.602668170000 5.417610807000 2.017356773000 7 N 7.239924675000 4.56263773000 5.051036423000 8 N 8.031916513000 8.9774819000 7.773417763000 9 N 9.598507450000 9.07595296000 3.431636829000 10 N 11.756021680000 5.96162094200 2.909270893000 12 C 8.065685108000 5.401268862000 5.000409349000 13 C 8.550806667000 8.350282651000 6.856958208000 14 C 10.974194920000 11.982636800000 2.419840142000 15 H 11.121156060000 11.982636800000 3.437404900000 16 H 10.059612840000 12.048602790000 2.014084114000 17 H 11.821582660000 11.927125010000 1.79969753000 18 C 10.762649740000 9.10027653000 0.41793893470 20 H 9.837230063009 9.467069318000 0.414311957300 21 H 10.78274090000 8.02054899900 0.580820469800 22 C 12.60447973000 9.1059115300 3.0	4 Si 12.7867/980000 8.260311010000 7.335744151000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 8 C 8.009716864000 8.707257677000 7.64661541000 9 N 9.566858336000 9.077103083000 3.432693486000 10 N 11.744628510000 6.948854107000 6.333396215000 11 N 10.98365520000 5.999355907000 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.995616850000 11.567895490000 2.42274965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.05009415000 2.02009364000 17 H 11.84977685000 11.88397338000 1.799798166000 18 C 10.73117891000 9.46783764700 0.150672302400 21 H 10.3865576000 8.005469083000 0.580779930500 22 C 12.57377553000 9.067089666003 3.01
55 12.469356030000 5.409775118000 6.41824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.563263773000 7.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 5.90195820000 6.318685332000 11C 11.05883660000 5.96162094200 2.909270893000 12C 8.065685108000 5.401268862000 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.589510660000 2.419840142000 15H 11.12115606000 11.92263680000 3.43740990000 16H 10.059612840000 12.048602790000 2.014084114000 17H 11.821582660000 11.922125010000 0.143111957300 21H 10.762649740000 9.10059115300 3.011435499000 22 C 12.60447973000 9.11059115300 3.011435499000 23 H 12.711945460000 8.019806302002 2.929423796000	4 Si 12.27867980000 8.260311010000 7.335784161000 5 Si 12.490135410000 5.384883170000 6.426952779000 6 C 114.49234590000 5.421042793000 2.110827894000 7 C 7.340282422000 4.581213136000 4.861991834000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 5.9935690700 3.034945521000 11 N 10.98365520000 5.9935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.56789549000 2.422744965000 15 H 1.156651270000 11.95890599000 3.44011507700 16 H 10.99188610000 12.0509415000 2.0209936400 17 H 11.84977685000 11.8397338000 0.62747629860 18 C 10.73117891000 9.475518206000 0.10801768000 21 H 10.736465750000 9.42242573200 4.02439016600 24 H 13.332435780000 9.472842573200 2.318540294000 </th
55 12.469356030000 5.409775118000 6.41824719000 6N 11.602668170000 5.417510807000 2.017356773000 7N 7.239924675000 4.563263773000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 6.991958200000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.40126882000 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.982636800000 2.419840142000 15H 11.121156060000 11.982636800000 3.437404900000 16H 10.059612840000 12.048602790000 2.014084114000 17H 11.82158266000 11.92712501000 0.625053507100 19H 11.61657752000 9.3077450000 0.041793893470 20H 9.837230063000 9.467069318000 0.4143111957300 21H 10.787204090000 8.1020548999000 2.35766895000 22H 12.83493819000 9.40100739800 2.35766895000<	4 Si 12.7867/980000 8.26031101000 7.335744151000 5 Si 12.490135410000 5.38488317000 6.426952779000 6 C 11.449234590000 5.421042793000 2.110827894000 8 C 8.009716864000 8.707257677000 7.646615481000 9 N 9.566858336000 5.99356907000 3.034945521000 10 N 11.744628510000 6.94885410700 6.339396215000 11 N 10.98365520000 5.9935690700 3.034945521000 12 N 8.1629952300 5.432470024000 4.863120685000 13 N 8.61235063800 8.266425377000 6.725793201000 14 C 10.99561685000 11.567895490000 2.422744965000 15 H 11.156651270000 11.95690599000 3.440115077000 16 H 10.091886100000 12.0509415000 2.02099364000 17 H 11.8497685000 11.8387338000 1.79979816600 18 C 10.73117891000 9.1051028300 0.627476298600 19 H 11.5887157000 9.47551820600 0.10801768000 21 H 10.736465570000 8.005469083000 0.58077993050 </th
55 12.46935603000 5.409775118000 6.411824719000 6N 11.602668170000 5.417610807000 2.017356773000 7N 7.239924675000 4.563263773000 5.051036423000 8N 8.031916513000 8.877748319000 7.773417763000 9N 9.598507450000 9.075952960000 3.431636829000 10N 11.756021680000 6.99195820000 6.318685332000 11C 11.05883660000 5.961620942000 2.909270893000 12C 8.065685108000 5.40126886200 5.000409349000 13C 8.550806667000 8.350282651000 6.856958208000 14C 10.974194920000 11.98263680000 2.419840142000 15H 11.1211560000 11.92712501000 1.799697953000 16C 10.6564974000 9.1022765300 0.625033507100 19H 11.61657725000 9.5037450000 0.580820469800 22C 12.60447973000 9.1002739800 4.045092749000 23H 12.83493819000 9.40100739800 4.045092749000 24H 13.36384755000 9.573027928000 2.35760689500	4 Si 12.2780/93000 8.2631101000 7.3374416100 5 Si 12.49013541000 5.38488317000 6.42695277900 6 C 11.44923459000 5.421042793000 2.110827894000 7 C 7.34028242200 4.58121313600 4.861991834000 8 C 8.00971686400 8.707257677000 7.646515481000 9 N 9.56685833600 9.07710308300 3.432693486000 10 N 11.744628510000 6.94854107000 6.339396215000 11 N 10.983655200000 5.999356907000 3.034945521000 12 N 8.162999523000 5.432470024000 4.863120685000 13 N 8.612350638000 8.266425377000 6.725793201000 14 C 10.995616850000 11.56789549000 2.422744955000 15 H 11.156651270000 11.8597388000 0.627476298600 17 H 18.49776850000 9.475518206000 0.40996553100 01 H 11.78917000 9.4578327000 2.318540294000 22 C 12.57377563000 9.05708966000 3.018001768000 23 H 12.4835780000 9.422425732000 2.318540294000

42 C	11.730087100000 8.109	861088000 9.142685905	000	42 C	11.732040630000	8.096269392000	9.151303571000	
43 H	10.629975370000 8.097	805299000 9.17693666	3000	43 H	10.632794710000	8.057727882000	9.197390146000	
44 H	12 08064/030000 8 963	059384000 9 74736440	000	лл н	12 067652000000	8 965756880000	9 7/1309173000	
	12.0000449300000 8.905				12.007052000000	8.505750880000	5.741505175000	
45 H	12.102386610000 7.185	991631000 9.60795237	0000	45 H	12.130798940000	7.187621685000	9.625526499000	
46 C	11.666583820000 9.990	972253000 6.788619355	000	46 C	11.624998340000	9.949587565000	6.774545114000	
47 H	11.985872460000 10.264	4256750000 5.77380729	1000	47 H	11.941404280000	10.219203740000	5.757344589000	
48 H	12.066566770000 10.751	1499210000 7.48184284	6000	48 H	12.013837680000	10.721060270000	7.461715818000	
49 H	10.569376230000 10.047	7410030000 6.83263402	8000	49 H	10.526771960000	9.989357699000	6.815505182000	
50.0	14.040656520000 5.250	402206000 5 25115070	2000	50.0	14.045320410000	5 25 77 075 20000	5 339175740000	
50 C	14.040050520000 5.259	492290000 5.55115079.	000	50 C	14.045559410000	5.257707529000	5.5561/5/40000	
51 H	13.784575530000 5.409	747127000 4.29149530	.000	51 H	13.771438830000	5.408278979000	4.282976061000	
52 H	14.495735350000 4.260	133720000 5.45377077	3000	52 H	14.517056390000	4.264899606000	5.430322863000	
53 H	14.794250500000 6.010	076109000 5.63294841	1000	53 H	14.791681060000	6.018930968000	5.611468572000	
54 C	11.284397900000 4.049	962053000 5.840519942	000	54 C	11.317274660000	4.000703302000	5.888419359000	
55 H	10 369249940000 4 000	760918000 6 44771437	1000	55 H	10 408787390000	3 960253336000	6 507141677000	
5511	10.505245540000 4.000				10.400707350000	3.300233330000	5.007041077000	
56 H	11.799891820000 3.077	228923000 5.92366758	5000	56 H	11.838141790000	3.032038231000	5.985947564000	
57 H	10.984852720000 4.160	700527000 4.78744915	6000	57 H	11.004483780000	4.096901364000	4.838514827000	
58 C	12.975412080000 4.883	225869000 8.183296729	000	58 C	13.045643450000	4.879294866000	8.191405054000	
59 H	13.729651270000 5.544	251612000 8.63526819	000	59 H	13.794073110000	5.560721524000	8.623335959000	
60 H	13.400656620000 3.865	824202000 8.14916292	5000	60 H	13.492926230000	3.871414693000	8.155376179000	
61 H	12 101713060000 / 858	955106000 8 85163044	1000	61 H	12 1865/3180000	4 841038155000	8 878317728000	
0111	12.101713000000 4.838	555100000 8.85105044.		0111	12.180343180000	4.841038133000	8.878317728000	/
[U(IV)N*₂CN₃] ¹⁻			[U	(IV)N*₂NC₃] ¹			
īυ	9.975453302000 7.30672	25179000 4.8791173400	00	1 U	9.937883397000	7.282841429000	4.899762000000	
2 Si	10.923643780000 9.6474	72487000 2.474381091	000	2 Si 💠	10.878127960000	9.641462564000	2.490337497000	
3 Si	7.985110042000 9.71043	32446000 3.3836632180	00	3 Si	7.944664927000	9.685712383000	3.391897049000	
4 Si	12 292233630000 8 3322	91992000 7 282584159	000	4 Si -	12 339154120000	8 333438082000	7 247289579000	
5.0	12.232233030000 0.3322	51552000 7.202501255	200		2 44255 4020000	5.200405456000	6 204024242000	
5 51	12.418904110000 5.3892	54442000 6.390207217	000	5 51 3	12.442554930000	5.399485456000	6.381924242000	
6 N	11.550533080000 5.4478	2.080727094	000	6C 1	11.287098220000	5.501948617000	2.116293070000	
7 N	7.411293603000 4.72146	55691000 4.8853661180	00	7 C	7.462449476000	4.774374789000	5.092484934000	
8 N	8.116595862000 8.80644	45081000 7.7150785380	00	8 C	8.241223468000	8.819900038000	7.639355200000	
9 N	9.620112956000 9.03298	86788000 3.4986772550	00	9 N	9.579527837000	9.017523200000	3.510735692000	
10 N	11 711527280000 7 000	770810000 6 26167741	2000	10 N	11 738020750000	7 01 2786464000	6 244544640000	
10 N	11.711557580000 7.009	0//0810000 0.2010//41		10 N	11.728930750000	7.012786464000	6.244544649000	
11 C	11.031294670000 6.017	238305000 2.967494680	000	11 N	10.925234080000	6.073770713000	3.089726674000	
12 C	8.238858808000 5.5557	4.886235477	000	12 N	8.287114587000	5.622317374000	5.003804731000	
13 C	8.662837513000 8.3309	6.790082339	000	13 N	8.786037057000	8.381209262000	6.682070248000	
14 C	11.005816400000 11.543	3292240000 2.53110804	4000	14 C	10.963278510000	11.536446630000	2.572413950000	
15 H	11 157185280000 11 90/	4638360000 3 55898142	0000	15 H	11 111560190000	11 882114820000	3 605849702000	
16.11	10.006227020000 12.010	0008660000 2 12841883	8000	1011	10.054640360000	12 018650440000	2 184156542000	
10 H	10.096257920000 12.015	990800000 2.13841887	8000	10 H	10.054640260000	12.018059440000	2.184150542000	
17 H	11.853113050000 11.896	6669430000 1.92216302	0000	17 H	11.811822550000	11.898277750000	1.970119082000	
18 C	10.752695000000 9.091	025722000 0.679310513	800	18 C	10.703208260000	9.120698887000	0.682675958300	
19 H	11.615878360000 9.444	656038000 0.09333283	2670	19 H	11.581897880000	9.459636321000	0.111134426300	
20 H	9.841626480000 9.4734	442893000 0.200476186	800	20 H	9.808683655000	9.538039345000	0.202299230600	
21 H	10.739136240000 7.992	243259000 0.62773236	1100	21 H	10.657926620000	8.024310478000	0.608095183500	
22.0	12 61 520 20 50000 0.026	222050000 2 050062066	000	22.0	12 571881840000	0.002200455000	3.047004609000	
22 C	12.015592050000 9.020	22/950000 5.05906506	000	22 C	12.571881840000	9.002290455000	5.047004608000	
23 H	12.863913100000 9.293	733913000 4.09453184	3000	23 H	12.802870190000	9.191260534000	4.102971052000	
24 H	13.374722650000 9.501	277989000 2.41607272	0000	24 H	13.334695520000	9.531041581000	2.452010902000	
25 H	12.728853860000 7.939	904347000 2.93903888	0000	25 H	12.691403060000	7.928400081000	2.853825874000	
26 C	7.508999560000 10.186	719310000 1.608260993	000	26 C	7.463935286000	10.146376060000	1.613166638000	
27 H	8 1/2008625000 10 975	373100000 1 17821132	1000	27 H	8 086878217000	10 942476080000	1 182267038000	
2711	0.142030023000 10.575			27.11	6.000070217000	10.5424700000000	1.102207030000	
28 H	6.473443694000 10.563	893150000 1.61583705	000	28 H	6.423157302000	10.508753510000	1.615477218000	
29 H	7.539043115000 9.3167	725114000 0.936799547	000	29 H	7.510398701000	9.274579585000	0.945248256500	
30 C	7.819335826000 11.248	447080000 4.467713796	000	30 C	7.757553777000	11.233882960000	4.459011072000	
31 H	7.959500377000 10.985	841940000 5.52634761	.000	31 H	7.925892826000	10.992118890000	5.518091154000	
32 H	6.815448401000 11.689	061020000 4.36063284	6000	32 H	6.740060077000	11.645152860000	4.364589470000	
33 H	8 556848342000 12 019	547740000 4 20340690	5000	33 H	8 467803167000	12 020854340000	4 168581698000	
3511	6.550048542000 12.015				6.407803107000	12.020034340000	4.100501050000	
34 C	6.707185876000 8.4378	369784000 3.933482535	000	34 C	6.671868273000	8.408750899000	3.947198631000	
35 H	6.693968939000 7.5406	551036000 3.299002979	000	35 H	6.684220081000	7.499138806000	3.330248463000	
36 H	5.714711296000 8.9127	721352000 3.857954399	000	36 H	5.673811136000	8.865439515000	3.841938728000	
37 H	6.816547201000 8.1134	499761000 4.978170557	000	37 H	6.771538873000	8.106867545000	4.998538778000	
38 C	14.186864430000 8.451	211589000 7.24411304	000	38 C	14.237713230000	8.407174444000	7.230349365000	
20 11	14 677091200000 7 555	484554000 7 65054704	0000	20.11	14 709067910000	7 514920100000	7 665705505000	
39 H	14.077681390000 7.555	HOHONO /.65054704		22 H	14.100901810000	7.514829100000	1.000/95595000	
40 H	14.516351500000 9.311	554339000 7.84848958	0000	40 H	14.573970580000	9.277420332000	7.816890421000	
41 H	14.556310560000 8.600	668234000 6.21882097	000	41 H	14.621890470000	8.525784881000	6.206530147000	
42 C	11.722975470000 8.160	763470000 9.072789230	000	42 C	11.759398590000	8.196014329000	9.039379236000	
43 H	10.624234610000 8 136	093085000 9.11644017	3000	43 H	10.660918380000	8,222601540000	9.086039148000	
	12.064500450000 0.110	247240000 0 0000	0000		12 1420020000	0.04505205000	0.636144333300	
44 H	12.004039150000 9.028	9.65947948		44 H	12.142082030000	9.045952063000	9.020141331000	
45 H	12.111737470000 7.254	550578000 9.55576086	5000	45 H	12.103165750000	7.271630159000	9.522256312000	
46 C	11.649540540000 10.008	6.67787041	1000	46 C	11.771195080000	10.028896930000	6.616441178000	
47 H	11.992629250000 10.284	4085380000 5.67185312	3000	47 H	12.307626380000	10.353648600000	5.715023900000	
48 H	12.039311830000 10.772	2991350000 7.37033007	1000	48 H	11.993816760000	10.763002820000	7.408191814000	
∆0 H	10.553487040000 10.091	1909530000 6 71110220	5000	49 H	10.690936170000	10.092224640000	6.428519194000	
45 1	10.000 10.000		000	-1211	12.0300000000	10.032224040000	5.420313134000	
50 C	13.905041900000 5.244	004225000 5.315645968	000	50 C	13.313888180000	5.245223140000	5.293421821000	

51 H	13.706939040000	5.376269313000	4.255120779000	51 H	13.718103030000	5.409900234000	4.238394348000	
52 H	14.423171350000	4.249100442000	5.429239968000	52 H	14.416042730000	4.237540702000	5.379136951000	
53 H	14.722190870000	5.996381754000	5.581823480000	53 H	14.754285730000	5.973535249000	5.572492748000	
54 C	11.169211080000	4.088020242000	5.840945254000	54 C	11.199518300000	4.077884871000	5.863985898000	
55 H	10.267775940000	4.065180439000	6.469290402000	55 H	10.293453760000	4.076617212000	6.486454376000	
56 H	11.658022820000	3.103274269000	5.927834961000	56 H	11.686705820000	3.096882433000	5.990996722000	
57 H	10.852167570000	4.182853704000	4.792470450000	57 H	10.890490600000	4.143589361000	4.812143151000	
58 C	12.893937930000	4.929667853000	8.170404929000	58 C	12.934891590000	4.951730030000	8.161325651000	
59 H	13.667416460000	5.580257000000	8.601904049000	59 H	13.694595160000	5.617496603000	8.593100472000	
60 H	13.292267810000	3.901915885000	8.169663511000	60 H	13.352556000000	3.931833652000	8.161769332000	
61 H	12.020154610000	4.945297538000	8.837154686000	61 H	12.061133200000	4.951238936000	8.828615668000	

[MCp*₂X₃]^q/q=2-,1-/X=CN,NC/ COSMO [Ce(III)Cp*₂CN₃]²⁻ 1 Ce 0.00000000000 0.000000000 0.599294960700 [Ce(III)Cp*₂NC₃]²⁻ 1 Ce 0.00000000000 0.000000000 0.640904058200 2 N 0.0000000000 0.000000000 4.414545948000 2 C 0.0000000000 0.000000000 4.354278349000 3 N -0.598670714500 3.658093434000 1.603483091000 3 C -0.357973822400 3.594981095000 1.557398063000 4 C 0.0000000000 0.000000000 3.238714979000 4 N 0.0000000000 0.000000000 3.177841918000

6C 2.034381957000 3.3633807400 -1.39145452000 7C 2.11370630000 1.51357110000 0.558827427200 7C 2.11390613000 0.51387110000 0.558827427200 7C 2.11370613000 0.558827427200 7C 2.11370613000 0.558827427200 7C 2.11370613000 0.558827427200 7C 2.13806317000 0.7583318800 0.604588414100 9C 2.8650817000 0.918558118800 0.592266166 11C 1.76607345000 0.30468877500 2.8666912000 11C 1.76607345000 0.91857278100 0.43252191500 13H 1.0589503000 0.6668775900 2.866904200 2.8756739800 1.068747500 3.180447500 14H 1.8569503000 0.66687759800 3.1664122000 14H 1.2569751000 2.8756379800 1.08247579900 15C 1.82670758000 0.26874513100 1.6H 1.74433717600 2.8756379800 1.8259491400 18H 2.8321367800 0.3628792000 1.4857476600 1.8274756600 1.8274756600 1.8274756600 1.8293951500 1.8284515700
7 C 2.13706.59900 1.5137911000 0.5882742720 7 C 2.81301193200 1.376916.152001 0.53489738700 8 C 2.61018311900 1.15317171000 0.693581442700 8 C 2.6596878900 0.43450421110 0.69030177130 10 C 2.47766314900 0.3046867750 2.865664100 10 C 2.455664400 0.4385113800 0.5922661616 11 C 1.7667345000 0.3046857750 2.865664100 0.4455530700 3.445577000 11 H 1.265921000 0.40819129200 3.44557170069500 13 H 1.0385072000 3.15640123200 1.0681754000 1.06847500 3.1864012300 1.6481754000 3.662141000 3.1864012300 14 H 1.5653430300 3.562240700 0.2687751500 1.8270755000 1.877475400 3.660214000 0.263321247 14 H 1.5653430300 3.562240700 0.268775500 1.877475400 3.1864012300 1.87848570 14 H 1.5653430300 3.562240700 0.2687742700 1.87848570 0.263221247 14 H 1.7323751000 0
BC 2.60133119000 1.132117715000 0.693581442700 8 C 2.6958678000 0.97724812200 0.60601771000 9C 2.83506877000 0.27017594600 0.68458404100 9C 2.80050114000 0.938381800 0.6640177100 0.66401771100 0.666017713100 1.0015127000 3.4352261666 12 1.7510745800 0.4685877500 2.8656640100 1.11 1.7665117000 0.2819179200 3.4322815500 13 H 1.0383656100 0.031577249120 3.4455727000 1.14 1.2502751000 0.24819759200 3.1751069500 14 H 1.3653430300 0.6653753000 1.0681743000 1.66 1.7443717000 3.460214100 0.263221247 17 H 1.16482250400 2.9628155000 1.6887451300 1.64 1.74433717600 3.46602481000 0.263221247 17 H 1.6482250400 2.962815500 1.85727056000 1.8274763000 3.4652481000 1.6383861000 17 H 1.6482250400 2.79474343000 2.9937558600 3.650234000 1.825740766000 1.825740766000 1.825740766
9 C 2.83036377000 0.270175294600 0.68458044100 9 C 2.80303142000 0.43840211100 0.66601771300 10 C 2.47746114900 0.07833319880 0.604268041000 11C 1.76601316000 0.1837527285100 2.85658402800 11 C 1.76107345000 0.30468577500 -2.86658212000 11E 1.76693117600 0.187727285100 2.8595402800 13 H 1.038566100 1.07319670200 -3.1750648500 12H 2.9993985100 0.6885733370 -3.44455727000 12H 2.90472848200 0.7897082700 -3.850447570 14 H 1.36509253000 0.6587159400 -1.68817943000 15E 2.40427848200 2.78965895000 -0.7893781300 15 C 1.8250752000 1.8320752000 1.83207625000 12H 2.999783900 2.889063000 1.8851082000 2.889563000 1.8993198800 16 L 1.548275000 1.82770765000 12H 2.999783700 1.825751500 1.8258951000 1.893791800 1.893791800 1.893791800 1.8258951000 1.445950106000 1.893791800 1
10 C 2.47746314900 -0.76839319800 -0.60426804010 10 C 2.41565064400 -0.93858113600 -0.592261616C 11 C 1.76107345800 0.30468867730 -2.66663112000 11 C 1.76861176200 0.18572785100 2.85945022000 12 H 2.68596642000 0.485553337100 3.4455727000 12 H 2.7093996100 0.10191524/000 3.1050413700990 13 H 1.3836566100 0.7395758000 -0.665871594300 -1.06817943000 15 C 2.04274882000 2.7806588000 -0.7249754300 16 H 1.955745000 2.91853758000 -0.68817943000 15 C 2.0427482000 2.460558000 -0.26374513100 17 H 1.6642250400 2.9028155000 -1.4856205000 18 H 2.937958000 1.8597016000 12 H 2.47967628700 1.45563072000 18 H 2.9379578000 1.8597105600 1.8284851500 14 H 2.32784754000 0.4665994000 1.77323779900 22 H 4.9995148100 1.9318187000 24 H 4.569747000 1.8284851500 21 H 2.2704584600
11 C 1.76107345800 0.304688677500 -2.86668211200 11 C 1.76863117600 0.185772785100 -2.8595402800 12 H 2.6856604200 0.4855333710 -3.44455727000 12 H 2.7098981000 0.28419179200 -3.1751069500 13 H 1.138036561000 1.073196702000 -3.17504365000 13 H 1.115499240000 0.74807482700 -3.1860467500 15 C 1.89267254000 2.91853758800 -1.6681794300 15 C 2.04278482000 2.7880589600 -0.7249754300 16 H 1.50534303300 3.6624240700 0.2683731300 16 H 1.7439758600 3.46502148100 -2.837959300 -1.8594914300 18 H 2.3219878000 3.66242447000 1.8570765000 18 H 2.9975586000 1.4989316800 1.4989316800 1.4989316800 1.4989316800 21 H 2.7866877500 1.5751068400 1.752106400 1.857076500 1.824845700 2.8034596000 1.4989316800 1.824845700 21 H 2.7868871000 1.58510682000 2.79947434000 2.74 4.3955148100 2.91956994000 1.7643310100 21 H 2.7866877100
12 H 2.685696042000 0.48555337100 3.444557270000 12 H 2.703399861000 0.28419179200 3.1320815500 13 H 1.03836561000 1.07319670200 3.17506435000 13 H 1.15499240000 1.01015247000 3.15510069500 14 H 1.365092530000 0.665871534300 -3.05641232000 14 H 1.2927071000 3.74907482700 3.86604487500 15 C 1.892672540000 2.96028155500 -1.692076250000 16 H 1.74337176000 3.46602144100 0.2633714310 16 H 1.64822504000 2.96028355000 -1.892076250000 17 H 1.278676287000 2.875963793000 -1.8594914300 17 H 1.164822504000 2.96642341200 1.8227470766000 2.01 H 2.9397858600 1.09409220000 2.8837598000 1.8258485700 21 H 2.7845846000 2.9498139400 1.8138187000 2.01 H 2.4212174600 2.80284397600 1.824581530 21 H 2.78458846000 -1.0685951400 1.78239709000 2.2 G 3.35351002 1.4743317600 1.824581530 21 H 2.7845846000 -1.06889514100 1.0125660070 2.16
13H 1.038365661000 1.073196702000 -3.1750.4365000 13H 1.115.499240000 1.01915.47000 -3.1750.069500 14H 1.3650253000 -0.66871594300 -1.066817943000 164 1.227501000 -0.749074827900 -3.1860448750 15C 1.89267254000 2.91853758000 -0.66837451310 164 1.72437582000 2.87805896000 -1.07249754300 16H 1.50534330300 3.5624407000 0.26837513100 18H 1.279676287000 2.879563793000 -1.88249744070 0.26837451310 17H 1.64822504000 2.90298387000 3.36288792000 1.4852506600 19C 3.034059601000 1.89297016000 1.8838483700 20H 2.37966887000 2.57966783000 2.57947434300 20H 2.421274800 2.80324976000 1.8845843500 21H 2.79668871000 1.57510684000 2.4913318170000 22H 4.0955148100 2.1915669400 1.845381500 21H 2.7945886000 2.40165994000 1.77323970900 22H 4.0955148100 2.1915669400 1.8253415600 22H 3.97898240000 2.4116459340000 1.6683951400 <td< td=""></td<>
14 H 1.36509253000 -0.668371594300 -3.196401232000 14 H 1.29267057100 -0.7497482790 -3.1860487500 15 C 1.89267254000 2.91853758800 -1.06881794300 15 C 2.04278482200 2.7880595600 -1.07249754300 16 H 1.50534030300 3.5624204700 -0.2683751100 16 H 1.743171600 2.8595373000 -1.8594914300 17 H 1.164822504000 2.9606423942000 1.8527065000 19 C 3.03405961000 1.59257055000 1.85849813600 19 C 2.929998307000 2.06642394200 1.82574766600 19 C 3.0405961000 1.992570165000 1.89257016500 1.8258435700 21 H 2.27845884600 2.94983139400 1.8131817000 21 H 2.411274800 2.09324397600 1.845381500 21 H 2.4784584600 2.4065994000 1.773239790900 22 H 4.3959148100 -1.0775727000 1.7634331000 21 H 3.4369419900 -1.06725727000 1.7653894200 24 H 4.49736001600 -1.30720280300 1.267184200 24 H 3.1269487300 -2.9079158700 -2.7848927000 27 H 2.3
15 C 1.892672540000 2.918537588000 -1.068817943000 15 C 2.042784882000 2.788065896000 -1.07249754300 16 H 1.505343033000 3.562424047000 -2.68374513100 16 H 1.744337176000 3.466021481000 -2.66323212470 17 H 1.164822504000 2.96028155500 1.892076255000 17 H 1.279676287000 2.875963793000 1.85949914300 19 C 2.9299880700 3.3628875000 1.44562066300 19 C 2.9309850000 1.892570155000 2.87595379300 1.85264837600 20 H 2.76668878100 1.57810648000 2.79917434300 20 H 2.8628805000 1.40949292000 2.80234397600 1.82574375600 21 H 2.27845884600 2.4065994000 1.773239709000 22 H 4.09595148100 2.18566397000 1.26771842000 1.8263815900 22 H 3.97898264000 2.4165994000 1.75639942000 22 H 4.459501600 -1.30370280300 1.26771842000 1.7823375100 21 H 3.456645195000 -2.166848915000 1.10122666000 27 C 2.56364582600 2.337154343400 1.08253657500 21 C 2
16 H 1.50534303000 3.562420407000 -0.268374513100 16 H 1.744337176000 3.466021481000 -0.2623212470 17 H 1.164822504000 2.9028155500 -1.892076250000 17 H 1.279676287000 2.87563793000 -1.85949914300 18 H 2.832130878000 3.62887920000 -1.44562063000 19 C 3.97976586600 3.155810082000 -1.48933166600 20 H 2.282998307000 1.578106848000 2.799474343000 20 H 2.8828053000 1.40404928000 2.8037516800 21 H 2.27845884600 2.4085994000 1.77323970900 22 H 4.095951481000 2.191566994000 1.7634301000 22 H 4.9595419600 -1.668859514000 1.8338187000 22 H 4.095951481000 1.26771842000 1.81381889100 24 H 4.5494573400 -0.47275279000 1.765099342000 24 H 4.45736016000 -3.03702803807 7.7843827000 27 C 2.7098215700 -2.166884915000 -1.91124586000 25 H 3.064483887000 -2.92731750700 1.7571227300 28 H 2.8054195000 -2.430497364000 -1.911245800 2.8828953000 <
17 H 1.164822504000 2.96028155500 -1.892076250000 17 H 1.279676287000 2.87596373000 -1.85949914300 18 H 2.832130878000 3.362887920000 -1.44562063000 18 H 2.993785886000 3.155810082000 -1.49933168600 19 C 2.929998307000 2.06642394200 1.825740766000 19 C 3.034059601000 1.892570165000 1.82854835700 20 H 2.78658878100 1.578106848000 2.999474343000 2.01 2.803243976000 2.803243976000 1.82537155000 21 H 2.4786846000 2.41065994000 1.773239709000 22 H 4.095951481000 2.191566994000 1.78253575100 22 H 3.35383402000 1.047275279000 1.756398942000 24 H 4.45736016000 1.30370289300 1.78253575100 24 H 4.5094573400 -1.0678858770 2.78489827000 25 H 2.97613413200 -2.9731450700 1.7825357500 25 H 3.11229533200 2.16610954000 1.9112786000 28 H 1.88447113000 -523892347000 1.92253875600 27 C 2.7008215700 2.36084515000 1.352125466000 33 C -2.3
18 H 2.832130878000 3.36288792000 -1.445620063000 18 H 2.99378558600 3.155810082000 -1.49893168600 19 C 2.929998307000 2.066423942000 1.825740766000 19 C 3.03405961000 1.892570165000 1.82854835700 20 H 2.786688781000 1.578106848000 2.799474343000 20 H 2.88288063000 1.409409280000 2.80374596600 21 H 2.78458846000 2.49483193400 1.81338187000 21 H 2.4212174800 2.803243976000 1.82453815300 22 H 3.97898264000 1.04027527900 1.756939342000 22 H 4.09595148100 -1.26771842000 1.81838890100 24 H 4.540945734000 -1.04727527900 1.76538902000 25 H 2.97613413200 -2.29731750700 1.7781227300 25 H 3.13600989700 -0.6780858070 2.784898270000 27 C 2.56364582600 -2.32716543400 -1.6820637500 28 H 2.8054005700 2.9709158700 -3.03602415200 26 H 3.06448388700 -0.2697364270 2.97846231000 31 K 0.598670714500 -5.2881958000 1.33225466000 31 C -3.57
19 C 2.92998307000 2.066423942000 1.825740766000 1.9 C 3.034059601000 1.892570165000 1.825483570 20 H 2.786688781000 1.57810644000 2.799474343000 2.0 H 2.88286063000 1.409409280000 2.8037516600 21 H 2.278458846000 2.41055904000 1.773239709000 22 H 4.095951481000 2.191566994000 1.7634301000 23 C 3.43695419600 -1.068859514000 1.803024417000 23 C 3.35333402000 -1.267718420000 1.81388890100 24 H 4.54994573400 -1.047275279000 1.756398042000 24 H 4.45736016000 -1.303702803000 1.7825357510 25 H 3.11229533200 -2.116610954000 1.76589942000 2.76 H 3.06448388700 0.86297364270 2.79846231200 26 H 3.136009897000 -2.66884915000 -1.0112686000 28 H 1.88447135000 -2.237163434000 -1.98526375500 27 C 2.700982157000 -2.9079158700 -3.03602415200 28 H 1.88447135000 -3.9570878600 0.2973813404 30 H 3.72400679000 -2.2812173000 -1.50201013200 30 H
20 H 2.786688781000 1.578106848000 2.799474343000 20 H 2.88286630000 1.40940928000 2.8037519600 21 H 2.27845884600 2.949831934000 1.813381870000 21 H 2.421212748000 2.803243976000 1.82453815300 22 H 3.978982640000 2.41065994000 1.773239709000 22 H 4.095951481000 2.191566994000 1.7634330100 23 C 3.436954196000 -1.047275279000 1.75609342000 24 H 4.45736016000 -1.303702803000 1.7852357510 25 H 3.112295332000 -2.116610954000 1.765389042000 25 H 2.976134132000 -2.297317507000 1.77511227300 27 C 2.700982157000 -2.16688915000 -1.01122686000 21 H 2.8447135000 -2.337516300 -0.8520637500 28 H 2.00541095000 -2.43049736400 -1.911417582000 28 H 1.88447135000 -2.53892347000 -1.92353875400 29 H 2.55546550700 -2.3070132000 -3.0570882100 -3.5979882400 -2.51520964100 -1.44478720700 31 N 0.5
21 H 2.278458846000 2.949831934000 1.813381870000 21 H 2.421212748000 2.803243976000 1.8245381530 22 H 3.979882640000 2.410659904000 1.773239709000 22 H 4.099591481000 2.191566994000 1.8245381530 23 C 3.3436954196000 1.068859514000 1.803024417000 23 C 3.3535340200 1.26771842000 1.8245381530 24 H 4.54094573400 1.047275279000 1.756099342000 24 H 4.4573601600 1.30370280300 1.7825357510 25 H 3.11229533200 -2.116610954000 1.765389042000 25 H 2.97613413200 -2.29731750700 1.7511227300 26 H 3.1360989700 -0.67808580700 2.784898270000 26 H 3.06448388700 -0.86297364270 2.79846231200 27 C 2.70982157000 -2.430497364000 -1.911417582000 28 H 1.8844713500 -2.53892347000 -1.9235875400 29 H 2.55546550700 -2.90709158700 -3.05200132000 31 C 0.357973822400 3.05720878600 -0.2973813194 30 H 3.72400679071450 -5.28389558000 1.33222546000 32 C <t< td=""></t<>
22 H 3.978982640000 2.410659904000 1.773239709000 22 H 4.095951481000 2.191566994000 1.7634301000 23 C 3.436954196000 -1.068859514000 1.803024417000 23 C 3.353533402000 -1.267718420000 1.8183889100 24 H 4.540945734000 -1.047275279000 1.75609342000 24 H 4.457360016000 -1.303702803000 1.7825357510C 25 H 3.112295332000 -2.116610954000 1.765389042000 26 H 3.064483887000 0.862973642700 2.7984623120C 27 C 2.700982157000 -2.166884915000 -1.011226860000 27 C 2.563645826000 -2.327163434000 -1.0822637540C 28 H 2.00541095000 -2.430497364000 -1.911417582000 28 H 1.88447135000 -2.538923470000 -1.9235387540C 29 H 2.555465507000 -2.907091587000 -0.30602415200 30 H 3.591644264000 -2.51209641000 -1.4447872070C 31 N 0.598670714500 -3.658093434000 1.603483091000 31 C 0.357973822400 -3.579386300 0.22451576200 32 C 0.41353165400 -2.528389585000 1.332225466000
23 C 3.436954196000 -1.068859514000 1.803024417000 23 C 3.353533402000 -1.267718420000 1.81838890100 24 H 4.540945734000 -1.047275279000 1.756099342000 24 H 4.45736001600 -1.30370280300 1.782537510C 25 H 3.112295332000 -2.116610954000 1.765389042000 25 H 2.976134132000 -2.297317507000 1.7751122730C 27 C 2.700982157000 -0.678008580700 2.784898270000 25 H 3.06443887000 -0.82973642700 2.7984623120 28 H 2.005410950000 -2.430497364000 -1.911417582000 28 H 1.88447135000 -2.538923470000 -1.92353875400 29 H 2.555465507000 -2.907091587000 -0.303602415200 30 H 3.591644264000 -2.515209641000 -1.44478720700 31 N 0.598670714500 -3.658093434000 1.603483091000 31 C 0.357973822400 -3.594981095000 1.22317567200 32 C 0.413534165400 -2.528389585000 1.33225466000 32 N 0.24458457700 -2.471195795000 1.23217567200 34 C -2.113706309000 -1.1351379110000 0.589827427200
24 H 4.540945734000 -1.047275279000 1.756099342000 24 H 4.457360016000 -1.303702803000 1.7825375100 25 H 3.112295332000 -2.116610954000 1.765389042000 25 H 2.976134132000 -2.297317507000 1.77511227300 26 H 3.13609897000 -0.678008580700 2.784898270000 2.6 H 3.06443887000 0.862973642700 2.79846231200 27 C 2.70982157000 -2.166884915000 -1.011226660000 2.8 H 1.88447135000 -2.83923470000 -1.08220637500 28 H 2.005410950000 -2.43049736400 -1.91147582000 2.8 H 1.88447135000 -2.53382547000 -1.9233875400 9 H 2.555465507000 -2.28812173000 -1.50201132000 30 H 3.59164426400 -2.51520964100 -1.44478720700 31 N 0.598670714500 -3.65809343400 1.603483091000 31 C 0.35797382400 -3.594981095000 1.55739806300 32 C 0.413534165400 -2.52838958500 1.332225466000 32 N 0.244858457700 -2.471195795000 1.22317567200 34 C -2.113706309000 -1.135217715000 0.693581442700
1411 4.10021517000 1.170035372000 1.170035372000 1.170035372000 1.170035372000 25 H 3.112295332000 -2.116610954000 1.765389042000 25 H 2.976134132000 -2.297317507000 1.77511227300 26 H 3.16009897000 -0.678008580700 2.784898270000 2.6 H 3.06443887000 -0.862973642700 2.79846231200 27 C 2.2005410950000 -2.430497364000 -1.911417582000 2.8 H 1.88444713500 -2.327163434000 -1.92353875400 29 H 2.555465507000 -2.907091587000 -0.303602415200 29 H 2.33775163300 -3.57208786000 -0.297381131940 30 H 3.724000679000 -2.8812173000 -1.502010132000 30 H 3.59164264000 -2.51520964100 -1.4478720700 31 N 0.598670714500 -3.658093434000 1.603483091000 31 C 0.357973822400 -3.594981095000 1.55739805300 32 C 0.413534165400 -2.52838958500 1.332225466000 32 N 0.248458457700 -2.471195795000 1.22317567200 33 C -2.03438195700 0.3633697400 -1.391454542000 33 C -2.03248999200
2-1.1 2-1.10213123000 1.1731122300 1.1731122300 1.1731122300 26 H 3.136009897000 -0.678008580700 2.784898270000 26 H 3.06448388700 -0.862973642700 2.79846231200 27 C 2.503645826000 -2.166884915000 -1.010226860000 28 H 1.884447135000 -2.538923470000 -1.92353875400 29 H 2.555465507000 -2.907091587000 -0.303602415200 29 H 2.337751653000 -3.597288200 -2.4247787000 31 N 0.598670714500 -2.52839344000 1.603483091000 31 C 0.35973822400 -2.515209641000 -1.44478720700 32 C 0.413534165400 -2.5283958500 1.332225466000 32 N 0.24458457700 -2.471195795000 1.2217567200 33 C -2.03438195700 0.3633697400 -1.51357911000 0.589827427200 34 C -2.183011932000 -1.376916152000 0.5848931870 34 C -2.11370630900 -1.135217715000 0.693581442700 35 C -2.65988678900 0.97724812290 0.70030910770 35 C -2.610183119000 -1.35217715000 0.6693581442700 36 C -2.803003142000 <t< td=""></t<>
21 3.1500051000 1.0800630000 2.1988221000 2.1988321000 2.1988423100 27 2.700982157000 -2.166884915000 -1.010226860000 28 1.88447135000 -2.327163434000 -1.92353875400 29 2.555465507000 -2.907091587000 -0.303602415200 29 2.33775165300 -3.05720876600 0.29738131940 30 H 3.724000679000 -2.88121730000 -1.502010132000 30 H 3.591644264000 -2.515209641000 -1.5739806300 31 0.598670714500 -3.658093434000 1.602010132000 31 0.357973822400 -3.594981095000 1.25739805300 32 C 0.41353416540 -2.5283958500 1.33225466000 32 N 0.248458457700 -2.47119579500 1.23217567200 33 C -2.03438195700 0.36330697400 -1.391454542000 33 C -2.03248999200 -0.204528477500 1.38295555300 34 C -2.113706309000 -1.135217715000 0.69358142700 35 C -2.659886789000 -0.977
27 C 2.0038213000 -2.1083213000 -1.101228800000 28 H 2.005410950000 -2.430497364000 -1.911417582000 28 H 1.884447135000 -2.538923470000 -1.92337875400 29 H 2.555465507000 -2.907091587000 -0.303602415200 29 H 2.337751653000 -3.057208786000 -0.29738131940 30 H 3.724000679000 -2.288121730000 -1.502010132000 30 H 3.59164264000 -2.5152964000 1.5573886300 31 N 0.598670714500 -2.58889585000 1.63343391000 31 C 0.357973822400 -3.594981095000 1.22317567500 32 C 0.413534165400 -2.52889585000 1.332225466000 32 N 0.2484597700 -2.471195795000 1.22317567500 34 C -2.113706309000 -1.513579110000 -0.589827427200 34 C -2.183011932000 -1.376916152000 -0.5848978170 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.659886789000 -0.977248122900 0.70030910770 36 C -2.747463149000 0.768393198800 -0.604268040100 37 C -2.416506044000 0.918358113800 -5.9226616160<
26 n 2.059-0590000 -2.4309-97364000 -1.9141/582000 28 h 1.8444/15000 -2.5382244/0.000 -1.92253875400 29 H 2.35751653000 -2.907911587000 -1.502010132000 29 H 2.337751653000 -3.057208786000 0.29738131940 30 H 3.724000679000 -2.288121730000 -1.502010132000 30 H 3.591644264000 -2.515209641000 1.4447872070 31 N 0.598670714500 -3.658093434000 1.63483091000 31 C 0.357973822400 -3.594981095000 1.5573986300 32 C 0.413534165400 -2.52839585000 1.332225466000 32 N 0.248458457700 -2.47119579500 1.5573981702 34 C -2.113706309000 -1.51357911000 -0.589827427200 34 C -2.18301193200 -1.37691615200 -0.58489738170 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.65988678000 -0.977248122900 0.70030910770 36 C -2.747463149000 0.768393198800 -0.604268040100 37 C -2.416506044000 .918358113800 -5.9226616160
29 Fi 2.3374635307000 -2.907491387000 -0.393802415200 -0.2973813194(30 H 3.724000679000 -2.288121730000 -1.502010132000 30 H 3.59464264000 -2.515209641000 -1.4447872070(31 N 0.598670714500 -3.658093434000 1.603483091000 31 C 0.357973822400 -3.594981095000 1.55739806300 32 C 0.413534165400 -2.528389585000 1.332225466000 32 N 0.248485857700 -2.471195795000 1.22317567200 33 C -2.034381957000 -0.336330697400 -1.391454542000 33 C -2.032489992000 -0.204528477500 -1.3829555300 34 C -2.113706309000 -1.513579110000 -0.589827427200 34 C -2.183011932000 -1.376916152000 -0.58489738170 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.680303142000 0.438402111100 0.69601777130 36 C -2.747463149000 0.768393198800 -0.604268040100 37 C -2.46566116600 38 C -1.76073458000 -0.394688677500 -2.856682112000 38 C -1.76863176000 -0.88497851500 -2.85954502800
30 H 3.724000073000 -2.28121730000 -1.502010132000 -1.44478720700 31 N 0.598670714500 -3.65809343000 1.603483091000 31 C 0.357973822400 -3.554981095000 1.55739806300 32 C 0.413534165400 -2.28389585000 1.332225466000 32 N 0.248458457700 -2.471195795000 1.22317567200 33 C -2.034381957000 -0.36330697400 -1.391454542000 33 C -2.032489992000 -0.204528477500 -1.3829555300 34 C -2.113706309000 -1.513579110000 -0.589827427200 34 C -2.16301132000 -1.376916152000 -0.58489738170 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.6886789000 -0.977248122900 0.7003910770 36 C -2.477463149000 0.768393198800 -0.604268040100 37 C -2.465661176000 -9.185772785100 -2.85954502800 39 H -2.68566642000 -0.486877500 -2.866682112000 38 C -1.76631176000 -0.84491972900 -3.43229815500 40 H -1.03836561000 -1.0
31 N 0.55867/0714500 -3.558093434000 1.603483091000 31 C 0.357973822400 -3.559481095000 1.55739806300 32 C 0.413534165400 -2.52838958000 1.332225466000 32 N 0.248458457700 -2.471195795000 1.2231756720C 33 C -2.03438195000 0.336330697400 -1.391454542000 33 C -2.032489992000 -0.204528477500 -1.3829555300 34 C -2.11370630000 -1.513579110000 -0.588827427200 34 C -2.183011932000 -1.376916152000 -0.5848973817C 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.659886789000 -0.977248122900 0.70030910770 36 C -2.835036877000 0.270175294600 0.68458404100 36 C -2.4656044000 0.91835811380 -0.59226616160 37 C -2.477463149000 0.768393198800 -0.604268040100 37 C -2.465661176000 -0.185772785100 -2.8594502800 38 C -1.7610734582000 -0.30468877500 -2.866682112000 38 C -1.76863176000 -0.819772785100 -2.8594502800
32 C 0.415541105400 -2.528389585000 1.332225466000 32 N 0.248458457700 -2.471195795000 1.22317567200 33 C -2.034381957000 -0.336330697400 -1.391454542000 33 C -2.032489992000 -0.204528477500 -1.3829555300 34 C -2.11370630000 -1.513579110000 -0.588827427200 34 C -2.183011932000 -1.376916152000 -0.58489738170 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.659886789000 -0.977248122900 0.70030910770 36 C -2.835036877000 0.270175294600 0.68458404100 36 C -2.80303142000 0.438402111100 0.69601777130 37 C -2.477463149000 0.768393198800 -0.604268040100 37 C -2.16566040000 0.918358113800 -0.59226616160 38 C -1.761073458000 -0.304688677500 -2.866682112000 38 C -1.768631176000 -0.81772785100 -2.8594502800 39 H -2.2659861000 -1.073196702000 -3.175064355000 40 H -1.115499240000 -1.010915247000 -3.12504487500<
33 C -2.03438195 / UUU -0.336330697400 -1.391454542000 33 C -2.032489992000 -0.204528477500 -1.38295555300 34 C -2.113706309000 -1.513579110000 -0.589827427200 34 C -2.183011932000 -1.376916152000 -0.5848973817 35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.659886789000 -0.977248122900 0.7003091077C 36 C -2.835036877000 0.270175294600 0.68458404100 36 C -2.803003142000 0.438402111100 0.69601777130 37 C -2.477463149000 0.76839319800 -0.604268040100 37 C -2.165664176000 0.918358113800 -0.59226616160 38 C -1.761073458000 -0.304688677500 -2.866682112000 38 C -1.768631176000 -0.8185772785100 -2.85954502800 39 H -2.685696042000 -0.43555337100 -3.444557270000 39 H -2.709399861000 -0.0284191792900 -3.43229815500 40 H -1.03836561000 -1.073196702000 -3.17506435000 40 H -1.115499240000 -1.01915247000 -3.18604487500 41 H -1.3626725540000 -2.918537588000
34 C -2.113706309000 -1.53579110000 -0.588827427200 34 C -2.183011932000 -1.376916152000 -0.588827817(35 C -2.610183119000 -1.135217715000 0.693581442700 35 C -2.659886789000 -0.977248122900 0.7003091077C 36 C -2.835036877000 0.270175294600 0.66458404100 36 C -2.803003142000 0.438402111100 0.69601777130 37 C -2.477463149000 0.768393198800 -0.604268040100 37 C -2.416566044000 0.918358113800 -0.59226616160 38 C -1.76073458000 -0.304688677500 -2.866682112000 38 C -1.768631176000 -0.81777285100 -2.85954502800 39 H -2.685696042000 -0.43553337100 -3.444557270000 39 H -2.79399861000 -0.284191792900 -3.43229815500 40 H -1.03836561000 -1.07319670200 -3.175064355000 40 H -1.11549924000 -1.0191524700 -3.18604487500 41 H -1.365072550000 -0.668371594300 -3.196401232000 41 H -1.2246757100 0.749074828900 -2.78806589000
35 C -2.659886789000 -0.977248122900 0.7003091077C 36 C -2.835036877000 0.270175294600 0.66458404100 36 C -2.83003142000 0.438402111100 0.69661777130 37 C -2.47763149000 0.768393198800 -0.604268040100 37 C -2.416506644000 0.91835811380 -0.59226616160 38 C -1.761073458000 -0.304688677500 -2.866682112000 38 C -1.76861176000 -0.185772785100 -2.85954502800 39 H -2.685666042000 -0.48555337100 -3.444557270000 39 H -2.70939861000 -0.284191792900 -3.43229815500 40 H -1.03836561000 -1.073196702000 -3.175064355000 40 H -1.115499240000 -1.010915247000 -3.18604487500 41 H -1.36509253000 0.665871594300 -3.196401232000 41 H -1.292670571000 0.74907482709 -3.18604487500 42 C -1.892670571000 2.918537588000 -3.166817943000 42 C -2.4784882000 -2.788065896000 -1.072497453400
36 C -2.835036877000 0.270175294600 0.684584044100 36 C -2.803003142000 0.438402111100 0.69601777130 37 C -2.477463149000 0.768393198800 -0.604268040100 37 C -2.416506044000 0.91835811380 -0.5922661616C 38 C -1.761073458000 -0.304688677500 -2.866682112000 38 C -1.768631176000 -0.8577278510 -2.8595450280C 39 H -2.685696042000 -0.48555333710 -3.444557270000 39 H -2.709399861000 -0.284191792900 -3.4322981550C 40 H -1.03836561000 -1.07319670200 -3.175064365000 40 H -1.115499240000 -1.01915247000 -3.1860448750C 41 H -1.36509253000 0.665871594300 -3.196401232000 41 H -1.29267057100 0.74907482790 -3.1860448750C 42 C -1.892670571000 2.91853758800 -3.166817943000 42 C -2.4784882000 -2.788065896000 -1.0724975430C 41 H -1.050207000 0.56531754300 0.566817943000 42 C -2.4784882000 -2.788065896000 -1.0724975430C
37 C -2.47463149000 0.768393198800 -0.604268040100 37 C -2.416506044000 0.918358113800 -0.5922661616C 38 C -1.76107345800 0.034688677500 -2.866682112000 38 C -1.768631176000 -0.185772785100 -2.8595450280C 39 H -2.685696042000 -0.485553337100 -3.444557270000 39 H -2.709399861000 -0.284191792900 -3.4322981550C 40 H -1.038365661000 -1.073196702000 -3.175064355000 40 H -1.115499240000 -1.010915247000 -3.1751006950C 41 H -1.362672540000 -2.91853758800 -3.196401232000 41 H -1.292670571000 0.74907482790 -3.1860448750C 42 C -1.61401290000 -2.918537588000 -0.60817943000 42 C -2.4784882000 -2.7880658960000 -1.0724975430C 41 H -1.26701202000 -1.60817943000 42 C -2.4784882000 -2.788065896000 -0.724975430C
38 C -1.761073458000 -0.304688677500 -2.866682112000 38 C -1.768631176000 -0.185772785100 -2.8595450280C 39 H -2.68569642000 -0.485553337100 -3.444557270000 39 H -2.709399861000 -0.284191792900 -3.4322981550C 40 H -1.038365661000 -1.073196702000 -3.175064355000 40 H -1.115499240000 -1.01915247000 -3.1751006950C 41 H -1.3690253000 0.665871594300 -3.196401232000 41 H -1.292670571000 0.749074827900 -3.1860448750C 42 C -1.6042748482000 -2.918537588000 -0.608817943000 41.07249754300C -1.07249754300C -1.07249754300C
39 H -2.685696042000 -0.485553337100 -3.444557270000 39 H -2.709399861000 -0.284191792900 -3.43229815500 40 H -1.038365661000 -1.073196702000 -3.175064365000 40 H -1.115499240000 -1.01915247000 -3.17510669500 41 H -1.365092530000 0.665871594300 -3.196401232000 41 H -1.292670571000 0.749074827900 -3.18604487500 42 C -1.892672540000 -2.918537588000 -1.068817943000 42 C -2.042784882000 -2.788065896000 -1.07249754300 41 H -1.507470000 -2.918537588000 -1.068817943000 42 C -2.042784882000 -2.788065896000 -1.07249754300
40 H -1.038365661000 -1.073196702000 -3.175064365000 41 H -1.365092530000 0.665871594300 -3.196401232000 42 C -1.892672540000 -2.918537588000 -1.068817943000 42 C -1.05714003000 -2.918537588000 -1.068817943000 42 L -1.05714003000 -2.918537588000 -1.068817943000
41 H -1.365092530000 0.6565871594300 -3.196401232000 41 H -1.292670571000 0.749074827900 -3.18604487500 42 C -1.892672540000 -2.918537588000 -1.068817943000 42 C -2.042784882000 -2.788065896000 -1.07249754300 41 H -1.505141032000 2.55141447000 0.56237411100 41 H -1.7449754300
42 C -1.892672540000 -2.918537588000 -1.068817943000 42 C -2.042784882000 -2.788065896000 -1.07249754300 41 L 1.56514002000 2.55244042000 -0.56324513100 43 LL -1.474373136000 -2.788065896000 -1.07249754300
A2 U 1 505242020200 2 553424047000 0 25524512100 A2 U 1 744227456000 2 455024404000 0 2552224247
43 H -1.744337176000 -3.466021481000 -0.26323212470
44 H -1.164822504000 -2.960281555000 -1.892076250000 44 H -1.279676287000 -2.875963793000 -1.85949914300
45 H -2.832130878000 -3.362887920000 -1.445620063000 45 H -2.993785886000 -3.155810082000 -1.49893168600
46 C -2.929998307000 -2.066423942000 1.825740766000 46 C -3.034059601000 -1.892570165000 1.82854835700
47 H -2.786688781000 -1.578106848000 2.799474343000 47 H -2.882880630000 -1.409409280000 2.80375196800
48 H -2.278458846000 -2.949831934000 1.813381870000 48 H -2.421212748000 -2.803243976000 1.82453815300
49 H -3.978982640000 -2.410659904000 1.773239709000 49 H -4.095951481000 -2.191566994000 1.76343301000
50 C -3.436954196000 1.068859514000 1.803024417000 50 C -3.353533402000 1.267718420000 1.81838890100
51 H -4.5540945734000 1.047275279000 1.756099342000 51 H -4.457360016000 1.303702803000 1.78253575100
52 H -3.112295332000 2.116610954000 1.765389042000 52 H -2.976134132000 2.297317507000 1.77511227300
53 H -3.136009897000 0.678008580700 2.784898270000 53 H -3.064483887000 0.862973642700 2.79846231200
54 C -2.700982157000 2.166884915000 -1.101226860000 54 C -2.563645826000 2.327163434000 -1.08520637500
55 H -2.005410950000 2.430497364000 -1.911417582000 55 H -1.884447135000 2.538973470000 -1.92353875407
56 H -2.555465507000 2.907091587000 -0.303602415200 56 H -2.337751653000 3.057208786000 -0.29738131940
70120120120120120120120120120120120120120

57 H	-3.724000679000	2.288121730000	-1.502010132000	57 H	-3.591644264000	2.515209641000	-1.444787207000
F1.1/	W C . * CN 12-						
		0.0000000000000000000000000000000000000	0 579911769800		0.000000000000000000000000000000000000	0.0000000000000000000000000000000000000	0.632549000000
2.0	0.0000000000000	0.0000000000000	4.350420240000	20	0.0000000000000	0.0000000000000	4.205505000000
2 N	0.000000000000	0.00000000000000	4.360438248000	20	0.000000000000	0.000000000000000	4.305505000000
3 N	-0.409575461800	3.580387961000	1.628155337000	3 C	-0.323763000000	3.547740000000	1.502163000000
4 C	0.000000000000	0.000000000000	3.184891866000	4 N	0.000000000000	0.000000000000	3.127746000000
5 C	-0.274055746700	2.447833806000	1.332904663000	5 N	-0.242201000000	2.410313000000	1.196694000000
6 C	2.351421602000	-0.907100117800	-0.625649931900	6 C	2.372926000000	-0.938348000000	-0.561304000000
7 C	1.969696628000	0.241507952700	-1.386657103000	7 C	1.973458000000	0.171150000000	-1.369432000000
80	2 124901975000	1 392868297000	-0 550878552000	80	2 133244000000	1 360683000000	-0.59240000000
0.0	2.000240728000	0.052008240200	0.721227810200	00	2.133211000000	0.083607000000	0.504370000000
90	2.000340728000	0.952008249200	0.721227810500	90	2.025014000000	0.985607000000	0.89437000000
10 C	2.752611768000	-0.465785304000	0.673137043100	10 C	2.770333000000	-0.433988000000	0.713505000000
11 C	2.477261201000	-2.304750947000	-1.158473425000	11 C	2.529574000000	-2.351079000000	-1.039098000000
12 H	1.741260528000	-2.505667487000	-1.952212177000	12 H	1.772842000000	-2.613123000000	-1.793693000000
13 H	2.310079990000	-3.051661349000	-0.370542882600	13 H	2.415952000000	-3.068147000000	-0.216162000000
14 H	3.479239138000	-2.477587096000	-1.593958236000	14 H	3.522115000000	-2.506425000000	-1.502334000000
15 C	1.741151936000	0.270133517100	-2.869763100000	15 C	1.743990000000	0.125427000000	-2.851718000000
16 1	1 002060402000	1 105241560000	2 172521071000	16 1	1 002480000000	0.940146000000	2 10645000000
47.0	1 272762402000	0.654403334403	2 226074206000	17.0	1 200002000000	0.010017000000	2 160874000000
1/H	1.2/3/02183000	-0.054403331100	-3.230974360000	1/H	1.260802000000	-0.01891/00000	-3.1036/400000
18 H	2.696599330000	0.388160032000	-3.416607750000	18 H	2.698856000000	0.218803000000	-3.40420200000
19 C	1.998142002000	2.818348615000	-1.003010422000	19 C	1.993188000000	2.761382000000	-1.108843000000
20 H	2.942504506000	3.181828089000	-1.450723774000	20 H	2.939552000000	3.117279000000	-1.557743000000
21 H	1.730194961000	3.481764677000	-0.170211319100	21 H	1.706601000000	3.457214000000	-0.309845000000
22 H	1.213148522000	2.935855657000	-1.765799995000	22 H	1.217679000000	2.832146000000	-1.885863000000
22.0	2 007651280000	1 922611212000	1 969640072000	22 C	2 00501 2000000	1 017299000000	1 805025000000
25 0	3.00/031303000	1.032011213000	1.000040072000	230	3.003512000000	1.51/388000000	2 790662000000
24 H	2.839798085000	1.332923783000	2.833486842000	24 H	2.84341400000	1.456053000000	2.78966200000
25 H	2.419829728000	2.760029252000	1.883910594000	25 H	2.40358000000	2.834901000000	1.779310000000
26 H	4.079427802000	2.101333586000	1.808275544000	26 H	4.072805000000	2.200603000000	1.738736000000
27 C	3.342680512000	-1.315818644000	1.759540943000	27 C	3.327132000000	-1.241997000000	1.848832000000
28 H	4.447895703000	-1.309722491000	1.710572206000	28 H	4.428160000000	-1.320174000000	1.781444000000
29 H	2.997258827000	-2.355286995000	1.686606445000	29 H	2.910193000000	-2.257821000000	1.856071000000
30 H	3 049470505000	-0 953406119200	2 755919585000	30 H	3 083371000000	-0 788742000000	2 82026100000
21 N	0.400575461800	2.590397061000	1 639155337000	21.0	0.222762000000	2 54774000000	1 502162000000
31 N	0.409575461800	-3.580387961000	1.628155337000	310	0.323763000000	-3.54774000000	1.502163000000
32 C	0.274055746700	-2.447833806000	1.332904663000	32 N	0.242201000000	-2.410313000000	1.196694000000
33 C	-2.351421602000	0.907100117800	-0.625649931900	33 C	-2.372926000000	0.938348000000	-0.56130400000
34 C	-1.969696628000	-0.241507952700	-1.386657103000	34 C	-1.973458000000	-0.171150000000	-1.369432000000
35 C	-2.124901975000	-1.392868297000	-0.550878552000	35 C	-2.133244000000	-1.360683000000	-0.59240000000
36 C	-2.606340728000	-0.952008249200	0.721227810300	36 C	-2.623614000000	-0.983607000000	0.694370000000
37 C	-2.752611768000	0.465785304000	0.673137043100	37 C	-2.770333000000	0.433988000000	0.713505000000
38 C	-2 477261201000	2 304750947000	-1 158473425000	38 C	-2 52957400000	2 35107900000	-1.039098000000
20 1	1 741260528000	2 505667487000	1 052212177000	20 1	1 772842000000	2 612122000000	1 70260200000
3511	-1.741200328000	2.303007487000	-1.932212177000	3911	-1.772842000000	2.013123000000	-1.75305300000
40 H	-2.310079990000	3.051661349000	-0.370542882600	40 H	-2.415952000000	3.068147000000	-0.216162000000
41 H	-3.479239138000	2.477587096000	-1.593958236000	41 H	-3.522115000000	2.506425000000	-1.502334000000
42 C	-1.741151936000	-0.270133517100	-2.869763100000	42 C	-1.743990000000	-0.125427000000	-2.851718000000
43 H	-1.093969402000	-1.105241560000	-3.173531971000	43 H	-1.092489000000	-0.940146000000	-3.196469000000
44 H	-1.273762183000	0.654403331100	-3.236974386000	44 H	-1.280802000000	0.818917000000	-3.169874000000
45 H	-2.696599330000	-0.388160032000	-3.416607750000	45 H	-2.698856000000	-0.21880300000	-3.404202000000
AF C	-1 998142002000	-2 8183/8615000	-1 003010422000	AFC	-1 993188000000	-2 761382000000	-1 108843000000
40 0	2.0425045002000	2.010340013000	1 450722774000	47	2.020552000000	2.101302000000	1 557743000000
4/H	-2.942504506000	-3.101828089000	-1.450/25//4000	4/H	-2.939552000000	-2.11/2/9000000	-1.357743000000
48 H	-1.730194961000	-3.481764677000	-0.1/0211319100	48 H	-1.706601000000	-3.457214000000	-0.309845000000
49 H	-1.213148522000	-2.935855657000	-1.765799995000	49 H	-1.217679000000	-2.832146000000	-1.885863000000
50 C	-3.007651389000	-1.832611213000	1.868640072000	50 C	-3.005912000000	-1.917388000000	1.805035000000
51 H	-2.839798085000	-1.332923783000	2.833486842000	51 H	-2.843414000000	-1.456053000000	2.789662000000
52 H	-2.419829728000	-2.760029252000	1.883910594000	52 H	-2.403580000000	-2.834901000000	1.779310000000
53 H	-4.079427802000	-2.101333586000	1.808275544000	53 H	-4.072805000000	-2.200603000000	1.738736000000
54 C	-3.342680512000	1.315818644000	1,759540943000	54 C	-3.327132000000	1.24199700000	1.848832000000
	4 44790570000	1 200723 404000	1 710573306000		4 43916000000	1 22017400000	1 781444000000
55 H	-4.447695703000	1.509722491000	1.710372200000	55 H	-4.42610000000	1.5201/400000	1.75144400000
56 H	-2.997258827000	2.355286995000	1.686606445000	56 H	-2.910193000000	2.257821000000	1.8560/1000000
57 H	-3.049470505000	0.953406119200	2.755919585000	57 H	-3.083371000000	0.788742000000	2.820261000000
[1]	IV)Cp*_CN_1 ¹⁻			[1]	IV)Cp*_NC_1 ¹⁻		
10	0.0000000000000000000000000000000000000	0.000000000000	0.423341000000	10	0.000000000000000	0.0000000000000000000000000000000000000	0.569583000000
2 N	-0.039158000000	-3.518341000000	1.560553000000	2 C	-0.001737000000	-3.480360000000	1.500258000000
R N	0.000000000000	0.000000000000	4.116776000000	30	0.0000000000000	0.000000000000	4.178328000000
	0.020159000000	2 E1924100000	1 560552000000	40	0.00172700000	2.49026000000	1 500258000000
4 N	0.039136000000	3.31834100000	1.50055500000	40	0.001/5/000000	3.480300000000	1.30023000000
5 C	-0.028795000000	-2.390420000000	1.22/27300000	5 N	-0.000431000000	-2.354196000000	1.146471000000
6 C	0.000000000000	0.000000000000	2.941015000000	6 N	0.000000000000	0.000000000000	2.998262000000
7 C	0.028795000000	2.390420000000	1.227273000000	7 N	0.000431000000	2.354196000000	1.146471000000
8 C	-2.696014000000	0.664290000000	0.814012000000	8 C	-2.676426000000	0.715516000000	0.639185000000
9 C	-2.660852000000	-0.757250000000	0.664620000000	9 C	-2.676843000000	-0.713623000000	0.639919000000
1							

10 C	-2.251310000000	-1.050415000000	-0.676298000000		10 C	-2.214792000000	-1.156785000000	-0.638784000000	
11 C	-2.042382000000	0.195957000000	-1.354274000000		11 C	-1.925714000000	-0.000329000000	-1.430184000000	
12 C	-2.328105000000	1.253744000000	-0.434616000000		12 C	-2.213961000000	1.157115000000	-0.639878000000	
13 C	-3.188608000000	1.398277000000	2.027653000000		13 C	-3.202465000000	1.587106000000	1.743857000000	
14 H	-4.286488000000	1.503204000000	1.999737000000		14 H	-4.295154000000	1.709610000000	1.652503000000	
15 H	-2.757476000000	2.404869000000	2.092502000000		15 H	-2.749923000000	2.585536000000	1.720012000000	
16 H	-2.931144000000	0.866288000000	2.952420000000		16 H	-3.004918000000	1.155098000000	2.733893000000	
17 C	-3.158025000000	-1.739007000000	1.686952000000		17 C	-3.203555000000	-1.583840000000	1.745436000000	
18 H	-2.851078000000	-1.458877000000	2.703622000000		18 H	-3.012096000000	-1.147241000000	2.734671000000	
19 H	-2.783229000000	-2.75040000000	1.495955000000		19 H	-2.746382000000	-2.580328000000	1.727322000000	
20 H	-4.260614000000	-1.775008000000	1.674248000000		20 H	-4.295292000000	-1.711719000000	1.650030000000	
21 C	-2.193075000000	-2.408282000000	-1.317968000000		21 C	-2.228072000000	-2.570123000000	-1.149228000000	
22 H	-3.139930000000	-2.629758000000	-1.839004000000		22 H	-3.164564000000	-2.771568000000	-1.697147000000	
23 H	-2.023131000000	-3.199154000000	-0.578172000000		23 H	-2.152539000000	-3.296321000000	-0.332016000000	
24 H	-1.395190000000	-2.481167000000	-2.071642000000		24 H	-1.400678000000	-2.767940000000	-1.845122000000	
25 C	-1.767820000000	0.368031000000	-2.822731000000		25 C	-1.696841000000	-0.000806000000	-2.915460000000	
26 H	-1.219699000000	-0.482210000000	-3.248611000000		26 H	-1.148383000000	-0.888614000000	-3.254262000000	
27 H	-1.195610000000	1.281490000000	-3.038303000000		27 H	-1.145259000000	0.885106000000	-3.254074000000	
28 H	-2.715147000000	0.450137000000	-3.382193000000		28 H	-2.663732000000	0.000938000000	-3.447898000000	
29 C	-2.413837000000	2.708707000000	-0.795397000000		29 C	-2.225506000000	2.569966000000	-1.151797000000	
30 H	-1.626680000000	3.012354000000	-1.499768000000		30 H	-1.396224000000	2.766800000000	-1.845746000000	
31 H	-2.329791000000	3.350430000000	0.088267000000		31 H	-2.151952000000	3.297084000000	-0.335199000000	
32 H	-3.380849000000	2.921181000000	-1.282068000000		32 H	-3.160475000000	2.771109000000	-1.702467000000	
33 C	2.696014000000	-0.664290000000	0.814012000000		33 C	2.676426000000	-0.715516000000	0.639185000000	
34 C	2.328105000000	-1.253744000000	-0.434616000000		34 C	2.213961000000	-1.157115000000	-0.639878000000	
35 C	2.042382000000	-0.195957000000	-1.354274000000		35 C	1.925714000000	0.000329000000	-1.430184000000	
36 C	2.251310000000	1.050415000000	-0.676298000000		36 C	2.214792000000	1.156785000000	-0.638784000000	
37 C	2.660852000000	0.757250000000	0.664620000000		37 C	2.676843000000	0.713623000000	0.639919000000	
38 C	3.188608000000	-1.398277000000	2.027653000000		38 C	3.202465000000	-1.587106000000	1.743857000000	
39 H	4.286488000000	-1.503204000000	1.999737000000		39 H	4.295154000000	-1.709610000000	1.652503000000	
40 H	2.757476000000	-2.404869000000	2.092502000000		40 H	2.749923000000	-2.585536000000	1.720012000000	
41 H	2.931144000000	-0.866288000000	2.952420000000		41 H	3.004918000000	-1.155098000000	2.733893000000	
42 C	2.413837000000	-2.708707000000	-0.795397000000		42 C	2.225506000000	-2.569966000000	-1.151797000000	
43 H	3.380849000000	-2.921181000000	-1.282068000000		43 H	3.160475000000	-2.771109000000	-1.702467000000	
44 H	1.626680000000	-3.012354000000	-1.499768000000		44 H	1.396224000000	-2.766800000000	-1.845746000000	
45 H	2.329791000000	-3.350430000000	0.088267000000		45 H	2.151952000000	-3.297084000000	-0.335199000000	
46 C	1.767820000000	-0.368031000000	-2.822731000000		46 C	1.696841000000	0.000806000000	-2.915460000000	
47 H	2.715147000000	-0.450137000000	-3.382193000000		47 H	2.663732000000	-0.000938000000	-3.447898000000	
48 H	1.219699000000	0.482210000000	-3.248611000000		48 H	1.148383000000	0.888614000000	-3.254262000000	
49 H	1.195610000000	-1.281490000000	-3.038303000000		49 H	1.145259000000	-0.885106000000	-3.254074000000	
50 C	2.193075000000	2.408282000000	-1.317968000000		50 C	2.228072000000	2.570123000000	-1.149228000000	
51 H	3.139930000000	2.629758000000	-1.839004000000		51 H	3.164564000000	2.771568000000	-1.697147000000	
52 H	2.023131000000	3.199154000000	-0.578172000000		52 H	2.152539000000	3.296321000000	-0.332016000000	
53 H	1.395190000000	2.481167000000	-2.071642000000		53 H	1.400678000000	2.767940000000	-1.845122000000	
54 C	3.158025000000	1.739007000000	1.686952000000		54 C	3.203555000000	1.583840000000	1.745436000000	
55 H	2.851078000000	1.458877000000	2.703622000000	1	55 H	3.012096000000	1.147241000000	2.734671000000	
56 H	2.783229000000	2.75040000000	1.495955000000		56 H	2.746382000000	2.580328000000	1.727322000000	
57 H	4.260614000000	1.775008000000	1.674248000000		57 H	4.295292000000	1.711719000000	1.650030000000	
			\checkmark						
			[MI]	/ -1, -1, q=2/ N* ₂ X ₃] ^q	X=CN	,NC /COSM	NO		

						vi0	
[Ce 1 Ce	(III)N* ₂ CN ₃] ²⁻ 13.559564290000	22.521889050000	0.051943346570	[Ce 1 Ce	(III)N*2NC3] ⁻² 13.486678810000	22.521595650000	0.134391228300
2 Si	16.212558330000	24.028828060000	1.855044953000	2 Si	16.197472770000	24.013942530000	1.835128911000
3 Si	15.993548290000	24.859317280000	-1.063391135000	3 Si	15.953057190000	24.831244070000	-1.075381884000
4 Si	11.574915010000	20.974231270000	-2.440758209000	4 Si	11.599864400000	20.988700370000	-2.424740108000
5 Si	14.457881690000	20.018650710000	-2.309504919000	5 Si	14.477681200000	20.050176810000	-2.274463870000
6 C	14.467503210000	20.503830970000	1.560492791000	6 N	14.410622880000	20.585414970000	1.491755763000
7 C	11.743510650000	22.567565290000	1.935807288000	7 N	11.758517600000	22.589010080000	1.927488858000
8 C	12.117275610000	24.597092330000	-0.833168929500	8 N	12.177778720000	24.488394980000	-0.804246529200
9 N	15.467092360000	23.924613320000	0.293495194900	9 N	15.425922080000	23.907224750000	0.288868706900
10 N	13.171753680000	21.042774620000	-1.770329730000	10 N	13.183534660000	21.061486580000	-1.728946322000
11 N	14.886311590000	19.597182350000	2.179893110000	11 C	14.760859110000	19.649361290000	2.117018449000
12 N	10.934145930000	22.597538400000	2.786920735000	12 C	10.941519950000	22.601381790000	2.776643702000
13 N	11.525677750000	25.524397590000	-1.247430322000	13 C	11.572956850000	25.432808310000	-1.167454591000
14 C	14.975566510000	23.612522400000	3.228358122000	14 C	14.980043510000	23.605926490000	3.230052393000
15 H	14.113842030000	24.296419970000	3.232703626000	15 H	14.118870160000	24.290616000000	3.241531438000
16 H	15.486206950000	23.705340880000	4.201694404000	16 H	15.504485350000	23.708908810000	4.194902899000
17 H	14.591615090000	22.583203100000	3.164434332000	17 H	14.596138090000	22.576128070000	3.183099757000
18 C	16.883619580000	25.759556300000	2.296696499000	18 C	16.877862350000	25.743851440000	2.266536666000
19 H	17.666857860000	26.104133100000	1.605178663000	19 H	17.647644380000	26.089164170000	1.560604634000
20 H	17.320788840000	25.731621640000	3.308633133000	20 H	17.334145240000	25.715063380000	3.269934926000

21 H	16.077179190000	26.507874670000	2.297269091000		21 H	16.071858950000	26.492646370000	2.282533264000	
22 C	17.671078460000	22.824012900000	2.031116451000		22 C	17.657073260000	22.808744270000	1.999243904000	
22.11	47 343344370000	24 700200460000	4 000000		22.11	47 200040550000	24 7725 4 44 20000	4 000227200000	
23 H	17.312341370000	21.788308460000	1.932217363000		23 H	17.299019660000	21.773544120000	1.896337268000	
24 H	18.155548800000	22.927756450000	3.015875866000		24 H	18.147292620000	22.907829410000	2.981550899000	
25 H	18.427896960000	23.000117300000	1.251774542000		25 H	18.409401430000	22.988545120000	1.216537838000	
26 C	15 572667060000	26 706818890000	-0.915816875000		26 C	15 533911880000	26 681135980000	-0 938097/35300	
20 C	13.372007000000	20.700818890000	-0.913810873000		20 C	13.333511880000	20.081133580000	-0.538057433300	
27 H	14.485489490000	26.820483050000	-0.785692056200		27 H	14.447093360000	26.797771040000	-0.809077284800	
28 H	15.868675140000	27.245661250000	-1.830824517000		28 H	15.830953350000	27.214708590000	-1.855882268000	
29 H	16 076483450000	27 179913830000	-0.060769553950		29 H	16 037704080000	27 158279770000	-0.085289245330	
2511	10.070105150000	2/11/3313030000	0.000703333350		2511	10.057701000000	2/11502/5//00000	0.005205245550	
30 C	17.869840360000	24.732960450000	-1.380425171000		30 C	17.833062550000	24.710255620000	-1.381459948000	
31 H	18.456221660000	25.118715200000	-0.532368747100		31 H	18.417256760000	25.099248820000	-0.533712254600	
32 H	18.151124510000	25.313460110000	-2.274283147000		32 H	18.114386160000	25.289259230000	-2.276445934000	
22.11	40 400005400000	22 60652206000	4 5 4000 455 5 6000		22.11	40 435000300000	22 66 42226 60000	4 5 4070070000	
33 H	18.169205120000	23.686533960000	-1.543904556000		33 H	18.135880300000	23.664322600000	-1.542782726000	
34 C	15.142835870000	24.283845840000	-2.659145057000		34 C	15.125642180000	24.258019320000	-2.682219083000	
35 H	15.317929560000	23.226301420000	-2.901490212000		35 H	15.306247460000	23.200769810000	-2.919369116000	
36 H	15 536352060000	24 877135590000	-3 500806235000		36 H	15 530786880000	24 854886210000	-3 516034041000	
5011	15.550552000000	2	5.5000002550000		5011	13.3507000000000	21.051000210000	5.510051011000	
37 H	14.055877110000	24.454205500000	-2.625718430000		37 H	14.038663610000	24.421580750000	-2.657969343000	
38 C	11.017727260000	19.228278330000	-2.970969516000		38 C	11.057099360000	19.246045680000	-2.981707392000	
39 H	11.654643530000	18,796488330000	-3.757276126000		39 H	11.707390260000	18.823606470000	-3,761998273000	Y
40.11	0.000000077740000	40.270406400000	2 264776402000		40.11	40.024246220000	40 200 4700 40000	2 2000007747000	
40 H	9.989032774000	19.278186400000	-3.364776192000		40 H	10.034346230000	19.296478940000	-3.390665747000	,
41 H	11.019082870000	18.537251510000	-2.114756249000		41 H	11.047712350000	18.546374560000	-2.132600205000	
42 C	11.392655190000	22.085622860000	-3.971028968000		42 C	11.425257200000	22.116374430000	-3.944228571000	
12 11	11 572242750000	22 125057010000	2 602607040000		12 11	11 606046610000	22 162202810000	2 654702502000	
45 T	11.575242750000	23.135057910000	-3.093007049000		45 H	11.000040010000	23.102302810000	-3.654703592000	
44 H	10.378335170000	22.012349490000	-4.396336023000		44 H	10.413628780000	22.048788390000	-4.376754421000	
45 H	12.116613740000	21.808721530000	-4.752202710000		45 H	12.154149830000	21.847221650000	-4.723478828000	
16 C	10 280699810000	21 547521450000	-1 182442323000		46 C	10 281695390000	21 532713320000	-1 175889360000	
40 C	10.280055810000	21.547521450000	-1.182442323000		40 C	10.281055550000	21.332713320000	-1.173889300000	
47 H	10.274719870000	20.922828390000	-0.277164063600		47 H	10.280455500000	20.904114750000	-0.272911288900	
48 H	9.283628253000	21.478723790000	-1.649453422000		48 H	9.290790255000	21.439361820000	-1.651458466000	
49 H	10.416516220000	22,594047510000	-0.870219052900		49 H	10.389498030000	22.581025210000	-0.860524657600	
-10-11	10.110510220000	22.551017510000				10.505 150050000	22.501025210000		
50 C	14.674621600000	20.021820220000	-4.204640817000		50 C	14.686025210000	20.060362350000	-4.171961134000	
51 H	13.780449110000	19.641545700000	-4.721986380000		51 H	13.791794570000	19.682490280000	-4.690484088000	
52 H	15.527014990000	19.387089610000	-4.497406069000		52 H	15.538163940000	19.426446660000	-4.467807897000	
52.11	14.864086350000	21 041285280000	4 573641830000		52.11	14 877050580000	21 000012570000	4 527775227000	
5511	14.804980330000	21.041285280000	-4.373041825000		5511	14.877035380000	21.080913370000	-4.537775337000	
54 C	14.256121630000	18.207878350000	-1.770772811000		54 C	14.283886600000	18.232627120000	-1.751327843000	
		18 161071/00000	-0 673045614800		CC 11	14 206656370000	18.176105840000	-0.654928271100	
55 H	14.188895550000	10.1013/1430000	0.07 50 1501 1000		2211	14.200030370000			
55 H	14.188895550000 15.126283810000	17 610294890000	-2 088268973000		56 H	15 161141350000	17 643826620000	-2 065926477000	
55 H 56 H	14.188895550000 15.126283810000	17.610294890000	-2.088268973000		56 H	15.161141350000	17.643826620000	-2.065926477000	
55 H 56 H 57 H	14.188895550000 15.126283810000 13.351412640000	17.610294890000 17.748257110000	-2.088268973000 -2.193988472000		56 H 57 H	15.161141350000 13.386392560000	17.643826620000 17.770297520000	-2.065926477000 -2.186661175000	
55 H 56 H 57 H 58 C	14.188895550000 15.126283810000 13.351412640000 16.123053720000	17.610294890000 17.748257110000 20.569342430000	-2.088268973000 -2.193988472000 -1.586013495000		56 H 57 H 58 C	15.161141350000 13.386392560000 16.150234240000	17.643826620000 17.770297520000 20.594053440000	-2.065926477000 -2.186661175000 -1.567184725000	
55 H 56 H 57 H 58 C 59 H	14.188895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000	17.610294890000 17.748257110000 20.569342430000 21.600596440000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000		56 H 57 H 58 C 59 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000	17.643826620000 17.770297520000 20.594053440000 21.626118530000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000	
55 H 56 H 57 H 58 C 59 H	14.188895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000	17.610294890000 17.748257110000 20.569342430000 21.600596440000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000		56 H 57 H 58 C 59 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000	17.643826620000 17.770297520000 20.594053440000 21.626118530000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000	
55 H 56 H 57 H 58 C 59 H 60 H	14.188895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000 16.913330620000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000		56 H 57 H 58 C 59 H 60 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.934155710000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H	14.188895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.934155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H	14.18895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.934155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H	14.18895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.934155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H	14.18895550000 15.126283810000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 13.38639250000 16.150234240000 16.422218860000 16.934155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H	14.1889555000 15.12628381000 13.35141264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000	D	56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.934155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H [U(I 1 U	14.18889555000 15.12628361000 13.35142640000 16.123053720000 16.400776630000 16.146472460000 16.146472460000 16.146472460000	17.61029489000 17.74825711000 20.569342430000 21.600596440000 19.912676460000 20.471248000000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.16114135000 13.38639256000 16.150234240000 16.422218860000 16.394155710000 16.179620460000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600	
55 H 56 H 57 H 58 C 59 H 60 H 61 H [U(I 1 U 2 Si	14.1889555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 16.193502 10.9865108125000 10.965692310000	10.1037143000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.16114135000 15.161141350000 13.386392560000 16.150234240000 16.422218860000 16.394155710000 16.179620460000 16.179620460000 10.33166490000 0.935166490000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 4.887482808000 2.490260305000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H [U(I 1 U 2 Si	14.18889555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956608125000 10.956692310000	10.1037143000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000	-2.088268973000 -2.19398472000 -1.586013495000 -1.845463558000 -0.489998860000 -0.489998860000		56 H 57 H 58 C 59 H 60 H 61 H	15.16114135000 15.16114135000 13.386392560000 16.150234240000 16.422218860000 16.3934155710000 16.179620460000 16.179620460000 10.935166490000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 4.887482808000 2.490260305000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H [U(I 1 U 2 Si 3 Si	14.18889550000 15.126283810000 13.351412640000 16.123053720000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000	17.102311930000 17.748257110000 20.569342430000 21.600556440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000 9.741004467000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000		56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si	12.5053570000 15.161141350000 16.150234240000 16.422218860000 16.934155710000 16.179620460000 16.179620460000 10.935166490000 8.031232992000	17.64382662000 17.77029752000 20.594053440000 21.62611853000 19.93627718000 20.498022320000 7.187468814000 9.627198803000 9.754262572000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 4.887482808000 2.490260305000 3.358834680000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H [U(I) 1 U 2 Si 3 Si 4 Si	14.18889555000 15.12628381000 13.3514264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000 10.956692310000 8.039157364000 12.234809420000	17.101291493000 17.74825711000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000 9.741004467000 8.361749759000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000		56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si	15.16114135000 13.38639256000 16.150234240000 16.422218860000 16.394155710000 16.179620460000 10.935166490000 8.031232992000 12.247827970000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000 9.754262572000 8.328156888000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si	14.1889555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.48296790000	10.103/14/3000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000 9.741004467000 8.361749759000 5.45637141000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.411009943000		56 H 57 H 58 C 59 H 60 H 61 H [U(1 1 U 2 Si 3 Si 4 Si 5 Si	15.16114135000 15.16114135000 13.38639256000 16.150234240000 16.422218860000 16.394155710000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.4728913000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000 9.754262572000 8.32815688000 5.43305015000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.40205490000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 5 Si	14.1889555000 15.12628381000 13.351412640000 16.123053720000 16.913330620000 16.913330620000 16.146472460000 16.146472460000 10.9566108125000 10.9566108125000 10.956623100000 12.234809420000 12.482969790000	17.10231493000 17.748257110000 20.65934230000 20.659342430000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.456371461000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.845463558000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.411009943000		56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 C	15.16114135000 15.16114135000 16.15023424000 16.15023424000 16.4222186000 16.17962046000 16.17962046000 10.93516649000 8.03123299200 12.24782797000 12.47829913000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000 9.754262572000 8.328156888000 5.433050715000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N	14.1889555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 12.2482969790000 11.270075660000	17.1023/143000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.614008972000 9.741004467000 8.361749759000 5.456371461000 5.222982565000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845433558000 -1.985261134000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000		56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 C	15.16114135000 15.161141350000 16.150234240000 16.42221886000 16.394155710000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.472899130000 11.200506960000	17.64382662000 17.77029752000 20.594053440000 21.62611853000 20.498022320000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.43050715000 5.325775487000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N	14.1889555000 15.12628381000 13.3511264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.248296390000 11.270075660000 7.291939496000	17.19191919000 17.74825711000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 7.196436014000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000		55 H 56 H 57 H 58 C 59 H 60 H 61 H 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C	15.16114135000 13.38639256000 16.150234240000 16.422218860000 16.394155710000 16.179620460000 10.935166490000 8.031232992000 12.2478299130000 11.200506560000 7.316433030000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 7.187468814000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000	-2.065926477000 -2.186661175000 1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N	14.1888555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 13.25075660000 7.291939496000 7.95759376000	10.103/143000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 7.196436014000 9.61400872000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 4.877864688000 7.771455120000		56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C	15.16114135000 15.16114135000 13.38639256000 16.150234240000 16.42221886000 16.3934155710000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.478299130000 1.200506960000 7.316433030000 7.904918961000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.754262572000 8.32815688000 5.433050715000 5.325775487000 8.429582887000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N	14.1889555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.24809420000 12.24809420000 7.291939496000 7.795759376000	17.10231493000 17.748257110000 20.569342430000 21.600556440000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.741004467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000	-2.088268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.283351697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000		55H 56H 57H 58C 59H 60H 61H 1U 2Si 3Si 4Si 5Si 6C 7C 8C 8N	II. 100000000000000000000000000000000000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.43050715000 5.325775487000 8.429582887000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N	14.1889555000 15.12628381000 13.3511264000 16.12305372000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 11.270075660000 7.29193496000 7.795759376000 9.632714523000	17.101291493000 17.748257110000 17.748257110000 20.569342430000 21.600596440000 19.912676660000 20.471248000000 7.196436014000 9.614008972000 9.741004467000 8.361749759000 5.222982565000 4.495111074000 8.515907391000 9.053138267000	-2.088268973000 -2.19398847000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000		55H 56H 57H 58C 59H 60H 61H 10 2Si 3Si 4Si 5Si 6C 7C 8C 9N	15.16114135000 15.16114135000 13.38639256000 16.150234240000 16.39415571000 16.379620460000 16.379620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247829910000 7.316433030000 7.904918961000 9.621600611000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 8.42958287000 9.063677926000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N	14.1889555000 15.12628381000 13.35112640000 16.123053720000 16.30776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 12.291939496000 7.291939496000 7.795759376000 9.632714523000 11.728840000000	17.1923483000 17.74825711000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.422982565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000 6.304944243000		56 H 57 H 58 C 59 H 60 H 61 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N	15.16114135000 15.16114135000 13.38639256000 16.150234240000 16.42221886000 16.394155710000 16.179620460000 10.935166490000 8.031232992000 12.2478299130000 12.2478299130000 12.2478299130000 7.316433030000 7.904918961000 9.621600611000 11.728919910000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 8.429582887000 9.063677926000 7.000131428000	-2.065926477000 -2.186661175000 1.567184725000 1.326940088000 1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 5 Si 5 Si 6 N 7 N 8 N 9 N 10 N	14.18889555000 15.12628381000 13.351412640000 16.123053720000 16.40776630000 16.913330620000 16.146472460000 10.95692310000 8.039157364000 12.234809420000 12.234809420000 12.7291393496000 7.795759376000 9.632714523000 11.728840000000 10.807435710000	17.1943480000 17.748257110000 20.56934230000 20.569342430000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.4256571461000 5.222982565000 4.495111074000 9.053183267000 7.020337594000 5.795962023000	-2.088268973000 -2.088268973000 -2.13988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285315697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000 6.304944243000 2.889803973000		5511 56H 57H 58C 59H 60H 61H 1U 2Si 3Si 4Si 5Si 6C 7C 8C 9N 10N	15.161141350000 15.161141350000 16.150234240000 16.42221860000 16.179620460000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.2478299130000 7.316433030000 7.904918961000 11.728919910000 10.854450240000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.75468814000 9.754262572000 8.328156888000 5.433050715000 8.429582887000 9.063677926000 7.000131428000 5.931849862000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.490260305000 2.039673269000 2.039673269000 2.039673269000 3.476051662000 6.297183921000 2.992004493000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C	14.1889555000 15.12628361000 13.351412640000 16.123053720000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 11.270075660000 7.291939496000 7.795759376000 9.632714523000 11.728840000000 10.807435710000	17.10234830000 17.748257110000 20.569342430000 21.600596440000 19.9126764660000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000 5.7595962023000 5.35373242400	-2.088268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.41109943000 1.972658145000 6.304944243000 2.889803973000 4.87261534000		551 56 57 59 59 60 61 61 10 25i 35i 45i 55i 60 70 80 70 80 90 100 110	15.161141350000 15.161141350000 16.150234240000 16.422218860000 16.3934155710000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.4728991300000 7.316433030000 7.904918961000 9.62160611000 11.7289199100000 10.854450240000 18.1378271000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 8.429582887000 9.063677926000 5.931849862000 5.931849862000 5.931849862000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.83028653000 7.73444115000 3.476051662000 6.2971839210000 2.992004493000 4.83102710000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C	14.1889555000 15.12628381000 13.3511264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.24809420000 12.24809420000 12.24809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 12.294809420000 13.251452300 13.251452300 13.251452300 13.251452300 14.27455942000 15.2745594200 15.274559459459459459459459459459455945945945	17.19143000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 9.014008972000 9.741004467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000 5.3536720300	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000 6.304944243000 2.889803973000 4.879621534000		53 h 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 9 N 10 N 11 N 12 N	15.161141350000 13.386392560000 16.150234240000 16.394155710000 16.394155710000 16.379620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.2478299130000 7.316433030000 7.904918961000 9.62160061100 11.728919910000 10.854450240000 8.137882219000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 8.429582887000 9.063677926000 7.00131428000 5.931849862000 5.931849862000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.99200493000 4.871857108000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C	14.18889555000 15.12628381000 13.35112640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.23480420000 12.23480420000 12.291939496000 7.291939496000 7.291939496000 1.72840000000 11.728840000000 10.807435710000 8.097369042000 8.390960971000	17.1943000 17.610294890000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.22282565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000 5.353732434000 8.93987375000	-2.088268973000 -2.0938268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 -0.489998860000 2.493877250000 6.411009943000 1.972658145000 1.972658145000 3.46724888500 6.304944243000 2.889803973000 4.879621534000 6.850029332000		53 H 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N	15.16114135000 15.16114135000 13.38639256000 16.150234240000 16.42221886000 16.394155710000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.2478299130000 1.205506960000 7.316433030000 7.904918961000 9.621600611000 11.728919910000 10.854450240000 8.137882219000 8.528716680000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.5427198803000 9.754262572000 8.328156888000 5.433050715000 8.429582887000 9.063677926000 9.063677926000 5.931849862000 5.934898 5.942700379000 8.11359607 5.94270 5	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 5 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C	14.1889555000 15.12628361000 13.351412640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.24809420000 12.24809420000 11.72075660000 9.632714523000 11.728840000000 8.03756902000 8.0395692000 11.728840000000 10.807435710000 8.03956921000 11.156560210000	17.192430000 17.748257110000 17.748257110000 20.569342430000 20.569342430000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.741004467000 8.351749759000 5.456371461000 5.22982565000 4.49511074000 8.515907391000 7.02033759000 7.02033759000 5.353732434000 8.090877375000 11.510196960000	-2.088268973000 -2.088268973000 -2.139308472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.283351697000 6.411009943000 1.972658145000 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000		556 567 576 587 597 607 617 10 258 358 607 10 258 358 607 70 807 70 807 70 80 70 80 10 80 11 10 11 10 11 10 10 10 10 10 10 10 10	II. 100000000000000000000000000000000000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 8.429584576000 8.42958487000 9.063677926000 9.063677926000 5.34270379000 8.113596097000 11.528242630000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.3358834680000 7.287802802000 4.833028653000 4.833028653000 6.297183921000 2.929204493000 4.871857108000 6.782748913000 2.501541327000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 12 C	14.1889555000 15.12628381000 13.3514264000 16.12305372000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 11.270075660000 7.29193496000 7.29193496000 7.29193496000 11.72884000000 10.807435710000 8.399360971000 8.399360971000 11.156560210000 11.32184410000	17.19234830000 17.748257110000 20.569342430000 20.569342430000 20.569342430000 20.47124800000 20.47124800000 20.47124800000 20.47124800000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000 9.053138267000 7.020337544000 8.5935732434000 8.090877375000 11.510196960000 11.85655010000	-2.088268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -1.84543558000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 6.304944243000 2.889803973000 4.877864588000 6.304944243000 2.889803973000 4.879621534000 2.547820917000 3.579540733000		53 fi 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 13 H 14 C 15 H 15 H 10 C 10	15.161141350000 13.386392560000 16.150234240000 16.150234240000 16.179620460000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.472899130000 12.247827970000 12.478299130000 12.247827970000 12.478829190000 1.128919910000 10.854450240000 8.137882219000 8.528716680000 11.102976450000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 8.429582887000 9.063677926000 7.000131428000 5.931849862000 5.931849862000 5.442700379000 8.113596097000 11.528242630000 11.528242630000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.83028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H	14.1889555000 15.12628381000 13.35114264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.248296390000 11.270075660000 9.632714523000 11.72884000000 10.807435710000 8.037369042000 8.330960971000 11.35560210000 11.32485510000	17.1923483000 17.74825711000 20.569342430000 21.600596440000 20.456342430000 20.47124800000 20.47124800000 20.47124800000 9.91267646000 9.91267646000 9.91267646000 9.01410467000 8.361749759000 5.426371461000 5.222982565000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.810196960000 11.810196960000	-2.088268973000 -2.19398847000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 4.887045754000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.59540233000		53 h 56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 15.161141350000 16.150234240000 16.422218860000 16.394155710000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.2478299308000 12.2478299308000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 12.2478299130000 11.22819910000 10.854450240000 8.337882219000 8.528716680000 11.12976450000 11.2297450000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 19.936277180000 20.498022320000 9.627198803000 9.754262572000 8.32815688000 5.433050715000 5.4320575087000 8.429582887000 9.063677926000 9.063677926000 9.063677926000 8.42958287000 9.13596097000 11.528242630000 11.528242630000 11.528242630000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 6.402059490000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.25038342000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H	14.1888555000 15.12628381000 13.351412640000 16.123053720000 16.400776630000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.24808420000 12.24808420000 12.24808420000 12.24808420000 1.2.7915759376000 9.632714523000 11.72884000000 11.72884000000 11.72884000000 11.72884000000 11.156560210000 11.121854510000 10.269855090000	17.19436000 17.748257110000 20.56934230000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 20.471248000000 9.64400872000 9.74100467000 8.361749759000 5.425371461000 5.222982565000 4.495111074000 5.053138267000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.856256010000 12.032964350000	-2.083268973000 -2.083268973000 -2.13988472000 -1.586013495000 -1.845463558000 -1.845463558000 -0.489998860000 2.48977250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 6.304944243000 2.889803973000 4.877864688000 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.579540233000 2.158578604000		55 H 56 H 57 H 58 C 59 H 60 H 61 H 61 H 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H	I	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.0498022320000 9.754262572000 9.754262572000 8.32156888000 5.433050715000 8.4295840576000 9.063677926000 7.000131428000 5.931849862000 5.442700379000 8.113596097000 11.528242630000 11.897302420000 12.031940060000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.287802802000 6.402059490000 4.833028653000 7.734344115000 6.297183921000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.10004008000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H	14.1889555000 15.12628361000 15.12628361000 13.351412640000 16.123053720000 16.146472460000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 11.270075660000 7.291939496000 7.795759376000 9.632714523000 11.728840000000 11.321854510000 10.269855090000 12.24300419000 12.2430041900000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.243004190000 12.2430041900000 12.2430041900000 12.24300419000000000000000000000000000000000	17.192430000 17.748257110000 20.569342430000 21.600596440000 20.471248000000 20.471248000000 20.471248000000 20.471248000000 9.74100467000 8.361749759000 5.46371461000 5.22282565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000 5.353732434000 15.5195966000 11.5101966000 11.85625601000 12.032964350000 11.820893680000	-2.083268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 6.304944243000 6.304944243000 6.304944243000 6.304944243000 6.304944243000 6.304944243000 2.889803973000 2.547820917000 3.579540233000 2.158578604000 1.941170055000		55 H 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 7 C 8 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 13 N 14 C 15 H 14 C	15.161141350000 15.161141350000 16.32234240000 16.422218860000 16.422218860000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.472899130000 1.20506960000 1.720919910000 8.528716680000 11.02976450000 11.102976450000 11.262164960000 10.210702440000 11.966411010000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.2498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 8.429584057000 8.429582887000 9.063677926000 5.931849862000 5.93184986097000 11.528242630000 11.897302420000 12.031940060000 11.837252440000	-2.065926477000 -2.186661175000 -1.567184725000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.99200493000 2.99200493000 6.782748913000 2.501541327000 3.526388342000 2.100040008000 1.889545146000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C	14.18889550000 15.126283810000 13.351142640000 16.623053720000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 11.2565500000 11.321854500000 12.23206042000 11.321854500000 12.23206042000 12.232060420000 12.23206042000 13.32184510000 10.269855090000 12.0320640000	17.610294890000 17.748257110000 20.569342430000 21.600596440000 21.600596440000 20.471248000000 20.471248000000 20.47124800000 20.47124800000 9.74100467000 8.361749759000 5.456371461000 5.22982565000 4.495111074000 8.515907391000 9.053138267000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.856256010000 12.032964350000 9.113053843000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.77145512000 3.467248885000 6.304944243000 2.889803973000 4.879621534000 6.80029332000 2.547820917000 3.579540233000 2.158578604000 1.941170055000 0.668807494400		53 fi 56 fi 57 fi 58 fi 60 fi 61 fi 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C	15.16114135000 15.16114135000 16.150234240000 16.150234240000 16.150234240000 16.39415571000 16.379620460000 16.379620460000 10.935166490000 8.031232992000 12.24782797000 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.2478279700 12.24782797000 12.24782797000 12.2478777000000 12.247877777777777777	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 8.429582887000 9.063677926000 7.000131428000 5.931849862000 5.931849862000 5.931849862000 11.528242630000 11.528242630000 11.837252440000 9.08730476800	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.67517297880	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C	14.1889555000 15.12628381000 13.3511264000 16.12305372000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.29689790000 11.270075660000 9.632714523000 11.72884000000 10.807435710000 8.097369042000 8.39056971000 11.321854510000 10.269855090000 12.02306190000 11.226850910000 11.226850910000 11.265655040000	17.196436014000 17.748257110000 20.56934230000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 7.020337594000 5.05318267000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.856256010000 12.032964350000 11.820893680000 9.131063843000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.845463558000 -0.489998860000 -0.489998860000 -0.489998860000 -0.489998860000 -0.489998860000 -0.48377250000 6.411009943000 6.411009943000 1.972658145000 0.4877864688000 -0.771455120000 3.46724888500 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.579540233000 2.158578604000 1.941170055000 0.668807494400		53 H 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N	15.161141350000 15.161141350000 16.150234240000 16.150234240000 16.150234240000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.478299130000 11.20556660000 11.728919910000 10.854450240000 8.137882219000 8.528716680000 11.102976450000 11.102976450000 11.262164960000 10.781474150000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 9.063677926000 7.000131428000 5.931849862000 5.931849862000 5.931849862000 1.528242630000 11.528242630000 11.83725240000 12.031940060000 11.837252440000 9.4152324263000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.490260305000 2.039673269000 2.039673269000 2.039673269000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.675172979800	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H	14.18895550001 15.12628361000 15.12628361000 13.351412640000 16.123053720000 16.913330620000 16.913330620000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.24809420000 12.24809420000 11.72075660000 11.728440000000 10.807435710000 11.728440000000 11.55560210000 11.155550210000 11.321854510000 10.269855090000 12.023006190000 10.796850540000 11.686241540000	17.192430000 17.748257110000 17.748257110000 20.563342430000 21.600536440000 20.471248000000 20.471248000000 20.47124800000 20.47124800000 9.614008972000 9.74104467000 8.361749759000 5.456371461000 5.22982565000 7.020337594000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.856256010000 12.032964350000 9.113063843000 9.434213457000	-2.083268973000 -2.083268973000 -2.133988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 6.304944243000 2.889803973000 4.877626814512000 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.579540233000 2.158578604000 1.941170055000 0.668807494400 0.102377867600		556 567 576 587 597 607 617 10 259 359 459 551 67 77 87 77 87 77 87 77 87 77 87 77 87 70 87 10 87 10 10 11 11 12 11 12 11 12 14 12 13 11 12 14 12 13 14 12 14 12 14 12 14 14 14 14 14 14 14 14 14 14 14 14 14	II. 100000000000000000000000000000000000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.0498022320000 9.627198803000 9.627198803000 9.75426257200 8.328156888000 5.433050715000 8.42958457600 9.063677926000 9.063677926000 5.931849862000 5.94270379000 8.113596097000 11.528242630000 11.528242630000 11.897302420000 11.87752440000 9.087304768000 9.087304768000 9.415333184000	-2.065926477000 -2.186661175000 1.567184725000 1.826940088000 1.977341531000 -0.472328148600 2.490260305000 3.358834680000 2.490260305000 4.833028653000 2.039673269000 4.833028653000 3.476051662000 6.297183921000 2.92204493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.675172979800 0.098783835570	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C	14.1889555000 15.12628361000 15.12628361000 13.351412640000 16.123053720000 16.146472460000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.956692310000 11.2482969790000 11.27075600000 7.291939496000 7.79579376000 9.632714523000 11.72884000000 11.72884000000 11.72884000000 11.72884000000 11.6566210000 11.321884510000 10.269855090000 12.02306190000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.26985090000 10.66241540000 9.909441615000	17.19234830000 17.748257110000 20.569342430000 21.600596440000 20.569342430000 20.471248000000 20.471248000000 20.471248000000 9.14008972000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 7.020337594000 5.795962023000 5.353732434000 8.090877375000 11.510196960000 11.510196960000 11.85625010000 11.820893680000 9.113063843000 9.434213457000 9.552173285000	-2.083268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -0.489998860000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 6.304944243000 2.889803973000 4.877864688000 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.579540233000 2.547820917000 3.57954023000 2.547820917000 3.57954023000 2.547820917000 3.57954023000 2.547820917000 3.57954023000 2.547820917000 3.57954023000 2.5478604000 1.94117055000 0.066807494400 0.102377867600 0.19180052100 0.09140052000 0.09140052000 0.09140052000 0.09140052000 0.09140052000 0.09140052000 0.091400520		53 H 56 H 57 H 58 C 59 H 61 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 7 C 8 C 7 C 8 C 7 C 8 C 9 N 10 N 11 N 13 N 14 C 15 H 16 H 17 H 12 SH 13 SH 12 SH 13 SH 12 SH 13 SH 14 SH 12 SH 14 SH 12 SH 14 SH 15 SH 10 SH	15.161141350000 15.161141350000 16.150234240000 16.422218860000 16.179620460000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.472899130000 1.2050650000 1.720919910000 10.854450240000 8.137882219000 8.528716680000 11.02976450000 11.02976450000 11.0210702440000 11.0210702440000 11.966411010000 10.781474150000 11.662098690000 9.882986827000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 8.429584057000 8.429584057000 1.5282487000 9.063677926000 1.528242630000 1.528242630000 1.5391498600000 1.539149060000 1.539140060000 1.539140060000 1.539140060000 1.539140060000 1.539140060000 1.539140060000 9.087304768000 9.41533184000	-2.065926477000 -2.186661175000 -1.567184725000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.83028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 2.99204493000 2.591541327000 3.52638842000 2.501541327000 3.52638842000 2.51543127000 3.52638842000 0.675172979800 0.098783835570 0.194374580300	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 12 H 18 C	14.18895550001 15.126283810000 13.351142640000 16.123053720000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.956692310000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 11.2506500000 10.7955937600 9.63271452300 11.72884000000 10.80743571000 8.390960971000 11.15660210000 11.321855090000 12.023006190000 12.02306190000 11.686241540000 9.099441615000 10.721291690000	17.1610294890000 17.748257110000 20.569342430000 21.600596440000 20.47124800000 20.47124800000 20.47124800000 20.47124800000 20.47124800000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 7.020337594000 5.353732434000 8.0597375000 11.510196960000 11.85626010000 12.032964350000 9.113663843000 9.13263843000 9.43213457000 5.5521732325000 8.016954084000	-2.088268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.77145512000 3.467248885000 6.304944243000 2.889803973000 4.879621534000 6.30029332000 2.547820917000 3.579540233000 2.158578604000 0.102377867600 0.102377867600 0.102377867600		53 fi 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 61 H 61 H 61 H 61 H 62 H 63 Si 6C 7C 8C 9N 10N 11N 12N 13N 14C 15H 16H 17H 17H 17H 17H 17H 17H 17H 17	15.161141350000 13.386392560000 16.150234240000 16.150234240000 16.39415571000 16.379620460000 16.379620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 11.26216490000 11.36204960000 9.882986827000 10.72863090000 10.72863090000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.627198803000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 8.429582887000 9.063677926000 9.063677926000 9.063677926000 11.528242630000 11.528242630000 11.837252440000 9.087304768000 9.415333184000 9.439333184000 9.439333184000 9.439333184000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.057517297800 0.098783835570 0.194374580300 0.627685684000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 21 C	14.18895550001 15.126283810000 13.351142640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.956692310000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 11.270075660000 11.27007560000 11.72884000000 11.72884000000 11.32566210000 11.321884510000 10.29685090000 12.23200190000 11.656241540000 10.796850940000 11.656241540000 10.796850940000 11.656241540000 10.796850940000 11.656241540000 10.796850940000 11.656241540000 10.796850940000 11.656241540000 10.796850940000 11.656241540000 10.721291690000 10.721291690000	17.192430000 17.748257110000 20.56934230000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 20.471248000000 9.61400872000 9.74100467000 8.361749759000 5.456371461000 5.22292555000 4.495111074000 9.053138267000 7.020337594000 5.353732434000 8.515907391000 9.053138267000 7.020337594000 5.353732434000 8.51590735000 11.510196960000 11.856256010000 12.032964350000 9.131063843000 9.434213457000 9.434213457000 9.434213457000 9.52173285000	-2.083268973000 -2.083268973000 -2.133988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 6.34044243000 2.889803973000 4.877864688000 0.534044243000 2.889803973000 4.879621534000 6.34044243000 2.547820917000 3.579540233000 2.158578604000 1.94170055000 0.668807494400 0.102377867600 0.19180052100 0.602195839300		55 H 56 H 57 H 58 C 59 H 61 H 61 H 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 C 19 H 22 C	15.161141350000 15.161141350000 16.150234240000 16.150234240000 16.179620460000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247829130000 1.20506960000 9.621600611000 11.728919910000 10.854450240000 8.137882219000 8.528716680000 11.262164960000 11.262164960000 11.966411010000 10.834474150000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 11.966420000 12.247827000 12.247827000 12.247827000 12.247827000 12.247827000 12.247827000 12.247827000 12.24782700 12.24782700 12.24782700 12.24782700 12.2478270 12.24782700 12.2478270 12.247870 12.2478770 12.2478770 12.2478770 12.2478770 12.24787770 12.247877	17.64382662000 17.77029752000 20.594053440000 21.626118530000 20.498022320000 9.7542625718000 9.754262572000 8.32815688000 5.433050715000 8.42958287000 9.063677926000 7.00131428000 5.931849862000 5.931849862000 1.528242630000 1.528242630000 1.5331840000 9.4153318400 9.4153318400 9.415552000 9.415552000 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.41555200 9.415555200 9.415555200 9.415555200 9.415555200 9.41555555555555555555555555555555555555	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.490260305000 2.039673269000 2.039673269000 4.833028653000 7.28780280200 6.402059490000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.675172979800 0.098783835570 0.194374580300	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C	14.18895550001 15.12628361000 15.12628361000 13.351412640000 16.123053720000 16.91330620000 16.91330620000 16.146472460000 10.956692310000 8.039157364000 11.254809420000 12.234809420000 12.234809420000 11.72075660000 7.291939496000 11.728840000000 10.807435710000 11.321854510000 11.32585090000 11.325855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 11.326855090000 12.62941615000 10.8074191260000 10.80741910000 10.721291690000 12.61875470000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6187547000 12.6	17.192430000 17.748257110000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 9.614008972000 9.741004467000 8.351749759000 5.456371461000 5.22282565000 7.020337594000 7.020337594000 5.353732434000 8.09087375000 11.510196960000 11.856256010000 11.820893680000 9.113063843000 9.434213457000 9.434213457000 9.552173285000 8.016954084000 8.899621241000	-2.083268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.283351697000 6.411009943000 1.972658145000 6.304944243000 2.889803973000 4.879621534000 6.304944243000 2.889803973000 4.879621534000 6.35002932000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.57954023300 3.57954023300 3.57954023300 3.57954023300 3.57954023300 3.57954023300 3.57954023300 3.57954023300 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200 3.579540200		55 H 56 H 57 H 58 C 59 H 61 H 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 13 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 10 C 11 H 12 N 12 N 13 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12	II. 1.0000000000000000000000000000000000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 9.936277180000 9.0498022320000 9.754262572000 8.328156888000 5.433050715000 8.429582887000 9.063677926000 9.063677926000 5.34270379000 8.113596097000 11.528242630000 11.83702420000 11.83702420000 11.837252440000 9.087304768000 9.41533184000 9.41533184000 9.49365523000 7.988897898000 8.970259121000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.49026030500 2.49026030500 3.35883468000 7.287802802000 4.0205949000 2.039673269000 4.833028653000 7.734344115000 6.297183921000 2.9200493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 0.675172979800 0.098783835570 0.194374580300 0.62785684000 3.063247584000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H	14.1889555000 15.12628361000 15.12628361000 13.3514264000 16.423053720000 16.430776630000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.956692310000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 12.234809420000 11.256500000 11.725793745000 11.156560210000 11.321854510000 10.269855090000 10.269855090000 10.796850540000 11.686241540000 9.909441615000 10.721291690000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 12.61875470000 1	17.610294890000 17.748257110000 20.569342430000 21.600596440000 20.471248000000 20.471248000000 20.471248000000 20.471248000000 20.471248000000 9.614008972000 9.74100467000 8.361749759000 5.456371461000 5.22282565000 4.495111074000 8.515907391000 9.053132647000 7.02337544000 1.55962023000 1.55962023000 1.55962023000 1.559562023000 1.559562023000 1.5595600300 1.5595600300 1.5595600300 1.55956003 1.55973735000 1.150196960000 1.1856256010000 1.182683580000 9.113063843000 9.434213457000 9.552173285000 8.016954084000 8.899621241000 9.143138645000	-2.0836268973000 -2.193988472000 -1.586013495000 -1.84543558000 -1.84543558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.41109943000 1.972658145000 4.877864688000 7.771455120000 3.467248885000 6.304944243000 2.889803973000 4.87786458000 1.972621534000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.158578604000 1.941170055000 0.668807494400 0.102377867600 0.191800652100 0.602195839300 3.058562736000 4.099905597000		53 fi 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 16 H 16 H 16 H 16 H 12 N 12 N 13 N 12 N 13 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12	15.161141350000 13.386392560000 16.150234240000 16.150234240000 16.150234240000 16.179620460000 16.379620460000 16.379620460000 10.935166490000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.472899130000 12.247827970000 12.478891901000 10.754630000 11.102976450000 11.262164960000 10.210702440000 11.262164960000 10.210702440000 11.662098690000 9.882986827000 10.728683090000 12.2618444970000 12.875558300000	17.64382662000 17.77029752000 20.594053440000 21.62611853000 20.498022320000 9.627198803000 9.627198803000 9.754262572000 8.328156888000 5.433050715000 5.325775487000 4.595540576000 9.063677926000 7.000131428000 5.931849862000 11.528242630000 11.528242630000 11.53752440000 11.83752440000 11.83752440000 9.087304768000 9.041533184000	-2.065926477000 -2.186661175000 -1.567184725000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.40205949000 2.039673269000 4.83028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.52639842000 1.889545146000 0.675172979800 0.098783835570 0.194374580300 0.627685684000 3.063247584000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H	14.18895550001 15.126283810000 13.351142640000 16.123053720000 16.400776630000 16.91330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.234809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 11.2565010000 11.25650210000 11.321854510000 12.023006190000 12.023006190000 11.686241540000 12.023006190000 12.023006190000 12.618754700000 12.618754700000 12.618754700000 13.414148210000 13.414148210000	17.196436014000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 20.471248000000 20.47124800000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 7.020337594000 5.353732434000 8.05937375000 11.510196960000 11.856256010000 12.032964350000 11.820893680000 9.434213457000 9.434213457000 8.016954084000 8.896621241000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213452000 11.8208936843000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213457000 9.434213452000 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.43454200 10.4345420 10.4345450 10.4345450 10.44556561 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.45454560 10.454560 10.4545660 10.454560 10.454560 10.4545660 10.4545660	-2.088268973000 -2.088268973000 -2.139388472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 7.271455120000 3.46724888500 6.304944243000 2.889803973000 4.877864688000 7.771455120000 3.4672488500 6.304944243000 2.889803973000 4.879621534000 6.850029332000 2.547820917000 3.579540233000 2.158578604000 1.941170055000 0.602195839300 3.058562736000 4.099905597000 2.41926423500		53 h 56 H 57 H 58 C 59 H 60 H 61 H	15.161141350000 15.161141350000 16.150234240000 16.150234240000 16.150234240000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827910000 12.247827910000 1.247827910000 1.247827910000 1.247827910000 1.247827910000 1.252164960000 1.102976450000 1.1262164960000 1.26264960000 1.26264960000 1.366411010000 1.781474150000 1.366411010000 1.728986827000 1.2618444970000 1.2487583800000 1.248758300000 1.24875880000 1.2488	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 9.542718803000 9.754262572000 8.328156880000 5.433050715000 8.328156880000 5.3325775487000 9.063677926000 8.42958287000 9.063677926000 1.528242630000 1.528242630000 1.528242630000 1.533184962000 1.83725240000 9.41533184000 9.41533184000 9.49936523000 7.9888788900 8.970259121000 9.271652427000 9.271652427000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.52638842000 2.50541327000 3.52638842000 1.889545146000 0.675172979800 0.098783835570 0.194374580300 0.627685684000 4.087567238000 2.39350605800	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 22 H 22 H	14.18895550001 15.12628361000 15.12628361000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 8.039157364000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 11.72075660000 11.72075660000 11.728440000000 10.807435710000 11.728440000000 10.807435710000 11.56560210000 11.321854510000 10.269855090000 12.023006190000 10.796850540000 12.688241540000 9.99441615000 10.721291690000 12.68824190000 12.6890000 12.6890000 12.6800000 12.6800000000 12.68000000 12.68000000 12.68000000 12.68000000000 12.680000000000 12.680000000000 12.6800000000000 13.4144820000000 13.4144820000000 13.4144820000000000000000000000000000000000	17.192430000 17.748257110000 17.748257110000 20.569342430000 21.600596440000 19.912676460000 20.471248000000 20.471248000000 20.47124800000 9.614008972000 9.74104467000 8.361749759000 5.456371461000 5.22982565000 7.020337594000 5.353732434000 8.090877375000 11.510196960000 11.856256010000 12.032964350000 9.13063843000 9.434213457000 9.552173285000 8.016954084000 8.899621241000 9.3139645000 9.13138645000 9.313947162000	-2.083268973000 -2.083268973000 -2.133988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 2.493877250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 6.304944243000 2.889803973000 4.877621534000 6.304944243000 2.889803973000 4.879621534000 6.304944243000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 0.668807494400 0.102377867600 0.191800652100 0.602195839300 3.05856273600 4.09905597000 2.419264235000 2.947264235000 2.947264235000		55 H 56 H 57 H 58 C 59 H 60 H 61 H 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 7 C 8 C 7 C 8 C 7 C 8 C 10 N 11 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 12 N 12 N 13 N 14 C 15 H 10 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12	II. 100000000000000000000000000000000000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 9.936277180000 9.0498022320000 9.754262572000 8.328156888000 5.433050715000 8.4295847000 9.063677926000 7.000131428000 5.931849862000 5.442700379000 8.113596097000 1.528242630000 1.528242630000 1.1528242630000 1.1528242630000 1.1533149600000 1.837252440000 9.087304768000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.415333184000 9.41533184000 9.415333184000 9.4153318400 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.4153318400 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.41533184000 9.4153318400 9.41545800 9.4154800 9.4154800 9.4154800 9.4154800	-2.065926477000 -2.186661175000 1.567184725000 1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.49026030500 2.35883468000 2.28780280200 6.402059490000 2.039673269000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.297183921000 2.99204493000 4.871857108000 6.297183921000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 1.889545146000 0.675172979800 0.098783835570 0.194374580300 1.94374580300 0.627685684000 3.063247584000 2.393506058000 2.393506058000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H	14.18895550001 15.12628361000 15.12628361000 13.351412640000 16.123053720000 16.146472460000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 10.956692310000 12.23480940000 12.24809420000 11.270075600000 12.23480940000 11.72884000000 10.8073579000 11.72884000000 11.72884000000 10.8073570000 11.56560210000 11.3218451000 10.269855090000 12.6895590000 10.271291690000 10.271291690000 10.271291690000 12.688821190000 13.41418210000 13.41418210000 13.41418210000 13.44148210000 13.4448210000 13.4448210000 13.44448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 13.4448210000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.444820000 14.4448200000 14.4448200000 14.44482000000 14.44482000000 14.44482000000000000000000000000000000000	17.192436000 17.748257110000 20.569342430000 21.600596440000 20.569342430000 20.471248000000 20.471248000000 20.471248000000 20.471248000000 9.14100467000 8.361749759000 5.46371461000 5.22282565000 7.020337594000 5.795962023000 5.353732434000 11.51019660000 11.856256010000 11.856256010000 11.85256010000 11.820893680000 9.113063843000 9.434213457000 9.552173285000 8.016954084000 8.899621241000 9.313047162000 7.89582710000	-2.083268973000 -2.193988472000 -1.84543558000 -1.84543558000 -1.84543558000 -1.84543558000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.41100943000 1.972658145000 6.3049442430000 6.3049442430000 2.889803973000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540233000 2.547820917000 3.579540235000 2.41926423500 2.41926423500		53 H 56 H 57 H 58 C 59 H 61 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 7 C 8 C 7 C 8 C 7 C 8 C 7 C 8 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 12 N 13 N 12 N 13 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12	I. 1.00000000000000000000000000000000000	17.64382662000 17.77029752000 20.594053440000 21.626118530000 9.936277180000 9.0498022320000 9.754262572000 8.328156888000 5.433050715000 8.328156888000 5.433050715000 8.429584057000 1.5282487000 9.063677926000 5.931849862000 5.442700379000 11.528242630000 11.528242630000 11.837304768000 9.087304768000 9.41533184000 9.087304768000 9.41533184000 9.49335523000 7.988897898000 8.970259121000 9.271652427000 9.375134952000 7.873781126000	-2.065926477000 -2.186661175000 -1.567184725000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 3.358834680000 7.287802802000 6.402059490000 2.039673269000 4.833028653000 2.9200493000 2.9200493000 2.9200493000 2.9920493000 2.501541327000 3.57638342000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 2.501541327000 0.675172979800 0.098783835570 0.194374580300 0.627685684000 3.063247584000 4.87567238000 2.393506058000 3.06022436000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 20 H 21 H 22 H 22 H 22 H 25 H 26 C	14.18895550001 15.126283810000 13.351142640000 16.123053720000 16.400776630000 16.31330620000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 12.234809420000 12.234809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 13.2565091000 11.156560210000 12.2291690000 12.2291690000 12.64854190000 12.64854190000 12.64854190000 13.414148210000 13.414148210000 13.414148210000 13.441448210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.444148210000 13.4444820000 13.4444820000 13.44448200000 13.44448200000 13.44448200000 13.44448200000 13.44448200000 13.44448200000 13.444482000000 13.44448200000000 13.444482000000000000000000000000000000000	17.512324830000 17.748257110000 20.569342430000 21.600596440000 21.600596440000 20.471248000000 20.471248000000 20.471248000000 20.47124800000 9.74100467000 8.361749759000 5.456371461000 5.222982565000 4.495111074000 8.515907391000 7.020337594000 5.75562023000 7.020337594000 5.353732434000 8.05957372000 11.510196960000 11.856256010000 12.032964350000 9.113658430000 9.13163843000 9.342213457000 9.552173285000 8.016954084000 8.819654084000 8.819654084000 9.343213457000 9.34213457000 9.34213457000 9.34213457000 9.34213457000 9.34213457000 9.34213457000 9.342142000 8.016954084000 8.819621241000 9.3423427000 9.342344000 9.3423427000 9.342347000 9.342347000 9.342347000 9.342347000 9.342347000	-2.0836268973000 -2.193988472000 -1.586013495000 -1.845463558000 -1.845463558000 -1.985261134000 -0.489998860000 2.493877250000 3.349834560000 7.285351697000 6.411009943000 1.972658145000 4.877864688000 7.77145512000 3.467248885000 6.304944243000 2.889803973000 4.879621534000 6.300944243000 2.5878604000 0.10237867600 0.102478675000 1.94117005507000 2.419264235000 2.947466775000 1.603464137000		53 h 56 H 57 H 58 C 59 H 60 H 61 H 61 H 61 H 61 H 61 H 7 C 8 C 9 N 10 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 15 H 16 H 17 H 20 H 21 H 22 C 23 H 24 H 22 C 23 H 24 H 22 C 23 H 24 H 22 C	15.16114135000 13.38639256000 16.150234240000 16.150234240000 16.39415571000 16.379620460000 16.379620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 11.262164960000 11.102976450000 11.102976450000 11.662098690000 9.882986827000 10.781474150000 11.662088690000 9.882986827000 10.784683090000 12.2618444970000 12.875558300000 13.395913820000 12.668887740000 2.541747195000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 9.936277180000 20.498022320000 9.754262572000 8.32815688000 5.433050715000 8.42958287000 4.59554057600 8.42958287000 9.063677926000 9.063677926000 9.063677926000 1.52824263000 1.52824263000 1.52824263000 1.531849862000 5.442700379000 1.1.897302420000 11.83725240000 9.08730476800 9.41533184000 9.4933523000 8.970259121000 9.271652427000 9.271652427000 9.375134952000 7.873781126000	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 4.837482808000 7.287802802000 4.833028653000 7.734344115000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.52638842000 2.501541327000 3.52638842000 1.89545146000 0.675172979800 0.098783835570 0.194374580300 0.627685684000 3.063247584000 3.063247584000 3.0632436000 1.89551525000	
55 H 56 H 57 H 58 C 59 H 60 H 61 H 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 21 C 19 H 22 C 13 C 14 C 15 H 16 H 17 H 18 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 12 C 13 C 14 C 15 H 16 H 17 H 10 N 11 C 12 C 13 C 14 C 12 C 13 C 14 C 14 C 15 C 14 C 15 C 16 C 16 H 17 H 10 C 16 C 16 C 17 H 10 C 16 C 16 C 16 C 17 H 10 C 16 C 16 C 16 C 16 C 17 H 10 C 16 C 16 C 16 C 16 C 16 C 16 C 16 C 17 C 16 C 16 C 16 C 16 C 16 C 16 C 16 C 16	14.18895550001 15.126283810000 13.351142640000 16.123053720000 16.400776630000 16.913330620000 16.146472460000 16.146472460000 10.956692310000 10.956692310000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.24809420000 12.2480942000 11.2707560000 10.795759376000 9.632714523000 11.72884000000 10.807435710000 8.39060971000 11.321854510000 10.26385090000 11.264894490000 12.64894490000 12.64894490000 15.64894490000 15.64894490000 15.64894490000	17. 10294890000 17. 748257110000 20. 56934230000 20. 56934240000 19. 912676460000 20. 471248000000 20. 471248000000 20. 471248000000 20. 47124800000 9. 61400872000 9. 74100467000 8. 361749759000 5. 4259255000 4. 495111074000 9. 053138267000 7. 020337594000 5. 353732434000 8. 515907391000 9. 053138267000 7. 020337594000 5. 353732434000 8. 5962023000 11. 510196960000 11. 856256010000 12. 032964350000 9. 113063843000 9. 434213457000 9. 43421345458000 11. 44251458000 11. 4425145800 11. 44251458	-2.083268973000 -2.133988472000 -1.586013495000 -1.845463558000 -1.985261134000 -0.489998860000 -0.489998860000 4.877854000 2.493877250000 3.349834560000 1.972658145000 6.41100943000 1.972658145000 6.34044243000 2.889803973000 4.877864688000 0.346724885000 6.34044243000 2.889803973000 4.879621534000 6.3579540233000 2.547820917000 3.579540233000 2.547820917000 3.57954023000 2.547820917000 0.668807494400 0.102377867600 0.911980652100 0.602195839300 3.058562736000 4.09905597000 2.419264235000 2.947466775000 1.60346137000 1.228274513000		53 ft 56 ft 57 ft 58 c 59 ft 60 ft 61 ft 10 2 si 3 si 4 si 5 si 6 c 7 c 8 c 9 N 11 N 12 N 13 N 14 c 15 ft 10 ft 13 N 14 c 15 ft 10 ft 10 ft 11 N 2 si 3 si 4 si 5 si 6 c 7 c 8 c 9 N 11 N 12 N 13 N 14 c 15 ft 10 N 12 N 12 N 12 N 12 N 12 N 12 N 12 N 12	15.161141350000 15.161141350000 16.150234240000 16.150234240000 16.179620460000 16.179620460000 16.179620460000 10.935166490000 8.031232992000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247827970000 12.247829130000 1.20516490000 1.728949130000 1.728949130000 1.7281474150000 1.261644960000 1.26208690000 9.8826827000 1.2618444970000 1.2.68847440000 1.2.6884740000 7.541471195000 8.205359953000	17.643826620000 17.770297520000 20.594053440000 21.626118530000 20.498022320000 9.75468814000 9.754262572000 8.32815688000 5.433050715000 8.32815688000 5.3325775487000 8.429582887000 9.063677926000 7.00131428000 5.931849862000 5.931849862000 5.442700379000 8.113596097000 1.528242630000 1.528242630000 1.837252440000 9.087304768000 9.41533184000 9.415456555000 9.41555555000 9.415555555000 9.41555555	-2.065926477000 -2.186661175000 -1.567184725000 -1.826940088000 -1.977341531000 -0.472328148600 2.490260305000 2.490260305000 2.490260305000 4.83028653000 7.287802802000 6.402059490000 4.833028653000 3.476051662000 6.297183921000 2.992004493000 4.871857108000 6.782748913000 2.501541327000 3.526398342000 2.501541327000 3.526398342000 2.10004008000 1.889545146000 0.675172979800 0.098783835570 0.194374580300 3.063247584000 2.39356058000 3.00822436000 1.59975152500	

ſ	28 H	6.545168059000	10.755795940000	1.630122695000	28 H	6.519971954000	10.725850710000	1.624797498000	
	29 H	7.584696360000	9.521146991000	0.879301630700	29 H	7.542984265000	9.459664547000	0.903226453100	
	30.0	7 82/10/00/00	11 22/2850/0000	4 515713632000	30.0	7 835609010000	11 27/251590000	4 481402260000	
	21 11	7.022825100000	10.804150630000	F FF0728F46000	21 11	7.090206602000	10.090507930000	5 520782211000	
	31 H	7.932835100000	10.894159630000	5.559728546000	31 H	7.989206692000	10.980507830000	5.530782211000	
	32 H	6.826107936000	11.677831440000	4.399491180000	32 H	6.827491984000	11.710322140000	4.387553937000	
	33 H	8.581555429000	11.998412780000	4.320966885000	33 H	8.573377044000	12.052054390000	4.233167325000	
	34 C	6.704853218000	8.473113322000	3.793767663000	34 C	6.685294763000	8.517177212000	3.855162484000	
	35 H	6.700526859000	7.621160798000	3.098095492000	35 H	6.683069802000	7.626676884000	3.209684705000	
	36 H	5,719701015000	8.967642925000	3.737456853000	36 H	5,705122204000	9.014850693000	3,752719475000	
	27 1	6 902742722000	9 074227205000	4 914920997000	27 Ц	6 769670219000	9 177727717000	4 997674540000	
	37.11	0.803742732000	8.074337393000	4.814850887000	37 11	0.708079318000	8.177727717000	4.897074540000	
	38 C	14.121063860000	8.639495064000	7.234647676000	38 C	14.139988220000	8.573844787000	7.256742311000	
	39 H	14.679406270000	7.772739842000	7.619014347000	39 H	14.682165470000	7.699198372000	7.647096312000	
	40 H	14.396320780000	9.514210584000	7.846421117000	40 H	14.422288250000	9.445228802000	7.870292046000	
	41 H	14.460589530000	8.824260407000	6.204017177000	41 H	14.490695500000	8.752769732000	6.228607586000	
	42 C	11.740563050000	8.176057727000	9.109753982000	42 C	11.734490730000	8.139079807000	9.107705630000	
	43 H	10.648168810000	8.060796859000	9.178300743000	43 H	10.640349510000	8.034714691000	9.165925848000	
	1 1 H	12 028166500000	9.075723073000	9 678559598000	11 H	12 027031470000	9.031476235000	9 6849622990000	
	44 11	12.028100300000	3.073723073000	500000000000000000000000000000000000000	44 11	12.027031470000	3.031470233000	9.084902299000	
	45 H	12.213226360000	7.304547605000	9.584255895000	45 H	12.192748990000	7.259087069000	9.580818062000	
	46 C	11.450644200000	9.993824705000	6.726508507000	46 C	11.510045860000	9.986303674000	6.739961043000	
	47 H	11.687479420000	10.260711270000	5.688026858000	47 H	11.762936720000	10.257399810000	5.706088315000	
	48 H	11.831168040000	10.803985440000	7.371392935000	48 H	11.908594520000	10.777627620000	7.397647243000	
	49 H	10.356095570000	9.975771427000	6.832632480000	49 H	10.414773520000	9.992702357000	6.834730331000	
	50 C	13.977531990000	5.311181608000	5.249440837000	50 C	13.993241080000	5.291748616000	5.272193400000	
	51 H	13 647829650000	5 408036102000	4 204157009000	51 H	13 689165080000	5 429359229000	4 223685762000	
	52.11	13.047623030000	4.222052200000	5.255262322000	52.0	13.003105000000	1.201000000000	4.223003702000	
	52 H	14.4/4233//0000	4.333952380000	5.365369273000	52 H	14.467526670000	4.301069969000	5.366623526000	
	53 H	14.716508560000	6.101250515000	5.449872917000	53 H	14.742793630000	6.060058122000	5.514707855000	
	54 C	11.273760840000	4.074119125000	5.951701317000	54 C	11.276488730000	4.050321723000	5.905510802000	
	55 H	10.415578450000	4.033928139000	6.638443202000	55 H	10.386443170000	4.022861361000	6.551188219000	
	56 H	11.806434540000	3.109262203000	6.011425286000	56 H	11.801447890000	3.084538790000	6.006467010000	
	57 H	10.881816120000	4.160651862000	4.926805078000	57 H	10.936148300000	4.126275913000	4.862744975000	
	58 C	13 10/010820000	5 003287922000	8 156773298000	58 C	13 056212950000	4 955213977000	8 155970984000	
	50 0	13.104515020000	5.005207522000	0.525022040000	50 0	13.030212550000	5.54022020000	0.5533703040000	
	59 H	13.870669040000	5.695935818000	8.535933949000	59 H	13.815236540000	5.640338286000	8.561237159000	
	60 H	13.551806560000	3.995636034000	8.128333279000	60 H	13.500130010000	3.946311949000	8.124329999000	
	61 H	12.275455440000	4.984009659000	8.879302002000	61 H	12.210517010000	4.929772629000	8.859467086000	
L	F1 1/1	1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1							
- 1					· [[]/]	VINI* NC 1"			
	10	V)N [*] 2CN3] 10.034757000000	7.375728000000	4.883747000000	[U(I	V)N*2NC3] ¹ 10.129239000000	7.415174000000	4.858136000000	
	1U 1U	V)N [*] 2CN3J 10.034757000000	7.375728000000	4.883747000000	[U(I 10	V)N*2NC3] ¹ 10.129239000000	7.415174000000	4.858136000000	
	1 U 2 Si	V)N [*] 2CN3J 10.034757000000 10.988535000000	7.375728000000	4.883747000000 2.507023000000	[U(I 1 U 2 Si	V)N*2NC3] ¹ 10.129239000000 10.843132000000	7.415174000000 9.658875000000	4.858136000000	
	1 U 2 Si 3 Si	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000	7.375728000000 9.659384000000 9.738781000000	4.883747000000 2.507023000000 3.370051000000	[U(I 1 U 2 Si 3 Si	V)N*2NC3 10.129239000000 10.843132000000 7.899819000000	7.415174000000 9.658875000000 9.754898000000	4.858136000000 2.448480000000 3.387831000000	
	1 U 2 Si 3 Si 4 Si	V)N [*] 2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000	7.375728000000 9.659384000000 9.738781000000 8.389186000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000	[U(I 1 U 2 Si 3 Si 4 Si	V)N*2NC3] ^{1*} 10.129239000000 10.843132000000 7.899819000000 12.374722000000	7.415174000000 9.658875000000 9.754898000000 8.341086000000	4.858136000000 2.448480000000 3.387831000000 7.246608000000	
	1 U 2 Si 3 Si 4 Si 5 Si	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.397459000000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si	V)N*2NC3] ¹ 10.12923900000 10.84313200000 7.89981900000 12.37472200000 12.50627100000	7.415174000000 9.65887500000 9.75489800000 8.34108600000 5.36087400000	4.858136000000 2.448480000000 3.387831000000 7.246608000000 6.440021000000	
	1 U 2 Si 3 Si 4 Si 5 Si 6 N	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000 5.287196000000	4.883747000000 2.50702300000 3.370051000000 7.25580600000 6.397459000000 1.971327000000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si 6 C	V)N*2NC3] ¹¹ 10.129239000000 10.843132000000 7.899819000000 12.374722000000 12.506271000000 11.220797000000	7.415174000000 9.658875000000 9.754898000000 8.341086000000 5.360874000000 5.353626000000	4.858136000000 2.448480000000 3.387831000000 7.246608000000 6.440021000000 2.096381000000	
	1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N	<pre>VJN*2LN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000</pre>	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000 5.287196000000 4.743698000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.971327000000 4.915227000000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C	V)N*2NC3] ¹ 10.129239000000 10.843132000000 12.374722000000 12.506271000000 11.220797000000 7.576979000000	7.415174000000 9.65887500000 9.75489800000 8.341086000000 5.360874000000 5.353626000000 4.92748000000	4.858136000000 2.448480000000 3.387831000000 7.246608000000 6.440021000000 2.096381000000 5.074283000000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N	<pre>VJN*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000 7.929479000000</pre>	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000 5.287196000000 4.743698000000 8.41228400000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 7.792674000000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C	V)N*2NC3] ¹ 10.129239000000 10.843132000000 12.374722000000 12.506271000000 11.220797000000 7.576979000000 8.184567000000	7.415174000000 9.65887500000 9.75489800000 8.341086000000 5.360874000000 4.92748000000 8.69994400000	4.858136000000 2.448480000000 3.387831000000 7.246608000000 6.440021000000 2.096381000000 5.074283000000 7.606587000000	
	LU(I 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N	<pre>V)N*2CN3] 10.03475700000 10.98853500000 8.00937900000 12.302155000000 12.448598000000 11.09155400000 7.46241100000 7.92947900000 9.649742000000</pre>	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000 4.743698000000 8.412284000000 9.050121000000	4.883747000000 2.507023000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 7.792674000000 5.1291600000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N	V)N*2NC3] ^{1*} 10.129239000000 10.843132000000 12.374722000000 12.506271000000 11.220797000000 8.184567000000 9.531602000000	7.415174000000 9.658875000000 9.754898000000 8.341086000000 5.360874000000 4.92748000000 8.699944000000 9.047924000000	4.85813600000 2.44848000000 3.38783100000 7.24660800000 6.44002100000 5.07428300000 7.60658700000 3.47266400000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N	<pre>V)N*2CN3] 10.03475700000 10.98853500000 8.00937900000 12.30215500000 12.44859800000 11.09155400000 7.46241100000 7.92947900000 9.64974200000 11.73246600000</pre>	7.375728000000 9.659384000000 9.738781000000 5.4389186000000 5.412881000000 4.743698000000 8.412284000000 9.050171000000	4.883747000000 2.507023000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 7.792674000000 3.512916000000	[U(I 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N	V)N*2NC3]* 10.129239000000 10.843132000000 12.899819000000 12.374722000000 12.266271000000 11.22097000000 8.184567000000 9.531602000000	7.415174000000 9.658875000000 9.754898000000 5.360874000000 4.927480000000 8.699944000000 9.047924000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.074283000000 3.47766400000 6.25051000000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N	V)N*2CN3J 10.03475/000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000 7.929479000000 9.649742000000 11.722496000000	7.375728000000 9.659384000000 9.738781000000 8.389186000000 5.412881000000 4.743698000000 8.412284000000 9.050171000000 7.036682000000	4.883747000000 2.507023000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 7.792674000000 3.512916000000 6.250258000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N	V)N*2NC3]** 10.129239000000 10.843132000000 12.8943132000000 12.374722000000 12.56271000000 11.220797000000 8.184567000000 9.531602000000 11.792882000000	7.415174000000 9.658875000000 9.754898000000 5.360874000000 5.35626000000 4.92748000000 8.699944000000 6.981742000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 3.47766400000 6.26206100000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C	V)N*2CN3 10.034757000000 10.034757000000 10.9853500000 8.00937900000 12.30215500000 12.44859800000 11.09155400000 7.46241100000 7.92947900000 9.64974200000 11.72249600000 10.777231000000	7.37572800000 9.65938400000 9.73878100000 5.41288100000 5.28719600000 4.74369800000 8.41228400000 5.05017100000 7.03668200000 5.91459900000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.971327000000 4.915227000000 7.792674000000 3.512916000000 6.250258000000 2.914040000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N	♥)№ ² , №C ₂] ^{**} 10.129239000000 10.843132000000 12.374722000000 12.506271000000 11.220797000000 11.220797000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.353562600000 4.92748000000 8.69994400000 9.04792400000 6.98174200000 6.02650100000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 3.47766400000 6.26206100000 3.01123000000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C	V)N*2CN3 10.034757000000 10.03475700000 10.9853500000 8.0937900000 12.30215500000 12.44859800000 11.09155400000 7.46241100000 7.92947900000 9.64974200000 11.72249600000 10.777231000000 8.28372500000	7,375728000000 9,559384000000 9,73878100000 5,41288100000 5,28719600000 4,74369800000 8,41228400000 9,05017100000 7,03668200000 5,91459900000 5,58585600000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.915227000000 7.792674000000 3.512916000000 6.250258000000 2.914040000000 4.905267000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N	♥)№ 2,№C,3]** 10.129239000000 10.843132000000 7.899819000000 12.37472200000 12.506271000000 11.220797000000 7.576979000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35352600000 4.92748000000 6.9994400000 6.98174200000 6.98174200000 5.73204800000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 7.60658700000 3.47766400000 6.26206100000 3.01123000000 4.91507200000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000 7.929479000000 9.649742000000 11.722496000000 10.777231000000 8.283725000000 8.567050000000	7.375728000000 9.559384000000 9.738781000000 5.412881000000 5.28719600000 4.743698000000 8.412284000000 9.050171000000 7.036682000000 5.914599000000 5.585856000000 8.109714000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 7.79267400000 3.512916000000 6.250258000000 2.914040000000 4.905267000000 6.852838000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N	V)N *2NC2]** 10.129239000000 10.843132000000 12.374722000000 12.50627100000 11.220797000000 7.576979000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.822177000000	7.41517400000 9.65887500000 9.75489800000 5.360874000000 5.350874000000 4.92748000000 6.9994400000 6.981742000000 6.026501000000 5.732048000000 8.332762000000	4.85813600000 2.44848000000 7.24660800000 6.44002100000 2.09638100000 5.07428300000 7.60658700000 3.47766400000 6.26206100000 3.01123000000 4.91507200000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C	<pre>V)N*2CN3J 10.034757000000 10.988535000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000 7.929479000000 9.649742000000 11.722496000000 10.777231000000 8.283725000000 8.567050000000 11.093493000000</pre>	7,375728000000 9,65938400000 9,73878100000 8,38918600000 5,41288100000 5,28719600000 4,74369800000 8,41228400000 7,036682000000 5,914599000000 5,58585600000 8,109714000000 11,538284000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 7.79267400000 6.250258000000 2.914040000000 4.905267000000 6.852838000000 2.630639000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C	V)N*2NC2]** 10.129239000000 10.843132000000 12.374722000000 12.56271000000 11.220797000000 11.220797000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.822177000000 10.989414000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35362600000 4.92748000000 6.924400000 6.94792400000 6.04792400000 6.02551000000 5.732048000000 8.332762000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 3.0742800000 6.26206100000 3.01123000000 4.91507200000 6.68094000000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H	V)N*2CN3J 10.034757000000 10.98853500000 12.30215500000 12.30215500000 11.09155400000 7.46241100000 7.92947900000 9.64974200000 11.72249600000 10.77723100000 8.283725000000 8.56705000000 11.09349300000 11.23662700000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 4.74369800000 8.41228400000 9.05017100000 5.91459900000 5.91459900000 8.10971400000 11.538284000000 11.86890800000	4.883747000000 2.507023000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 3.512916000000 6.250258000000 2.91404000000 4.905267000000 6.852838000000 2.630639000000 3.672134000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H	V)N*2NC2]** 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.20797000000 11.220797000000 8.184567000000 9.53160200000 10.891767000000 8.42875800000 8.42875800000 8.42875800000 10.98941400000 11.14754900000	7.415174000000 9.658875000000 9.754898000000 5.360874000000 4.92748000000 9.047924000000 6.02650100000 6.02650100000 8.33276200000 11.540756000000 11.87590600000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 5.074283000000 3.47766400000 6.26206100000 4.91507200000 6.6809400000 2.54675100000 3.5823600000	
	LU(1 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H	V)N*2CN3J 10.03475/000000 10.9885355000000 8.009379000000 12.302155000000 12.448598000000 11.091554000000 7.462411000000 9.649742000000 11.722496000000 10.777231000000 8.263725000000 11.093493000000 11.26627000000 10.191066000000	7.375728000000 9.55338400000 9.73878100000 5.41288100000 4.74369800000 8.41228400000 9.05017100000 7.03682000000 5.91459900000 5.5858600000 11.53828400000 11.868908000000 12.03652700000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.397459000000 4.915227000000 3.512916000000 6.250258000000 2.91404000000 4.905267000000 6.852838000000 2.630639000000 3.672134000000 3.24244000000	[U(1 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H	V)N*2NC2]** 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.20797000000 11.220797000000 8.184567000000 11.792882000000 10.891767000000 8.428758000000 10.89144000000 10.49544000000 10.98128000000	7.415174000000 9.658875000000 9.754898000000 5.360874000000 4.92748000000 9.047924000000 6.981742000000 6.02650100000 5.732048000000 11.540756000000 11.87590600000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 7.60658700000 3.477664000000 6.26206100000 4.91507200000 4.91507200000 2.54675100000 3.58236000000 2.15617500000	
	1 U 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.44859800000 11.09155400000 7.46241100000 9.64974200000 11.72249600000 10.77723100000 8.28372500000 8.56705000000 11.0349300000 11.23662700000 10.191006000000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 5.41288100000 4.74369800000 8.41228400000 5.05017100000 7.036682000000 5.91459900000 5.8585600000 8.10971400000 11.538284000000 11.63892800000 12.03652700000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 7.792674000000 3.512916000000 4.90526700000 6.85283800000 2.63063900000 3.672134000000 2.242340000000 2.03866600000	LU(1 1U 2Si 3Si 4Si 5Si 6C 7C 8C 9N 10N 11N 12N 13N 14C 15H 16H	♥)№ ² ,№C ₂) ^{**} 10.129239000000 10.843132000000 12.374722000000 12.506271000000 11.220797000000 1.220797000000 8.184567000000 8.184567000000 1.792882000000 10.891767000000 8.822177000000 10.98914000000 11.147549000000 11.145206200000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.04792400000 6.02650100000 6.02650100000 5.73204800000 8.33276200000 11.540756000000 12.052747000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 5.07428300000 7.60658700000 6.26206100000 3.01123000000 4.91507200000 6.68094000000 2.54675100000 3.8236000000 2.15617500000	
	LUU 1 U 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.44859800000 11.09155400000 7.462411000000 9.649742000000 11.722496000000 10.777231000000 8.283725000000 11.093493000000 11.236627000000 11.93355000000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 5.28719600000 4.74369800000 9.05017100000 5.05017100000 5.91459900000 5.91459900000 1.53828400000 11.8690800000 11.8697200000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 7.792674000000 3.512916000000 6.250258000000 2.914040000000 2.63063900000 3.672134000000 2.63966000000 2.038966000000	10 10 25i 35i 45i 55i 6C 7C 8C 9N 11N 12N 13N 14C 15H 16H 17H	♥)№ 2,№C,3] ^{**} 10.129239000000 10.843132000000 12.898219000000 12.506271000000 12.506271000000 12.576979000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.822177000000 10.892414000000 11.47549000000 11.47549000000 10.998128000000 11.85263000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35352600000 4.92748000000 9.047924000000 6.026501000000 5.732048000000 1.87590600000 1.87590600000 1.87464500000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 3.47766400000 6.26206100000 4.91507200000 6.68094000000 2.54675100000 3.823600000 2.15617500000 1.94794700000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.448598000000 11.09155400000 7.462411000000 9.649742000000 11.722496000000 11.722496000000 8.283725000000 8.56705000000 11.093493000000 11.236627000000 11.953355000000 11.953355000000 10.817372000000	7,375728000000 9,559384000000 9,738781000000 8,38918600000 5,41288100000 4,74369800000 8,41228400000 7,03668200000 5,91459900000 5,91459900000 1,53828400000 11,53828400000 11,86890800000 11,86527000000 1,897872000000 9,12926500000	4.883747000000 2.507023000000 7.25580600000 6.39745900000 1.97132700000 7.792674000000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 2.63063900000 3.672134000000 2.24234000000 2.0386600000 0.707444000000	10 10 25i 35i 45i 55i 6C 7C 8C 9N 11N 12N 13N 14C 15H 16H 17H 18C	V)N * 2NC_3]** 10.12939000000 10.843132000000 7.899819000000 12.374722000000 12.374722000000 12.506271000000 11.220797000000 8.184567000000 9.531602000000 10.891767000000 8.428758000000 8.428758000000 8.428758000000 10.989414000000 11.147549000000 10.98128000000 11.485206300000 10.655580800000 10.655580800000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35087400000 4.92748000000 6.9994400000 6.98174200000 6.026501000000 5.732048000000 1.540756000000 1.87590600000 1.87590600000 1.874645000000 9.12161300000	4.85813600000 2.44848000000 7.24668000000 6.44002100000 5.07428300000 7.60658700000 3.47766400000 6.26206100000 3.01123000000 4.915072000000 6.68094000000 2.546751000000 3.58236000000 1.94794700000 0.6508700000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H	V)N*2CN3 10.33475700000 10.33475700000 10.3345700000 10.3853500000 8.09339900000 12.30215500000 12.44859800000 12.44859800000 1.09155400000 7.46241100000 7.92947900000 9.64974200000 10.77723100000 8.28372500000 11.09349300000 11.23662700000 10.19100600000 11.95335500000 11.95335500000 11.70321500000	7,375728000000 9,559384000000 9,738781000000 5,412881000000 5,28719600000 4,743698000000 9,050171000000 7,036682000000 5,914599000000 5,914599000000 11,538284000000 11,538284000000 11,85972000000 9,129265000000 9,46667900000	4.883747000000 2.507023000000 7.255806000000 6.337405900000 1.971327000000 4.91522700000 7.79267400000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 6.85283800000 2.63063900000 3.672134000000 2.03896600000 0.707444000000 0.707444000000 0.14180900000	25i 35i 45i 55i 6C 7C 8C 9N 11N 12N 13N 14C 15H 16H 17H 18C 19H	♥)№ 2,№C,3]** 10.129239000000 10.843132000000 12.374722000000 12.506271000000 12.506271000000 12.20797000000 7.576979000000 8.184567000000 11.792882000000 10.891767000000 8.428758000000 10.989414000000 11.47549000000 11.45263000000 11.548163000000 11.548163000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35087400000 4.92748000000 6.92148000000 6.94792400000 6.026501000000 5.732048000000 11.540756000000 11.87590600000 11.87590600000 9.121613000000 9.423724000000	4.85813600000 2.44848000000 7.24660800000 6.44002100000 5.07428300000 7.60658700000 3.47766400000 6.26206100000 4.91507200000 6.68094000000 1.5475100000 0.55475100000 0.6508700000	
	LUI 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H	V)N*2CN3 10.3347500000 10.33475000000 10.388535000000 8.0937900000 12.30215500000 12.30215500000 12.30215500000 12.44859800000 7.46241100000 7.92947900000 9.64974200000 10.77723100000 8.5670500000 11.23662700000 10.1910600000 11.9333500000 10.81737200000 11.70221500000	7,375728000000 9,53934000000 8,38918600000 5,4128100000 5,28719600000 4,74369800000 8,41228400000 5,91459900000 5,58585600000 8,10971400000 11,538284000000 11,86890800000 11,86972000000 9,129265000000 9,46667900000	4.883747000000 2.507023000000 7.255806000000 6.397459000000 1.971327000000 4.915227000000 5.51291600000 6.250258000000 2.91404000000 4.905267000000 6.852838000000 2.630639000000 3.672134000000 2.038966000000 0.707444000000 0.707444000000 0.141809000000 0.221343000000	10 10 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H	V)N *2NC2]** 10.129239000000 10.843132000000 12.374722000000 12.56271000000 12.20797000000 11.220797000000 8.184567000000 8.184567000000 11.79288200000 10.891767000000 8.428758000000 10.989414000000 11.47549000000 11.452063000000 11.548163000000 9.778301000000 9.778301000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 4.92748000000 9.04792400000 6.98174200000 6.98174200000 6.026501000000 5.73204800000 11.540756000000 11.87590600000 11.874645000000 9.121613000000 9.423724000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 7.60658700000 3.47766400000 6.26206100000 3.01123000000 4.91507200000 0.56804000000 2.546751000000 1.94794700000 0.65008700000 0.07654100000	
	LUI 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H	V)N*2CN3J 10.03475/000000 110.03475/000000 110.03475/000000 12.302155000000 12.302155000000 12.44859800000 7.46241100000 7.92947900000 9.64974200000 11.72249600000 11.777231000000 11.23627000000 11.93355000000 11.93355000000 11.93355000000 11.73215000000 9.924346000000 10.770227000000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 4.74369800000 8.41228400000 9.05017100000 7.03668200000 5.91459900000 1.58585600000 11.5878400000 11.89787200000 9.12926500000 9.4667900000 9.4667900000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 4.915227000000 7.792674000000 3.512916000000 6.250258000000 2.91404000000 4.905267000000 3.672134000000 2.038966000000 0.707444000000 0.14180900000 0.221343000000 0.221343000000	251 10 253 353 453 60 70 80 90 100 110 120 130 140 154 164 174 180 194 204 214	V)N*2,NC2]** 10.129239000000 10.843132000000 10.843132000000 12.374722000000 12.374722000000 12.506271000000 12.506271000000 12.506271000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.822177000000 10.98914000000 10.098128000000 11.485263000000 11.548163000000 9.778301000000 10.567176000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 4.92748000000 9.047924000000 6.98174200000 6.92551000000 5.73204800000 11.540756000000 11.87950600000 9.12161300000 9.42372400000 9.2591000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 5.07428300000 7.60658700000 6.626206100000 4.91507200000 4.91507200000 6.6894000000 1.94794700000 0.6508700000 0.07654100000 0.07654100000	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C	V)N*2CN3J 10.034757000000 110.034757000000 110.034757000000 12.302155000000 12.302155000000 12.44859800000 7.46241100000 9.64974200000 10.777231000000 8.28372500000 11.0349300000 11.23662700000 11.95335500000 10.81737200000 11.70321500000 10.77022700000 12.65053400000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 5.28719600000 4.74369800000 5.05017100000 7.03668200000 5.91459900000 5.91459900000 11.53828400000 11.63828400000 11.6362700000 9.12926500000 9.5489600000 8.03019000000 8.5958600000	4.883747000000 2.507023000000 3.370051000000 6.39745900000 1.971327000000 4.915227000000 3.512916000000 6.250258000000 2.914040000000 4.905267000000 6.852838000000 2.630639000000 3.672134000000 0.221433000000 0.221343000000 0.221343000000 0.221343000000 0.537321000000 3.3105524000000	100 100 25i 35i 45i 55i 6C 7C 8C 9N 10N 12N 13N 14C 15H 16H 16H 17H 18C 19H 20H 21H 20H 21H 20H 20H 20H 20H 20H 20H 20H 20	♥)№ 2,№C,3) [™] 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.506271000000 11.220797000000 8.184567000000 9.531602000000 10.891767000000 10.891767000000 10.989414000000 11.47548000000 10.657508000000 11.548163000000 11.548163000000 10.567176000000 12.493747000000	7.41517400000 9.55887500000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.047924000000 6.02650100000 6.026501000000 8.33276200000 11.540756000000 11.87590600000 11.874645000000 9.42372400000 9.56901000000 8.027366000000 8.027366000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 5.07428300000 7.60658700000 6.26206100000 4.91507200000 6.6809400000 6.6809400000 2.54675100000 1.94794700000 0.650870000 0.1664600000 0.58594700000 0.58594700000	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 21 H 21 H 21 H 21 H 21 H 21 H 21	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.302155000000 12.44859800000 7.462411000000 9.649742000000 10.777231000000 8.283725000000 11.93493000000 11.93355000000 11.93355000000 11.73215000000 9.924346000000 12.857030000000	7,375728000000 9,55938400000 9,73878100000 5,41288100000 4,74369800000 8,41228400000 5,05017100000 5,05017100000 5,914599000000 5,58585600000 11,53828400000 11,538284000000 11,897872000000 9,46667900000 9,54899600000 8,03019000000 9,184575000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.915227000000 3.512916000000 6.250258000000 2.914040000000 2.630639000000 3.672134000000 2.038966000000 0.707444000000 0.14180900000 0.637321000000 3.105524000000 3.105524000000	LUU 1U 2 Si 3 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 21 C 23 H	V)N*2,NCG]** 10.129239000000 10.8123000000 10.843132000000 12.898219000000 12.506271000000 12.506271000000 12.506271000000 12.20797000000 531602000000 11.792882000000 10.891767000000 8.822177000000 10.892414000000 11.47549000000 10.982414000000 11.45549000000 11.548163000000 9.778301000000 12.493747000000 12.75142000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35352600000 4.92748000000 9.047924000000 6.981742000000 6.026501000000 1.87590600000 1.87590600000 1.87590600000 9.12161300000 9.1261300000 9.56901000000 8.02736600000 9.25445000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 7.66658700000 3.47766400000 6.26206100000 4.91507200000 6.68094000000 6.68094000000 2.54675100000 3.58236000000 0.58594700000 0.6664600000 0.58594700000 3.06030500000	
	EUT 10 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 22 H	V)N*2CN3J 10.034757000000 10.988535000000 8.009379000000 12.302155000000 12.44859800000 12.44859800000 7.46241100000 9.64974200000 9.64974200000 11.72249600000 10.777231000000 8.283725000000 11.93493000000 11.93355000000 11.953355000000 11.953355000000 11.702270000000 10.770227000000 12.650534000000 12.4897090000000	7,375728000000 9,55938400000 9,73878100000 8,38918600000 5,41288100000 4,74369800000 8,41228400000 9,05017100000 5,51459900000 5,58585600000 11,53828400000 11,53828400000 11,86890800000 11,867900000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 3.51291600000 6.25025800000 2.91404000000 2.91404000000 2.63063900000 2.63063900000 2.4234000000 0.77744400000 0.14180900000 0.22134300000 0.22134300000 0.22134300000 0.33752400000 1.4151835000000 2.4288600000	LUU 1 U 2 Si 3 Si 5 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H	♥)№ 2,№C,2) ^{**} 10.12929000000 10.843132000000 12.374722000000 12.374722000000 12.374722000000 12.3747200000 11.22097000000 12.576979000000 11.22097000000 10.891767000000 10.891767000000 10.989414000000 11.147549000000 10.98128000000 11.548163000000 11.548163000000 11.548163000000 11.548163000000 11.548163000000 11.2493747000000 12.493747000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.35352600000 4.92748000000 6.6994400000 6.98174200000 6.98174200000 6.026501000000 1.540756000000 1.540756000000 1.87590600000 9.12161300000 9.12161300000 9.42372400000 9.56901000000 8.8027366000000 8.8027366000000 9.255000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 5.07428300000 7.66658700000 3.47766400000 3.01123000000 4.915072000000 4.915072000000 0.56894000000 1.94794700000 0.6508700000 0.07654100000 0.1666400000 0.1666400000 3.0003500000 2.3919200000	
	EUT 10 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 22 H 22 H	V)N*2CN3 20034757000000 10.034757000000 10.034757000000 10.98533500000 8.09337900000 12.30215500000 12.30215500000 12.44859800000 11.09155400000 7.46241100000 7.46241100000 9.64974200000 10.777231000000 8.28372500000 11.0349300000 11.3662700000 11.9335500000 11.70321500000 9.92434600000 10.77022700000 12.8970900000 13.43254000000	7,375728000000 9,55938400000 9,73878100000 5,41288100000 5,41288100000 4,74369800000 9,05017100000 5,91459900000 5,91459900000 11,53828400000 11,53828400000 11,86890800000 11,867500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000 9,12926500000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.39745900000 1.971327000000 4.915227000000 3.512916000000 6.250258000000 2.914040000000 4.905267000000 2.630639000000 2.630639000000 2.42340000000 2.242340000000 2.038966000000 0.707444000000 0.221343000000 0.637321000000 0.637321000000 3.105524000000 4.151835000000 2.478786000000	LUU 1 U 2 Si 3 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 24 H 24 H 27 H	♥)№ *2№C2]** 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.50627100000 12.50627100000 11.220797000000 7.576979000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.428758000000 10.989414000000 11.47549000000 10.989414000000 11.457508000000 11.45508000000 11.45508000000 11.548163000000 10.567176000000 12.493747000000 12.775142000000 13.271643000000	7.41517400000 9.65887500000 9.75489800000 8.34108600000 5.36037400000 6.353532600000 9.04792400000 6.98174200000 6.026501000000 1.540756000000 1.874645000000 9.12161300000 9.12161300000 9.42372400000 9.5591000000 8.027366000000 8.9468100000 9.5545000000 9.5545000000 9.5575000000	4.85813600000 2.44848000000 7.2466800000 6.44002100000 2.09638100000 5.07428300000 7.60658700000 3.47766400000 3.01123000000 4.91507200000 0.5854700000 1.94794700000 0.5854700000 0.5854700000 0.58594700000 3.07616100000 2.3910200000	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 13 C 13 C 13 C 13 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H	V)N*2CN3J 10.33475000000 110.3845535000000 110.3885355000000 12.302155000000 12.302155000000 12.44859800000 7.46241100000 7.46241100000 9.64974200000 10.777231000000 11.722496000000 11.23662700000 11.23662700000 11.93355000000 11.93355000000 11.702215000000 11.70227000000 12.650534000000 12.89709000000 12.89709000000 12.74778000000	7,375728000000 9,73878100000 9,73878100000 5,41288100000 5,41288100000 4,74369800000 8,41228400000 7,03668200000 5,91459900000 5,91459900000 11.53828400000 11.53828400000 11.86890800000 9,129265000000 9,12926500000000 9,1292650000000 9,1292650000000 9,1292650000000 9,12926500000000000000000000000000000000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.39745900000 1.97132700000 4.91522700000 7.79267400000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 6.85283800000 2.63063900000 2.4234000000 2.03896600000 0.707444000000 0.21343000000 0.221343000000 0.637321000000 3.10552400000 3.10552400000 4.15183500000 2.47878600000 2.47878600000	2 C C C C C C C C C C C C C C C C C C C	♥)№ 2,№C,]** 10.12939000000 10.843132000000 12.374722000000 12.374722000000 12.506271000000 12.506271000000 12.506271000000 12.20797000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.428758000000 8.428758000000 10.989414000000 11.47549000000 10.989414000000 11.47549000000 10.657508000000 11.548163000000 9.778301000000 10.56717600000 12.5491700000 12.5491700000 12.5491700000 12.75142000000 13.271643000000 12.54914000000 12.54914000000 12.54914000000 13.271643000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 5.36087400000 6.92748000000 6.92748000000 6.981742000000 6.026501000000 5.732048000000 11.540756000000 11.87590600000 9.121613000000 9.423724000000 9.423724000000 9.56901000000 8.027366000000 8.946481000000 9.55445000000 9.552750000000 7.852276000000	4.85813600000 2.44848000000 3.38783100000 7.24660800000 2.09638100000 5.07428300000 7.60658700000 3.47766400000 3.01123000000 4.91507200000 4.91507200000 0.58594000000 1.94794700000 0.58594700000 0.58594700000 3.6030500000 4.07616100000 2.39190200000	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 25 H 26 C	V)N*2CN3 20037500000 10.3475700000 10.3475700000 10.3475700000 10.38853500000 8.0937900000 12.30215500000 12.30215500000 12.44859800000 1.09155400000 7.46241100000 7.92947900000 9.64974200000 11.72249600000 11.7723100000 8.5670500000 11.9349300000 11.9345500000 11.9335500000 11.7321500000 11.7321500000 12.7434600000 12.7503400000 12.7879000000 13.43254000000 13.43254000000 12.72477800000	7.37572800000 9.65938400000 9.73878100000 5.41288100000 4.74369800000 8.41228400000 9.05017100000 7.03668200000 5.91459900000 15.58585000000 11.89787200000 9.1292500000 9.1292500000 9.4667900000 9.54899600000 9.1292500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000 9.18457500000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 4.915227000000 7.792674000000 3.512916000000 2.91404000000 4.905267000000 2.91404000000 3.672134000000 2.038966000000 0.707444000000 0.41819900000 0.41819900000 0.4151835000000 3.105524000000 4.151835000000 2.478786000000 2.957967000000 1.597846000000	LUU 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 16 H 20 H	♥)● *, NC_3) ** 10.129239000000 10.843132000000 10.843132000000 12.374722000000 12.506271000000 12.506271000000 12.506271000000 8.184567000000 8.184567000000 9.531602000000 10.9891767000000 8.428758000000 10.98914000000 10.98914000000 11.147549000000 11.548163000000 9.778301000000 10.567176000000 11.548163000000 12.493747000000 12.775142000000 12.75142000000 12.75643000000 12.75643000000 12.75643000000 7.438903000000	7.41517400000 9.65887500000 9.75489800000 5.36087400000 4.92748000000 9.04792400000 6.98174200000 6.98174200000 6.9250100000 11.54075600000 11.8790600000 9.12161300000 9.12161300000 9.2574700000 9.25445000000 9.25445000000 9.25445000000 1.874648100000 9.25445000000 1.8506000000 9.25276000000 1.8506000000 9.25276000000 9.25276000000 1.85276000000 1.85276000000	 4.85813600000 2.44848000000 3.8783100000 6.44002100000 6.44002100000 7.7428300000 7.7428300000 7.7428300000 6.6605400000 6.6605400000 6.5605400000 6.5605400000 6.5605400000 6.56594700000 6.56594700000 6.56594700000 6.56594700000 6.56594700000 6.565547000000 6.565547000000 6.565547000000 6.565547000000 6.565547000000 6.565547000000 6.565547000000 6.565547000000 6.5655470000000 6.5655470000000 6.5655470000000 6.5655470000000 6.56554700000000 6.565547000000000 6.565547000000000 	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 20 H 20 H 22 C 23 H 24 H 25 H 26 C 27 H	V)N*2CN3J 10.03475/000000 110.03475/000000 110.03475/000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 9.64974200000 10.777231000000 11.72249600000 11.0349300000 11.23662700000 11.93355000000 11.7321500000 11.7321500000 11.7321500000 11.7321500000 11.7321500000 12.650534000000 12.650534000000 12.459790000000 13.43254000000 13.43254000000 12.724778000000 12.724778000000	7.37572800000 9.55938400000 9.73878100000 5.41288100000 5.28719600000 4.74369800000 5.28719600000 5.0017100000 7.03668200000 5.91459900000 5.5885600000 11.53828400000 11.538284000000 11.63652700000 9.14295000000 9.54899600000 9.54899600000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000 9.54895000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.971327000000 3.512916000000 3.512916000000 4.905267000000 4.905267000000 3.672134000000 2.24234000000 0.21343000000 0.221343000000 0.437321000000 3.105524000000 3.105524000000 4.151835000000 2.3957967000000 1.597846000000 1.597846000000	LUU 1 U 2 Si 3 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 18 C 19 H 20 H 20 H 21 H 22 C 23 H 24 H 25 H 25 H 26 C 27 H 26 C 27 H	♥)№ 2,№C,2) [™] 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.506271000000 12.506271000000 8.184567000000 9.531602000000 10.891767000000 10.891767000000 10.891767000000 10.892414000000 11.47549000000 11.548163000000 10.567176000000 10.567176000000 12.493747000000 12.775142000000 12.75142000000 12.756414000000 7.438903000000 8.885428000000	7.41517400000 9.55887500000 9.75489800000 5.36087400000 4.92748000000 9.047924000000 6.026501000000 6.026501000000 11.540756000000 11.87590600000 11.87590600000 9.12161300000 9.42372400000 9.5901000000 8.02736600000 9.5901000000 9.59501000000 9.59501000000 9.59501000000 9.52445000000 9.5595000000 8.02736600000 8.02736600000 8.02736600000 9.5595000000 9.5595000000 9.5595000000	 4.85813600000 2.44848000000 3.8783100000 4.4402100000 4.402100000 4.402100000 5.07428300000 5.07428300000 4.7766400000 4.7766400000 4.91507200000 4.91507200000 5.54675100000 4.91507200000 1.5417500000 0.5859400000 0.6508700000 0.6508700000 0.54594700000 0.54594700000 0.54594700000 0.54594700000 0.54594700000 0.54594700000 0.54594700000 0.5459400000 0.5459400000 1.40504800000 1.41389700000 	
	2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 26 C 27 H 28 H	V)N*2CN3J 10.034757000000 110.034757000000 110.034757000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 9.64974200000 10.777231000000 10.777231000000 11.23662700000 11.93355000000 11.93355000000 11.7321500000 10.817372000000 12.650534000000 12.650534000000 12.650534000000 13.43254000000 13.43254000000 12.724778000000 12.724778000000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.41288100000 4.74369800000 9.5017100000 5.5145900000 5.5145900000 5.5145900000 5.5385600000 11.53828400000 11.8689080000 9.12926500000 9.4667900000 9.5489600000 9.5489600000 9.48457500000 9.48457500000 9.48457500000 9.48457500000 9.4202800000 9.4202800000 11.02958000000	4.883747000000 2.50702300000 3.37005100000 7.25580600000 6.39745900000 1.97132700000 1.97132700000 3.51291600000 3.51291600000 2.91404000000 2.91404000000 2.91404000000 2.63063900000 3.672134000000 2.4234000000 0.70744000000 0.14180900000 0.63732100000 3.1052400000 1.5183500000 2.47878600000 1.59784600000 1.59784600000 1.58704900000	100 2 Si 3 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 H 25 H 26 C 27 H 28 H	V)N*2,NCG]** 10.129239000000 10.843132000000 7.899819000000 12.89627100000 12.506271000000 12.506271000000 12.506271000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.428758000000 8.428758000000 10.892414000000 11.47549000000 10.6957508000000 11.548163000000 10.567176000000 12.493747000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 12.75142000000 13.271643000000 2.69414000000 7.4389030000000 6.40963400000000	7.41517400000 9.55887500000 9.75489800000 5.36087400000 5.35352600000 4.92748000000 6.98174200000 6.98174200000 6.98174200000 6.32501000000 11.87590600000 11.87590600000 11.87590600000 9.42372400000 9.42372400000 9.42372400000 9.5691000000 9.5545000000 9.35275000000 10.2682900000 10.2682900000	4.85813600000 2.44848000000 3.8783100000 6.44002100000 2.09638100000 7.7426600000 7.760658700000 3.47766400000 6.26206100000 4.91507200000 6.68094000000 2.54675100000 0.58594700000 0.7654100000 0.58594700000 0.58594700000 4.97616100000 0.58594700000 0.58594700000 0.585947000000 1.625048000000 1.625048000000	
	EUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 S 23 H 25 H 25 H 25 H 26 C 27 H 28 H 29 H	V)N*2CN3J 10.034757000000 110.034757000000 110.034757000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 9.64974200000 9.64974200000 10.777231000000 8.283725000000 11.236627000000 11.93493000000 11.93355000000 11.7321500000 10.770227000000 12.650534000000 12.650534000000 12.74778000000 13.43254000000 12.724778000000 7.58766000000 8.23886800000 6.55238100000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.41288100000 4.74369800000 9.5017100000 5.5145900000 5.9145900000 5.9145900000 5.9145900000 1.5382600000 1.6392800000 1.8690800000 9.4667900000 9.5489600000 9.36457500000 9.18457500000 9.3745100000 1.02958000000 9.4202800000 1.02958000000 9.4202800000 9.4202800000 1.02958000000 9.4202800000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 7.79267400000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 2.63063900000 2.63063900000 2.63063900000 2.03896600000 0.707444000000 0.14180900000 0.4151835000000 2.47878600000 2.47878600000 1.9668900000 1.9668900000 1.58704900000 1.58704900000 0.91253000000	10 10 2 Si 3 Si 5 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 H 24 H 25 H 26 H 27 H 28 H 29 H	♥)● *, NC_3)** 10.12939000000 10.8123000000 12.85627100000 12.37472200000 12.37472200000 12.37472200000 12.5627100000 12.5627100000 12.20797000000 5.31602000000 11.4254700000 0.53160200000 10.89176700000 8.42875800000 8.42875800000 10.8914700000 10.9894400000 11.4754900000 10.9814800000 11.4754900000 11.45546300000 12.49374700000 12.56941400000 12.56941400000 7.4389300000 8.88542800000 6.40963400000 7.45547500000	7.41517400000 9.65887500000 9.75489800000 9.75489800000 5.3607400000 5.3637400000 4.92748000000 4.92748000000 9.04792400000 6.026501000000 6.026501000000 5.732048000000 1.540756000000 1.87596000000 9.12161300000 9.42372400000 9.25445000000 9.25275000000 7.85275000000 7.85275000000 1.0.56715000000 9.32445000000	4.85813600000 2.44848000000 3.38783100000 6.44002100000 2.09638100000 2.09638100000 3.07428300000 3.47766400000 3.477664000000 3.01123000000 4.915072000000 4.915072000000 2.546751000000 0.56547000000 0.6508700000 0.076541000000 0.076541000000 0.585947000000 3.06030500000 0.585947000000 0.585947000000 1.231897000000 1.231897000000 1.213897000000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 13 C 13 C 13 C 13 C 13	V)N*2CN3J 10.33475000000 110.33475000000 110.3885355000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 7.46241100000 9.64974200000 10.7723100000 10.777231000000 11.23662700000 11.23662700000 11.93355000000 11.70227000000 12.650534000000 12.89709000000 12.3724778000000 12.724778000000 12.724778000000 6.552381000000 7.630879000000 7.630879000000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.41288100000 4.74369800000 9.5017100000 5.91459800000 5.91459900000 5.91459900000 5.91459900000 1.53828400000 1.153828400000 1.86890800000 9.1295500000 9.1295500000 9.1295500000 9.1895700000 9.1895700000 9.18499600000 9.18457500000 9.18457500000 9.18457500000 10.23746100000 11.0258000000 11.0258000000 11.24898000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.39745900000 1.971327000000 4.915227000000 3.512916000000 6.250258000000 2.914040000000 2.91404000000 2.91404000000 2.630639000000 2.4234000000 0.707444000000 0.221343000000 0.221343000000 0.637321000000 0.637321000000 1.415835000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.59784000000 1	100 100 25i 35i 55i 6C 7C 8C 9N 11N 12N 13N 14C 15H 16H 17H 18C 19H 20H 21H 20H 21H 22C 23H 24H 25H 26H 27H 26H 27H 26H 27H 27H 28H 29H 29H 20H 29H 20H 20H 20H 20H 20H 20H 20H 20	V)N *2,NCG]** 10.129239000000 10.843132000000 7.899819000000 12.374722000000 12.374722000000 12.5627100000 11.220797000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 10.989414000000 11.47549000000 11.485263000000 11.548163000000 11.548163000000 11.548163000000 11.548163000000 12.493747000000 12.755142000000 7.438903000000 7.4389000000 7.455475000000 7.455475000000 7.455475000000	7.41517400000 9.65887500000 9.75489800000 8.34108600000 5.3687500000 5.35352600000 4.92748000000 6.69994400000 6.03174200000 6.026501000000 6.026501000000 5.732048000000 1.540756000000 1.87590600000 9.12161300000 9.42372400000 9.56901000000 8.02736600000 9.35275000000 10.26862900000 11.056715000000 9.4213000000	 4.85813600000 2.44848000000 3.8783100000 7.2466800000 6.44002100000 2.09638100000 5.07428300000 5.07428300000 4.0766400000 3.01123000000 4.91507200000 4.915072000000 5.5475100000 3.58236000000 2.15617500000 0.6508700000 0.6508700000 0.7654100000 0.58594700000 3.6814000000 2.3914000000 4.07616100000 1.6389700000 1.639700000 1.639700000 1.639500000 1.639500000 	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 14 C 13 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 28 H 28 H 29 H 29 H 29 H 20 H 21 H 21 H 21 H 21 H 21 H 21 H 21 H 21	V)N*2CN3J 10.33475000000 110.33475000000 110.388535000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 7.46241100000 9.64974200000 10.777231000000 10.777231000000 11.23657000000 11.23657000000 11.933355000000 10.817372000000 11.933355000000 11.933355000000 12.89709000000 12.89709000000 12.89709000000 12.724778000000 12.72478888000000 12.72478888000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.5588000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000 12.55880000000000000000000000000000000000	7.375728000000 9.65938400000 9.73878100000 5.41288100000 5.41288100000 5.28719600000 4.74369800000 8.41228400000 9.05017100000 7.0368200000 5.91459900000 5.91459900000 5.9385600000 11.53828400000 9.1292500000 9.1292500000 9.4667900000 9.1292500000 9.13457500000 9.1457500000 9.18457500000 10.23746100000 11.62274100000 9.376233000000 11.24898000000	4.883747000000 2.507023000000 3.370051000000 7.255806000000 6.39745900000 1.971327000000 4.915227000000 6.250258000000 2.914040000000 4.905267000000 2.91404000000 2.630639000000 2.4234000000 0.707444000000 0.72134000000 0.21343000000 0.221343000000 0.637321000000 1.4151835000000 1.597846000000 1.597846000000 1.587049000000 0.91253000000 0.91253000000 0.91253000000 0.91255000000 0.91255000000 1.58784000000 0.91255000000 1.58784000000 0.91255000000 1.58784000000 1.58784000000 0.91253000000 1.58784000000 0.91253000000 1.58784000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91255000000 0.91253000000 0.91255000000 0.91253000000 0.91254000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.91253000000 0.912540000000 0.912540000000 0.912540000000 0.91254000000000	LUU 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 16 H 20 H 20 H 22 Si 23 H 26 C 27 H 28 H 29 H 20 H	♥)№ 2,№C,3) [™] 10.129239000000 10.843132000000 12.374722000000 12.374722000000 12.506271000000 12.506271000000 8.184567000000 9.53160200000 10.89176700000 10.89176700000 10.89176700000 10.9812800000 10.9812800000 11.54816300000 10.55751800000 11.54816300000 12.49374700000 12.77514200000 12.75514200000 12.75514200000 12.55941400000 7.43890300000 7.43890300000 7.43547500000 7.95215500000	7.41517400000 9.65887500000 9.75489800000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.04792400000 9.04792400000 9.04792400000 6.0255100000 5.73204800000 11.54075600000 11.8795060000 9.12161300000 9.12461300000 9.12541000000 9.25445000000 9.25445000000 9.35275000000 10.26862900000 11.66374400000 9.35275000000 10.66374400000 9.35275000000 11.27269100000	4.85813600000 2.44848000000 3.38783100000 7.24660800000 6.44002100000 2.09638100000 5.07428300000 7.4666800000 3.47766400000 6.6206100000 3.0112300000 4.91507200000 3.5873600000 2.54675100000 3.5823600000 0.6508700000 0.6508700000 0.5854700000 0.5854700000 2.3919020000 1.6250480000 1.6250480000 1.21389700000 1.535200000 3.5326000000 1.52542800000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 13 C 13 C 13 C 13 C 13	V)N*2CN3 V)N*2CN3 10.34757000000 10.34757000000 10.34757000000 11.03475700000 12.302155000000 12.302155000000 12.302155000000 1.091554000000 7.462411000000 7.462411000000 9.649742000000 10.777231000000 8.56705000000 11.03457000000 11.9349300000 11.9335500000 11.7321500000 12.65053400000 12.72477800000 12.8709000000 13.43254000000 12.72477800000 7.58766000000 6.552381000000 7.844169000000 7.86483000000 7.86483000000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.28719600000 4.74369800000 8.41228400000 9.05017100000 7.03668200000 5.91459900000 5.91459900000 5.9385600000 11.5828400000 11.8382400000 9.126500000 9.4267900000 9.4567900000 9.4267900000 9.4567500000 11.8378700000 9.4262800000 11.8787200000 9.1245500000 11.8787200000 9.12457500000 9.12457500000 11.025800000 11.025800000 11.0258000000 11.0258000000 11.24898000000 11.24898000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 7.79267400000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 6.85283800000 2.63663900000 2.6326600000 2.03896600000 0.70744000000 0.70744000000 0.415183500000 2.47878600000 2.95796700000 1.95784600000 1.968900000 1.958704900000 1.9583000000 3.5974900000 3.5974900000 3.5974900000 3.5974900000 3.5974900000 3.5974900000 3.5974900000 3.5974900000	LUU 1 U 2 Si 3 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 17 H 20 H	♥)● *,NC_3)** 10.129239000000 10.843132000000 10.843132000000 12.374722000000 12.506271000000 12.506271000000 12.506271000000 8.184567000000 9.531602000000 11.792882000000 10.881767000000 8.428758000000 8.428758000000 8.428758000000 10.98914000000 10.098128000000 11.4581563000000 11.54815300000 9.778301000000 10.567176000000 12.75142000000 12.75142000000 12.75142000000 12.569414000000 7.43893000000 8.825475000000 7.962165000000 7.962165000000 7.962165000000	7.415174000000 9.658875000000 9.75489800000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.04792400000 6.02551000000 6.02551000000 5.73204800000 11.54075600000 11.874060000 9.12161300000 9.25747000000 9.2574000000 9.2574000000 9.25445000000 9.25445000000 10.26862900000 10.26862900000 10.2776000000 9.35275000000 10.26862900000 11.05671500000 10.272691000000 9.41219300000 11.37464500000	4.85813600000 2.44848000000 3.38783100000 7.24660800000 6.44002100000 2.09638100000 5.07428300000 7.46658700000 6.4602100000 3.47766400000 6.26206100000 3.01123000000 4.91507200000 2.5675100000 2.5675100000 0.5854700000 0.6608700000 0.07654100000 0.0765400000 0.3693700000 1.94794700000 0.36935000000 0.3650400000 0.3650400000 1.947947000000 0.3650400000 0.3650400000 0.3650400000 0.3650400000 1.400000000 1.62504800000 1.62504800000 1.63990700000 1.63990700000 1.63935200000 1.5342800000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 13 C 13 C 13 C 14 C 15 H 16 H 17 H 20 H 20 H 20 H 20 H 20 H 22 Si 23 H 26 C 27 H 28 H 29 H 30 C 31 H 32 H	V)N*2CN3J 10.33475000000 110.33475000000 110.388535000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 9.64974200000 9.64974200000 11.72249600000 11.72249600000 11.0349300000 11.0349300000 11.9335500000 11.9335500000 11.7322500000 11.7321500000 11.7322500000 12.65053400000 12.65053400000 12.877000000 12.4747800000 12.72477800000 13.43254000000 12.72477800000 12.72477800000 12.72477800000 13.43254000000 13.4325400000 13.4325400000 13.4325400000 13.4325400000 13.4325400000 13.43254000000 13.43254000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.4325400000000000000000000000000000000000	7.375728000000 9.659384000000 9.73878100000 8.38918600000 5.41288100000 5.28719600000 4.74369800000 8.1228400000 5.05017100000 5.91459900000 5.91459900000 5.91459900000 5.91459900000 11.53828400000 11.63828400000 11.83787200000 9.12926500000 9.5489600000 9.5489600000 9.4667900000 9.5489600000 9.12926500000 9.5489600000 11.83772000000 9.4667900000 9.5489600000 9.129265000000 9.3623000000 9.36233000000 11.029580000000 11.24888000000 11.24889000000 11.24775000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.971327000000 3.512916000000 3.512916000000 4.905267000000 4.905267000000 2.914040000000 2.63063900000 3.672134000000 2.24234000000 0.707444000000 0.221343000000 0.437321000000 3.105524000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 1.597846000000 3.574854000000 3.554854000000 3.	LUU 1 U 2 Si 3 Si 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 20 H	♥)● *, NC_3)** 10.129239000000 10.843132000000 10.843132000000 12.374722000000 12.506271000000 12.506271000000 12.506271000000 12.506271000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 8.428758000000 8.428758000000 11.792882000000 11.792882000000 11.47549000000 11.4554000000 11.6557508000000 12.569414000000 12.775142000000 12.569414000000 12.775142000000 12.569414000000 7.438903000000 6.409634000000 7.78362000000 7.785475000000 7.79362000000 7.79262000000 7.922165000000	7.41517400000 9.55887500000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.047924000000 6.026501000000 6.026501000000 11.540756000000 11.540756000000 11.87590600000 9.12161300000 9.12161300000 9.352750000000 9.352750000000 9.352750000000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.26862900000 10.268744000000 9.41213000000 11.272691000000 11.272691000000 11.272691000000	4.85813600000 2.44848000000 3.8783100000 3.8783100000 6.4402100000 2.09638100000 5.07428300000 5.07428300000 5.07428300000 6.26206100000 3.01123000000 6.26206100000 6.26206100000 6.26304000000 2.54675100000 1.94794700000 0.65008700000 0.56594700000 0.56594700000 0.56594700000 1.62504800000 1.62504800000 1.62504800000 1.6399700000 1.63990700000 1.63990700000 1.6390700000 1.6390700000 1.6390700000 1.4397000000 1.4397000000 1.4397000000 1.4397000000 1.43937000000 1.43937000000 1.4397000000 1.4397000000 1.4397000000 1.4397000000	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 25 H 26 C 27 H 28 H 29 H 30 C 31 H 32 H 33 H	V)N*2CN3J 10.034757000000 110.034757000000 110.034757000000 110.034757000000 12.302155000000 12.44859800000 12.44859800000 9.64974200000 1.72249600000 10.77723100000 8.28372500000 11.0349300000 11.0349300000 11.9349300000 11.7321500000 10.81737200000 11.7321500000 10.77022700000 12.650534000000 12.450534000000 12.450534000000 12.724778000000 13.43254000000 13.43254000000 15.52381000000 7.58766000000 7.58766000000 7.58766000000 7.58468300000 7.5848300000 7.588300000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.41288100000 4.74369800000 4.74369800000 5.0517100000 5.0517100000 5.91459900000 5.91459900000 5.91459900000 1.53828400000 11.53828400000 9.12925500000 9.4667900000 9.5489600000 9.1457500000 9.1457500000 1.0295800000 9.466736100000 9.1457500000 9.34637600000 9.34637600000 9.34637600000 9.34637600000 9.34637600000 9.34637600000 9.346376000000 9.346376000000 9.346376000000 9.346376000000 9.37623000000 1.029580000000 1.32989000000 1.32989000000 1.34989000000 1.34989000000 1.34989000000 1.30375000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.971327000000 3.512916000000 3.512916000000 2.914040000000 2.914040000000 2.91404000000 2.63063900000 2.63063900000 2.63063900000 2.03896600000 0.70744000000 0.415183500000 1.5178500000 1.59784600000 1.59784600000 1.58704900000 1.58704900000 1.58704900000 1.58704900000 1.58704900000 1.58704900000 1.58704900000 1.58704900000 3.4356500000 3.4356500000 3.4369500000 3.4369500000 3.4369500000 3.43695000000 3.458744000000 3.4369500000 3.4369500000 3.4369500000 3.4369500000 3.4587400000 3.4369500000 3.4369500000 3.4587400000 3.4369500000 3.4369500000 3.4587400000 3.4587400000 3.4369500000 3.4587400000 3.4597400000 3.4587400000 3.4587400000 3.4587400000 3.45874000000 3.45874000000 3.45874000000 3.4587400000 3.45874000000 3.458747400000 3.4587474747474747474747474	2 S H 2 S H 2 S H 4 S H 5 S H 6 C 7 C 8 C 9 N 10 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 16 H 17 H 18 C 19 H 20 H 20 H 21 C 23 H 26 C 27 H 28 H 29 H 20 C 31 H 32 H 33 H	V)N*2,NCG]** I0.129239000000 I0.81239000000 I0.843132000000 I2.89821900000 I2.50627100000 I1.220797000000 I2.50627100000 I1.220797000000 S3160200000 I1.4256700000 8.18456700000 I.179288200000 I0.89176700000 8.42875800000 8.42875800000 8.42875800000 8.42875800000 I1.4754900000 I1.4754900000 I1.4754900000 I1.54816300000 I1.54816300000 I2.49374700000 I2.7514200000 I2.7514200000 I2.7514200000 I2.7514200000 I2.7514200000 I2.7542800000	7.41517400000 9.65887500000 9.75489800000 9.75489800000 5.36087400000 5.36087400000 4.92748000000 9.04792400000 6.02650100000 6.026501000000 6.026501000000 6.026501000000 1.54075600000 1.8790600000 1.8790600000 9.4237400000 9.42372400000 9.5690100000 9.5690100000 9.5275000000 9.5275000000 9.35275000000 9.4219300000 9.41219300000 9.41219300000 1.171448500000 1.204815600000	4.85813600000 2.44848000000 3.8783100000 6.44002100000 2.09638100000 3.47766400000 6.26206100000 4.91507200000 6.68094000000 2.54675100000 0.58594700000 0.07654100000 0.07654100000 0.07654100000 0.07654100000 0.1664600000 0.1664600000 1.62504800000 0.076541000000 0.162504800000 0.076541000000 0.076541000000 0.076541000000 0.076541000000 0.076541000000 0.0765410000000 0.076540000000 0.0765400000000000000000000000000000000000	
	IU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 12 C 13 C 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 26 C 27 H 28 H 29 H 30 C 31 H 32 H 33 H 34 C	V)N*2CN3J 10.034757000000 110.034757000000 110.034757000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 10.77231000000 10.777231000000 8.283725000000 11.23657000000 11.93493000000 11.9335500000 10.19106000000 11.953355000000 10.770227000000 12.650534000000 12.650534000000 12.78766000000 12.78766000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.432540000000 13.4325400000000000000000000000000000000000	7.375728000000 9.65938400000 9.73878100000 8.38918600000 5.41288100000 5.41288100000 4.74369800000 9.5017100000 5.5145900000 5.5145900000 5.91459900000 5.5145900000 1.5382400000 1.5382400000 1.6392800000 9.4667900000 9.4667900000 9.45499600000 9.45499600000 9.4545700000 9.1457500000 1.02958000000 9.4202800000 1.02958000000 9.4202800000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.02958000000 1.0295938000000	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.9386600000 2.03896600000 0.707444000000 0.4180900000 2.47878600000 2.47878600000 1.9587000000 1.9587000000 1.9668900000 1.9158000000 1.9158000000 1.9158000000 1.9158000000 1.9158000000 1.9200000 1.9158000000 1.9158000000 1.9158000000 1.9158000000 1.9158000000 1.9156000000 1.92000000 1.9200000 1.92000000 1.92000000 1.92000000 1.9158000000	10 10 2 Si 3 Si 5 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 H 23 H 26 H 26 H 27 H 26 H 27 H 26 H 27 H 27 H 26 H 27 H 27 H 26 H 27	V)N*2,NCG]** 10.129239000000 10.8123000000 7.899819000000 12.806271000000 12.506271000000 12.506271000000 12.5076979000000 8.184567000000 9.531602000000 11.792882000000 10.891767000000 8.428758000000 10.891767000000 10.989414000000 11.47549000000 10.981428000000 11.47549000000 11.47549000000 11.457508000000 11.548163000000 12.493747000000 12.569414000000 12.493747000000 12.569414000000 7.43893000000 6.409634000000 7.455475000000 7.79362000000 6.772028000000 6.611827000000	7.41517400000 9.65887500000 9.75489800000 9.34108600000 5.3607400000 5.35362600000 4.92748000000 6.03994400000 9.04792400000 6.026501000000 5.732048000000 1.540756000000 1.8750600000 1.8750600000 9.12161300000 9.25445000000 9.2545000000 9.2545000000 9.25275000000 7.82275000000 7.82275000000 1.056715000000 9.25445000000 9.25445000000 9.2545000000 1.056715000000 1.1.272691000000 1.1.27465000000 1.1.27485000000 9.412193000000 9.42358000000	 4.85813600000 2.44848000000 3.8783100000 4.2402100000 4.402100000 5.07428300000 5.07428300000 4.0766400000 4.01507200000 4.01507200000 4.01507200000 5.5475100000 3.5823600000 2.15617500000 0.6508700000 0.6508700000 0.6508700000 0.6508700000 0.07654100000 0.5854700000 2.391700000 2.34000000 2.354000000 1.21389700000 1.63990700000 1.6395200000 3.55442800000 4.4097500000 3.52384000000 	
	LUU 2 Si 3 Si 4 Si 5 Si 6 N 7 N 8 N 9 N 10 N 11 C 13 C 13 C 13 C 13 C 13 C 13 C 13 C	V)N*2CN3J 10.33475000000 110.33475000000 110.388535000000 12.302155000000 12.302155000000 12.44859800000 12.44859800000 7.46241100000 9.64974200000 10.77023100000 11.72249600000 11.23657000000 11.2367000000 11.23657000000 11.33355000000 11.73215000000 12.650534000000 12.8709000000 12.8709000000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 12.72477800000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.5528100000 10.55281000000 10.55281000000 10.55281000000 10.55281000000	7.375728000000 9.53938400000 9.73878100000 8.38918600000 5.41288100000 5.28719600000 4.74369800000 9.5017100000 5.5145900000 5.5145900000 5.5145900000 5.5145900000 1.53828400000 1.53828400000 1.6390800000 9.12926500000 9.12926500000 9.12926500000 9.12926500000 9.14667900000 9.12926500000 9.12926500000 9.14957000000 9.14957000000 9.12926500000 9.12926500000 9.12926500000 9.12926500000 9.12926500000 9.129265000000 9.129265000000 9.12926500000 9.12926500000 9.12926500000 9.12927000000 9.12927000000 9.12927000000 9.12927000000 9.12927000000 9.12927000000 9.12927000000 <td>4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.4234000000 2.4234000000 2.0386600000 0.70744400000 0.14180900000 1.4151835000000 2.478786000000 1.597846000000 1.597846000000 1.58704900000 1.58704900000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 3.69655000000 3.69655000000 3.69658000000 3.69658000000 3.890628000000 </td> <td>2 Si 3 Si 3 Si 5 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 26 H 26 C 27 H 26 H 27 H 26 C 27 H 26 H 27 H 26 C 27 H 27 H</td> <td>V)N * 2,NCG]** 10.12939000000 10.1239000000 7.899819000000 12.374722000000 12.374722000000 12.3747200000 12.5627100000 11.220797000000 7.576979000000 8.184567000000 9.531602000000 10.389414000000 10.389414000000 11.4754900000 10.389414000000 11.4754900000 10.56750800000 11.54816300000 11.54816300000 12.49374700000 12.77514200000 13.271643000000 7.4380700000 7.4380400000 7.4380400000 7.4380400000 7.438054200000 6.409634000000 7.7962165000000 6.572028000000 6.611842000000 6.61164000000</td> <td>7.41517400000 9.65887500000 9.75489800000 9.35087400000 5.3607400000 5.35362600000 4.92748000000 6.03994400000 6.03174200000 6.026501000000 5.732048000000 1.540756000000 1.540756000000 1.540756000000 9.12161300000 9.42372400000 9.56901000001 9.35275000000 10.2682900000 10.56755000000 10.56755000000 10.5675000000 10.5675000000 10.56874000000 9.35275000000 10.56874000000 9.41219300000 11.272691000000 11.27485000000 12.048156000000 9.41219300000 1.059758000000 1.2048156000000</td> <td> 4.85813600000 2.44848000000 3.8783100000 6.44002100000 6.44002100000 6.4002100000 5.07428300000 4.0766400000 4.01507200000 6.62094000000 4.91507200000 6.62094000000 6.5087400000 0.5547500000 0.1664600000 0.1664600000 0.3693700000 3.5894700000 4.076161000000 1.62542800000 1.6399700000 1.6399700000 1.6355500000 1.6399700000 1.6393700000 1.6393700000 1.6399700000 1.6393700000 1.6393700000 1.6399700000 1.6393700000 1.6393700000 1.6393700000 1.6393700000 1.6393700000 1.55442800000 1.55442800000 1.529384000000 3.20062000000 </td> <td></td>	4.883747000000 2.507023000000 3.370051000000 7.25580600000 6.39745900000 1.97132700000 4.91522700000 3.51291600000 6.25025800000 2.91404000000 4.90526700000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.91404000000 2.4234000000 2.4234000000 2.0386600000 0.70744400000 0.14180900000 1.4151835000000 2.478786000000 1.597846000000 1.597846000000 1.58704900000 1.58704900000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 1.58744000000 3.69655000000 3.69655000000 3.69658000000 3.69658000000 3.890628000000	2 Si 3 Si 3 Si 5 Si 4 Si 5 Si 6 C 7 C 8 C 9 N 11 N 12 N 13 N 14 C 15 H 16 H 17 H 18 C 19 H 20 H 21 H 22 C 23 H 24 H 26 H 26 C 27 H 26 H 27 H 26 C 27 H 26 H 27 H 26 C 27 H 27 H	V)N * 2,NCG]** 10.12939000000 10.1239000000 7.899819000000 12.374722000000 12.374722000000 12.3747200000 12.5627100000 11.220797000000 7.576979000000 8.184567000000 9.531602000000 10.389414000000 10.389414000000 11.4754900000 10.389414000000 11.4754900000 10.56750800000 11.54816300000 11.54816300000 12.49374700000 12.77514200000 13.271643000000 7.4380700000 7.4380400000 7.4380400000 7.4380400000 7.438054200000 6.409634000000 7.7962165000000 6.572028000000 6.611842000000 6.61164000000	7.41517400000 9.65887500000 9.75489800000 9.35087400000 5.3607400000 5.35362600000 4.92748000000 6.03994400000 6.03174200000 6.026501000000 5.732048000000 1.540756000000 1.540756000000 1.540756000000 9.12161300000 9.42372400000 9.56901000001 9.35275000000 10.2682900000 10.56755000000 10.56755000000 10.5675000000 10.5675000000 10.56874000000 9.35275000000 10.56874000000 9.41219300000 11.272691000000 11.27485000000 12.048156000000 9.41219300000 1.059758000000 1.2048156000000	 4.85813600000 2.44848000000 3.8783100000 6.44002100000 6.44002100000 6.4002100000 5.07428300000 4.0766400000 4.01507200000 6.62094000000 4.91507200000 6.62094000000 6.5087400000 0.5547500000 0.1664600000 0.1664600000 0.3693700000 3.5894700000 4.076161000000 1.62542800000 1.6399700000 1.6399700000 1.6355500000 1.6399700000 1.6393700000 1.6393700000 1.6399700000 1.6393700000 1.6393700000 1.6399700000 1.6393700000 1.6393700000 1.6393700000 1.6393700000 1.6393700000 1.55442800000 1.55442800000 1.529384000000 3.20062000000 	

36 H	5.735429000000	8.897216000000	3.776096000000	36 H	5.616761000000	8.958020000000	3.857822000000	
37 H	6.815837000000	8.127469000000	4.942958000000	37 H	6.746153000000	8.155298000000	4.967082000000	
38 C	14.180391000000	8.523966000000	7.150696000000	38 C	14.261309000000	8.471087000000	7.222738000000	
39 H	14.690956000000	7.632656000000	7.548497000000	39 H	14.753942000000	7.608722000000	7,694941000000	
40 H	14 518570000000	9 393094000000	7 741487000000	40 H	14 569269000000	9 372548000000	7 776889000000	
41 H	14 519304000000	8 668474000000	6 112018000000	<u>л1 н</u>	14 643110000000	8 562641000000	6 19/977000000	
42.0	11 756527000000	8 21/771000000	9.050334000000	42.0	11 777951000000	8 225471000000	9.031385000000	
42 0	10 657027000000	8 164120000000	0.110992000000	42 0	10.679934000000	8 17070000000	9.051555000000	
4311	12.097217000000	0.100272000000	0.620420000000	4311	12 10152000000	0.11789000000	9.008034000000	
44 1	12.08/21/000000	9.100273000000	9.62042000000	44 1	12.101339000000	9.117889000000	9.590201000000	
45 H	12.174526000000	7.321838000000	9.538121000000	45 H	12.178428000000	7.342127000000	9.547007000000	
46 C	11.586487000000	10.039652000000	6.640731000000	46 C	11.73192000000	9.982403000000	6.528132000000	
47 H	11.877718000000	10.306283000000	5.614908000000	47 H	12.399876000000	10.389616000000	5.757196000000	
48 H	11.989661000000	10.823787000000	7.307347000000	48 H	11.718014000000	10.708814000000	7.357906000000	
49 H	10.489252000000	10.086034000000	6.719107000000	49 H	10.702846000000	9.982696000000	6.134531000000	
50 C	13.961485000000	5.280307000000	5.275187000000	50 C	14.040476000000	5.200830000000	5.350868000000	
51 H	13.668814000000	5.388484000000	4.218582000000	51 H	13.781200000000	5.342136000000	4.291064000000	
52 H	14.436816000000	4.291352000000	5.395031000000	52 H	14.483238000000	4.197943000000	5.460440000000	
53 H	14.714384000000	6.050404000000	5.505226000000	53 H	14.810024000000	5.940679000000	5.615543000000	
54 C	11.184180000000	4.104054000000	5.882347000000	54 C	11.252170000000	4.050674000000	5.919894000000	
55 H	10.280972000000	4.103329000000	6.511238000000	55 H	10.361211000000	4.052802000000	6.563504000000	
56 H	11.669759000000	3.117943000000	5.996019000000	56 H	11.733698000000	3.063739000000	6.017768000000	
57 H	10.864638000000	4.173723000000	4.830998000000	57 H	10.924268000000	4.149509000000	4.876240000000	
58 C	12.957259000000	5.008165000000	8.171102000000	58 C	12.983063000000	4.969110000000	8.228492000000	
59 H	13.727273000000	5.684086000000	8.574283000000	59 H	13.757675000000	5.636298000000	8.632024000000	
60 H	13.375223000000	3.985644000000	8.183449000000	60 H	13.384275000000	3.942745000000	8.261537000000	
61 H	12.093445000000	5.024263000000	8.854382000000	61 H	12.110656000000	5.006633000000	8.896714000000	
		5						