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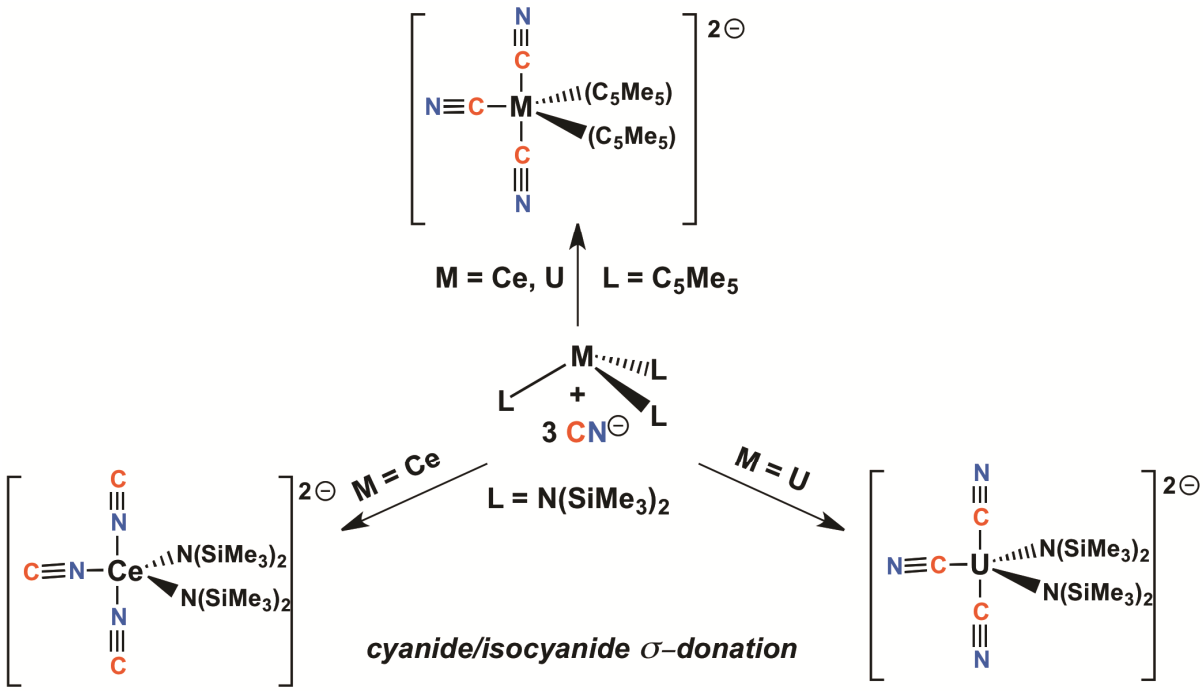
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Cyanide linkage isomerism in cerium(III) and uranium(III) complexes. A relativistic DFT study

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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, $N(SiMe_3)_2$; X = CN, NC), using relativistic DFT computations, focusing on cyanide (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

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

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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* = C_5Me_5) 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 $[(MN^*_3)_2(\mu\text{-}CN)]^-$ (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

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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 = C_5H_5) [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 6*d*/5*f* 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].

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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 = Ce^{3+}/U^{3+}; 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 = Ce^{3+}, $U^{3+/4+}$; q = 2, 1) (**1a**) and (**1b**) (complexes **6** and **5** in ref. 2b) , and their hypothetical isomers $[MCp^*_2(NC)_3]^{q-}$. The computed parameters for the isocyanide cerium(III) $[CeN^*_2(NC)_3]^{2-}$ (**2a**) and cyanide uranium(III) $[UN^*_2(CN)_3]^{2-}$ (**2b**) complexes (respectively

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

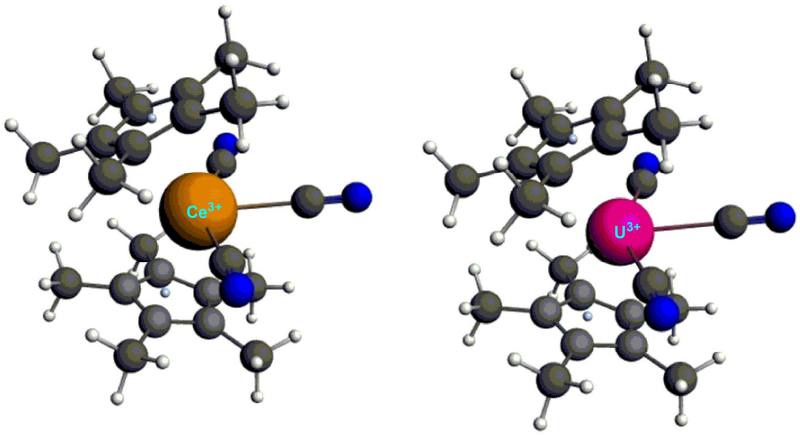


Fig. 1. ZORA/BP86/DZP optimized geometry of the bis(cyclopentadienyl) tris(cyanide) $[MCp^*_2X_3]^{2-}$ complexes (M = Ce^{3+}, U^{3+} ; X = CN) **1a** (left) and **1b** (right). The blue, black, and white spheres are nitrogen, carbon, and hydrogen atoms, respectively.

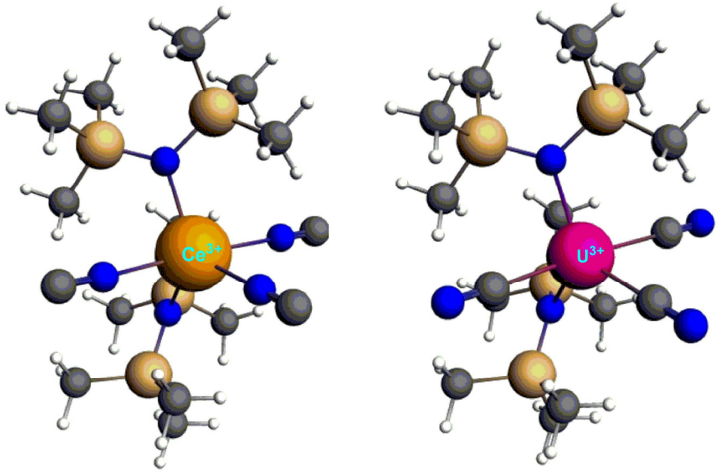


Fig. 2. ZORA/BP86/DZP optimized structures of the bis(silylamide) tris(cyanide/isocyanide) complexes $[MN^*_2X_3]^{2-}$ complexes (M = Ce^{3+}, U^{3+} ; X = CN, NC), **2a** (left) and **2b** (right). The orange, blue, black, and white spheres are silicon, nitrogen, carbon, and hydrogen atoms, respectively.

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

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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 = Ce^{3+}, U^{3+} and U^{4+}; X = CN/NC; L = Cp*/N*; q = 2, 1) in the gas phase and in solution (in italics).

Complex	<M–C/N>	Δ (Å)[a]	<C–N/N–C>	<M–L>
$[MCp^*_2X_3]^{q-}$				
Ce^{3+}	2.665/2.535		1.178/1.182	2.621/2.638
	2.655/2.546		*1.176/1.177*	*2.586/2.583*
	2.666/-		**1.158/ -**	**2.562/ -**
U^{3+}	2.612/2.492	0.053/0.043	1.178/1.183	2.571/2.560
	2.585/2.489	*0.070/0.057*	*1.177/1.180*	*2.509/2.534*
	2.640/ -		**1.156/ -**	**2.534/ -**
U^{4+}	2.501/2.389		1.175/1.185	2.482/2.507
	2.520/2.424		*1.176/1.180*	*2.476/2.493*
	2.520/ -		**1.158/ -**	**2.446 / -**
$[MN^*_2X_3]^{q-}$				
Ce^{3+}	2.666/2.511		1.176/1.183	2.413/2.427
	2.657/2.523		*1.175/1.179*	*2.379/2.387*
	- /2.580		**- /1.164**	**- /2.390**
U^{3+}	2.605/2.462	0.061/0.049	1.178/1.185	2.377/2.394/
	2.593/2.472	*0.064/0.051*	*1.176/1.181*	*2.348/2.358*
	2.600/ -		**1.148/ -**	**2.334/ -**
U^{4+}	2.512/2.374		1.175/1.186	2.239/2.253
	2.543/2.416		*1.175/1.182*	*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 metal-ligand 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

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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→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 $U^{III}(5f^3)$ 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 $[UN^*_3X_2]^{2-/1-}$ 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 = Ce^{3+}, U^{3+}; 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 Ce^{3+} and (+0.73/+1.03 for U^{3+}) which are consistent with the slightly stronger σ-donation of the cyanide ligand to the U(III) ion, since

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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 $[MCp^*_2X_3]^{2-}$ and $[MN^*_2X_3]^{2-}$ (M = Ce^{3+}, U^{3+}, X = CN/NC) complexes in the gas phase and in solution (in italics).

M–(CN/NC) Structure	NPA spin population		NPA net charge	
	ρ_M	q_M	<C–N>	<N–C>
		$[MCp^*_2X_3]^{2-}$		
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*
		$[MN^*_2X_3]^{2-}$		
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) MN_2* 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

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the MN_2* 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 MN_2* 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 UN_2* 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 = Ce^{3+}, U^{3+}; L = Cp*, N*; X = CN/NC) complexes in the gas phase and in solution (in italics).

Compound		M–(CN/NC) (Å)	Mayer bond order		NM bond index	
			<M–C/N>	<C–N/N–C>	<M–C/N>	<C–N/N–C>
$[MCp^*_2X_3]^{2-}$	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.

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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 = Ce^{3+} or U^{3+}; 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^1) 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.

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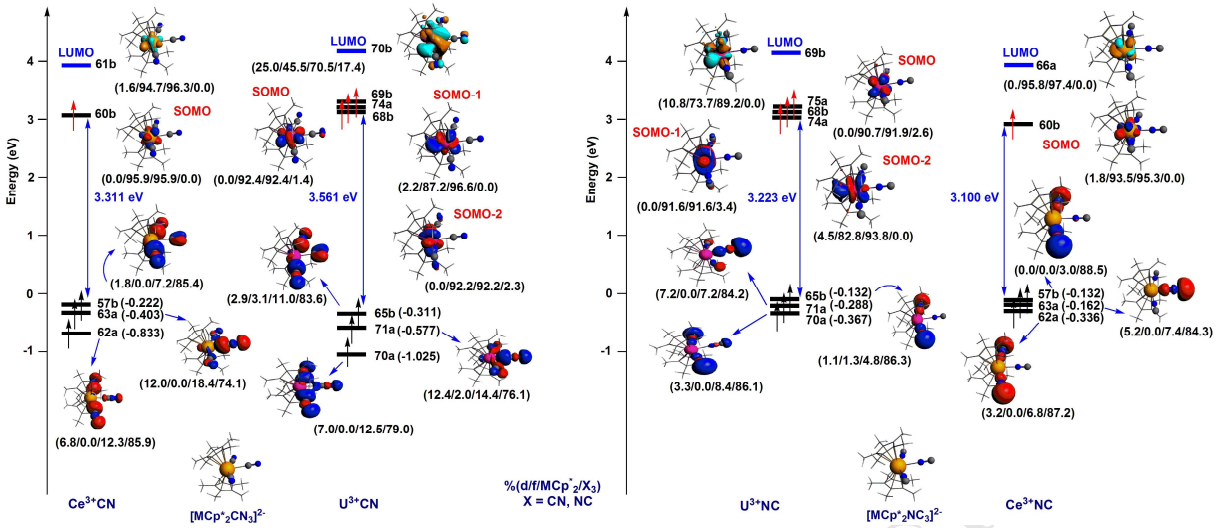


Fig. 3. ZORA/BP86/DZP α spin-MO diagram for M–CN (left) and M–NC (right) $[MCp^*_2X_3]^{2-}$ (X = CN/NC) complexes (C_2 symmetry). From the left to the right, the M *d*, M *f*, ML_2, and X_3 percentage contributions are given in brackets. Contour values are ±0.03 $(e/bohr^3)^{1/2}$.

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 $[MCp^*_2X_3]^{2-}$ 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 6*d*/5*f* U(III) orbitals and C-cyanide ones due to a better energy matching [11].

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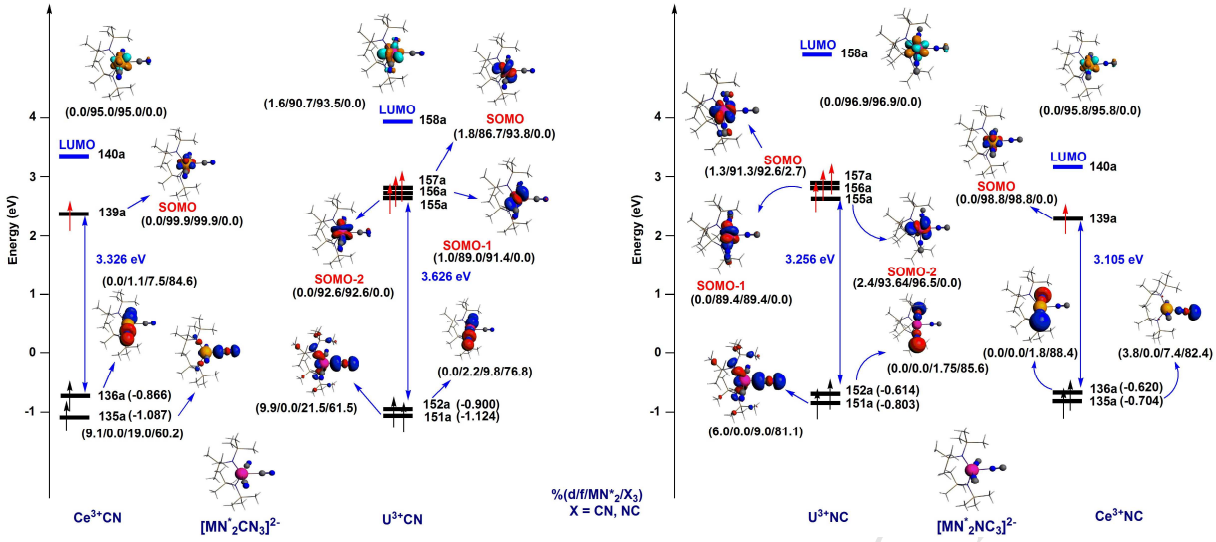


Fig. 4. ZORA/BP86/DZP α spin-MO diagram for M–CN (left) and M–NC (right) $[MN^*_2X_3]^{2-}$ (X = CN/NC) complexes (C_1 symmetry). From the left to the right, the M *d*, M *f*, ML_2, and X_3 percentage contributions are given in brackets. Contour values are ±0.03 $(e/bohr^3)^{1/2}$.

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

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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 = Ce^{3+} or U^{3+}; 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 = Ce^{3+} or U^{3+}; L = Cp* or N*; X = CN(left)/NC(right)) in the gas phase and in solution (in italics).

ion	E_{Pauli} (eV)	E_{elstat} (eV)	E_{st} (eV)	E_{orb} (eV)	E_{solvat} (eV)	TBE_{frag} (eV)	ΔE (kcal/mol)
	$[MCp^*_2X_3]^{2-}$						
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

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	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
	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*
			$[MN^*_2X_3]^{2-}$				
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
	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*
U^{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
	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

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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 = Ce^{3+}/U^{3+}; 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

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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*/*f* metallic 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 Δ*E*, 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].

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Appendix A. Computational details

All molecular geometries of the tris(cyanide) complexes $[ML_2X_3]^{2-}$ (M = Ce^{3+}/U^{3+}; 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^1) 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.*, ML_2 and X_3 (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 ($Cp^* = C_5Me_5$ and $N^* = N(SiMe_3)_2$) 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

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E_{Pauli}, the electronic repulsion due to the Pauli principle, and E_{elstat}, the stabilizing electrostatic energy between the two fragments $E_{steric} = E_{Pauli} + E_{elstat}$. 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

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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.

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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

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Cartesian coordinates of DFT optimized geometries.

$[MCp^*_2X_3]^q$ / q=2- ,1- /X=CN ,NC/ GAZ

$[Ce(III)Cp^*_2CN_3]^{2-}$

1 Ce	0.000000000000	0.000000000000	0.662157345200
2 N	0.000000000000	0.000000000000	4.473082654000
3 N	-0.603426950800	3.736948879000	1.406183130000
4 C	0.000000000000	0.000000000000	3.295433151000
5 C	-0.417392077300	2.585003675000	1.241293223000
6 C	2.047694898000	0.343201361900	-1.382503998000
7 C	2.130878989000	1.521198489000	-0.581825116900
8 C	2.628106787000	1.141088081000	0.701578806600
9 C	2.853257207000	-0.265610856700	0.690675451800
10 C	2.493862205000	-0.762946573500	-0.598896747200
11 C	1.763758775000	0.309156840900	-2.856446193000
12 H	2.680382217000	0.494954075400	-3.449472830000
13 H	1.030792118000	1.071770170000	-3.158556435000
14 H	1.369676232000	-0.665466803000	-3.178561441000
15 C	1.916794684000	2.926203279000	-1.065870868000
16 H	1.514268595000	3.573179139000	-0.274856437100
17 H	1.198637064000	2.965456791000	-1.898583752000
18 H	2.861825480000	3.371929563000	-1.433355235000
19 C	2.930879266000	2.072843034000	1.839840410000
20 H	2.782777209000	1.582003551000	2.812127215000
21 H	2.269486591000	2.949340862000	1.825595948000
22 H	3.977936681000	2.430004259000	1.800274464000
23 C	3.439587092000	-1.069484386000	1.815420425000
24 H	4.545724150000	-1.073911782000	1.771362271000
25 H	3.091512981000	-2.110833485000	1.787791054000
26 H	3.147052070000	-0.665089863100	2.794494635000
27 C	2.720429876000	-2.159634770000	-1.100494159000
28 H	2.020262807000	-2.423856496000	-1.907678999000
29 H	2.575483748000	-2.904209797000	-0.306837864500
30 H	3.743248668000	-2.278947694000	-1.508034534000
31 N	0.603426950800	-3.736948879000	1.406183130000
32 C	0.417392077300	-2.585003675000	1.241293223000
33 C	-2.047694898000	-0.343201361900	-1.382503998000
34 C	-2.130878989000	-1.521198489000	-0.581825116900
35 C	-2.628106787000	-1.141088081000	0.701578806600
36 C	-2.853257207000	0.265610856700	0.690675451800
37 C	-2.493862205000	0.762946573500	-0.598896747200
38 C	-1.763758775000	-0.309156840900	-2.856446193000
39 H	-2.680382217000	-0.494954075400	-3.449472830000
40 H	-1.030792118000	-1.071770170000	-3.158556435000
41 H	-1.369676232000	0.665466803000	-3.178561441000
42 C	-1.916794684000	-2.926203279000	-1.065870868000
43 H	-1.514268595000	-3.573179139000	-0.274856437100
44 H	-1.198637064000	-2.965456791000	-1.898583752000
45 H	-2.861825480000	-3.371929563000	-1.433355235000
46 C	-2.930879266000	-2.072843034000	1.839840410000
47 H	-2.782777209000	-1.582003551000	2.812127215000
48 H	-2.269486591000	-2.949340862000	1.825595948000
49 H	-3.977936681000	-2.430004259000	1.800274464000
50 C	-3.439587092000	1.069484386000	1.815420425000
51 H	-4.545724150000	1.073911782000	1.771362271000
52 H	-3.091512981000	2.110833485000	1.787791054000
53 H	-3.147052070000	0.665089863100	2.794494635000
54 C	-2.720429876000	2.159634770000	-1.100494159000
55 H	-2.020262807000	2.423856496000	-1.907678999000
56 H	-2.575483748000	2.904209797000	-0.306837864500
57 H	-3.743248668000	2.278947694000	-1.508034534000

$[Ce(III)Cp^*_2NC_3]^{2-}$

1 Ce	0.000000000000	0.000000000000	0.768988710600
2 C	0.000000000000	0.000000000000	4.446721466000
3 C	-0.369424745800	3.662852699000	1.420315226000
4 N	0.000000000000	0.000000000000	3.264089134000
5 N	-0.253396091900	2.503149597000	1.223800742000
6 C	2.039385842000	0.200771171200	-1.376836986000
7 C	2.187950419000	1.379417240000	-0.590108161000
8 C	2.669558318000	0.987747457600	0.695479695500
9 C	2.817518516000	-0.430856334500	0.698246513500
10 C	2.430028796000	-0.918002202200	-0.586246219300
11 C	1.754127382000	0.169934613600	-2.849472099000
12 H	2.684186600000	0.271383501500	-3.441961765000
13 H	1.088167717000	0.987568192300	-3.159991866000
14 H	1.279571213000	-0.771541507400	-3.160577215000
15 C	2.046311331000	2.788255056000	-1.085146770000
16 H	1.695030545000	3.462182308000	-0.292950408300
17 H	1.316559507000	2.860820959000	-1.905139388000
18 H	3.008713897000	3.177968823000	-1.470937402000
19 C	3.046120978000	1.915449612000	1.814296221000
20 H	2.919127271000	1.436812229000	2.795402331000
21 H	2.416256343000	2.815095989000	1.817348475000
22 H	4.102987391000	2.234978837000	1.734084785000
23 C	3.375816230000	1.258270554000	1.820024837000
24 H	4.478192557000	1.335862379000	1.754326657000
25 H	2.961021238000	2.275037557000	1.810327466000
26 H	3.132332912000	0.827100924000	2.801233902000
27 C	2.585843711000	-2.327725755000	-1.074191927000
28 H	1.913818845000	-2.543422017000	-1.917979387000
29 H	2.348655216000	-3.057660065000	-0.288874733400
30 H	3.618698961000	-2.518689391000	-1.424370678000
31 C	0.369424745800	-3.662852699000	1.420315226000
32 N	0.253396091900	-2.503149597000	1.223800742000
33 C	-2.039385842000	-0.200771171200	-1.376836986000
34 C	-2.187950419000	-1.379417240000	-0.590108161000
35 C	-2.669558318000	-0.987747457600	0.695479695500
36 C	-2.817518516000	0.430856334500	0.698246513500
37 C	-2.430028796000	0.918002202200	-0.586246219300
38 C	-1.754127382000	-0.169934613600	-2.849472099000
39 H	-2.684186600000	-0.271383501500	-3.441961765000
40 H	-1.088167717000	-0.987568192300	-3.159991866000
41 H	-1.279571213000	0.771541507400	-3.160577215000
42 C	-2.046311331000	-2.788255056000	-1.085146770000
43 H	-1.695030545000	-3.462182308000	-0.292950408300
44 H	-1.316559507000	-2.860820959000	-1.905139388000
45 H	-3.008713897000	-3.177968823000	-1.470937402000
46 C	-3.046120978000	-1.915449612000	1.814296221000
47 H	-2.919127271000	-1.436812229000	2.795402331000
48 H	-2.416256343000	-2.815095989000	1.817348475000
49 H	-4.102987391000	-2.234978837000	1.734084785000
50 C	-3.375816230000	1.258270554000	1.820024837000
51 H	-4.478192557000	1.335862379000	1.754326657000
52 H	-2.961021238000	2.275037557000	1.810327466000
53 H	-3.132332912000	0.827100924000	2.801233902000
54 C	-2.585843711000	2.327725755000	-1.074191927000
55 H	-1.913818845000	2.543422017000	-1.917979387000
56 H	-2.348655216000	3.057660065000	-0.288874733400
57 H	-3.618698961000	2.518689391000	-1.424370678000

$[U(III)Cp^*_2CN_3]^{2-}$

1 U	0.000000000000	0.000000000000	0.693105122500
2 N	0.000000000000	0.000000000000	4.456691964000
3 N	-0.397896091000	3.690327760000	1.515900192000
4 C	0.000000000000	0.000000000000	3.278936557000
5 C	-0.254902033200	2.536504041000	1.323045130000
6 C	2.368842994000	-0.921176233800	-0.605739074300
7 C	1.976424121000	0.212236714200	-1.381308185000
8 C	2.148022431000	1.379076393000	-0.576063082800

$[U(III)Cp^*_2NC_3]^{2-}$

1 U	0.000000000000	0.000000000000	0.664625353000
2 C	0.000000000000	0.000000000000	4.319730655000
3 C	-0.387448409300	3.590307312000	1.404297020000
4 N	0.000000000000	0.000000000000	3.137208501000
5 N	-0.280052445400	2.439791998000	1.149287192000
6 C	2.369944770000	-0.891760090600	-0.606668924500
7 C	1.980304733000	0.258166036900	-1.361038308000
8 C	2.164071410000	1.409075622000	-0.534932961900

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9 C	2.646523899000	0.965499386700	0.696375330900
10 C	2.783486533000	-0.452699697700	0.678056838400
11 C	2.493121756000	-2.327449838000	-1.116241867000
12 H	1.756929473000	-2.537286360000	-1.906811341000
13 H	2.318651656000	-3.064254534000	-0.320989344100
14 H	3.496228466000	-2.512212720000	-1.548513178000
15 C	1.727054677000	0.210613090100	-2.860127156000
16 H	1.079352277000	1.042645681000	-3.170092250000
17 H	1.247166951000	-0.718308643000	-3.199123445000
18 H	2.674238336000	0.310463056600	-3.428608545000
19 C	2.003768574000	2.795448616000	-1.050808283000
20 H	2.936306663000	3.158107351000	-1.526229732000
21 H	1.749241946000	3.473785938000	-0.226398547800
22 H	1.199337394000	2.895438300000	-1.795439488000
23 C	3.039607845000	1.867050548000	1.830940262000
24 H	2.890782213000	1.376174611000	2.802861891000
25 H	2.433863666000	2.782933925000	1.843928191000
26 H	4.105523584000	2.158486432000	1.762000830000
27 C	3.351280454000	-1.290282041000	1.787255845000
28 H	4.457413109000	-1.313605179000	1.745736130000
29 H	2.983213090000	-2.322979698000	1.737479598000
30 H	3.063722520000	-0.901022300500	2.774549461000
31 N	0.397896091000	-3.690327760000	1.515900192000
32 C	0.254902033200	-2.536504041000	1.323045130000
33 C	-2.368842994000	0.921176233800	-0.605739074300
34 C	-1.976424121000	-0.212236714200	-1.381308185000
35 C	-2.148022431000	-1.379076393000	-0.576063082800
36 C	-2.646523899000	-0.965499386700	0.696375330900
37 C	-2.783486533000	0.452699697700	0.678056838400
38 C	-2.493121756000	2.327449838000	-1.116241867000
39 H	-1.756929473000	2.537286360000	-1.906811341000
40 H	-2.318651656000	3.064254534000	-0.320989344100
41 H	-3.496228466000	2.512212720000	-1.548513178000
42 C	-1.727054677000	-0.210613090100	-2.860127156000
43 H	-1.079352277000	-1.042645681000	-3.170092250000
44 H	-1.247166951000	0.718308643000	-3.199123445000
45 H	-2.674238336000	-0.310463056600	-3.428608545000
46 C	-2.003768574000	-2.795448616000	-1.050808283000
47 H	-2.936306663000	-3.158107351000	-1.526229732000
48 H	-1.749241946000	-3.473785938000	-0.226398547800
49 H	-1.199337394000	-2.895438300000	-1.795439488000
50 C	-3.039607845000	-1.867050548000	1.830940262000
51 H	-2.890782213000	-1.376174611000	2.802861891000
52 H	-2.433863666000	-2.782933925000	1.843928191000
53 H	-4.105523584000	-2.158486432000	1.762000830000
54 C	-3.351280454000	1.290282041000	1.787255845000
55 H	-4.457413109000	1.313605179000	1.745736130000
56 H	-2.983213090000	2.322979698000	1.737479598000
57 H	-3.063722520000	0.901022300500	2.774549461000

9 C	2.651100472000	0.971260239100	0.731526509300
10 C	2.783244111000	-0.448290372900	0.687293182600
11 C	2.512063446000	-2.282511665000	-1.151083997000
12 H	1.772090349000	-2.487573038000	-1.939912690000
13 H	2.356988820000	-3.038797109000	-0.370709183000
14 H	3.514094643000	-2.441693440000	-1.596054335000
15 C	1.737864494000	0.285648155000	-2.841716736000
16 H	1.100223011000	1.130819928000	-3.138835065000
17 H	1.249391645000	-0.631489810800	-3.199481124000
18 H	2.687728868000	0.386424910100	-3.405919230000
19 C	2.036996262000	2.832018480000	-0.991524179400
20 H	2.961560847000	3.173712719000	-1.496276135000
21 H	1.829416700000	3.508129872000	-0.152701927000
22 H	1.208775025000	2.961707716000	-1.704665955000
23 C	3.029797979000	1.856227814000	1.883017532000
24 H	2.910141544000	1.335949993000	2.843519408000
25 H	2.392715090000	2.749966842000	1.924544408000
26 H	4.083743004000	2.187142527000	1.809446979000
27 C	3.346869970000	-1.310371413000	1.779111497000
28 H	4.448766930000	-1.387721653000	1.701942406000
29 H	2.927882378000	-2.324668596000	1.743591448000
30 H	3.110855741000	-0.905355151300	2.773161912000
31 C	0.387448409300	-3.590307312000	1.404297020000
32 N	0.280052445400	-2.439791998000	1.149287192000
33 C	-2.369944770000	0.891760090600	0.606668924500
34 C	-1.980304733000	-0.258166036900	-1.361038308000
35 C	-2.164071410000	-1.409075622000	-0.534932961900
36 C	-2.651100472000	-0.971260239100	0.731526509300
37 C	-2.783244111000	0.448290372900	0.687293182600
38 C	-2.512063446000	2.282511665000	-1.151083997000
39 H	-1.772090349000	2.487573038000	-1.939912690000
40 H	-2.356988820000	3.038797109000	-0.370709183000
41 H	-3.514094643000	2.441693440000	-1.596054335000
42 C	-1.737864494000	-0.285648155000	-2.841716736000
43 H	-1.100223011000	-1.130819928000	-3.138835065000
44 H	-1.249391645000	0.631489810800	-3.199481124000
45 H	-2.687728868000	-0.386424910100	-3.405919230000
46 C	-2.036996262000	-2.832018480000	-0.991524179400
47 H	-2.961560847000	-3.173712719000	-1.496276135000
48 H	-1.829416700000	-3.508129872000	-0.152701927000
49 H	-1.208775025000	-2.961707716000	-1.704665955000
50 C	-3.029797979000	-1.856227814000	1.883017532000
51 H	-2.910141544000	-1.335949993000	2.843519408000
52 H	-2.392715090000	-2.749966842000	1.924544408000
53 H	-4.083743004000	-2.187142527000	1.809446979000
54 C	-3.346869970000	1.310371413000	1.779111497000
55 H	-4.448766930000	1.387721653000	1.701942406000
56 H	-2.927882378000	2.324668596000	1.743591448000
57 H	-3.110855741000	0.905355151300	2.773161912000

$[U(IV)Cp^*_2CN_3]^{1-}$

1 U	0.000000000000	0.000000000000	0.498247659300
2 N	-0.006121805906	-3.596980631000	1.269106245000
3 N	0.000000000000	0.000000000000	4.171972244000
4 N	0.006121805906	3.596980631000	1.269106245000
5 C	-0.009639042411	-2.439685628000	1.059658680000
6 C	0.000000000000	0.000000000000	2.997217064000
7 C	0.009639042411	2.439685628000	1.059658680000
8 C	-2.667769700000	0.712457745500	0.745934941600
9 C	-2.668050356000	-0.714247608400	0.730830216300
10 C	-2.275947090000	-1.143844297000	-0.573170776300
11 C	-2.019662334000	0.021287448080	-1.361539616000
12 C	-2.276253382000	1.169769389000	-0.548906811300
13 C	-3.109315756000	1.567249268000	1.896421385000
14 H	-4.207119027000	1.682650979000	1.890345956000
15 H	-2.658040153000	2.565864142000	1.855182271000
16 H	-2.826465783000	1.124382182000	2.860664679000
17 C	-3.110530665000	-1.592779751000	1.862876005000
18 H	-2.817501567000	-1.176304580000	2.835698150000
19 H	-2.669213834000	-2.594263470000	1.794874757000
20 H	-4.209326609000	-1.697590965000	1.861140125000
21 C	-2.324782642000	-2.547916531000	-1.097389569000

$[U(IV)Cp^*_2NC_3]^{1-}$

1 U	0.000000000000	0.000000000000	0.530890778500
2 C	0.012301319410	-3.545588480000	1.061853406000
3 C	0.000000000000	0.000000000000	4.081818081000
4 C	-0.012301319410	3.545588480000	1.061853406000
5 N	0.003140854492	-2.383955272000	0.828748276200
6 N	0.000000000000	0.000000000000	2.896467294000
7 N	-0.003140854492	2.383955272000	0.828748276200
8 C	-2.657116844000	0.719974661500	0.770092334400
9 C	-2.658319790000	-0.708038772100	0.777365803700
10 C	-2.316890683000	-1.154846233000	-0.537087348300
11 C	-2.077947405000	-0.005562485418	-1.347685065000
12 C	-2.314772174000	1.152357206000	-0.549290486600
13 C	-3.077674098000	1.600039448000	1.908817966000
14 H	-4.171481773000	1.749516208000	1.901360640000
15 H	-2.596923398000	2.584762020000	1.856004983000
16 H	-2.807602339000	1.160744176000	2.877877024000
17 C	-3.080251472000	-1.576936010000	1.923845886000
18 H	-2.846473903000	-1.109629338000	2.889053509000
19 H	-2.570447974000	-2.548297252000	1.902850304000
20 H	-4.168670305000	-1.758999353000	1.893938093000
21 C	-2.407735286000	-2.559213812000	-1.050313443000

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22 H	-3.296189704000	-2.737472924000	-1.587310447000
23 H	-2.188837746000	-3.285727271000	-0.298752673300
24 H	-1.541846946000	-2.739980285000	-1.844823252000
25 C	-1.795823978000	0.038190528340	-2.845315079000
26 H	-1.246112610000	-0.847171464300	-3.192166812000
27 H	-1.236040911000	0.925774336600	-3.170476317000
28 H	-2.759127166000	0.050792277940	-3.386303545000
29 C	-2.332184466000	2.583892064000	-1.044242142000
30 H	-1.545072981000	2.799171998000	-1.780269176000
31 H	-2.208236675000	3.305334660000	-0.228740314500
32 H	-3.301726522000	2.775655072000	-1.537050363000
33 C	2.667769700000	-0.712457745500	0.745934941600
34 C	2.276253382000	-1.169769389000	-0.548906811300
35 C	2.019662334000	-0.021287448080	-1.361539616000
36 C	2.275947090000	1.143844297000	-0.573170776300
37 C	2.668050356000	0.714247608400	0.730830216300
38 C	3.109315756000	-1.567249268000	1.896421385000
39 H	4.207119027000	-1.682650979000	1.890345956000
40 H	2.658040153000	-2.565864142000	1.855182271000
41 H	2.826465783000	-1.124382182000	2.860664679000
42 C	2.332184466000	-2.583892064000	-1.044242142000
43 H	3.301726522000	-2.775655072000	-1.537050363000
44 H	1.545072981000	-2.799171998000	-1.780269176000
45 H	2.208236675000	-3.305334660000	-0.228740314500
46 C	1.795823978000	-0.038190528340	-2.845315079000
47 H	2.759127166000	-0.050792277940	-3.386303545000
48 H	1.246112610000	0.847171464300	-3.192166812000
49 H	1.236040911000	-0.925774336600	-3.170476317000
50 C	2.324782642000	2.547916531000	-1.097389569000
51 H	3.296189704000	2.737472924000	-1.587310447000
52 H	2.188837746000	3.285727271000	-0.298752673300
53 H	1.541846946000	2.739980285000	-1.844823252000
54 C	3.110530665000	1.592779751000	1.862876005000
55 H	2.817501567000	1.176304580000	2.835698150000
56 H	2.669213834000	2.594263470000	1.794874757000
57 H	4.209326609000	1.697590965000	1.861140125000

22 H	-3.366636630000	-2.704123019000	-1.578714393000
23 H	-2.346689957000	-3.293110021000	-0.239695619500
24 H	-1.602857477000	-2.800192006000	-1.758591963000
25 C	-1.853483917000	-0.013989423750	-2.830915273000
26 H	-1.290312087000	-0.898607150200	-3.158042188000
27 H	-1.304583077000	0.875102772200	-3.169780338000
28 H	-2.814059476000	-0.025472879730	-3.377141667000
29 C	-2.398653819000	2.551669350000	-1.077650250000
30 H	-1.589873781000	2.782296804000	-1.784893325000
31 H	-2.338065400000	3.294014941000	-0.274711533100
32 H	-3.354547996000	2.694731973000	-1.611881410000
33 C	2.657116844000	-0.719974661500	0.770092334400
34 C	2.314772174000	-1.152357206000	-0.549290486600
35 C	2.077947405000	0.005562485418	-1.347685065000
36 C	2.316890683000	1.154846233000	-0.537087348300
37 C	2.658319790000	0.708038772100	0.777365803700
38 C	3.077674098000	-1.600039448000	1.908817966000
39 H	4.171481773000	-1.749516208000	1.901360640000
40 H	2.596923398000	-2.584762020000	1.856004983000
41 H	2.807602339000	-1.160744176000	2.877877024000
42 C	2.398653819000	-2.551669350000	-1.077650250000
43 H	3.354547996000	-2.694731973000	-1.611881410000
44 H	1.589873781000	-2.782296804000	-1.784893325000
45 H	2.338065400000	-3.294014941000	-0.274711533100
46 C	1.853483917000	0.013989423750	-2.830915273000
47 H	2.814059476000	0.025472879730	-3.377141667000
48 H	1.290312087000	0.898607150200	-3.158042188000
49 H	1.304583077000	-0.875102772200	-3.169780338000
50 C	2.407735286000	2.559213812000	-1.050313443000
51 H	3.366636630000	2.704123019000	-1.578714393000
52 H	2.346689957000	3.293110021000	-0.239695619500
53 H	1.602857477000	2.800192006000	-1.758591963000
54 C	3.080251472000	1.576936010000	1.923845886000
55 H	2.846473903000	1.109629338000	2.889053509000
56 H	2.570447974000	2.548297252000	1.902850304000
57 H	4.168670305000	1.758999353000	1.893938093000

$[MN^*_2X_3]^q$ /q=2- ,1- /X=CN ,NC /GAZ

$[Ce(III)N^*_2CN_3]^{2-}$

1 Ce	13.490106620000	22.521990030000	0.130086868600
2 Si	16.183970060000	24.031669560000	1.867627026000
3 Si	16.000453060000	24.858052630000	-1.036970627000
4 Si	11.569644710000	20.979705460000	-2.409344487000
5 Si	14.431817110000	20.009631850000	-2.320757126000
6 C	14.608299590000	20.486856770000	1.490309387000
7 C	11.685862530000	22.601184380000	2.024665652000
8 C	12.180530040000	24.589817230000	-0.990801766500
9 N	15.442192240000	23.927297210000	0.307092500100
10 N	13.166854510000	21.035876060000	-1.744084474000
11 N	15.120157300000	19.575999270000	2.031710109000
12 N	10.870267570000	22.629245990000	2.871789423000
13 N	11.654547110000	25.505325190000	-1.510362883000
14 C	14.968927980000	23.564149590000	3.242300904000
15 H	14.075454980000	24.205785870000	3.257827189000
16 H	15.473633220000	23.672297340000	4.217356126000
17 H	14.632029430000	22.518055830000	3.176960965000
18 C	16.799336890000	25.784694750000	2.334174613000
19 H	17.575395600000	26.163449470000	1.652083936000
20 H	17.229854790000	25.762303000000	3.349581831000
21 H	15.969138580000	26.506817850000	2.336243794000
22 C	17.692250120000	22.887038500000	2.048232925000
23 H	17.377856760000	21.838449770000	1.935614470000
24 H	18.159969350000	22.997066110000	3.040931610000
25 H	18.454768920000	23.100921560000	1.284058291000
26 C	15.568923480000	26.707623750000	-0.922181641900
27 H	14.476536370000	26.822435220000	-0.853927899600
28 H	15.911769390000	27.245173160000	-1.822140483000
29 H	16.023880640000	27.188378010000	-0.044317531080
30 C	17.898015150000	24.760233380000	-1.279242689000
31 H	18.449094280000	25.156375750000	-0.412481745200
32 H	18.205144820000	25.341487160000	-2.164931301000

$[Ce(III)N^*_2NC_3]^{2-}$

1 Ce	13.466098780000	22.519003230000	0.156744398900
2 Si	16.202908360000	24.024249040000	1.862358691000
3 Si	15.997065980000	24.865717960000	-1.024682780000
4 Si	11.553493270000	20.974560370000	-2.412704224000
5 Si	14.409736670000	20.007919270000	-2.300370781000
6 N	14.524235740000	20.592630810000	1.420146387000
7 N	11.746333320000	22.631010720000	1.920673239000
8 N	12.289375080000	24.459234590000	-0.970115351800
9 N	15.445746030000	23.919774630000	0.311563038000
10 N	13.140988870000	21.030997440000	-1.729664804000
11 C	14.958356150000	19.654137750000	1.994709667000
12 C	10.921811340000	22.684377160000	2.767911719000
13 C	11.751158850000	25.400367520000	-1.443529654000
14 C	15.018705030000	23.525188870000	3.253836382000
15 H	14.108578690000	24.142866800000	3.278353814000
16 H	15.532077720000	23.652253430000	4.222054591000
17 H	14.710751330000	22.470967180000	3.191098854000
18 C	16.792925900000	25.783871150000	2.341035436000
19 H	17.547954600000	26.188210970000	1.650208060000
20 H	17.241844080000	25.758531200000	3.348446402000
21 H	15.947557770000	26.487979150000	2.366539423000
22 C	17.735930820000	22.906155160000	2.017799619000
23 H	17.443309590000	21.854857540000	1.877097928000
24 H	18.201022110000	22.999565750000	3.013428973000
25 H	18.494340460000	23.154423600000	1.260103933000
26 C	15.513286660000	26.703524490000	-0.912934310300
27 H	14.417308250000	26.790587680000	-0.859569545900
28 H	15.855975610000	27.254388950000	-1.805026826000
29 H	15.943039300000	27.191018610000	-0.025534835790
30 C	17.901455220000	24.827309250000	-1.242809859000
31 H	18.434450870000	25.239416950000	-0.372316266100
32 H	18.196908810000	25.418768620000	-2.126000465000

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33	H	18.219074290000	23.717954720000	-1.429129147000
34	C	15.251289010000	24.281973060000	-2.681458937000
35	H	15.443209750000	23.223961320000	-2.904976551000
36	H	15.691449430000	24.877996950000	-3.498520421000
37	H	14.164089590000	24.446437410000	-2.702862778000
38	C	10.980229670000	19.227371550000	-2.910378424000
39	H	11.603087170000	18.772497470000	-3.695238988000
40	H	9.948231816000	19.285955500000	-3.295703389000
41	H	10.978096200000	18.548577370000	-2.044403772000
42	C	11.380122100000	22.056429070000	-3.966069510000
43	H	11.568247570000	23.110722810000	-3.712900569000
44	H	10.360610780000	21.983652150000	-4.380267658000
45	H	12.091361990000	21.759734290000	-4.751553127000
46	C	10.280286310000	21.585665330000	-1.162540074000
47	H	10.274730200000	20.998053400000	-0.232573943400
48	H	9.278347138000	21.498952650000	-1.616228020000
49	H	10.411692990000	22.644717150000	-0.891713034300
50	C	14.579848920000	20.001362430000	-4.230931745000
51	H	13.668076340000	19.623558200000	-4.718578077000
52	H	15.419373820000	19.360957240000	-4.550053266000
53	H	14.764213880000	21.017315990000	-4.612512126000
54	C	14.243487960000	18.191602660000	-1.791657411000
55	H	14.230596640000	18.131635670000	-0.692832765500
56	H	15.092898840000	17.589368350000	-2.155180181000
57	H	13.317118320000	17.739883880000	-2.174374335000
58	C	16.140837760000	20.532277690000	-1.686343719000
59	H	16.415280920000	21.558511860000	-1.965910813000
60	H	16.899544910000	19.857423320000	-2.117169797000
61	H	16.205180490000	20.443959840000	-0.592038388900

33	H	18.255316770000	23.795447110000	-1.392609522000
34	C	15.307324020000	24.270609030000	-2.688530971000
35	H	15.586655690000	23.235182310000	-2.927748454000
36	H	15.709507300000	24.915739200000	-3.487993117000
37	H	14.211202090000	24.348730390000	-2.719686415000
38	C	10.970202050000	19.220150180000	-2.917387932000
39	H	11.603555590000	18.763613280000	-3.692962506000
40	H	9.943170421000	19.276427640000	-3.316280682000
41	H	10.957942490000	18.543380920000	-2.049731922000
42	C	11.375593310000	22.044936090000	-3.976063569000
43	H	11.570123310000	23.099069150000	-3.727570095000
44	H	10.357226700000	21.975816070000	-4.393693540000
45	H	12.088069450000	21.740050180000	-4.757274189000
46	C	10.245259660000	21.579576030000	-1.183834044000
47	H	10.235996410000	20.994015890000	-0.252533786800
48	H	9.248533407000	21.483904120000	-1.647089275000
49	H	10.371795790000	22.638806240000	-0.914561003600
50	C	14.570017850000	20.003926100000	-4.210492384000
51	H	13.665574120000	19.618818320000	-4.706088416000
52	H	15.418016520000	19.372364380000	-4.524793764000
53	H	14.747775610000	21.022748950000	-4.587833060000
54	C	14.222260100000	18.185171360000	-1.781308826000
55	H	14.203222490000	18.117780970000	-0.683015324000
56	H	15.074038610000	17.585940270000	-2.144626239000
57	H	13.297954170000	17.734544500000	-2.170831618000
58	C	16.117992670000	20.525028540000	-1.659497078000
59	H	16.393378620000	21.552855750000	-1.932562829000
60	H	16.876538500000	19.851873880000	-2.093538856000
61	H	16.178334010000	20.433524310000	-0.565709433600

$[U(III)N^*_2CN_3]^{2-}$

1	U	9.870916846000	7.217636646000	4.891487284000
2	Si	10.886976370000	9.675800247000	2.439903953000
3	Si	7.988545376000	9.718245472000	3.321013915000
4	Si	12.295229180000	8.288082051000	7.336557932000
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
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	0.041793893470
20	H	9.837230063000	9.467069318000	0.143111957300
21	H	10.787204090000	8.020548999000	0.580820469800
22	C	12.604479730000	9.110591153000	3.011435499000
23	H	12.834938190000	9.401007398000	4.045092749000
24	H	13.363847550000	9.573027928000	2.357606895000
25	H	12.711945460000	8.019806302000	2.929423796000
26	C	7.459677648000	10.211000840000	1.546099335000
27	H	8.088094371000	11.001224450000	1.108993647000
28	H	6.421718659000	10.584043570000	1.569014770000
29	H	7.488766898000	9.342360429000	0.871043788200
30	C	7.751521257000	11.273796890000	4.388446754000
31	H	7.902729238000	11.020432290000	5.448600948000
32	H	6.732263481000	11.680013630000	4.276882442000
33	H	8.467178778000	12.064719930000	4.117992211000
34	C	6.683532848000	8.463154380000	3.868964124000
35	H	6.667800543000	7.565398086000	3.234337637000
36	H	5.688889096000	8.938415864000	3.807476946000
37	H	6.811763174000	8.133020203000	4.911316078000
38	C	14.203063480000	8.455312279000	7.369952233000
39	H	14.699210880000	7.555074008000	7.763452891000
40	H	14.500225830000	9.306346244000	8.005799677000
41	H	14.595098960000	8.636278250000	6.357322464000

$[U(III)N^*_2NC_3]^{2-}$

1	U	9.861076137000	7.194637680000	4.882952268000
2	Si	10.864918380000	9.655939107000	2.443029080000
3	Si	7.978844037000	9.768608085000	3.332980513000
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
10	N	11.744628510000	6.948854107000	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	11.567895490000	2.422744965000
15	H	11.156651270000	11.956905990000	3.440115077000
16	H	10.091886100000	12.050094150000	2.020099364000
17	H	11.849776850000	11.883973380000	1.799798166000
18	C	10.731178910000	9.105100283000	0.627476298600
19	H	11.588717570000	9.475518206000	0.040996553100
20	H	9.809261594000	9.467837647000	0.150672302400
21	H	10.736465750000	8.005469083000	0.580779930500
22	C	12.573775630000	9.067089666000	3.018001768000
23	H	12.833968700000	9.422425732000	4.024390106000
24	H	13.332435780000	9.458974327000	2.318540294000
25	H	12.648557680000	7.970463954000	3.008290122000
26	C	7.464558171000	10.300177420000	1.563997034000
27	H	8.124132922000	11.067177560000	1.130865838000
28	H	6.443191157000	10.716180060000	1.594054513000
29	H	7.455437998000	9.437073710000	0.881339882300
30	C	7.792885756000	11.322395350000	4.415217856000
31	H	7.954747913000	11.058448350000	5.471198736000
32	H	6.782446512000	11.754781610000	4.322690981000
33	H	8.524109404000	12.096916430000	4.138699513000
34	C	6.629610730000	8.554156659000	3.867919867000
35	H	6.620480341000	7.642910714000	3.251964685000
36	H	5.646112249000	9.045055988000	3.762963436000
37	H	6.728712541000	8.248109647000	4.919570303000
38	C	14.185111000000	8.457786813000	7.358781077000
39	H	14.697552100000	7.569944219000	7.759323255000
40	H	14.470877870000	9.320141099000	7.984616152000
41	H	14.569604120000	8.635111627000	6.342296132000

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42 C	11.730087100000	8.109861088000	9.142685905000
43 H	10.629975370000	8.097805299000	9.176936668000
44 H	12.080644930000	8.963059384000	9.747364409000
45 H	12.102386610000	7.185991631000	9.607952370000
46 C	11.666583820000	9.990972253000	6.788619355000
47 H	11.985872460000	10.264256750000	5.773807291000
48 H	12.066566770000	10.751499210000	7.481842846000
49 H	10.569376230000	10.047410030000	6.832634028000
50 C	14.040656520000	5.259492296000	5.351150797000
51 H	13.784575530000	5.409747127000	4.291495301000
52 H	14.495735350000	4.260133720000	5.453770778000
53 H	14.794250500000	6.010076109000	5.632948414000
54 C	11.284397900000	4.049962053000	5.840519942000
55 H	10.369249940000	4.000760918000	6.447714374000
56 H	11.799891820000	3.077228923000	5.923667585000
57 H	10.984852720000	4.160700527000	4.787449155000
58 C	12.975412080000	4.883225869000	8.183296729000
59 H	13.729651270000	5.544251612000	8.635268194000
60 H	13.400656620000	3.865824202000	8.149162926000
61 H	12.101713060000	4.858955106000	8.851630443000

42 C	11.732040630000	8.096269392000	9.151303571000
43 H	10.632794710000	8.057727882000	9.197390146000
44 H	12.067652000000	8.965756880000	9.741309173000
45 H	12.130798940000	7.187621685000	9.625526499000
46 C	11.624998340000	9.949587565000	6.774545114000
47 H	11.941404280000	10.219203740000	5.757344589000
48 H	12.013837680000	10.721060270000	7.461715818000
49 H	10.526771960000	9.989357699000	6.815505182000
50 C	14.045339410000	5.257707529000	5.338175740000
51 H	13.771438830000	5.408278979000	4.282976061000
52 H	14.517056390000	4.264899606000	5.430322863000
53 H	14.791681060000	6.018930968000	5.611468572000
54 C	11.317274660000	4.000703302000	5.888419359000
55 H	10.408787390000	3.960253336000	6.507141677000
56 H	11.838141790000	3.032038231000	5.985947564000
57 H	11.004483780000	4.096901364000	4.838514827000
58 C	13.045643450000	4.879294866000	8.191405054000
59 H	13.794073110000	5.560721524000	8.623335959000
60 H	13.492926230000	3.871414693000	8.155376179000
61 H	12.186543180000	4.841038155000	8.878317728000

$[U(IV)N^*_2CN_3]^{1-}$

1 U	9.975453302000	7.306725179000	4.879117340000
2 Si	10.923643780000	9.647472487000	2.474381091000
3 Si	7.985110042000	9.710432446000	3.383663218000
4 Si	12.292233630000	8.332291992000	7.282584159000
5 Si	12.418904110000	5.389254442000	6.390207217000
6 N	11.550533080000	5.447871223000	2.080727094000
7 N	7.411293603000	4.721465691000	4.885366118000
8 N	8.116595862000	8.806445081000	7.715078538000
9 N	9.620112956000	9.032986788000	3.498677255000
10 N	11.711537380000	7.009770810000	6.261677412000
11 C	11.031294670000	6.017238305000	2.967494680000
12 C	8.238858808000	5.555772963000	4.886235477000
13 C	8.662837513000	8.330911455000	6.790082339000
14 C	11.005816400000	11.543292240000	2.531108044000
15 H	11.157185280000	11.904638360000	3.558981429000
16 H	10.096237920000	12.019908660000	2.138418878000
17 H	11.853113050000	11.896669430000	1.922163020000
18 C	10.752695000000	9.091025722000	0.679310513800
19 H	11.615878360000	9.444656038000	0.093332832670
20 H	9.841626480000	9.473442893000	0.200476186800
21 H	10.739136240000	7.992243259000	0.627732364100
22 C	12.615392050000	9.026227950000	3.059063069000
23 H	12.863913100000	9.293733913000	4.094531848000
24 H	13.374722650000	9.501277989000	2.416072720000
25 H	12.728853860000	7.939904347000	2.939038889000
26 C	7.508999560000	10.186719310000	1.608260992000
27 H	8.142098625000	10.975323190000	1.178211324000
28 H	6.473443694000	10.563893150000	1.615837058000
29 H	7.539043115000	9.316725114000	0.936799547000
30 C	7.819335826000	11.248447080000	4.467713796000
31 H	7.959500377000	10.985841940000	5.526347611000
32 H	6.815448401000	11.689061020000	4.360632846000
33 H	8.556848342000	12.019547740000	4.203406906000
34 C	6.707185876000	8.437869784000	3.933482535000
35 H	6.693968939000	7.540651036000	3.299002979000
36 H	5.714711296000	8.912721352000	3.857954399000
37 H	6.816547201000	8.113499761000	4.978170557000
38 C	14.186864430000	8.451211589000	7.244113047000
39 H	14.677881390000	7.555484554000	7.650547040000
40 H	14.516351500000	9.311554339000	7.848489580000
41 H	14.556310560000	8.600668234000	6.218820972000
42 C	11.722975470000	8.160763470000	9.072789230000
43 H	10.624234610000	8.136093085000	9.116440178000
44 H	12.064599150000	9.028347240000	9.659479480000
45 H	12.111737470000	7.254550578000	9.555760865000
46 C	11.649540540000	10.008485850000	6.677870411000
47 H	11.992629250000	10.284085380000	5.671853123000
48 H	12.039311830000	10.772991350000	7.370330071000
49 H	10.553487040000	10.081909530000	6.711193285000
50 C	13.965641900000	5.244664225000	5.315645968000

$[U(IV)N^*_2NC_3]^{1-}$

1 U	9.937883397000	7.282841429000	4.899762000000
2 Si	10.878127960000	9.641462564000	2.490337497000
3 Si	7.944664927000	9.685712383000	3.391897049000
4 Si	12.339154120000	8.333438082000	7.247289579000
5 Si	12.442554930000	5.399485456000	6.381924242000
6 C	11.287098220000	5.501948617000	2.116293070000
7 C	7.462449476000	4.774374789000	5.092484934000
8 C	8.241223468000	8.819900038000	7.639355200000
9 N	9.579527837000	9.017523200000	3.510735692000
10 N	11.728930750000	7.012786464000	6.244544649000
11 N	10.925234080000	6.073770713000	3.089726674000
12 N	8.287114587000	5.622317374000	5.003804731000
13 N	8.786037057000	8.381209262000	6.682070248000
14 C	10.963278510000	11.536446630000	2.572413950000
15 H	11.111560190000	11.882114820000	3.605849702000
16 H	10.054640260000	12.018659440000	2.184156542000
17 H	11.811822550000	11.898277750000	1.970119082000
18 C	10.703208260000	9.120698887000	0.682675958300
19 H	11.581897880000	9.459636321000	0.111134426300
20 H	9.808683655000	9.538039345000	0.202299230600
21 H	10.657926620000	8.024310478000	0.608095183500
22 C	12.571881840000	9.002290455000	3.047004608000
23 H	12.802870190000	9.191260534000	4.102971052000
24 H	13.334695520000	9.531041581000	2.452010902000
25 H	12.691403060000	7.928400081000	2.853825874000
26 C	7.463935286000	10.146376060000	1.613166638000
27 H	8.086878217000	10.942476080000	1.182267038000
28 H	6.423157302000	10.508753510000	1.615477218000
29 H	7.510398701000	9.274579585000	0.945248256500
30 C	7.757553777000	11.233882960000	4.459011072000
31 H	7.925892826000	10.992118890000	5.518091154000
32 H	6.740060077000	11.645152860000	4.364589470000
33 H	8.467803167000	12.020854340000	4.168581698000
34 C	6.671868273000	8.408750899000	3.947198631000
35 H	6.684220081000	7.499138806000	3.330248463000
36 H	5.673811136000	8.865439515000	3.841938728000
37 H	6.771538873000	8.106867545000	4.998538778000
38 C	14.237713230000	8.407174444000	7.230349365000
39 H	14.708967810000	7.514829100000	7.665795595000
40 H	14.573970580000	9.277420332000	7.816890421000
41 H	14.621890470000	8.525784881000	6.206530147000
42 C	11.759398590000	8.196014329000	9.039379236000
43 H	10.660918380000	8.222601540000	9.086039148000
44 H	12.142682630000	9.045952063000	9.626141331000
45 H	12.103165750000	7.271630159000	9.522256312000
46 C	11.771195080000	10.028896930000	6.616441178000
47 H	12.307626380000	10.353648600000	5.715023900000
48 H	11.993816760000	10.763002820000	7.408191814000
49 H	10.690936170000	10.092224640000	6.428519194000
50 C	13.979888180000	5.245223140000	5.293421821000

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51 H	13.706939040000	5.376269313000	4.255120779000
52 H	14.423171350000	4.249100442000	5.429239968000
53 H	14.722190870000	5.996381754000	5.581823480000
54 C	11.169211080000	4.088020242000	5.840945254000
55 H	10.267775940000	4.065180439000	6.469290402000
56 H	11.658022820000	3.103274269000	5.927834961000
57 H	10.852167570000	4.182853704000	4.792470450000
58 C	12.893937930000	4.929667853000	8.170404929000
59 H	13.667416460000	5.580257000000	8.601904049000
60 H	13.292267810000	3.901915885000	8.169663511000
61 H	12.020154610000	4.945297538000	8.837154686000

51 H	13.718103030000	5.409900234000	4.238394348000
52 H	14.416042730000	4.237540702000	5.379136951000
53 H	14.754285730000	5.973535249000	5.572492748000
54 C	11.199518300000	4.077884871000	5.863985898000
55 H	10.293453760000	4.076617212000	6.486454376000
56 H	11.686705820000	3.096882433000	5.990996722000
57 H	10.890490600000	4.143589361000	4.812143151000
58 C	12.934891590000	4.951730030000	8.161325651000
59 H	13.694595160000	5.617496603000	8.593100472000
60 H	13.352556000000	3.931833652000	8.161769332000
61 H	12.061133200000	4.951238936000	8.828615668000

$[MCp^*_2X_3]^q$ /q=2- ,1- /X=CN ,NC/ COSMO

$[Ce(III)Cp^*_2CN_3]^{2-}$

1 Ce	0.000000000000	0.000000000000	0.599294960700
2 N	0.000000000000	0.000000000000	4.414545948000
3 N	-0.598670714500	3.658093434000	1.603483091000
4 C	0.000000000000	0.000000000000	3.238714979000
5 C	-0.413534165400	2.528389585000	1.332225466000
6 C	2.034381957000	0.336330697400	-1.391454542000
7 C	2.113706309000	1.513579110000	-0.589827427200
8 C	2.610183119000	1.135217715000	0.693581442700
9 C	2.835036877000	-0.270175294600	0.684584044100
10 C	2.477463149000	-0.768393198800	-0.604268040100
11 C	1.761073458000	0.304688677500	-2.866682112000
12 H	2.685696042000	0.485553337100	-3.444557270000
13 H	1.038365661000	1.073196702000	-3.175064365000
14 H	1.365092530000	-0.665871594300	-3.196401232000
15 C	1.892672540000	2.918537588000	-1.068817943000
16 H	1.505343033000	3.562424047000	-0.268374513100
17 H	1.164822504000	2.960281555000	-1.892076250000
18 H	2.832130878000	3.362887920000	-1.445620063000
19 C	2.929998307000	2.066423942000	1.825740766000
20 H	2.786688781000	1.578106848000	2.799474343000
21 H	2.278458846000	2.949831934000	1.813381870000
22 H	3.978982640000	2.410659904000	1.773239709000
23 C	3.436954196000	-1.068859514000	1.803024417000
24 H	4.540945734000	-1.047275279000	1.756099342000
25 H	3.112295332000	-2.116610954000	1.765389042000
26 H	3.136009897000	-0.678008580700	2.784898270000
27 C	2.700982157000	-2.166884915000	-1.101226860000
28 H	2.005410950000	-2.430497364000	-1.911417582000
29 H	2.555465507000	-2.907091587000	-0.303602415200
30 H	3.724000679000	-2.288121730000	-1.502010132000
31 N	0.598670714500	-3.658093434000	1.603483091000
32 C	0.413534165400	-2.528389585000	1.332225466000
33 C	-2.034381957000	-0.336330697400	-1.391454542000
34 C	-2.113706309000	-1.513579110000	-0.589827427200
35 C	-2.610183119000	-1.135217715000	0.693581442700
36 C	-2.835036877000	0.270175294600	0.684584044100
37 C	-2.477463149000	0.768393198800	-0.604268040100
38 C	-1.761073458000	-0.304688677500	-2.866682112000
39 H	-2.685696042000	-0.485553337100	-3.444557270000
40 H	-1.038365661000	-1.073196702000	-3.175064365000
41 H	-1.365092530000	0.665871594300	-3.196401232000
42 C	-1.892672540000	-2.918537588000	-1.068817943000
43 H	-1.505343033000	-3.562424047000	-0.268374513100
44 H	-1.164822504000	-2.960281555000	-1.892076250000
45 H	-2.832130878000	-3.362887920000	-1.445620063000
46 C	-2.929998307000	-2.066423942000	1.825740766000
47 H	-2.786688781000	-1.578106848000	2.799474343000
48 H	-2.278458846000	-2.949831934000	1.813381870000
49 H	-3.978982640000	-2.410659904000	1.773239709000
50 C	-3.436954196000	1.068859514000	1.803024417000
51 H	-4.540945734000	1.047275279000	1.756099342000
52 H	-3.112295332000	2.116610954000	1.765389042000
53 H	-3.136009897000	0.678008580700	2.784898270000
54 C	-2.700982157000	2.166884915000	-1.101226860000
55 H	-2.005410950000	2.430497364000	-1.911417582000
56 H	-2.555465507000	2.907091587000	-0.303602415200

$[Ce(III)Cp^*_2NC_3]^{2-}$

1 Ce	0.000000000000	0.000000000000	0.640904058200
2 C	0.000000000000	0.000000000000	4.354278349000
3 C	-0.357973822400	3.594981095000	1.557398063000
4 N	0.000000000000	0.000000000000	3.177841918000
5 N	-0.248458457700	2.471195795000	1.223175672000
6 C	2.032489992000	0.204528477500	-1.382955553000
7 C	2.183011932000	1.376916152000	-0.584897381700
8 C	2.659886789000	0.977248122900	0.700309107700
9 C	2.803003142000	-0.438402111100	0.696017771300
10 C	2.416506044000	-0.918358113800	-0.592266161600
11 C	1.768631176000	0.185772785100	-2.859545028000
12 H	2.709399861000	0.284191792900	-3.432298155000
13 H	1.115499240000	1.010915247000	-3.175100695000
14 H	1.292670571000	-0.749074827900	-3.186044875000
15 C	2.042784882000	2.788065896000	-1.072497543000
16 H	1.744337176000	3.466021481000	-0.263232124700
17 H	1.279676287000	2.875963793000	-1.859499143000
18 H	2.993785886000	3.155810082000	-1.498931686000
19 C	3.034059601000	1.892570165000	1.828548357000
20 H	2.882880630000	1.409409280000	2.803751968000
21 H	2.421212748000	2.803243976000	1.824538153000
22 H	4.095951481000	2.191566994000	1.763433010000
23 C	3.353533402000	-1.267718420000	1.818388901000
24 H	4.457360016000	-1.303702803000	1.782535751000
25 H	2.976134132000	-2.297317507000	1.775112273000
26 H	3.064483887000	-0.862973642700	2.798462312000
27 C	2.563645826000	-2.327163434000	-1.085206375000
28 H	1.884447135000	-2.538923470000	-1.923538754000
29 H	2.337751653000	-3.057208786000	-0.297381319400
30 H	3.591644264000	-2.515209641000	-1.444787207000
31 C	0.357973822400	-3.594981095000	1.557398063000
32 N	0.248458457700	-2.471195795000	1.223175672000
33 C	-2.032489992000	-0.204528477500	-1.382955553000
34 C	-2.183011932000	-1.376916152000	-0.584897381700
35 C	-2.659886789000	-0.977248122900	0.700309107700
36 C	-2.803003142000	0.438402111100	0.696017771300
37 C	-2.416506044000	0.918358113800	-0.592266161600
38 C	-1.768631176000	-0.185772785100	-2.859545028000
39 H	-2.709399861000	-0.284191792900	-3.432298155000
40 H	-1.115499240000	-1.010915247000	-3.175100695000
41 H	-1.292670571000	0.749074827900	-3.186044875000
42 C	-2.042784882000	-2.788065896000	-1.072497543000
43 H	-1.744337176000	-3.466021481000	-0.263232124700
44 H	-1.279676287000	-2.875963793000	-1.859499143000
45 H	-2.993785886000	-3.155810082000	-1.498931686000
46 C	-3.034059601000	-1.892570165000	1.828548357000
47 H	-2.882880630000	-1.409409280000	2.803751968000
48 H	-2.421212748000	-2.803243976000	1.824538153000
49 H	-4.095951481000	-2.191566994000	1.763433010000
50 C	-3.353533402000	1.267718420000	1.818388901000
51 H	-4.457360016000	1.303702803000	1.782535751000
52 H	-2.976134132000	2.297317507000	1.775112273000
53 H	-3.064483887000	0.862973642700	2.798462312000
54 C	-2.563645826000	2.327163434000	-1.085206375000
55 H	-1.884447135000	2.538923470000	-1.923538754000
56 H	-2.337751653000	3.057208786000	-0.297381319400

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57	H	-3.724000679000	2.288121730000	-1.502010132000

57	H	-3.591644264000	2.515209641000	-1.444787207000

$[U(III)Cp^*_2CN_3]^{2-}$

1	U	0.000000000000	0.000000000000	0.579911769800
2	N	0.000000000000	0.000000000000	4.360438248000
3	N	-0.409575461800	3.580387961000	1.628155337000
4	C	0.000000000000	0.000000000000	3.184891866000
5	C	-0.274055746700	2.447833806000	1.332904663000
6	C	2.351421602000	-0.907100117800	-0.625649931900
7	C	1.969696628000	0.241507952700	-1.386657103000
8	C	2.124901975000	1.392868297000	-0.550878552000
9	C	2.606340728000	0.952008249200	0.721227810300
10	C	2.752611768000	-0.465785304000	0.673137043100
11	C	2.477261201000	-2.304750947000	-1.158473425000
12	H	1.741260528000	-2.505667487000	-1.952212177000
13	H	2.310079990000	-3.051661349000	-0.370542882600
14	H	3.479239138000	-2.477587096000	-1.593958236000
15	C	1.741151936000	0.270133517100	-2.869763100000
16	H	1.093969402000	1.105241560000	-3.173531971000
17	H	1.273762183000	-0.654403331100	-3.236974386000
18	H	2.696599330000	0.388160032000	-3.416607750000
19	C	1.998142002000	2.818348615000	-1.003010422000
20	H	2.942504506000	3.181828089000	-1.450723774000
21	H	1.730194961000	3.481764677000	-0.170211319100
22	H	1.213148522000	2.935855657000	-1.765799995000
23	C	3.007651389000	1.832611213000	1.868640072000
24	H	2.839798085000	1.332923783000	2.833486842000
25	H	2.419829728000	2.760029252000	1.883910594000
26	H	4.079427802000	2.101333586000	1.808275544000
27	C	3.342680512000	-1.315818644000	1.759540943000
28	H	4.447895703000	-1.309722491000	1.710572206000
29	H	2.997258827000	-2.355286995000	1.686606445000
30	H	3.049470505000	-0.953406119200	2.755919585000
31	N	0.409575461800	-3.580387961000	1.628155337000
32	C	0.274055746700	-2.447833806000	1.332904663000
33	C	-2.351421602000	0.907100117800	-0.625649931900
34	C	-1.969696628000	-0.241507952700	-1.386657103000
35	C	-2.124901975000	-1.392868297000	-0.550878552000
36	C	-2.606340728000	-0.952008249200	0.721227810300
37	C	-2.752611768000	0.465785304000	0.673137043100
38	C	-2.477261201000	2.304750947000	-1.158473425000
39	H	-1.741260528000	2.505667487000	-1.952212177000
40	H	-2.310079990000	3.051661349000	-0.370542882600
41	H	-3.479239138000	2.477587096000	-1.593958236000
42	C	-1.741151936000	-0.270133517100	-2.869763100000
43	H	-1.093969402000	-1.105241560000	-3.173531971000
44	H	-1.273762183000	0.654403331100	-3.236974386000
45	H	-2.696599330000	-0.388160032000	-3.416607750000
46	C	-1.998142002000	-2.818348615000	-1.003010422000
47	H	-2.942504506000	-3.181828089000	-1.450723774000
48	H	-1.730194961000	-3.481764677000	-0.170211319100
49	H	-1.213148522000	-2.935855657000	-1.765799995000
50	C	-3.007651389000	-1.832611213000	1.868640072000
51	H	-2.839798085000	-1.332923783000	2.833486842000
52	H	-2.419829728000	-2.760029252000	1.883910594000
53	H	-4.079427802000	-2.101333586000	1.808275544000
54	C	-3.342680512000	1.315818644000	1.759540943000
55	H	-4.447895703000	1.309722491000	1.710572206000
56	H	-2.997258827000	2.355286995000	1.686606445000
57	H	-3.049470505000	0.953406119200	2.755919585000

$[U(III)Cp^*_2NC_3]^{2-}$

1	U	0.000000000000	0.000000000000	0.632549000000
2	C	0.000000000000	0.000000000000	4.305505000000
3	C	-0.323763000000	3.547740000000	1.502163000000
4	N	0.000000000000	0.000000000000	3.127746000000
5	N	-0.242201000000	2.410313000000	1.196694000000
6	C	2.372926000000	-0.938348000000	-0.561304000000
7	C	1.973458000000	0.171150000000	-1.369432000000
8	C	2.133244000000	1.360683000000	-0.592400000000
9	C	2.623614000000	0.983607000000	0.694370000000
10	C	2.770333000000	-0.433988000000	0.713505000000
11	C	2.529574000000	-2.351079000000	-1.039098000000
12	H	1.772842000000	-2.613123000000	-1.793693000000
13	H	2.415952000000	-3.068147000000	-0.216162000000
14	H	3.522115000000	-2.506425000000	-1.502334000000
15	C	1.743990000000	0.125427000000	-2.851718000000
16	H	1.092489000000	0.940146000000	-3.196469000000
17	H	1.280802000000	-0.818917000000	-3.169874000000
18	H	2.698856000000	0.218803000000	-3.404202000000
19	C	1.993188000000	2.761382000000	-1.108843000000
20	H	2.939552000000	3.117279000000	-1.557743000000
21	H	1.706601000000	3.457214000000	-0.309845000000
22	H	1.217679000000	2.832146000000	-1.885863000000
23	C	3.005912000000	1.917388000000	1.805035000000
24	H	2.843414000000	1.456053000000	2.789662000000
25	H	2.403580000000	2.834901000000	1.779310000000
26	H	4.072805000000	2.200603000000	1.738736000000
27	C	3.327132000000	-1.241997000000	1.848832000000
28	H	4.428160000000	-1.320174000000	1.781444000000
29	H	2.910193000000	-2.257821000000	1.856071000000
30	H	3.083371000000	-0.788742000000	2.820261000000
31	C	0.323763000000	-3.547740000000	1.502163000000
32	N	0.242201000000	-2.410313000000	1.196694000000
33	C	-2.372926000000	0.938348000000	-0.561304000000
34	C	-1.973458000000	-0.171150000000	-1.369432000000
35	C	-2.133244000000	-1.360683000000	-0.592400000000
36	C	-2.623614000000	-0.983607000000	0.694370000000
37	C	-2.770333000000	0.433988000000	0.713505000000
38	C	-2.529574000000	2.351079000000	-1.039098000000
39	H	-1.772842000000	2.613123000000	-1.793693000000
40	H	-2.415952000000	3.068147000000	-0.216162000000
41	H	-3.522115000000	2.506425000000	-1.502334000000
42	C	-1.743990000000	-0.125427000000	-2.851718000000
43	H	-1.092489000000	-0.940146000000	-3.196469000000
44	H	-1.280802000000	0.818917000000	-3.169874000000
45	H	-2.698856000000	-0.218803000000	-3.404202000000
46	C	-1.993188000000	-2.761382000000	-1.108843000000
47	H	-2.939552000000	-3.117279000000	-1.557743000000
48	H	-1.706601000000	-3.457214000000	-0.309845000000
49	H	-1.217679000000	-2.832146000000	-1.885863000000
50	C	-3.005912000000	-1.917388000000	1.805035000000
51	H	-2.843414000000	-1.456053000000	2.789662000000
52	H	-2.403580000000	-2.834901000000	1.779310000000
53	H	-4.072805000000	-2.200603000000	1.738736000000
54	C	-3.327132000000	1.241997000000	1.848832000000
55	H	-4.428160000000	1.320174000000	1.781444000000
56	H	-2.910193000000	2.257821000000	1.856071000000
57	H	-3.083371000000	0.788742000000	2.820261000000

$[U(IV)Cp^*_2CN_3]^{1-}$

1	U	0.000000000000	0.000000000000	0.423341000000
2	N	-0.039158000000	-3.518341000000	1.560553000000
3	N	0.000000000000	0.000000000000	4.116776000000
4	N	0.039158000000	3.518341000000	1.560553000000
5	C	-0.028795000000	-2.390420000000	1.227273000000
6	C	0.000000000000	0.000000000000	2.941015000000
7	C	0.028795000000	2.390420000000	1.227273000000
8	C	-2.696014000000	0.664290000000	0.814012000000
9	C	-2.660852000000	-0.757250000000	0.664620000000

$[U(IV)Cp^*_2NC_3]^{1-}$

1	U	0.000000000000	0.000000000000	0.569583000000
2	C	-0.001737000000	-3.480360000000	1.500258000000
3	C	0.000000000000	0.000000000000	4.178328000000
4	C	0.001737000000	3.480360000000	1.500258000000
5	N	-0.000431000000	-2.354196000000	1.146471000000
6	N	0.000000000000	0.000000000000	2.998262000000
7	N	0.000431000000	2.354196000000	1.146471000000
8	C	-2.676426000000	0.715516000000	0.639185000000
9	C	-2.676843000000	-0.713623000000	0.639919000000

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10 C	-2.251310000000	-1.050415000000	-0.676298000000	
11 C	-2.042382000000	0.195957000000	-1.354274000000	
12 C	-2.328105000000	1.253744000000	-0.434616000000	
13 C	-3.188608000000	1.398277000000	2.027653000000	
14 H	-4.286488000000	1.503204000000	1.999737000000	
15 H	-2.757476000000	2.404869000000	2.092502000000	
16 H	-2.931144000000	0.866288000000	2.952420000000	
17 C	-3.158025000000	-1.739007000000	1.686952000000	
18 H	-2.851078000000	-1.458877000000	2.703622000000	
19 H	-2.783229000000	-2.750400000000	1.495955000000	
20 H	-4.260614000000	-1.775008000000	1.674248000000	
21 C	-2.193075000000	-2.408282000000	-1.317968000000	
22 H	-3.139930000000	-2.629758000000	-1.839004000000	
23 H	-2.023131000000	-3.199154000000	-0.578172000000	
24 H	-1.395190000000	-2.481167000000	-2.071642000000	
25 C	-1.767820000000	0.368031000000	-2.822731000000	
26 H	-1.219699000000	-0.482210000000	-3.248611000000	
27 H	-1.195610000000	1.281490000000	-3.038303000000	
28 H	-2.715147000000	0.450137000000	-3.382193000000	
29 C	-2.413837000000	2.708707000000	-0.795397000000	
30 H	-1.626680000000	3.012354000000	-1.499768000000	
31 H	-2.329791000000	3.350430000000	0.088267000000	
32 H	-3.380849000000	2.921181000000	-1.282068000000	
33 C	2.696014000000	-0.664290000000	0.814012000000	
34 C	2.328105000000	-1.253744000000	-0.434616000000	
35 C	2.042382000000	-0.195957000000	-1.354274000000	
36 C	2.251310000000	1.050415000000	-0.676298000000	
37 C	2.660852000000	0.757250000000	0.664620000000	
38 C	3.188608000000	-1.398277000000	2.027653000000	
39 H	4.286488000000	-1.503204000000	1.999737000000	
40 H	2.757476000000	-2.404869000000	2.092502000000	
41 H	2.931144000000	-0.866288000000	2.952420000000	
42 C	2.413837000000	-2.708707000000	-0.795397000000	
43 H	3.380849000000	-2.921181000000	-1.282068000000	
44 H	1.626680000000	-3.012354000000	-1.499768000000	
45 H	2.329791000000	-3.350430000000	0.088267000000	
46 C	1.767820000000	-0.368031000000	-2.822731000000	
47 H	2.715147000000	-0.450137000000	-3.382193000000	
48 H	1.219699000000	0.482210000000	-3.248611000000	
49 H	1.195610000000	-1.281490000000	-3.038303000000	
50 C	2.193075000000	2.408282000000	-1.317968000000	
51 H	3.139930000000	2.629758000000	-1.839004000000	
52 H	2.023131000000	3.199154000000	-0.578172000000	
53 H	1.395190000000	2.481167000000	-2.071642000000	
54 C	3.158025000000	1.739007000000	1.686952000000	
55 H	2.851078000000	1.458877000000	2.703622000000	
56 H	2.783229000000	2.750400000000	1.495955000000	
57 H	4.260614000000	1.775008000000	1.674248000000	

10 C	-2.214792000000	-1.156785000000	-0.638784000000	
11 C	-1.925714000000	-0.000329000000	-1.430184000000	
12 C	-2.213961000000	1.157115000000	-0.639878000000	
13 C	-3.202465000000	1.587106000000	1.743857000000	
14 H	-4.295154000000	1.709610000000	1.652503000000	
15 H	-2.749923000000	2.585536000000	1.720012000000	
16 H	-3.004918000000	1.155098000000	2.733893000000	
17 C	-3.203555000000	-1.583840000000	1.745436000000	
18 H	-3.012096000000	-1.147241000000	2.734671000000	
19 H	-2.746382000000	-2.580328000000	1.727322000000	
20 H	-4.295292000000	-1.711719000000	1.650030000000	
21 C	-2.228072000000	-2.570123000000	-1.149228000000	
22 H	-3.164564000000	-2.771568000000	-1.697147000000	
23 H	-2.152539000000	-3.296321000000	-0.332016000000	
24 H	-1.400678000000	-2.767940000000	-1.845122000000	
25 C	-1.696841000000	-0.000806000000	-2.915460000000	
26 H	-1.148383000000	-0.888614000000	-3.254262000000	
27 H	-1.145259000000	0.885106000000	-3.254074000000	
28 H	-2.663732000000	0.000938000000	-3.447898000000	
29 C	-2.225506000000	2.569966000000	-1.151797000000	
30 H	-1.396224000000	2.766800000000	-1.845746000000	
31 H	-2.151952000000	3.297084000000	-0.335199000000	
32 H	-3.160475000000	2.771109000000	-1.702467000000	
33 C	2.676426000000	-0.715516000000	0.639185000000	
34 C	2.213961000000	-1.157115000000	0.639878000000	
35 C	1.925714000000	0.000329000000	-1.430184000000	
36 C	2.214792000000	1.156785000000	-0.638784000000	
37 C	2.676843000000	0.713623000000	0.639919000000	
38 C	3.202465000000	-1.587106000000	1.743857000000	
39 H	4.295154000000	-1.709610000000	1.652503000000	
40 H	2.749923000000	-2.585536000000	1.720012000000	
41 H	3.004918000000	-1.155098000000	2.733893000000	
42 C	2.225506000000	-2.569966000000	-1.151797000000	
43 H	3.160475000000	-2.771109000000	-1.702467000000	
44 H	1.396224000000	-2.766800000000	-1.845746000000	
45 H	2.151952000000	-3.297084000000	-0.335199000000	
46 C	1.696841000000	0.000806000000	-2.915460000000	
47 H	2.663732000000	-0.000938000000	-3.447898000000	
48 H	1.148383000000	0.888614000000	-3.254262000000	
49 H	1.145259000000	-0.885106000000	-3.254074000000	
50 C	2.228072000000	2.570123000000	-1.149228000000	
51 H	3.164564000000	2.771568000000	-1.697147000000	
52 H	2.152539000000	3.296321000000	-0.332016000000	
53 H	1.400678000000	2.767940000000	-1.845122000000	
54 C	3.203555000000	1.583840000000	1.745436000000	
55 H	3.012096000000	1.147241000000	2.734671000000	
56 H	2.746382000000	2.580328000000	1.727322000000	
57 H	4.295292000000	1.711719000000	1.650030000000	

$[MN^*_2X_3]^q$ /q=2- ,1- /X=CN ,NC /COSMO

$[Ce(III)N^*_2CN_3]^{2-}$

1 Ce	13.559564290000	22.521889050000	0.051943346570	
2 Si	16.212558330000	24.028828060000	1.855044953000	
3 Si	15.993548290000	24.859317280000	-1.063391135000	
4 Si	11.574915010000	20.974231270000	-2.440758209000	
5 Si	14.457881690000	20.018650710000	-2.309504919000	
6 C	14.467503210000	20.503830970000	1.560492791000	
7 C	11.743510650000	22.567565290000	1.935807288000	
8 C	12.117275610000	24.597092330000	-0.833168929500	
9 N	15.467092360000	23.924613320000	0.293495194900	
10 N	13.171753680000	21.042774620000	-1.770329730000	
11 N	14.886311590000	19.597182350000	2.179893110000	
12 N	10.934145930000	22.597538400000	2.786920735000	
13 N	11.525677750000	25.524397590000	-1.247430322000	
14 C	14.975566510000	23.612522400000	3.228358122000	
15 H	14.113842030000	24.296419970000	3.232703626000	
16 H	15.486206950000	23.705340880000	4.201694404000	
17 H	14.591615090000	22.583203100000	3.164434332000	
18 C	16.883619580000	25.759556300000	2.296696499000	
19 H	17.666857860000	26.104133100000	1.605178663000	
20 H	17.320788840000	25.731621640000	3.308633133000	

$[Ce(III)N^*_2NC_3]^{-2}$

1 Ce	13.486678810000	22.521595650000	0.134391228300	
2 Si	16.197472770000	24.013942530000	1.835128911000	
3 Si	15.953057190000	24.831244070000	-1.075381884000	
4 Si	11.599864400000	20.988700370000	-2.424740108000	
5 Si	14.477681200000	20.050176810000	-2.274463870000	
6 N	14.410622880000	20.585414970000	1.491755763000	
7 N	11.758517600000	22.589010080000	1.927488858000	
8 N	12.177778720000	24.488394980000	-0.804246529200	
9 N	15.425922080000	23.907224750000	0.288868706900	
10 N	13.183534660000	21.061486580000	-1.728946322000	
11 C	14.760859110000	19.649361290000	2.117018449000	
12 C	10.941519950000	22.601381790000	2.776643702000	
13 C	11.572956850000	25.432808310000	-1.167454591000	
14 C	14.980043510000	23.605926490000	3.230052393000	
15 H	14.118870160000	24.290616000000	3.241531438000	
16 H	15.504485350000	23.708908810000	4.194902899000	
17 H	14.596138090000	22.576128070000	3.183099757000	
18 C	16.877862350000	25.743851440000	2.266536666000	
19 H	17.647644380000	26.089164170000	1.560604634000	
20 H	17.334145240000	25.715063380000	3.269934926000	

ACCEPTED MANUSCRIPT

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
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	-0.938097435300
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
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
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
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
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
43	H	11.573242750000	23.135057910000	-3.693607049000	43 H	11.606046610000	23.162302810000	-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
46	C	10.280699810000	21.547521450000	-1.182442323000	46 C	10.281695390000	21.532713320000	-1.175889360000
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
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
53	H	14.864986350000	21.041285280000	-4.573641829000	53 H	14.877059580000	21.080913570000	-4.537775337000
54	C	14.256121630000	18.207878350000	-1.770772811000	54 C	14.283886600000	18.232627120000	-1.751327843000
55	H	14.188895550000	18.161971490000	-0.673045614800	55 H	14.206656370000	18.176105840000	-0.654928271100
56	H	15.126283810000	17.610294890000	-2.088268973000	56 H	15.161141350000	17.643826620000	-2.065926477000
57	H	13.351412640000	17.748257110000	-2.193988472000	57 H	13.386392560000	17.770297520000	-2.186661175000
58	C	16.123053720000	20.569342430000	-1.586013495000	58 C	16.150234240000	20.594053440000	-1.567184725000
59	H	16.400776630000	21.600596440000	-1.845463558000	59 H	16.422218860000	21.626118530000	-1.826940088000
60	H	16.913330620000	19.912676460000	-1.985261134000	60 H	16.934155710000	19.936277180000	-1.977341531000
61	H	16.146472460000	20.471248000000	-0.489998860000	61 H	16.179620460000	20.498022320000	-0.472328148600

$[U(III)N^*_2CN_3]^{2-}$

1	U	9.865108125000	7.196436014000	4.887045754000
2	Si	10.956692310000	9.614008972000	2.493877250000
3	Si	8.039157364000	9.741004467000	3.349834560000
4	Si	12.234809420000	8.361749759000	7.285351697000
5	Si	12.482969790000	5.456371461000	6.411009943000
6	N	11.270075660000	5.222982565000	1.972658145000
7	N	7.291939496000	4.495111074000	4.877864688000
8	N	7.795759376000	8.515907391000	7.771455120000
9	N	9.632714523000	9.053138267000	3.467248885000
10	N	11.728840000000	7.020337594000	6.304944243000
11	C	10.807435710000	5.795962023000	2.889803973000
12	C	8.097369042000	5.353732434000	4.879621534000
13	C	8.390960971000	8.090877375000	6.850029332000
14	C	11.156560210000	11.510196960000	2.547820917000
15	H	11.321854510000	11.856256010000	3.579540233000
16	H	10.269855090000	12.032964350000	2.158578604000
17	H	12.023006190000	11.820893680000	1.941170055000
18	C	10.796850540000	9.113063843000	0.668807494400
19	H	11.686241540000	9.434213457000	0.102377867600
20	H	9.909441615000	9.552173285000	0.191800652100
21	H	10.721291690000	8.016954084000	0.602195839300
22	C	12.618754700000	8.899621241000	3.058562736000
23	H	12.868821190000	9.143138645000	4.099905597000
24	H	13.414148210000	9.319047162000	2.419264235000
25	H	12.648944940000	7.805828710000	2.947466775000
26	C	7.569831394000	10.349232980000	1.603464137000
27	H	8.232764536000	11.142514580000	1.228274513000

$[U(III)N^*_2NC_3]^{2-}$

1	U	9.848699368000	7.187468814000	4.887482808000
2	Si	10.935166490000	9.627198803000	2.490260305000
3	Si	8.031232992000	9.754262572000	3.358834680000
4	Si	12.247827970000	8.328156888000	7.287802802000
5	Si	12.472899130000	5.433050715000	6.402059490000
6	C	11.200506960000	5.325775487000	2.039673269000
7	C	7.316433030000	4.595540576000	4.833028653000
8	C	7.904918961000	8.429582887000	7.734344115000
9	N	9.621600611000	9.063677926000	3.476051662000
10	N	11.728919910000	7.000131428000	6.297183921000
11	N	10.854450240000	5.931849862000	2.992004493000
12	N	8.137882219000	5.442700379000	4.871857108000
13	N	8.528716680000	8.113596097000	6.782748913000
14	C	11.102976450000	11.528242630000	2.501541327000
15	H	11.262164960000	11.897302420000	3.526398342000
16	H	10.210702440000	12.031940060000	2.100040008000
17	H	11.966411010000	11.837252440000	1.889545146000
18	C	10.781474150000	9.087304768000	0.675172979800
19	H	11.662098690000	9.415333184000	0.098783835570
20	H	9.882986827000	9.499365523000	0.194374580300
21	H	10.728683090000	7.988897898000	0.627685684000
22	C	12.618444970000	8.970259121000	3.063247584000
23	H	12.875558300000	9.271652427000	4.087567238000
24	H	13.395913820000	9.375134952000	2.393506058000
25	H	12.668887740000	7.873781126000	3.008022436000
26	C	7.541747195000	10.311602390000	1.599751525000
27	H	8.205359953000	11.087536390000	1.190685345000

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28 H	6.545168059000	10.755795940000	1.630122695000
29 H	7.584696360000	9.521146991000	0.879301630700
30 C	7.824106005000	11.224285040000	4.515713632000
31 H	7.932835100000	10.894159630000	5.559728546000
32 H	6.826107936000	11.677831440000	4.399491180000
33 H	8.581555429000	11.998412780000	4.320966885000
34 C	6.704853218000	8.473113322000	3.793767663000
35 H	6.700526859000	7.621160798000	3.098095492000
36 H	5.719701015000	8.967642925000	3.737456853000
37 H	6.803742732000	8.074337395000	4.814830887000
38 C	14.121063860000	8.639495064000	7.234647676000
39 H	14.679406270000	7.772739842000	7.619014347000
40 H	14.396320780000	9.514210584000	7.846421117000
41 H	14.460589530000	8.824260407000	6.204017177000
42 C	11.740563050000	8.176057727000	9.109753982000
43 H	10.648168810000	8.060796859000	9.178300743000
44 H	12.028166500000	9.075723073000	9.678559598000
45 H	12.213226360000	7.304547605000	9.584255895000
46 C	11.450644200000	9.993824705000	6.726508507000
47 H	11.687479420000	10.260711270000	5.688026858000
48 H	11.831168040000	10.803985440000	7.371392935000
49 H	10.356095570000	9.975771427000	6.832632480000
50 C	13.977531990000	5.311181608000	5.249440837000
51 H	13.647829650000	5.408036102000	4.204157009000
52 H	14.474233770000	4.333952380000	5.365369273000
53 H	14.716508560000	6.101250515000	5.449872917000
54 C	11.273760840000	4.074119125000	5.951701317000
55 H	10.415578450000	4.033928139000	6.638443202000
56 H	11.806434540000	3.109262203000	6.011425286000
57 H	10.881816120000	4.160651862000	4.926805078000
58 C	13.104919820000	5.003287922000	8.156773298000
59 H	13.870669040000	5.695935818000	8.535933949000
60 H	13.551806560000	3.995636034000	8.128333279000
61 H	12.275455440000	4.984009659000	8.879302002000

28 H	6.519971954000	10.725850710000	1.624797498000
29 H	7.542984265000	9.459664547000	0.903226453100
30 C	7.835609010000	11.274251590000	4.481402260000
31 H	7.989206692000	10.980507830000	5.530782211000
32 H	6.827491984000	11.710322140000	4.387553937000
33 H	8.573377044000	12.052054390000	4.233167325000
34 C	6.685294763000	8.517177212000	3.855162484000
35 H	6.683069802000	7.626676884000	3.209684705000
36 H	5.705122204000	9.014850693000	3.752719475000
37 H	6.768679318000	8.177727717000	4.897674540000
38 C	14.139988220000	8.573844787000	7.256742311000
39 H	14.682165470000	7.699198372000	7.647096312000
40 H	14.422288250000	9.445228802000	7.870292046000
41 H	14.490695500000	8.752769732000	6.228607586000
42 C	11.734490730000	8.139079807000	9.107705630000
43 H	10.640349510000	8.034714691000	9.165925848000
44 H	12.027031470000	9.031476235000	9.684962299000
45 H	12.192748990000	7.259087069000	9.580818062000
46 C	11.510045860000	9.986303674000	6.739961043000
47 H	11.762936720000	10.257399810000	5.706088315000
48 H	11.908594520000	10.777627620000	7.397647243000
49 H	10.414773520000	9.992702357000	6.834730331000
50 C	13.993241080000	5.291748616000	5.272193400000
51 H	13.689165080000	5.429359229000	4.223685762000
52 H	14.467526670000	4.301069969000	5.366623526000
53 H	14.742793630000	6.060058122000	5.514707855000
54 C	11.276488730000	4.050321723000	5.905510802000
55 H	10.386443170000	4.022861361000	6.551188219000
56 H	11.801447890000	3.084538790000	6.006467010000
57 H	10.936148300000	4.126275913000	4.862744975000
58 C	13.056212950000	4.955213977000	8.155970984000
59 H	13.815236540000	5.640338286000	8.561237159000
60 H	13.500130010000	3.946311949000	8.124329999000
61 H	12.210517010000	4.929772629000	8.859467086000

$[U(IV)N^*_2CN_3]^{1-}$

1 U	10.034757000000	7.375728000000	4.883747000000
2 Si	10.988535000000	9.659384000000	2.507023000000
3 Si	8.009379000000	9.738781000000	3.370051000000
4 Si	12.302155000000	8.389186000000	7.255806000000
5 Si	12.448598000000	5.412881000000	6.397459000000
6 N	11.091554000000	5.287196000000	1.971327000000
7 N	7.462411000000	4.743698000000	4.915227000000
8 N	7.929479000000	8.412284000000	7.792674000000
9 N	9.649742000000	9.050171000000	3.512916000000
10 N	11.722496000000	7.036682000000	6.250258000000
11 C	10.777231000000	5.914599000000	2.914040000000
12 C	8.283725000000	5.585856000000	4.905267000000
13 C	8.567050000000	8.109714000000	6.852838000000
14 C	11.093493000000	11.538284000000	2.630639000000
15 H	11.236627000000	11.868908000000	3.672134000000
16 H	10.191006000000	12.036527000000	2.242340000000
17 H	11.953355000000	11.897872000000	2.038966000000
18 C	10.817372000000	9.129265000000	0.707444000000
19 H	11.703215000000	9.466679000000	0.141809000000
20 H	9.924346000000	9.548996000000	0.221343000000
21 H	10.770227000000	8.030190000000	0.637321000000
22 C	12.650534000000	8.955986000000	3.105524000000
23 H	12.897090000000	9.184575000000	4.151835000000
24 H	13.432540000000	9.422028000000	2.478786000000
25 H	12.724778000000	7.867361000000	2.957967000000
26 C	7.587660000000	10.237461000000	1.597846000000
27 H	8.238868000000	11.029580000000	1.196689000000
28 H	6.552381000000	10.622741000000	1.587049000000
29 H	7.630879000000	9.376233000000	0.912530000000
30 C	7.844169000000	11.248980000000	4.491556000000
31 H	7.956883000000	10.959398000000	5.548544000000
32 H	6.845899000000	11.703775000000	4.369695000000
33 H	8.598914000000	12.017451000000	4.262044000000
34 C	6.735383000000	8.441352000000	3.890628000000
35 H	6.760498000000	7.536231000000	3.264821000000

$[U(IV)N^*_2NC_3]^{1-}$

1 U	10.129239000000	7.415174000000	4.858136000000
2 Si	10.843132000000	9.658875000000	2.448480000000
3 Si	7.899819000000	9.754898000000	3.387831000000
4 Si	12.374722000000	8.341086000000	7.246608000000
5 Si	12.506271000000	5.360874000000	6.440021000000
6 C	11.220797000000	5.353626000000	2.096381000000
7 C	7.576979000000	4.927480000000	5.074283000000
8 C	8.184567000000	8.699944000000	7.606587000000
9 N	9.531602000000	9.047924000000	3.477664000000
10 N	11.792882000000	6.981742000000	6.262061000000
11 N	10.891767000000	6.026501000000	3.011230000000
12 N	8.428758000000	5.732048000000	4.915072000000
13 N	8.822177000000	8.332762000000	6.680940000000
14 C	10.989414000000	11.540756000000	2.546751000000
15 H	11.147549000000	11.875906000000	3.582360000000
16 H	10.098128000000	12.052747000000	2.156175000000
17 H	11.852063000000	11.874645000000	1.947947000000
18 C	10.657508000000	9.121613000000	0.650087000000
19 H	11.548163000000	9.423724000000	0.076541000000
20 H	9.778301000000	9.569010000000	0.166646000000
21 H	10.567176000000	8.027366000000	0.585947000000
22 C	12.493747000000	8.946481000000	3.060305000000
23 H	12.775142000000	9.254450000000	4.076161000000
24 H	13.271643000000	9.352750000000	2.391902000000
25 H	12.569414000000	7.852276000000	2.981400000000
26 C	7.438903000000	10.268629000000	1.625048000000
27 H	8.085428000000	11.056715000000	1.213897000000
28 H	6.409634000000	10.663744000000	1.639907000000
29 H	7.455475000000	9.412193000000	0.935352000000
30 C	7.779362000000	11.272691000000	4.505365000000
31 H	7.962165000000	10.997586000000	5.554428000000
32 H	6.772028000000	11.714485000000	4.440975000000
33 H	8.506025000000	12.048156000000	4.222205000000
34 C	6.611827000000	8.488458000000	3.929384000000
35 H	6.611614000000	7.600943000000	3.280620000000

ACCEPTED MANUSCRIPT

36	H	5.735429000000	8.897216000000	3.776096000000	5.616761000000	8.958020000000	3.857822000000
37	H	6.815837000000	8.127469000000	4.942958000000	6.746153000000	8.155298000000	4.967082000000
38	C	14.180391000000	8.523966000000	7.150696000000	14.261309000000	8.471087000000	7.222738000000
39	H	14.690956000000	7.632656000000	7.548497000000	14.753942000000	7.608722000000	7.694941000000
40	H	14.518570000000	9.393094000000	7.741487000000	14.569269000000	9.372548000000	7.776889000000
41	H	14.519304000000	8.668474000000	6.112018000000	14.643110000000	8.562641000000	6.194977000000
42	C	11.756527000000	8.214771000000	9.050334000000	11.777951000000	8.225471000000	9.031385000000
43	H	10.657027000000	8.164120000000	9.110883000000	10.679924000000	8.179799000000	9.068654000000
44	H	12.087217000000	9.100273000000	9.620420000000	12.101539000000	9.117889000000	9.590201000000
45	H	12.174526000000	7.321838000000	9.538121000000	12.178428000000	7.342127000000	9.547007000000
46	C	11.586487000000	10.039652000000	6.640731000000	11.731920000000	9.982403000000	6.528132000000
47	H	11.877718000000	10.306283000000	5.614908000000	12.399876000000	10.389616000000	5.757196000000
48	H	11.989661000000	10.823787000000	7.307347000000	11.718014000000	10.708814000000	7.357906000000
49	H	10.489252000000	10.086034000000	6.719107000000	10.702846000000	9.982696000000	6.134531000000
50	C	13.961485000000	5.280307000000	5.275187000000	14.040476000000	5.200830000000	5.350868000000
51	H	13.668814000000	5.388484000000	4.218582000000	13.781200000000	5.342136000000	4.291064000000
52	H	14.436816000000	4.291352000000	5.395031000000	14.483238000000	4.197943000000	5.460440000000
53	H	14.714384000000	6.050404000000	5.505226000000	14.810024000000	5.940679000000	5.615543000000
54	C	11.184180000000	4.104054000000	5.882347000000	11.252170000000	4.050674000000	5.919894000000
55	H	10.280972000000	4.103329000000	6.511238000000	10.361211000000	4.052802000000	6.563504000000
56	H	11.669759000000	3.117943000000	5.996019000000	11.733698000000	3.063739000000	6.017768000000
57	H	10.864638000000	4.173723000000	4.830998000000	10.924268000000	4.149509000000	4.876240000000
58	C	12.957259000000	5.008165000000	8.171102000000	12.983063000000	4.969110000000	8.228492000000
59	H	13.727273000000	5.684086000000	8.574283000000	13.757675000000	5.636298000000	8.632024000000
60	H	13.375223000000	3.985644000000	8.183449000000	13.384275000000	3.942745000000	8.261537000000
61	H	12.093445000000	5.024263000000	8.854382000000	12.110656000000	5.006633000000	8.896714000000

ACCEPTED MANUSCRIPT