

Theoretical Investigation on the Ligands Constructed from Phenanthroline and Five-Membered N-Heterocyclic Rings for Separation of Am(III) and Eu(III)

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Isolated phenanthroline and N-heterocyclic rings

The molecular properties of isolated phenanthroline and five-membered N-heterocyclic rings $R_1\sim R_8$ were evaluated by using electronic structure calculations. Several indicators are used to describe the molecular properties of Ph and $R_1\sim R_8$, including electrostatic potential (ESP), natural atomic charges of coordinating N atoms, HOMO energy, and protonation energy, which are calculated at the PBE0/6-311G(d) level and listed in **Table S1**. It is notable that $R_1\sim R_3$ are constitutional isomers, $R_2(R_3)$ are more stable than R_1 by 9.98 kcal/mol, and that $R_4\sim R_8$ are also constitutional isomers, among which $R_7(R_8)$ is the most stable, and from R_4 to R_5 to R_6 to $R_7(R_8)$ their energies go down successively by 5.33, 4.71 and 7.53 kcal/mol, respectively. Thus, the N-N and N-N-N structures are not conducive to molecular stabilization. Since the bonding interaction between the *f*-element and ligand is mainly ionic in nature, the ESP of the ligand can be used to measure coordination ability of the ligand with the lanthanides and actinides. The ESP values of the ligand are mapped onto electron density isosurface ($0.002e/\text{\AA}^3$) by various colors in **Fig.S1**. The ESP minimum of $R_1\sim R_8$ is located at the site of the N atom, and the ESP minimum of Ph is situated at the intersection of the two symmetry axes of the two pyridines through the N atom, as shown in **Fig.S1**, which are deemed as the coordination sites with the metal. The bidentate ligand Ph has much more negative ESP minimum than the monodentate ligand $R_1\sim R_8$, owing to the synergistic effect between the two pyridine N atoms, so its coordination capacity is certainly much stronger than $R_1\sim R_8$. And the coordination ability of the monodentate ligand $R_1\sim R_8$ reduces according to the order of $R_6 > R_2(R_3) > R_4 > R_7(R_8) > R_1 > R_5$, as shown by the ESP minima in **Table S1**. The charge on the coordinated N atom is the highest in $R_7(R_8)$, followed by $R_2(R_3)$, the third is Ph, and the charges on the coordinated N atom of the other ligands are close to each other. There is no apparent relationship between the ESP and $q(N)$. ESP is a physical observable and determined by the overall charge distribution of the molecule and reflects the ability of a molecule participating in electrostatic interaction, while the atomic charges have none of these properties.

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The extraction process of lanthanides and actinides is carried out under acidic conditions, the weakly alkaline extractants are easy to protonate. Protonation free energy ΔG was evaluated for the reaction equation $L + [H_3O]^+ = [LH]^+ + H_2O$ in aqueous phase, and listed in **Table S1**. It can be observed that the N atoms on Ph are more prone to protonation than $R_1 \sim R_8$. The protonation energy of the coordination N atoms on R_1 to R_8 is very close, so their protonation tendency is similar. In general, these monodentate ligands $R_1 \sim R_8$ and bidentate ligand Ph have a high protonation tendency.

The most important indicator reflecting property of the ligands is the interaction energy between the ligands and the Am(III) and Eu(III) ions in their complexes. In the gas phase, the 1:1 complexes of the monodentate ligands $R_1 \sim R_8$ with Am/Eu are unstable, so we calculate the 1:2 complexes $R_iMR_i^{3+}$ formed by M^{3+} with two identical ring R_i ($i = 1 \sim 8$). The complexes $R_iMR_i^{3+}$ have *cis-trans* isomers, here we only consider the *trans*-isomers. The geometry structures optimized for MPh^{3+} and $R_iMR_i^{3+}$ at the PBE0/6-311G(d)-RECP level are shown in **Fig.S2**. The interaction energy in $R_iMR_i^{3+}$ is $\Delta E = [E(R_iMR_i^{3+}) - E(M^{3+}) - 2E(R_i)]/2$. The calculated energy for each M-N interaction is about 128 ~ 200 kcal/mol, as shown in **Table S2**. It is found that $R_2(R_3)$ has the most strong interaction with both Am(III) and Eu(III) ions, the interaction strength of these ligands with Am and Eu follows the same order $R_2(R_3) > R_6 > R_1 > R_4 > R_7(R_8) > R_5$. It is notable that the Am-N bond length is significantly smaller than the corresponding Eu-N bond length and the Am-N bond order (WBI values) is also larger than that of the corresponding Eu-N bond, while the interaction energy of Am(III) ion with the N-donor is smaller than that of Eu(III) ion by about 20kcal/mol for R_1 to R_4 , or 17kcal/mol for R_6 to R_8 . This inconsistency between bond length, bond order, and interaction energy will be explained later.

It has been shown that the solvation has significant effects on the interaction of lanthanides and actinides with ligand. Here we consider two solvents, water and n-Octanol, for the 1:1 complexes MR_i^{3+} of the Am(III) and Eu(III) with the monodentate ligands R_i ($i = 1 \sim 8$). The model chemistry also has great influence on the prediction of the metal-ligand interaction, here we consider three quantum chemistry theoretical methods, DFT methods with quasi-relativistic effective core potentials (QRECP), ZORA (Zero Order Regular Approximation) and DKH (Douglas Kroll Hess) methods.

In the DFT calculation with QRECP, the functionals also have significant effects on the calculated results, so we take a series of functionals to perform DFT calculation, including the exchange- correlation functionals BP86 and PBE, and the hybridized functionals TPSSH, B3LYP, PBE0 and M06-2X. For the 1:1 complexes MR_i^{3+} ($i = 1 \sim 8$) of the metal with the monodentate ligands R_i , we consider two structures, one is the global minima, the other is the constrained minima, thus the minima with the M-N-C angle constrained to approximate the M^{3+} location observed in the complex $M(PhR_i)^{3+}$ of M^{3+} with the tridentate ligand PhR_i . For MR_6^{3+} the two structures have obvious difference, while for the other complexes MR_i^{3+} ($i \neq 6$) the two structures have small difference. For the global minima, the M-N bond length and the interaction energy between M^{3+} and R_i in the optimized structure by the various functionals in the aqueous phase were listed in **Tables S3 and S4** and shown in **Fig.S3**. For the constrained minima, we optimized the structures of the complexes MR_i^{3+} ($i = 1 \sim 8$) in the aqueous phase and n-octanol phase using DFT method with various functionals, the results of the aqueous phase are shown in **Fig.S4** and in **Tables S5 and S6**, and the results of the n-octanol phase are shown in **Fig.S5** and in **Tables S7 and S8**.

We first consider the results of the **constrained** minima in the **aqueous** phase. For the Am complexes AmR_i^{3+} , the bond lengths and bonding energies given by various functionals are quite consistent with the ESP of the ligands, thus AmR_2^{3+} and AmR_6^{3+} have the shortest Am-N bond length and the greatest bonding energy, while AmR_5^{3+} has the longest Am-N bond length and the least bonding energy, as shown in **Fig.S4** and **Tables S5-S6**. Moreover the variation law of the bond length and bonding

energy across the series of $R_1\sim R_8$ are also consistent for various functionals, except that B3LYP gives a quite large Am-N bond length for AmR_5^{3+} . For the Eu complexes EuR_i^{3+} , there are some obvious difference from the AmR_i^{3+} complexes. The variation laws of the bonding energies given by various functionals are consistent with each other, EuR_2^{3+} has the greatest bonding energy and EuR_5^{3+} has the least bonding energy, while the bonding energy of EuR_6^{3+} is always less than that of EuR_1^{3+} for the various functionals except for PBE0. The Eu-N bond lengths given by various functionals are very inconsistent, only the BP86 and PBE functionals produce Eu-N bond lengths consistent with the ESP of the ligands, all the hybridized functionals can not give bond lengths consistent with ESP. It is worth noting that although the bonding energy in the solution phase is much smaller than that in the gas phase due to the solvent effect, in the solution phase the bonding energy of Am-ligand bond is still less than that of Eu-ligand bond, similar to the gas phase. This should be a general feature of DFT calculations with quasi-relativistic effective potentials, regardless of the functional used. For the results of the global minima of the aqueous phase in **Fig.S3** and in **Tables S3 and S4**, except that the bond lengths have some inconsistent with the results of the constrained minima in the aqueous phase, the bonding energies of the global minima and constrained minima are consistent with each other. The influence of solvent effect on bond length and bond energy is obvious. For the constrained minima, although the results of the n-octanol phase have much similar characters to the results of the aqueous phase, we can still observe their obvious difference. For example, the consistency between the different functionals in the n-octanol phase gets worse, and the bond energy of the n-octanol phase is more than 10kcal/mol higher than that of the aqueous phase, as shown in **Fig.S5** and in **Tables S5 and S6**.

That the Am-ligand bonding energy predicted by DFT-RECP method is smaller than the Eu-ligand bond energy is quite unreasonable and inconsistent with the bond lengths, bond order and electron density topological properties (QTAIM parameters). To improve this situation, we perform relativistic quantum chemistry calculations using the ZORA and DKH methods. The calculated bond lengths and bonding energies of the Am-N and Eu-N bonds are shown in **Tables S9 and S10**, and also plotted in **Fig.S6**, and the corresponding QTAIM parameters are listed in **Table S11**. For comparison purposes, we have also included the results of DFT-RECP with PBE0 functional in these graphs and tables. The ZORA and DKH methods predicted much larger bonding energy than DFT-RECP-PBE0 method. For the Eu complexes EuR_i^{3+} , the DKH bonding energy is very close to the ZORA bonding energy, the former is only 2kcal/mol less than the later. However, for the Am complexes AmR_i^{3+} , the DKH bonding energy is much larger than the ZORA bonding energy, by at least 200 kcal/mol. It can be seen that the ZORA bonding energy of the Am-ligand bond is still less than the ZORA bonding energy of the Eu-ligand bond, similar to the DFT-RECP method, while the Am-ligand bonding energy predicted by DKH method is much larger than the corresponding Eu-ligand bonding energy. Therefore, DKH method predicted bonding energy consistent with bond length, while the ZORA and DFT-RECP methods fail to do this. From **Fig.S6(a) and (c)** and **Table S9**, we can see that the ZORA and DKH methods predicted much shorter Am-N bond than the DFT-RECP method except for the AmR_2^{3+} complex, while the Eu-N bond length predicted by ZORA and DKH methods is larger than that by DFT-RECP method except for the EuR_1^{3+} complex. It is worth noting that the Eu-N bond lengths predicted by ZORA and DKH are very close to each other, while the Am-N bond length predicted by DKH is smaller than that predicted by ZORA. So we note that there are significant differences in the treatment of Am and Eu by ZORA and DKH methods.

The QTAIM parameters, ρ and $\nabla^2\rho$ and H at the Am-N BCPs calculated by the ZORA and DKH methods, are much larger than those by DFT-RECP method, and the ZORA and DKH methods give very

close results, as shown in **Table S11**. The ZORA and DKH methods predict stronger and more covalent Am-N bond than the DFT-RECP method. However, for the Eu-N bond, the ZORA and DKH give a BCP electron density something less than that of DFT-RECP. Anyway, the three methods are consistent in predicting the nature of Am-N and Eu-N bonds, that is, both Am-N and Eu-N bonds are mainly ionic in nature, and the covalence of Am-N bond is higher than that of Eu-N bond.

Effects of spin-orbit coupling on compounds

To understand the impact of spin-orbit coupling in the interaction between Americium and the ligands, optimizations of the $\text{AmR}_4\text{PhR}_4(\text{NO}_3)_3$ compound were performed at the PBE0/ZORA theoretical level considering both spin-orbit coupling (SOC) and non-spin-orbit coupling (NOSOC) interactions. The obtained N-Am bond lengths, QTAIM properties, and Mayer bond orders are summarized in the **Table S12**. Notably, considering SOC interactions resulted in an average bond length for N-Am that was shorter by 0.0006 Å compared to when SOC interactions were not considered. However, the differences in QTAIM properties such as ρ , $\nabla^2\rho$, $H(r)$, and Mayer bond orders were not significantly distinct. Overall, the covalency of N-Am under SOC consideration appeared slightly higher than without SOC, although this increase in covalency was not distinctly pronounced. Additionally, single-point energies $E(\text{a.u.})$ and free energies $G(\text{a.u.})$ were calculated for the $\text{AmR}_4\text{PhR}_4(\text{NO}_3)_3$ compound under both spin-orbit coupling (SOC) and non-spin-orbit coupling (NOSOC) interactions (**Table S13**). The energy difference (ΔE in kcal/mol) and free energy difference (ΔG in kcal/mol) indicate that spin-orbit interactions contribute minimally to energy and Gibbs free energy calculations. Kaneko et al. also confirmed the negligible contribution of spin-orbit coupling effects to Gibbs energy calculations for complex formation reactions (less than 0.005 kcal/mol) (Inorg. Chem. 2018, 57, 14513-14523)

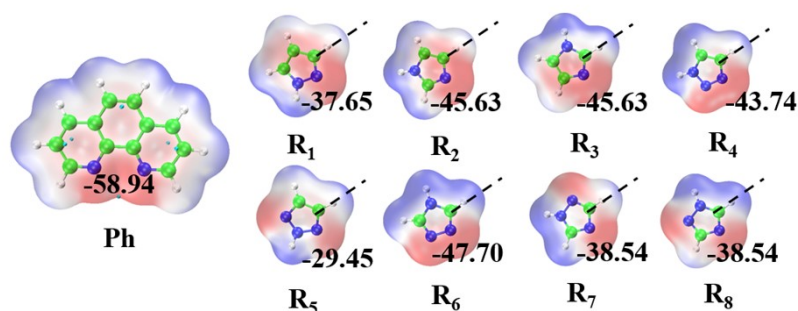


Fig. S1 ESP (kcal/mol) mapped onto the electron density isosurface ($0.002\text{e}/\text{\AA}^3$) for the free ligands phenanthroline and $\text{R}_1\text{-R}_8$

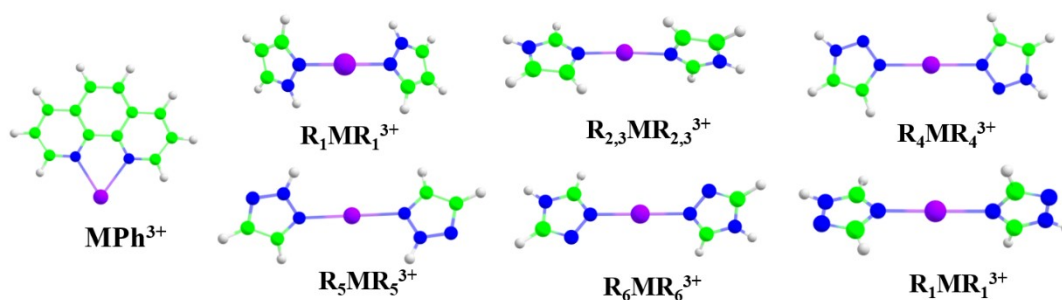


Fig. S2 Optimized structures of MPh^{3+} and $R_iMR_i^{3+}$ in gas phase at PBE0/6-311G(d)-RECP

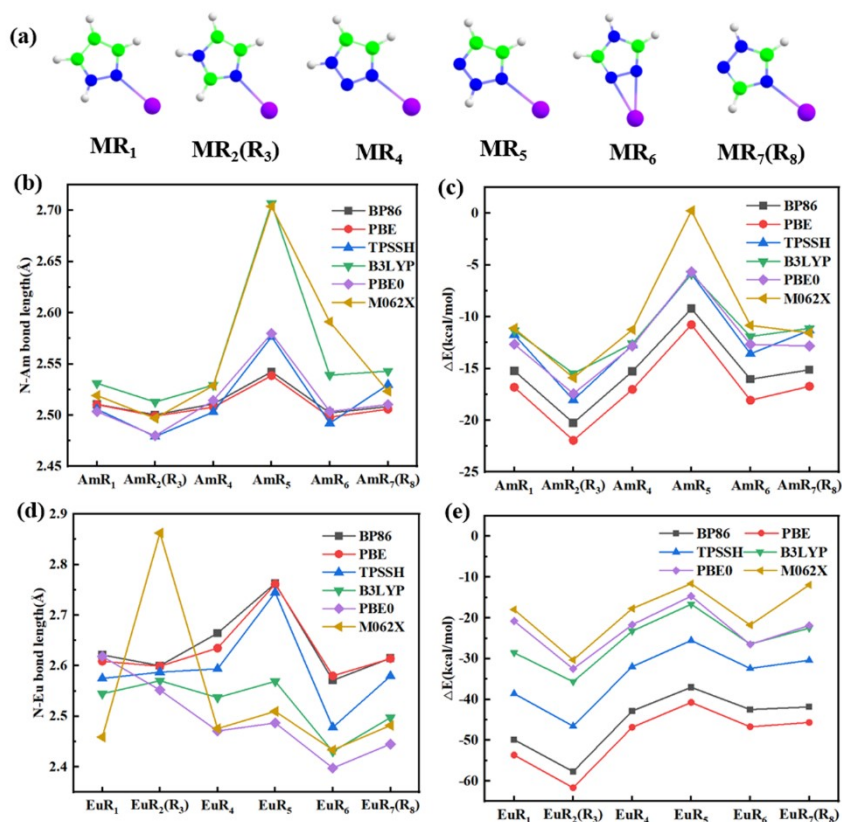


Fig. S3 (a) Optimized geometries, (b, d) N-M (M=Am, Eu) bond length and (c, e) interaction energies (kcal/mol) for **global minima** of the complexes MR_i^{3+} ($i = 1\sim 8$) calculated by using several DFT methods with the 6-311G(d)/RECP basis set using the CPCM solvation model in aqueous phase

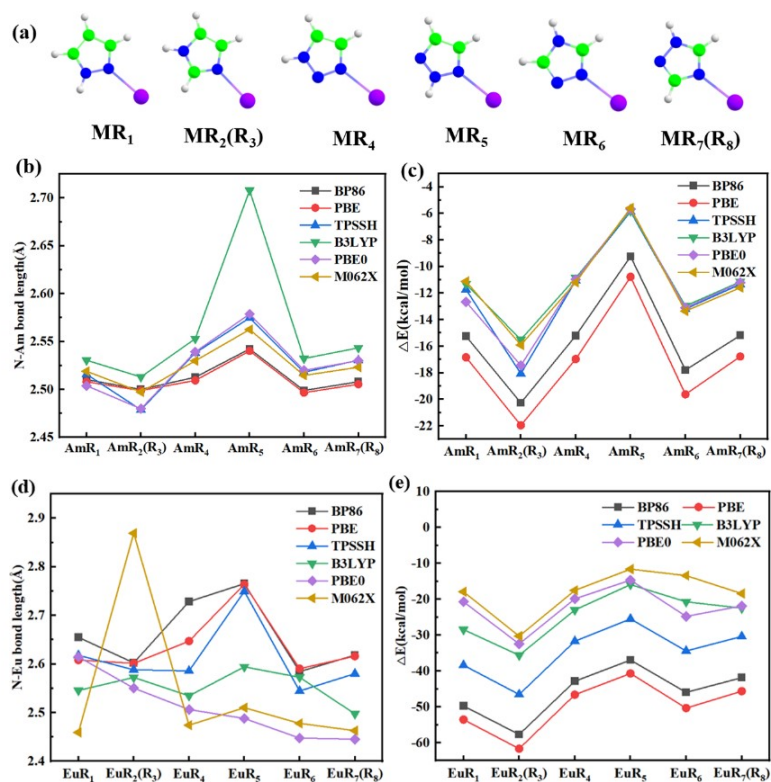


Fig. S4 (a) Optimized geometries, (b, d) N-M (M=Am, Eu) bond length (Å) and (c, e) interaction energies (kcal/mol) for the **constrained** minima of the complexes MR_i^{3+} ($i = 1\sim 8$) with the M-N-C angle to approximate the M^{3+} location observed in the complex $M(\text{PhR}_i)^{3+}$ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set and the CPCM solvation model in **aqueous** phase

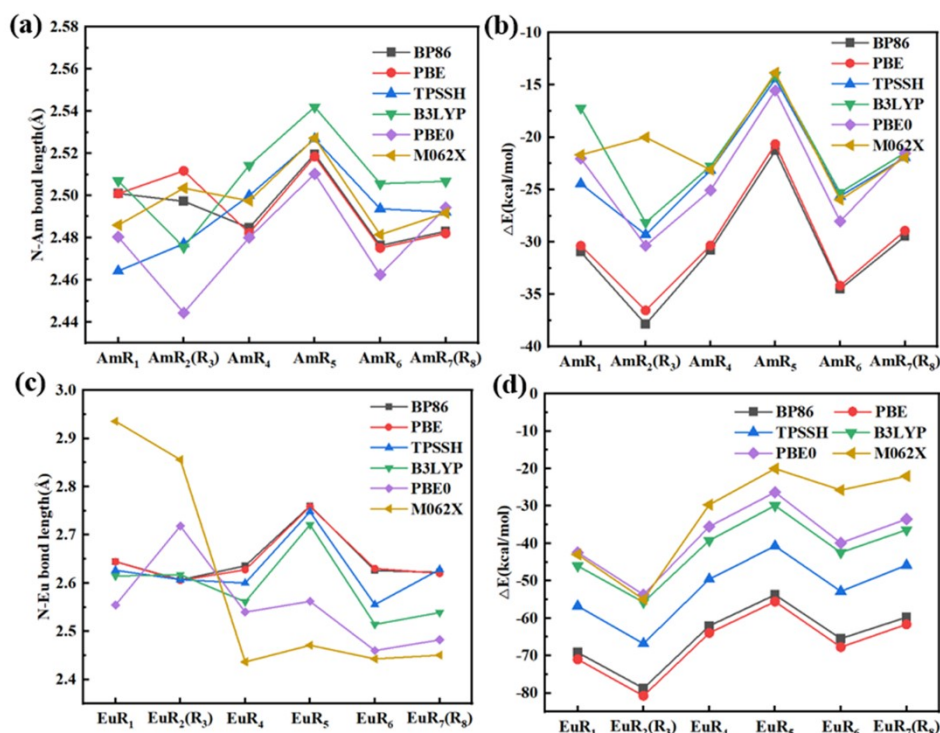


Fig. S5 (a, c) N-M (M=Am, Eu) bond length and (b, d) interaction energies (kcal/mol) for the **constrained** minima of the complexes MR_i^{3+} ($i = 1\sim 8$) with the M-N-C angle to approximate the M^{3+} location observed in the complex $M(\text{PhR}_i)^{3+}$ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set using the CPCM solvation model in **n-octanol** phase

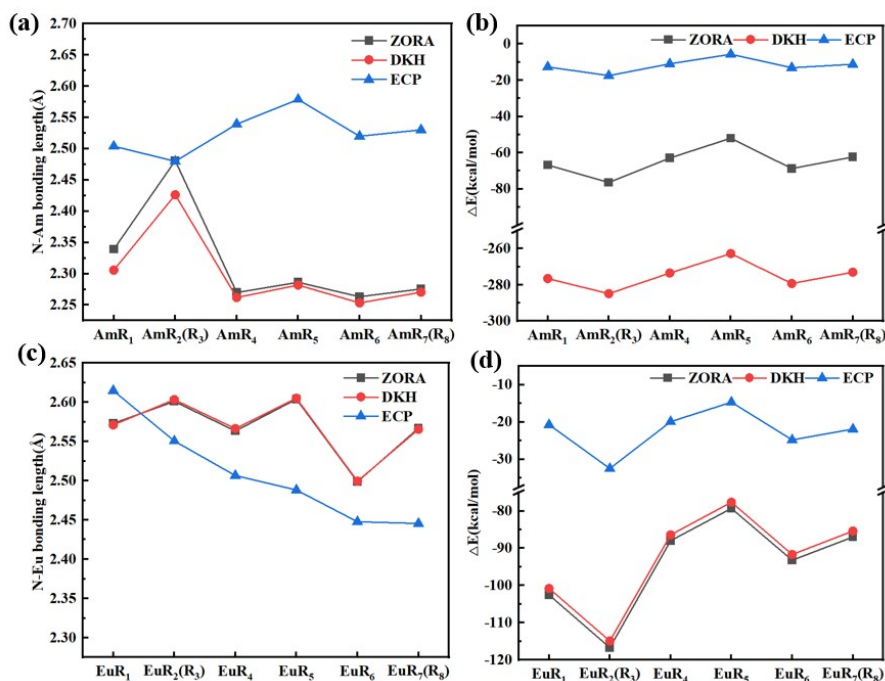


Fig. S6 (a, c) Am-N and Eu-N bond lengths (Å) and (b, d) bonding energies (kcal/mol) of the M-ligand interaction for the constrained minima of the MR_i^{3+} complexes ($i = 1\sim 8$) with the M-N-C angle constrained to approximate the M^{3+} location observed in the complex $M(\text{PhR}_i)^{3+}$ calculated by using the PBE0/ZORA/DKH/6-311G(d)-RECP methods and the CPCM solvation model in aqueous phase

Table S1 Molecular energy, the ESP minima, natural atomic charges $q(\text{N})$ of the N atom, the energy levels of HOMO and LUMO and their gap, and protonation energies of Ph and R₁~R₈ in the gas phase calculated at the PBE0/6-311G(d) level. Protonation free energy ΔG is the free energy change of the reaction equation $\text{L} + [\text{H}_3\text{O}]^+ = [\text{LH}]^+ + \text{H}_2\text{O}$ in aqueous phase.

	E(a.u.)	HOMO	LUMO	gap	ESP(kcal/mol)	$q(\text{N})$	$\Delta\text{G}(\text{kcal/mol})$
Ph	-571.051755	-6.6969	-1.4919	5.2050	-58.94	-0.4201	-189.8
R ₁	-225.987774	-7.1055	0.7012	7.8067	-37.65	-0.2892	-157.4
R ₂ (R ₃)	-226.003750	-6.5677	0.9357	7.5034	-45.63	-0.4952	-154.3
R ₄	-242.004456	-7.6516	0.0386	7.6903	-43.74	-0.2612	-159.2
R ₅	-242.012921	-7.9209	-0.0335	7.8875	-29.45	-0.2641	-159.3
R ₆	-242.020442	-7.3524	0.5187	7.8711	-47.70	-0.2993	-153.7
R ₇ (R ₈)	-242.032402	-7.8042	0.2508	8.0550	-38.54	-0.5140	-154.6

Table S2 Interaction energies ΔE (kcal/mol), bond lengths $r(\text{N-M})$ (Å), and bond orders (WBIs) between M and N in the complexes MPh^{3+} and $\text{R}_i\text{MR}_i^{3+}$ in the gas phase calculated at PBE0/6-311G(d)-RECP.

Ligands	$\Delta\text{E}(\text{Am})$	$\Delta\text{E}(\text{Eu})$	$r(\text{N-Am})$	$r(\text{N-Eu})$	WBI(N-Am)	WBI(N-Eu)
Ph	-345.6	-388.3	2.549	2.565	0.0903	0.0651
R ₁	-165.1	-184.5	2.437	2.616	0.1764	0.0655
R ₂ (R ₃)	-179.5	-200.4	2.541	2.603	0.0994	0.0645
R ₄	-164.1	-183.4	2.306	2.630	0.2898	0.0549
R ₅	-138.3	-159.2	2.600	2.705	0.0928	0.0536
R ₆	-171.7	-188.7	2.309	2.600	0.2732	0.0600
R ₇ (R ₈)	-155.2	-171.6	2.334	2.663	0.2684	0.0568

Table S3 N-M (M=Am, Eu) bond length for global minima of the complexes MR_i^{3+} ($i = 1\sim 8$) calculated by using several DFT methods with the 6-311G(d)/RECP basis set using the CPCM solvation model in aqueous phase

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁	2.511	2.510	2.506	2.531	2.504	2.519
AmR ₂ (R ₃)	2.500	2.499	2.479	2.513	2.480	2.497
AmR ₄	2.511	2.508	2.503	2.529	2.514	2.529
AmR ₅	2.542	2.539	2.577	2.707	2.580	2.704
AmR ₆	2.502	2.498	2.492	2.539	2.504	2.591
AmR ₇ (R ₈)	2.508	2.506	2.530	2.543	2.510	2.523
Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	2.621	2.609	2.575	2.545	2.619	2.459
EuR ₂ (R ₃)	2.600	2.599	2.587	2.570	2.552	2.862
EuR ₄	2.665	2.635	2.594	2.537	2.471	2.476
EuR ₅	2.763	2.761	2.745	2.569	2.487	2.510
EuR ₆	2.571	2.580	2.478	2.430	2.398	2.434

EuR ₇ (R ₈)	2.615	2.614	2.580	2.498	2.445	2.482
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Table S4 N-M (M=Am, Eu) interaction energies (kcal/mol) for **global minima** of the complexes MR_{*i*}³⁺ (*i* = 1~8) calculated by using several DFT methods with the 6-311G(d)/RECP basis set using the CPCM solvation model in **aqueous phase**

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁	-15.2	-16.8	-11.7	-11.3	-12.7	-11.1
AmR ₂ (R ₃)	-20.3	-21.9	-18.0	-15.5	-17.4	-15.9
AmR ₄	-15.3	-17.0	-12.7	-12.6	-12.8	-11.2
AmR ₅	-9.2	-10.8	-5.9	-5.9	-5.7	0.2
AmR ₆	-16.0	-18.1	-13.6	-11.9	-12.7	-10.8
AmR ₇ (R ₈)	-15.1	-16.7	-11.3	-11.1	-12.8	-11.6
Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	-49.9	-53.7	-38.6	-28.6	-20.8	-18.0
EuR ₂ (R ₃)	-57.7	-61.7	-46.6	-35.7	-32.5	-30.3
EuR ₄	-42.8	-46.8	-32.0	-23.2	-21.7	-17.7
EuR ₅	-37.0	-40.7	-25.6	-16.7	-14.7	-11.6
EuR ₆	-42.5	-46.7	-32.4	-26.4	-26.5	-21.8
EuR ₇ (R ₈)	-41.8	-45.6	-30.4	-22.5	-21.9	-11.9

Table S5 Am-M and Eu-N bond lengths for the **constrained** minima of the complexes MR_{*i*}³⁺ (*i* = 1~8) with the M-N-C angle to approximate the M³⁺ location observed in the complex M(PhR_{*i*})³⁺ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set and the CPCM solvation model in **aqueous phase**

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁ ³⁺	2.510	2.508	2.516	2.531	2.504	2.519
AmR ₂ (R ₃)	2.500	2.499	2.479	2.513	2.480	2.497
AmR ₄	2.513	2.510	2.538	2.553	2.539	2.530
AmR ₅	2.542	2.540	2.575	2.708	2.579	2.563
AmR ₆	2.499	2.497	2.518	2.532	2.520	2.515
AmR ₇ (R ₈)	2.508	2.506	2.531	2.544	2.530	2.523
Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	2.655	2.608	2.618	2.546	2.615	2.459
EuR ₂ (R ₃)	2.602	2.601	2.588	2.573	2.551	2.869
EuR ₄	2.729	2.647	2.586	2.535	2.507	2.474
EuR ₅	2.765	2.764	2.749	2.594	2.488	2.510
EuR ₆	2.584	2.591	2.545	2.573	2.448	2.478
EuR ₇ (R ₈)	2.618	2.616	2.580	2.498	2.446	2.463

Table S6 The metal-ligand interaction energies (kcal/mol) for the **constrained** minima of the complexes MR_i^{3+} ($i = 1\sim 8$) with the M-N-C angle constrained to approximate the M^{3+} location observed in the complex $M(PhR_i)^{3+}$ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set and the CPCM solvation model in **aqueous** phase

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁	-15.3	-16.8	-11.7	-11.3	-12.7	-11.1
AmR ₂ (R ₃)	-20.3	-22.0	-18.1	-15.5	-17.5	-15.9
AmR ₄	-15.2	-17.0	-11.1	-10.9	-11.0	-11.2
AmR ₅	-9.2	-10.8	-5.9	-5.8	-5.7	-5.6
AmR ₆	-17.8	-19.6	-13.2	-13.0	-13.1	-13.4
AmR ₇ (R ₈)	-15.2	-16.8	-11.3	-11.2	-11.2	-11.6
	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	-49.8	-53.6	-38.4	-28.5	-20.7	-17.9
EuR ₂ (R ₃)	-57.7	-61.7	-46.6	-35.6	-32.5	-30.3
EuR ₄	-42.9	-46.6	-31.7	-23.0	-19.9	-17.6
EuR ₅	-37.0	-40.7	-25.5	-15.9	-14.7	-11.6
EuR ₆	-46.0	-50.4	-34.5	-20.7	-24.8	-13.4
EuR ₇ (R ₈)	-41.9	-45.7	-30.4	-22.5	-21.9	-18.4

Table S7 Am-M and Eu-N bond lengths for the **constrained** minima of the complexes MR_i^{3+} ($i = 1\sim 8$) with the M-N-C angle to approximate the M^{3+} location observed in the complex $M(PhR_i)^{3+}$ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set using the CPCM solvation model in **n-octanol** phase

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁	2.501	2.501	2.464	2.507	2.480	2.486
AmR ₂ (R ₃)	2.497	2.512	2.477	2.476	2.444	2.504
AmR ₄	2.485	2.482	2.500	2.514	2.480	2.498
AmR ₅	2.520	2.519	2.527	2.542	2.510	2.527
AmR ₆	2.476	2.475	2.494	2.506	2.462	2.482
AmR ₇ (R ₈)	2.483	2.482	2.492	2.507	2.494	2.492
	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	2.645	2.644	2.627	2.615	2.554	2.936
EuR ₂ (R ₃)	2.607	2.606	2.607	2.618	2.718	2.856
EuR ₄	2.636	2.628	2.600	2.561	2.540	2.437
EuR ₅	2.760	2.759	2.748	2.721	2.562	2.471
EuR ₆	2.626	2.630	2.555	2.515	2.460	2.443
EuR ₇ (R ₈)	2.623	2.620	2.628	2.539	2.483	2.451

Table S8 The metal-ligand interaction energies (kcal/mol) for the **constrained** minima of the complexes MR_i^{3+} ($i = 1\sim 8$) with the M-N-C angle constrained to approximate the M^{3+} location observed in the complex $M(PhR_i)^{3+}$ calculated by using several DFT functionals with the 6-311G(d)/RECP basis set using the CPCM solvation model in **n-octanol** phase

Complexes	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
AmR ₁	-31.0	-30.4	-24.4	-17.2	-22.0	-21.7
AmR ₂ (R ₃)	-37.9	-36.5	-29.3	-28.1	-30.4	-20.0
AmR ₄	-30.8	-30.3	-23.2	-22.8	-25.1	-23.1
AmR ₅	-21.3	-20.7	-14.5	-14.1	-15.5	-13.8
AmR ₆	-34.5	-34.2	-25.6	-25.3	-28.0	-26.0
AmR ₇ (R ₈)	-29.5	-28.9	-21.9	-21.5	-21.5	-21.9
	BP86	PBE	TPSSH	B3LYP	PBE0	M062X
EuR ₁	-69.1	-71.0	-56.7	-46.0	-42.4	-43.0
EuR ₂ (R ₃)	-78.7	-80.7	-66.8	-55.7	-53.7	-54.9
EuR ₄	-62.0	-63.9	-49.5	-39.2	-35.5	-29.7
EuR ₅	-53.7	-55.5	-40.7	-29.9	-26.3	-20.0
EuR ₆	-65.4	-67.7	-52.8	-42.4	-39.9	-25.7
EuR ₇ (R ₈)	-59.7	-61.6	-45.8	-36.4	-33.5	-22.0

Table S9 Am-N and Eu-N bond lengths (Å) for the constrained minima of the MR_i³⁺ complexes (*i* = 1~8) with the M-N-C angle constrained to approximate the M³⁺ location observed in the complex M(PhR_i)³⁺ calculated by using the PBE0/ZORA/DKH/6-311G(d)-RECP methods and the CPCM solvation model in aqueous phase

	ECP	ZORA	DKH		ECP	ZORA	DKH
AmR ₁	2.504	2.339	2.306	EuR ₁	2.615	2.573	2.571
AmR ₂ (R ₃)	2.480	2.481	2.426	EuR ₂ (R ₃)	2.551	2.601	2.603
AmR ₄	2.539	2.270	2.262	EuR ₄	2.507	2.563	2.566
AmR ₅	2.579	2.286	2.282	EuR ₅	2.488	2.604	2.605
AmR ₆	2.520	2.263	2.253	EuR ₆	2.448	2.499	2.500
AmR ₇ (R ₈)	2.530	2.276	2.271	EuR ₇ (R ₈)	2.446	2.567	2.565

Table S10 Bonding energies (kcal/mol) of the M-ligand interaction for the constrained minima of the MR_i³⁺ complexes (*i* = 1~8) with the M-N-C angle constrained to approximate the M³⁺ location observed in the complex M(PhR_i)³⁺ calculated by using the PBE0/ZORA/DKH/6-311G(d)-RECP methods and the CPCM solvation model in aqueous phase

	ECP	ZORA	DKH		ECP	ZORA	DKH
AmR ₁	-12.7	-66.8	-276.6	EuR ₁	-20.7	-102.5	-100.8
AmR ₂ (R ₃)	-17.5	-76.4	-284.9	EuR ₂ (R ₃)	-32.5	-116.7	-114.9
AmR ₄	-11.0	-62.9	-273.5	EuR ₄	-19.9	-88.0	-86.4
AmR ₅	-5.7	-52.0	-262.8	EuR ₅	-14.7	-79.3	-77.7
AmR ₆	-13.1	-68.7	-279.3	EuR ₆	-24.8	-93.2	-91.7
AmR ₇ (R ₈)	-11.2	-62.3	-273.0	EuR ₇ (R ₈)	-21.9	-87.0	-85.4

Table S11 Electron density ρ , Laplacian $\nabla^2\rho$, and local electron Energy density $H(r)$ at the N-M BCPs in the MR_i³⁺ complexes (*i* = 1~8) with the M-N-C angle constrained to approximate the M³⁺ location observed in the complex M(PhR_i)³⁺ calculated by using the PBE0/ZORA/DKH/6-311G(d)-RECP methods and the CPCM solvation model in aqueous phase.

ρ	ECP	ZORA	DKH	ρ	ECP	ZORA	DKH
AmR ₁	0.0548	0.0810	0.0878	EuR ₁	0.0364	0.0397	0.0399

AmR ₂ (R ₃)	0.0593	0.0581	0.0663	EuR ₂ (R ₃)	0.0430	0.0377	0.0375
AmR ₄	0.0527	0.1005	0.1017	EuR ₄	0.0496	0.0416	0.0412
AmR ₅	0.0467	0.0937	0.0941	EuR ₅	0.0517	0.0369	0.0367
AmR ₆	0.0551	0.1020	0.1037	EuR ₆	0.0586	0.0486	0.0485
AmR ₇ (R ₈)	0.0532	0.0974	0.0980	EuR ₇ (R ₈)	0.0583	0.0408	0.0409
$\nabla^2\rho$	ECP	ZORA	DKH	$\nabla^2\rho$	ECP	ZORA	DKH
AmR ₁	0.1550	0.2679	0.2733	EuR ₁	0.1235	0.1508	0.1514
AmR ₂ (R ₃)	0.1567	0.2021	0.2205	EuR ₂ (R ₃)	0.1416	0.1393	0.1385
AmR ₄	0.1480	0.2192	0.2275	EuR ₄	0.1451	0.1484	0.1488
AmR ₅	0.1396	0.2304	0.2373	EuR ₅	0.1368	0.1359	0.1357
AmR ₆	0.1534	0.2219	0.2305	EuR ₆	0.1399	0.1775	0.1770
AmR ₇ (R ₈)	0.1510	0.2242	0.2315	EuR ₇ (R ₈)	0.1429	0.1484	0.1488
$H(r)$	ECP	ZORA	DKH	$H(r)$	ECP	ZORA	DKH
AmR ₁	-0.0069	-0.0134	-0.0175	EuR ₁	0.0002	0.0016	0.0016
AmR ₂ (R ₃)	-0.0091	-0.0038	-0.0069	EuR ₂ (R ₃)	-0.0016	0.0015	0.0016
AmR ₄	-0.0064	-0.0264	-0.0272	EuR ₄	-0.0044	0.0010	0.0011
AmR ₅	-0.0040	-0.0217	-0.0219	EuR ₅	-0.0054	0.0019	0.0019
AmR ₆	-0.0074	-0.0275	-0.0286	EuR ₆	-0.0085	-0.0001	-0.0001
AmR ₇ (R ₈)	-0.0066	-0.0244	-0.0248	EuR ₇ (R ₈)	-0.0084	0.0012	0.0012

Table S12 Under the PBE0/ZORA theoretical level, considering the interactions of spin-orbit coupling (SOC) and non-spin-orbit coupling (NOSOC), the values of the N-Am bond length in the AmR₄PhR₄(NO₃)₃ compound, along with ρ , $\nabla^2\rho$, $H(r)$, and Mayer bond order. ^a

Bond length	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am
PBE0/ZORA(SOC)	2.6271	2.6717	2.6729	2.6380	2.6524
PBE0/ZORA(NOSOC)	2.6262	2.6733	2.6745	2.6379	2.6530
ρ	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am
PBE0/ZORA(SOC)	0.0409	0.0374	0.0375	0.0399	0.0389
PBE0/ZORA(NOSOC)	0.0408	0.0375	0.0376	0.0399	0.0389
$\nabla^2\rho$	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am
PBE0/ZORA(SOC)	0.1410	0.1249	0.1250	0.1374	0.1321
PBE0/ZORA(NOSOC)	0.1408	0.1254	0.1254	0.1374	0.1323
$H(r)*10^2$	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am
PBE0/ZORA(SOC)	-0.1640	-0.1418	-0.1483	-0.1463	-0.1501
PBE0/ZORA(NOSOC)	-0.1622	-0.1440	-0.1501	-0.1460	-0.1506
Mayer bond orders	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am
PBE0/ZORA(SOC)	0.2003	0.1952	0.1935	0.2013	0.1976
PBE0/ZORA(NOSOC)	0.2001	0.1952	0.1934	0.2012	0.1975

^a:ZORA employs the ZORA-def2-TZVP basis set for C, H, O, and N elements, with the Am and Eu atoms utilizing the SARC-ZORA-TZVP basis set.

Table S13 The single-point energies and free energies of the AmR₄PhR₄(NO₃)₃ compound under spin-orbit coupling (SOC) and non-spin-orbit coupling (NOSOC) interactions at the PBE0/ZORA theoretical level, along with the differences in single-point energies and free energies between SOC and NOSOC.

AmR ₄ PhR ₄ (NO ₃) ₃	E(a.u.)	ΔE (kcal/mol)	G(a.u.)	ΔG (kcal/mol)
PBE0/ZORA(SOC)	-33979.25585481	0.0069	-33979.01355248	0.0055
PBE0/ZORA(NOSOC)	-33979.25584385		-33979.01356119	

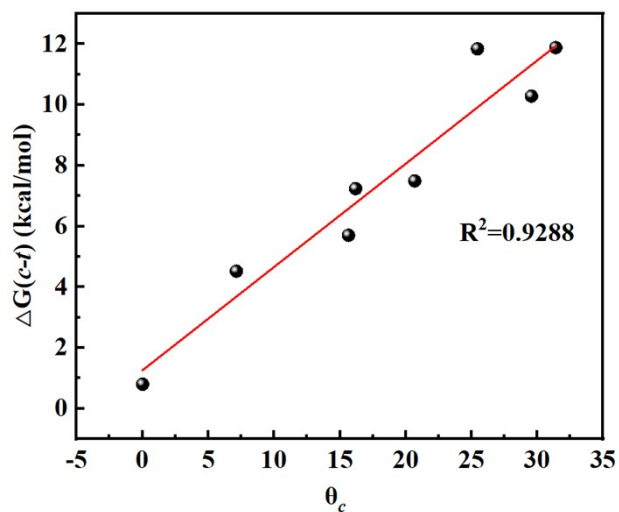
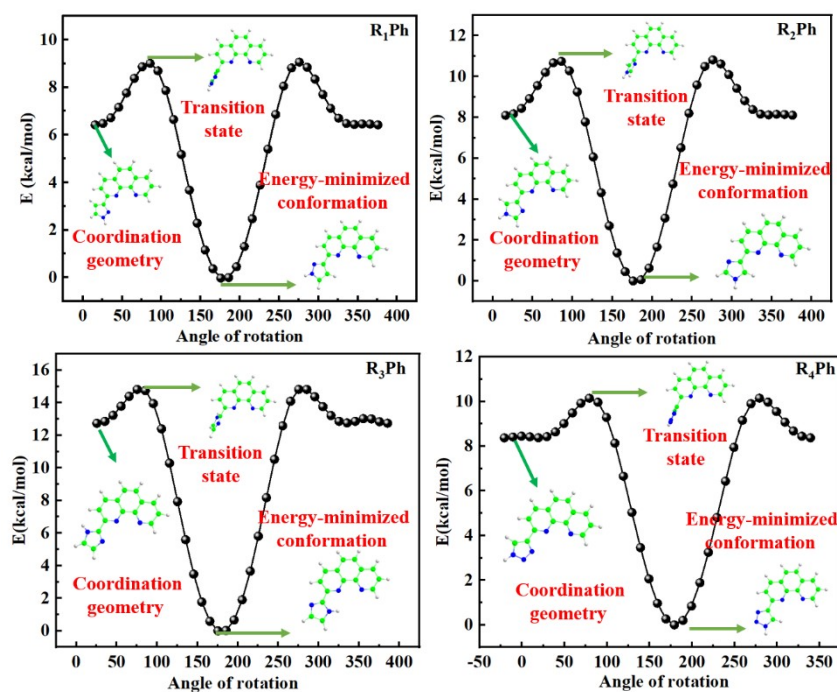


Fig.S7 The angle θ_c versus the free energy $\Delta G(c-t)$ required to convert from the trans- to cis- conformations



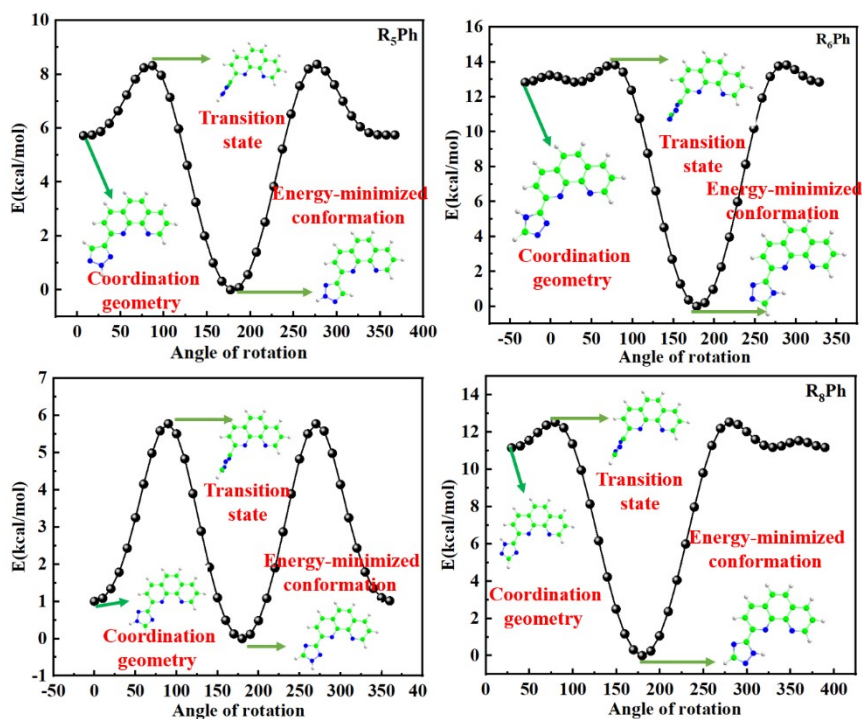


Fig. S8 The potential energy curve of the R_lPh rotating around the C-C single bond

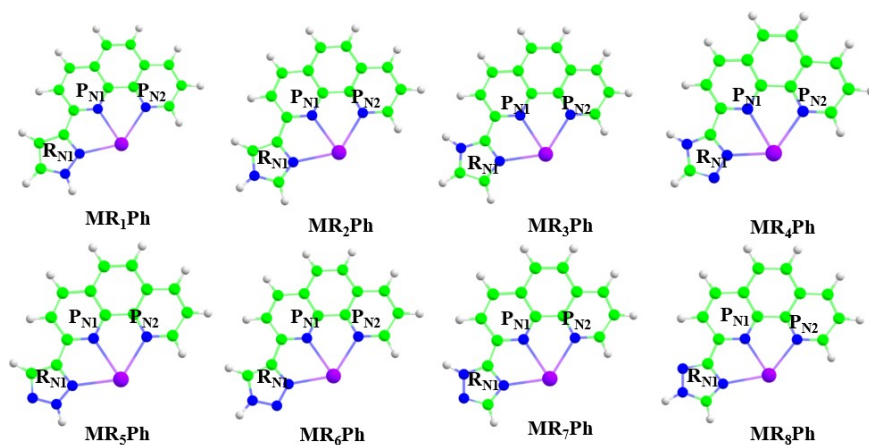


Fig. S9 Geometric configuration of $M(R_lPh)^{3+}$ ($l = 1-8$)

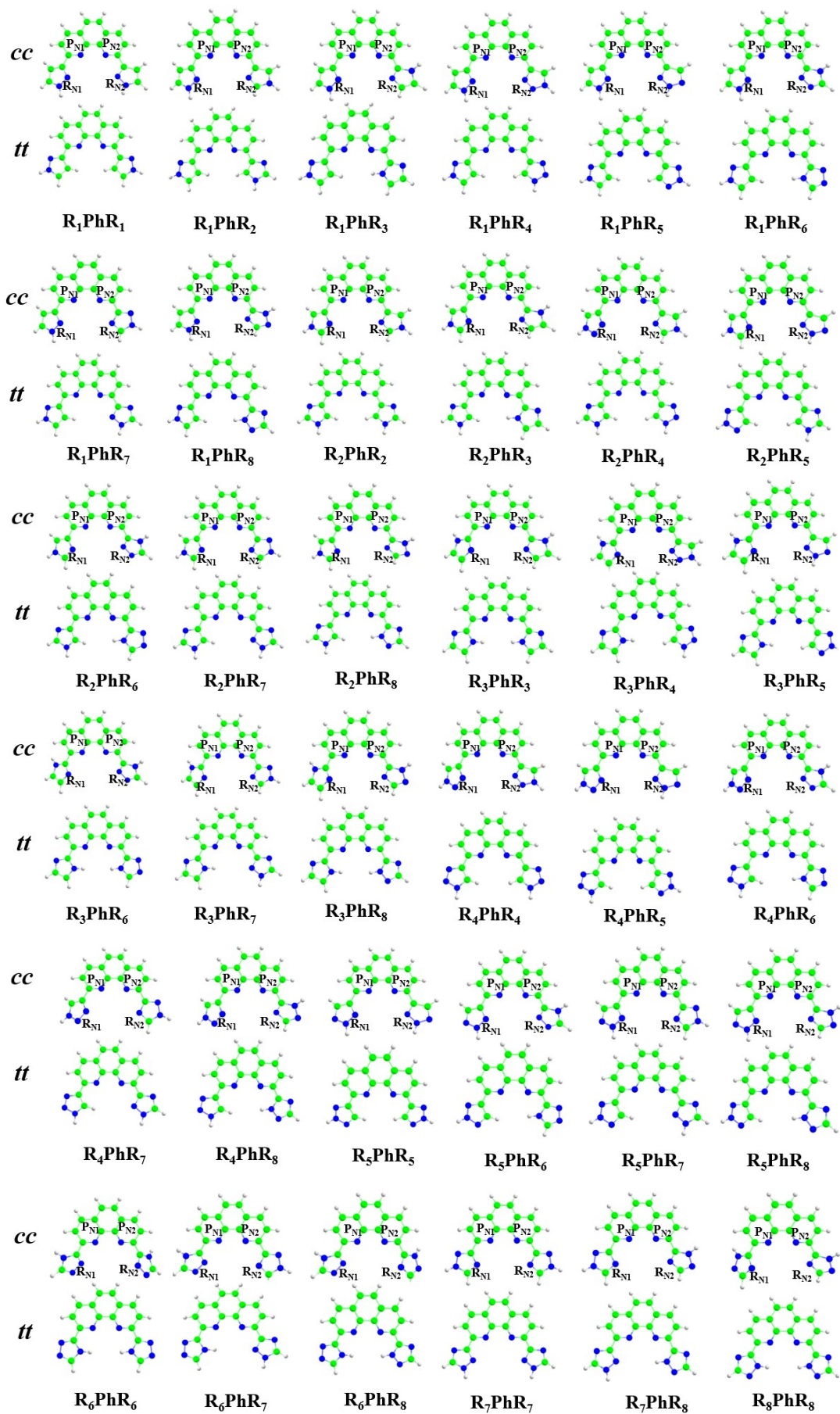


Fig. S10 The molecular structures of the ligands $R_l\text{PhR}_r$ ($l, r = 1\sim 8$)

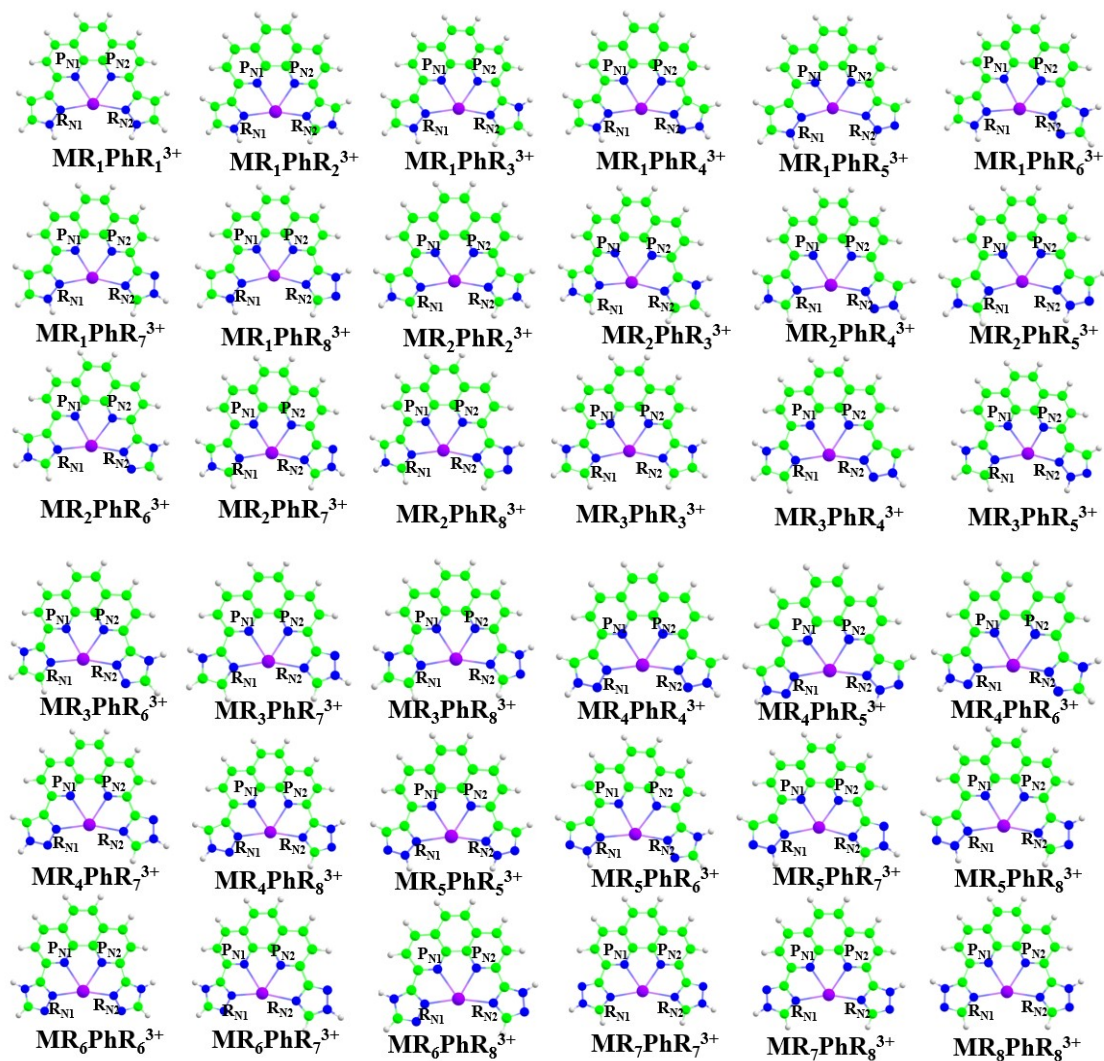


Fig. S11 optimized geometric structures of the complexes $\text{M}(\text{R}_l\text{PhR}_r)^{3+}$ ($\text{M} = \text{Am}, \text{Eu}$)

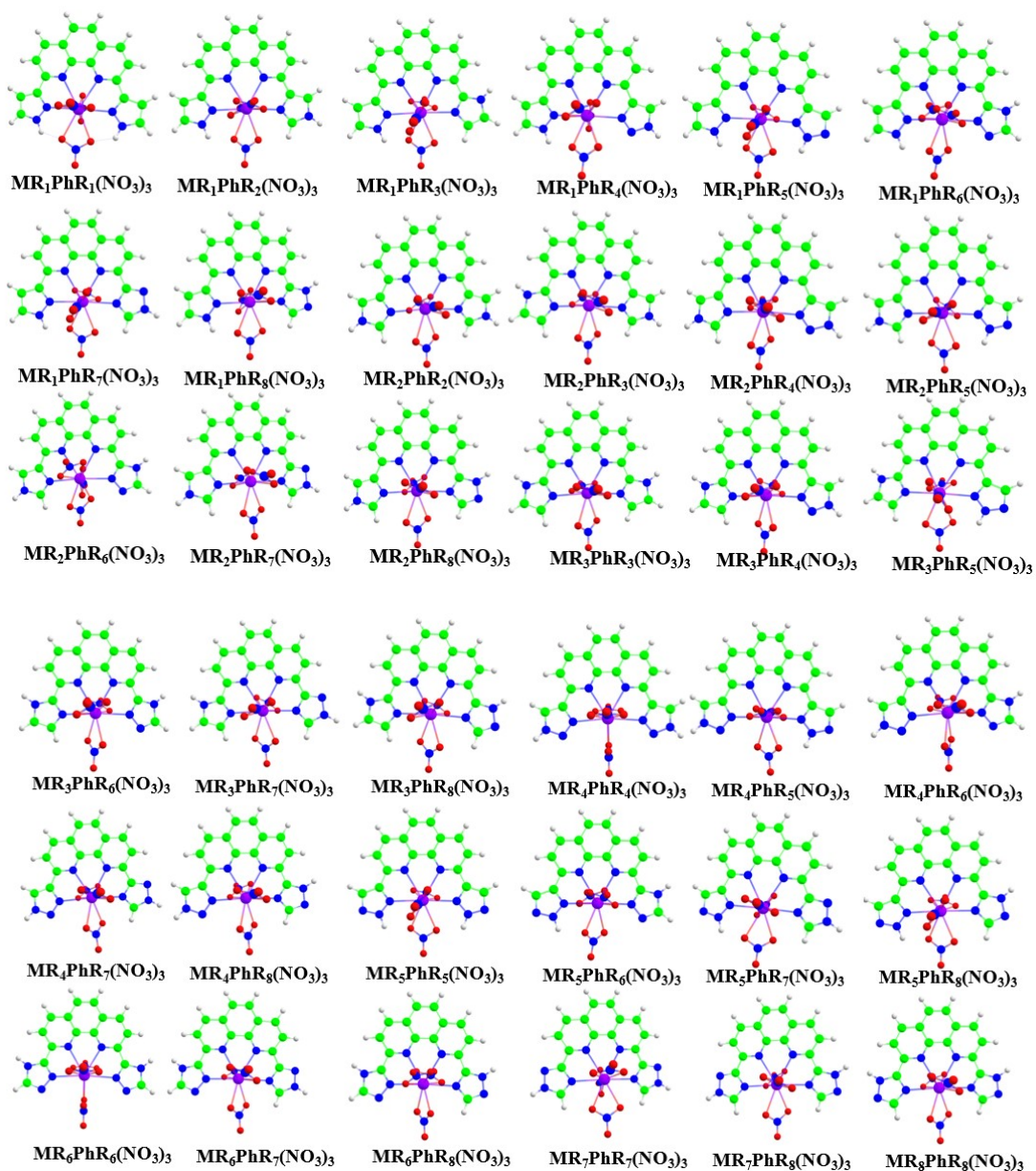


Fig. S12 Geometric structures of $M(R_lPhR_r)(NO_3)_3$ at the PBE0/6-311G(d)-RECP level

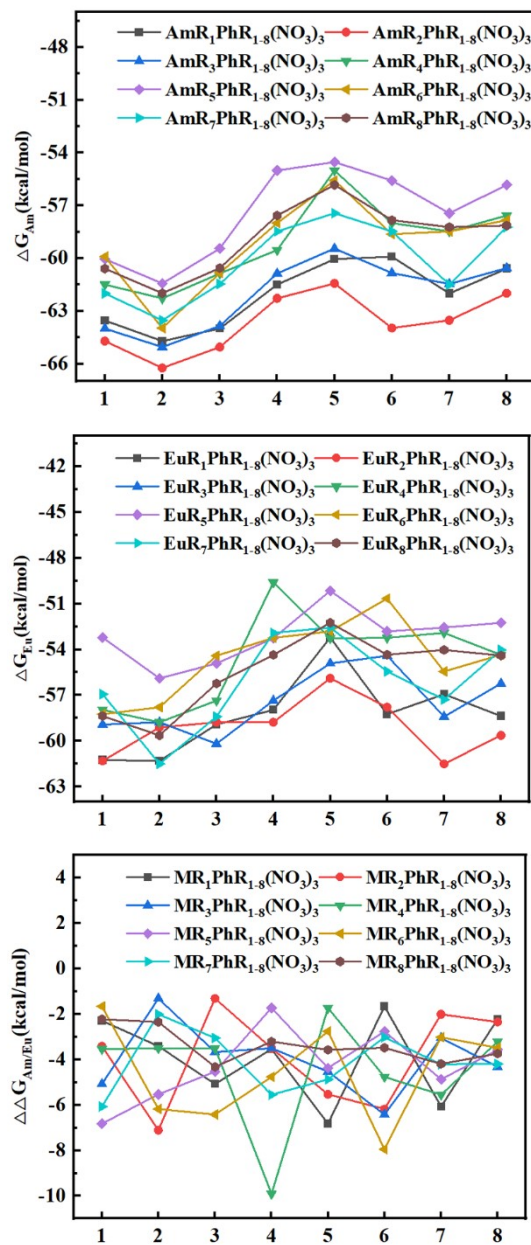


Fig. S13 Gibbs free energy (a) ΔG_{Am} , (b) ΔG_{Eu} , and (c) $\Delta\Delta G_{\text{Am/Eu}}$ (kcal/mol) of the solvent extraction process between the aqueous phase and n-octanol phase for $\text{M}(\text{R}_l\text{PhR}_r)(\text{NO}_3)_3$ ($l, r = 1-8$) calculated by the PBE0/6-311G(d)-RECP method.

Table S14 ESP values of $R_l\text{Ph}$ and the sum of ESPs of R_l and Ph and their scaling relationship. $\text{ESP}(\text{PhR}) \sim [\text{ESP}(\text{Ph}) + \text{ESP}(\text{R})]$ calculated by PBE0/6-311G(d) method

	ESP		ESP		ESP(Ph+R)/ESP(R)
$R_1\text{Ph}$	-70.67	$R_1+\text{Ph}$	-96.59	$(R_1+\text{Ph})/R_1$	1.37
$R_2\text{Ph}$	-74.66	$R_2+\text{Ph}$	-104.57	$(R_2+\text{Ph})/R_2$	1.40
$R_3\text{Ph}$	-70.03	$R_3+\text{Ph}$	-104.57	$(R_3+\text{Ph})/R_3$	1.49
$R_4\text{Ph}$	-70.11	$R_4+\text{Ph}$	-102.68	$(R_4+\text{Ph})/R_4$	1.46
$R_5\text{Ph}$	-65.62	$R_5+\text{Ph}$	-88.39	$(R_5+\text{Ph})/R_5$	1.35
$R_6\text{Ph}$	-66.39	$R_6+\text{Ph}$	-106.64	$(R_6+\text{Ph})/R_6$	1.61
$R_7\text{Ph}$	-70.81	$R_7+\text{Ph}$	-97.48	$(R_7+\text{Ph})/R_7$	1.38
$R_8\text{Ph}$	-64.01	$R_8+\text{Ph}$	-97.48	$(R_8+\text{Ph})/R_8$	1.52

Table S15 The averaged bond lengths (r), Mayer bond orders (m), and WBI bond orders (w) of the M-N bonds and the bonding energies ΔE_M (kcal/mol) in $M(R_l\text{Ph})^{3+}$ ($l=1-8$) calculated by PBE0/6-311G(d)-RECP method

	$r(\text{N-Am})$	$r(\text{N-Eu})$	$w(\text{N-Am})$	$w(\text{N-Eu})$	$m(\text{N-Am})$	$m(\text{N-Eu})$	ΔE_{Am}	ΔE_{Eu}
MR_1Ph	2.489	2.576	0.1231	0.0619	0.3622	0.2641	-409.2	-449.2
MR_2Ph	2.510	2.574	0.1100	0.0614	0.3387	0.2655	-423.7	-464.5
MR_3Ph	2.516	2.579	0.1077	0.0601	0.3322	0.2603	-419.5	-460.2
MR_4Ph	2.486	2.591	0.1224	0.0573	0.3516	0.2434	-411.7	-451.2
MR_5Ph	2.531	2.593	0.1038	0.0588	0.3175	0.2516	-389.6	-430.8
MR_6Ph	2.442	2.596	0.1503	0.0567	0.4028	0.2393	-414.3	-450.4
MR_7Ph	2.510	2.593	0.1135	0.0594	0.3469	0.2577	-405.5	-446.1
MR_8Ph	2.480	2.594	0.1281	0.0582	0.3760	0.2526	-398.3	-437.2

Table S16 The averaged bond lengths (r), Mayer bond orders (m), and WBI bond orders (w) of the M-N bonds and the bond length (r') after subtracting the ionic radius (the ionic radius of Am^{3+} is 0.975 Å, and the ionic radius of Eu^{3+} is 0.947 Å) in $\text{MRPh}(\text{NO}_3)_3$ ($l=1-8$) calculated by PBE0/6-311G(d)-RECP method

	$r(\text{N-Am})$	$r(\text{N-Eu})$	$w(\text{N-Am})$	$w(\text{N-Eu})$	$m(\text{N-Am})$	$m(\text{N-Eu})$	$r'(\text{N-Am})$	$r'(\text{N-Eu})$
$\text{MR}_1\text{Ph}(\text{NO}_3)_3$	2.598	2.580	0.0897	0.0760	0.1608	0.1594	1.623	1.633
$\text{MR}_2\text{Ph}(\text{NO}_3)_3$	2.600	2.582	0.0879	0.0741	0.1628	0.1643	1.625	1.635
$\text{MR}_3\text{Ph}(\text{NO}_3)_3$	2.611	2.594	0.0855	0.0713	0.1583	0.1591	1.636	1.647
$\text{MR}_4\text{Ph}(\text{NO}_3)_3$	2.627	2.609	0.0810	0.0647	0.1414	0.1380	1.652	1.662
$\text{MR}_5\text{Ph}(\text{NO}_3)_3$	2.610	2.592	0.0864	0.0731	0.1516	0.1577	1.635	1.645
$\text{MR}_6\text{Ph}(\text{NO}_3)_3$	2.633	2.607	0.0792	0.0619	0.1396	0.1376	1.658	1.660
$\text{MR}_7\text{Ph}(\text{NO}_3)_3$	2.610	2.592	0.0886	0.0719	0.1566	0.1544	1.635	1.645

MR₈Ph(NO₃)₃ 2.620 2.603 0.0831 0.0667 0.1522 0.1476 1.645 1.656

Table S17 The free energy and bond dissociation energy ($M^{3+}+L+3NO_3^-=ML(NO_3)_3$) in the gas phase (a) and in n-octanol phase (b) calculated by PBE0/6-311G(d) -RECP method

	ΔG_{Am}^a	ΔG_{Eu}^a	ΔE_{Am}^a	ΔE_{Eu}^a	ΔG_{Am}^b	ΔG_{Eu}^b	ΔE_{Am}^b	ΔE_{Eu}^b
MR ₁ Ph(NO ₃) ₃	-1034.0	-1046.3	-1081.6	-1094.5	-263.4	-272.3	-332.6	-342.1
MR ₂ Ph(NO ₃) ₃	-1034.6	-1046.8	-1082.0	-1095.0	-266.3	-278.2	-335.3	-347.9
MR ₃ Ph(NO ₃) ₃	-1031.7	-1043.9	-1078.7	-1091.6	-265.0	-276.9	-333.6	-346.2
MR ₄ Ph(NO ₃) ₃	-1026.7	-1038.9	-1074.0	-1086.8	-261.1	-273.0	-329.9	-342.5
MR ₅ Ph(NO ₃) ₃	-1028.0	-1040.4	-1076.0	-1089.0	-258.2	-266.9	-327.7	-337.0
MR ₆ Ph(NO ₃) ₃	-1026.2	-1034.2	-1073.0	-1081.8	-261.2	-271.2	-329.6	-340.4
MR ₇ Ph(NO ₃) ₃	-1031.2	-1043.5	-1078.3	-1091.3	-264.7	-271.1	-333.3	-340.4
MR ₈ Ph(NO ₃) ₃	-1027.7	-1039.9	-1074.5	-1087.5	-261.4	-273.3	-329.8	-342.4

Table S18 The Gibbs free energy ΔG_M of the extraction process $M(H_2O)_9^{3+}+L+3NO_3^-=ML(NO_3)_3+9H_2O$ in gas phase and the difference $\Delta\Delta G_{Am/Eu}$ calculated by PBE0/6-311G(d) -RECP method

	$\Delta G_{Am}(\text{gas})$	$\Delta G_{Eu}(\text{gas})$	$\Delta\Delta G_{Am/Eu}$
MR ₁ P(NO ₃) ₃	-533.5	-535.1	1.6
MR ₂ P(NO ₃) ₃	-534.1	-535.7	1.5
MR ₃ P(NO ₃) ₃	-531.3	-532.7	1.4
MR ₄ P(NO ₃) ₃	-526.3	-527.8	1.5
MR ₅ P(NO ₃) ₃	-527.6	-529.3	1.7
MR ₆ P(NO ₃) ₃	-525.8	-523.0	-2.8
MR ₇ P(NO ₃) ₃	-530.8	-532.3	1.6
MR ₈ P(NO ₃) ₃	-527.3	-528.8	1.5

Table S19 The twist angles $\angle R_i\text{Ph}$ and $\angle R_r\text{Ph}$ between the R_i or R_r plane and the Ph plane in the *cc*- and *tt*- configurations for the $R_i\text{PhR}_r$ ligand.

	$R_1\text{PhR}_1$	$R_1\text{PhR}_2$	$R_1\text{PhR}_3$	$R_1\text{PhR}_4$	$R_1\text{PhR}_5$	$R_1\text{PhR}_6$
$\angle R_i\text{P}(\text{cc})$	19.80	20.21	19.08	18.86	18.71	17.93
$\angle R_r\text{P}(\text{cc})$	19.78	20.38	28.08	24.31	15.75	34.25
$\angle R_i\text{P}(\text{tt})$	0.02	0.02	0.06	0.04	0.06	0.08
$\angle R_r\text{P}(\text{tt})$	0.02	0.00	0.00	0.01	0.00	0.03
	$R_1\text{PhR}_7$	$R_1\text{PhR}_8$	$R_2\text{PhR}_2$	$R_2\text{PhR}_3$	$R_2\text{PhR}_4$	$R_2\text{PhR}_5$
$\angle R_i\text{P}(\text{cc})$	19.08	18.01	21.74	21.02	21.36	18.99
$\angle R_r\text{P}(\text{cc})$	0.86	32.30	21.77	29.20	27.02	16.22
$\angle R_i\text{P}(\text{tt})$	0.01	0.04	0.02	0.02	0.03	0.00
$\angle R_r\text{P}(\text{tt})$	0.00	0.01	0.02	0.01	0.04	0.00
	$R_2\text{PhR}_6$	$R_2\text{PhR}_7$	$R_2\text{PhR}_8$	$R_3\text{PhR}_3$	$R_3\text{PhR}_4$	$R_3\text{PhR}_5$

$\angle R_rP(cc)$	20.94	19.89	19.65	28.55	28.70	27.03
$\angle R_rP(cc)$	36.66	1.54	33.48	28.55	27.31	14.74
$\angle R_rP(tt)$	0.03	0.01	0.06	0.00	0.00	0.03
$\angle R_rP(tt)$	0.01	0.07	0.02	0.01	0.02	0.01
	R_3PhR_6	R_3PhR_7	R_3PhR_8	R_4PhR_4	R_4PhR_5	R_4PhR_6
$\angle R_rP(cc)$	28.34	28.13	27.34	28.19	22.87	28.67
$\angle R_rP(cc)$	37.06	1.86	33.09	28.21	14.30	37.64
$\angle R_rP(tt)$	0.01	0.02	0.02	0.01	0.00	0.00
$\angle R_rP(tt)$	0.00	0.00	0.01	0.01	0.00	0.00
	R_4PhR_7	R_4PhR_8	R_5PhR_5	R_5PhR_6	R_5PhR_7	R_5PhR_8
$\angle R_rP(cc)$	24.92	25.53	13.71	12.84	14.53	13.08
$\angle R_rP(cc)$	2.17	33.20	10.32	33.06	0.56	31.30
$\angle R_rP(tt)$	0.00	0.00	0.00	0.01	0.00	0.00
$\angle R_rP(tt)$	0.00	0.00	0.01	0.01	0.00	0.01
	R_6PhR_6	R_6PhR_7	R_6PhR_8	R_7PhR_7	R_7PhR_8	R_8PhR_8
$\angle R_rP(cc)$	38.17	35.28	35.65	0.00	1.77	31.97
$\angle R_rP(cc)$	38.15	2.54	33.02	0.01	32.48	31.96
$\angle R_rP(tt)$	0.00	0.02	0.00	0.01	0.00	0.00
$\angle R_rP(tt)$	0.00	0.04	0.00	0.01	0.00	0.00

Table S20 The HOMO-LUMO orbital energy levels, Ph_{N1} , Ph_{N2} , R_{N1} , and R_{N2} , protonation energies (ΔG_{RN1} , ΔG_{PN1} , ΔG_{PN2}) in R_lPhR_r ($l, r = 1-8$)

Ligands	HOMO	LUMO	gap	ΔG_{PN1}	ΔG_{PN2}	ΔG_{RN1}	ΔG_{RN2}
R_1PhR_1	-5.9579	-1.3875	4.5704	-89.3	-89.3	-70.1	-70.1
R_1PhR_2	-5.8064	-1.3053	4.5011	-91.6	-93.1	-72.6	-79.7
R_1PhR_3	-5.9092	-1.5556	4.3536	-88.6	-88.0	-71.0	-81.9
R_1PhR_4	-6.0808	-1.5004	4.5805	-88.3	-86.3	-71.2	-71.0
R_1PhR_5	-6.1524	-1.5909	4.5614	-85.3	-82.6	-66.9	-56.2
R_1PhR_6	-6.2457	-1.7310	4.5147	-85.7	-82.0	-70.0	-77.8
R_1PhR_7	-6.0457	-1.4688	4.5769	-86.6	-88.2	-69.2	-69.8
R_1PhR_8	-6.3080	-1.7952	4.5128	-84.4	-80.3	-67.6	-71.5
R_2PhR_2	-5.6916	-1.2213	4.4703	-95.3	-95.3	-82.1	-82.1
R_2PhR_3	-5.8058	-1.4786	4.3272	-92.5	-90.2	-80.7	-84.3
R_2PhR_4	-5.9070	-1.4209	4.4861	-92.1	-88.5	-80.9	-73.3
R_2PhR_5	-5.9704	-1.5112	4.4592	-89.2	-85.0	-76.6	-58.8
R_2PhR_6	-6.0525	-1.6548	4.3977	-89.7	-84.2	-79.8	-80.1
R_2PhR_7	-5.8665	-1.3867	4.4798	-92.0	-88.8	-79.5	-71.7
R_2PhR_8	-6.1015	-1.7182	4.3833	-87.9	-82.6	-77.5	-74.0
R_3PhR_3	-5.9065	-1.7117	4.1948	-87.4	-87.4	-82.8	-82.8
R_3PhR_4	-5.9818	-1.6641	4.3177	-87.0	-85.5	-82.8	-71.7
R_3PhR_5	-6.0531	-1.7479	4.3052	-84.0	-81.9	-78.8	-57.1

R ₃ PhR ₆	-6.1048	-1.8798	4.2250	-84.6	-81.3	-81.5	-78.5
R ₃ PhR ₇	-5.9568	-1.6306	4.3262	-87.0	-85.9	-81.7	-70.3
R ₃ PhR ₈	-6.1543	-1.9415	4.2127	-83.2	-79.7	-79.6	-72.4
R ₄ PhR ₄	-6.2620	-1.6143	4.6477	-85.0	-85.0	-71.7	-71.7
R ₄ PhR ₅	-6.2990	-1.6989	4.6001	-82.3	-81.6	-67.8	-57.3
R ₄ PhR ₆	-6.4393	-1.8379	4.6014	-82.6	-80.7	-70.4	-78.3
R ₄ PhR ₇	-6.2049	-1.5784	4.6264	-85.2	-85.5	-70.7	-70.5
R ₄ PhR ₈	-6.4869	-1.9005	4.5865	-81.6	-79.2	-68.5	-72.5
R ₅ PhR ₅	-6.3640	-1.7884	4.5756	-76.8	-76.8	-51.2	-51.2
R ₅ PhR ₆	-6.4731	-1.9198	4.5533	-78.8	-77.9	-56.0	-74.5
R ₅ PhR ₇	-6.2672	-1.6660	4.6012	-81.5	-82.4	-55.9	-66.0
R ₅ PhR ₈	-6.5430	-1.9829	4.5601	-77.2	-76.1	-53.4	-68.2
R ₆ PhR ₆	-6.6072	-2.0468	4.5604	-78.5	-78.5	-76.9	-76.9
R ₆ PhR ₇	-6.3876	-1.8034	4.5843	-80.9	-82.9	-77.4	-69.4
R ₆ PhR ₈	-6.6572	-2.1088	4.5484	-77.3	-76.7	-75.2	-71.2
R ₇ PhR ₇	-6.1638	-1.5412	4.6226	-85.5	-85.5	-69.0	-69.0
R ₇ PhR ₈	-6.4513	-1.8648	4.5865	-81.8	-79.2	-66.9	-71.3
R ₈ PhR ₈	-6.7230	-2.1703	4.5527	-75.4	-75.4	-69.0	-69.0

Table S21 N-M Bond lengths (Å) in the complexes $\mathbf{M}(\mathbf{R}_l\mathbf{PhR}_r)^{3+}$ ($l, r=1-8$) calculated by the PBE0/6-311G(d)-RECP method in the gas phase

	R _{N1} -Am	Ph _{N1} -Am	Ph _{N2} -Am	R _{N2} -Am	N _{aver} -Am	R _{N1} -Eu	Ph _{N1} -Eu	Ph _{N2} -Eu	R _{N2} -Eu	N _{aver} -Eu
MR ₁ PhR ₁	2.448	2.413	2.413	2.448	2.431	2.621	2.580	2.580	2.621	2.600
MR ₁ PhR ₂	2.471	2.376	2.383	2.447	2.419	2.606	2.566	2.599	2.635	2.601
MR ₁ PhR ₃	2.451	2.425	2.441	2.405	2.431	2.593	2.558	2.612	2.647	2.603
MR ₁ PhR ₄	2.436	2.412	2.468	2.415	2.433	2.621	2.595	2.627	2.576	2.605
MR ₁ PhR ₅	2.447	2.386	2.403	2.529	2.441	2.617	2.584	2.593	2.658	2.613
MR ₁ PhR ₆	2.442	2.430	2.503	2.353	2.432	2.620	2.598	2.634	2.524	2.594
MR ₁ PhR ₇	2.442	2.409	2.423	2.483	2.439	2.634	2.604	2.589	2.623	2.612
MR ₁ PhR ₈	2.464	2.375	2.405	2.460	2.426	2.630	2.600	2.607	2.589	2.606
MR ₂ PhR ₂	2.442	2.419	2.419	2.442	2.431	2.614	2.585	2.585	2.614	2.600
MR ₂ PhR ₃	2.443	2.431	2.442	2.407	2.431	2.601	2.579	2.603	2.628	2.602
MR ₂ PhR ₄	2.429	2.417	2.468	2.418	2.433	2.637	2.612	2.613	2.567	2.607
MR ₂ PhR ₅	2.443	2.388	2.397	2.530	2.439	2.631	2.600	2.577	2.644	2.613
MR ₂ PhR ₆	2.435	2.437	2.502	2.356	2.432	2.645	2.623	2.627	2.520	2.604
MR ₂ PhR ₇	2.473	2.389	2.395	2.500	2.439	2.646	2.619	2.575	2.613	2.613
MR ₂ PhR ₈	2.432	2.427	2.455	2.428	2.435	2.652	2.621	2.594	2.577	2.611
MR ₃ PhR ₃	2.453	2.386	2.386	2.453	2.420	2.610	2.596	2.596	2.610	2.603
MR ₃ PhR ₄	2.397	2.440	2.481	2.420	2.434	2.650	2.624	2.605	2.555	2.608
MR ₃ PhR ₅	2.415	2.432	2.431	2.521	2.450	2.646	2.613	2.568	2.632	2.615
MR ₃ PhR ₆	2.405	2.458	2.515	2.360	2.434	2.659	2.637	2.620	2.510	2.606
MR ₃ PhR ₇	2.396	2.441	2.437	2.474	2.437	2.660	2.632	2.568	2.602	2.616
MR ₃ PhR ₈	2.400	2.449	2.466	2.431	2.436	2.665	2.632	2.585	2.566	2.612
MR ₄ PhR ₄	2.409	2.467	2.467	2.408	2.438	2.582	2.650	2.650	2.582	2.616

MR ₄ PhR ₅	2.400	2.457	2.417	2.488	2.440	2.573	2.636	2.609	2.658	2.619
MR ₄ PhR ₆	2.416	2.487	2.503	2.349	2.439	2.577	2.650	2.652	2.527	2.601
MR ₄ PhR ₇	2.407	2.468	2.423	2.460	2.439	2.589	2.657	2.607	2.623	2.619
MR ₄ PhR ₈	2.410	2.478	2.453	2.417	2.439	2.586	2.652	2.626	2.594	2.614
MR ₅ PhR ₅	2.530	2.409	2.411	2.513	2.466	2.653	2.597	2.597	2.653	2.625
MR ₅ PhR ₆	2.493	2.436	2.494	2.338	2.440	2.663	2.620	2.649	2.527	2.615
MR ₅ PhR ₇	2.506	2.405	2.399	2.490	2.450	2.671	2.619	2.594	2.618	2.625
MR ₅ PhR ₈	2.492	2.428	2.444	2.410	2.443	2.667	2.616	2.616	2.589	2.622
MR ₆ PhR ₆	2.396	2.430	2.430	2.396	2.413	2.524	2.652	2.652	2.524	2.588
MR ₆ PhR ₇	2.345	2.504	2.443	2.465	2.439	2.538	2.664	2.612	2.623	2.609
MR ₆ PhR ₈	2.350	2.513	2.471	2.424	2.440	2.528	2.651	2.622	2.587	2.597
MR ₇ PhR ₇	2.463	2.423	2.423	2.463	2.443	2.634	2.615	2.615	2.634	2.624
MR ₇ PhR ₈	2.463	2.434	2.454	2.417	2.442	2.630	2.611	2.636	2.605	2.620
MR ₈ PhR ₈	2.420	2.463	2.463	2.420	2.441	2.599	2.627	2.627	2.599	2.613

Table S22 Bond energies ΔE_M (kcal/mol) in $M(\mathbf{R}_l\text{PhR}_r)^{3+}$ ($l, r = 1-8$) calculated by the PBE0/6-311G(d)-RECP method in the gas phase

	ΔE_{Am}	ΔE_{Eu}		ΔE_{Am}	ΔE_{Eu}		ΔE_{Am}	ΔE_{Eu}
MR ₁ PhR ₁	-472.4	-499.9	MR ₂ PhR ₆	-495.7	-515.4	MR ₄ PhR ₇	-475.1	-499.5
MR ₁ PhR ₂	-487.7	-513.6	MR ₂ PhR ₇	-482.9	-511.7	MR ₄ PhR ₈	-470.5	-491.0
MR ₁ PhR ₃	-482.6	-509.3	MR ₂ PhR ₈	-479.0	-503.4	MR ₅ PhR ₅	-434.3	-466.6
MR ₁ PhR ₄	-477.5	-502.0	MR ₃ PhR ₃	-487.2	-517.3	MR ₅ PhR ₆	-463.4	-484.5
MR ₁ PhR ₅	-454.2	-483.5	MR ₃ PhR ₄	-487.8	-512.2	MR ₅ PhR ₇	-451.3	-480.8
MR ₁ PhR ₆	-482.1	-501.2	MR ₃ PhR ₅	-463.6	-493.5	MR ₅ PhR ₈	-446.3	-472.3
MR ₁ PhR ₇	-470.1	-497.5	MR ₃ PhR ₆	-492.1	-511.6	MR ₆ PhR ₆	-483.9	-502.8
MR ₁ PhR ₈	-463.8	-489.0	MR ₃ PhR ₇	-480.4	-507.6	MR ₆ PhR ₇	-480.0	-498.7
MR ₂ PhR ₂	-499.1	-526.5	MR ₃ PhR ₈	-475.7	-499.8	MR ₆ PhR ₈	-475.0	-490.5
MR ₂ PhR ₃	-496.1	-521.8	MR ₄ PhR ₄	-482.4	-503.9	MR ₇ PhR ₇	-467.5	-495.0
MR ₂ PhR ₄	-491.0	-516.0	MR ₄ PhR ₅	-458.5	-485.5	MR ₇ PhR ₈	-463.1	-486.4
MR ₂ PhR ₅	-468.3	-497.6	MR ₄ PhR ₆	-486.9	-503.3	MR ₈ PhR ₈	-458.4	-478.1

Table S23 Bond lengths and average bond lengths of the M-N bonds in $\mathbf{M}(\mathbf{R}_l\mathbf{PhR}_r)(\mathbf{NO}_3)_3$ ($l, r=1-8$) at the PBE0/6-311G(d)-RECP level

	R _{N1} -Am	P _{N1} -Am	P _{N2} -Am	R _{N2} -Am	N _{aver} -Am	R _{N1} -Eu	P _{N1} -Eu	P _{N2} -Eu	R _{N2} -Eu	N _{aver} -Eu
MR ₁ PhR ₁ (NO ₃) ₃	2.544	2.687	2.687	2.544	2.615	2.564	2.686	2.699	2.542	2.623
MR ₁ PhR ₂ (NO ₃) ₃	2.608	2.698	2.675	2.604	2.646	2.550	2.736	2.701	2.555	2.636
MR ₁ PhR ₃ (NO ₃) ₃	2.571	2.750	2.711	2.587	2.655	2.549	2.736	2.695	2.552	2.633
MR ₁ PhR ₄ (NO ₃) ₃	2.558	2.678	2.688	2.614	2.634	2.537	2.678	2.705	2.596	2.629
MR ₁ PhR ₅ (NO ₃) ₃	2.539	2.694	2.703	2.588	2.631	2.529	2.687	2.690	2.582	2.622
MR ₁ PhR ₆ (NO ₃) ₃	2.562	2.711	2.706	2.602	2.645	2.550	2.737	2.733	2.584	2.651
MR ₁ PhR ₇ (NO ₃) ₃	2.556	2.730	2.713	2.581	2.645	2.544	2.740	2.709	2.568	2.640
MR ₁ PhR ₈ (NO ₃) ₃	2.563	2.750	2.727	2.588	2.657	2.549	2.736	2.704	2.577	2.641
MR ₂ PhR ₂ (NO ₃) ₃	2.575	2.693	2.693	2.575	2.634	2.575	2.679	2.679	2.575	2.627
MR ₂ PhR ₃ (NO ₃) ₃	2.578	2.702	2.691	2.589	2.640	2.566	2.743	2.730	2.575	2.654
MR ₂ PhR ₄ (NO ₃) ₃	2.558	2.683	2.700	2.622	2.641	2.550	2.658	2.678	2.621	2.627
MR ₂ PhR ₅ (NO ₃) ₃	2.554	2.688	2.716	2.585	2.636	2.542	2.701	2.731	2.583	2.639
MR ₂ PhR ₆ (NO ₃) ₃	2.566	2.689	2.706	2.611	2.643	2.536	2.701	2.737	2.598	2.643
MR ₂ PhR ₇ (NO ₃) ₃	2.567	2.705	2.710	2.583	2.641	2.556	2.730	2.733	2.573	2.648
MR ₂ PhR ₈ (NO ₃) ₃	2.572	2.709	2.708	2.593	2.646	2.553	2.776	2.749	2.579	2.664
MR ₃ PhR ₃ (NO ₃) ₃	2.623	2.691	2.692	2.623	2.657	2.589	2.682	2.682	2.589	2.635
MR ₃ PhR ₄ (NO ₃) ₃	2.570	2.684	2.711	2.624	2.647	2.571	2.657	2.680	2.628	2.634
MR ₃ PhR ₅ (NO ₃) ₃	2.573	2.708	2.761	2.594	2.659	2.540	2.706	2.751	2.570	2.641
MR ₃ PhR ₆ (NO ₃) ₃	2.575	2.697	2.716	2.611	2.650	2.567	2.672	2.693	2.605	2.635
MR ₃ PhR ₇ (NO ₃) ₃	2.582	2.703	2.719	2.586	2.648	2.582	2.690	2.714	2.588	2.643
MR ₃ PhR ₈ (NO ₃) ₃	2.583	2.706	2.718	2.595	2.650	2.583	2.704	2.708	2.596	2.648
MR ₄ PhR ₄ (NO ₃) ₃	2.613	2.662	2.662	2.613	2.638	2.571	2.676	2.676	2.571	2.624
MR ₄ PhR ₅ (NO ₃) ₃	2.634	2.697	2.713	2.605	2.662	2.601	2.694	2.698	2.572	2.641
MR ₄ PhR ₆ (NO ₃) ₃	2.611	2.713	2.705	2.594	2.656	2.597	2.688	2.679	2.579	2.636
MR ₄ PhR ₇ (NO ₃) ₃	2.616	2.715	2.701	2.568	2.650	2.615	2.694	2.678	2.562	2.637
MR ₄ PhR ₈ (NO ₃) ₃	2.618	2.720	2.703	2.577	2.654	2.614	2.699	2.680	2.569	2.640
MR ₅ PhR ₅ (NO ₃) ₃	2.574	2.707	2.714	2.560	2.639	2.570	2.694	2.708	2.554	2.631
MR ₅ PhR ₆ (NO ₃) ₃	2.582	2.734	2.715	2.592	2.656	2.565	2.737	2.736	2.571	2.652
MR ₅ PhR ₇ (NO ₃) ₃	2.578	2.744	2.712	2.567	2.651	2.575	2.737	2.709	2.552	2.643
MR ₅ PhR ₈ (NO ₃) ₃	2.586	2.764	2.726	2.576	2.663	2.573	2.772	2.714	2.559	2.655
MR ₆ PhR ₆ (NO ₃) ₃	2.609	2.693	2.694	2.609	2.651	2.551	2.705	2.705	2.551	2.628
MR ₆ PhR ₇ (NO ₃) ₃	2.602	2.722	2.715	2.575	2.653	2.617	2.687	2.685	2.587	2.644
MR ₆ PhR ₈ (NO ₃) ₃	2.605	2.724	2.715	2.582	2.657	2.607	2.688	2.686	2.590	2.643
MR ₇ PhR ₇ (NO ₃) ₃	2.587	2.727	2.727	2.587	2.657	2.565	2.740	2.740	2.565	2.653
MR ₇ PhR ₈ (NO ₃) ₃	2.580	2.727	2.722	2.586	2.654	2.557	2.786	2.787	2.572	2.676
MR ₈ PhR ₈ (NO ₃) ₃	2.589	2.724	2.724	2.589	2.656	2.586	2.709	2.709	2.586	2.648

Table S24 Bond lengths and average bond lengths of the M-N bonds in $\mathbf{M}(\mathbf{R}_l\mathbf{PhR}_r)(\mathbf{NO}_3)_3$ ($l, r = 1-8$) at the PBE0/6-311G(d)-RECP level after subtracting the radius of the metals

	R _{N1} -Am	P _{N1} -Am	P _{N2} -Am	R _{N2} -Am	N _{aver} -Am	R _{N1} -Eu	P _{N1} -Eu	P _{N2} -Eu	R _{N2} -Eu	N _{aver} -Eu
MR ₁ PhR ₁ (NO ₃) ₃	1.569	1.712	1.712	1.569	1.640	1.617	1.739	1.752	1.595	1.676
MR ₁ PhR ₂ (NO ₃) ₃	1.633	1.723	1.700	1.629	1.671	1.603	1.789	1.754	1.608	1.689
MR ₁ PhR ₃ (NO ₃) ₃	1.596	1.775	1.736	1.612	1.680	1.602	1.789	1.748	1.605	1.686
MR ₁ PhR ₄ (NO ₃) ₃	1.583	1.703	1.713	1.639	1.659	1.590	1.731	1.758	1.649	1.682
MR ₁ PhR ₅ (NO ₃) ₃	1.564	1.719	1.728	1.613	1.656	1.582	1.740	1.743	1.635	1.675
MR ₁ PhR ₆ (NO ₃) ₃	1.587	1.736	1.731	1.627	1.670	1.603	1.790	1.786	1.637	1.704
MR ₁ PhR ₇ (NO ₃) ₃	1.581	1.755	1.738	1.606	1.670	1.597	1.793	1.762	1.621	1.693
MR ₁ PhR ₈ (NO ₃) ₃	1.588	1.775	1.752	1.613	1.682	1.602	1.789	1.757	1.630	1.694
MR ₂ PhR ₂ (NO ₃) ₃	1.600	1.718	1.718	1.600	1.659	1.628	1.732	1.732	1.628	1.680
MR ₂ PhR ₃ (NO ₃) ₃	1.603	1.727	1.716	1.614	1.665	1.619	1.796	1.783	1.628	1.707
MR ₂ PhR ₄ (NO ₃) ₃	1.583	1.708	1.725	1.647	1.666	1.603	1.711	1.731	1.674	1.680
MR ₂ PhR ₅ (NO ₃) ₃	1.579	1.713	1.741	1.610	1.661	1.595	1.754	1.784	1.636	1.692
MR ₂ PhR ₆ (NO ₃) ₃	1.591	1.714	1.731	1.636	1.668	1.589	1.754	1.790	1.651	1.696
MR ₂ PhR ₇ (NO ₃) ₃	1.592	1.730	1.735	1.608	1.666	1.609	1.783	1.786	1.626	1.701
MR ₂ PhR ₈ (NO ₃) ₃	1.597	1.734	1.733	1.618	1.671	1.606	1.829	1.802	1.632	1.717
MR ₃ PhR ₃ (NO ₃) ₃	1.648	1.716	1.717	1.648	1.682	1.642	1.735	1.735	1.642	1.688
MR ₃ PhR ₄ (NO ₃) ₃	1.595	1.709	1.736	1.649	1.672	1.624	1.710	1.733	1.681	1.687
MR ₃ PhR ₅ (NO ₃) ₃	1.598	1.733	1.786	1.619	1.684	1.593	1.759	1.804	1.623	1.694
MR ₃ PhR ₆ (NO ₃) ₃	1.600	1.722	1.741	1.636	1.675	1.620	1.725	1.746	1.658	1.688
MR ₃ PhR ₇ (NO ₃) ₃	1.607	1.728	1.744	1.611	1.673	1.635	1.743	1.767	1.641	1.696
MR ₃ PhR ₈ (NO ₃) ₃	1.608	1.731	1.743	1.620	1.675	1.636	1.757	1.761	1.649	1.701
MR ₄ PhR ₄ (NO ₃) ₃	1.638	1.687	1.687	1.638	1.663	1.624	1.729	1.729	1.624	1.677
MR ₄ PhR ₅ (NO ₃) ₃	1.659	1.722	1.738	1.630	1.687	1.654	1.747	1.751	1.625	1.694
MR ₄ PhR ₆ (NO ₃) ₃	1.636	1.738	1.730	1.619	1.681	1.650	1.741	1.732	1.632	1.689
MR ₄ PhR ₇ (NO ₃) ₃	1.641	1.740	1.726	1.593	1.675	1.668	1.747	1.731	1.615	1.690
MR ₄ PhR ₈ (NO ₃) ₃	1.643	1.745	1.728	1.602	1.679	1.667	1.752	1.733	1.622	1.693
MR ₅ PhR ₅ (NO ₃) ₃	1.599	1.732	1.739	1.585	1.664	1.623	1.747	1.761	1.607	1.684
MR ₅ PhR ₆ (NO ₃) ₃	1.607	1.759	1.740	1.617	1.681	1.618	1.790	1.789	1.624	1.705
MR ₅ PhR ₇ (NO ₃) ₃	1.603	1.769	1.737	1.592	1.676	1.628	1.790	1.762	1.605	1.696
MR ₅ PhR ₈ (NO ₃) ₃	1.611	1.789	1.751	1.601	1.688	1.626	1.825	1.767	1.612	1.708
MR ₆ PhR ₆ (NO ₃) ₃	1.634	1.718	1.719	1.634	1.676	1.604	1.758	1.758	1.604	1.681
MR ₆ PhR ₇ (NO ₃) ₃	1.627	1.747	1.740	1.600	1.678	1.670	1.740	1.738	1.640	1.697
MR ₆ PhR ₈ (NO ₃) ₃	1.630	1.749	1.740	1.607	1.682	1.660	1.741	1.739	1.643	1.696
MR ₇ PhR ₇ (NO ₃) ₃	1.612	1.752	1.752	1.612	1.682	1.618	1.793	1.793	1.618	1.706
MR ₇ PhR ₈ (NO ₃) ₃	1.605	1.752	1.747	1.611	1.679	1.610	1.839	1.840	1.625	1.729
MR ₈ PhR ₈ (NO ₃) ₃	1.614	1.749	1.749	1.614	1.681	1.639	1.762	1.762	1.639	1.701

Table S25 Gibbs free energy ΔG_M and $\Delta\Delta G_{Am/Eu}$ (kcal/mol) of the solvent extraction process in the gas phase calculated by the PBE0/6-311G(d)-RECP method

	$\Delta G_{Am}(\text{gas})$	$\Delta G_{Eu}(\text{gas})$	$\Delta\Delta G_{Am/Eu}$		$\Delta G_{Am}(\text{gas})$	$\Delta G_{Eu}(\text{gas})$	$\Delta\Delta G_{Am/Eu}$
MR ₁ PhR ₁ (NO ₃) ₃	-546.9	-548.7	1.8	MR ₃ PhR ₆ (NO ₃) ₃	-536.5	-536.1	-0.4
MR ₁ PhR ₂ (NO ₃) ₃	-547.3	-548.8	1.5	MR ₃ PhR ₇ (NO ₃) ₃	-541.9	-541.9	0.0
MR ₁ PhR ₃ (NO ₃) ₃	-545.4	-542.2	-3.2	MR ₃ PhR ₈ (NO ₃) ₃	-538.5	-538.6	0.2
MR ₁ PhR ₄ (NO ₃) ₃	-540.4	-541.5	1.0	MR ₄ PhR ₄ (NO ₃) ₃	-534.3	-527.3	-7.0
MR ₁ PhR ₅ (NO ₃) ₃	-543.6	-542.3	-1.3	MR ₄ PhR ₅ (NO ₃) ₃	-534.7	-535.8	1.2
MR ₁ PhR ₆ (NO ₃) ₃	-539.3	-539.0	-0.3	MR ₄ PhR ₆ (NO ₃) ₃	-532.6	-532.4	-0.2
MR ₁ PhR ₇ (NO ₃) ₃	-545.5	-546.1	0.7	MR ₄ PhR ₇ (NO ₃) ₃	-537.3	-537.2	-0.1
MR ₁ PhR ₈ (NO ₃) ₃	-541.6	-540.4	-1.3	MR ₄ PhR ₈ (NO ₃) ₃	-533.8	-533.7	0.0
MR ₂ PhR ₂ (NO ₃) ₃	-547.5	-545.6	-1.9	MR ₅ PhR ₅ (NO ₃) ₃	-537.6	-536.6	-1.0
MR ₂ PhR ₃ (NO ₃) ₃	-544.6	-545.6	1.0	MR ₅ PhR ₆ (NO ₃) ₃	-534.5	-535.6	1.1
MR ₂ PhR ₄ (NO ₃) ₃	-540.1	-539.8	-0.3	MR ₅ PhR ₇ (NO ₃) ₃	-540.3	-541.0	0.7
MR ₂ PhR ₅ (NO ₃) ₃	-543.6	-543.9	0.3	MR ₅ PhR ₈ (NO ₃) ₃	-536.5	-535.0	-1.5
MR ₂ PhR ₆ (NO ₃) ₃	-539.7	-538.1	-1.6	MR ₆ PhR ₆ (NO ₃) ₃	-532.2	-527.0	-5.2
MR ₂ PhR ₇ (NO ₃) ₃	-545.5	-545.7	0.2	MR ₆ PhR ₇ (NO ₃) ₃	-536.4	-535.4	-1.0
MR ₂ PhR ₈ (NO ₃) ₃	-541.3	-542.0	0.7	MR ₆ PhR ₈ (NO ₃) ₃	-533.3	-531.7	-1.6
MR ₃ PhR ₃ (NO ₃) ₃	-540.8	-541.3	0.5	MR ₇ PhR ₇ (NO ₃) ₃	-543.1	-520.0	-1.1
MR ₃ PhR ₄ (NO ₃) ₃	-537.2	-534.9	-2.3	MR ₇ PhR ₈ (NO ₃) ₃	-538.4	-539.2	0.8
MR ₃ PhR ₅ (NO ₃) ₃	-540.4	-537.2	-3.2	MR ₈ PhR ₈ (NO ₃) ₃	-536.1	-535.1	-1.0

Table S26 Averaged electron density (ρ), Laplacian ($\nabla^2\rho$), local electron energy density ($H(r)$) and delocalization indices δ at the N-M and O-M BCPs for the MR_iPh (NO₃)₃ calculated in the PBE0/6-311G(d)-RECP level

	N_{R-M}	N_{Ph-M}	O-M	N_{R-M}	N_{Ph-M}	O-M
Complexes		$\rho(\text{Am/Eu})$			$\nabla^2\rho(\text{Am/Eu})$	
MR ₁ Ph (NO ₃) ₃	0.049/0.045	0.041/0.038	0.051/0.051	0.176/0.160	0.138/0.127	0.198/0.193
MR ₂ Ph(NO ₃) ₃	0.046/0.042	0.042/0.038	0.052/0.051	0.159/0.145	0.141/0.131	0.200/0.194
MR ₃ Ph(NO ₃) ₃	0.045/0.043	0.041/0.037	0.052/0.051	0.154/0.143	0.139/0.129	0.201/0.195
MR ₄ Ph(NO ₃) ₃	0.042/0.038	0.040/0.037	0.053/0.052	0.152/0.137	0.136/0.126	0.203/0.197
MR ₅ Ph(NO ₃) ₃	0.042/0.038	0.041/0.039	0.053/0.052	0.152/0.141	0.138/0.129	0.203/0.196
MR ₆ Ph(NO ₃) ₃	0.044/0.043	0.039/0.035	0.053/0.052	0.153/0.143	0.133/0.123	0.203/0.197
MR ₇ Ph(NO ₃) ₃	0.047/0.043	0.040/0.037	0.052/0.052	0.168/0.153	0.136/0.125	0.200/0.195
MR ₈ Ph(NO ₃) ₃	0.047/0.043	0.039/0.036	0.052/0.052	0.164/0.149	0.134/0.123	0.202/0.196
		$H(r)*10^2(\text{Am/Eu})$			$\delta(\text{Am/Eu})$	
MR ₁ Ph (NO ₃) ₃	-0.353/-0.150	-0.186/-0.016	-0.235/-0.212	0.268/0.221	0.240/0.197	0.286/0.250
MR ₂ Ph(NO ₃) ₃	-0.249/-0.095	-0.209/-0.015	-0.239/-0.219	0.261/0.216	0.240/0.198	0.288/0.259
MR ₃ Ph(NO ₃) ₃	-0.247/-0.134	-0.182/0.008	-0.246/-0.222	0.259/0.225	0.233/0.194	0.290/0.257
MR ₄ Ph(NO ₃) ₃	-0.169/0.026	-0.167/0.009	-0.262/-0.256	0.234/0.190	0.231/0.190	0.294/0.265
MR ₅ Ph(NO ₃) ₃	-0.117/0.033	-0.201/-0.035	-0.261/-0.235	0.227/0.185	0.238/0.205	0.293/0.250
MR ₆ Ph(NO ₃) ₃	-0.222/-0.104	-0.132/0.050	-0.258/-0.249	0.246/0.221	0.221/0.178	0.294/0.262

MR ₇ Ph(NO ₃) ₃	-0.300/-0.096	-0.165/0.007	-0.246/-0.230	0.263/0.216	0.233/0.189	0.290/0.261
MR ₈ Ph(NO ₃) ₃	-0.297/-0.093	-0.137/0.038	-0.255/-0.245	0.263/0.216	0.225/0.184	0.293/0.264

Table S27 Averaged electron density (ρ), Laplacian ($\nabla^2\rho$), local electron energy density ($H(r)$) and delocalization indices δ at the N-M and O-M BCPs for the MR_rPhR_r(NO₃)₃ calculated in the PBE0/6-311G(d)-RECP level

	N _R -M	N _{Ph} -M	O-M	N _R -M	N _{Ph} -M	O-M
Complexes		$\rho(\text{Am/Eu})$			$\nabla^2\rho(\text{Am/Eu})$	
MR ₁ PhR ₁ (NO ₃) ₃	0.048/0.041	0.036/0.031	0.067/0.046	0.161/0.144	0.118/0.108	0.177/0.143
MR ₂ PhR ₂ (NO ₃) ₃	0.045/0.040	0.036/0.032	0.047/0.045	0.146/0.134	0.121/0.113	0.176/0.170
MR ₃ PhR ₃ (NO ₃) ₃	0.042/0.039	0.036/0.032	0.049/0.046	0.137/0.130	0.121/0.113	0.177/0.171
MR ₄ PhR ₄ (NO ₃) ₃	0.042/0.040	0.038/0.032	0.050/0.047	0.144/0.138	0.130/0.115	0.185/0.174
MR ₅ PhR ₅ (NO ₃) ₃	0.045/0.040	0.035/0.031	0.049/0.047	0.154/0.142	0.115/0.106	0.183/0.178
MR ₆ PhR ₆ (NO ₃) ₃	0.043/0.042	0.035/0.030	0.050/0.046	0.144/0.141	0.123/0.109	0.185/0.173
MR ₇ PhR ₇ (NO ₃) ₃	0.044/0.040	0.033/0.028	0.050/0.047	0.152/0.144	0.109/0.097	0.184/0.177
MR ₈ PhR ₈ (NO ₃) ₃	0.044/0.038	0.034/0.030	0.049/0.047	0.143/0.132	0.115/0.107	0.181/0.146
		$H(r)*10^2(\text{Am/Eu})$			$\delta(\text{Am/Eu})$	
MR ₁ PhR ₁ (NO ₃) ₃	-0.374/-0.081	-0.129/0.095	-0.253/-0.104	0.265/0.205	0.209/0.163	0.253/0.229
MR ₂ PhR ₂ (NO ₃) ₃	-0.316/-0.061	-0.130/0.097	-0.254/-0.091	0.251/0.202	0.201/0.165	0.258/0.230
MR ₃ PhR ₃ (NO ₃) ₃	-0.270/-0.043	-0.103/0.118	-0.284/-0.108	0.222/0.199	0.201/0.158	0.266/0.234
MR ₄ PhR ₄ (NO ₃) ₃	-0.224/-0.020	-0.140/0.115	-0.320/-0.141	0.219/0.194	0.212/0.159	0.275/0.244
MR ₅ PhR ₅ (NO ₃) ₃	-0.275/-0.022	-0.112/0.103	-0.306/-0.139	0.239/0.192	0.197/0.160	0.265/0.237
MR ₆ PhR ₆ (NO ₃) ₃	-0.266/-0.102	-0.069/0.157	-0.322/-0.135	0.227/0.212	0.194/0.144	0.276/0.236
MR ₇ PhR ₇ (NO ₃) ₃	-0.302/-0.038	-0.054/0.141	-0.303/-0.141	0.241/0.200	0.189/0.145	0.268/0.239
MR ₈ PhR ₈ (NO ₃) ₃	-0.269/-0.022	-0.065/0.148	-0.299/-0.135	0.241/0.195	0.181/0.147	0.269/0.240

Table S28 The $\Delta E_{ij}^{(2)}$ of N-M interactions and the occupation numbers (ON) of the MR_rPh(NO₃)₃(Am/Eu) were calculated using the PBE0/6-311G(d)-RECP method.

	ON(α -spin)	ON(β -spin)	ON($\alpha+\beta$)	$\Delta E_{ij}^{(2)}$ (α -spin)	$\Delta E_{ij}^{(2)}$ (β -spin)	$\Delta E_{ij}^{(2)}$ ($\alpha+\beta$)
AmR ₁ Ph(NO ₃) ₃	0.2946	0.2504	0.5450	27.55	25.81	53.36
EuR ₁ Ph(NO ₃) ₃	0.2633	0.1959	0.4592	22.11	22.55	44.66
AmR ₂ Ph(NO ₃) ₃	0.2693	0.2493	0.5186	29.30	25.93	55.23
EuR ₂ Ph(NO ₃) ₃	0.2635	0.1957	0.4592	21.92	21.91	43.83
AmR ₃ Ph(NO ₃) ₃	0.2642	0.1953	0.4595	25.74	24.08	49.82
EuR ₃ Ph(NO ₃) ₃	0.2642	0.1953	0.4595	22.57	21.01	43.58
AmR ₄ Ph(NO ₃) ₃	0.2952	0.2602	0.5554	24.11	22.05	46.16
EuR ₄ Ph(NO ₃) ₃	0.2568	0.1961	0.4529	20.77	18.50	39.27
AmR ₅ Ph(NO ₃) ₃	0.2976	0.2611	0.5587	26.79	23.53	50.32
EuR ₅ Ph(NO ₃) ₃	0.2653	0.1954	0.4607	21.28	21.37	42.65
AmR ₆ Ph(NO ₃) ₃	0.2938	0.2585	0.5523	22.74	22.17	44.91

EuR ₆ Ph(NO ₃) ₃	0.2596	0.195	0.4546	19.61	18.30	37.91
AmR ₇ Ph(NO ₃) ₃	0.2953	0.2602	0.5555	20.22	24.41	44.63
EuR ₇ Ph(NO ₃) ₃	0.2651	0.1953	0.4604	21.54	21.44	42.98
AmR ₈ Ph(NO ₃) ₃	0.2956	0.2601	0.5557	24.67	22.51	47.18
EuR ₈ Ph(NO ₃) ₃	0.2565	0.1957	0.4522	20.43	18.48	38.91

Table S29 The second-order stabilization energy ($\Delta E_{ij}^{(2)}$) of donor-acceptor interactions and the ON on the $7s/6s$, $6d/5d$ and $5f/4f$ orbitals of the Am/Eu for MR_{*i*}Ph (NO₃)₃ calculated by the PBE0/6-311G*-RECP method

		$\Delta E_{ij}^{(2)} s$	$\Delta E_{ij}^{(2)} d$	$\Delta E_{ij}^{(2)} f$	ON <i>s</i>	ON <i>d</i>	ON <i>f</i>
AmR ₁ Ph(NO ₃) ₃	α -spin	20.15	4.82	2.58	0.1176	0.0975	0.0795
	β -spin	19.25	1.84	4.72	0.1090	0.0468	0.0946
EuR ₁ Ph(NO ₃) ₃	α -spin	17.82	3.95	0.34	0.1039	0.1072	0.0522
	β -spin	17.17	4.00	1.38	0.0997	0.0737	0.0225
AmR ₂ Ph(NO ₃) ₃	α -spin	20.22	6.65	2.43	0.1176	0.0984	0.0533
	β -spin	18.84	2.37	4.72	0.1097	0.0491	0.0905
EuR ₂ Ph(NO ₃) ₃	α -spin	17.41	4.08	0.43	0.1038	0.1069	0.0528
	β -spin	16.74	3.89	1.28	0.0996	0.0740	0.0221
AmR ₃ Ph(NO ₃) ₃	α -spin	19.36	4.62	1.76	0.1031	0.1074	0.0537
	β -spin	18.15	1.80	4.13	0.0989	0.0747	0.0217
EuR ₃ Ph(NO ₃) ₃	α -spin	16.97	5.12	0.48	0.1031	0.1074	0.0537
	β -spin	16.32	3.61	1.08	0.0989	0.0747	0.0217
AmR ₄ Ph(NO ₃) ₃	α -spin	18.79	3.94	1.38	0.1162	0.0989	0.0801
	β -spin	17.52	1.29	3.24	0.1078	0.0559	0.0965
EuR ₄ Ph(NO ₃) ₃	α -spin	16.61	2.68	1.48	0.1027	0.1094	0.0447
	β -spin	16.05	2.07	0.38	0.0985	0.0762	0.0214
AmR ₅ Ph(NO ₃) ₃	α -spin	19.52	4.84	2.43	0.1170	0.0976	0.0830
	β -spin	18.63	0.75	4.15	0.1086	0.0540	0.0985
EuR ₅ Ph(NO ₃) ₃	α -spin	17.33	3.63	0.32	0.1034	0.1076	0.0543
	β -spin	16.72	3.38	1.27	0.0992	0.0735	0.0227
AmR ₆ Ph(NO ₃) ₃	α -spin	18.41	3.09	1.24	0.1156	0.0996	0.0786
	β -spin	17.11	1.54	3.52	0.1070	0.0567	0.0948
EuR ₆ Ph(NO ₃) ₃	α -spin	16.48	1.77	1.36	0.1020	0.1094	0.0482
	β -spin	16.02	1.86	0.42	0.0978	0.0770	0.0202
AmR ₇ Ph(NO ₃) ₃	α -spin	13.46	4.75	2.01	0.1172	0.0976	0.0805
	β -spin	18.43	1.71	4.27	0.1088	0.0545	0.0969
EuR ₇ Ph(NO ₃) ₃	α -spin	17.17	3.96	0.41	0.1035	0.1072	0.0544
	β -spin	16.53	4.08	0.83	0.0992	0.0740	0.0221
AmR ₈ Ph(NO ₃) ₃	α -spin	19.04	3.95	1.68	0.1168	0.0986	0.0802
	β -spin	17.85	0.86	3.80	0.1082	0.0554	0.0965
EuR ₈ Ph(NO ₃) ₃	α -spin	16.77	1.83	1.83	0.1030	0.1088	0.0447

β -spin 16.18 2.01 0.29 0.0988 0.0760 0.0209

Table S30 The second-order stabilization energy ($\Delta E_{ij}^{(2)}$) of donor-acceptor interactions and the ON on the $7s/6s$, $6d/5d$ and $5f/4f$ orbitals of the Am/Eu for $MR_nPhR_n(NO_3)_3$ calculated by the PBE0/6-311G*-

		RECP method					
		$\Delta E_{ij}^{(2)}s$	$\Delta E_{ij}^{(2)}d$	$\Delta E_{ij}^{(2)}f$	ON s	ON d	ON f
AmR ₁ PhR ₁ (NO ₃) ₃	α -spin	29.13	10.78	7.54	0.1258	0.0936	0.0727
	β -spin	27.10	3.31	7.80	0.1181	0.0446	0.0953
EuR ₁ PhR ₁ (NO ₃) ₃	α -spin	25.20	6.26	0.17	0.1129	0.1021	0.0511
	β -spin	24.43	3.30	1.92	0.1089	0.0736	0.0239
AmR ₂ PhR ₂ (NO ₃) ₃	α -spin	26.86	8.38	5.25	0.1241	0.0909	0.0786
	β -spin	24.98	4.87	5.31	0.1166	0.0446	0.0918
EuR ₂ PhR ₂ (NO ₃) ₃	α -spin	23.63	8.16	0.08	0.1120	0.1001	0.0607
	β -spin	22.87	5.62	0.97	0.1080	0.0720	0.0243
AmR ₃ PhR ₃ (NO ₃) ₃	α -spin	25.43	7.94	4.24	0.1230	0.0915	0.0816
	β -spin	23.65	3.74	5.05	0.1154	0.0441	0.0926
EuR ₃ PhR ₃ (NO ₃) ₃	α -spin	22.85	9.42	0.07	0.1108	0.1001	0.0670
	β -spin	22.12	5.59	0.67	0.1067	0.0722	0.0242
AmR ₄ PhR ₄ (NO ₃) ₃	α -spin	26.91	8.42	0.34	0.1236	0.0963	0.0820
	β -spin	24.91	4.78	10.71	0.1157	0.0476	0.0978
EuR ₄ PhR ₄ (NO ₃) ₃	α -spin	23.59	8.40	0.09	0.1104	0.1028	0.0856
	β -spin	22.84	6.15	0.90	0.1062	0.0739	0.0268
AmR ₅ PhR ₅ (NO ₃) ₃	α -spin	27.28	8.42	4.90	0.1248	0.0943	0.0715
	β -spin	25.57	3.67	4.96	0.1173	0.0440	0.0956
EuR ₅ PhR ₅ (NO ₃) ₃	α -spin	24.40	6.02	0.12	0.1125	0.1037	0.0530
	β -spin	23.73	4.32	0.79	0.1085	0.0746	0.0241
AmR ₆ PhR ₆ (NO ₃) ₃	α -spin	25.88	8.44	0.32	0.1220	0.0966	0.0779
	β -spin	23.93	3.28	10.00	0.1142	0.0471	0.0971
EuR ₆ PhR ₆ (NO ₃) ₃	α -spin	22.98	6.24	0.03	0.1090	0.1046	0.0565
	β -spin	22.34	5.96	0.80	0.1049	0.0756	0.0239
AmR ₇ PhR ₇ (NO ₃) ₃	α -spin	26.70	7.80	0.29	0.1251	0.0937	0.0687
	β -spin	24.78	4.14	4.52	0.1175	0.0455	0.0920
EuR ₇ PhR ₇ (NO ₃) ₃	α -spin	23.57	5.13	0.03	0.1126	0.1023	0.0546
	β -spin	22.88	4.07	1.06	0.1086	0.0737	0.0239
AmR ₈ PhR ₈ (NO ₃) ₃	α -spin	25.38	5.86	4.34	0.1228	0.0920	0.0823
	β -spin	23.59	4.13	5.02	0.1152	0.0446	0.0934
EuR ₈ PhR ₈ (NO ₃) ₃	α -spin	22.49	4.73	0.01	0.1106	0.1009	0.0683
	β -spin	21.83	3.98	0.14	0.1065	0.0733	0.0237

Cartesian coordinates

X Y Z
30

R₁AmR₁³⁺ (PBE0/6-311G*-RECP)

C	3.98950200	1.50980600	0.66786400
N	2.11286300	0.47514800	0.01553300
C	2.95283700	0.55181400	-1.03986600
C	4.13810600	1.18626900	-0.69970800
H	4.66231600	2.01574400	1.35141100
H	2.40152700	1.17900600	1.97206600
H	2.68185300	0.15314200	-2.01053700
H	4.99076500	1.39627500	-1.33149000
N	2.80114200	1.07485300	1.04886200
Am	-0.00004700	-0.73858500	0.00007300
C	-3.98950000	1.50947900	-0.66824400
N	-2.11269300	0.47533400	-0.01559700
C	-2.95258900	0.55244100	1.03986700
C	-4.13794700	1.18655900	0.69948600
H	-4.66240300	2.01500200	-1.35200800
H	-2.40155000	1.17827100	-1.97241600
H	-2.68145900	0.15437200	2.01075900
H	-4.99060000	1.39665100	1.33124300
N	-2.80108500	1.07450700	-1.04913900

R_{2,3}AmR_{2,3}³⁺ (PBE0/6-311G*-RECP)

C	-3.83547200	1.91977000	0.57054100
C	-2.49555800	1.56844900	0.75242900
H	-4.42701200	2.71874800	0.99829300
H	-5.27783100	0.99604000	-0.66701900
H	-1.78035300	2.07015900	1.38984400
N	-4.32401600	1.02383800	-0.31661400
C	-3.34623900	0.17006300	-0.65736700
H	-3.49907900	-0.64526100	-1.35262600
N	-2.20062600	0.47924400	-0.01675900
Am	-0.00003400	-0.79181800	0.00001300
C	3.83538200	1.92011000	-0.57024900
C	2.49539000	1.56885800	-0.75186300
H	4.42678700	2.71932700	-0.99774400
H	5.27816300	0.99563500	0.66631200
H	1.78001300	2.07094500	-1.38879700
N	4.32422400	1.02364300	0.31625000
C	3.34660300	0.16968600	0.65683300
H	3.49959100	-0.64603700	1.35158200
N	2.20075400	0.47921000	0.01668800

R₄AmR₄³⁺ (PBE0/6-311G*-RECP)

C	4.39486000	0.66906400	-0.00001300
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N	3.05064100	-1.08975300	-0.00000100
C	3.10332800	1.11798800	-0.00001300
H	5.34500800	1.18720500	-0.00001800
H	5.02415600	-1.37399100	-0.00000600
H	2.74313400	2.13892100	-0.00001800
N	4.27703400	-0.67957200	-0.00000700
N	2.30546200	-0.01054500	-0.00000300
Am	0.00000000	0.00010800	0.00000600
C	-4.39476400	-0.66948200	-0.00001200
N	-3.05080000	1.08953100	-0.00000200
C	-3.10316600	-1.11821800	-0.00001500
H	-5.34483600	-1.18776000	-0.00001500
H	-5.02435600	1.37348200	-0.00000600
H	-2.74282400	-2.13909900	-0.00002000
N	-4.27713400	0.67917200	-0.00000700
N	-2.30546400	0.01043100	-0.00000300

R₅AmR₅³⁺ (PBE0/6-311G*-RECP)

C	4.38070400	-1.16640600	0.47669700
C	3.27421500	-0.43681100	0.98644700
H	5.35003800	-1.37249200	0.91427400
H	3.18884200	0.06742800	1.94062600
N	2.30292700	-0.45998500	0.08161200
Am	0.00006000	0.74308800	0.00018100
N	2.85550700	-1.19787800	-0.94464800
H	2.37477900	-1.42565000	-1.81013900
N	4.04184900	-1.62027200	-0.74788400
C	-4.38105300	-1.16580400	-0.47704500
C	-3.27491800	-0.43510200	-0.98606000
H	-5.35053000	-1.37144300	-0.91452300
H	-3.19019900	0.07063200	-1.93951400
N	-2.30324700	-0.45946400	-0.08176900
N	-2.85523300	-1.19928100	0.94361500
H	-2.37416900	-1.42801600	1.80866800
N	-4.04153600	-1.62156600	0.74667200

R₆AmR₆³⁺ (PBE0/6-311G*-RECP)

C	-3.15421500	0.93661100	-0.28257100
H	-2.93827400	1.87413600	-0.78150400
N	-3.00126300	-1.02476400	0.68098100
Am	0.00000000	-0.00008600	-0.17767600
C	-4.24891800	-0.67696500	0.66411000
H	-5.07220300	-1.25976800	1.05853100
N	-4.37143900	0.55058400	0.06826800

H	-5.23494600	1.06850100	-0.08269000
N	-2.29225700	-0.03003600	0.10158300
C	3.15430100	-0.93652400	-0.28236000
H	2.93844400	-1.87418500	-0.78107000
N	3.00116800	1.02503300	0.68079000
C	4.24885800	0.67735800	0.66396800
H	5.07209100	1.26032700	1.05825200
N	4.37149100	-0.55030100	0.06837800
H	5.23504600	-1.06816300	-0.08248600
N	2.29225100	0.03011400	0.10160900

R_{7,8}AmR_{7,8}³⁺(PBE0/6-311G*-RECP)

N	2.30425100	0.11488200	-0.00043200
Am	-0.00000500	-0.25621900	-0.00010900
C	3.29814200	-0.52633000	0.67389500
H	3.20591400	-1.35982100	1.35961000
N	4.43203900	0.04535600	0.35155500
H	5.37191800	-0.18211800	0.67320500
C	2.98652700	1.09201700	-0.73587000
N	4.25869600	1.05453900	-0.51789800
H	2.53210200	1.81174200	-1.40567300
N	-2.30418500	0.11539200	0.00007200
C	-3.29844300	-0.52725300	-0.67234500
H	-3.20650100	-1.36170000	-1.35694000
N	-4.43225300	0.04458300	-0.34996400
H	-5.37232700	-0.18367200	-0.67049000
C	-2.98615900	1.09352100	0.73448000
N	-4.25850100	1.05524900	0.51769800
H	-2.53135300	1.81468500	1.40246900

AmPh³⁺(PBE0/6-311G*-RECP)

C	-1.47912700	-0.73224300	0.00039700
C	-1.48369000	-3.50226000	0.00086900
H	-1.41890300	-4.58508700	0.00122400
C	-1.47905200	0.73235200	0.00041100
C	-2.71630400	1.43136800	-0.00048200
C	-2.69866600	2.84746200	-0.00028800
C	-1.48263200	3.50240100	0.00083000
H	-3.63196800	3.40463100	-0.00113000
H	-1.41775200	4.58522100	0.00110500
N	-0.30528200	1.38450800	0.00140400
C	-2.71655100	-1.43082500	-0.00021500
N	-0.30551200	-1.38470500	0.00100100
C	-2.69952800	-2.84698500	-0.00003900

H	-3.63305500	-3.40376000	-0.00044300
C	-3.92426700	0.70694800	-0.00124500
H	-4.87376500	1.23688100	-0.00189300
C	-3.92433000	-0.70609200	-0.00105100
H	-4.87388800	-1.23592600	-0.00165000
C	-0.32327300	-2.73708800	0.00137900
H	0.64154500	-3.23856500	0.00225000
C	-0.32245600	2.73688400	0.00171600
H	0.64254700	3.23800700	0.00282700
Am	1.83515900	-0.00012200	-0.00034500

R₁EuR₁³⁺ (PBE0/6-311G*-RECP)

C	4.50914900	0.75148700	-0.32607800
N	2.33240700	0.27906600	-0.00722200
C	2.64000000	1.33103000	0.74399200
C	3.99640400	1.69168900	0.59812000
H	5.50411500	0.63751800	-0.74071100
H	3.56325500	-0.82406800	-1.29725600
H	1.90603600	1.81969400	1.37265100
H	4.53131000	2.50125800	1.07680800
N	3.51291400	-0.04903500	-0.64858000
Eu	-0.00160400	-0.90163000	-0.00016800
C	-4.50516600	0.75536900	0.32932600
N	-2.32995000	0.27886200	0.00750900
C	-2.63909100	1.32719400	-0.74896800
C	-3.99432000	1.68964700	-0.60127400
H	-5.49898400	0.64440300	0.74742700
H	-3.55793200	-0.81505900	1.30764200
H	-1.90652700	1.81149000	-1.38262900
H	-4.52979600	2.49698000	-1.08300500
N	-3.50855600	-0.04432200	0.65385900

R_{2,3}EuR_{2,3}³⁺ (PBE0/6-311G*-RECP)

C	-3.96891400	1.82739300	0.18107100
C	-2.59364300	1.57348300	0.28148300
H	-4.54036700	2.73182400	0.34449300
H	-5.50968000	0.48769800	-0.35004400
H	-1.82922100	2.28776000	0.55514400
N	-4.52013800	0.65391900	-0.18834800
C	-3.54455000	-0.26694300	-0.30685300
H	-3.74567700	-1.29103100	-0.59342500
N	-2.34365100	0.26809000	-0.02431600

Eu	-0.01044200	-0.88309600	0.03971200
C	4.36034400	1.00182200	0.62285800
C	3.14032800	0.46133700	1.04979300
H	5.24418700	1.28924300	1.17744600
H	4.96285600	1.47755600	-1.34157500
H	2.86580500	0.22948100	2.07017100
N	4.24767600	1.11842800	-0.71533700
C	3.03207000	0.67537000	-1.08980400
H	2.71171700	0.66951100	-2.12335500
N	2.32246200	0.26217100	-0.02514500

R₄EuR₄³⁺ (PBE0/6-311G*-RECP)

C	-4.54431400	0.66222100	-0.09930800
N	-2.54710800	1.54587200	0.22379000
C	-3.54848800	-0.33361200	-0.19638100
H	-5.62301300	0.62357800	-0.19421500
H	-4.19099000	2.71574900	0.29967100
H	-3.69096600	-1.38755500	-0.39680400
N	-3.84790400	1.76703900	0.15654000
N	-2.34988400	0.26111400	0.00919300
Eu	-0.00002700	-0.91864100	-0.00117000
C	4.54394400	0.66243100	0.10578200
N	2.54792700	1.54472700	-0.22817100
C	3.54769700	-0.33284100	0.20421100
H	5.62231300	0.62414200	0.20449200
H	4.19217900	2.71407700	-0.30412200
H	3.68939000	-1.38583700	0.41009200
N	3.84851200	1.76609200	-0.15761900
N	2.34984600	0.26101400	-0.00819200

R₅EuR₅³⁺ (PBE0/6-311G*-RECP)

C	4.60732400	0.82571100	-0.44611600
C	3.47810000	0.09425800	-0.93470400
H	5.60064400	0.94513600	-0.86181300
H	3.40567300	-0.49489300	-1.83994700
N	2.47931000	0.24530100	-0.07926100
Eu	0.00000000	-0.83342700	0.00007200
N	3.02766400	1.05133900	0.88886000
H	2.52652700	1.37385600	1.71148700
N	4.24435600	1.40474500	0.71137900
C	-4.60722200	0.82599800	0.44614400
C	-3.47800000	0.09460300	0.93481400

H	-5.60048100	0.94563400	0.86192500
H	-3.40548400	-0.49420600	1.84027200
N	-2.47927700	0.24535700	0.07924000
N	-3.02779300	1.05086200	-0.88923200
H	-2.52678800	1.37294100	-1.71210900
N	-4.24444500	1.40439800	-0.71172800

R₆EuR₆³⁺ (PBE0/6-311G*-RECP)

C	-3.21325500	0.46436300	-1.05522600
H	-3.12931400	0.20311800	-2.10288000
N	-2.80063600	0.71384700	1.05967100
Eu	0.00194500	-0.92960000	0.01537500
C	-4.00696200	1.23235200	0.79406100
H	-4.66121700	1.69701700	1.52244000
N	-4.27314900	1.08200800	-0.51940300
H	-5.11525100	1.37795100	-1.00887900
N	-2.30389700	0.23645800	-0.07518100
C	3.52760400	-0.23706300	0.10127800
H	3.76654800	-1.28636100	0.22542300
N	2.46395500	1.62979500	-0.17454400
C	3.77705800	1.88824500	-0.11424800
H	4.22275300	2.87314200	-0.19036500
N	4.44977600	0.73124400	0.04668100
H	5.45853700	0.61558600	0.12038200
N	2.29663200	0.32050400	-0.03578600

R_{7,8}EuR_{7,8}³⁺ (PBE0/6-311G*-RECP)

N	-2.40645400	-0.25199800	-0.00526600
Eu	0.00004500	0.88742200	-0.00002700
C	-3.52161300	0.06191000	-0.68347700
H	-3.66090200	0.84696600	-1.41674800
N	-4.50753900	-0.78302200	-0.30670900
H	-5.47414800	-0.81080700	-0.63209000
C	-2.80193900	-1.30094800	0.76375200
N	-4.09567100	-1.63806100	0.58641000
H	-2.18606000	-1.84657700	1.46711400
N	2.40633300	-0.25201700	0.00534900
C	3.52086700	0.06078400	0.68500500
H	3.65948800	0.84461800	1.41972900
N	4.50713300	-0.78347200	0.30762000
H	5.47345800	-0.81180500	0.63377800
C	2.80251500	-1.29964400	-0.76526100
N	4.09607200	-1.63694700	-0.58741700

H	2.18721600	-1.84399800	-1.47011000
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EuPh³⁺ (PBE0/6-311G*-RECP)

C	-1.11054600	-0.73337900	-0.00011400
C	-1.11945900	-3.50303500	0.00004200
H	-1.05499300	-4.58582800	0.00008900
C	-1.11027900	0.73355700	-0.00004800
C	-2.34887800	1.43191300	-0.00006300
C	-2.33344600	2.84792400	-0.00009700
C	-1.11811900	3.50323100	-0.00001200
H	-3.26745200	3.40377700	-0.00010900
H	-1.05340300	4.58600800	0.00001700
N	0.06218900	1.38529800	0.00002000
C	-2.34932800	-1.43123700	0.00006900
N	0.06174500	-1.38557300	-0.00027300
C	-2.33451000	-2.84729300	0.00019500
H	-3.26877500	-3.40270300	0.00039000
C	-3.55611800	0.70759700	-0.00000800
H	-4.50586800	1.23710000	-0.00002200
C	-3.55633700	-0.70649900	0.00008800
H	-4.50624900	-1.23571000	0.00025800
C	0.04095600	-2.73719800	-0.00022200
H	1.00479000	-3.24065200	-0.00053900
Eu	2.22068200	-0.00024600	0.00003500
C	0.04196900	2.73699000	0.00005600
H	1.00602300	3.24002000	0.00017700

The constrained minima of the MR_{*i*}³⁺ complexes (*i* = 1~8) with the M-N-C angle constrained to approximate the M³⁺ location observed in the complex M(PhR_{*i*})³⁺ calculated by using the PBE0/ZORA/DKH/6-311G(d)-RECP methods and the CPCM solvation model in aqueous phase

AmR_{*i*}³⁺ (PBE0/ZORA, CPCM)

C	-3.59317109053145	-0.65243220524473	0.01646684744366
N	-1.48403740747615	-0.00696034198305	-0.06247312863906
C	-2.24641033528238	1.11150572297188	-0.02596798097495
C	-3.58481207263012	0.76699084982897	0.01654502986641
H	-4.41872163982981	-1.35875093732072	0.03779378833608
H	-1.99758438231406	-2.01507108325887	-0.04692987280630
H	-1.78888375798354	2.09752384882039	-0.04403917337942
H	-4.44655238206647	1.42468822821407	0.03688753886941
N	-2.33713247495571	-1.05504984899748	-0.02209287971909

Am 0.84987054306972 -0.01388623303048 0.09381283100324

AmR_{2,3}³⁺(PBE0/ZORA, CPCM)

C 3.90700501329906 0.75843069530366 0.06332286951709
C 3.76398529036766 -0.64515647561840 -0.08254050621127
H 4.79614514405424 1.37908162767024 0.12579491957752
H 2.39183775827272 2.22300333604187 0.23670541894254
H 4.55592026563123 -1.38626664844743 -0.15491149965493
N 2.65408102075230 1.24297149509693 0.13397567435533
C 1.78967420465190 0.22105188468949 0.03274819651278
H 0.70838236399690 0.33949031120012 0.04239041516474
N 2.45705158185407 -0.94758762013281 -0.09577913370853
Am 1.50084825711988 -3.20568744580368 -0.47126174449527

AmR₄³⁺(PBE0/ZORA, CPCM)

C 3.94082638594658 0.40560497019354 -0.65758629004182
N 2.20013518445051 0.75985313150840 0.65911170845092
C 3.54487222814445 -0.80496426186625 -0.14098142878190
H 4.73568532141004 0.68539454131359 -1.33964624769643
H 3.05319292045398 2.30901285897517 -0.28082868411327
H 3.94118369029366 -1.80595849088891 -0.28298861567502
N 3.07712154680431 1.30031987396441 -0.12543261978241
N 2.47738666733810 -0.50887706721606 0.65880287695786
Am 1.16395340515835 -2.04474931598388 1.69241023068205

AmR₅³⁺(PBE0/ZORA, CPCM)

C 4.03725471632764 0.80437103827217 -0.01094189706640
C 3.83887043263716 -0.57083847750175 -0.01908690940001
H 4.96219030310669 1.36807506895320 -0.05616794330244
H 4.54351273328927 -1.39769073876806 -0.07212835514721
N 2.50710732308181 -0.76354693039828 0.05262568041904
Am 1.45580311558214 -2.79167846656003 -0.04103517478215
N 1.97140744878683 0.45764494694646 0.10084959220820
H 0.96661379676865 0.62391016818406 0.17129622606832
N 2.84228116041980 1.39946134087223 0.06589021100265

AmR₆³⁺(PBE0/ZORA, CPCM)

C 3.47139605151698 0.85449800784518 -0.13451711406874
H 4.24697109801819 1.54812887497043 -0.45172095172070
N 2.18167172369846 -0.92541147856962 0.00666077239596
Am 4.24953104364358 -1.30417081334779 -2.40353629559214
C 1.81184149613454 -0.06898573371527 0.91618097272392

H	1.00267359539723	-0.20312680087369	1.62696784529646
N	2.59747094610509	1.04465137430826	0.85016317613779
H	2.53195402610229	1.86899846351766	1.44549710787480
N	3.20386700938365	-0.35183836413515	-0.63680901304735

AmR_{7,8}³⁺(PBE0/ZORA, CPCM)

N	2.45092742136390	-0.78597580259769	-0.08576045498904
Am	1.41821284716703	-2.75719779795724	-0.56194667230387
C	1.90933347325795	0.37359535675974	0.33639930472544
H	0.86640136682125	0.56372918742583	0.57793617211827
N	2.88118498944274	1.25454997457328	0.40074471143091
H	2.80283251202967	2.23135359968770	0.68018810585878
C	3.79541719727051	-0.50505974542936	-0.25051717978600
N	4.06227891410936	0.73288309388167	0.04165195874826
H	4.53488614853758	-1.22998899634392	-0.58074358580275

EuR₁³⁺(PBE0/ZORA, CPCM)

C	-3.62847629145701	-0.67903048134465	-0.00157530329333
N	-1.50649078035948	0.01879700553171	0.00171094870051
C	-2.22919793753539	1.10704822719297	-0.00011363473861
C	-3.61995717105975	0.76718474985933	-0.00241788495623
H	-4.45935312836994	-1.38130928359064	-0.00277727709551
H	-2.01758221260624	-2.00247569961470	0.00181694775997
H	-1.78456769458923	2.09963333180065	0.00012088823221
H	-4.48348177317834	1.42718449662674	-0.00439284075851
N	-2.38462349332201	-1.04879344455178	0.00085477687256
Eu	1.06629548247740	-0.00968090190966	0.00677637927694

EuR_{2,3}³⁺(PBE0/ZORA, CPCM)

C	3.90718875124501	0.78727242028326	0.07662295586835
C	3.75546343146484	-0.64567403934208	-0.08232904872979
H	4.80319341347548	1.40091403400125	0.13992449134737
H	2.39960539775054	2.24137345780459	0.24412474381099
H	4.55569048138087	-1.37846136406713	-0.16898807389434
N	2.66967584441732	1.26207899949356	0.13532614067576
C	1.80022854583374	0.22239557973804	0.02323049381981
H	0.71892658183348	0.34731900059693	0.04024764534575
N	2.45895017518433	-0.94224118611814	-0.11123670729946
Eu	1.45600827741435	-3.31564574239028	-0.46647803094445

EuR₄³⁺(PBE0/ZORA, CPCM)

C	3.95897095091202	0.46464795464079	-0.68743679528921
N	2.22401396217802	0.76933522694202	0.63304433981839
C	3.52608125184958	-0.79024879844482	-0.12607127811827
H	4.76374332378073	0.71170883753470	-1.37711992862237
H	3.09318235364826	2.35452124803302	-0.30952601285800
H	3.94161160695484	-1.78495386863619	-0.27540953987964
N	3.12719434012220	1.34208262283526	-0.15943979030058
N	2.48693197516075	-0.51107809675584	0.66433760391976
Eu	1.01262758539358	-2.26037888614895	1.82048233132991

EuR₅³⁺(PBE0/ZORA, CPCM)

C	4.05373232835110	0.86224581219440	-0.02563052225869
C	3.82438143999236	-0.57130441480317	0.00489942626540
H	4.98657650207489	1.41630198438129	-0.09759879186389
H	4.54493796609702	-1.38569010473891	-0.03715466968130
N	2.53333388673730	-0.75607855720358	0.09284085481386
Eu	1.32212299365645	-3.05297684716317	-0.10060402361319
N	2.01412122459697	0.50085489471072	0.11582117722206
H	0.99961089747706	0.65532426365931	0.18698020291979
N	2.84622379101685	1.46103091896310	0.05174777619598

EuR₆³⁺(PBE0/ZORA, CPCM)

C	3.44912438793128	0.86376216778257	-0.10652120168374
H	4.22488510002869	1.55694505919221	-0.42954832142333
N	2.18845988849373	-0.91517126143023	-0.00346637512832
Eu	4.36182608413090	-1.41185610727431	-2.57905580075777
C	1.80191751849597	-0.03067559819291	0.94999730856293
H	0.99169752717065	-0.18401843454477	1.66007047262359
N	2.58174002585800	1.06538509673782	0.88333397685208
H	2.51808251846077	1.89244790913924	1.48180410757784
N	3.17964393943001	-0.37407530140963	-0.63772766662328

EuR_{7,8}³⁺(PBE0/ZORA, CPCM)

N	2.46437195571219	-0.76647666775870	-0.11237187455551
Eu	1.31818624779041	-3.01664585804470	-0.57319554026785
C	1.92888236370098	0.38093950010104	0.31586858011634
H	0.88538690529071	0.58708406372382	0.55077287606972
N	2.93170229694954	1.30311423965250	0.41872122071466
H	2.83984386458765	2.27791165906889	0.72329186439581
C	3.76151414741234	-0.49782047920910	-0.25635194250220
N	4.06548809894514	0.80829726453213	0.07736702348155
H	4.52609898961102	-1.19851485206587	-0.58614984745253

AmR₁³⁺(PBE0/DKH, CPCM)

C	-3.58900409370430	-0.64802986600577	0.02005738705349
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N	-1.47921233349917	-0.00939317244844	-0.07374801724114
C	-2.24625040914606	1.11143520965051	-0.02752642379880
C	-3.58192225306530	0.76457647306811	0.01971547889954
H	-4.41349247942303	-1.35538849019172	0.04029019497944
H	-1.99473776000154	-2.01586694164266	-0.05143636272951
H	-1.78955688095655	2.09816011752649	-0.04749920278402
H	-4.44234756834624	1.42368345541538	0.03928963268573
N	-2.33071550009076	-1.05496914871283	-0.02204118127297
Am	0.81980427823296	-0.01564963665908	0.10290149420824

AmR_{2,3}³⁺(PBE0/DKH, CPCM)

C	3.90713045653896	0.74738906868988	0.05639019424160
C	3.76853613179780	-0.64350312831470	-0.08868950489742
H	4.79463615970611	1.36869417269913	0.12485717161639
H	2.38780284864063	2.21378772396742	0.23888861154419
H	4.55769319946828	-1.38809194875346	-0.15149972248837
N	2.64828967179564	1.23388277627495	0.13619536809440
C	1.78439938937826	0.21799809202169	0.03487338617545
H	0.70336909882721	0.33719902706318	0.03661171640783
N	2.45377795720830	-0.94987357037791	-0.09349342450910
Am	1.51929598663878	-3.15815105327018	-0.46368918618498

AmR₄³⁺(PBE0/DKH, CPCM)

C	3.94053785372285	0.40473134902036	-0.65721807102316
N	2.19839856834022	0.75990193637814	0.65836682200641
C	3.54361842487956	-0.80619991937891	-0.14173051892900
H	4.73678672563653	0.68562983839448	-1.33724109625270
H	3.05295171358290	2.30859860072068	-0.27948700352262
H	3.94113396453114	-1.80687975296759	-0.28405360059118
N	3.07654388116253	1.29957121602687	-0.12540882627049
N	2.47523184418486	-0.50978186072551	0.65775541191196
Am	1.16915437395940	-2.03993516746852	1.69187781267077

AmR₅³⁺(PBE0/DKH, CPCM)

C	4.03753333894363	0.80410455497513	-0.00648662722247
C	3.83806219012479	-0.57128831429952	-0.02455837914210
H	4.96241530095912	1.36857349063181	-0.04598670447630
H	4.54191193780966	-1.39874694564600	-0.08230420629052
N	2.50584338029583	-0.76392031049895	0.04210502789515
Am	1.45867127906880	-2.79012244617011	-0.02499508479241
N	1.97146820069168	0.45761571659023	0.09703626122205
H	0.96638973100295	0.62378687308547	0.16535034798537
N	2.84274567110354	1.39970533133193	0.07114079482124

AmR₆³⁺(PBE0/DKH, CPCM)

C	3.47510740019745	0.85189085643399	-0.13199660661203
H	4.25100726325080	1.54591160085164	-0.44838164540084
N	2.18628339104045	-0.93107174324036	0.01185867207360
Am	4.23681220465067	-1.29405131247377	-2.40590030883341
C	1.81280832263653	-0.07001225485871	0.91540555225958
H	1.00054363866135	-0.20134001191250	1.62332946662265
N	2.59685567021379	1.04518857650226	0.84794632859808
H	2.52614181204441	1.87303386512306	1.43808595947847
N	3.21181728730456	-0.35680604642562	-0.63146091818607

AmR_{7,8}³⁺(PBE0/DKH, CPCM)

N	2.44917589242301	-0.78619832848955	-0.08973447327742
Am	1.42250936847391	-2.75672350257978	-0.55659166721919
C	1.90862089364629	0.37387195180682	0.33436493372379
H	0.86568896619636	0.56574279723554	0.57514827746475
N	2.88166306514177	1.25379589620096	0.40174532442466
H	2.80346826935160	2.23009690705210	0.68372231124012
C	3.79417655324396	-0.50483485279398	-0.25153253925310
N	4.06314794732395	0.73226354922229	0.04373010013604
H	4.53302391419914	-1.23012554765439	-0.58289990723965

EuR₁³⁺(PBE0/DKH, CPCM)

C	-3.62626039695111	-0.67855145961887	-0.00140075759527
N	-1.50559154062386	0.01870852004106	0.00200291517124
C	-2.22838017483626	1.10797945451371	0.00011203471804
C	-3.61796398340414	0.76730961993539	-0.00214080589425
H	-4.45583817633871	-1.38215156230733	-0.00265748692943
H	-2.01434686223587	-2.00251213242192	0.00200898551003
H	-1.78153372552834	2.09978757496160	0.00032535003472
H	-4.48123547337421	1.42722420360294	-0.00410917789646
N	-2.38182557047151	-1.04873645025628	0.00106184394788
Eu	1.04554090376404	-0.01049976845031	0.00480009893351

EuR_{2,3}³⁺(PBE0/DKH, CPCM)

C	3.90767875192985	0.78745504421209	0.07824674312513
C	3.75556918968282	-0.64501670851972	-0.08628548927390
H	4.80384752676041	1.40067146372535	0.14519384084812
H	2.39984669392982	2.24161363635174	0.24890861782976
H	4.55527482340521	-1.37826201110491	-0.17537259005528
N	2.66976218617421	1.26234291044230	0.13692753888647
C	1.80005260004258	0.22336008625265	0.01961560354990
H	0.71856532512936	0.34828631107013	0.03455950753614
N	2.45890101666216	-0.94128674084800	-0.11789023101469
Eu	1.45543278628359	-3.31983283158163	-0.45345893143166

EuR₄³⁺(PBE0/DKH, CPCM)

C	3.96052166923364	0.46569606876066	-0.68593752301678
N	2.22774721530379	0.77137975829145	0.63813560797169
C	3.52796952989833	-0.78944570320081	-0.12341802333616
H	4.76441370656952	0.71160964658353	-1.37724683800048
H	3.08930009308407	2.35478892589184	-0.31552228813472
H	3.93894148809944	-1.78530444474534	-0.27836566351231
N	3.12297292850976	1.34217990623269	-0.16494744068344
N	2.48603733874181	-0.51134883279608	0.66307794324172
Eu	1.01645338055962	-2.26391908501794	1.82708515547048

EuR₅³⁺(PBE0/DKH, CPCM)

C	4.05619286193817	0.86210228479250	-0.00125697610888
C	3.82092991905050	-0.57096703341232	-0.03032041450741
H	4.99251042824361	1.41420518004248	-0.03320671366837
H	4.53967250900641	-1.38566404993921	-0.09530896625250
N	2.52761625067577	-0.75282665786644	0.03135944757099
Eu	1.32549278559512	-3.06364899102331	-0.00792559638276
N	2.01345082301679	0.50408189746089	0.09414267378302
H	0.99829178544482	0.65935634917239	0.15541027639657
N	2.85088366702882	1.46306897077303	0.07840769916934

EuR₆³⁺(PBE0/DKH, CPCM)

C	3.47149627445978	0.84075117824697	-0.14133807900797
H	4.24585120574970	1.54058180313039	-0.45011989414597
N	2.16984570220391	-0.93984840149046	0.04152245661423
Eu	4.28068471502059	-1.29625146272157	-2.45655120320639
C	1.79737126166254	-0.06405252092401	0.92617229893933
H	0.98749276319053	-0.18329266506623	1.64012302432878
N	2.58570465536714	1.04824365257017	0.84744808154113
H	2.53356784068925	1.87296466948000	1.44915245101839
N	3.22536257165655	-0.35635272322526	-0.63752263608152

EuR_{7,8}³⁺(PBE0/DKH, CPCM)

N	2.46421567984451	-0.76670994287868	-0.11224402862674
Eu	1.31826047854429	-3.01514422867699	-0.57349855220273
C	1.92883718695779	0.38148449246495	0.31610192582849
H	0.88506431082784	0.58731408333433	0.55055315624944
N	2.93162380889641	1.30287543467212	0.41881061009446
H	2.84000627386675	2.27787308837027	0.72335787804706
C	3.76150394706992	-0.49813696406604	-0.25651456436947
N	4.06592774008732	0.80764637276952	0.07725141445822
H	4.52603544390515	-1.19931346598949	-0.58586547947874

AmR₁³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.61591100	-0.63360000	0.00000200
N	-1.49073900	-0.01058200	-0.00000200
C	-2.24653400	1.09067100	0.00000000
C	-3.60008300	0.74912300	0.00000000
H	-4.42730700	-1.34474300	0.00000300
H	-1.99461600	-1.98846500	-0.00000200
H	-1.78311900	2.06670000	0.00000000
H	-4.45142000	1.41050600	0.00000000
N	-2.34097800	-1.04235900	-0.00000100
Am	1.01319600	-0.00011100	0.00000000

AmR_{2,3}³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.57248800	0.71763000	0.00000100
C	-2.26924100	1.11295000	-0.00000100
H	-4.49575000	1.27262200	0.00000300
H	-4.34817300	-1.26263000	0.00000300
H	-1.85990700	2.11101500	-0.00000200
N	-3.54511900	-0.65342000	0.00000100
C	-2.26992700	-1.05587600	-0.00000100
H	-1.96505800	-2.09048900	-0.00000200
N	-1.46504300	-0.00552500	-0.00000200
Am	1.01484200	-0.00069600	0.00000000

AmR₄³⁺(PBE0/6-311G*-RECP, CPCM)

C	3.59919000	0.67373100	0.00000200
N	2.25106800	-1.08504700	-0.00000200
C	2.29749700	1.10110500	-0.00000200
H	4.54564900	1.18736100	0.00000500
H	4.24386700	-1.35036800	0.00000300
H	1.88764500	2.09791500	-0.00000300

N	3.49797000	-0.66978000	0.00000100
N	1.51889300	-0.00918200	-0.00000200
Am	-1.02034500	-0.00248300	0.00000000

AmR₅³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.64901900	0.64914600	-0.00001900
C	-2.32475700	1.08432000	0.00001800
H	-4.56666700	1.21500900	-0.00003300
H	-1.90391900	2.07734000	0.00003400
N	-1.55091800	-0.00179600	-0.00000500
Am	1.02785800	0.00185100	0.00000000
N	-2.39738000	-1.01407500	0.00000300
H	-2.08975600	-1.97489500	0.00000800
N	-3.65791600	-0.68328000	0.00000800

AmR₆³⁺(PBE0/6-311G*-RECP, CPCM)

C	2.27381200	1.04359000	-0.00005600
H	1.95594300	2.07406200	-0.00005100
N	2.27549700	-1.14009400	-0.00002800
Am	-1.01820200	-0.00180800	0.00000600
C	3.50988400	-0.72418100	0.00002000
H	4.38581500	-1.35295600	0.00010100
N	3.55262200	0.63374600	0.00005900
H	4.37655700	1.21584800	0.00015000
N	1.50169000	-0.01960500	-0.00010800

AmR_{7,8}³⁺(PBE0/6-311G*-RECP, CPCM)

N	1.50583000	-0.02153800	-0.00001200
Am	-1.02416900	-0.00263600	0.00000100
C	2.34572900	-1.04838400	-0.00000700
H	2.08761000	-2.09566600	-0.00001100
N	3.58409000	-0.57473400	0.00000700
H	4.44797200	-1.09508300	0.00001800
C	2.32127500	1.07134700	-0.00000500
N	3.59552900	0.76982600	0.00000600
H	1.96027500	2.08854200	-0.00000900

EuR₁³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.36193800	-0.64655900	-0.00009400
N	-1.23285500	0.00051800	-0.00000100
C	-1.97477900	1.09345100	-0.00009500
C	-3.34129300	0.76216400	0.00012000
H	-4.18392400	-1.34543400	-0.00014600
H	-1.75275400	-1.98974000	0.00007800
H	-1.51391900	2.06995400	-0.00014600
H	-4.19159000	1.42498200	0.00020500
N	-2.10268900	-1.04289600	0.00004400
Eu	1.38189000	-0.00186400	0.00000200

EuR_{2,3}³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.30357900	0.71037600	0.00451900
C	-1.96222100	1.10119200	0.00186200
H	-4.21594500	1.28428400	-0.00245200
H	-4.09343400	-1.24733300	0.00207600
H	-1.56242300	2.10340800	-0.00983200
N	-3.28526400	-0.64147500	-0.00104500
C	-2.00114600	-1.04770800	-0.00108500
H	-1.70496000	-2.08520700	0.00792000
N	-1.17867600	0.00243100	-0.00566500
Eu	1.37184200	-0.00261900	0.00027800

EuR₄³⁺(PBE0/6-311G*-RECP, CPCM)

C	3.25180700	0.67264200	-0.00000300
N	1.90652700	-1.08456100	0.00000300
C	1.93910300	1.10017200	0.00000300
H	4.19459200	1.19359900	-0.00000800
H	3.90055400	-1.34779600	-0.00000600
H	1.53238600	2.09842700	0.00000200
N	3.15262800	-0.66792300	-0.00000300
N	1.16746500	-0.00540900	0.00000600
Eu	-1.33903700	-0.00437900	-0.00000100

EuR₅³⁺(PBE0/6-311G*-RECP, CPCM)

C	-3.25618500	0.64743400	0.00000300
C	-1.93577600	1.08836200	-0.00000300
H	-4.17503400	1.21081800	0.00000800
H	-1.51717500	2.08228400	-0.00000400
N	-1.16247100	0.00129200	-0.00000700
Eu	1.32567800	0.00296500	0.00000100
N	-2.00333000	-1.01839100	-0.00000200
H	-1.69344800	-1.97905300	-0.00000200
N	-3.25995600	-0.68513400	0.00000300

EuR₆³⁺(PBE0/6-311G*-RECP, CPCM)

C	1.90215600	1.05017500	0.00012700
H	1.58692200	2.08120600	0.00011600
N	1.88152200	-1.13088900	0.00009700
Eu	-1.31786000	-0.00265900	-0.00002900
C	3.12282900	-0.73221600	-0.00011700
H	3.99156100	-1.37012100	-0.00031600
N	3.17349100	0.62541300	-0.00013500
H	4.00239100	1.20194300	-0.00049300
N	1.12990600	-0.01642100	0.00039000

EuR_{7,8}³⁺(PBE0/6-311G*-RECP, CPCM)

N	1.12256300	-0.01723900	-0.00003600
Eu	-1.32291000	-0.00425600	-0.00000200
C	1.95801500	-1.05174400	-0.00003000
H	1.69446900	-2.09754700	0.00009300
N	3.19248500	-0.57791800	0.00002600
H	4.05705400	-1.09808500	0.00033000
C	1.93670200	1.07883000	0.00015500
N	3.20600200	0.76737400	-0.00016400
H	1.57616300	2.09574500	0.00016700

AmR₁Ph³⁺ (PBE0/6-311G*-RECP)

C	2.22681600	0.20808500	0.06889800
C	4.02345900	-1.85675300	0.32459900
H	4.68662900	-2.70737000	0.43611800
C	1.27079800	1.29164800	-0.01918900
C	1.72982000	2.63388700	-0.11509700
C	0.75016200	3.65871000	-0.14220400
C	-0.58099000	3.33557200	-0.05543200
H	1.05860600	4.69738500	-0.21956500
H	-1.33587300	4.11279200	-0.05700400
N	-0.03426700	0.98795300	0.02860500
C	3.60686800	0.50070400	0.05332800
C	-0.95446200	1.98401700	0.02681700
C	-3.51484000	2.30700500	0.16053400
C	-4.52513500	1.37014200	0.26430700
H	-3.64288900	3.37837700	0.12134900
H	-4.42102900	-0.72244600	0.37880200
H	-5.59902400	1.48140400	0.33466800
C	-2.33454900	1.55765100	0.12045200
N	-2.60920300	0.22501800	0.19553500
N	1.75401400	-1.05118000	0.18991500

C	4.51444900	-0.57318400	0.17862300
H	5.58486100	-0.38746400	0.16878500
N	-3.94172600	0.16259700	0.27607300
C	3.11323000	2.89227000	-0.14500100
H	3.46745300	3.91651100	-0.21456600
C	4.03204100	1.85170400	-0.06615500
H	5.09533900	2.07378200	-0.08152900
C	2.64473600	-2.04985400	0.32583200
H	2.24655900	-3.05502500	0.44065400
Am	-0.72986100	-1.36556100	-0.12653100

AmR₂Ph³⁺ (PBE0/6-311G*-RECP)

C	1.26677400	1.30834500	0.01114900
C	-0.95817300	1.99530400	-0.02616700
C	-0.58272900	3.35492100	0.02341700
H	-1.33761800	4.13246000	0.02371200
C	2.22993900	0.22891900	-0.04174400
C	3.60655400	0.52924800	-0.02872000
C	4.52033300	-0.54120900	-0.10163800
C	4.03891300	-1.83377400	-0.19313400
H	5.58936600	-0.34834100	-0.09229500
H	4.70853600	-2.68405300	-0.25845700
N	1.76580400	-1.03776400	-0.11518500
C	1.72539500	2.65737000	0.07531600
C	-2.32476200	1.56521700	-0.07344500
C	-3.50284000	2.29992400	-0.11349600
H	-3.69766000	3.36286500	-0.11796200
H	-5.48975700	1.59884800	-0.19243900
H	-4.56447100	-0.74785600	-0.16523100
N	-2.64263100	0.21356100	-0.08677200
N	-0.03690800	0.99744500	-0.02857100
C	0.74323700	3.68183800	0.08497900
H	1.05191100	4.72185700	0.13480900
C	-3.96056800	0.14927700	-0.13370400
N	-4.49765000	1.38896400	-0.14967800
C	3.10514700	2.92337700	0.09854600
H	3.45251900	3.95105800	0.14334300
C	4.02604500	1.88869700	0.05206400
H	5.08864100	2.11328800	0.07076300
C	2.66123200	-2.03486500	-0.20086900
H	2.27000000	-3.04657000	-0.27714300
Am	-0.72377600	-1.40025800	0.07154800

AmR₃Ph³⁺ (PBE0/6-311G*-RECP)

C	1.26206500	1.30631500	0.01284100
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C	-0.95772000	1.99826700	-0.02443800
C	-0.58642400	3.35515500	0.03356300
H	-1.33136600	4.14289100	0.03702600
C	2.22276800	0.22532000	-0.04449700
C	3.59812300	0.52633900	-0.03154600
C	4.51200800	-0.54392700	-0.11335700
C	4.03067400	-1.83444600	-0.21265700
H	5.58096600	-0.35093500	-0.10451100
H	4.69989500	-2.68444900	-0.28557200
N	1.75699500	-1.04171900	-0.12611300
C	1.72341600	2.65670500	0.07999400
C	-2.31278200	1.53782000	-0.08650800
H	-3.52791900	3.28405500	-0.11002400
H	-5.53382700	1.78770300	-0.20784000
H	-4.52673100	-0.78045900	-0.20821700
N	-2.63198500	0.22424200	-0.11869900
N	-0.03869300	0.99865600	-0.02539100
C	0.74384700	3.67918700	0.09587400
H	1.05229400	4.71910500	0.14959900
C	-3.97927000	0.15081700	-0.16194200
C	-4.51047000	1.43989700	-0.16381800
N	-3.45330800	2.27381700	-0.11679700
C	3.10562600	2.92143000	0.10564100
C	4.01967600	1.88721500	0.05402000
H	3.45394900	3.94836300	0.15653300
H	5.08316700	2.10776200	0.07048400
C	2.65173900	-2.03659000	-0.21773600
H	2.26183300	-3.04854900	-0.29778400
Am	-0.73455800	-1.40976300	0.07954400

AmR₄Ph³⁺ (PBE0/6-311G*-RECP)

C	2.21592600	0.18575500	0.05147800
C	3.95456400	-1.93805100	0.24884400
H	4.59340400	-2.80991300	0.33583900
C	1.29081000	1.29544500	-0.01629100
C	1.78941400	2.62323300	-0.09657700
C	0.84443300	3.67818000	-0.09861200
C	-0.49769700	3.39540100	-0.01257500
H	1.18489500	4.70794200	-0.15953400
H	-1.22873100	4.19586100	-0.00030300
N	-0.02402500	1.02751300	0.03500100
C	3.60445300	0.43718100	0.03003600
C	-0.90810300	2.05628400	0.04126700
H	-3.81738800	3.31531900	0.16475400

H	-5.41607000	1.32270000	0.23393600
C	-2.29203200	1.63761200	0.10096700
N	-2.55669800	0.29553300	0.11328700
N	1.70909900	-1.06264900	0.15269400
C	4.48074300	-0.66657600	0.12394100
H	5.55604000	-0.51181400	0.10799500
N	-3.83304300	0.08017400	0.16378300
N	-4.40188000	1.26586400	0.18611900
C	-3.51628600	2.27750000	0.15174400
C	4.07008100	1.77510000	-0.07616200
H	5.13928200	1.96476200	-0.10452600
C	3.18251200	2.84156900	-0.13037900
H	3.56508100	3.85653000	-0.18401300
C	2.57106200	-2.08955300	0.26692600
H	2.14507500	-3.08421500	0.37741600
Am	-0.76542200	-1.36059700	-0.09300400

AmR₅Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.26717400	1.30569800	-0.01551200
C	0.95403400	1.99795700	0.02037600
C	0.58664000	3.35113800	-0.04567600
H	1.34405700	4.12640300	-0.04815900
C	-2.23227100	0.22179400	0.05388000
C	-3.61249600	0.52188200	0.04065000
C	-4.52958600	-0.54756200	0.13718400
C	-4.04715400	-1.83781200	0.25265200
H	-5.59864700	-0.35356000	0.12783700
H	-4.71549400	-2.68743800	0.33932800
N	-1.77029400	-1.04033600	0.14819200
C	-1.72334700	2.65226500	-0.09398000
C	2.33598400	1.57874400	0.09172400
H	3.73077200	3.36834800	0.12136700
N	2.65341400	0.26200900	0.14130900
N	0.03485100	0.99827900	0.02475000
C	-0.74480000	3.67823100	-0.11573900
H	-1.05297200	4.71806600	-0.17909100
N	4.53992900	1.43940800	0.21101100
C	3.53724700	2.30510000	0.13612300
C	-3.10355400	2.91637700	-0.11891900
H	-3.45556600	3.94254100	-0.17490600
C	-4.03131400	1.87412800	-0.05668800
H	-5.09338700	2.10333600	-0.07334800
N	3.97354500	0.27022900	0.20758700
H	4.53809600	-0.57009400	0.27318800

C	-2.66982000	-2.03673300	0.25638100
H	-2.27787300	-3.04653600	0.34977000
Am	0.73522700	-1.39995200	-0.09600700

AmR₆Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.30501300	1.27796900	-0.01934800
C	0.87896000	2.07278300	0.05145300
C	0.45432700	3.40070000	0.00040100
H	1.16518000	4.21936900	0.02184600
C	-2.20213800	0.15371800	0.04798300
C	-3.59313000	0.37546900	0.02522900
C	-4.44127200	-0.75081300	0.12380400
C	-3.88560000	-2.00785500	0.25517200
H	-5.52009600	-0.62310800	0.10760100
H	-4.50417700	-2.89371100	0.34748100
N	-1.66189200	-1.08453500	0.15615200
C	-1.82590700	2.59652700	-0.09784000
C	2.25600700	1.61269400	0.11820800
H	3.65608900	3.21394400	0.14638300
H	5.45641000	1.39595100	0.20870700
N	2.48248000	0.30188200	0.14322500
N	0.01352500	1.03209100	0.03438800
C	-0.89944700	3.66080300	-0.09264400
H	-1.25276800	4.68642600	-0.15116400
N	3.80427300	0.05340200	0.16947200
C	4.38838600	1.22410100	0.17623700
N	3.45331200	2.22065000	0.14651800
C	-4.08770300	1.70667200	-0.08378600
H	-5.16102400	1.86996600	-0.11241900
C	-3.23031700	2.78593100	-0.13612300
H	-3.63156800	3.79340300	-0.18929100
C	-2.49784500	-2.13041700	0.27650700
H	-2.05117800	-3.11530000	0.39661900
Am	0.79100400	-1.32716900	-0.09679500

AmR₇Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.26666800	1.30063000	0.01562000
C	0.95067100	1.98248500	-0.02902000
C	0.60292600	3.33826900	0.02828100
H	1.38124200	4.09353900	0.02137800
C	-2.23036500	0.22129900	-0.05088400
C	-3.60983600	0.52317400	-0.03185900

C	-4.52624500	-0.54777000	-0.12353700
C	-4.04377400	-1.83745400	-0.24180800
H	-5.59537900	-0.35477400	-0.10948000
H	-4.71243100	-2.68699100	-0.32565600
N	-1.76646500	-1.04144800	-0.14773200
C	-1.71211100	2.64753800	0.09380300
C	2.32709800	1.53439300	-0.09127700
N	2.65871300	0.19785000	-0.11541300
N	0.03627800	0.98612800	-0.03032700
C	-0.72869600	3.66993800	0.10466200
H	-1.03272400	4.71110700	0.16567000
C	3.98862800	0.21861100	-0.17849000
H	4.66213700	-0.62700800	-0.22130100
C	-3.09494300	2.91463300	0.12269900
H	-3.44333800	3.94212600	0.17473200
C	-4.02419200	1.87660800	0.06730000
H	-5.08546600	2.10812800	0.08987000
N	3.36755100	2.33292100	-0.13511100
N	4.39101600	1.49134400	-0.19053000
H	5.33985500	1.85101700	-0.24102500
C	-2.66630000	-2.03724600	-0.25492200
H	-2.27537100	-3.04684700	-0.35535000
Am	0.73847000	-1.39566900	0.09001600

AmR₈Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.27396900	1.29126300	-0.01782600
C	0.93838900	2.00633200	0.03690100
C	0.56076000	3.35157700	-0.03399500
H	1.30041200	4.14455700	-0.03079000
C	-2.21608800	0.19845200	0.05928200
C	-3.59946100	0.47516500	0.03853300
C	-4.49423900	-0.61349300	0.14793500
C	-3.98796300	-1.89126300	0.28615500
H	-5.56699700	-0.44157700	0.13333300
H	-4.64077600	-2.75142900	0.38609200
N	-1.72723300	-1.05646000	0.17271000
C	-1.74511600	2.62800700	-0.10897900
C	2.30619100	1.53149600	0.11364500
H	3.63020400	3.20484400	0.18884400
N	2.60185700	0.21739700	0.13574600
N	0.03454200	0.99947200	0.03619500
C	-0.77910000	3.66072300	-0.12275900
H	-1.09582000	4.69752000	-0.19355700
N	3.45781800	2.20523800	0.17511900

C	3.96425600	0.18718100	0.20548200
H	4.56622000	-0.71042000	0.24593400
N	4.50118000	1.38624800	0.23617900
C	-3.13659700	2.87123200	-0.14331700
H	-3.50155900	3.89222800	-0.20507900
C	-4.04079200	1.82092400	-0.07738100
H	-5.10669300	2.02926200	-0.10188100
C	-2.60640900	-2.06723800	0.29992900
H	-2.19765700	-3.06808600	0.41816500
Am	0.74943500	-1.36802400	-0.10773000

EuR₁Ph³⁺ (PBE0/6-311G*-RECP)

C	2.13180000	0.13211600	0.00035500
C	4.10699600	-1.78523800	0.00110900
H	4.84001100	-2.58429000	0.00137500
C	1.08128800	1.15212500	-0.00000100
C	1.44726200	2.53716000	-0.00037700
C	0.39997300	3.49620000	-0.00075700
C	-0.90105500	3.07552600	-0.00071500
H	0.63925000	4.55565000	-0.00131300
H	-1.71025500	3.79542000	-0.00107500
N	-0.18887400	0.75790400	0.00010500
C	3.48518600	0.53751500	0.00039500
C	-1.17793600	1.69301700	-0.00010300
C	-3.74258500	1.91911700	0.00048600
C	-4.72719300	0.95593700	0.00110600
H	-3.90053900	2.98700100	0.00001700
H	-4.55811700	-1.13734500	0.00220000
H	-5.80611900	1.03097600	0.00133300
C	-2.53321000	1.19844700	0.00040900
N	-2.77515800	-0.13977400	0.00127500
N	1.77272600	-1.16139100	0.00074500
C	4.48561500	-0.45603100	0.00072900
H	5.53536600	-0.17627800	0.00073300
N	-4.10095900	-0.23445900	0.00143900
C	2.79694500	2.89942400	-0.00038800
H	3.07605400	3.94929500	-0.00067300
C	3.80132800	1.92160400	0.00000300
H	4.84352600	2.23000300	0.00000600
C	2.74840100	-2.08708500	0.00113800
H	2.43596000	-3.12817600	0.00155300
Eu	-0.77406600	-1.73360700	-0.00078500

EuR₂Ph³⁺ (PBE0/6-311G*-RECP)

C	1.07208700	1.15753500	0.00002100
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C	-1.18911200	1.69070500	0.00010200
C	-0.91311200	3.07923200	0.00027300
H	-1.72141800	3.80084100	0.00035900
C	2.12344500	0.14407200	-0.00003800
C	3.47178500	0.55527100	-0.00011700
C	4.47454000	-0.43319100	-0.00026300
C	4.10286200	-1.76404900	-0.00023700
H	5.52299400	-0.14917300	-0.00037300
H	4.84025600	-2.55895400	-0.00037500
N	1.76845500	-1.15455900	0.00010900
C	1.43564200	2.54681500	0.00006700
C	-2.52350400	1.17881700	-0.00006500
C	-3.73823100	1.87033600	0.00011700
H	-3.97507500	2.92484300	0.00029100
H	-5.69328700	1.09354500	-0.00058700
H	-4.66912500	-1.21579900	-0.00078800
N	-2.78849400	-0.18384800	-0.00027600
N	-0.19785300	0.75835800	0.00001500
C	0.38388000	3.50126400	0.00026500
H	0.62085600	4.56096900	0.00036400
C	-4.09866300	-0.29632900	-0.00043400
N	-4.69233000	0.92510800	-0.00037200
C	2.78468900	2.91493200	-0.00012200
H	3.05702900	3.96607600	-0.00006800
C	3.78397800	1.94630200	-0.00012400
H	4.82629100	2.25333100	-0.00032100
C	2.74517700	-2.07434800	-0.00001200
H	2.43890500	-3.11745000	0.00012100
Eu	-0.75188300	-1.74726700	0.00013400

EuR₃Ph³⁺ (PBE0/6-311G*-RECP)

C	1.05253200	1.16123700	0.00000300
C	-1.20824400	1.68387900	-0.00003700
C	-0.94451200	3.07104800	0.00044300
H	-1.74791900	3.79886900	0.00071600
C	2.10823300	0.15508400	-0.00029000
C	3.45304200	0.57591100	-0.00025500
C	4.46234800	-0.40676700	-0.00066200
C	4.10031200	-1.73898800	-0.00107700
H	5.50873400	-0.11537500	-0.00063500
H	4.84301400	-2.52892300	-0.00142700
N	1.76166500	-1.14773700	-0.00060200
C	1.40891400	2.55303000	0.00038000

C	-2.52784200	1.13678900	-0.00043900
H	-3.83143100	2.82821600	-0.00072600
H	-5.76223000	1.24000200	-0.00104600
H	-4.62834200	-1.28055300	-0.00100800
N	-2.78685800	-0.19130700	-0.00068300
N	-0.21421100	0.75618700	-0.00011800
C	0.35395900	3.49912500	0.00062700
H	0.58382400	4.56041000	0.00105000
C	-4.12186000	-0.32487000	-0.00093900
C	-4.72133200	0.94431600	-0.00092500
N	-3.70859300	1.82278200	-0.00070900
C	2.75868600	2.93052700	0.00051300
C	3.75795500	1.96993000	0.00019400
H	3.02347000	3.98349400	0.00082300
H	4.79932300	2.28023200	0.00019500
C	2.74401100	-2.05952000	-0.00099700
H	2.44610600	-3.10520300	-0.00131200
Eu	-0.74056800	-1.76579400	0.00061800

EuR₄Ph³⁺ (PBE0/6-311G*-RECP)

C	2.12394000	0.10711400	0.00030100
C	4.04797100	-1.86479200	0.00123100
H	4.75758600	-2.68474400	0.00166400
C	1.10373500	1.15992000	-0.00002300
C	1.51031100	2.53299300	-0.00047100
C	0.49416700	3.52482800	-0.00055300
C	-0.82109600	3.14554100	-0.00018400
H	0.76700600	4.57620900	-0.00092800
H	-1.60864000	3.89031200	-0.00019500
N	-0.17655800	0.80420700	0.00017800
C	3.49006800	0.47418500	0.00011400
C	-1.13306700	1.77345800	0.00015300
H	-4.05403600	2.93155200	0.00117000
H	-5.60859100	0.90714800	0.00135900
C	-2.48732100	1.28255100	0.00049400
N	-2.72152500	-0.06765600	0.00031600
N	1.72960300	-1.17525800	0.00086200
C	4.46359900	-0.54715800	0.00056500
H	5.52060900	-0.29611600	0.00034200
N	-3.98858200	-0.30280600	0.00070400
N	-4.59265900	0.87587500	0.00102300
C	-3.73153100	1.90006800	0.00088500
C	3.84679600	1.84588500	-0.00039600
H	4.89754500	2.12402400	-0.00048200

C	2.87050900	2.85509000	-0.00070900
H	3.18207200	3.89591700	-0.00098900
C	2.68122200	-2.12706600	0.00131200
H	2.34052800	-3.15935400	0.00184400
Eu	-0.83653700	-1.73811400	-0.00066100

EuR₅Ph³⁺ (PBE0/6-311G*-RECP)

C	1.07377100	1.15719200	0.00017200
C	-1.18442000	1.69529400	0.00007400
C	-0.91526900	3.07642200	0.00091500
H	-1.72670700	3.79461600	0.00106100
C	2.12765000	0.13904200	-0.00043500
C	3.48154000	0.54840900	-0.00056900
C	4.48631400	-0.44247000	-0.00162900
C	4.11163100	-1.77285800	-0.00243300
H	5.53515900	-0.15891700	-0.00175000
H	4.84657700	-2.57026900	-0.00337200
N	1.77351500	-1.15497100	-0.00097900
C	1.43476800	2.54200900	0.00091700
C	-2.53893300	1.19592000	-0.00085100
H	-4.01235200	2.92705400	-0.00124200
N	-2.80364500	-0.13315300	-0.00160700
N	-0.19649000	0.75991800	-0.00011200
C	0.38712100	3.49977700	0.00141000
H	0.62421800	4.55988600	0.00209000
N	-4.74125600	0.96747300	-0.00156800
C	-3.77432300	1.87281900	-0.00144200
C	2.78438100	2.90809200	0.00095200
H	3.06177100	3.95865900	0.00143900
C	3.79417400	1.93070300	0.00020200
H	4.83523000	2.24349000	-0.00005200
N	-4.11983600	-0.17718200	-0.00273600
H	-4.65016200	-1.04203900	-0.00410200
C	2.75412600	-2.07798700	-0.00195000
H	2.44525100	-3.12019700	-0.00237300
Eu	-0.76952700	-1.74700100	0.00135400

EuR₆Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.11288000	1.15720600	0.00005700
C	1.11433000	1.79139000	0.00016800
C	0.79714700	3.15755500	-0.00010300
H	1.57150600	3.91642200	-0.00017700
C	-2.12200900	0.09287200	0.00031600

C	-3.49251700	0.44847700	0.00002600
C	-4.45741500	-0.58285400	0.00026200
C	-4.02882400	-1.89543300	0.00091500
H	-5.51672900	-0.34163100	-0.00007400
H	-4.73001000	-2.72267000	0.00120900
N	-1.71498300	-1.18455100	0.00086800
C	-1.53163000	2.52656000	-0.00036500
C	2.46122500	1.27012400	0.00042700
H	3.87227900	2.87808400	0.00188000
H	5.66196500	1.06297400	0.00081100
N	2.68595800	-0.04411700	0.00019300
N	0.16722700	0.81428800	0.00020600
C	-0.52624500	3.52518100	-0.00042000
H	-0.80651200	4.57470700	-0.00077200
N	3.99789500	-0.28051600	0.00013800
C	4.59228400	0.89876500	0.00062800
N	3.66680200	1.88626600	0.00094300
C	-3.86209300	1.81521500	-0.00031900
H	-4.91566800	2.08281600	-0.00080700
C	-2.89737800	2.83537000	-0.00068700
H	-3.22032200	3.87277600	-0.00106900
C	-2.65895400	-2.14445400	0.00115900
H	-2.30902600	-3.17360100	0.00168900
Eu	0.87495200	-1.74389400	-0.00050000

EuR₇Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.08055900	1.15247100	-0.00000500
C	1.17086300	1.68204700	-0.00008800
C	0.92275100	3.06545600	-0.00035400
H	1.75534900	3.76020700	-0.00051700
C	-2.13493900	0.13629100	0.00007600
C	-3.48788900	0.54944300	0.00020100
C	-4.49449400	-0.43968000	0.00035400
C	-4.12097000	-1.77041700	0.00031400
H	-5.54295800	-0.15483400	0.00040400
H	-4.85703100	-2.56671900	0.00039000
N	-1.78094000	-1.15711000	0.00007900
C	-1.43144800	2.53888600	-0.00011800
C	2.51911300	1.15943000	0.00011300
N	2.81341300	-0.18408700	0.00124200
N	0.18735000	0.74904900	0.00004400
C	-0.37875400	3.49365700	-0.00031900
H	-0.61236400	4.55452500	-0.00051200
C	4.13903500	-0.19892600	0.00068900

H	4.79018200	-1.06291700	0.00128000
C	-2.78068600	2.90778700	-0.00002300
H	-3.05589600	3.95894400	-0.00007400
C	-3.79436300	1.93244500	0.00016100
H	-4.83408400	2.24962400	0.00029600
N	3.58824100	1.93225400	-0.00029700
N	4.58410100	1.06615200	0.00024000
H	5.54468000	1.39668000	0.00005000
C	-2.76375900	-2.07775300	0.00015200
H	-2.45654100	-3.12033700	0.00007000
Eu	0.79079500	-1.75628300	-0.00027700

EuR₈Ph³⁺ (PBE0/6-311G*-RECP)

C	-1.08606900	1.15545600	-0.00000800
C	1.16192500	1.71696500	0.00002900
C	0.88437300	3.09444200	-0.00042600
H	1.68035500	3.83049900	-0.00064900
C	-2.12698500	0.12412500	0.00023400
C	-3.48551600	0.51970500	0.00025700
C	-4.47965200	-0.48286300	0.00055800
C	-4.08941300	-1.80817500	0.00084600
H	-5.53165400	-0.21128400	0.00056500
H	-4.81509000	-2.61406200	0.00109400
N	-1.75716800	-1.16476100	0.00050600
C	-1.46162100	2.53643800	-0.00034500
C	2.50003700	1.17584300	0.00041500
H	3.86788600	2.83036200	0.00042900
N	2.77408000	-0.14194100	0.00073000
N	0.18583900	0.77221000	0.00015200
C	-0.42475200	3.50354100	-0.00056500
H	-0.67143200	4.56145200	-0.00097800
N	3.67487100	1.83463700	0.00046300
C	4.12433300	-0.19406900	0.00086800
H	4.71382000	-1.10072600	0.00118800
N	4.69567300	1.00345000	0.00082600
C	-2.81696200	2.88735600	-0.00040900
H	-3.10709000	3.93444400	-0.00064500
C	-3.81331100	1.89789000	-0.00008800
H	-4.85806100	2.19827900	-0.00008300
C	-2.72782900	-2.09786100	0.00080100
H	-2.40754500	-3.13657000	0.00104500
Eu	0.81213400	-1.75540200	-0.00053500

AmR₁Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.70362700	-0.54468200	0.04112000
C	3.15456200	-3.23634700	0.22797800
H	3.27306000	-4.31144400	0.29506800
C	2.45498500	0.87035100	-0.08082600
C	3.54676100	1.76535300	-0.08286700
C	3.25477800	3.13198800	-0.24574500
C	1.95642400	3.54077900	-0.40793300
H	4.06509300	3.85504000	-0.25131000
H	1.71538700	4.58773500	-0.54980100
N	1.18242200	1.28584200	-0.20940000
C	4.03136800	-1.00076300	0.17881000
C	0.92991900	2.57935100	-0.38601700
C	-1.12658300	4.17097900	-0.73490100
C	-2.46401800	3.84495400	-0.82846000
H	-0.70068800	5.16100600	-0.77776400
H	-3.35476800	1.89244600	-0.70772200
H	-3.34263200	4.45749300	-0.95914000
C	-0.47396900	2.93632600	-0.56539100
N	-1.36323000	1.94544600	-0.56639800
N	1.65145500	-1.38912900	-0.00479500
C	4.23322800	-2.38967200	0.27992400
H	5.24180900	-2.77694300	0.39143300
N	-2.54807600	2.50739600	-0.72128900
C	4.87558300	1.26770300	0.06966900
H	5.69875800	1.97567100	0.07645900
C	5.10825100	-0.06195200	0.19916500
H	6.12094700	-0.43650900	0.31282500
C	1.87348500	-2.68813600	0.07918200
H	1.00016000	-3.32903400	0.00982200
Am	-0.79223500	-0.44581900	0.04980500
N	-3.63626500	-1.08254900	0.34425800
O	-3.21150900	-0.10611300	-0.37625400
O	-4.80194300	-1.30337500	0.47814000
O	-2.72955000	-1.77045600	0.88877600
N	-0.43182600	-1.71923700	-2.53970100
O	-0.21821400	-2.28127100	-3.57378900
O	-0.78214100	-2.35257200	-1.48517300
O	-0.32286800	-0.46286900	-2.40518600
N	-0.52496300	0.05627000	2.90338600
O	-0.43721400	0.22141500	4.08396500
O	-1.07905000	0.90086100	2.13089200
O	-0.05648500	-0.97915400	2.32412400

AmR₂Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.45794200	0.78512200	-0.12113500
C	0.98654900	2.53906800	-0.44254700
C	2.04537000	3.46894500	-0.45718800
H	1.84207300	4.52390200	-0.60184800
C	2.66129900	-0.63640100	0.00183300
C	3.97352200	-1.13330400	0.14922800
C	4.13185200	-2.52810200	0.24966100
C	3.02847900	-3.34090400	0.18622100
H	5.12717500	-2.94609100	0.36955900
H	3.11329500	-4.41930600	0.25198800
N	1.58405300	-1.44822300	-0.05359300
C	3.57636900	1.64489600	-0.11512700
C	-0.40110400	2.93091300	-0.63654900
C	-0.97948300	4.15939500	-0.83460200
H	-0.57487000	5.15641500	-0.89925100
H	-3.03667900	4.60394600	-1.09370700
H	-3.48475000	2.09934500	-0.84477900
N	-1.37968700	1.96772500	-0.63529700
N	1.19878400	1.24055800	-0.26156200
C	3.32726800	3.02091600	-0.28262500
H	4.15960300	3.71862400	-0.28178300
C	-2.51901200	2.58172800	-0.81817000
N	-2.31948100	3.91333600	-0.94834500
C	4.88764900	1.10774300	0.04837900
H	5.73207900	1.79020600	0.06236700
C	5.07841000	-0.22885600	0.17929000
H	6.07814200	-0.63444700	0.30131100
C	1.76550100	-2.75325000	0.02821900
H	0.87256200	-3.36557700	-0.05032300
Am	-0.82420700	-0.41193300	0.06608100
N	-0.35424900	0.30000400	2.85708900
O	-1.00545900	1.06370200	2.07709900
O	-0.17349800	0.55946400	4.01125100
O	0.10569100	-0.75887300	2.31808800
N	-3.58716800	-1.18084600	0.53767100
O	-3.26839500	-0.19037000	-0.20735800
O	-4.72522200	-1.49806000	0.71737600
O	-2.61015400	-1.78902100	1.06849300
N	-0.58271600	-1.75035400	-2.51168100
O	-0.44122800	-0.49475400	-2.40635500
O	-0.91186600	-2.35506900	-1.43523500
O	-0.41604600	-2.33654400	-3.54217600

AmR₃Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.45156300	0.74407500	-0.12573300
C	0.99973900	2.51071200	-0.44740200
C	2.06315900	3.43240500	-0.46503100
H	1.88325900	4.49196400	-0.61141300
C	2.63759900	-0.68039700	-0.00098100
C	3.94394600	-1.18999800	0.14665400
C	4.08696100	-2.58622100	0.24990100
C	2.97352700	-3.38552300	0.18858300
H	5.07714000	-3.01592200	0.37043100
H	3.04573400	-4.46469900	0.25675900
N	1.55023800	-1.47714000	-0.05506100
C	3.57970500	1.59442400	-0.12170400
C	-0.39219000	2.88210700	-0.64205200
H	-0.37364000	4.98809800	-0.85714400
H	-2.87936700	4.87799200	-1.13236000
H	-3.47867600	2.17156700	-0.89110200
N	-1.37257800	1.99653600	-0.65839300
N	1.20105900	1.21106200	-0.26489400
C	3.34283600	2.97060300	-0.29051700
H	4.18063500	3.66148500	-0.29165600
C	-2.52891400	2.68251600	-0.85758900
C	-2.24891700	4.01844100	-0.97186100
N	-0.89213500	4.12700500	-0.83342300
C	4.88507700	1.04257000	0.04205500
C	5.05873800	-0.29615000	0.17473800
H	5.73787900	1.71437900	0.05514600
H	6.05384900	-0.71275200	0.29745400
C	1.71687000	-2.78397600	0.02940000
H	0.81679600	-3.38590500	-0.04772700
Am	-0.85886000	-0.39786500	0.06882500
N	-3.60154900	-1.18278900	0.56397200
O	-3.29693800	-0.18263200	-0.17225900
O	-4.73315300	-1.51980500	0.74320800
O	-2.61330300	-1.78229700	1.08975000
N	-0.57836700	-1.75276400	-2.49519700
O	-0.38907200	-2.34773900	-3.51658200
O	-0.41632400	-0.49943500	-2.39143700
O	-0.95262500	-2.34476300	-1.42647100
N	-0.28020500	0.35474000	2.83109800
O	-0.04719300	0.64016200	3.96985100
O	-0.92659800	1.12337300	2.05122500

O	0.11578700	-0.73675500	2.30843900
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AmR₄Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.58040200	-0.80096100	-0.04341300
C	2.78092200	-3.52497800	0.09804600
H	2.79906700	-4.60743300	0.14696400
C	2.46832100	0.63295400	-0.14553500
C	3.63844200	1.42274500	-0.11156600
C	3.47918500	2.81287200	-0.25698500
C	2.22929000	3.34452500	-0.44123600
H	4.35328600	3.45675900	-0.23113900
H	2.09496100	4.41284900	-0.56746500
N	1.24426100	1.16994400	-0.29647800
C	3.85790500	-1.37898900	0.10714500
C	1.11953800	2.48023400	-0.45778100
H	-0.30771900	5.20008300	-0.97563800
H	-2.80443000	4.66956700	-1.22099700
C	-0.23823500	2.96374900	-0.67430800
N	-1.28729800	2.09466900	-0.69426300
N	1.45622100	-1.54386600	-0.12116200
C	3.93089800	-2.78227000	0.18553800
H	4.89765100	-3.26181000	0.30844600
N	-2.38848900	2.72247200	-0.91520500
N	-2.07059000	4.00233800	-1.04400500
C	-0.74839000	4.21952700	-0.90424900
C	5.01648000	-0.54486300	0.16510400
H	5.98733100	-1.01438800	0.29110600
C	4.91225800	0.80281300	0.05755400
H	5.79705000	1.43093700	0.09432800
C	1.55730300	-2.85894300	-0.06053700
H	0.62883400	-3.41321800	-0.15580600
Am	-0.88392300	-0.35885600	0.07668300
N	-3.52743100	-1.24006100	0.79267600
O	-3.33139500	-0.22714400	0.04372200
O	-4.62082700	-1.63853800	1.05963300
O	-2.46990500	-1.79468400	1.24005700
N	-0.13824900	0.54745500	2.74981600
O	0.17064400	0.90886900	3.84819000
O	-0.88154500	1.24255800	1.98601000
O	0.26660500	-0.55245100	2.25521900
N	-0.80595100	-1.67193100	-2.51860200
O	-0.70854000	-2.24414700	-3.56484900
O	-0.61576700	-0.42257500	-2.39990800

O	-1.10384500	-2.28184000	-1.43692600
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AmR₅Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.45401300	0.85781500	-0.09261800
C	0.93723200	2.57009300	-0.40425700
C	1.96327000	3.52999500	-0.43579000
H	1.72468900	4.57689800	-0.58369800
C	2.69863900	-0.55732500	0.03892500
C	4.02585900	-1.01525400	0.17408300
C	4.22587300	-2.40383500	0.28343200
C	3.14545200	-3.24874800	0.24134500
H	5.23416600	-2.79220600	0.39316900
H	3.26213300	-4.32361400	0.31456300
N	1.64443300	-1.39991100	0.00364700
C	3.54830800	1.75068500	-0.10408500
C	-0.46558200	2.92458700	-0.58247000
H	-0.81581400	5.14566800	-0.82339400
N	-1.37115200	1.94775100	-0.57741400
N	1.18282000	1.27677100	-0.22086200
C	3.26106700	3.11704700	-0.27493600
H	4.07384700	3.83705000	-0.28777200
N	-2.46336500	3.85180600	-0.85307400
C	-1.16524400	4.12680800	-0.76149400
C	4.87645300	1.25050900	0.04699700
H	5.70164800	1.95600600	0.04623000
C	5.10524100	-0.07890700	0.18402600
H	6.11729700	-0.45558200	0.29609300
N	-2.51809600	2.54974400	-0.73601100
H	-3.37498200	2.00692300	-0.72989900
C	1.86491200	-2.69886600	0.09467300
H	0.99060900	-3.33927400	0.03310700
Am	-0.80298700	-0.45922000	0.06127100
N	-3.64746000	-1.05791600	0.35729800
O	-3.21524600	-0.06988000	-0.34172000
O	-4.81304000	-1.27515000	0.48778700
O	-2.74352500	-1.76457900	0.88763200
N	-0.44692200	-1.71391500	-2.53169800
O	-0.34548400	-0.45679000	-2.38813600
O	-0.23552500	-2.26622900	-3.57034000
O	-0.78696900	-2.35617300	-1.47906700
N	-0.48383100	0.12381500	2.89011900
O	-1.02156800	0.95934700	2.09425300

O	-0.06356000	-0.94846200	2.34230700
O	-0.36980500	0.33033700	4.06100900

AmR₆Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.47018900	0.58046500	-0.13402200
C	1.16030700	2.45054500	-0.45142300
C	2.28106600	3.29670400	-0.43851200
H	2.17819200	4.36846100	-0.56946700
C	2.55066100	-0.85586400	-0.02675800
C	3.81548200	-1.45767200	0.12930200
C	3.85959700	-2.86167100	0.21607200
C	2.69348300	-3.57929400	0.13128900
H	4.81546500	-3.36128700	0.34354700
H	2.68820800	-4.66155100	0.18729400
N	1.41060300	-1.57226000	-0.10426800
C	3.65642300	1.34995100	-0.10163200
C	-0.20138500	2.92226600	-0.66993400
H	-0.07703200	5.03740700	-0.87816000
H	-2.61915300	4.94182800	-1.22138100
N	-1.24382200	2.12303400	-0.72263600
N	1.26089600	1.13921100	-0.28654300
C	3.52278300	2.74060800	-0.25156000
H	4.40790000	3.36908000	-0.22808500
N	-2.35511900	2.85448600	-0.95383600
C	-1.97263900	4.09708000	-1.04046800
N	-0.62609700	4.19478800	-0.87031300
C	4.99067200	-0.64519600	0.18492700
H	5.95146000	-1.13402900	0.31482800
C	4.91696600	0.70405600	0.07149300
H	5.81536000	1.31244500	0.10709400
C	1.48405300	-2.88870700	-0.03487400
H	0.54433800	-3.42383600	-0.12914700
Am	-0.92414800	-0.32674400	0.06660900
N	-3.55299200	-1.23870400	0.78519200
O	-3.36973400	-0.21508400	0.04833200
O	-2.48710300	-1.78362000	1.22749900
O	-4.64015800	-1.65621200	1.04702300
N	-0.76429100	-1.67176600	-2.50970300
O	-0.53956400	-0.42816200	-2.39579400
O	-0.62511800	-2.26268800	-3.54094000
O	-1.14334300	-2.25550700	-1.43896300
N	-0.11231500	0.57478500	2.72824200

O	-0.83661900	1.29113300	1.96599100
O	0.23585900	-0.54773000	2.24338700
O	0.23144300	0.93881200	3.81587900

AmR₇Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.46259800	0.76917100	-0.11258800
C	1.00728300	2.52320700	-0.44211500
C	2.05409800	3.45901400	-0.46538100
H	1.82787700	4.50755800	-0.61728000
C	2.66027000	-0.65199900	0.02149500
C	3.97103900	-1.15026000	0.17100000
C	4.12643900	-2.54436000	0.28220300
C	3.02034800	-3.35453200	0.22658500
H	5.12062800	-2.96437400	0.40394200
H	3.10237200	-4.43258900	0.30055300
N	1.57986600	-1.45991200	-0.02630700
C	3.58113300	1.63101500	-0.11379700
C	-0.38651900	2.91166900	-0.63650200
N	-1.37041900	1.97473800	-0.64263200
N	1.20608900	1.22629200	-0.25598100
C	3.33668500	3.00648300	-0.28966500
H	4.17141200	3.70111400	-0.29390600
C	-2.47004400	2.66885300	-0.82548500
H	-3.47101600	2.26559900	-0.86708300
C	4.89140700	1.08998800	0.05230200
H	5.73822100	1.76934900	0.06057000
C	5.07742300	-0.24616700	0.19255800
H	6.07647400	-0.65301800	0.31620200
N	-0.81844400	4.14233000	-0.81552300
N	-2.14104100	3.96336600	-0.93379600
H	-2.74371000	4.75701500	-1.07611100
C	1.75881600	-2.76498100	0.06547800
H	0.86484600	-3.37652100	-0.00734400
Am	-0.83810400	-0.41987800	0.06407300
N	-3.62072300	-1.12394900	0.50125100
O	-3.27029300	-0.13103400	-0.22685100
O	-2.66236000	-1.76681600	1.02683700
O	-4.76717900	-1.41242700	0.67108400
N	-0.56532300	-1.74497900	-2.51230900
O	-0.42583700	-0.48897500	-2.39832300
O	-0.38701300	-2.32492900	-3.54339600
O	-0.90603300	-2.35486500	-1.44213700
N	-0.38915800	0.30679800	2.85091200

O	-1.00148400	1.08272200	2.04954200
O	0.04389500	-0.77279000	2.33124100
O	-0.22106700	0.57397800	4.00421200

AmR₈Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.45400100	0.73321000	-0.12840700
C	1.01583100	2.50482700	-0.45503100
C	2.07647800	3.42501400	-0.47408700
H	1.89603600	4.48402200	-0.62263200
C	2.63337300	-0.69190600	0.00131200
C	3.93771600	-1.20474900	0.15167000
C	4.07732300	-2.60092400	0.25919600
C	2.96143100	-3.39694000	0.19914700
H	5.06606200	-3.03314100	0.38189200
H	3.03021800	-4.47610400	0.27034300
N	1.54343500	-1.48477000	-0.05070900
C	3.58499800	1.58172200	-0.12467300
C	-0.38043700	2.87741600	-0.65255300
H	-0.44992500	4.99390600	-0.89022100
N	-1.36837100	1.99719900	-0.66964700
N	1.20644400	1.20563300	-0.27160500
C	3.35535400	2.95783600	-0.29675400
H	4.19594700	3.64504600	-0.29797700
N	-0.90385100	4.09695900	-0.85071000
C	-2.47645500	2.74353600	-0.87444100
H	-3.46720500	2.31865600	-0.92443200
N	-2.23530500	4.03200000	-0.99397900
C	4.88839400	1.02527800	0.04265400
H	5.74390400	1.69337000	0.05556200
C	5.05530000	-0.31371300	0.17867600
H	6.04870400	-0.73368400	0.30378400
C	1.70673500	-2.79202500	0.03751900
H	0.80519400	-3.39191800	-0.03837000
Am	-0.87045200	-0.40324100	0.07229700
N	-3.61817600	-1.14433300	0.57351100
O	-3.29974700	-0.14070000	-0.15293700
O	-2.63556400	-1.76779300	1.08463400
O	-4.75309300	-1.46358100	0.75702400
N	-0.57968900	-1.75239300	-2.48916400
O	-0.41975600	-0.49835500	-2.38192700
O	-0.38379400	-2.34508200	-3.50968200
O	-0.95921500	-2.34585500	-1.42269200
N	-0.25985900	0.38291500	2.81630800

O	-0.89609000	1.15040100	2.02545000
O	0.10867600	-0.72623300	2.31087100
O	-0.01249500	0.68517000	3.94681600

EuR₁Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.62191700	-0.53411500	0.02823900
C	3.14285900	-3.21258800	0.20614600
H	3.28913600	-4.28453400	0.26950800
C	2.33747700	0.87457900	-0.09039500
C	3.40485000	1.79863700	-0.08594600
C	3.07703900	3.15657700	-0.25365400
C	1.76945100	3.53009500	-0.42880400
H	3.86760200	3.90123400	-0.25409600
H	1.50132100	4.56961300	-0.57698300
N	1.05578600	1.25610800	-0.22594500
C	3.96019700	-0.95474300	0.17505800
C	0.76952500	2.54112900	-0.41107200
C	-1.33797100	4.06330700	-0.78432100
C	-2.66236800	3.68898100	-0.88551100
H	-0.94701900	5.06767900	-0.82851300
H	-3.48182600	1.70537900	-0.75641600
H	-3.56157800	4.26887700	-1.02467700
C	-0.64336300	2.85303500	-0.60455500
N	-1.49609700	1.83116000	-0.60815100
N	1.59262300	-1.40509200	-0.03333700
C	4.19830300	-2.33828500	0.27219100
H	5.21574100	-2.69919900	0.39152900
N	-2.69843300	2.34944500	-0.77327500
C	4.74508500	1.33605600	0.07676900
H	5.54944200	2.06526100	0.09052700
C	5.01140400	0.01268400	0.20665500
H	6.03274900	-0.33503500	0.32811800
C	1.84879500	-2.69778600	0.04683600
H	0.99297400	-3.36070400	-0.03551400
N	-3.61703900	-1.20905900	0.43647700
O	-3.23870700	-0.28838800	-0.37548500
O	-4.77265700	-1.45602300	0.61116400
O	-2.67989200	-1.81463400	1.02327900
N	-0.55845700	-1.84900200	-2.44231500
O	-0.36868000	-2.44376300	-3.46289600
O	-0.87966300	-2.44830700	-1.35995700
O	-0.45110100	-0.58963100	-2.35165700
N	-0.60864300	0.06947300	2.84438000
O	-0.52904800	0.25937000	4.02221800

O	-1.26862500	0.82776200	2.06948800
O	-0.02185100	-0.90854000	2.27295700
Eu	-0.85593900	-0.50806300	0.05734800

EuR₂Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.33551200	0.79804000	-0.13217200
C	0.81485000	2.50818200	-0.45760300
C	1.84504700	3.46972400	-0.46165000
H	1.61114000	4.51859100	-0.60454200
C	2.57874200	-0.61805000	-0.01944100
C	3.90358200	-1.07736900	0.13495100
C	4.10144400	-2.46791700	0.22544600
C	3.02227400	-3.31101300	0.14498800
H	5.10723000	-2.85822100	0.35135600
H	3.13739600	-4.38711400	0.20277900
N	1.52542900	-1.45885300	-0.09311500
C	3.42774500	1.69061800	-0.11414700
C	-0.58373800	2.85321000	-0.66210100
C	-1.20467600	4.05939800	-0.86807600
H	-0.83600200	5.07028800	-0.93345300
H	-3.27505400	4.42686900	-1.14331600
H	-3.63189900	1.90788700	-0.88672900
N	-1.52550300	1.85450500	-0.66439400
N	1.06489800	1.21658500	-0.27746100
C	3.13846300	3.05932800	-0.27756700
H	3.94940500	3.78173900	-0.26674600
C	-2.68475700	2.42558200	-0.85645000
N	-2.53402000	3.76372900	-0.99008000
C	4.75275300	1.19066500	0.05706000
H	5.57704700	1.89703000	0.08244800
C	4.98102100	-0.14078500	0.18119200
H	5.99118200	-0.51766100	0.30943500
C	1.74398400	-2.75847000	-0.02019200
H	0.86887400	-3.39445000	-0.11266300
N	-0.43101700	0.29574400	2.79589500
O	-1.18513000	0.97546400	2.03491400
O	-0.25328100	0.57493500	3.94644100
O	0.13812200	-0.70200300	2.24444400
N	-3.55538100	-1.30126800	0.64778000
O	-3.29116300	-0.37232200	-0.18991000
O	-4.67667600	-1.64471300	0.88029000
O	-2.54618800	-1.82020800	1.20970700
N	-0.72867300	-1.86950900	-2.41767800

O	-0.60315400	-0.61016900	-2.35380700
O	-1.00474500	-2.44734900	-1.31316700
O	-0.59395100	-2.48225800	-3.43760800
Eu	-0.89069200	-0.47316400	0.07268200

EuR₃Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.32466900	0.76683300	-0.13189300
C	0.81685900	2.48495100	-0.45648000
C	1.84792300	3.44277800	-0.45812100
H	1.63286800	4.49654400	-0.59880500
C	2.55635700	-0.65204900	-0.02066000
C	3.87736600	-1.11933900	0.13440300
C	4.06539000	-2.51128500	0.22411300
C	2.97920100	-3.34536900	0.14229700
H	5.06782700	-2.90976100	0.35060000
H	3.08602700	-4.42235000	0.19971600
N	1.49604600	-1.48214800	-0.09638700
C	3.42330500	1.65472200	-0.11187400
C	-0.58603200	2.80426500	-0.66506500
H	-0.64878700	4.90852900	-0.89301200
H	-3.14609400	4.69647600	-1.18838600
H	-3.63769900	1.96886900	-0.93708200
N	-1.52913800	1.87995700	-0.68606700
N	1.06086000	1.19236200	-0.27741400
C	3.14092100	3.02328800	-0.27292500
H	3.95452700	3.74242400	-0.26016600
C	-2.70963700	2.51798900	-0.89869200
C	-2.48308700	3.86383600	-1.01745900
N	-1.13300200	4.02772800	-0.86682300
C	4.74468100	1.14476900	0.05997300
C	4.96118600	-0.18875400	0.18248100
H	5.57479700	1.84403000	0.08738000
H	5.96848500	-0.57297800	0.31145900
C	1.70480800	-2.78338000	-0.02395500
H	0.82469700	-3.41225000	-0.11736800
N	-3.56763000	-1.30851000	0.67679800
O	-3.32002000	-0.37108300	-0.15501500
O	-4.68091400	-1.67251400	0.91233100
O	-2.54635200	-1.81598300	1.23263700
N	-0.71992400	-1.86641600	-2.40911700
O	-0.55679400	-2.48345400	-3.42221600
O	-0.58328100	-0.60817300	-2.34423700
O	-1.03778800	-2.43802100	-1.31262900

N	-0.37410200	0.34094300	2.77234000
O	-0.15216100	0.64131200	3.91006100
O	-1.12944500	1.02707600	2.01815000
O	0.14698500	-0.68596400	2.22805700
Eu	-0.92720200	-0.46336600	0.07299100

EuR₄Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.50634100	-0.74555000	-0.04507900
C	2.81447100	-3.45861000	0.08937000
H	2.87525800	-4.53967400	0.13534700
C	2.33682600	0.68278800	-0.14317200
C	3.47385800	1.51927300	-0.10758400
C	3.25792200	2.90194200	-0.25186100
C	1.98742400	3.38218900	-0.43742600
H	4.10486600	3.58114000	-0.22483900
H	1.80929900	4.44401200	-0.56434500
N	1.09204800	1.16924000	-0.29282600
C	3.80566200	-1.27215600	0.10647000
C	0.91404700	2.47299800	-0.45464700
H	-0.63431800	5.13024800	-0.96021700
H	-3.10318200	4.48508700	-1.21888100
C	-0.46283500	2.89747000	-0.67333500
N	-1.46950200	1.98016800	-0.70275600
N	1.41260200	-1.53110600	-0.12867400
C	3.93426700	-2.67163300	0.18121900
H	4.91900600	-3.11287100	0.30489500
N	-2.59768800	2.55726200	-0.92363300
N	-2.33948800	3.85193400	-1.04334800
C	-1.02941500	4.12986800	-0.89711000
C	4.92951100	-0.39201100	0.16824000
H	5.91834300	-0.82219000	0.29507500
C	4.77142700	0.95062600	0.06231000
H	5.63026900	1.61367200	0.10126500
C	1.56553900	-2.84099500	-0.07045500
H	0.65943600	-3.43065000	-0.16955600
N	-3.49827000	-1.38350000	0.81846800
O	-3.34452900	-0.42385600	-0.00478000
O	-4.57369800	-1.81764000	1.10365500
O	-2.42142100	-1.84367300	1.31944800
N	-0.29464000	0.49857200	2.71702800
O	-0.02516600	0.86449200	3.82488100
O	-1.10009300	1.13199900	1.96610300
O	0.21872700	-0.54518500	2.20254100

N	-0.87544900	-1.77703200	-2.43793800
O	-0.77901800	-2.36160100	-3.47793000
O	-0.70915900	-0.52263200	-2.34082200
O	-1.14691500	-2.37610800	-1.34552400
Eu	-0.95184600	-0.43001800	0.08118700

EuR₅Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.33391200	0.86264100	-0.10317600
C	0.77273800	2.53088900	-0.43422300
C	1.77125400	3.51943300	-0.45890800
H	1.50517900	4.55872700	-0.61372000
C	2.61565000	-0.54604000	0.02441600
C	3.95352300	-0.96701700	0.17220200
C	4.19107700	-2.35016900	0.27652000
C	3.13506200	-3.22407500	0.21542100
H	5.20830900	-2.71110000	0.39704700
H	3.28062300	-4.29578000	0.28378300
N	1.58542600	-1.41648800	-0.03083100
C	3.40272800	1.78596800	-0.10476200
C	-0.63920100	2.83810000	-0.62962100
H	-1.07043700	5.04322600	-0.88853200
N	-1.50710400	1.82799500	-0.62603300
N	1.05334800	1.24624500	-0.24168700
C	3.07837500	3.14332000	-0.28115000
H	3.87057100	3.88604400	-0.28633900
N	-2.66790100	3.68792000	-0.92251300
C	-1.38164500	4.01232200	-0.82246500
C	4.74244700	1.32242500	0.06043300
H	5.54804400	2.05018000	0.06970900
C	5.00603500	-0.00059300	0.19771700
H	6.02686800	-0.34922600	0.32059000
N	-2.67360600	2.38518500	-0.79727400
H	-3.50938200	1.81100600	-0.78802000
C	1.84127900	-2.70906500	0.05491900
H	0.98531000	-3.37231900	-0.02366000
N	-3.62401200	-1.18528000	0.47152200
O	-3.24387100	-0.26316700	-0.33682600
O	-4.77831400	-1.42810700	0.65247300
O	-2.68511000	-1.80034200	1.05106400
N	-0.58375100	-1.85541000	-2.43101000
O	-0.48271700	-0.59485800	-2.33584700
O	-0.39947500	-2.44430500	-3.45488200
O	-0.89212000	-2.46003600	-1.34756900
N	-0.56447700	0.14527900	2.82809800

O	-1.22311000	0.88692600	2.03415100
O	-0.00856000	-0.86626800	2.28530100
O	-0.46047600	0.38009700	3.99502200
Eu	-0.86539600	-0.52471800	0.07032100

EuR₆Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.33592500	0.65512000	-0.14770900
C	0.91947000	2.44219400	-0.48325900
C	1.98662200	3.35463300	-0.47074900
H	1.82004200	4.41757700	-0.60800500
C	2.50001500	-0.77392300	-0.03882000
C	3.79756900	-1.29925400	0.12371400
C	3.92447600	-2.69827600	0.20851300
C	2.80330400	-3.48320900	0.11409900
H	4.90740800	-3.14076700	0.34132800
H	2.86209600	-4.56408800	0.16711500
N	1.40447500	-1.55502200	-0.12531700
C	3.47397900	1.49421300	-0.11444200
C	-0.46955700	2.81908200	-0.71274500
H	-0.49577500	4.93099000	-0.97276800
H	-3.02529200	4.64510700	-1.31211000
N	-1.45219600	1.94617400	-0.74774100
N	1.09726600	1.14106200	-0.30696300
C	3.25820400	2.87372800	-0.27266500
H	4.10405400	3.55408800	-0.24736300
N	-2.61243900	2.58928700	-0.99556800
C	-2.32010900	3.85360800	-1.11091600
N	-0.98395800	4.05215400	-0.94215500
C	4.92198000	-0.41806800	0.18545400
H	5.90938500	-0.84870300	0.32186900
C	4.76961200	0.92429000	0.06769200
H	5.63051600	1.58447900	0.10626700
C	1.55596600	-2.86474900	-0.05854900
H	0.64919100	-3.45311400	-0.16080600
N	-3.52703500	-1.33911300	0.85494400
O	-3.37709700	-0.44758500	-0.03985800
O	-2.44899100	-1.73669800	1.40992200
O	-4.59793600	-1.77173600	1.15918300
N	-0.87567300	-1.83597100	-2.39331500
O	-0.69404500	-0.58108100	-2.32385500
O	-0.75547200	-2.44707300	-3.41585000
O	-1.18550600	-2.40349400	-1.29542200
N	-0.25673500	0.58209300	2.68853800
O	-1.08702500	1.20021700	1.95596100

O	0.24950000	-0.46561600	2.17174100
O	0.04738500	0.96305800	3.78322800
Eu	-0.98204400	-0.41184900	0.08189500

EuR₇Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.33590200	0.78416300	-0.12540500
C	0.82831500	2.49144700	-0.46468300
C	1.84444600	3.46064100	-0.47612100
H	1.58654300	4.50176700	-0.62867800
C	2.57630400	-0.63119000	-0.00018000
C	3.90036200	-1.08879100	0.15988800
C	4.09823800	-2.47833900	0.26200100
C	3.01844000	-3.32154900	0.18662700
H	5.10353300	-2.86825400	0.39246900
H	3.13307000	-4.39717600	0.25300700
N	1.52184000	-1.47082600	-0.06850800
C	3.42620600	1.68127700	-0.11277800
C	-0.57665500	2.82927400	-0.67310900
N	-1.52257600	1.85449800	-0.68290000
N	1.06732300	1.20172400	-0.27717500
C	3.13906400	3.04877300	-0.28688200
H	3.95092700	3.76999700	-0.27982200
C	-2.64625500	2.50437400	-0.87744400
H	-3.63074300	2.06295300	-0.92357300
C	4.75098500	1.18062400	0.06498800
H	5.57610400	1.88592800	0.08634700
C	4.97711100	-0.14996600	0.19999600
H	5.98711500	-0.52574300	0.33283400
N	-1.05393200	4.04173100	-0.86172000
N	-2.36759300	3.81062300	-0.99003300
H	-2.99951800	4.57936900	-1.14152900
C	1.74066700	-2.77010100	0.01507100
H	0.86613500	-3.40742500	-0.07375400
N	-3.58920500	-1.24897100	0.62859200
O	-3.29823500	-0.32244900	-0.20341600
O	-2.59393100	-1.79784800	1.18871500
O	-4.71876700	-1.56366500	0.85798600
N	-0.71192200	-1.87796000	-2.41418800
O	-0.58606200	-0.61806500	-2.34702900
O	-0.56334900	-2.48942300	-3.43197700
O	-1.00444900	-2.45589100	-1.31355200
N	-0.45916300	0.31759700	2.78324500
O	-1.19008600	1.00112200	2.00140400

O	0.09534700	-0.69985600	2.25316400
O	-0.29070800	0.61059100	3.93074500
Eu	-0.90545100	-0.48508400	0.07049800

EuR₈Ph(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.32494600	0.75823700	-0.13450300
C	0.82806200	2.47901400	-0.46735400
C	1.85509000	3.43666600	-0.47289800
H	1.63812100	4.48914300	-0.61897700
C	2.55217800	-0.66092900	-0.01559500
C	3.87194900	-1.12911400	0.14367300
C	4.05874700	-2.52067300	0.24060700
C	2.97135500	-3.35345600	0.16124900
H	5.06039400	-2.91981600	0.37056400
H	3.07639300	-4.43027800	0.22390200
N	1.49049600	-1.48910500	-0.08800900
C	3.42512700	1.64611500	-0.11645700
C	-0.57957300	2.79719300	-0.67934600
H	-0.73348500	4.90831900	-0.92794500
N	-1.52911400	1.87657700	-0.70165500
N	1.06320400	1.18718400	-0.28486500
C	3.14803400	3.01410400	-0.28391500
H	3.96353800	3.73085300	-0.27310400
N	-1.15054600	3.99366100	-0.88728200
C	-2.66476400	2.57543200	-0.91896700
H	-3.63665600	2.10977100	-0.97501300
N	-2.47687000	3.87267700	-1.04238400
C	4.74541500	1.13397500	0.06035400
H	5.57722100	1.83102200	0.08628300
C	4.95719300	-0.19945400	0.18912200
H	5.96342400	-0.58528600	0.32164100
C	1.69798600	-2.79040200	-0.00911800
H	0.81746400	-3.41904100	-0.10032200
N	-3.58676700	-1.27148400	0.68557600
O	-3.32573600	-0.33473900	-0.14355300
O	-2.57027000	-1.79796600	1.23527800
O	-4.70367300	-1.61830600	0.92413400
N	-0.71467700	-1.87656800	-2.39823000
O	-0.57833400	-0.61760000	-2.33350900
O	-0.54121100	-2.49489000	-3.40782900
O	-1.04367100	-2.44569300	-1.30323000
N	-0.35912900	0.37528000	2.75594800
O	-1.10637000	1.05958800	1.99065500
O	0.13961000	-0.67196700	2.22941300

O	-0.12524600	0.69518800	3.88503900
Eu	-0.93958500	-0.47145100	0.07661900

AmR₁PhR₁³⁺(PBE0/6-311G*-RECP)

C	0.71004300	2.08354400	0.00002500
C	2.66923200	0.82681500	-0.00033600
C	3.44215400	1.99409500	-0.00041500
H	4.52377000	1.92950700	-0.00062400
C	-0.71007900	2.08353500	0.00003700
C	-1.41189700	3.30255300	-0.00002400
C	-2.81968600	3.22390800	-0.00018700
C	-3.44218900	1.99405800	-0.00036300
H	-3.41343500	4.13323600	-0.00022200
H	-4.52380400	1.92945400	-0.00056100
N	-1.32494600	0.87264400	-0.00003300
C	1.41184800	3.30256900	-0.00005300
C	3.25215400	-0.50807300	-0.00061600
C	4.57762600	-0.92649200	-0.00089500
H	5.47754200	-0.33041200	-0.00096400
C	4.51453200	-2.31070700	-0.00108900
H	5.29668900	-3.05819300	-0.00135900
H	2.86203800	-3.59557000	-0.00112100
C	-2.66925300	0.82678700	-0.00030900
C	-4.57762000	-0.92655900	-0.00087700
C	-4.51449600	-2.31077100	-0.00112400
H	-5.47754800	-0.33049700	-0.00089600
H	-2.86197300	-3.59559400	-0.00125500
H	-5.29663400	-3.05827600	-0.00141500
C	-3.25215700	-0.50810900	-0.00061500
N	-2.40968000	-1.57664300	-0.00068100
N	2.40970200	-1.57663000	-0.00062700
N	1.32492300	0.87266000	-0.00004600
C	2.81963700	3.22394000	-0.00024100
H	3.41337900	4.13327300	-0.00029700
N	3.22384000	-2.65297600	-0.00088800
N	-3.22379400	-2.65300700	-0.00096700
C	-0.68048100	4.52979700	0.00001100
H	-1.22814300	5.46651400	0.00001600
C	0.68041700	4.52980600	-0.00000500
H	1.22806800	5.46652800	-0.00001400
Am	0.00001100	-1.14396300	0.00077800

AmR₁PhR₂³⁺(PBE0/6-311G*-RECP)

C	-0.72757500	2.07213600	-0.00684200
C	-2.66161800	0.77628800	0.15090300
C	-3.44961300	1.93951000	0.18058300
H	-4.52708400	1.86365100	0.27112300
C	0.69011600	2.08092800	0.00477500
C	1.39286100	3.29572200	0.05008800
C	2.79965500	3.20176600	0.13296900
C	3.41202000	1.96674800	0.20136000
H	3.40180200	4.10513700	0.16367200
H	4.48961200	1.89783000	0.29213700
N	1.29861600	0.86919700	0.03045400
C	-1.43963600	3.27941900	0.02756100
C	-3.17301200	-0.57181700	0.29272500
C	-4.43502400	-1.06161900	0.49895400
H	-5.39818600	-0.58045300	0.58022600
H	-5.04393600	-3.07104400	0.78209100
C	2.63399100	0.80142400	0.16288900
C	4.48837200	-0.97144100	0.51562800
C	4.40248900	-2.35065000	0.60571200
H	5.38708600	-0.38136900	0.61177500
H	2.73793600	-3.61553500	0.46843900
H	5.16183600	-3.10143100	0.77804400
C	3.18265100	-0.54466600	0.29438500
N	2.33175700	-1.60696500	0.24285100
N	-2.27287300	-1.63758400	0.28230800
N	-1.32563300	0.85109100	0.02036800
C	-2.84856600	3.17546300	0.10191800
H	-3.45699300	4.07484100	0.12232500
N	3.11886800	-2.68104900	0.43774900
C	0.65315100	4.51724800	0.03574000
H	1.19181100	5.45909600	0.04882700
C	-0.71141000	4.50847700	0.02629300
H	-1.26109100	5.44406400	0.03688400
C	-2.99979000	-2.73245200	0.48236800
H	-2.63550500	-3.74833900	0.54395400
N	-4.29169900	-2.41309300	0.61334300
Am	0.00721100	-1.07697400	-0.40670600

AmR₁PhR₃³⁺(PBE0/6-311G*-RECP)

C	0.77169100	2.06696900	0.00025800
C	2.70187900	0.77173600	-0.00287300
C	3.50508100	1.91775100	-0.00333800
H	4.58665500	1.84139400	-0.00502000

C	-0.65024200	2.09957900	0.00029100
C	-1.32015500	3.33594800	-0.00017200
C	-2.72987700	3.29443400	-0.00157800
C	-3.38325300	2.08156800	-0.00309500
H	-3.29965400	4.21895000	-0.00185600
H	-4.46614700	2.04477600	-0.00467200
N	-1.29554600	0.90459400	-0.00040500
C	1.50268200	3.27141000	-0.00023100
C	3.19124200	-0.59306900	-0.00533700
H	5.29692400	-0.51342300	-0.00866100
C	4.41342000	-2.42816400	-0.00920700
H	5.31064200	-3.02924500	-0.01168100
H	2.67028700	-3.76963200	-0.00809200
C	-2.64006900	0.89417900	-0.00270600
C	-4.59961400	-0.80178000	-0.00732300
C	-4.57887100	-2.18732600	-0.00920900
H	-5.48128400	-0.17908100	-0.00761900
H	-2.96516100	-3.52141300	-0.01030600
H	-5.38334000	-2.91070100	-0.01150300
C	-3.26175100	-0.42380800	-0.00523000
N	-2.45317000	-1.51768600	-0.00570400
N	2.33177100	-1.62607400	-0.00510400
N	1.35814900	0.84622300	-0.00044000
C	2.90766800	3.16082700	-0.00171900
H	3.52141500	4.05673400	-0.00197500
N	-3.29916400	-2.56839900	-0.00793300
C	-0.55933400	4.54584400	0.00026400
H	-1.08516800	5.49501300	0.00034800
C	0.80114200	4.51520200	0.00022500
H	1.37001700	5.43918200	0.00026700
C	3.09355700	-2.77582700	-0.00730600
N	4.44606000	-1.06114100	-0.00777400
Am	-0.02824300	-1.16303200	0.00644200

AmR₁PhR₄³⁺(PBE0/6-311G*-RECP)

C	0.81632000	2.06264900	-0.00014600
C	2.74584700	0.76710200	-0.00028400
C	3.55164100	1.90900600	-0.00050300
H	4.63180500	1.81659000	-0.00068800
C	-0.60627600	2.10598100	0.00004900
C	-1.26648500	3.34886400	0.00025200
C	-2.67614800	3.32309300	0.00047000
C	-3.34398000	2.11835500	0.00035100

H	-3.23466400	4.25447200	0.00071800
H	-4.42718800	2.09367700	0.00045300
N	-1.26823400	0.91800500	0.00001100
C	1.55278200	3.26427600	-0.00027100
C	3.25640500	-0.59437100	-0.00014600
C	4.48705200	-1.21033400	-0.00012500
H	5.50420000	-0.84704200	-0.00034300
H	4.83040200	-3.31330300	0.00025800
C	-2.61443600	0.92383300	0.00008400
C	-4.59658200	-0.74670600	-0.00030400
C	-4.59291600	-2.13293500	-0.00065900
H	-5.47084800	-0.11362600	-0.00014100
H	-2.99587700	-3.48789900	-0.00095700
H	-5.40668700	-2.84596400	-0.00090800
C	-3.25456100	-0.38518100	-0.00018400
N	-2.46025700	-1.48980600	-0.00039200
N	2.32870200	-1.59438900	0.00007000
N	1.40025200	0.83783700	-0.00016900
C	2.95731000	3.15317300	-0.00051900
H	3.57115200	4.04901500	-0.00074600
N	-3.31867600	-2.53071400	-0.00060400
C	-0.49912200	4.55384100	0.00017500
H	-1.01946000	5.50600000	0.00030200
C	0.86019600	4.51333500	-0.00012000
H	1.43660900	5.43264100	-0.00023800
N	2.89984400	-2.76500800	0.00020700
N	4.18593200	-2.52773000	0.00008600
Am	-0.04689100	-1.16132400	0.00020100

AmR₁PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.73524800	2.06391000	-0.00037900
C	-2.66802100	0.77095000	-0.13441800
C	-3.46122100	1.92486800	-0.15664400
H	-4.53981600	1.84425500	-0.22812000
C	0.68652500	2.07838500	0.00500700
C	1.37936400	3.30161200	-0.01620300
C	2.78842900	3.22859400	-0.08889900
C	3.41533900	2.00299000	-0.16928500
H	3.37820800	4.14057400	-0.10220100
H	4.49425400	1.94607000	-0.25382200
N	1.30999600	0.87434800	-0.03232300
C	-1.45405800	3.27144600	-0.02776200
C	-3.21186800	-0.57563500	-0.24766600

C	-4.50971100	-1.05376500	-0.44354500
H	-5.45233500	-0.53498800	-0.54007600
H	-2.90424000	-3.64553700	-0.39384900
C	2.64936700	0.82949400	-0.14376400
C	4.52644900	-0.94168500	-0.39480700
C	4.43868900	-2.32093200	-0.49219400
H	5.43365300	-0.35711600	-0.42387200
H	2.76247900	-3.57634600	-0.49654600
H	5.20369400	-3.07553500	-0.61845200
C	3.21128000	-0.50871500	-0.26158600
N	2.35230600	-1.56566800	-0.27083800
N	-2.38339200	-1.64742300	-0.20023300
N	-1.32859500	0.84628700	-0.02598900
C	-2.86046200	3.16636800	-0.09303700
H	-3.47150300	4.06423200	-0.11001800
N	3.14502900	-2.64554300	-0.40867900
C	0.63237900	4.51789300	-0.00516700
H	1.16630100	5.46270800	-0.01311200
C	-0.73391400	4.50401900	-0.00808000
H	-1.28751000	5.43745700	-0.00977000
N	-3.20745800	-2.67996300	-0.36787700
N	-4.45698800	-2.38074900	-0.51563500
Am	0.02779600	-1.10393200	0.33696200

AmR₁PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.89477800	2.04122200	0.00004400
C	2.78033500	0.69302800	0.00031000
C	3.62796400	1.79990500	0.00043600
H	4.70578600	1.68036700	0.00068500
C	-0.52934900	2.12602300	0.00003200
C	-1.14614700	3.38904100	-0.00007800
C	-2.55614600	3.41131100	-0.00012100
C	-3.26194300	2.22922600	-0.00002700
H	-3.08372500	4.36053900	-0.00025900
H	-4.34537900	2.24008900	-0.00002500
N	-1.22715700	0.95942200	0.00008800
C	1.67311200	3.22238100	0.00004200
C	3.18739800	-0.70519900	0.00023300
H	5.29411900	-0.96589500	0.00024200
C	4.05668300	-2.69447700	0.00009900
H	4.79940900	-3.48076300	0.00012400
C	-2.57174200	1.01009200	0.00007400
C	-4.61542800	-0.58374700	0.00011400
C	-4.66631600	-1.96902700	0.00032600

H	-5.46459200	0.08260700	-0.00024700
H	-3.12220000	-3.38455200	0.00121700
H	-5.50717300	-2.64985700	0.00036000
C	-3.25980700	-0.27509100	0.00022000
N	-2.51037500	-1.40976300	0.00056200
N	2.23160500	-1.62481500	0.00007900
N	1.43844500	0.80746400	0.00010000
C	3.07055000	3.06565200	0.00025700
H	3.71379200	3.94059700	0.00027300
N	-3.40827600	-2.41557400	0.00061700
C	-0.33875300	4.57038800	-0.00013200
H	-0.83024900	5.53789600	-0.00020600
C	1.01858100	4.49174200	-0.00008400
H	1.62099800	5.39418400	-0.00015300
N	2.76496200	-2.86641400	-0.00005100
N	4.35945200	-1.35679700	0.00026100
Am	-0.07898900	-1.18257600	-0.00025300

AmR₁PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.76202000	2.05831700	0.00848000
C	-2.68347000	0.76140400	-0.07041400
C	-3.49635100	1.89868100	-0.08581300
H	-4.57370800	1.78411100	-0.13201400
C	0.65810900	2.09135100	0.00666800
C	1.33115100	3.32657100	-0.00846400
C	2.74038000	3.27960100	-0.05490000
C	3.38964600	2.06440400	-0.10245500
H	3.31358000	4.20201000	-0.06531800
H	4.47127500	2.02488400	-0.15441000
N	1.30029600	0.89559000	-0.01705100
C	-1.49721800	3.25725400	-0.00721600
C	-3.21077900	-0.59266300	-0.13980900
H	-5.31016500	-2.76788400	-0.37542100
H	-2.95728000	-3.77253700	-0.24613300
C	2.64361400	0.87928700	-0.08613100
C	4.58015000	-0.83872600	-0.21115200
C	4.53965100	-2.22246100	-0.26537300
H	5.46976500	-0.22727700	-0.21392600
H	2.90697400	-3.53302000	-0.30415800
H	5.33319900	-2.95526100	-0.32802600
C	3.24846800	-0.44350500	-0.15616800
N	2.42355700	-1.52727300	-0.17425200
N	-2.36422700	-1.68413000	-0.12098100
N	-1.34382600	0.83281100	-0.00584600

C	-2.90375400	3.14388900	-0.04613900
H	-3.51942000	4.03854600	-0.05624500
N	3.25480300	-2.58746100	-0.23411200
C	0.56832200	4.53395600	0.00186300
H	1.09136200	5.48470600	-0.00187500
C	-0.79395300	4.50103000	0.00345900
H	-1.36262700	5.42523600	0.00451700
N	-4.47145800	-0.91468500	-0.24113200
C	-3.20476500	-2.72017500	-0.22200000
N	-4.44236000	-2.24824200	-0.29180000
Am	0.03954200	-1.14672700	0.19034300

AmR₁PhR₈³⁺(PBE0/6-311G*-RECP)

C	0.80502900	2.03045000	-0.00389700
C	2.70589600	0.69310200	0.17598600
C	3.53181500	1.82134900	0.21638500
H	4.60732700	1.72653700	0.31760600
C	-0.62154800	2.08342800	-0.01156500
C	-1.27838200	3.32412000	0.01005700
C	-2.69114200	3.28729900	0.09004800
C	-3.35469600	2.08144000	0.18100800
H	-3.25530100	4.21546300	0.10171200
H	-4.43436300	2.05935600	0.27205000
N	-1.28419700	0.90190500	0.03441600
C	1.55747600	3.22063300	0.02794100
C	3.13088300	-0.69763700	0.28895900
H	5.23487500	-0.75902300	0.59581000
H	2.66088000	-3.84755000	0.40572500
C	-2.62183700	0.88501800	0.15859900
C	-4.53179200	-0.83487300	0.47674900
C	-4.48496800	-2.21589400	0.57726100
H	-5.41771300	-0.22123500	0.54148500
H	-2.84984800	-3.52423500	0.50331600
H	-5.26801500	-2.94534100	0.73568200
C	-3.21002800	-0.44379400	0.28881200
N	-2.38497400	-1.53223800	0.26697800
N	2.24974000	-1.71894900	0.22241400
N	1.37483300	0.80565300	0.04020300
C	2.95884000	3.07702100	0.12423600
H	3.59220400	3.95921500	0.14698000
N	-3.20643200	-2.58064600	0.44455400
C	-0.49727600	4.51967400	-0.00417200
H	-1.00464300	5.47914600	0.00198900
C	0.86906500	4.47087200	0.00492200

H	1.44508700	5.39057500	0.01870600
N	4.29552600	-2.55180900	0.56120500
N	4.33820900	-1.21930900	0.48934200
C	3.02952200	-2.83149200	0.39642200
Am	-0.05021700	-1.08515200	-0.37938300

AmR₂PhR₂³⁺(PBE0/6-311G*-RECP)

C	-0.70969400	2.08387600	-0.00021400
C	-2.67683600	0.83285100	0.00836200
C	-3.44561400	2.00638000	0.00910400
H	-4.52774000	1.94739600	0.01339200
C	0.70958500	2.08389600	-0.00007800
C	1.40876900	3.30351300	0.00133300
C	2.81889800	3.22992900	0.00549500
C	3.44551900	2.00651900	0.00991900
H	3.40736000	4.14258000	0.00630300
H	4.52764400	1.94754400	0.01439800
N	1.33088500	0.87151100	0.00168300
C	-1.40892700	3.30346800	0.00091000
C	-3.25273900	-0.49621500	0.01596300
C	-4.54697800	-0.93981400	0.02721600
H	-5.49461100	-0.42279300	0.03259300
H	-5.26068300	-2.93590200	0.04078100
H	-2.87052500	-3.70651500	0.02602000
C	2.67678600	0.83297500	0.00860200
C	4.54696000	-0.93971900	0.02683600
H	5.49459100	-0.42269700	0.03228200
H	2.87050300	-3.70642700	0.02527200
H	5.26064300	-2.93581000	0.04041500
C	3.25272300	-0.49609800	0.01584100
N	2.40048200	-1.59707300	0.01369000
N	-2.40050000	-1.59719000	0.01399400
N	-1.33094000	0.87146900	0.00172900
C	-2.81904500	3.22980700	0.00464500
H	-3.40755300	4.14242800	0.00511500
C	-3.18624900	-2.67261100	0.02401400
C	3.18621500	-2.67251900	0.02348400
N	-4.46918300	-2.30301600	0.03206700
N	4.46914800	-2.30291700	0.03158300
C	-0.68077800	4.52994900	-0.00017800
H	-1.22921200	5.46613600	-0.00033000
C	0.68058500	4.52996100	0.00007500
H	1.22900800	5.46615500	0.00017000
Am	0.00006600	-1.14861500	-0.02092200

AmR₂PhR₃³⁺(PBE0/6-311G*-RECP)

C	-0.65158900	2.10056600	0.00005700
C	-2.64779500	0.90066100	0.00003900
C	-3.38584100	2.09506100	-0.00014100
H	-4.46917400	2.06429400	-0.00022000
C	0.76984700	2.06651400	0.00009500
C	1.50346100	3.27087100	0.00016100
C	2.90818500	3.15948300	0.00022700
C	3.50540600	1.91669700	0.00021300
H	3.52175200	4.05547000	0.00029600
H	4.58689400	1.83972500	0.00020100
N	1.35772100	0.84585800	0.00010100
C	-1.31640000	3.33746600	-0.00003400
C	-3.26028000	-0.41196700	0.00018000
C	-4.56706100	-0.81834400	0.00042300
H	-5.49956300	-0.27430900	0.00029400
H	-5.33817700	-2.79288300	0.00110300
H	-2.97075500	-3.63210700	0.00094500
C	2.70127600	0.77155400	0.00018300
H	5.29809500	-0.50677600	0.00077400
H	2.68038500	-3.77030500	-0.00007400
H	5.31919500	-3.02276900	0.00080800
C	3.19276000	-0.59270000	0.00025600
N	2.33654200	-1.62796200	-0.00005700
N	-2.44039700	-1.53731700	0.00036800
N	-1.30166600	0.90410500	0.00007900
C	-2.72857500	3.30177000	-0.00018700
H	-3.29328500	4.22931200	-0.00033800
C	-3.25673400	-2.58946500	0.00073000
C	3.10150800	-2.77562600	0.00012800
N	-4.52871000	-2.18287200	0.00079400
C	-0.55520400	4.54603500	0.00001400
H	-1.08052500	5.49548900	-0.00002000
C	0.80554400	4.51497500	0.00012800
H	1.37559700	5.43814500	0.00021500
N	4.44906700	-1.05709500	0.00059600
C	4.42024400	-2.42439800	0.00050100
Am	-0.02600900	-1.16580200	-0.00036800

AmR₂PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.60916400	2.10624800	-0.00014100
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C	-2.62310400	0.92861000	0.00014200
C	-3.34801600	2.12969900	0.00004600
H	-4.43158400	2.11040200	0.00021100
C	0.81286800	2.06229200	0.00000800
C	1.55118700	3.26427800	0.00016100
C	2.95558200	3.15330200	0.00059200
C	3.55053500	1.90990300	0.00075700
H	3.56859100	4.04967300	0.00080900
H	4.63065300	1.81751800	0.00110200
N	1.39914000	0.83781100	0.00008800
C	-1.26496800	3.34916100	-0.00026800
C	-3.25347500	-0.37536400	0.00046300
C	-4.56492800	-0.76627800	0.00087600
H	-5.49106600	-0.21143700	0.00101100
H	-5.35957900	-2.73175800	0.00107800
H	-3.00204900	-3.60004800	0.00094600
C	2.74462100	0.76828000	0.00044200
C	4.49191300	-1.20260100	0.00077600
H	5.50735200	-0.83479800	0.00116600
H	4.84418000	-3.30396800	0.00036000
C	3.25856900	-0.59197500	0.00049900
N	2.33525100	-1.59579300	0.00011500
N	-2.44801600	-1.51074900	0.00048000
N	-1.27532700	0.91624700	-0.00004600
C	-2.67704100	3.32853300	-0.00022700
H	-3.23089400	4.26261400	-0.00039600
C	-3.27651400	-2.55421400	0.00082000
N	-4.54268600	-2.13148400	0.00099000
N	4.19655000	-2.52120100	0.00038300
C	-0.49804000	4.55330400	-0.00030200
H	-1.01842500	5.50543600	-0.00049900
C	0.86156300	4.51320100	-0.00005800
H	1.43856800	5.43205000	-0.00002000
N	2.91139000	-2.76400900	-0.00000900
Am	-0.04378300	-1.16389200	-0.00049800

AmR₂PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.68923000	2.07718000	-0.00663300
C	-2.65285200	0.82606500	0.15759700
C	-3.41745800	2.00538300	0.18242200
H	-4.49642000	1.95225200	0.27144800
C	0.73168700	2.06241400	0.00301800
C	1.45276700	3.26897100	0.03706900

C	2.85815000	3.16075100	0.11441000
C	3.45683500	1.91843400	0.18602000
H	3.47050600	4.05757600	0.13669900
H	4.53442600	1.83639500	0.26960900
N	1.32480900	0.84440000	0.03183600
C	-1.37953900	3.29964900	0.01696100
C	-3.19563100	-0.50891900	0.28845700
C	-4.47203900	-0.97076800	0.48018300
H	-5.42377400	-0.46698500	0.56137800
H	-5.13206500	-2.96752600	0.73085400
H	-2.73965800	-3.70147500	0.49551000
C	2.66195900	0.76591900	0.15708800
C	4.49177200	-1.06491100	0.50330600
H	5.43471800	-0.54907100	0.61112300
H	2.87462500	-3.64926700	0.44998400
C	3.19903500	-0.58268800	0.28444800
N	2.36713300	-1.65144100	0.23260900
N	-2.32289800	-1.59651700	0.26656600
N	-1.31331700	0.87048000	0.03273100
C	-2.79096700	3.22684900	0.09454500
H	-3.37935100	4.13963800	0.10790700
C	-3.07790600	-2.67580700	0.44519700
N	-4.36294100	-2.32575200	0.57420200
C	-0.63261900	4.51490800	0.00774500
H	-1.16625200	5.45987300	0.01524900
C	0.73408300	4.50147900	0.01484100
H	1.28770800	5.43482400	0.01952100
N	3.18371300	-2.68579800	0.41971900
N	4.43254000	-2.39100000	0.58461700
Am	-0.02206300	-1.09417200	-0.38384500

AmR₂PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.88983800	2.04159800	-0.00009000
C	2.77831000	0.69603500	-0.00001600
C	3.62543600	1.80318900	-0.00015500
H	4.70328200	1.68426500	-0.00015700
C	-0.53379400	2.12617100	0.00001400
C	-1.14710700	3.38879400	0.00010800
C	-2.55936500	3.41517700	0.00039600
C	-3.26723800	2.23852200	0.00049300
H	-3.08294100	4.36653400	0.00054100
H	-4.35088100	2.25410400	0.00072300
N	-1.23490900	0.95745500	0.00004600
C	1.66931300	3.22354700	-0.00019700

C	3.18976200	-0.70069200	0.00019500
H	5.29790700	-0.94880800	0.00005200
H	4.81778300	-3.46666700	0.00052800
C	-2.58095300	1.01340800	0.00024700
C	-4.58355600	-0.60754800	0.00033500
H	-5.48773100	-0.01755900	0.00073800
H	-3.13060400	-3.49892600	-0.00081400
H	-5.45395600	-2.54042300	0.00001800
C	-3.25747700	-0.26752600	0.00014500
N	-2.49730000	-1.43328700	-0.00028000
N	2.23923300	-1.62548600	0.00039400
N	1.43638600	0.80841400	-0.00002900
C	3.06675600	3.06784500	-0.00025800
H	3.70868400	3.94370300	-0.00036400
C	-3.36495400	-2.44331300	-0.00040600
N	-4.61452400	-1.97210600	0.00001200
C	1.01686700	4.49220700	-0.00020200
H	1.61929100	5.39455700	-0.00031700
C	-0.34088500	4.56967800	-0.00004100
H	-0.83292700	5.53690600	-0.00001800
N	2.78013800	-2.86425300	0.00052600
C	4.07063300	-2.68468300	0.00043100
N	4.36580600	-1.34539300	0.00022500
Am	-0.07538100	-1.18546900	-0.00013900

AmR₂PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.66335500	2.07152400	-0.00626000
C	2.65039400	0.85129700	0.17419700
C	3.39671700	2.04354900	0.19688200
H	4.47597600	2.01121500	0.29088400
C	-0.76276700	2.03739300	-0.00175300
C	-1.50196900	3.23450200	0.01772000
C	-2.90838100	3.11356700	0.11430300
C	-3.49795100	1.86916700	0.21516500
H	-3.52639300	4.00666200	0.12974600
H	-4.57139600	1.75754900	0.32021600
N	-1.35001600	0.81820800	0.05161500
C	1.33518100	3.30498300	0.00906900
C	3.21164900	-0.47793400	0.29594200
C	4.49711100	-0.90616000	0.51016500
H	5.43100700	-0.37538800	0.62055300
H	5.21215300	-2.88557200	0.73566900
H	2.84743500	-3.68491200	0.42645400
C	-2.68205400	0.73298500	0.18071400

H	-2.85642700	-3.80447400	0.44158400
H	-5.21465900	-2.83539000	0.71976400
C	-3.17272000	-0.63405800	0.29833700
N	-2.30984400	-1.71500700	0.23855700
N	2.37133800	-1.59378600	0.23126800
N	1.31053600	0.88016300	0.04500800
C	2.74903800	3.25291400	0.09678300
H	3.32231000	4.17535800	0.10570900
C	3.15537100	-2.64882000	0.40832700
C	-3.12406200	-2.75724000	0.41489300
N	4.42761200	-2.26389300	0.57656200
N	-4.36445800	-2.30422500	0.56342200
C	0.57153600	4.50671600	-0.01447900
H	1.08928300	5.46057200	-0.01009500
C	-0.79856500	4.47387700	-0.01016800
H	-1.36261500	5.40105200	-0.00115300
N	-4.41879500	-0.97401900	0.49177800
Am	0.02944600	-1.09019300	-0.38490300

AmR₂PhR_g³⁺(PBE0/6-311G*-RECP)

C	0.61048500	2.10750800	0.00014100
C	2.62863800	0.94347600	-0.00040200
C	3.34481700	2.15115200	-0.00022800
H	4.42857200	2.13999600	-0.00037800
C	-0.81109300	2.05058300	-0.00007200
C	-1.56639100	3.24443200	-0.00029400
C	-2.96788300	3.11241900	-0.00084900
C	-3.54636100	1.85848500	-0.00127500
H	-3.59559600	3.99863200	-0.00097600
H	-4.62635500	1.76097600	-0.00182700
N	-1.37961700	0.82250700	-0.00029700
C	1.25305500	3.35538800	0.00013000
C	3.26418000	-0.35752300	-0.00132400
C	4.57738300	-0.74274300	-0.00254300
H	5.50112000	-0.18369400	-0.00295800
H	5.38088900	-2.70444400	-0.00418600
H	3.02842300	-3.58336800	-0.00281500
C	-2.72110200	0.73193700	-0.00102100
H	-5.31522000	-0.68136100	-0.00233800
H	-2.77972300	-3.80976800	-0.00186000
C	-3.18994800	-0.64483700	-0.00149100
N	-2.32241600	-1.67444100	-0.00136500
N	2.46285200	-1.49668100	-0.00131100
N	1.28182200	0.92235400	0.00000400

C	2.66597700	3.34572900	0.00009300
H	3.21377800	4.28342000	0.00016700
C	3.29678200	-2.53591700	-0.00242400
C	-3.13114800	-2.78736800	-0.00178300
N	4.56118700	-2.10769200	-0.00311300
C	0.47107900	4.55167300	0.00009400
H	0.98114900	5.50952200	0.00017000
C	-0.88879000	4.49984600	-0.00010900
H	-1.47343500	5.41386300	-0.00022200
N	-4.40014800	-2.49054100	-0.00224800
N	-4.41778200	-1.15192400	-0.00206300
Am	0.05281100	-1.17067700	0.00179100

AmR₃PhR₃³⁺(PBE0/6-311G*-RECP)

C	0.00000000	0.71337900	-2.05617400
C	0.00016900	2.68786100	-0.79715900
C	0.00019100	3.45688100	-1.96941000
H	0.00031900	4.54024600	-1.92752600
C	0.00000000	-0.71337900	-2.05617400
C	-0.00002900	-1.41339900	-3.27601100
C	-0.00007800	-2.82371900	-3.19469700
C	-0.00019100	-3.45688100	-1.96941000
H	-0.00009200	-3.41521600	-4.10561000
H	-0.00031900	-4.54024600	-1.92752600
N	0.00003200	-1.34360500	-0.85293600
C	0.00002900	1.41339900	-3.27601100
C	0.00041100	3.21028100	0.55866100
H	0.00063500	5.31347000	0.38344000
H	0.00101900	5.44438300	2.89102600
H	0.00112200	2.83500500	3.75137500
C	-0.00016900	-2.68786100	-0.79715900
H	-0.00063500	-5.31347000	0.38344000
H	-0.00112200	-2.83500500	3.75137500
H	-0.00101900	-5.44438300	2.89102600
C	-0.00041100	-3.21028100	0.55866100
N	-0.00060000	-2.39833900	1.63592600
N	0.00060000	2.39833900	1.63592600
N	-0.00003200	1.34360500	-0.85293600
C	0.00007800	2.82371900	-3.19469700
H	0.00009200	3.41521600	-4.10561000
C	0.00093200	3.21429100	2.74020800
C	-0.00093200	-3.21429100	2.74020800
C	0.00095700	4.51999800	2.33269900
C	-0.00095700	-4.51999800	2.33269900

N	0.00046600	4.48844600	0.96911000
N	-0.00046600	-4.48844600	0.96911000
C	0.00003200	0.68118200	-4.50227100
C	-0.00003200	-0.68118200	-4.50227100
H	0.00003700	1.22713300	-5.44003600
H	-0.00003700	-1.22713300	-5.44003600
Am	0.00000000	0.00000000	1.11931700

AmR₃PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.67156900	2.09129500	-0.00002700
C	-2.64986800	0.86627300	0.00004100
C	-3.41232300	2.03958400	0.00004100
H	-4.49584700	2.00105200	0.00006400
C	0.75375200	2.08294700	-0.00004500
C	1.45705200	3.30377800	0.00001200
C	2.86453500	3.23168000	0.00000400
C	3.49165000	2.00464800	-0.00006400
H	3.45351700	4.14403800	0.00005900
H	4.57391500	1.94136100	-0.00012700
N	1.37014800	0.87404600	-0.00007400
C	-1.36334900	3.31946100	-0.00000400
C	-3.19744500	-0.47628100	0.00008000
H	-5.29818900	-0.30482700	-0.00012900
H	-5.42248700	-2.81689700	-0.00032100
H	-2.81583000	-3.67373200	0.00010600
C	2.71656700	0.84067000	-0.00008200
H	5.52481800	-0.67907200	-0.00006600
H	4.93681800	-3.16734200	-0.00004000
C	3.26947500	-0.50451700	-0.00006600
N	2.37711600	-1.53619300	0.00001600
N	-2.38583400	-1.54699200	0.00012000
N	-1.30318400	0.89105300	-0.00001400
C	-2.77142200	3.25952400	0.00000700
H	-3.35192300	4.17731200	-0.00003700
C	-3.19639100	-2.66267300	0.00000500
C	-4.49954400	-2.25600900	-0.00016500
N	-4.47180800	-0.88890900	-0.00012700
C	-0.62719000	4.54290500	0.00002600
C	0.73268700	4.53520800	0.00004700
H	-1.17049500	5.48214100	0.00002400
H	1.28612900	5.46854500	0.00008600
N	2.98853700	-2.68567500	0.00005600
C	4.52088900	-1.07734900	-0.00006900

N	4.26587900	-2.40427300	0.00001600
Am	-0.01696200	-1.18253500	0.00002100

AmR₃PhR₅³⁺(PBE0/6-311G*-RECP)

C	0.73811100	2.06896900	0.00351400
C	2.68148000	0.79761700	-0.12449000
C	3.47065000	1.95543300	-0.14611600
H	4.55106800	1.89386100	-0.21430200
C	-0.68629600	2.08204400	0.01181600
C	-1.37487400	3.30759300	0.00138300
C	-2.78349000	3.24381000	-0.03741300
C	-3.41748500	2.01993000	-0.08908400
H	-3.36882400	4.15868500	-0.04030600
H	-4.49907700	1.96685800	-0.13620000
N	-1.31150500	0.87907200	-0.00952600
C	1.45387900	3.28388100	-0.01525300
C	3.17788200	-0.56003200	-0.20788300
H	5.28263400	-0.45454900	-0.31379900
H	5.32227800	-2.96654300	-0.40149000
H	2.69110300	-3.73947100	-0.29074100
C	-2.65375700	0.84586800	-0.08463600
H	-5.49612500	-0.37049700	-0.37072600
H	-3.04178200	-3.55954600	-0.33939100
C	-3.24688800	-0.48096400	-0.18009600
N	-2.45180500	-1.57666000	-0.16962700
N	2.33006100	-1.60656800	-0.19905300
N	1.33963300	0.85839900	-0.03157900
C	2.86026600	3.18993300	-0.08053000
H	3.46307000	4.09322300	-0.09392800
C	3.10230900	-2.74091900	-0.26079000
C	4.42122900	-2.37621900	-0.31943100
N	4.43861400	-1.01255000	-0.28397400
C	0.73461100	4.51526700	0.00520500
C	-0.62916500	4.52695000	0.01530500
H	1.28829900	5.44853000	0.00062000
H	-1.16616800	5.46999700	0.02370700
N	-4.55791400	-2.24593500	-0.39074000
N	-3.31357900	-2.58506200	-0.29872400
C	-4.56635400	-0.91781000	-0.31716600
Am	-0.00035400	-1.15245800	0.24013800

AmR₃PhR₆³⁺(PBE0/6-311G*-RECP)

C	-0.59663800	2.11331200	0.00005400
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C	-2.60947700	0.95088200	-0.00026400
C	-3.33419900	2.14940800	-0.00020400
H	-4.41840100	2.14548900	-0.00042200
C	0.83120100	2.06461200	-0.00003400
C	1.57606900	3.26635500	-0.00002800
C	2.97778100	3.14923800	-0.00031500
C	3.56920700	1.89990000	-0.00060700
H	3.59623300	4.04185900	-0.00039300
H	4.64990300	1.80994600	-0.00097100
N	1.40822200	0.84577400	-0.00017800
C	-1.24641300	3.36194700	0.00017200
C	-3.20557700	-0.37127400	-0.00049700
H	-5.29919500	-0.11691600	-0.00122800
H	-5.52297500	-2.62088500	-0.00163100
H	-2.95127300	-3.58037200	-0.00051800
C	2.75211100	0.76940600	-0.00049600
H	5.31953800	-0.79835800	-0.00148300
H	4.91743700	-3.32953500	-0.00094300
C	3.20416600	-0.61547600	-0.00071200
N	2.28307900	-1.56939600	-0.00017500
N	-2.43829300	-1.47358500	-0.00033400
N	-1.26318000	0.93262600	-0.00011400
C	-2.65617300	3.34825700	0.00003700
H	-3.20735900	4.28394000	0.00006400
C	-3.29172200	-2.55505400	-0.00065200
C	-4.57854900	-2.09695100	-0.00115500
C	4.14665100	-2.57074600	-0.00062500
N	-4.49635000	-0.73287600	-0.00098200
C	-0.47051900	4.56337900	0.00032300
C	0.88834100	4.51855800	0.00022300
H	-0.98601600	5.51829600	0.00043300
H	1.46752600	5.43611100	0.00029500
N	2.86194200	-2.79002400	-0.00008800
N	4.39991400	-1.22326800	-0.00106900
Am	-0.04831900	-1.20409300	0.00059000

AmR₃PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.71623600	2.07844900	0.00008600
C	2.68056700	0.83501800	0.00000600
C	3.45281900	2.00181700	0.00012400
H	4.53603200	1.95409000	0.00006300
C	-0.70590500	2.07563500	-0.00003800
C	-1.41087500	3.29321500	-0.00015600
C	-2.82040700	3.21856700	-0.00043900

C	-3.44588900	1.99028000	-0.00051700
H	-3.41128600	4.12978900	-0.00058100
H	-4.52678100	1.90293800	-0.00074500
N	-1.31981900	0.86444100	-0.00004700
C	1.41513500	3.30182400	0.00018200
C	3.20646100	-0.51608900	-0.00016800
H	5.30893900	-0.38153900	0.00003300
H	5.38904100	-2.89612900	-0.00072900
H	2.76935800	-3.70673400	-0.00077600
C	-2.66220000	0.83216800	-0.00026000
H	-3.08473400	-3.69393000	0.00015300
H	-5.40994600	-2.61821900	-0.00003800
C	-3.23516000	-0.50479300	-0.00017600
N	-2.42336700	-1.62144800	0.00000100
N	2.37434100	-1.57210200	-0.00055900
N	1.33479300	0.87288700	0.00002800
C	2.82261200	3.22877200	0.00023100
H	3.41245600	4.14062600	0.00034300
C	3.16629700	-2.70205400	-0.00060800
C	-3.29904500	-2.63392500	0.00003900
C	4.47611600	-2.31906400	-0.00054100
N	4.47256900	-0.95139500	-0.00023000
C	0.68021700	4.52640500	0.00016100
C	-0.68075500	4.52205200	-0.00001900
H	1.22448500	5.46511700	0.00027100
H	-1.23056600	5.45756800	-0.00002800
N	-4.50877900	-0.78914000	-0.00019600
N	-4.52317700	-2.12439200	-0.00006600
Am	0.01094500	-1.17763400	0.00023300

AmR₃PhR₈³⁺(PBE0/6-311G*-RECP)

C	0.67025400	2.09359600	0.00002400
C	2.65478900	0.88417600	-0.00097300
C	3.40703100	2.06533900	-0.00140600
H	4.49091600	2.03642600	-0.00208100
C	-0.75496900	2.07011200	0.00027200
C	-1.47720300	3.28201700	0.00031800
C	-2.88224000	3.18655900	0.00035500
C	-3.49124600	1.94755100	-0.00003900
H	-3.48761400	4.08820200	0.00059700
H	-4.57342100	1.87758400	-0.00002700
N	-1.35188200	0.85608300	0.00022100
C	1.34712200	3.32782600	-0.00025700
C	3.20941200	-0.45548300	-0.00137900

H	5.30961600	-0.27344700	-0.00288000
H	5.44686500	-2.78429400	-0.00208400
H	2.84581000	-3.65505200	-0.00022100
C	-2.69476600	0.79934300	-0.00022000
H	-5.32739400	-0.54013200	-0.00245800
H	-2.88321800	-3.74038700	-0.00254600
C	-3.20131700	-0.56475700	-0.00121100
N	-2.36451200	-1.61934900	-0.00136900
N	2.40269700	-1.53069600	-0.00059100
N	1.30876000	0.89877700	-0.00021800
C	2.75646400	3.28042200	-0.00095400
H	3.32997300	4.20265700	-0.00112100
C	3.21956400	-2.64141500	-0.00061200
C	-3.20488500	-2.70816100	-0.00212000
C	4.52102300	-2.22801100	-0.00157500
N	4.48592400	-0.86162500	-0.00203100
N	-4.44360200	-1.03600200	-0.00210100
C	0.59390100	4.54278000	-0.00005000
C	-0.76645300	4.52138300	0.00023200
H	1.12562100	5.48877200	-0.00011900
H	-1.32901600	5.44926500	0.00033600
N	-4.46502800	-2.37389900	-0.00303000
Am	0.02743700	-1.18844500	0.00141100

AmR₄PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.71286000	2.08948200	-0.00005700
C	-2.69277500	0.86811400	0.00021800
C	-3.45591300	2.03866900	0.00022000
H	-4.53872100	1.98600400	0.00024300
C	0.71344500	2.08935900	-0.00013700
C	1.40898700	3.31607800	-0.00009200
C	2.81664000	3.25812500	0.00010500
C	3.45650000	2.03805500	0.00032200
H	3.39568600	4.17683100	0.00014200
H	4.53929900	1.98519100	0.00052500
N	1.34472800	0.88588200	-0.00001000
C	-1.40815700	3.31630000	0.00001100
C	-3.26435500	-0.46873300	0.00033000
H	-5.52189800	-0.61487500	0.00122000
H	-4.96517300	-3.11060600	0.00103400
C	2.69313400	0.86766700	0.00028500
H	5.52186300	-0.61652100	0.00076300
H	4.96406800	-3.11195500	0.00071800
C	3.26438000	-0.46934500	0.00047000

N	2.38561800	-1.51213200	0.00023500
N	-2.38604700	-1.51190700	-0.00020800
N	-1.34436000	0.88608800	0.00004700
C	-2.81583800	3.25860100	0.00012700
H	-3.39468700	4.17743200	0.00014300
N	-3.01162800	-2.65417800	0.00019500
N	3.01067100	-2.65470000	0.00030700
N	-4.28453200	-2.35592500	0.00071100
N	4.28370900	-2.35701900	0.00051700
C	-4.52297700	-1.02560300	0.00085700
C	4.52275300	-1.02679700	0.00068900
C	-0.67894500	4.54408400	-0.00007300
H	-1.22846600	5.47970300	-0.00007300
C	0.67997600	4.54397900	-0.00013300
H	1.22965700	5.47950300	-0.00016100
Am	-0.00013400	-1.18254400	-0.00037900

AmR₄PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.64217900	2.09106300	-0.00001000
C	-2.63298300	0.88164700	0.00043600
C	-3.38171400	2.06310500	0.00021100
H	-4.46481700	2.02215700	0.00030000
C	0.78082400	2.06946200	0.00012000
C	1.49790100	3.28276100	0.00020000
C	2.90429500	3.19517600	0.00053800
C	3.51942700	1.96093200	0.00079500
H	3.50322500	4.10114100	0.00066300
H	4.60104100	1.88656200	0.00114500
N	1.38553100	0.85350100	0.00027300
C	-1.32220000	3.32442000	-0.00015400
C	-3.25540500	-0.43370800	0.00089400
H	-5.51088000	-0.29564600	0.00150200
C	2.73337300	0.80583200	0.00063400
H	5.51605200	-0.77432600	0.00154300
H	4.87040900	-3.24838400	0.00142100
C	3.26532900	-0.54695600	0.00090500
N	2.34970200	-1.55824800	0.00058600
N	-2.47672800	-1.54121800	0.00093300
N	-1.28591200	0.89303400	0.00016600
C	-2.73094300	3.27827400	-0.00011800
H	-3.30338100	4.20126200	-0.00031400
N	2.93408600	-2.72270700	0.00086000
N	4.21652300	-2.47006800	0.00126700

C	-4.58647900	-0.85459400	0.00136100
C	4.50285300	-1.14895600	0.00128200
C	-0.57386900	4.54119600	-0.00023900
H	-1.10877100	5.48529300	-0.00039800
C	0.78589900	4.52113100	-0.00001500
H	1.34820600	5.44918900	0.00000200
N	-3.35926400	-2.54368200	0.00148900
H	-3.10550600	-3.52425400	0.00191900
N	-4.60009700	-2.18518200	0.00169300
Am	-0.01765500	-1.16385000	-0.00104900

AmR₄PhR₆³⁺(PBE0/6-311G*-RECP)

C	-0.79354800	2.07171400	0.00005700
C	-2.73016500	0.79494400	0.00044500
C	-3.53730900	1.93133600	0.00085200
H	-4.61869700	1.85039700	0.00131400
C	0.63557500	2.11436500	-0.00025100
C	1.28731100	3.36284400	-0.00031800
C	2.69651400	3.35359000	-0.00057600
C	3.37554500	2.15569000	-0.00059300
H	3.24456400	4.29111100	-0.00069500
H	4.45953400	2.13909400	-0.00093600
N	1.30398300	0.93180700	-0.00024500
C	-1.53228000	3.27900800	0.00031400
C	-3.20022400	-0.58311400	0.00028700
H	-5.31741400	-0.74138700	0.00000000
C	2.65149200	0.95910800	-0.00032500
H	5.53454200	-0.40868600	0.00060200
H	5.08136800	-2.92522500	0.00115100
C	3.27257500	-0.35598400	0.00010100
N	2.43812700	-1.43456600	0.00019500
N	-2.29095300	-1.54834400	-0.00012000
N	-1.38390900	0.85733800	0.00007600
C	-2.93446000	3.17473700	0.00072400
H	-3.54404800	4.07343100	0.00094800
N	3.11032000	-2.54895200	0.00099000
N	4.37049000	-2.19897600	0.00101400
C	4.55340100	-0.86022100	0.00059000
C	-0.84141300	4.52864500	0.00020500
H	-1.41809400	5.44774800	0.00031700
C	0.51667500	4.56776600	-0.00010700
H	1.03714900	5.51998300	-0.00014900
N	-2.88329600	-2.76243100	-0.00049800
H	-4.94467000	-3.27757300	-0.00012100

C	-4.16503100	-2.52777900	-0.00013500
N	-4.40263100	-1.17685300	0.00003000
Am	0.03287300	-1.20633600	-0.00021200

AmR₄PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.66432500	2.08210300	0.00000900
C	-2.63775400	0.85889500	0.00006300
C	-3.40962300	2.02356700	0.00018100
H	-4.49130800	1.94672600	0.00024400
C	0.75871400	2.07616400	-0.00006200
C	1.46153300	3.29779700	-0.00008000
C	2.86866900	3.22607400	-0.00012400
C	3.49741500	1.99878600	-0.00011200
H	3.45742500	4.13863000	-0.00018400
H	4.57975000	1.93653900	-0.00012800
N	1.37641000	0.86721000	-0.00008000
C	-1.36137900	3.30558300	0.00009300
C	-3.22826100	-0.47019400	0.00003700
C	2.72403800	0.83497000	-0.00008700
H	5.52653900	-0.70311700	0.00007800
H	4.92023200	-3.18700000	0.00040500
C	3.27277900	-0.51142300	-0.00003800
N	2.37293700	-1.53690800	0.00005400
N	-2.43049000	-1.59666000	-0.00003600
N	-1.29335900	0.87650100	-0.00000600
C	-2.77116700	3.24492900	0.00019100
H	-3.35213500	4.16252100	0.00025800
N	2.97581300	-2.69188500	0.00028500
N	4.25436200	-2.41924100	0.00030400
C	4.51958200	-1.09390800	0.00014500
C	-0.62623400	4.53061900	0.00008800
H	-1.17186400	5.46854400	0.00012100
C	0.73383400	4.52691100	-0.00000500
H	1.28449200	5.46189700	-0.00001600
H	-5.42783400	-2.55811600	0.00001000
C	-3.31788300	-2.59976800	-0.00006900
H	-3.11515800	-3.66216600	-0.00012500
N	-4.53507700	-2.07489500	0.00000900
N	-4.50494200	-0.73953000	0.00009100
Am	-0.00673000	-1.17666600	-0.00006700

AmR₄PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.71396300	2.07714000	-0.00008100
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C	-2.67081700	0.82646500	-0.00010700
C	-3.45587000	1.98123300	-0.00012600
H	-4.53864000	1.92163900	-0.00005400
C	0.71242000	2.09269400	0.00000900
C	1.39285800	3.32567000	0.00013200
C	2.80174700	3.28042700	0.00022300
C	3.45157000	2.06527500	0.00011300
H	3.37362100	4.20367900	0.00038800
H	4.53488400	2.02227900	0.00010000
N	1.35087900	0.89501400	-0.00002400
C	-1.42865500	3.29507900	-0.00014500
C	-3.19557800	-0.53028800	-0.00007200
C	2.69848300	0.88700400	-0.00000900
H	5.53393800	-0.58696900	-0.00015200
H	4.98528400	-3.08436700	-0.00045300
C	3.27588900	-0.44763500	-0.00011400
N	2.40038400	-1.49386100	-0.00010500
N	-2.37200200	-1.59529800	0.00002800
N	-1.32571900	0.86844200	-0.00009900
C	-2.83408300	3.21354600	-0.00018100
H	-3.42971000	4.12167300	-0.00025800
N	3.02984800	-2.63372300	-0.00020700
N	4.30199800	-2.33182300	-0.00026500
C	4.53616200	-1.00079200	-0.00020800
C	-0.71321000	4.53094800	-0.00008300
H	-1.27199100	5.46108500	-0.00019200
C	0.64632000	4.54493200	0.00008900
H	1.18406200	5.48752300	0.00019800
C	-3.22509600	-2.67530700	0.00010500
H	-2.91499200	-3.71115700	0.00016800
N	-4.44306800	-0.98673300	-0.00010500
H	-5.32114400	-0.48063700	-0.00021500
N	-4.48035600	-2.32467200	-0.00004400
Am	0.01012500	-1.18878400	0.00009400

AmR₅PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.71014700	2.06705400	0.00336400
C	-2.66526800	0.80539400	-0.11697800
C	-3.44303600	1.97038000	-0.12426900
H	-4.52335300	1.90543000	-0.18511400
C	0.71630600	2.06419200	-0.00272500
C	1.42227300	3.28241300	-0.01977100
C	2.83049200	3.20082000	-0.10022900

C	3.44738700	1.97036200	-0.18449600
H	3.42676800	4.10867900	-0.11276000
H	4.52597600	1.90431200	-0.27034100
N	1.32795500	0.85699300	-0.05063200
C	-1.41422400	3.28505100	-0.01252000
C	-3.23042900	-0.53042200	-0.24029200
H	-5.47144100	-0.44681900	-0.52834200
C	2.66945800	0.80533800	-0.15608600
H	5.48093800	-0.48659600	-0.45811900
C	3.22925400	-0.53284500	-0.25571500
N	2.40239200	-1.60648500	-0.23934600
N	-2.42097700	-1.61788500	-0.20779600
N	-1.32195100	0.86111300	-0.01751800
C	-2.82384500	3.20203100	-0.06176000
H	-3.42095300	4.10945500	-0.06779000
N	-4.50808400	-2.30930000	-0.52980200
N	4.48933200	-2.33458900	-0.46604100
C	-4.53752100	-0.98287700	-0.44055700
C	4.53620000	-1.00730200	-0.39750300
C	-0.68087300	4.50673500	0.00725100
H	-1.22178900	5.44775900	0.01538400
C	0.69015700	4.50491200	-0.00049200
H	1.23315300	5.44473500	-0.01164800
N	-3.26317500	-2.63176300	-0.38843600
H	-2.97708600	-3.60262100	-0.42689900
N	3.23502500	-2.63691600	-0.36578400
H	2.93530300	-3.60318800	-0.41578400
Am	0.00222900	-1.12122900	0.32563700

AmR₅PhR₆³⁺(PBE0/6-311G*-RECP)

C	-0.56832200	2.11168400	0.00010100
C	-2.59319900	0.96631800	-0.00015800
C	-3.30431800	2.17219500	-0.00031400
H	-4.38818900	2.16564900	-0.00050800
C	0.85724000	2.05054700	-0.00004400
C	1.61498300	3.24520100	-0.00000200
C	3.01513700	3.11399300	-0.00018400
C	3.59553400	1.85834700	-0.00050600
H	3.64245700	4.00050600	-0.00006500
H	4.67537900	1.75817900	-0.00069500
N	1.42350400	0.82609000	-0.00031700
C	-1.20652000	3.36518900	0.00005800

C	-3.26223200	-0.32659800	-0.00050000
H	-5.51153100	-0.10491400	-0.00053500
C	2.76842900	0.73659100	-0.00061600
H	5.30875500	-0.89040500	-0.00126200
C	3.19935600	-0.65420600	-0.00071600
N	2.25508000	-1.58640000	-0.00032300
N	-2.52622700	-1.46237300	-0.00067600
N	-1.24719700	0.93379400	0.00012500
C	-2.61634400	3.36583500	-0.00013100
H	-3.15893100	4.30666500	-0.00017800
N	-4.67185500	-2.02665400	-0.00105500
C	-4.60830700	-0.69747800	-0.00069100
C	-0.41919700	4.55999400	0.00011700
H	-0.92672600	5.51922700	0.00015000
C	0.93919100	4.50356500	0.00015500
H	1.52658800	5.41591700	0.00031600
N	-3.44482100	-2.43049700	-0.00095300
H	-3.22693200	-3.41984400	-0.00132800
N	2.80225900	-2.82147600	-0.00046300
N	4.37825600	-1.29198200	-0.00091900
C	4.09178700	-2.63397700	-0.00069500
H	4.84406400	-3.41140100	-0.00081600
Am	-0.04828600	-1.18680300	0.00065000

AmR₅PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.70134400	2.06868800	0.00810700
C	2.65975700	0.81747200	-0.13915800
C	3.43047500	1.98683000	-0.16277800
H	4.50969300	1.92658300	-0.24483700
C	-0.72071400	2.06161900	0.00713400
C	-1.43780800	3.27008300	-0.02227600
C	-2.84673000	3.17285100	-0.08865300
C	-3.45483300	1.93509600	-0.15151900
H	-3.45168500	4.07480200	-0.10893700
H	-4.53200200	1.83667400	-0.23026700
N	-1.31964800	0.84683400	-0.01248400
C	1.39849900	3.29051600	-0.01094500
C	3.22555400	-0.51810700	-0.25149900
H	5.47656400	-0.46333000	-0.44801700
C	-2.65820500	0.78566700	-0.12274100
C	-3.19168100	-0.56420500	-0.23695600
N	-2.36284600	-1.67081300	-0.19808100
N	2.40131100	-1.59378400	-0.25265500
N	1.31895200	0.86190800	-0.03445200

C	2.80667000	3.21498200	-0.08325700
H	3.39918800	4.12525500	-0.09555200
N	4.48981200	-2.31395300	-0.48531200
C	4.53323900	-0.98747000	-0.39707500
C	0.65478400	4.50866600	0.00085000
H	1.19141400	5.45200500	-0.00744500
C	-0.71249500	4.49944100	-0.00244900
H	-1.26209500	5.43530400	-0.00334100
N	3.23680800	-2.62178000	-0.39271300
H	2.93938100	-3.58755900	-0.45878600
C	-3.21194900	-2.68821800	-0.37251600
H	-2.97845500	-3.74348600	-0.41002900
N	-4.43797500	-2.19468600	-0.49840900
H	-5.30742300	-2.69838600	-0.64322100
N	-4.44985800	-0.86388000	-0.41568400
Am	0.00867500	-1.12242400	0.32456200

AmR₅PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.64563000	2.09222100	-0.00010200
C	-2.64025300	0.89576700	0.00073300
C	-3.38097700	2.08354200	0.00064000
H	-4.46442800	2.05019300	0.00102700
C	0.77721900	2.05819700	0.00007300
C	1.51084100	3.26398900	0.00019600
C	2.91472500	3.15612100	0.00076500
C	3.51417300	1.91134800	0.00135100
H	3.52798700	4.05253700	0.00082100
H	4.59577700	1.83229500	0.00187400
N	1.36493300	0.83863700	0.00035300
C	-1.31290600	3.33042800	-0.00017500
C	-3.26747800	-0.41713300	0.00161300
H	-5.52240000	-0.27102500	0.00304500
C	2.70898100	0.77071200	0.00113800
H	5.32289100	-0.61581600	0.00290200
C	3.19737400	-0.59886500	0.00169100
N	2.33912400	-1.63769300	0.00120900
N	-2.49159400	-1.52738600	0.00144800
N	-1.29412700	0.89853500	0.00017800
C	-2.72269800	3.29483900	0.00012100
H	-3.28945700	4.22138500	0.00005100
N	-4.61784000	-2.16378300	0.00326200
C	-4.59977300	-0.83308600	0.00264200
C	-0.54988100	4.54000700	-0.00033600

H	-1.07498900	5.48974400	-0.00052900
C	0.81027300	4.50880200	-0.00012300
H	1.37993500	5.43238200	-0.00015800
N	-3.37840800	-2.52640400	0.00246400
H	-3.12967400	-3.50831000	0.00295500
N	4.42908300	-1.09428200	0.00241400
C	3.15900900	-2.74427800	0.00199000
H	2.81864300	-3.77061100	0.00197000
N	4.42408400	-2.43296900	0.00264800
Am	-0.02556900	-1.17127400	-0.00194900

AmR₆PhR₆³⁺(PBE0/6-311G*-RECP)

C	-0.71636300	2.07221300	-0.04321200
C	-2.66492700	0.81378900	0.18009800
C	-3.44390500	1.97292500	0.23920200
H	-4.51892800	1.92080600	0.37183700
C	0.71625000	2.07224600	-0.04317600
C	1.41840900	3.29113600	0.01510100
C	2.82213000	3.20488500	0.13265900
C	3.44378300	1.97308500	0.23936500
H	3.41789600	4.11232700	0.17084900
H	4.51880100	1.92101700	0.37206000
N	1.33443900	0.87239100	-0.00123400
C	-1.41858200	3.29107100	0.01502500
C	-3.12430100	-0.56525600	0.33672200
H	-5.22153800	-0.64130800	0.66559000
H	-4.92057100	-3.17936200	0.81796300
C	2.66486800	0.81391100	0.18019500
H	5.22157900	-0.64104500	0.66553900
H	4.92078000	-3.17913000	0.81777500
C	3.12432300	-0.56511000	0.33676300
N	2.24284600	-1.56425400	0.28532200
N	-2.24274000	-1.56433600	0.28541100
N	-1.33449800	0.87233600	-0.00128700
C	-2.82230500	3.20475300	0.13250500
H	-3.41811700	4.11216700	0.17064900
N	-2.87002100	-2.74592700	0.46746400
N	2.87020500	-2.74581600	0.46728500
C	-4.13136000	-2.46168100	0.63905200
C	4.13152100	-2.46148900	0.63891400
N	-4.32987600	-1.11065400	0.56265600
N	4.32994900	-1.11044600	0.56257700
C	0.68144900	4.51748400	0.00055700
H	1.22472300	5.45685100	0.01758800

C	-0.68167900	4.51745300	0.00051900
H	-1.22499700	5.45679500	0.01751900
Am	0.00002500	-1.11379600	-0.42617300

AmR₆PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.83373800	2.05906300	-0.00015600
C	2.75885400	0.76802800	-0.00062300
C	3.57287100	1.89956500	-0.00075100
H	4.65378700	1.81212300	-0.00102800
C	-0.59210900	2.10358000	0.00002700
C	-1.24910000	3.34706100	0.00021600
C	-2.66042900	3.33128100	0.00035800
C	-3.33478900	2.13011100	0.00016500
H	-3.21306500	4.26620100	0.00054000
H	-4.41834500	2.08603100	0.00017300
N	-1.25497200	0.91705500	-0.00007900
C	1.57661300	3.26297900	-0.00021500
C	3.20789800	-0.61705100	-0.00072500
H	5.32097300	-0.81553400	-0.00061400
H	4.90111400	-3.34438700	-0.00020900
C	-2.59832400	0.94123500	-0.00010400
H	-5.51289000	-2.36889400	-0.00145800
C	-3.23432900	-0.36735100	-0.00054900
N	-2.48082900	-1.52317500	-0.00104100
N	2.27970800	-1.56535900	-0.00068500
N	1.41347600	0.84134000	-0.00031600
C	2.97807100	3.14838300	-0.00052100
H	3.59503000	4.04208100	-0.00061000
N	2.84947000	-2.79070100	-0.00039100
C	4.13529600	-2.58046800	-0.00035200
N	4.39812900	-1.23392500	-0.00055200
C	-0.47554600	4.55106500	0.00021300
H	-0.99453400	5.50413100	0.00038200
C	0.88370000	4.51191200	-0.00001200
H	1.45888800	5.43198900	-0.00004500
C	-3.40557900	-2.49122300	-0.00122600
H	-3.24298200	-3.56055900	-0.00164700
N	-4.60233000	-1.92014800	-0.00119600
N	-4.52065200	-0.58730300	-0.00063400
Am	-0.03687400	-1.20007000	0.00067700

AmR₆PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.78985400	2.07650500	0.00005000
C	-2.73529000	0.81786900	0.00031900
C	-3.53069000	1.96356600	0.00081300
H	-4.61294700	1.89410500	0.00116400
C	0.64000000	2.10089600	-0.00010500
C	1.31338400	3.33979000	-0.00027700
C	2.72118700	3.30399900	-0.00060300
C	3.38022000	2.09191500	-0.00050800
H	3.28809200	4.23033500	-0.00086200
H	4.46433700	2.06643100	-0.00065000
N	1.28678000	0.91107600	0.00000100
C	-1.51175900	3.29142000	0.00036000
C	-3.21320600	-0.55838500	0.00023900
H	-5.33121200	-0.70934600	0.00077900
H	-4.96819200	-3.24642900	0.00009700
C	2.63184300	0.91169500	-0.00009700
C	3.20509900	-0.42627500	0.00033700
N	2.42511300	-1.52282300	0.00138300
N	-2.30742000	-1.52736600	-0.00008300
N	-1.38944800	0.86854600	-0.00003300
C	-2.91570000	3.20157500	0.00080900
H	-3.51713800	4.10582900	0.00115600
N	-2.90428300	-2.73862400	-0.00023400
C	-4.18559700	-2.49957100	0.00006000
N	-4.41766400	-1.14786900	0.00044000
C	0.55805800	4.55464500	-0.00010600
H	1.08955500	5.50077500	-0.00023600
C	-0.80095600	4.53190300	0.00024200
H	-1.36440200	5.45934000	0.00043500
C	3.31929300	-2.56753100	0.00157100
H	3.04987500	-3.61473700	0.00244100
N	4.47038100	-0.83309900	0.00020700
H	5.32808300	-0.29320100	-0.00065800
N	4.56058000	-2.16775800	0.00090900
Am	0.02094200	-1.21149200	-0.00042600

AmR₇PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.70983000	2.06898400	-0.00005500
C	2.66884400	0.82633100	0.00012600
C	3.45041500	1.98454100	0.00022200
H	4.53144800	1.89856500	0.00034200
C	-0.70982500	2.06898200	-0.00005000

C	-1.41412600	3.28737700	-0.00000300
C	-2.82336600	3.21308200	0.00009200
C	-3.45041100	1.98454100	0.00019300
H	-3.41406400	4.12448100	0.00012000
H	-4.53144300	1.89856400	0.00031700
N	-1.32506800	0.85757800	-0.00000700
C	1.41413100	3.28737900	-0.00000500
C	3.23876200	-0.51119700	0.00026600
C	-2.66883900	0.82633000	0.00016800
C	-3.23876700	-0.51119400	0.00035100
N	-2.42063800	-1.62455300	0.00002400
N	2.42063000	-1.62455100	0.00001100
N	1.32507100	0.85758100	-0.00001900
C	2.82337000	3.21308400	0.00012300
H	3.41407000	4.12448200	0.00017800
C	3.29211100	-2.64192200	0.00032600
H	3.07331000	-3.70102300	0.00030800
C	-3.29212800	-2.64191600	0.00044100
H	-3.07333600	-3.70101900	0.00044600
C	0.68059700	4.51373500	-0.00000400
H	1.22743200	5.45099500	0.00001600
C	-0.68059400	4.51373400	-0.00003500
H	-1.22743000	5.45099300	-0.00002700
N	4.51034500	-0.80238400	0.00066700
N	-4.51035100	-0.80237000	0.00058100
N	-4.51787900	-2.13798200	0.00075200
H	-5.40248600	-2.63606800	0.00103300
N	4.51786500	-2.13799600	0.00076800
H	5.40246800	-2.63608900	0.00114800
Am	0.00000200	-1.17118300	-0.00038200

AmR₇PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.66525600	2.08403000	0.00000500
C	-2.64363500	0.87516200	-0.00003600
C	-3.40666100	2.04693300	-0.00006500
H	-4.48903100	1.97868700	-0.00011500
C	0.75771000	2.06413600	-0.00001700
C	1.47841900	3.27768100	0.00001300
C	2.88320000	3.18406200	-0.00004400
C	3.49498600	1.94537300	-0.00010500
H	3.48744500	4.08651900	-0.00004300
H	4.57730000	1.87730300	-0.00019400
N	1.35702500	0.85069900	-0.00006500

C	-1.34864100	3.31309900	0.00002000
C	-3.23985600	-0.45127800	-0.00005500
C	2.70113900	0.79657300	-0.00010100
C	3.20482100	-0.56778800	-0.00007800
N	2.36125400	-1.61839800	0.00001000
N	-2.44659300	-1.58167000	-0.00011800
N	-1.30018200	0.88333900	0.00000600
C	-2.75962400	3.26403000	-0.00002400
H	-3.33426700	4.18565600	-0.00003100
C	-3.33959800	-2.58009600	-0.00010100
H	-3.14337700	-3.64374700	-0.00012900
C	3.19650900	-2.71287600	-0.00000200
H	2.86987000	-3.74357900	0.00003900
C	-0.59743200	4.53030800	0.00006800
H	-1.13227900	5.47458000	0.00010600
C	0.76320600	4.51405000	0.00007000
H	1.32215700	5.44412100	0.00011500
N	-4.51754000	-0.71454000	-0.00007300
N	-4.55436700	-2.04942100	-0.00012700
H	-5.44965200	-2.52839100	-0.00015100
N	4.45742000	-2.38482400	-0.00008200
N	4.44355300	-1.04612600	-0.00014000
H	5.33019200	-0.55494900	-0.00018400
Am	-0.01598000	-1.18368400	0.00007800

AmR₈PhR₈³⁺(PBE0/6-311G*-RECP)

C	0.71326000	2.08001300	-0.00025900
C	2.67653400	0.84495000	-0.00046100
C	3.45153600	2.00766200	-0.00006400
H	4.53486400	1.95773900	0.00021200
C	-0.71333400	2.07999500	-0.00026500
C	-1.41308200	3.30420300	-0.00007900
C	-2.81994500	3.23520200	0.00003300
C	-3.45161000	2.00756700	-0.00004500
H	-3.40864800	4.14791100	0.00024100
H	-4.53493500	1.95759900	0.00003900
N	-1.33212600	0.87662900	-0.00035200
C	1.41297100	3.30423600	0.00007900
C	3.20812700	-0.50953700	-0.00055600
H	5.33366200	-0.44997800	-0.00085700
C	-2.67655900	0.84488300	-0.00033700
H	-5.33364800	-0.45009400	-0.00103800
C	-3.20811900	-0.50962000	-0.00035100
N	-2.38887900	-1.57871800	0.00014800

N	2.38891300	-1.57865700	-0.00021600
N	1.33208300	0.87665100	-0.00057400
C	2.81983700	3.23528000	0.00020100
H	3.40850500	4.14801200	0.00054700
N	4.45766100	-0.96009500	-0.00053900
N	-4.45764300	-0.96020500	-0.00064800
C	3.24773000	-2.65405200	-0.00048700
H	2.94406400	-3.69184700	-0.00037500
C	-3.24767500	-2.65412000	0.00005300
H	-2.94398100	-3.69190700	0.00040400
N	4.50146800	-2.29732200	-0.00025200
N	-4.50143100	-2.29743300	-0.00076400
C	0.68001400	4.53183400	0.00027400
H	1.22710000	5.46905300	0.00051000
C	-0.68015800	4.53181900	0.00015100
H	-1.22726600	5.46902500	0.00025700
Am	0.00003000	-1.19487800	0.00037000

EuR₁PhR₁³⁺(PBE0/6-311G*-RECP)

C	-0.73325800	1.90204300	-0.00005300
C	-2.71857600	0.70465300	0.00019300
C	-3.48101100	1.88779800	0.00022600
H	-4.56287500	1.84123900	0.00035900
C	0.73325800	1.90204300	-0.00004900
C	1.42680100	3.14288400	-0.00001000
C	2.84210300	3.10012200	0.00008900
C	3.48101100	1.88779800	0.00022300
H	3.41218800	4.02442400	0.00009300
H	4.56287500	1.84123900	0.00034600
N	1.36193700	0.72936300	0.00000200
C	-1.42680100	3.14288400	-0.00001100
C	-3.35229600	-0.59748100	0.00046400
C	-4.72473500	-0.90639300	0.00091700
H	-5.57373300	-0.24031900	0.00108400
C	-4.77663500	-2.28118200	0.00111600
H	-5.61074500	-2.96873000	0.00144000
H	-3.20901400	-3.68027500	0.00069400
C	2.71857500	0.70465300	0.00021000
C	4.72473500	-0.90639300	0.00081700
C	4.77663600	-2.28118200	0.00107800
H	5.57373300	-0.24031900	0.00090200
H	3.20901400	-3.68027500	0.00099700
H	5.61074500	-2.96873000	0.00140300

C	3.35229600	-0.59748100	0.00046800
N	2.60652600	-1.73161400	0.00047400
N	-2.60652600	-1.73161400	0.00046200
N	-1.36193700	0.72936300	-0.00000900
C	-2.84210300	3.10012200	0.00009500
H	-3.41218800	4.02442400	0.00010500
N	-3.50228600	-2.71333300	0.00070900
N	3.50228600	-2.71333300	0.00085200
C	0.70015300	4.34508400	-0.00004700
H	1.23128600	5.29263700	-0.00005300
C	-0.70015300	4.34508400	-0.00004600
H	-1.23128700	5.29263700	-0.00005100
Eu	0.00000000	-1.46174800	-0.00093400

EuR₁PhR₂³⁺(PBE0/6-311G*-RECP)

C	0.75960400	1.89362400	0.00356200
C	2.73432000	0.67806700	-0.01781300
C	3.51185500	1.85943300	-0.02106400
H	4.59382600	1.80560600	-0.03193700
C	-0.70509100	1.90918700	0.00386200
C	-1.37970200	3.15274800	0.00023600
C	-2.79216600	3.12820800	-0.00848400
C	-3.44757000	1.92220600	-0.01969000
H	-3.35173700	4.05885300	-0.00939400
H	-4.52990800	1.89053500	-0.03072900
N	-1.34931300	0.74017600	-0.00019100
C	1.46934300	3.13324700	-0.00083400
C	3.32998700	-0.62548800	-0.03780800
C	4.68184200	-0.96708000	-0.07395200
H	5.58307800	-0.37181500	-0.09069400
H	5.55251000	-2.88175600	-0.11618500
C	-2.70216000	0.73068600	-0.01783800
C	-4.73108000	-0.85385200	-0.07106300
C	-4.80382200	-2.22890800	-0.09058900
H	-5.56993900	-0.17529300	-0.07990600
H	-3.25860900	-3.65129900	-0.08110300
H	-5.64880100	-2.90231300	-0.11719400
C	-3.35682500	-0.56667600	-0.04004800
N	-2.62876700	-1.70927900	-0.04004500
N	2.57460900	-1.78981700	-0.03156800
N	1.37622200	0.71560000	0.00046700
C	2.88693700	3.07299600	-0.01019000
H	3.46479300	3.99221900	-0.01147800

N	-3.53891700	-2.68123000	-0.07057600
C	-0.63472600	4.35258800	0.00288700
H	-1.15901800	5.30392100	0.00332200
C	0.76009600	4.34053200	0.00218500
H	1.30178100	5.28161900	0.00188500
C	3.43960400	-2.77677200	-0.06280200
H	3.21235100	-3.83401800	-0.06832700
N	4.71529900	-2.31079600	-0.08907600
Eu	-0.03741200	-1.46344900	0.07945000

EuR₁PhR₃³⁺(PBE0/6-311G*-RECP)

C	0.80589400	1.86836100	0.00064800
C	2.75396200	0.61584700	-0.00343500
C	3.55819900	1.77555500	-0.00407200
H	4.64027200	1.71241700	-0.00606100
C	-0.65569300	1.91460700	0.00076600
C	-1.30020200	3.17211700	0.00029400
C	-2.71239900	3.17967400	-0.00129300
C	-3.39535400	1.98926100	-0.00350500
H	-3.25070900	4.12273900	-0.00130000
H	-4.47821200	1.98281400	-0.00549400
N	-1.32756400	0.75830100	-0.00016900
C	1.54288100	3.09448200	-0.00008400
C	3.29320200	-0.71085200	-0.00712000
H	5.40870900	-0.42415800	-0.01670900
C	4.71593100	-2.39089300	-0.01671300
H	5.66378800	-2.91132300	-0.02216300
H	3.08533100	-3.90108400	-0.01147100
C	-2.67821800	0.78005800	-0.00333300
C	-4.74613900	-0.75505000	-0.01343400
C	-4.85317200	-2.12844100	-0.01697000
H	-5.56811700	-0.05610200	-0.01527500
H	-3.34454600	-3.58927800	-0.01448900
H	-5.71510800	-2.78057900	-0.02195000
C	-3.36589500	-0.50183500	-0.00749100
N	-2.66614500	-1.66209900	-0.00746300
N	2.54308500	-1.83373600	-0.00558100
N	1.39814500	0.67934500	-0.00003000
C	2.95580600	3.00369100	-0.00192100
H	3.55386800	3.90988600	-0.00210700
N	-3.60046100	-2.61249000	-0.01292500
C	-0.52814300	4.35882000	0.00091800
H	-1.03511500	5.31943700	0.00116600
C	0.85989500	4.31981400	0.00070400

H	1.42299200	5.24800600	0.00077600
C	3.40021400	-2.86697400	-0.01124100
N	4.61527200	-1.05203200	-0.01379300
Eu	-0.07974700	-1.47433800	0.01457900

EuR₁PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.77587800	1.90506700	0.00000300
C	-2.75609100	0.70346900	0.00151500
C	-3.52681600	1.87766600	0.00227700
H	-4.60940300	1.82670200	0.00339100
C	0.69240500	1.91315900	-0.00042700
C	1.37619000	3.16301700	-0.00030300
C	2.79288500	3.13488600	-0.00047900
C	3.44310800	1.93051400	-0.00025900
H	3.35274100	4.06540000	-0.00043800
H	4.52529500	1.89452600	-0.00003700
N	1.33315700	0.74722000	-0.00046600
C	-1.47624600	3.14034800	0.00062300
C	-3.34818400	-0.61643200	0.00206700
C	-4.66020400	-1.06182300	0.00314400
H	-5.61867900	-0.56410300	0.00417100
H	-5.27856300	-3.09270000	0.00389200
C	2.69224800	0.73836800	0.00006200
C	4.72648700	-0.83593800	0.00105600
C	4.80359400	-2.20896600	0.00407700
H	5.56351200	-0.15485800	-0.00186700
H	3.25979400	-3.63662100	0.01070400
H	5.64977200	-2.88166300	0.00468700
C	3.34686000	-0.55158100	0.00171100
N	2.62350200	-1.70081700	0.00578000
N	-2.55275200	-1.73127500	0.00078700
N	-1.39981600	0.72947800	0.00016000
C	-2.89017700	3.09330100	0.00166500
H	-3.46317200	4.01583000	0.00209600
N	3.53621700	-2.66411000	0.00671100
C	0.64342600	4.35889800	-0.00005900
H	1.16866800	5.30968400	-0.00014700
C	-0.75619100	4.34967700	0.00045800
H	-1.29412000	5.29347900	0.00086200
N	-3.27920300	-2.79695900	0.00259000
N	-4.54089200	-2.39573700	0.00304400
Eu	0.01171700	-1.48558800	-0.00413200

EuR₁PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.74813500	1.89537600	-0.00012000
C	-2.72701800	0.69148500	0.00006700
C	-3.49641800	1.86682100	-0.00001500
H	-4.57864300	1.81543400	0.00004500
C	0.71921100	1.90312400	-0.00003400
C	1.40699800	3.15087800	0.00013500
C	2.82395400	3.11697900	0.00038300
C	3.46996800	1.90971300	0.00048200
H	3.38761800	4.04527600	0.00051500
H	4.55212100	1.86971500	0.00072400
N	1.35545000	0.73579500	-0.00002900
C	-1.44730100	3.13029600	-0.00014000
C	-3.35433700	-0.61479300	0.00040200
C	-4.71424300	-0.97601200	0.00076300
H	-5.61243000	-0.37583300	0.00077700
H	-3.33589400	-3.68583600	0.00121000
C	2.71441900	0.72091800	0.00026300
C	4.73233400	-0.87405100	0.00065500
C	4.79390300	-2.24825900	0.00075800
H	5.57681500	-0.20208600	0.00068100
H	3.23646800	-3.65889700	0.00060500
H	5.63262500	-2.93039600	0.00099300
C	3.35658700	-0.57449700	0.00037000
N	2.61907600	-1.71531300	0.00032100
N	-2.62944300	-1.75652600	0.00054900
N	-1.37202500	0.71856000	-0.00007600
C	-2.86082300	3.08369400	-0.00014800
H	-3.43509800	4.00552100	-0.00021300
N	3.52194900	-2.68909400	0.00053900
C	0.67617200	4.34744900	0.00007900
H	1.20137600	5.29833900	0.00018600
C	-0.72513900	4.33907500	-0.00009000
H	-1.26179100	5.28372100	-0.00015300
N	-3.55157000	-2.69647900	0.00094300
N	-4.79252600	-2.29758500	0.00114800
Eu	0.01364600	-1.47253400	-0.00082500

EuR₁PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.80731300	1.89528600	-0.00531600
C	2.76442000	0.66400800	0.04602900
C	3.55595100	1.81886100	0.06282000
H	4.63809000	1.76044400	0.09275100
C	-0.65866800	1.92079400	-0.01391400
C	-1.32499400	3.18013200	-0.01266600

C	-2.74229000	3.16851800	-0.00574300
C	-3.40635100	1.97234100	0.01566200
H	-3.29141600	4.10538700	-0.01069400
H	-4.48888400	1.94981600	0.03005900
N	-1.31201500	0.76151400	-0.00694500
C	1.52641300	3.11948900	0.00968000
C	3.28809400	-0.68863000	0.07723000
H	5.42155100	-0.61892500	0.17948300
C	4.46670800	-2.49995500	0.14968900
H	5.31672000	-3.16690300	0.19648900
C	-2.67032900	0.76939600	0.02162200
C	-4.72100100	-0.77894400	0.13485000
C	-4.81298300	-2.14968500	0.18311300
H	-5.54968900	-0.08782100	0.14884700
H	-3.28558900	-3.59614000	0.17068800
H	-5.66547000	-2.81198500	0.24092300
C	-3.33916300	-0.51103100	0.07050500
N	-2.62858600	-1.67045100	0.07770600
N	2.47959700	-1.74394700	0.04893900
N	1.41183000	0.71245200	0.00310300
C	2.93559100	3.04834600	0.03960900
H	3.52541700	3.96021100	0.04929500
N	-3.55085400	-2.62051200	0.14574100
C	-0.57516400	4.36739700	-0.01360900
H	-1.08912600	5.32425100	-0.01883700
C	0.82009700	4.34189000	-0.00162300
H	1.37044900	5.27839600	0.00263900
N	3.20642900	-2.86916600	0.09273300
N	4.55933500	-1.14665200	0.14120300
Eu	-0.02450900	-1.49029600	-0.14518400

EuR₁PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.74334300	1.89287500	0.00018400
C	-2.71054300	0.68482200	-0.00126100
C	-3.49658200	1.84690400	-0.00177400
H	-4.57744800	1.76294800	-0.00270300
C	0.72206900	1.90334800	0.00037200
C	1.40674700	3.15372700	0.00031500
C	2.82417500	3.12194000	0.00005000
C	3.47117700	1.91558600	-0.00063000
H	3.38666500	4.05090200	0.00018600
H	4.55333600	1.87689700	-0.00111900
N	1.35836900	0.73655800	0.00013900
C	-1.45106900	3.12079700	-0.00025400

C	-3.31713400	-0.63469000	-0.00229700
H	-5.66486100	-2.55420300	-0.00611300
H	-3.41853700	-3.80591300	-0.00400200
C	2.71712400	0.72473700	-0.00078300
C	4.73935600	-0.86406700	-0.00420800
C	4.80555400	-2.23746700	-0.00561000
H	5.58134300	-0.18904700	-0.00464900
H	3.25129700	-3.65252400	-0.00523300
H	5.64619900	-2.91709100	-0.00733100
C	3.36182200	-0.56882900	-0.00228000
N	2.62829500	-1.71215200	-0.00246000
N	-2.59962600	-1.80658000	-0.00197900
N	-1.36058400	0.71222700	-0.00002600
C	-2.86564500	3.06747000	-0.00110800
H	-3.44379500	3.98686200	-0.00140500
N	3.53423300	-2.68204100	-0.00446300
C	0.67087700	4.34627100	0.00036100
H	1.19169300	5.29951400	0.00050000
C	-0.73106000	4.33269500	0.00003800
H	-1.27042700	5.27580500	-0.00010100
N	-4.62206200	-0.81270700	-0.00396700
C	-3.54748000	-2.73247800	-0.00357900
N	-4.74349200	-2.13023400	-0.00475600
Eu	0.00416400	-1.48748400	0.00459300

EuR₁PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.77368600	1.88962200	0.00408500
C	-2.73543200	0.66458500	-0.02490000
C	-3.52130300	1.82602800	-0.03231300
H	-4.60398200	1.77432400	-0.04821900
C	0.69280600	1.90975000	0.00706500
C	1.36663900	3.16609900	0.00482400
C	2.78436500	3.14639800	-0.00192700
C	3.44155500	1.94627300	-0.01533400
H	3.33872100	4.08024600	-0.00039000
H	4.52400700	1.91728100	-0.02595800
N	1.33895600	0.74825000	0.00255300
C	-1.48653800	3.11588900	-0.00322500
C	-3.28970100	-0.67570700	-0.04669700
H	-5.42183800	-0.47041300	-0.10997400
H	-3.24098000	-3.84481900	-0.07377700
C	2.69823200	0.74787700	-0.01674400
C	4.73723500	-0.81744700	-0.08525000
C	4.81832100	-2.18942200	-0.11235500

H	5.57176800	-0.13322300	-0.09524300
H	3.27956500	-3.62245100	-0.10200400
H	5.66584600	-2.85970700	-0.14698700
C	3.35633300	-0.53755000	-0.04572200
N	2.63576000	-1.69041600	-0.04772100
N	-2.55002000	-1.79621900	-0.03456700
N	-1.38383900	0.70739600	-0.00080800
C	-2.89718400	3.05183800	-0.01853700
H	-3.48343400	3.96606700	-0.02254700
N	3.55159100	-2.64854700	-0.08800500
C	0.62313600	4.35543400	0.00663900
H	1.13985600	5.31090000	0.00862600
C	-0.77474600	4.33476200	0.00227900
H	-1.32090800	5.27385500	0.00077000
N	-4.71700800	-2.35325700	-0.10458000
N	-4.58331600	-1.03783100	-0.08852600
C	-3.47065500	-2.78876500	-0.07111300
Eu	0.01730500	-1.48843900	0.09274000

EuR₂PhR₂³⁺(PBE0/6-311G*-RECP)

C	0.73296900	1.90239600	0.00154800
C	2.72115100	0.70653000	-0.00687400
C	3.48144900	1.89575000	-0.00792400
H	4.56399600	1.85586800	-0.01208600
C	-0.73294800	1.90239900	0.00160500
C	-1.42389200	3.14440600	0.00002200
C	-2.84026000	3.10273900	-0.00340600
C	-3.48142800	1.89576500	-0.00759500
H	-3.40724100	4.02870900	-0.00385000
H	-4.56397600	1.85588900	-0.01166700
N	-1.36442500	0.72875000	0.00025900
C	1.42392000	3.14440200	-0.00005800
C	3.33814400	-0.59279800	-0.01485000
C	4.68901800	-0.91570600	-0.02930400
H	5.58334300	-0.31052900	-0.03641900
H	5.58528200	-2.82197500	-0.04583600
H	3.25860700	-3.80357400	-0.02590800
C	-2.72113600	0.70654100	-0.00668400
C	-4.68902900	-0.91567000	-0.02812300
H	-5.58336100	-0.31048600	-0.03350000
H	-3.25863200	-3.80354700	-0.02889900
H	-5.58532600	-2.82192000	-0.04504300
C	-3.33813700	-0.59278300	-0.01484000
N	-2.59653400	-1.76615000	-0.01366600

N	2.59653700	-1.76615700	-0.01174900
N	1.36444100	0.72874600	0.00022400
C	2.84028700	3.10272800	-0.00362900
H	3.40727200	4.02869500	-0.00400900
C	3.47433500	-2.74415900	-0.02422100
C	-3.47435700	-2.74413400	-0.02573900
N	4.74057200	-2.26277400	-0.03494100
N	-4.74059800	-2.26273300	-0.03479900
C	0.69728700	4.34628200	0.00103500
H	1.23012800	5.29253900	0.00103900
C	-0.69725400	4.34628400	0.00103600
H	-1.23009200	5.29254200	0.00095600
Eu	-0.00001100	-1.46707700	0.03041100

EuR₂PhR₃³⁺(PBE0/6-311G*-RECP)

C	-0.68104400	1.91057900	-0.00006000
C	-2.69585000	0.76053400	0.00005600
C	-3.42567200	1.96848900	0.00008600
H	-4.50890900	1.95538800	0.00017600
C	0.78291000	1.87784800	-0.00005600
C	1.50474500	3.10669700	-0.00005500
C	2.91733700	3.03083800	-0.00000600
C	3.53289700	1.80797300	0.00007500
H	3.50654600	3.94281400	-0.00001900
H	4.61545500	1.75591900	0.00012800
N	1.38698400	0.69288100	-0.00001300
C	-1.33903200	3.16679500	-0.00005700
C	-3.34806200	-0.52373800	0.00022000
C	-4.70488400	-0.81211100	0.00061900
H	-5.58403700	-0.18519700	0.00079000
H	-5.64928300	-2.69614200	0.00018100
H	-3.34897000	-3.73647800	0.00046600
C	2.74212600	0.64145100	0.00008500
H	5.40658700	-0.37289000	0.00049000
H	3.12504500	-3.87495100	0.00028300
H	5.69014500	-2.85755900	0.00084000
C	3.29700400	-0.68328800	0.00022800
N	2.56044500	-1.81126900	0.00022100
N	-2.63596400	-1.71559800	0.00022900
N	-1.34103000	0.74996000	-0.00003200
C	-2.75517400	3.15991800	0.00000200
H	-3.29995100	4.09910800	0.00001000
C	-3.53843200	-2.67210000	0.00045500

C	3.43140200	-2.83861600	0.00031900
N	-4.79057100	-2.15873100	0.00026000
C	-0.58226100	4.35489600	-0.00008800
H	-1.09616600	5.31160400	-0.00009900
C	0.80714500	4.32646300	-0.00009000
H	1.36200800	5.25973700	-0.00010400
N	4.62033100	-1.00888800	0.00042100
C	4.73600800	-2.34973700	0.00062300
Eu	-0.04614000	-1.47995500	-0.00039500

EuR₂PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.71811100	1.90386200	-0.00014100
C	-2.70839900	0.71238800	0.00030400
C	-3.47318300	1.90334100	0.00023900
H	-4.55570000	1.86171200	0.00046000
C	0.74818100	1.91066400	-0.00004200
C	1.42951600	3.14979700	0.00007100
C	2.84062000	3.12185600	0.00055800
C	3.49426300	1.91328600	0.00096400
H	3.40233000	4.05120600	0.00068000
H	4.57744900	1.87759100	0.00139800
N	1.38851700	0.73872900	0.00023800
C	-1.41702100	3.15280900	-0.00017400
C	-3.32726600	-0.57923300	0.00096300
C	-4.68983000	-0.89301700	0.00242500
H	-5.57864600	-0.27894200	0.00343800
H	-5.60141600	-2.78766500	0.00401100
H	-3.27910300	-3.78957000	0.00136300
C	2.74103600	0.72962300	0.00077400
C	4.67464700	-1.00585800	0.00191000
H	5.62469000	-0.49280800	0.00229900
H	5.32766200	-3.02721800	0.00279900
C	3.35776600	-0.58392300	0.00113200
N	2.58160600	-1.71027400	0.00071900
N	-2.59906900	-1.75934200	0.00045000
N	-1.34847200	0.73269300	-0.00014600
C	-2.83523600	3.10889500	-0.00010100
H	-3.40203300	4.03493200	-0.00025500
C	-3.48447200	-2.72760000	0.00159600
N	-4.75186100	-2.23407600	0.00284700
N	4.57803900	-2.34384600	0.00217100
C	-0.70041800	4.35530700	-0.00033300
H	-1.23665900	5.29941300	-0.00059400
C	0.69182400	4.35767100	-0.00010100

H	1.22395400	5.30465400	0.00007100
N	3.32610900	-2.76594000	0.00156900
Eu	0.02428400	-1.48949400	-0.00207700

EuR₂PhR₅³⁺(PBE0/6-311G*-RECP)

C	0.74286700	1.89471600	-0.00006300
C	2.72875600	0.69643200	0.00019700
C	3.49760500	1.88454800	0.00037800
H	4.58006300	1.83925300	0.00063300
C	-0.72185800	1.90096800	-0.00009400
C	-1.40344300	3.13874900	-0.00007600
C	-2.81410100	3.10924200	0.00002900
C	-3.46531700	1.89855300	0.00018300
H	-3.37838100	4.03711900	0.00003800
H	-4.54810500	1.86118900	0.00036000
N	-1.36074300	0.72699900	-0.00005100
C	1.44497300	3.14179500	0.00004600
C	3.33558100	-0.60008100	0.00033600
C	4.69358100	-0.93007600	0.00060800
H	5.58947000	-0.32618400	0.00067500
H	5.58249300	-2.83578700	0.00092200
H	3.25030300	-3.81015200	0.00070700
C	-2.71178900	0.71461300	0.00014500
C	-4.72304900	-0.92691700	0.00063800
H	-5.61224300	-0.31385200	0.00064200
H	-3.38589600	-3.65752400	0.00103500
C	-3.36015000	-0.58630800	0.00039100
N	-2.65244100	-1.73674800	0.00051300
N	2.59214300	-1.77171800	0.00032100
N	1.36903400	0.72210400	-0.00005400
C	2.86342700	3.09267800	0.00025900
H	3.43374400	4.01662500	0.00037800
C	3.46693100	-2.75045600	0.00061300
N	4.73945000	-2.27199800	0.00074400
C	0.72917500	4.34446500	-0.00003200
H	1.26499900	5.28887700	0.00000300
C	-0.66428900	4.34683600	-0.00010900
H	-1.19602000	5.29414300	-0.00015600
N	-3.58842000	-2.66598700	0.00082200
N	-4.82138700	-2.24824600	0.00086300
Eu	-0.02154400	-1.47449400	-0.00076300

EuR₂PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.77763400	1.90275300	0.00827600
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C	2.74741800	0.69358300	-0.06232000
C	3.52179300	1.85886000	-0.08323800
H	4.60427000	1.81582800	-0.12428500
C	-0.68731700	1.91227500	0.01872300
C	-1.36916100	3.16990300	0.01637000
C	-2.78746700	3.14233200	0.00566300
C	-3.43854900	1.94372400	-0.02242200
H	-3.34445900	4.07427800	0.01148700
H	-4.52141700	1.91516500	-0.04137900
N	-1.32877200	0.74726700	0.01112600
C	1.47768700	3.13235500	-0.00920800
C	3.29553000	-0.65342800	-0.10472100
H	5.42511700	-0.53814800	-0.22539200
H	5.37332900	-3.08843400	-0.25123600
C	-2.68763800	0.74278500	-0.02771200
C	-4.68499600	-0.83684500	-0.18105700
H	-5.56521700	-0.21121800	-0.21445400
H	-3.30677800	-3.74879200	-0.20640300
H	-5.61478300	-2.71726000	-0.31077100
C	-3.31949300	-0.54049500	-0.08799800
N	-2.60604500	-1.72930000	-0.08857800
N	2.50982900	-1.72177100	-0.07469000
N	1.39856600	0.72442300	-0.00578000
C	2.88462800	3.08090300	-0.04976700
H	3.46268200	4.00013900	-0.06151000
C	-3.50018500	-2.68480400	-0.17892600
N	-4.76098700	-2.17477200	-0.23713200
C	0.75334100	4.35224100	0.00620900
H	1.29710300	5.29250200	0.00147700
C	-0.63516300	4.36505200	0.02006900
H	-1.16093100	5.31498800	0.02724800
N	3.26091400	-2.83530200	-0.12783900
C	4.50965800	-2.44057400	-0.19400300
N	4.57498500	-1.08390700	-0.18165200
Eu	0.01373600	-1.49903600	0.18862500

EuR₂PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.74271600	1.89545600	-0.00004000
C	-2.72981600	0.70297000	-0.00003300
C	-3.49569700	1.89400500	-0.00001900
H	-4.57824800	1.85151600	-0.00000400
C	0.71976600	1.89722800	-0.00003000
C	1.41124400	3.12799800	0.00002700
C	2.82305000	3.09068200	0.00006200

C	3.46856500	1.87594200	0.00005000
H	3.39187600	4.01576800	0.00010700
H	4.55033000	1.80501000	0.00008700
N	1.35105800	0.71881500	-0.00005500
C	-1.44014500	3.14574900	-0.00000900
C	-3.34118100	-0.59131100	-0.00000200
C	-4.70132900	-0.91428800	-0.00001100
H	-5.59391200	-0.30561600	-0.00006400
H	-5.60008400	-2.81510700	0.00006100
H	-3.27209200	-3.80093900	0.00017800
C	2.69725200	0.70523100	-0.00000800
H	3.46702400	-3.77847700	0.00010800
H	5.69592600	-2.49816100	-0.00000900
C	3.32486000	-0.60863300	-0.00000400
N	2.62282900	-1.78930900	0.00004600
N	-2.60382600	-1.76653500	0.00006000
N	-1.37077600	0.72399800	-0.00005700
C	-2.85884500	3.10061000	-0.00000700
H	-3.42689600	4.02590800	0.00001400
C	-3.48345400	-2.74021900	0.00011300
C	3.58339400	-2.70375800	0.00006300
N	-4.75431800	-2.25571400	0.00005500
N	4.76931600	-2.08714000	0.00000500
C	-0.71775000	4.34431200	0.00002300
H	-1.24853000	5.29151400	0.00004100
C	0.67585500	4.34008700	0.00004200
H	1.21154300	5.28515200	0.00007200
N	4.62988100	-0.76856600	-0.00004000
Eu	0.02754900	-1.49012300	-0.00003200

EuR₂PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.71800600	1.90101900	0.00001000
C	-2.71442900	0.72406000	-0.00026200
C	-3.47062200	1.92175300	-0.00027400
H	-4.55352600	1.88852000	-0.00044100
C	0.74657100	1.89536900	0.00010300
C	1.44135400	3.12589700	0.00000800
C	2.84966000	3.08075200	-0.00003100
C	3.49051700	1.86195000	0.00004900
H	3.42469400	4.00196300	-0.00021200
H	4.57390200	1.82500100	-0.00004000
N	1.37297100	0.71668400	0.00021400
C	-1.40590600	3.15664500	0.00007200

C	-3.33991800	-0.56271900	-0.00014100
C	-4.70730800	-0.86832100	-0.00029400
H	-5.59191400	-0.24783800	-0.00109100
H	-5.63071800	-2.75599200	-0.00107700
H	-3.31457200	-3.77275100	0.00158900
C	2.72132800	0.69066900	0.00022300
H	5.42753200	-0.39907900	0.00106800
H	3.30947600	-3.81296800	-0.00116400
C	3.30113100	-0.64391200	0.00012000
N	2.58199900	-1.77527600	-0.00105800
N	-2.61971200	-1.74736000	0.00089300
N	-1.35458200	0.73428400	-0.00011800
C	-2.82432900	3.12321000	-0.00005000
H	-3.38502200	4.05297300	0.00008300
C	-3.51183900	-2.70912900	0.00084100
C	3.52299400	-2.75366400	-0.00071800
N	-4.77757100	-2.20724800	-0.00033300
C	-0.67692300	4.35358000	0.00009700
H	-1.20521100	5.30217400	0.00014900
C	0.71255100	4.34398700	-0.00000200
H	1.25404900	5.28566300	-0.00008400
N	4.75830200	-2.29782200	0.00024300
N	4.59975100	-0.98144600	0.00026900
Eu	0.02003600	-1.49694100	0.00003100

EuR₃PhR₃³⁺(PBE0/6-311G*-RECP)

C	0.00000600	0.73162000	-1.88876200
C	0.00002700	2.71739500	-0.69634200
C	0.00007500	3.47887100	-1.88177600
H	0.00010300	4.56241700	-1.85610300
C	-0.00000600	-0.73162000	-1.88876200
C	-0.00003200	-1.42099400	-3.13229100
C	-0.00007400	-2.83420200	-3.09027700
C	-0.00007500	-3.47887100	-1.88177600
H	-0.00010500	-3.40224000	-4.01559100
H	-0.00010300	-4.56241700	-1.85610300
N	0.00000600	-1.36344000	-0.71605400
C	0.00003200	1.42099400	-3.13229100
C	-0.00000600	3.30601900	0.61650000
H	-0.00000700	5.40593700	0.25604400
H	0.00039400	5.74888600	2.73375900
H	-0.00033300	3.20996600	3.81202300
C	-0.00002700	-2.71739500	-0.69634200

H	0.00000700	-5.40593700	0.25604400
H	0.00033300	-3.20996600	3.81202300
H	-0.00039400	-5.74888600	2.73375900
C	0.00000600	-3.30601900	0.61650000
N	0.00018200	-2.59627400	1.76073800
N	-0.00018200	2.59627400	1.76073800
N	-0.00000600	1.36344000	-0.71605400
C	0.00007400	2.83420200	-3.09027700
H	0.00010500	3.40224000	-4.01559100
C	-0.00023500	3.49254500	2.76904200
C	0.00023500	-3.49254500	2.76904200
C	0.00019300	4.78259000	2.24976000
C	-0.00019300	-4.78259000	2.24976000
N	-0.00003500	4.63488100	0.91019700
N	0.00003500	-4.63488100	0.91019700
C	0.00002100	0.69263700	-4.33883800
C	-0.00002100	-0.69263700	-4.33883800
H	0.00003700	1.22851500	-5.28318600
H	-0.00003700	-1.22851500	-5.28318600
Eu	0.00000000	0.00000000	1.49291400

EuR₃PhR₄³⁺(PBE0/6-311G*-RECP)

C	0.76556000	1.87928000	0.01179600
C	2.72659700	0.64695400	-0.02722200
C	3.52020800	1.81500500	-0.02518700
H	4.60275500	1.76277400	-0.04047200
C	-0.69713100	1.91791300	0.00720300
C	-1.34810900	3.17161300	-0.00349000
C	-2.75913500	3.17530700	-0.02985700
C	-3.43979200	1.98239400	-0.05413600
H	-3.29966600	4.11708000	-0.03618800
H	-4.52319600	1.97158200	-0.08192400
N	-1.36489000	0.75874200	-0.00245600
C	1.49296700	3.11325400	0.00932000
C	3.28514900	-0.67009800	-0.07191600
H	5.39533600	-0.34633500	-0.15954500
H	5.69149500	-2.82698200	-0.23199200
H	3.12965400	-3.86301300	-0.14338500
C	-2.71436300	0.78086400	-0.04236700
H	-5.62257400	-0.37976900	-0.17911300
H	-5.37818000	-2.92004700	-0.19755700
C	-3.36098500	-0.51884700	-0.07780900
N	-2.60919900	-1.66131100	-0.05789700
N	2.55536900	-1.80723500	-0.06764900

N	1.36976400	0.69554600	0.00376000
C	2.90664500	3.03643900	-0.00212300
H	3.49548400	3.94861100	0.00151500
C	3.42704900	-2.82355500	-0.13020800
C	4.73618100	-2.32296700	-0.17581300
N	4.61313300	-0.98793400	-0.13711100
C	0.80312400	4.33495900	0.01427000
C	-0.58260400	4.36559900	0.00728700
H	1.36167400	5.26579700	0.01863700
H	-1.09651900	5.32250700	0.00608400
N	-3.37467200	-2.70172100	-0.10355600
C	-4.68429900	-0.91269300	-0.14167500
N	-4.61524900	-2.25293500	-0.15449200
Eu	-0.06727700	-1.49496500	0.14398900

EuR₃PhR₅³⁺(PBE0/6-311G*-RECP)

C	0.78921500	1.86960200	0.00022600
C	2.74880600	0.63453700	-0.00093200
C	3.54403700	1.80128200	-0.00101200
H	4.62663900	1.74719500	-0.00155300
C	-0.67256700	1.90622700	0.00021100
C	-1.32488900	3.15825700	0.00003100
C	-2.73573000	3.16005900	-0.00052000
C	-3.41394200	1.96490800	-0.00116900
H	-3.27902200	4.10033400	-0.00058800
H	-4.49731600	1.95212300	-0.00181300
N	-1.33883700	0.74484000	-0.00006100
C	1.51787300	3.10306700	0.00007800
C	3.30044200	-0.68546900	-0.00208800
H	5.41477400	-0.37987900	-0.00449100
H	5.69248700	-2.86391900	-0.00627300
H	3.12183000	-3.87838200	-0.00389300
C	-2.68774300	0.76323000	-0.00102000
H	-5.61251400	-0.19611900	-0.00472600
H	-3.46784900	-3.59297300	-0.00399200
C	-3.36811000	-0.52241600	-0.00214900
N	-2.68824200	-1.68955000	-0.00195400
N	2.56055400	-1.81662600	-0.00191000
N	1.39156400	0.68574500	0.00001200
C	2.93179800	3.02403600	-0.00037200
H	3.52209400	3.93534000	-0.00036700
C	3.42593600	-2.84081600	-0.00355500
C	4.73999800	-2.35132300	-0.00480100

N	4.62668200	-1.01500100	-0.00383100
C	0.82755300	4.32403200	0.00028800
C	-0.55935900	4.35318500	0.00026000
H	1.38471200	5.25578500	0.00035300
H	-1.07402400	5.30978900	0.00030000
N	-4.86823600	-2.14911600	-0.00482800
N	-3.64646800	-2.59686800	-0.00357700
C	-4.73820600	-0.83019800	-0.00396500
Eu	-0.06415200	-1.48454700	0.00417500

EuR₃PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.73510600	1.88731900	-0.00029900
C	2.71169500	0.68224200	0.00054200
C	3.48781400	1.86255900	0.00060400
H	4.57116100	1.82685800	0.00118700
C	-0.72767400	1.90901100	-0.00021100
C	-1.39739900	3.15460200	0.00008100
C	-2.80558600	3.13744600	0.00063300
C	-3.47286400	1.93222200	0.00111500
H	-3.36079800	4.07067300	0.00079900
H	-4.55683600	1.91543500	0.00162100
N	-1.37878500	0.74388100	-0.00002500
C	1.44318200	3.13156100	-0.00022100
C	3.29577500	-0.62490000	0.00158900
H	5.40181800	-0.25870900	0.00181200
H	5.75077800	-2.73315100	0.00415500
H	3.20762200	-3.82155600	0.00454500
C	-2.72736900	0.74749700	0.00086500
H	-5.44434100	-0.40687900	0.00461100
H	-5.46833100	-2.95820100	0.00470300
C	-3.31616900	-0.58400500	0.00159700
N	-2.56160300	-1.67427000	0.00080300
N	2.58958200	-1.77779900	0.00239600
N	1.35456700	0.71055900	-0.00010800
C	2.85706900	3.07565300	0.00009000
H	3.43316700	3.99591100	0.00010700
C	3.48266900	-2.77573000	0.00348200
C	4.78395700	-2.24792100	0.00338400
C	-4.58410400	-2.33606900	0.00350300
N	4.63220600	-0.91587300	0.00236100
C	0.73537600	4.34650400	-0.00027900
C	-0.64639800	4.36135100	-0.00014500
H	1.28377500	5.28334700	-0.00030700
H	-1.17316000	5.31113900	-0.00013700

N	-3.34666200	-2.76697200	0.00186500
N	-4.60928000	-0.97710900	0.00339500
Eu	-0.05611900	-1.51710900	-0.00310900

EuR₃PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.78739500	1.87086900	-0.00003700
C	-2.74937700	0.64295700	-0.00006400
C	-3.54072900	1.81318000	-0.00018900
H	-4.62350500	1.76284900	-0.00024800
C	0.67239400	1.90196600	-0.00007000
C	1.33568200	3.14702700	-0.00036500
C	2.74793000	3.14029200	-0.00054200
C	3.41983200	1.94072900	-0.00047600
H	3.29626800	4.07762300	-0.00074400
H	4.50291300	1.89375100	-0.00065100
N	1.33044100	0.73568700	0.00010000
C	-1.51049100	3.10787100	-0.00023800
C	-3.30672300	-0.67457200	-0.00016200
H	-5.41924300	-0.35581800	-0.00055500
H	-5.71214900	-2.83820800	-0.00067800
H	-3.14710900	-3.86768200	-0.00037400
C	2.67479400	0.75225400	-0.00016000
H	3.54842900	-3.71352800	0.00062600
H	5.74690500	-2.38249900	-0.00086000
C	3.33384800	-0.54693500	-0.00015400
N	2.65897300	-1.74370000	-0.00001500
N	-2.57368600	-1.81007000	-0.00009900
N	-1.39262700	0.68852500	0.00009800
C	-2.92477100	3.03399800	-0.00025500
H	-3.51213400	3.94714600	-0.00035500
C	-3.44526400	-2.82842300	-0.00033100
C	3.64043300	-2.63643900	0.00030400
C	-4.75665800	-2.33140300	-0.00048100
N	-4.63540000	-0.99594200	-0.00042800
C	-0.81255300	4.32447800	-0.00041500
C	0.57474300	4.34626600	-0.00049100
H	-1.36420000	5.25946600	-0.00052500
H	1.09394800	5.30040700	-0.00065300
N	4.64160900	-0.67721400	-0.00067500
N	4.81111900	-1.99283700	-0.00054400
Eu	0.06845600	-1.50062400	0.00064600

EuR₃PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.76440600	1.87673300	-0.00841500
C	-2.73399200	0.66160300	0.02156500
C	-3.51705000	1.83757100	0.02215200
H	-4.60015800	1.79554200	0.03483100
C	0.69719100	1.90144000	-0.00645900
C	1.36325900	3.14661600	0.00013500
C	2.77229100	3.13182200	0.01716900
C	3.43966100	1.92819900	0.03477200
H	3.32689000	4.06543500	0.02018000
H	4.52348200	1.91534700	0.05260400
N	1.35061300	0.73498000	0.00085500
C	-1.47874500	3.11810400	-0.00521400
C	-3.30343100	-0.65038500	0.05352100
H	-5.41287600	-0.30951400	0.12081700
H	-5.73013000	-2.78795300	0.17178000
H	-3.17527000	-3.84510200	0.10211300
C	2.69684300	0.73923600	0.02847900
H	5.42520900	-0.29043100	0.13112100
H	3.38464800	-3.75100700	0.09250800
C	3.30708300	-0.58237300	0.05639900
N	2.61300300	-1.72936300	0.04365000
N	-2.58222600	-1.79447900	0.04815800
N	-1.37712300	0.69789600	-0.00247500
C	-2.89285900	3.05416300	0.00518700
H	-3.47409000	3.97123300	0.00389400
C	-3.46216100	-2.80249200	0.09404700
C	3.57527400	-2.68735100	0.08797800
C	-4.77029300	-2.29058900	0.12990600
N	-4.63559500	-0.95767300	0.10277900
N	4.61095800	-0.89096300	0.10614100
C	-0.77485100	4.33409700	-0.00972200
C	0.60838300	4.35150900	-0.00690100
H	-1.32454300	5.27022300	-0.01201100
H	1.13264100	5.30277700	-0.00709700
N	4.79847700	-2.20444500	0.12691200
Eu	0.06197200	-1.50374000	-0.10762700

EuR₄PhR₄³⁺(PBE0/6-311G*-RECP)

C	-0.73523100	1.91802100	0.00006100
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C	-2.73012500	0.74029000	0.00084400
C	-3.48928100	1.92348900	0.00117000
H	-4.57226100	1.88307500	0.00195600
C	0.73522300	1.91802200	-0.00024300
C	1.42562300	3.16274700	-0.00029100
C	2.84122800	3.13089200	-0.00077900
C	3.48927200	1.92349600	-0.00114900
H	3.40357300	4.05994500	-0.00085300
H	4.57225300	1.88308400	-0.00183600
N	1.37132100	0.74941000	-0.00046800
C	-1.42563300	3.16274500	0.00004800
C	-3.34493400	-0.56694500	0.00099900
H	-5.61559000	-0.46511800	-0.00023200
H	-5.33117400	-3.00021900	-0.00025200
C	2.73012000	0.74029500	-0.00076100
H	5.61558800	-0.46509400	0.00093200
H	5.33119000	-3.00019700	0.00127900
C	3.34493300	-0.56693800	-0.00066300
N	2.57505300	-1.69976400	-0.00113000
N	-2.57504600	-1.69976500	0.00151200
N	-1.37132700	0.74940800	0.00040300
C	-2.84123900	3.13088700	0.00061700
H	-3.40358500	4.05993900	0.00063200
N	-3.32461700	-2.74782200	0.00092400
N	3.32463200	-2.74781500	-0.00027100
N	-4.57875300	-2.31887800	0.00013000
N	4.57876500	-2.31886200	0.00066800
C	-4.66827600	-0.98396000	0.00022000
C	4.66827800	-0.98394400	0.00039600
C	-0.70001900	4.36521300	-0.00005400
H	-1.23149500	5.31262200	0.00013900
C	0.70000600	4.36521400	-0.00030600
H	1.23148000	5.31262400	-0.00057300
Eu	0.00000200	-1.51776500	-0.00022600

EuR₄PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.70580400	1.90796800	-0.00719300
C	-2.69901400	0.72669700	0.01658500
C	-3.45705200	1.91083700	0.01499300
H	-4.53961000	1.86997300	0.02579400
C	0.76366100	1.90738300	-0.00397300
C	1.45874300	3.14943300	0.00299100
C	2.87455200	3.11045400	0.01867000
C	3.51761300	1.89954500	0.03311800

H	3.44157100	4.03674500	0.02241500
H	4.60037200	1.85444900	0.04980400
N	1.39438200	0.73722000	0.00094600
C	-1.39510000	3.15197400	-0.00581600
C	-3.34661700	-0.56771800	0.04508200
H	-5.60117400	-0.28690200	0.09576300
C	2.75296400	0.72035800	0.02573100
H	5.62196800	-0.53161600	0.11176600
H	5.29312900	-3.06158300	0.12155100
C	3.35104700	-0.59403100	0.04729200
N	2.56127200	-1.71346400	0.03390300
N	-2.64471400	-1.72418900	0.04799700
N	-1.34163500	0.73803500	-0.00220700
C	-2.81030100	3.11980400	0.00105900
H	-3.37445300	4.04786200	-0.00075200
N	3.29217700	-2.77455500	0.06187200
N	4.55270400	-2.36743600	0.09471600
C	-4.71421400	-0.90353300	0.08394100
C	4.66598600	-1.03400800	0.08768200
C	-0.66680900	4.35370400	-0.00826100
H	-1.19681000	5.30207300	-0.01112500
C	0.73508100	4.35267900	-0.00336500
H	1.26664600	5.30013600	-0.00216500
N	-3.58318600	-2.64474000	0.08647900
H	-3.38509800	-3.63823600	0.10160200
N	-4.81708800	-2.22258500	0.10960000
Eu	0.00043900	-1.49778100	-0.08950800

EuR₄PhR₆³⁺(PBE0/6-311G*-RECP)

C	-0.76579900	1.90895000	-0.01332600
C	-2.73610100	0.69923500	0.05585900
C	-3.51746900	1.86251500	0.07060200
H	-4.59978200	1.81372100	0.10888800
C	0.70152100	1.92687200	-0.01797100
C	1.37470900	3.18035700	-0.01052200
C	2.79104300	3.16409300	0.00888000
C	3.45214500	1.96439500	0.03810600
H	3.34332000	4.09916000	0.00866600
H	4.53528100	1.93656600	0.06421500
N	1.34997700	0.76426600	-0.00965200
C	-1.47590700	3.14178900	-0.00099300
C	-3.28058900	-0.64223000	0.10262900
H	-5.41308500	-0.53177900	0.21238100
C	2.70692800	0.77102200	0.03625000

H	5.59806300	-0.40871000	0.23520300
H	5.33082000	-2.94527300	0.28851200
C	3.33243200	-0.52932200	0.09378000
N	2.57153500	-1.66901400	0.07843100
N	-2.49267200	-1.71517600	0.08274400
N	-1.38155900	0.73191800	0.00211500
C	-2.88701400	3.08436800	0.03445800
H	-3.46728700	4.00236700	0.04089200
N	3.32689000	-2.71005600	0.15411000
N	4.57531200	-2.27037700	0.22160300
C	4.65618000	-0.93539400	0.18789200
C	-0.76423900	4.35761600	-0.01342200
H	-1.30846100	5.29765200	-0.01125500
C	0.63159100	4.37418500	-0.01969500
H	1.15170300	5.32780300	-0.02586300
N	-3.23990700	-2.82346200	0.13634100
H	-5.35636500	-3.08034900	0.25082200
C	-4.49453800	-2.42925500	0.19446300
N	-4.56083700	-1.07579400	0.17560100
Eu	0.01262300	-1.51638800	-0.18322900

EuR₄PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.70216000	1.90555300	0.00012700
C	-2.68334200	0.71947300	-0.00035400
C	-3.45873500	1.89006400	-0.00042000
H	-4.54028500	1.81574100	-0.00069800
C	0.76552300	1.90864100	0.00010600
C	1.45695300	3.15353300	0.00006300
C	2.87336800	3.11734700	-0.00017000
C	3.51817200	1.90764800	-0.00049200
H	3.43875800	4.04459600	-0.00015000
H	4.60110100	1.86446000	-0.00071600
N	1.39701400	0.73946300	-0.00007600
C	-1.40067600	3.14240000	0.00004100
C	-3.31086200	-0.58887900	-0.00089400
C	2.75555900	0.72612200	-0.00049000
H	5.62911400	-0.51027000	-0.00266800
H	5.31567400	-3.04211400	-0.00294200
C	3.35754900	-0.58618900	-0.00097600
N	2.57377700	-1.71029800	-0.00051800
N	-2.61872900	-1.77528800	-0.00051900
N	-1.33084300	0.73144400	0.00007200
C	-2.81704000	3.10303300	-0.00015800
H	-3.38537800	4.02852500	-0.00017100

N	3.31149500	-2.76642900	-0.00132100
N	4.57106300	-2.35221900	-0.00221200
C	4.67603600	-1.01860500	-0.00205000
C	-0.67520400	4.34737400	0.00014300
H	-1.20827700	5.29404300	0.00019100
C	0.72762900	4.35229400	0.00013900
H	1.25418300	5.30249700	0.00012700
H	-5.69865100	-2.45974900	-0.00310200
C	-3.58408800	-2.68151200	-0.00149600
H	-3.47637200	-3.75746400	-0.00151100
N	-4.76880400	-2.05413900	-0.00230700
N	-4.62088400	-0.74095500	-0.00203600
Eu	-0.00826300	-1.51541400	0.00183100

EuR₄PhR₈³⁺(PBE0/6-311G*-RECP)

C	0.73454800	1.90125200	-0.00025500
C	2.71078300	0.69792600	0.00064800
C	3.48612200	1.86788800	0.00088200
H	4.56929100	1.82626700	0.00153900
C	-0.73416300	1.91522500	-0.00024400
C	-1.41330200	3.16692300	0.00000200
C	-2.83012900	3.14495200	0.00034200
C	-3.48684100	1.94251700	0.00067100
H	-3.38591600	4.07799700	0.00046700
H	-4.57019000	1.91040400	0.00106900
N	-1.37749300	0.75189700	-0.00021400
C	1.43885900	3.13633500	-0.00010600
C	3.28822500	-0.63047500	0.00135500
C	-2.73663500	0.75243000	0.00051200
H	-5.62706800	-0.44424500	0.00301200
H	-5.34833000	-2.97987800	0.00391100
C	-3.35570300	-0.55105300	0.00129000
N	-2.58801500	-1.68645600	0.00131600
N	2.57416500	-1.76793900	0.00177100
N	1.35609100	0.72512600	-0.00005400
C	2.85146100	3.08606800	0.00037200
H	3.42800500	4.00645300	0.00047400
N	-3.34022100	-2.73185300	0.00222300
N	-4.59427100	-2.29993300	0.00306700
C	-4.68092100	-0.96556900	0.00248700
C	0.72296800	4.34891200	-0.00015700
H	1.26380000	5.29105100	-0.00006100
C	-0.67568200	4.36195400	-0.00015900
H	-1.19763900	5.31468300	-0.00022500

C	3.51454400	-2.73940200	0.00263100
H	3.30813100	-3.80040500	0.00323000
N	4.59198700	-0.96557600	0.00211300
H	5.41899600	-0.38082100	0.00200500
N	4.75404200	-2.27557300	0.00280000
Eu	-0.00790300	-1.51880400	-0.00266900

EuR₅PhR₅³⁺(PBE0/6-311G*-RECP)

C	-0.73412400	1.89721400	0.00030700
C	-2.72271100	0.70806300	-0.00095100
C	-3.48557800	1.88864500	-0.00102300
H	-4.56811300	1.84346900	-0.00166300
C	0.73431000	1.89717700	0.00026200
C	1.42803700	3.13868800	-0.00014700
C	2.84340700	3.10059000	-0.00073300
C	3.48576800	1.88848400	-0.00130900
H	3.41155900	4.02628800	-0.00095300
H	4.56830100	1.84324700	-0.00207600
N	1.36539600	0.72557300	0.00014100
C	-1.42779000	3.13875300	0.00002900
C	-3.35798300	-0.59212700	-0.00242400
H	-5.61590100	-0.33885400	-0.00424900
C	2.72284100	0.70794300	-0.00103700
H	5.61595600	-0.33932500	-0.00373200
C	3.35800700	-0.59229300	-0.00238800
N	2.64069400	-1.73986100	-0.00307400
N	-2.64082700	-1.73980800	-0.00295900
N	-1.36526600	0.72563500	0.00013400
C	-2.84316000	3.10072200	-0.00040500
H	-3.41127100	4.02644500	-0.00047800
N	-4.80786200	-2.26546200	-0.00543500
N	4.80768200	-2.26582300	-0.00521500
C	-4.72134100	-0.94468900	-0.00403500
C	4.72131900	-0.94504500	-0.00373400
C	-0.70151700	4.34140400	0.00005300
H	-1.23185200	5.28969000	0.00002000
C	0.70182400	4.34137100	-0.00005700
H	1.23220100	5.28963300	-0.00019900
N	-3.56924000	-2.67253200	-0.00474300
H	-3.36100300	-3.66402700	-0.00595100
N	3.56899400	-2.67270000	-0.00467900
H	3.36063200	-3.66416700	-0.00598100

Eu	-0.00008500	-1.48296700	0.00494600
EuR ₅ PhR ₆ ³⁺ (PBE0/6-311G*-RECP)			
C	0.67468200	1.91475000	-0.00013000
C	2.68196400	0.75945300	0.00089400
C	3.42459500	1.95508700	0.00050400
H	4.50765000	1.92801000	0.00081600
C	-0.79393700	1.89783800	0.00003400
C	-1.50584200	3.13007600	0.00014600
C	-2.91744800	3.07138100	0.00086800
C	-3.54769800	1.84819000	0.00160700
H	-3.49883300	3.98878700	0.00094300
H	-4.63067100	1.79820500	0.00230600
N	-1.40822700	0.72172100	0.00039000
C	1.34713700	3.16920900	-0.00035900
C	3.34939800	-0.52372200	0.00213900
H	5.60068700	-0.20569300	0.00355900
C	-2.76483400	0.68648600	0.00134200
H	-5.44082300	-0.56487300	0.00520000
C	-3.30426500	-0.65755800	0.00223300
N	-2.50764300	-1.72390800	0.00133700
N	2.66758600	-1.69318900	0.00240500
N	1.32412900	0.75235500	0.00029500
C	2.76333700	3.15509100	-0.00019900
H	3.31558900	4.09026200	-0.00048100
N	4.84955900	-2.15390300	0.00474800
C	4.72409900	-0.83720000	0.00340300
C	0.60362300	4.36192100	-0.00062700
H	1.12323700	5.31600100	-0.00093300
C	-0.79486300	4.34554500	-0.00033900
H	-1.33841400	5.28614300	-0.00041200
N	3.62183000	-2.59679300	0.00431200
H	3.44116300	-3.59402300	0.00522700
N	-3.24703200	-2.83834600	0.00222600
N	-4.58304000	-1.10171600	0.00405500
C	-4.50677200	-2.45447200	0.00423600
H	-5.36501100	-3.11283800	0.00550900
Eu	0.01057500	-1.51469800	-0.00404200
EuR ₅ PhR ₇ ³⁺ (PBE0/6-311G*-RECP)			
C	0.73763000	1.89787400	-0.00010200

C	2.72607900	0.71233200	-0.00009600
C	3.48748500	1.89478600	-0.00039600
H	4.57003200	1.85087000	-0.00057100
C	-0.72913600	1.89517400	0.00002400
C	-1.43157100	3.12977300	0.00027300
C	-2.84814900	3.08490200	0.00049900
C	-3.48587000	1.86909300	0.00047100
H	-3.42015700	4.00821200	0.00071800
H	-4.56726100	1.79117800	0.00065400
N	-1.35359500	0.71989200	-0.00005900
C	1.42820200	3.14198300	-0.00020600
C	3.36355300	-0.58631300	0.00026600
H	5.62094500	-0.32591600	0.00060500
C	-2.70601700	0.70191200	0.00017900
C	-3.32009100	-0.61197000	0.00018200
N	-2.61154200	-1.78952600	0.00005600
N	2.65013200	-1.73629000	0.00048700
N	1.36873200	0.72696600	-0.00006200
C	2.84409300	3.10601300	-0.00043700
H	3.41105000	4.03239700	-0.00061400
N	4.81960900	-2.25494700	0.00094800
C	4.72854500	-0.93485700	0.00059300
C	0.69688000	4.34042000	-0.00004600
H	1.22270800	5.29116400	-0.00012300
C	-0.70754600	4.33526500	0.00023800
H	-1.24044700	5.28213000	0.00041800
N	3.58127100	-2.66525700	0.00083600
H	3.37557200	-3.65715700	0.00106900
C	-3.56577500	-2.70838400	0.00021400
H	-3.44536400	-3.78298600	0.00020200
N	-4.75816500	-2.09636100	0.00035700
H	-5.68287000	-2.51413000	0.00048300
N	-4.62740700	-0.78130800	0.00035900
Eu	-0.01011600	-1.49914200	-0.00052800

EuR₅PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.70734300	1.90434800	-0.00040900
C	-2.70766800	0.73766400	-0.00006200
C	-3.45751500	1.92838500	-0.00043500
H	-4.54045600	1.89493600	-0.00035500
C	0.76108700	1.89136900	-0.00027600
C	1.46863300	3.12455600	-0.00032200
C	2.88140900	3.06976700	-0.00006900
C	3.51275200	1.84903500	0.00028500

H	3.46110900	3.98825700	-0.00013200
H	4.59584800	1.80389600	0.00053900
N	1.37878800	0.71469500	-0.00008000
C	-1.38650000	3.15508000	-0.00066000
C	-3.36147700	-0.55205500	0.00049100
H	-5.61630600	-0.26123700	-0.00305800
C	2.73348900	0.68205000	0.00028600
H	5.43157700	-0.42926500	0.00249000
C	3.29813500	-0.65144200	0.00074700
N	2.56861400	-1.77979700	0.00016700
N	-2.66455000	-1.71259100	0.00273600
N	-1.34961000	0.73938900	-0.00015700
C	-2.80294000	3.13265700	-0.00072200
H	-3.36075200	4.06458600	-0.00089500
N	-4.84109600	-2.20045400	0.00068600
C	-4.73205700	-0.88206700	-0.00096000
C	-0.64751800	4.34966200	-0.00079700
H	-1.16892600	5.30286000	-0.00099000
C	0.75329600	4.33700300	-0.00064600
H	1.29323800	5.27978900	-0.00077700
N	-3.60821600	-2.62789400	0.00288200
H	-3.41631900	-3.62292700	0.00520600
N	4.59695800	-1.00358100	0.00159000
C	3.49674500	-2.76342500	0.00082300
H	3.27798300	-3.82196200	0.00059300
N	4.74195100	-2.31537700	0.00166900
Eu	-0.00527000	-1.50436800	-0.00083700

EuR₆PhR₆³⁺(PBE0/6-311G*-RECP)

C	0.73305200	1.91688200	0.01671500
C	2.71797100	0.73211300	-0.03599500
C	3.48366800	1.90684600	-0.04274200
H	4.56691800	1.87221000	-0.06955200
C	-0.73216300	1.91705600	0.01528400
C	-1.42425600	3.15986500	0.00484100
C	-2.83652500	3.12079300	-0.02390000
C	-3.48270800	1.90777400	-0.05550500
H	-3.40491300	4.04619400	-0.02839000
H	-4.56581700	1.87336900	-0.08761900
N	-1.36274100	0.74658700	0.00228000
C	1.42521900	3.15937900	0.00677900
C	3.28173900	-0.60105600	-0.08515700
H	5.41143200	-0.46117000	-0.20851600
H	5.38913300	-3.01047600	-0.26074000

C	-2.71718700	0.73278000	-0.04480200
H	-5.41192500	-0.45948100	-0.19407800
H	-5.39159600	-3.00898200	-0.23570400
C	-3.28127300	-0.60014100	-0.08958500
N	-2.50824400	-1.68562700	-0.07187700
N	2.50856200	-1.68588400	-0.06317100
N	1.36345800	0.74618600	0.00851100
C	2.83748900	3.12012600	-0.01551200
H	3.40609200	4.04540400	-0.01843200
N	3.26988500	-2.78312800	-0.13139900
N	-3.27109100	-2.78249000	-0.12615600
C	4.51888900	-2.37129800	-0.19615300
C	-4.52046900	-2.37006800	-0.18086100
N	4.56686600	-1.01701400	-0.16775300
N	-4.56728400	-1.01565300	-0.15966200
C	-0.69509500	4.36725400	0.01452300
H	-1.22856800	5.31336700	0.01433500
C	0.69609600	4.36704400	0.01641700
H	1.22982100	5.31301700	0.02018900
Eu	-0.00036700	-1.52343500	0.16201600

EuR₆PhR₇³⁺(PBE0/6-311G*-RECP)

C	-0.79565300	1.89983300	0.00919200
C	-2.76430200	0.68917300	-0.03608700
C	-3.54678000	1.85204600	-0.04589600
H	-4.62947900	1.80249400	-0.07091200
C	0.67013000	1.91321100	0.01299900
C	1.35255900	3.15956300	0.00804700
C	2.77004400	3.13597000	-0.00549200
C	3.42471800	1.93098900	-0.02487600
H	3.32799300	4.06775400	-0.00631900
H	4.50692900	1.86924500	-0.04463600
N	1.31099800	0.74543500	0.00733900
C	-1.50489000	3.13378900	0.00038500
C	-3.30120000	-0.65512900	-0.06727300
H	-5.43618200	-0.56095300	-0.14139300
H	-5.36105000	-3.10896700	-0.16827200
C	2.66305000	0.74972900	-0.02164400
H	5.71239700	-2.39140700	-0.19024900
C	3.30469600	-0.55008300	-0.05953400
N	2.62681300	-1.74547000	-0.05810200
N	-2.50450800	-1.72222200	-0.05361300
N	-1.40886800	0.72359100	-0.00054500
C	-2.91688000	3.07514400	-0.02279900

H	-3.49836800	3.99243600	-0.02746400
N	-3.24422200	-2.83555200	-0.09058900
C	-4.50338700	-2.45107300	-0.13000700
N	-4.57943600	-1.09870100	-0.11670900
C	0.61125500	4.35563300	0.01292600
H	1.13358900	5.30822800	0.01615800
C	-0.78806700	4.34508700	0.00841100
H	-1.32646300	5.28857000	0.00660500
C	3.60157800	-2.63936800	-0.11452600
H	3.50653300	-3.71644400	-0.13367300
N	4.77856200	-1.99696300	-0.14604900
N	4.61615600	-0.68679100	-0.11225700
Eu	0.01959400	-1.52224300	0.12080700

EuR₆PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.76397800	1.90668400	-0.01141500
C	-2.74296800	0.71249800	0.05022400
C	-3.51463600	1.88320700	0.06555800
H	-4.59751800	1.84334500	0.10016000
C	0.70164700	1.90964400	-0.01773500
C	1.39002600	3.15307300	-0.01191400
C	2.80365800	3.11711800	0.00231700
C	3.45065000	1.90604200	0.02693800
H	3.37095700	4.04322700	0.00089300
H	4.53411000	1.87613500	0.04654200
N	1.33483900	0.73873300	-0.01102500
C	-1.46194700	3.14658100	0.00188800
C	-3.29357000	-0.62561100	0.08947200
H	-5.42649000	-0.51156200	0.18891700
H	-5.37510600	-3.06029200	0.21891800
C	2.68816600	0.72631400	0.02677400
C	3.27619000	-0.59602700	0.07909200
N	2.57044100	-1.74010000	0.07190300
N	-2.50718600	-1.70160700	0.06862200
N	-1.38792500	0.73479100	0.00175700
C	-2.87440000	3.09997200	0.03486400
H	-3.44768900	4.02239900	0.04251200
N	-3.25646000	-2.80721900	0.11538400
C	-4.51177800	-2.41039700	0.16909800
N	-4.57485100	-1.05719800	0.15460400
C	0.65735600	4.35753300	-0.01752600
H	1.18761300	5.30557900	-0.02325300
C	-0.73689900	4.35483200	-0.00911400
H	-1.27121500	5.30057600	-0.00529400

C	3.51555600	-2.70331900	0.15430300
H	3.31688000	-3.76571500	0.17387200
N	4.57984300	-0.92066100	0.16125700
H	5.40159200	-0.32912300	0.19341800
N	4.75016500	-2.22861200	0.20935000
Eu	0.00391100	-1.51556100	-0.16089800

EuR₇PhR₇³⁺(PBE0/6-311G*-RECP)

C	0.73258000	1.89617600	-0.00013200
C	2.70880800	0.70577800	-0.00021800
C	3.48754600	1.87465900	-0.00031200
H	4.56893400	1.79764500	-0.00042400
C	-0.73258000	1.89617600	-0.00005000
C	-1.43217000	3.13304400	-0.00006300
C	-2.84927800	3.08988800	0.00010900
C	-3.48754600	1.87466000	0.00029400
H	-3.42047700	4.01364800	0.00003500
H	-4.56893400	1.79764600	0.00049200
N	-1.35652600	0.72131300	0.00006000
C	1.43217000	3.13304400	-0.00018100
C	3.32461700	-0.60703600	-0.00007700
C	-2.70880800	0.70577800	0.00025100
C	-3.32461700	-0.60703600	0.00033600
N	-2.61970800	-1.78659400	-0.00023600
N	2.61970900	-1.78659400	0.00058100
N	1.35652600	0.72131200	-0.00013500
C	2.84927800	3.08988800	-0.00028500
H	3.42047700	4.01364800	-0.00026600
C	3.57623500	-2.70200800	0.00036200
H	3.45885200	-3.77689900	0.00068000
C	-3.57623400	-2.70200800	0.00017000
H	-3.45885200	-3.77689900	-0.00007600
C	0.70280600	4.33419900	-0.00025700
H	1.23117200	5.28357500	-0.00048900
C	-0.70280600	4.33419900	-0.00008900
H	-1.23117200	5.28357500	0.00007600
N	4.63319800	-0.77249500	-0.00013500
N	-4.63319800	-0.77249500	0.00066000
N	-4.76769500	-2.08669200	0.00101400
H	-5.69343400	-2.50178200	0.00162400
N	4.76769500	-2.08669200	-0.00034200
H	5.69343500	-2.50178200	-0.00077100
Eu	0.00000000	-1.51406700	-0.00016400

EuR₇PhR₈³⁺(PBE0/6-311G*-RECP)

C	0.70226600	1.90238100	0.00038000
C	2.69017800	0.73024200	-0.00078900
C	3.45775900	1.90732500	-0.00115300
H	4.53988600	1.84042600	-0.00193500
C	-0.76413900	1.89245100	0.00039300
C	-1.46863900	3.12793900	0.00009000
C	-2.88192200	3.07477700	-0.00038600
C	-3.51404800	1.85464200	-0.00091100
H	-3.46079900	3.99374000	-0.00055000
H	-4.59716800	1.81067100	-0.00148300
N	-1.38156300	0.71617600	0.00021900
C	1.39073000	3.14589400	0.00007600
C	3.32200400	-0.57416700	-0.00181200
C	-2.73604300	0.68594100	-0.00075500
C	-3.30219600	-0.64646500	-0.00189000
N	-2.57626800	-1.77713100	-0.00266200
N	2.63404400	-1.76369300	-0.00110200
N	1.33722100	0.73313200	0.00022200
C	2.80846700	3.11577100	-0.00054100
H	3.37078200	4.04497900	-0.00066600
C	3.60289300	-2.66569900	-0.00268900
H	3.50056900	-3.74225100	-0.00246700
C	-3.50722800	-2.75691000	-0.00432700
H	-3.29178500	-3.81608000	-0.00548000
C	0.65405900	4.34341000	0.00014800
H	1.17814300	5.29515800	0.00003100
C	-0.74783100	4.33616500	0.00018000
H	-1.28305100	5.28159000	0.00015000
N	4.63348700	-0.72177200	-0.00416300
N	4.78604400	-2.03315600	-0.00480600
H	5.71762100	-2.43561500	-0.00654400
N	-4.75199200	-2.30545000	-0.00462200
N	-4.60277300	-0.99459700	-0.00312200
H	-5.43521000	-0.41733300	-0.00268100
Eu	0.01548800	-1.51860300	0.00390100

EuR₈PhR₈³⁺(PBE0/6-311G*-RECP)

C	-0.73352300	1.89858700	0.00002500
C	-2.71699900	0.70963400	0.00054800
C	-3.48384200	1.88642500	0.00050000
H	-4.56736300	1.85269300	0.00065200
C	0.73352300	1.89858700	-0.00015500
C	1.42686600	3.14034600	-0.00008000

C	2.84078400	3.09989500	-0.00017700
C	3.48384200	1.88642500	-0.00034800
H	3.41099900	4.02426300	-0.00004300
H	4.56736300	1.85269300	-0.00038000
N	1.36209000	0.72727900	-0.00035800
C	-1.42686500	3.14034600	-0.00005300
C	-3.29921400	-0.61516500	0.00078600
H	-5.43009500	-0.35990200	0.00373000
C	2.71700000	0.70963300	-0.00038000
H	5.43009600	-0.35990200	-0.00269100
C	3.29921400	-0.61516600	-0.00033600
N	2.58788500	-1.75578300	0.00103900
N	-2.58788600	-1.75578300	-0.00064300
N	-1.36209000	0.72727900	0.00032000
C	-2.84078400	3.09989500	0.00015200
H	-3.41099800	4.02426400	-0.00000800
N	-4.60451200	-0.94723000	0.00193600
N	4.60451300	-0.94723000	-0.00107100
C	-3.53049700	-2.72366400	-0.00034100
H	-3.32887400	-3.78565900	-0.00142400
C	3.53049700	-2.72366500	0.00115300
H	3.32887400	-3.78565900	0.00233100
N	-4.77002100	-2.25543200	0.00123600
N	4.77002100	-2.25543200	-0.00013300
C	-0.69860600	4.34547500	-0.00011500
H	-1.23006900	5.29298600	-0.00011800
C	0.69860700	4.34547400	-0.00010200
H	1.23007000	5.29298600	-0.00013800
Eu	0.00000000	-1.51921900	-0.00039200

AmR₁PhR₁(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.73009800	-0.72239800	-0.12004900
C	1.52967300	-2.68639600	-0.20698400
C	2.70943600	-3.45286500	-0.22661600
H	2.65167200	-4.53386600	-0.27537700
C	2.73053700	0.72109400	-0.12018100
C	3.96578700	1.40669600	-0.13457400
C	3.92114000	2.81142900	-0.18002900
C	2.71157600	3.45155400	-0.22718600
H	4.84804200	3.37734600	-0.18790700
H	2.65448200	4.53258300	-0.27611600
N	1.54807100	1.35922800	-0.13745300
C	3.96491900	-1.40877100	-0.13427700
C	0.21425000	-3.31191700	-0.26537600

C	-0.18609900	-4.65857500	-0.34099800
H	0.42702300	-5.54478700	-0.38508000
C	-1.56446800	-4.60930700	-0.34151800
H	-2.30911600	-5.38921100	-0.38079900
H	-2.81852000	-2.87530300	-0.17872800
C	1.53134000	2.68582600	-0.20728400
C	-0.18316200	4.65911700	-0.34113000
C	-1.56156000	4.61078400	-0.34109700
H	0.43053200	5.54491300	-0.38561100
H	-2.81675200	2.87764900	-0.17766600
H	-2.30568300	5.39119800	-0.38019900
C	0.21630400	3.31220300	-0.26542600
N	-0.85185700	2.51837300	-0.23061800
N	-0.85339900	-2.51738000	-0.23100300
N	1.54724100	-1.35980100	-0.13726900
C	3.91939400	-2.81348700	-0.17945300
H	4.84594500	-3.37998200	-0.18714800
N	-1.90873900	-3.31219400	-0.27835700
N	-1.90669500	3.31392000	-0.27761600
N	-0.02499700	-0.00087500	2.96559300
N	-1.20103300	-0.00061600	-2.79641200
N	-3.69664800	0.00128500	0.61276200
O	-2.16811500	-0.00068500	-1.97528400
O	-1.36847000	-0.00127500	-3.98549700
O	-0.04025100	0.00018800	-2.27784000
O	-0.20800000	-1.07573600	2.31285000
O	-0.20598100	1.07466400	2.31338800
O	0.30265900	-0.00146900	4.12041000
O	-3.00874100	-1.06361400	0.60767200
O	-3.00797300	1.06574000	0.60719300
O	-4.89287200	0.00174900	0.62890000
C	5.19122000	0.67662000	-0.11798800
H	6.12568000	1.22956700	-0.11483000
C	5.19080200	-0.67945300	-0.11783300
H	6.12492100	-1.23297600	-0.11454800
Am	-0.75607400	0.00042000	0.11589800

AmR₁PhR₂(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.78572600	0.37035000	-0.05153200
C	-1.85291500	2.48373000	-0.06714500
C	-3.12938400	3.08415300	-0.08555200
H	-3.22023400	4.16388200	-0.11244200
C	-2.60419900	-1.06396100	-0.05992000
C	-3.74743300	-1.89630300	-0.07710500

C	-3.53398500	-3.28687100	-0.07110800
C	-2.25881300	-3.77913700	-0.02831200
H	-4.38745200	-3.95848000	-0.08795400
H	-2.07264800	-4.84627600	-0.00116100
N	-1.35241800	-1.55995700	-0.04477800
C	-4.09952900	0.88939600	-0.07530500
C	-0.64675600	3.29316300	-0.12812600
C	-0.48901700	4.65824800	-0.12433500
H	-1.18670700	5.47698100	-0.05376800
H	1.31813000	5.75773600	-0.25238200
C	-1.17632400	-2.87838700	-0.00665300
C	0.74699200	-4.65636500	0.06491200
C	2.10245500	-4.45650100	0.21517600
H	0.24568400	-5.60399200	-0.05509100
H	3.13363800	-2.57873100	0.44301900
H	2.92938000	-5.14859700	0.25256100
C	0.19617400	-3.35883100	0.09221200
N	1.15729500	-2.45664400	0.25237900
N	0.58116300	2.69576500	-0.23412300
N	-1.69582400	1.16438800	-0.02695900
C	-4.24063300	2.29008500	-0.08056900
H	-5.23498600	2.72679100	-0.09389300
N	2.28846600	-3.12723200	0.32184800
C	-5.05472400	-1.32981400	-0.09670600
H	-5.91092400	-1.99745500	-0.11115400
C	-5.22449400	0.01530800	-0.09623700
H	-6.21984600	0.44898300	-0.11223500
C	1.46471100	3.65454600	-0.29187800
H	2.53072100	3.50926300	-0.37879400
N	0.85687100	4.86410600	-0.22892300
Am	0.76251400	0.11253400	0.03702500
N	3.76658900	0.35215900	0.02159900
O	4.96361700	0.39446600	-0.04428500
O	3.01979100	1.23195000	-0.49031100
O	3.15601800	-0.59247900	0.62188700
N	0.75471300	-0.23655000	-2.87946800
O	1.37471500	-1.02253200	-2.09562400
O	0.10263000	0.68915100	-2.30572200
O	0.77926900	-0.36544800	-4.07076500
N	0.38172500	0.40853500	2.93551700
O	0.22957000	0.54272400	4.11664800
O	0.66391000	1.38709500	2.17015400
O	0.26897500	-0.71113900	2.35243700

AmR₁PhR₃(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.79931400	-0.31203500	-0.08925500
C	-1.89103700	-2.42604700	-0.17544000
C	-3.16809900	-3.01941700	-0.19917800
H	-3.28361200	-4.09596400	-0.26274800
C	-2.59587500	1.11843000	-0.07716700
C	-3.72545900	1.96773200	-0.07563000
C	-3.48832800	3.35414900	-0.06894000
C	-2.20229100	3.82191900	-0.05215900
H	-4.32887400	4.04191800	-0.07015500
H	-1.99554100	4.88555500	-0.03285800
N	-1.33755400	1.58611000	-0.07346800
C	-4.12041000	-0.81705700	-0.11183000
C	-0.67041900	-3.20506200	-0.28146700
H	-1.33390600	-5.21440000	-0.20968500
C	0.74150100	-4.88648200	-0.43928900
H	1.07742100	-5.91006200	-0.47829500
H	2.47472300	-3.51088800	-0.57895900
C	-1.13874600	2.89917800	-0.04755100
C	0.83705600	4.61888700	-0.00053800
C	2.18891300	4.37684200	0.12732800
H	0.36075900	5.58201700	-0.09529500
H	3.16698700	2.47235300	0.35343900
H	3.03577200	5.04432200	0.16660000
C	0.24882000	3.33995900	0.01726900
N	1.18688800	2.40535000	0.14518400
N	0.52998600	-2.66830500	-0.39749100
N	-1.72123200	-1.11206900	-0.09532300
C	-4.27407300	-2.21365100	-0.15434200
H	-5.27151700	-2.64276600	-0.16834300
N	2.33990700	3.04380900	0.20722200
C	-5.04119300	1.41705600	-0.08319700
H	-5.88843300	2.09620700	-0.07714400
C	-5.23260000	0.07474000	-0.10077900
H	-6.23505200	-0.34224800	-0.11087300
C	1.41620700	-3.69659200	-0.49351300
N	-0.57909600	-4.55782000	-0.30681600
Am	0.80369300	-0.13537700	0.04906000
N	0.99906700	0.29731300	-2.84137400
O	1.06911100	0.46944200	-4.02597400
O	1.93845200	0.61320200	-2.04975900
O	-0.02942300	-0.21271500	-2.29010700
N	0.07917800	-0.46607700	2.89443400
O	0.44532700	-1.44092600	2.16375500

O	0.06736200	0.66653700	2.32350000
O	-0.24209000	-0.61206400	4.04172300
N	3.74959600	-0.44607900	0.40807500
O	3.13459900	0.58504800	0.83797300
O	4.94371200	-0.53596900	0.43778900
O	3.00237000	-1.35707700	-0.04457500

AmR₁PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.76497900	-0.33776400	0.01223500
C	1.89351700	-2.46713300	-0.03929700
C	3.17072500	-3.04194200	0.09691600
H	3.28662700	-4.11949100	0.12753400
C	2.54872100	1.08877800	-0.06923000
C	3.66664900	1.95251300	-0.05379300
C	3.41767200	3.32941200	-0.19934200
C	2.13390900	3.77614300	-0.36515300
H	4.24973600	4.02737800	-0.19180100
H	1.92358600	4.83069700	-0.49953600
N	1.28993900	1.54278300	-0.18686200
C	4.08627400	-0.82324900	0.13857100
C	0.69929800	-3.29279700	-0.17206000
C	0.51860800	-4.65522400	-0.22828300
H	1.18822200	-5.49780000	-0.17880300
H	-1.35690200	-5.63553600	-0.45615700
C	1.07876500	2.84436300	-0.35332700
C	-0.90969100	4.53008500	-0.60765600
C	-2.26196000	4.26914800	-0.67708300
H	-0.44112600	5.50156800	-0.60595700
H	-3.23881600	2.36415200	-0.55908700
H	-3.11567900	4.92578500	-0.74247400
C	-0.31024500	3.25932900	-0.51851700
N	-1.24264300	2.31005800	-0.55019300
N	-0.52980400	-2.72005400	-0.28844800
N	1.70215800	-1.15700600	-0.06613100
C	4.25959300	-2.21769200	0.19109400
H	5.25866500	-2.62969200	0.29771100
N	-2.40318900	2.93219400	-0.64315100
C	4.98240100	1.42223000	0.09471000
H	5.82083200	2.11170600	0.12195300
C	5.18467300	0.08508800	0.19283800
H	6.18732300	-0.31687400	0.30232100
N	-1.43946800	-3.62377700	-0.41098800
N	-0.81399500	-4.79061800	-0.37665300
Am	-0.78284300	-0.13820300	0.03039300

N	-0.15384700	0.45693200	2.84616900
O	0.08417500	0.65627100	4.00528300
O	-0.87129800	1.23486600	2.15203800
O	0.31530500	-0.55293100	2.22614300
N	-3.49932300	-0.40362800	1.10803300
O	-4.60614600	-0.46483400	1.56022200
O	-2.58616600	-1.22609600	1.39596600
O	-3.15506300	0.51189200	0.28635000
N	-0.99642800	-0.45250600	-2.88470600
O	0.11706400	-0.23122500	-2.31272100
O	-2.00250800	-0.50302200	-2.11404800
O	-1.08655900	-0.60254000	-4.07276400

AmR₁PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.76019100	-0.61131200	-0.06397600
C	-1.65092700	-2.62906200	-0.16730000
C	-2.86089700	-3.34427000	-0.20695100
H	-2.85088800	-4.42569100	-0.27933000
C	-2.70127200	0.83273600	-0.03527900
C	-3.91069600	1.56402400	-0.01750500
C	-3.81726700	2.96675100	0.01175300
C	-2.58664500	3.56595800	0.02897100
H	-4.72453400	3.56346700	0.02538600
H	-2.49121100	4.64485100	0.06271300
N	-1.49749200	1.43166000	-0.03333600
C	-4.02360200	-1.24545400	-0.09776400
C	-0.36580700	-3.30910800	-0.25303900
C	0.02639200	-4.65581200	-0.24075900
H	-0.55668100	-5.56088700	-0.17081100
H	2.67730200	-3.13679800	-0.39964400
C	-1.43448000	2.75880800	0.00948400
C	0.35392700	4.67471900	0.05360600
C	1.72736300	4.57304500	0.13346200
H	-0.22265100	5.58467000	-0.00042400
H	2.90958200	2.78339900	0.26537800
H	2.50052700	5.32504700	0.16360000
C	-0.09812800	3.34187500	0.05548500
N	0.93641400	2.50872600	0.13052000
N	0.74520300	-2.58181800	-0.35017700
N	-1.60797100	-1.30450700	-0.07232900
C	-4.04046400	-2.65016700	-0.15942300
H	-4.99175400	-3.17341600	-0.18340600
N	2.01970700	3.26185000	0.17403800
C	-5.16474300	0.88467900	-0.03374800

H	-6.07558700	1.47545600	-0.01664100
C	-5.21985900	-0.46902200	-0.07495300
H	-6.17515000	-0.98456400	-0.09394300
N	1.71481000	-3.45554000	-0.38293100
N	1.35212200	-4.71154600	-0.32047500
Am	0.76974000	-0.02241800	0.02922700
N	0.32530500	-0.43241000	2.91398200
O	0.14014900	-0.60570400	4.08532100
O	0.81645200	-1.33427600	2.16245200
O	0.03790700	0.66027000	2.33326600
N	3.74970000	-0.17712700	0.28086900
O	3.09753000	0.83408800	0.68788900
O	3.03096500	-1.13307500	-0.14229400
O	4.94448000	-0.22571700	0.29708500
N	0.88562900	0.36731200	-2.86688300
O	-0.07656300	-0.23883500	-2.29089600
O	1.80032600	0.78741500	-2.09404200
O	0.91819900	0.53053400	-4.05313200

AmR₁PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.76894800	-0.01455800	0.02385700
C	-2.12949600	-2.22453700	0.05543100
C	-3.46332100	-2.66194800	0.12380900
H	-3.70356500	-3.71731800	0.19454600
C	-2.39153200	1.38137700	0.01281700
C	-3.40907100	2.36051400	0.02930300
C	-3.00563400	3.70779500	-0.00950100
C	-1.67456200	4.01573400	-0.09216200
H	-3.75591500	4.49272800	0.01070300
H	-1.34334600	5.04596500	-0.14928700
N	-1.08667300	1.69468300	-0.02585500
C	-4.14117700	-0.35705300	0.08462400
C	-1.00125600	-3.14356500	0.11582100
H	-1.81588900	-5.09217700	-0.15617900
C	0.27417500	-4.88232100	0.14723400
H	0.60406100	-5.90901500	0.11001300
C	-0.72861900	2.97198900	-0.11099100
C	1.42963700	4.43630700	-0.35849600
C	2.73428600	4.02894600	-0.54090100
H	1.07594600	5.45332000	-0.29287800
H	3.47051500	2.00474800	-0.66762300
H	3.65015500	4.58730300	-0.65708700
C	0.69511000	3.23767300	-0.27298900
N	1.50881300	2.19365400	-0.40048900

N	0.24034400	-2.75978000	0.29887800
N	-1.80091100	-0.94280100	-0.01863100
C	-4.46345300	-1.72392300	0.12369900
H	-5.50478600	-2.02773300	0.17291500
N	2.72213100	2.68356700	-0.55741600
C	-4.78114900	1.97311600	0.08157100
H	-5.53917700	2.75046700	0.09809100
C	-5.13602500	0.66468500	0.11046000
H	-6.18117300	0.37428200	0.15430200
N	1.04388700	-3.84444800	0.31610500
N	-1.02439400	-4.49774100	0.02098100
Am	0.81241600	-0.23946600	-0.00511700
N	0.23457300	-0.64372100	-2.87903600
O	-0.01812800	-0.83103700	-4.03766900
O	0.62511300	-1.58042400	-2.11150400
O	0.11897700	0.49125900	-2.33003300
N	3.70997200	-0.72603700	0.28126100
O	3.23378800	0.04009800	-0.63578800
O	4.89063700	-0.84392800	0.44448900
O	2.85021100	-1.32137100	0.97837900
N	0.42346900	0.40729300	2.84177400
O	1.21535900	1.05727500	2.09133100
O	0.27995300	0.66764800	4.00381200
O	-0.21698900	-0.52794700	2.26998900

AmR₁PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.79844600	-0.38863700	-0.08877700
C	-1.84842800	-2.47794500	-0.18060100
C	-3.10253000	-3.11153900	-0.19905800
H	-3.15007700	-4.19246600	-0.25296400
C	-2.63033700	1.04544600	-0.07157500
C	-3.78109300	1.86606900	-0.06238900
C	-3.58049400	3.25779800	-0.04890700
C	-2.30717600	3.76005000	-0.03399400
H	-4.43904000	3.92294800	-0.04358200
H	-2.12878300	4.82867100	-0.00974700
N	-1.38388200	1.54777600	-0.07004800
C	-4.10436400	-0.92998700	-0.10880200
C	-0.61510800	-3.24994000	-0.28038500
H	1.11709800	-5.72615300	-0.42954300
H	2.52109700	-3.53747700	-0.50163700
C	-1.22016600	2.86603500	-0.03843800
C	0.71040400	4.63781300	0.00062900

C	2.06961500	4.43174700	0.11437600
H	0.20775800	5.58814500	-0.08659100
H	3.10255900	2.55569900	0.31882600
H	2.89844600	5.12182900	0.14700200
C	0.15620700	3.34402900	0.01977800
N	1.12053200	2.43477900	0.13583800
N	0.59223900	-2.63684800	-0.37388900
N	-1.69963200	-1.16400500	-0.10192000
C	-4.22662200	-2.33127200	-0.15188400
H	-5.21476600	-2.78166500	-0.16069700
N	2.25747100	3.10320000	0.18865300
C	-5.08196400	1.28117600	-0.06893400
H	-5.94649400	1.93815000	-0.05767300
C	-5.23860600	-0.06539900	-0.09164700
H	-6.23010100	-0.50772200	-0.10041100
N	-0.55262800	-4.56580200	-0.29860000
C	1.44751000	-3.63196600	-0.44157500
N	0.76469500	-4.78388400	-0.40236100
Am	0.79115600	-0.09802700	0.04504500
N	0.16365800	-0.46406400	2.90547400
O	-0.10013200	-0.62230000	4.06466700
O	0.55934400	-1.41921600	2.16290800
O	0.06076000	0.66274000	2.33097200
N	3.74654700	-0.38977800	0.38489400
O	3.00363500	-1.31645100	-0.04724300
O	3.12695600	0.64557100	0.79242700
O	4.94102000	-0.47465900	0.41475400
N	1.01209000	0.29273900	-2.84863700
O	1.09356800	0.44495800	-4.03491500
O	-0.00808900	-0.23842200	-2.30126900
O	1.93099500	0.65064400	-2.05042100

AmR₁PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.80094400	-0.30787700	0.09086700
C	-1.90450600	-2.42317400	0.16908600
C	-3.17768900	-3.01711200	0.20411700
H	-3.29070900	-4.09380600	0.26842600
C	-2.59098700	1.12195200	0.07363100
C	-3.71794000	1.97381900	0.07322400
C	-3.47749200	3.35963400	0.05764100
C	-2.19015900	3.82353300	0.03243300
H	-4.31596500	4.04982500	0.05895500
H	-1.98088400	4.88648200	0.00664000

N	-1.33127000	1.58539500	0.06299200
C	-4.12360700	-0.81120000	0.12195100
C	-0.67710000	-3.20215100	0.26212500
H	-1.24907100	-5.25314400	0.17592000
H	2.42614700	-3.63787700	0.53708600
C	-1.12866300	2.89818600	0.02939000
C	0.84912800	4.61457100	-0.02986100
C	2.20127800	4.37033900	-0.14964700
H	0.37362800	5.57911400	0.05354900
H	3.18030500	2.46371000	-0.34816700
H	3.04878300	5.03682900	-0.19115100
C	0.25971600	3.33614700	-0.03806900
N	1.19791900	2.39969200	-0.15348500
N	0.52629400	-2.66864900	0.38160900
N	-1.72696000	-1.11218900	0.09136800
C	-4.28237900	-2.20647700	0.16756900
H	-5.28101800	-2.63203900	0.18943900
N	2.35162800	3.03645000	-0.21667400
C	-5.03525200	1.42602900	0.09031500
H	-5.88027400	2.10796900	0.08598400
C	-5.23295600	0.08487400	0.11454500
H	-6.23699000	-0.32762400	0.13178100
N	0.73850200	-4.89621700	0.38873000
N	-0.54781500	-4.53848900	0.27092000
C	1.35562000	-3.73539700	0.45032800
Am	0.81388000	-0.13232300	-0.04692700
N	0.08295700	-0.46309200	-2.88965400
O	-0.24481600	-0.61120000	-4.03397500
O	0.10399200	0.67381300	-2.32809400
O	0.42429500	-1.44144500	-2.14976000
N	0.96158500	0.28954100	2.84532800
O	1.00968600	0.45931200	4.03051500
O	1.90536200	0.62668300	2.06785100
O	-0.04867200	-0.23955400	2.27626500
N	3.75270200	-0.47984500	-0.35878500
O	4.94487400	-0.58253100	-0.37298100
O	3.15391400	0.56037500	-0.79288800
O	2.98789100	-1.38434100	0.07998100

AmR₂PhR₂(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.69189600	-0.72315500	-0.00605300
C	-1.49693500	-2.69534700	0.05106700
C	-2.68310300	-3.45837400	0.03745700
H	-2.63355300	-4.54076000	0.07191500

C	-2.69244700	0.72109100	0.00533100
C	-3.92965700	1.40343100	0.00522600
C	-3.88979500	2.81090900	0.00091000
C	-2.68574300	3.45634100	-0.03816200
H	-4.81970100	3.37214100	0.00996600
H	-2.63701700	4.53876500	-0.07258900
N	-1.51166200	1.36802500	0.00264100
C	-3.92858200	-1.40643300	-0.00618300
C	-0.19199700	-3.32309800	0.17809500
C	0.17073800	-4.64725500	0.18657800
H	-0.39007600	-5.56050400	0.07057100
H	2.11336400	-5.46093300	0.43062100
H	2.95935100	-3.05654600	0.63596500
C	-1.49899300	2.69423100	-0.05141300
C	0.16737800	4.64737400	-0.18644600
H	-0.39416000	5.56029000	-0.07132300
H	2.95738600	3.05842000	-0.63346200
H	2.10955800	5.46231500	-0.42976500
C	-0.19443800	3.32295900	-0.17763300
N	0.92088000	2.54716800	-0.36163600
N	0.92263200	-2.54657700	0.36327700
N	-1.51061800	-1.36917500	-0.00311700
C	-3.88764200	-2.81388100	-0.00193000
H	-4.81711600	-3.37582400	-0.01121200
N	0.44015600	-0.53203200	-2.87695800
N	0.43903600	0.53350800	2.87701400
N	3.77387000	0.00034600	-0.00108900
O	-0.04038600	-0.50046600	2.32426600
O	0.30757400	0.75863700	4.04952900
O	1.06148300	1.32541400	2.10132800
O	1.05672100	-1.32728200	-2.09993100
O	-0.03396700	0.50498400	-2.32546800
O	0.30924300	-0.75696100	-4.04959500
O	3.09549000	0.75744700	-0.75988900
O	3.09571300	-0.75621400	0.75852400
O	4.97467800	-0.00024400	-0.00178800
C	1.93615200	-3.36230700	0.47954700
C	1.93390000	3.36352700	-0.47763400
N	1.52346400	-4.64790700	0.37890300
N	1.52023000	4.64888600	-0.37788700
Am	0.80763300	0.00034400	0.00032600
C	-5.15441000	-0.68020700	-0.00422500
H	-6.08804400	-1.23478800	-0.00616600
C	-5.15493100	0.67626700	0.00309000

H	-6.08898800	1.23013400	0.00491700
AmR ₂ PhR ₃ (NO ₃) ₃ (PBE0/6-311G*-RECP)			
C	2.61654500	0.91467200	0.01994200
C	1.28317800	2.79454200	0.07385300
C	2.41321500	3.63931200	0.06736100
H	2.28729700	4.71552000	0.10077700
C	2.71940800	-0.52625800	0.02710400
C	4.00177600	-1.12351800	0.02029000
C	4.05602700	-2.52870100	0.00130900
C	2.89679500	-3.25590800	-0.04357400
H	5.02086400	-3.02719700	-0.00002700
H	2.93543800	-4.33843500	-0.09998000
N	1.58917900	-1.25048800	0.02612900
C	3.80183700	1.68155500	0.02432100
C	-0.06475800	3.32536600	0.18960100
C	-0.52053100	4.62023400	0.22279500
H	-0.02428500	5.57348100	0.13837600
H	-2.51831000	5.28877500	0.46006300
H	-3.19364800	2.82604400	0.60420800
C	1.66447800	-2.57337200	-0.04217900
H	0.86734000	-5.30998400	0.02524900
H	-2.73778400	-3.30030100	-0.70401900
H	-1.57308500	-5.80853500	-0.38705100
C	0.39078300	-3.25720500	-0.18181500
N	-0.74652200	-2.62637000	-0.40290000
N	-1.12402300	2.46805700	0.34031400
N	1.39259200	1.47263900	0.01954500
C	3.66113400	3.08260500	0.03205500
H	4.54792600	3.70968100	0.02644200
C	-2.19375800	3.20692300	0.46237900
C	-1.71154200	-3.57615100	-0.51953000
N	-1.87183100	4.52082800	0.39597200
C	5.07562100	1.04122200	0.02449900
H	5.96819200	1.65973800	0.02616900
C	5.17322100	-0.31184000	0.02317400
H	6.14437700	-0.79738600	0.02094000
N	0.18257000	-4.59736400	-0.15817900
C	-1.15098700	-4.81677500	-0.36752200
Am	-0.82710900	-0.06762600	-0.01623900
N	-0.38680600	-0.56414700	2.86807200
O	-0.21353600	-0.77884300	4.03727300
O	-0.09909200	0.54539000	2.32964200
O	-0.86161600	-1.44339500	2.08171700

N	-3.78227400	-0.25598300	-0.01050400
O	-4.98051200	-0.32041700	-0.02461600
O	-3.15399100	0.51409800	0.78160900
O	-3.05466700	-0.94798600	-0.78468700
N	-0.37314700	0.53771100	-2.87209600
O	-0.19590500	0.79325900	-4.03196300
O	-1.14069700	1.23095200	-2.13450800
O	0.20229600	-0.43322700	-2.29413200

AmR₂PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.53761000	1.07417100	0.01173500
C	-1.07876000	2.85880200	-0.09050500
C	-2.14726000	3.77942600	-0.06586300
H	-1.94907600	4.84417600	-0.11275200
C	-2.73979100	-0.35689100	0.01649400
C	-4.05980100	-0.86146800	0.06061700
C	-4.21609700	-2.25915600	0.08452700
C	-3.11167900	-3.06707400	0.09131700
H	-5.21455800	-2.68530300	0.11461500
H	-3.21346100	-4.14534400	0.14013800
N	-1.66231700	-1.16261300	-0.01259600
C	-3.66659100	1.92238100	0.03106800
C	0.29973300	3.29595800	-0.24306400
C	0.84094900	4.55636600	-0.30527200
H	0.41182400	5.54198500	-0.22526300
H	2.87381400	5.08735900	-0.58922700
H	3.38163100	2.58209400	-0.70812400
C	-1.83447000	-2.47534100	0.05049500
C	-0.42901200	-4.64610600	0.06071900
H	-1.08803800	-5.48877200	-0.06748500
H	1.45943600	-5.61721700	0.19781300
C	-0.62627800	-3.28640300	0.11872200
N	0.59441100	-2.70918500	0.28460300
N	1.29762900	2.36896900	-0.40215400
N	-1.27948800	1.54847300	-0.02157400
C	-3.42916600	3.31020100	0.00606400
H	-4.27016900	3.99716700	0.02775800
C	2.41205300	3.03200500	-0.55569200
N	2.17925800	4.36487900	-0.50305200
N	0.90473400	-4.77676300	0.19256400
C	-4.98117600	1.37269600	0.06999300
H	-5.82841800	2.05178000	0.08701700
C	-5.17183800	0.03000300	0.08465800
H	-6.17363900	-0.38755900	0.11609900

N	1.51453000	-3.60574400	0.32675700
Am	0.82586400	-0.11376800	-0.00936000
N	0.29537800	-0.59861600	-2.88205300
O	0.08561100	-0.81689600	-4.04449100
O	0.04507500	0.51801500	-2.34178800
O	0.77556600	-1.48321000	-2.10433800
N	3.73358900	-0.40156200	0.24317700
O	4.92522300	-0.46870100	0.36670400
O	3.19271400	0.21462700	-0.73676500
O	2.92918000	-0.92086300	1.06727300
N	0.36298400	0.45060400	2.85073700
O	0.19834200	0.67923200	4.01796000
O	0.98045300	1.25255400	2.08309500
O	-0.07849000	-0.59962000	2.29456200

AmR₂PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.75502000	0.53768000	-0.00191500
C	1.69935700	2.58887300	-0.04462100
C	2.93550800	3.26695400	-0.05579500
H	2.96124900	4.34989700	-0.09575800
C	2.65842100	-0.90402200	-0.00944200
C	3.84690100	-1.67103900	-0.01092400
C	3.71350100	-3.07098000	0.00357100
C	2.46717700	-3.63607800	0.04626100
H	4.60368400	-3.69299600	-0.00448400
H	2.34131400	-4.71207800	0.08249500
N	1.43884300	-1.47011300	-0.00353500
C	4.03552800	1.13354700	-0.01933200
C	0.43931500	3.30784800	-0.13898900
C	0.16999300	4.65376400	-0.12198000
H	0.79647500	5.52384100	-0.01092300
H	-1.71642100	5.60524700	-0.29886900
H	-2.73760800	3.27204800	-0.50135000
C	1.34069600	-2.79379300	0.05220200
C	-0.55278500	-4.62277000	0.19536100
H	-0.08109400	-5.59051800	0.12400700
H	-2.99374400	-2.79670700	0.48927800
C	-0.00873400	-3.32987600	0.16191700
N	-1.02409900	-2.47940700	0.28813000
N	-0.73333300	2.61462000	-0.30044500
N	1.62100100	1.26435500	0.01146600
C	4.09278700	2.54011300	-0.03171200
H	5.05897400	3.03607200	-0.03970500
C	-1.69049100	3.50151000	-0.37637400

N	-1.18423600	4.75188800	-0.27413000
C	5.20937400	0.32461700	-0.02843200
H	6.17821900	0.81472900	-0.03994700
C	5.11918100	-1.02823500	-0.02363600
H	6.01356900	-1.64379900	-0.02840500
N	-2.08358400	-3.23239800	0.38300400
N	-1.87108600	-4.52384500	0.33684500
Am	-0.79175300	0.07911500	0.00172400
N	-0.48843700	0.46188600	2.90716400
O	-0.37361600	0.62879900	4.08908100
O	-1.01746800	1.33402000	2.14636900
O	-0.08308400	-0.58937900	2.32414100
N	-0.54121900	-0.42328600	-2.88553100
O	-0.46105600	-0.62778800	-4.06414600
O	0.10320200	0.50552800	-2.30894100
O	-1.27288000	-1.13046500	-2.12178000
N	-3.77480900	0.12543000	-0.04251700
O	-3.12379900	-0.75439300	0.60950100
O	-4.97100100	0.12259900	-0.10002900
O	-3.06352800	0.99930000	-0.61922100

AmR₂PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.73941200	-0.39904900	-0.04829000
C	1.83473600	-2.51022300	-0.11623100
C	3.09935100	-3.11216000	0.00254700
H	3.20854300	-4.19123900	0.02590600
C	2.53958400	1.03028900	-0.11445200
C	3.66560800	1.87862400	-0.07501600
C	3.42943800	3.26183800	-0.19690600
C	2.15296200	3.72140100	-0.37408000
H	4.26644300	3.95316100	-0.16428700
H	1.95776500	4.78129500	-0.49181100
N	1.28657700	1.49443800	-0.24709200
C	4.05453900	-0.90783900	0.06988300
C	0.59970500	-3.27624700	-0.23222300
H	1.17432600	-5.32566500	-0.31429600
H	-1.34063700	-5.80456000	-0.50965200
C	1.08671100	2.79797800	-0.40051400
C	-0.85189100	4.45450400	-0.76273200
H	-0.43809100	5.44986100	-0.75453900
H	-3.37472600	2.42732100	-0.94750000
H	-2.89738600	4.93420700	-1.04923300
C	-0.29125200	3.20975700	-0.61644900
N	-1.27677500	2.25856200	-0.69901300

N	-0.59184700	-2.72549200	-0.28044600
N	1.66709800	-1.19802300	-0.12973800
C	4.20368300	-2.30464100	0.10157800
H	5.19528900	-2.73585800	0.20057800
C	-2.40347600	2.89320300	-0.87890100
N	-2.18971900	4.22921500	-0.92945500
C	5.16321600	-0.01337900	0.14216200
H	6.16157400	-0.42685900	0.24715200
C	4.97389200	1.32816900	0.07071000
H	5.82056500	2.00668200	0.11638600
N	-1.52686800	-3.69508700	-0.39864900
C	-0.88732000	-4.82925700	-0.42144600
N	0.45455100	-4.62342000	-0.31766700
Am	-0.81912400	-0.14776900	0.06550400
N	0.07926700	0.73438900	2.74242800
O	-0.74968000	1.41241100	2.07083300
O	0.52164800	-0.31414500	2.17059500
O	0.44407500	1.05885400	3.84039900
N	-3.35591500	-0.44045000	1.45581100
O	-4.39324300	-0.52546200	2.04922000
O	-2.36977600	-1.20313600	1.68581900
O	-3.16531700	0.42783500	0.54470900
N	-1.19054600	-0.43858500	-2.83683100
O	-1.35301200	-0.53803700	-4.02373400
O	-2.15625300	-0.44819500	-2.01581500
O	-0.03606800	-0.31223900	-2.32139000

AmR₂PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.67657600	0.81842800	0.00163700
C	-1.41603000	2.74866800	-0.03469900
C	-2.57645000	3.55025900	-0.02724200
H	-2.49067100	4.63053700	-0.05466500
C	-2.72711800	-0.62439800	-0.01373200
C	-3.98482900	-1.27075100	-0.01850500
C	-3.99209500	-2.67860300	-0.01467700
C	-2.80879200	-3.36571600	0.02614400
H	-4.94021900	-3.20812100	-0.02773000
H	-2.76812700	-4.44789100	0.05578300
N	-1.56938700	-1.30875300	-0.00818200
C	-3.88966900	1.54129000	-0.00212600
C	-0.08971200	3.33393000	-0.13887600
C	0.31540500	4.64576000	-0.14151500
H	-0.21798600	5.57670200	-0.03743100

H	2.28665200	5.39671700	-0.35315200
H	3.05932400	2.96647200	-0.54263900
C	-1.61016800	-2.63163100	0.04159100
H	2.81061900	-3.30399800	0.57145500
H	1.61566000	-5.61294200	0.39320700
C	-0.31895000	-3.29809200	0.16803000
N	0.82209200	-2.58245500	0.32559700
N	1.00304400	2.52216800	-0.30274500
N	-1.47370700	1.42277300	0.00955200
C	-3.80253200	2.94639500	-0.00085600
H	-4.71263800	3.53911000	0.00429200
C	2.04420000	3.30505500	-0.40227700
C	1.75724800	-3.49632100	0.43472600
N	1.67041100	4.60285700	-0.30976700
N	1.18326300	-4.70538700	0.35011900
C	-5.13839900	0.85383300	-0.01194300
H	-6.05330400	1.43883600	-0.01323600
C	-5.18537600	-0.50171600	-0.02082700
H	-6.13765500	-1.02318300	-0.02742400
N	-0.14137500	-4.60396600	0.18055900
Am	0.81449000	-0.02012300	0.00122900
N	0.51200800	0.43795300	2.89965000
O	0.40872300	0.62746400	4.08016600
O	-0.02279700	-0.55512600	2.31980800
O	1.15821000	1.22667800	2.13986900
N	3.78188700	-0.16402700	-0.03650100
O	4.98005600	-0.22451900	-0.05727200
O	3.07477600	-0.93898600	0.67773600
O	3.13239100	0.67868500	-0.72892200
N	0.46212500	-0.49219600	-2.89176300
O	1.00469000	-1.33960700	-2.11191100
O	0.04485600	0.56589800	-2.33371700
O	0.34639300	-0.69069500	-4.06950000

AmR₂PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.60670500	0.94771500	-0.01548800
C	-1.25049800	2.81063900	-0.06543600
C	-2.37033600	3.66910500	-0.05989200
H	-2.23131200	4.74369300	-0.09171800
C	-2.72994400	-0.49185200	-0.02318600
C	-4.02005300	-1.07477700	-0.01575700
C	-4.09397300	-2.47822100	0.00434000
C	-2.94334200	-3.22162900	0.04874300

H	-5.06528700	-2.96356100	0.00615000
H	-2.99135700	-4.30376000	0.10321000
N	-1.61042600	-1.23172000	-0.02162200
C	-3.78227400	1.72867100	-0.02029400
C	0.10372500	3.32587800	-0.17525800
C	0.57422700	4.61569500	-0.20641500
H	0.08833300	5.57452700	-0.12519700
H	2.58006900	5.26202100	-0.43441500
H	3.22928500	2.79235500	-0.57503000
C	-1.70777800	-2.55127700	0.04423500
H	-0.84840000	-5.33247800	0.00624700
H	2.66113100	-3.46476900	0.68043500
C	-0.43594100	-3.24891400	0.18320800
N	0.71341200	-2.63451900	0.39943900
N	1.15447000	2.45695800	-0.32046600
N	-1.37589500	1.48968900	-0.01328000
C	-3.62508500	3.12797400	-0.02706200
H	-4.50404000	3.76588000	-0.02207700
C	2.23296700	3.18405400	-0.43751700
C	1.61133900	-3.63879500	0.50344000
N	1.92483200	4.50118300	-0.37280100
C	-5.06405400	1.10364700	-0.02125600
H	-5.94845100	1.73380700	-0.02351000
C	-5.18110700	-0.24762100	-0.01933100
H	-6.15871800	-0.71964600	-0.01722600
N	1.08806300	-4.84000300	0.36986100
N	-0.21009300	-4.57268600	0.16979700
Am	0.83694300	-0.07289700	0.01386200
N	3.78064000	-0.32899200	-0.02575500
O	3.04285900	-1.03513200	0.72647600
O	3.16125900	0.48375100	-0.78330500
O	4.97618400	-0.41720800	-0.02315000
N	0.40715000	0.50679400	2.87423900
O	0.23550000	0.75262300	4.03617600
O	-0.20441300	-0.43349800	2.28037200
O	1.20351900	1.17880100	2.14782600
N	0.35008100	-0.55807000	-2.86335200
O	0.15471700	-0.77075200	-4.02854700
O	0.79826400	-1.45318300	-2.07738200
O	0.11417100	0.56396500	-2.32578900

AmR₃PhR₃(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.67106700	-0.72052300	0.00642600
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C	1.47273400	-2.68970300	-0.02428600
C	2.65824400	-3.45286900	-0.01694000
H	2.62303800	-4.53646500	-0.04522000
C	2.66957700	0.72593900	-0.00730200
C	3.90615000	1.41059400	-0.00944800
C	3.85968200	2.81656000	-0.00967200
C	2.65118500	3.45826200	0.01605900
H	4.78593700	3.38344300	-0.01514900
H	2.61379300	4.54178200	0.04438600
N	1.48871200	1.36461400	-0.01199500
C	3.90904700	-1.40264000	0.00784200
C	0.15842200	-3.29824100	-0.12199300
H	0.53081700	-5.38293300	0.01876300
H	-1.94490300	-5.73882100	-0.29617400
H	-2.98229400	-3.16400000	-0.53087700
C	1.46723500	2.69267900	0.02401900
H	0.51999700	5.38402800	-0.01865400
H	-2.98862500	3.15818600	0.53169300
H	-1.95632900	5.73505400	0.29692700
C	0.15175500	3.29859200	0.12222900
N	-0.95601100	2.60381400	0.28557900
N	-0.95073000	-2.60562200	-0.28507400
N	1.49152800	-1.36160600	0.01178600
C	3.86544600	-2.80870200	0.00813000
H	4.79285200	-3.37370600	0.01311000
N	-0.40683000	-0.39616800	2.88182000
N	-0.40899300	0.39445700	-2.88117300
N	-3.79387600	-0.00337500	-0.00120500
O	-0.18680900	-0.71706600	-2.31722100
O	-0.24519600	0.56975100	-4.05662900
O	-0.81057200	1.32060300	-2.10582300
O	-0.80598900	-1.32313800	2.10616200
O	-0.18871800	0.71646100	2.31844500
O	-0.24150000	-0.57172900	4.05702200
O	-3.11587400	0.72684600	0.78609800
O	-3.11384500	-0.73268000	-0.78747500
O	-4.99422800	-0.00412800	-0.00202700
C	-1.96729900	-3.49803900	-0.38196600
C	-1.97430900	3.49424200	0.38267500
C	-1.46954500	-4.77136800	-0.27339300
C	-1.47907300	4.76853800	0.27398600
N	-0.12018000	-4.62844600	-0.11213800
N	-0.12947500	4.62825800	0.11242400
C	5.13381300	-0.67307600	0.00331700

C	5.13241600	0.68355500	-0.00565600
H	6.06874200	-1.22520300	0.00581400
H	6.06620400	1.23760700	-0.00873100
Am	-0.83058600	-0.00076400	0.00054100

AmR₃PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.58898100	0.90260600	-0.03150900
C	-1.24698300	2.77279600	0.07647600
C	-2.36733600	3.62693300	0.06567700
H	-2.24982100	4.70336200	0.12864700
C	-2.69705200	-0.53917400	-0.04118800
C	-3.98097300	-1.12658500	-0.08945000
C	-4.04488700	-2.53159200	-0.11915900
C	-2.88916500	-3.26473400	-0.12500000
H	-5.01252200	-3.02346100	-0.15278000
H	-2.92046100	-4.34726400	-0.17530500
N	-1.56902000	-1.27013700	-0.01108800
C	-3.77026500	1.67925000	-0.04434100
C	0.11227800	3.26207600	0.23162700
H	-0.06355900	5.36947800	0.10772900
H	2.42208300	5.49680500	0.52186500
H	3.21493800	2.83678000	0.74742800
C	-1.65290900	-2.59137000	-0.07739300
H	-0.71020600	-5.55113100	-0.00574900
H	1.84421100	-5.50571500	-0.22191600
C	-0.39245400	-3.31913100	-0.13707000
N	0.79059000	-2.65950100	-0.26712700
N	1.14878600	2.46849600	0.42420800
N	-1.36696300	1.45368300	-0.00097100
C	-3.61941700	3.07706400	-0.00770600
H	-4.50087400	3.71124800	-0.01945000
C	2.23962000	3.26394000	0.57244400
C	1.86247700	4.57701100	0.46759400
N	0.51175200	4.55850400	0.25551700
C	-5.04676800	1.04558300	-0.08666700
C	-5.14817300	-0.30671600	-0.10988400
H	-5.93694000	1.66725900	-0.09917200
H	-6.12098800	-0.78769800	-0.14435800
N	1.76813500	-3.49231900	-0.30910700
C	-0.10639300	-4.66400600	-0.10217900
N	1.23499200	-4.70389900	-0.21025800
Am	0.85375300	-0.05330800	0.02664700
N	0.34444900	0.46071500	-2.83951600
O	0.15259900	0.67397500	-4.00583700

O	0.86055600	1.32800600	-2.06802700
O	0.03274500	-0.63732200	-2.28884300
N	3.76132900	-0.17356300	-0.20303500
O	3.17490200	0.37602000	0.78928800
O	2.99372300	-0.69223900	-1.06541900
O	4.95560700	-0.18718200	-0.30575700
N	0.22666900	-0.58760600	2.87260300
O	-0.02978400	-0.82782800	4.02120000
O	-0.10267900	0.50012900	2.31426700
O	0.83693800	-1.41727100	2.12780400

AmR₃PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.78655300	0.34681400	-0.05892000
C	-1.85739000	2.45345400	-0.10524000
C	-3.12857300	3.05929400	-0.13360200
H	-3.23305900	4.13752100	-0.18638000
C	-2.59970700	-1.08654800	-0.05959800
C	-3.73840600	-1.92435700	-0.06638400
C	-3.51770700	-3.31334800	-0.05582400
C	-2.23744200	-3.79758300	-0.02180100
H	-4.36631600	-3.99091100	-0.06486100
H	-2.04333700	-4.86370600	0.00408000
N	-1.34732600	-1.57043900	-0.05000000
C	-4.10221600	0.86507300	-0.08605600
C	-0.62871900	3.22280700	-0.19175700
H	-1.26772800	5.23618600	-0.04879000
H	1.14899600	5.91287300	-0.31361300
H	2.51784500	3.50156300	-0.50797500
C	-1.16628600	-2.88545600	-0.01181700
H	0.42779600	-5.58752500	0.05690300
H	3.16208700	-2.61341100	0.39025800
C	0.21561000	-3.33535400	0.07485000
N	1.17770000	-2.42166100	0.17946800
N	0.56524700	2.67727100	-0.33322200
N	-1.70104200	1.13676200	-0.04206500
C	-4.24239500	2.26364200	-0.11106000
H	-5.23552300	2.70237100	-0.12965600
C	1.46274700	3.69746600	-0.40281900
C	0.80171300	4.89239800	-0.30519800
N	-0.52156000	4.57445400	-0.17456100
C	-5.22383600	-0.01515900	-0.09345800
C	-5.04820600	-1.35954100	-0.08272900
H	-6.22152400	0.41286200	-0.10932300
H	-5.90294500	-2.02907900	-0.08740400

N	2.15009800	-4.40905300	0.23891900
N	2.28286000	-3.10692000	0.26917800
C	0.83916000	-4.59158900	0.11250500
Am	0.81669900	0.14200800	0.02463200
N	0.20201000	0.41810100	2.89745400
O	-0.07261800	0.54603200	4.05784800
O	0.16567600	-0.70416700	2.30767000
O	0.54074900	1.40423900	2.16721700
N	3.77763800	0.37435500	0.21189000
O	3.16026900	-0.61713400	0.72227200
O	3.02921700	1.27723200	-0.26280900
O	4.97218900	0.44214600	0.18914600
N	0.79907400	-0.32023700	-2.86735500
O	0.79493300	-0.49968100	-4.05193400
O	1.71809400	-0.76592000	-2.11266600
O	-0.12304600	0.32599800	-2.27396500

AmR₃PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.51448200	-1.06194500	-0.00010200
C	-1.05353600	-2.83859200	-0.11335300
C	-2.11828800	-3.76221700	-0.11281100
H	-1.93267000	-4.82877800	-0.17960600
C	-2.71492200	0.37033200	0.01756200
C	-4.03285100	0.88020000	0.07478500
C	-4.17930500	2.27713000	0.12243700
C	-3.06742900	3.07986000	0.13458300
H	-5.17363400	2.71095500	0.16824900
H	-3.17294500	4.15677100	0.21056900
N	-1.63680500	1.16587500	-0.01320500
C	-3.64422900	-1.90987000	0.00487800
C	0.33529500	-3.23786100	-0.26163600
H	0.28990400	-5.35511100	-0.18741200
H	2.78190100	-5.31851500	-0.57455200
H	3.40990300	-2.61042300	-0.73683200
C	-1.79804000	2.47801500	0.06967100
H	-1.11665100	5.28506200	-0.10657600
H	1.38709600	5.77934700	0.16881100
C	-0.56091000	3.24363100	0.14289000
N	0.62067300	2.70110300	0.32225700
N	1.32267200	-2.37768300	-0.42519300
N	-1.25954700	-1.53025100	-0.02892000
C	-3.40383700	-3.29519600	-0.04032400
H	-4.24194800	-3.98567100	-0.03445600
C	2.46133000	-3.10014600	-0.57933300

C	2.16558500	-4.43666600	-0.50630300
C	0.92747000	4.80345000	0.19475400
N	0.81502100	-4.50655200	-0.30823100
C	-4.95791100	-1.35496800	0.05138800
C	-5.14625100	-0.01207600	0.08788900
H	-5.80773800	-2.03086700	0.05826600
H	-6.14790900	0.40480000	0.12792200
N	1.55660900	3.67264100	0.35228600
N	-0.40929300	4.59105000	0.06416900
Am	0.87079700	0.12277800	-0.00530100
N	0.25573000	-0.52102500	2.81997100
O	0.00695000	-0.79016500	3.96417500
O	0.92767200	-1.29494200	2.07193100
O	-0.14991000	0.54708500	2.27035200
N	3.75692600	0.41101500	0.24314900
O	2.95585900	0.83793800	1.12442800
O	3.20803200	-0.12743400	-0.77819800
O	4.94731200	0.49295500	0.35271000
N	0.20302700	0.61140400	-2.85760000
O	-0.08821800	0.83308900	-4.00232100
O	0.03093400	-0.52095100	-2.31861400
O	0.69108700	1.50580500	-2.09864500

AmR₃PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.70243100	0.63699000	0.02342100
C	1.56711600	2.63986900	-0.02650100
C	2.77192500	3.36994800	-0.03376800
H	2.76772600	4.45339300	-0.08442100
C	2.65760900	-0.80661700	0.01182300
C	3.86947200	-1.53274400	0.01090600
C	3.78337700	-2.93802600	0.01908200
C	2.55630100	-3.54434200	0.05803700
H	4.69382000	-3.52996100	0.00945200
H	2.44406000	-4.62141700	0.08971300
N	1.45694500	-1.41000900	0.01501400
C	3.96006000	1.28268300	0.01186500
C	0.26650200	3.27466300	-0.14862600
H	0.66681800	5.34336200	0.06143100
H	-1.79531100	5.75037000	-0.31874800
H	-2.86791200	3.20170300	-0.63518500
C	1.40831700	-2.73252900	0.06654900
H	-3.05196900	-3.09866300	0.56006300
H	-2.01113400	-5.48504400	0.44869800

C	0.07379900	-3.30902000	0.18577000
N	-1.01896300	-2.51589600	0.31034100
N	-0.84907400	2.60224000	-0.35975500
N	1.54384300	1.31437900	0.03391300
C	3.95960800	2.68892100	-0.00120800
H	4.90380900	3.22537400	-0.00676700
C	-1.85080400	3.51518900	-0.46057000
C	-2.01291700	-3.36305400	0.43387600
C	-1.33564600	4.77532300	-0.30876800
N	0.00738800	4.60565300	-0.11574500
C	5.16122600	0.51412500	0.00596400
C	5.11758600	-0.84163500	0.00568500
H	6.11321000	1.03633300	-0.00034000
H	6.03405600	-1.42386800	0.00199600
N	-0.18964200	-4.59973700	0.22895900
N	-1.51937000	-4.60939300	0.38552800
Am	-0.84104900	0.04321600	-0.01639300
N	-0.37023700	-0.51280300	-2.87600900
O	-0.19438800	-0.74441200	-4.04001400
O	-1.09969600	-1.24943000	-2.13981700
O	0.16743800	0.47446500	-2.28886600
N	-3.79765600	0.07374100	-0.04243800
O	-3.09620800	0.84934700	-0.76099700
O	-3.13916000	-0.70573200	0.71561300
O	-4.99631700	0.07348000	-0.07622300
N	-0.44550800	0.48897500	2.87876400
O	-0.29029500	0.68322200	4.05315300
O	-0.12067500	-0.60073200	2.31954100
O	-0.93787600	1.37033800	2.10514000

AmR₃PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.64773500	0.75895800	0.01005900
C	-1.41918200	2.70537500	0.06270600
C	-2.58975700	3.49017900	0.07012500
H	-2.53565200	4.57246000	0.11556100
C	-2.67101400	-0.68663100	0.01902400
C	-3.91701400	-1.35563600	0.01246300
C	-3.89257400	-2.76116800	-0.00694700
C	-2.69203800	-3.42156500	-0.05118200
H	-4.82696800	-3.31419600	-0.00756700
H	-2.66412000	-4.50448300	-0.10339600
N	-1.50248200	-1.34375600	0.01893300
C	-3.87377100	1.46085500	0.02226900
C	-0.08987600	3.27686100	0.18090700

H	-0.39641900	5.37078700	0.06536500
H	2.08655500	5.64713000	0.41363500
H	3.04298500	3.04088900	0.62245900
C	-1.50565400	-2.66688600	-0.04662300
H	-0.45090500	-5.38231100	-0.04300200
H	2.91802800	-3.26014800	-0.67977800
C	-0.18686800	-3.27134300	-0.18533100
N	0.91674600	-2.57421300	-0.38833400
N	0.99664700	2.54704300	0.34810900
N	-1.45932200	1.37980200	0.00099300
C	-3.80801300	2.86585100	0.03685800
H	-4.72594000	3.44598500	0.04039500
C	2.04012700	3.40734900	0.46892500
C	1.88333200	-3.51033200	-0.50495900
C	1.58190300	4.69539600	0.37249400
N	0.23070300	4.59554400	0.19287800
N	0.13232600	-4.57618200	-0.18994900
C	-5.10970600	0.74852000	0.02395200
C	-5.13192200	-0.60771500	0.01845800
H	-6.03602600	1.31502400	0.03012700
H	-6.07508700	-1.14532900	0.01682000
N	1.44619000	-4.74768200	-0.38994600
Am	0.86385400	-0.00766500	-0.00880300
N	0.32867700	-0.55078500	2.85011900
O	0.10991900	-0.78792600	4.00627200
O	0.90132200	-1.38808300	2.08274800
O	-0.00679200	0.54156500	2.30305500
N	3.80417200	-0.08043300	0.01619100
O	3.13375100	0.65968600	0.80292300
O	3.11186700	-0.78880000	-0.78027400
O	5.00177900	-0.10741600	0.02462800
N	0.30180200	0.54076800	-2.85934100
O	0.06716900	0.78061500	-4.01187800
O	-0.13534000	-0.49842500	-2.27814500
O	0.99229400	1.31918700	-2.13071900

AmR₄PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.63882900	-0.72237900	-0.00008500
C	-1.43916900	-2.69193900	-0.00024700
C	-2.62280100	-3.45584000	-0.00024900
H	-2.57469800	-4.53882200	-0.00029500
C	-2.63831900	0.72415500	-0.00000800
C	-3.87389300	1.40885500	-0.00000400

C	-3.82888400	2.81493900	0.00000700
C	-2.62036800	3.45760200	-0.00000600
H	-4.75592400	3.38058500	0.00001900
H	-2.57150300	4.54055100	-0.00000300
N	-1.45770500	1.36731100	0.00003100
C	-3.87488700	-1.40620800	-0.00010300
C	-0.12988800	-3.33382000	-0.00031800
H	-0.32279900	-5.58472000	-0.00073000
H	2.23187500	-5.38947500	-0.00062000
C	-1.43727500	2.69287100	0.00000200
H	-0.31889600	5.58487700	-0.00061400
H	2.23564400	5.38785000	-0.00044600
C	-0.12754800	3.33384300	-0.00004300
N	1.02223700	2.60557000	0.00016000
N	1.02040400	-2.60634900	-0.00015100
N	-1.45867000	-1.36636800	-0.00016700
C	-3.83086400	-2.81232500	-0.00018000
H	-4.75830000	-3.37732100	-0.00018000
N	0.28888000	-0.00012500	-2.89087200
N	0.28846500	-0.00014200	2.89100300
N	3.73252700	-0.00108500	0.00018600
O	0.39909100	-1.07075100	2.22023600
O	0.08331500	-0.00006700	4.07389500
O	0.40011900	1.07042400	2.22028900
O	0.39981400	-1.07075200	-2.22015200
O	0.40000100	1.07042000	-2.22009100
O	0.08392500	-0.00008000	-4.07380300
O	3.05217200	0.00212800	-1.07380600
O	3.05215000	-0.00391300	1.07416900
O	4.93150400	-0.00141900	0.00019900
Am	0.82564300	-0.00028300	0.00015200
N	2.04495700	-3.38052200	-0.00026500
N	2.04732600	3.37902900	0.00002400
N	1.57801300	-4.62348700	-0.00051500
N	1.58124800	4.62231800	-0.00027400
C	0.23273900	-4.66157900	-0.00054700
C	0.23600100	4.66135000	-0.00033800
C	-5.10017600	-0.67640600	-0.00005400
H	-6.03486200	-1.22898600	-0.00006100
C	-5.09969700	0.67991900	-0.00001600
H	-6.03399200	1.23316100	0.00000500

AmR₄PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.44572700	1.34085400	-0.03277100
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C	-0.81993300	2.97524200	0.03545200
C	-1.78588100	3.99766400	-0.01363800
H	-1.47616700	5.03620700	0.00252500
C	-2.79311700	-0.06355100	-0.02309500
C	-4.15841700	-0.42708100	-0.06618800
C	-4.46135700	-1.80046700	-0.06782300
C	-3.44874000	-2.71952400	-0.04640500
H	-5.49882400	-2.11992100	-0.09875000
H	-3.66464600	-3.78148900	-0.07011100
N	-1.80457100	-0.97790500	0.02358000
C	-3.48303200	2.30075200	-0.07629100
C	0.59684300	3.28519300	0.15914200
H	1.02563800	5.50793500	0.19974100
C	-2.11536500	-2.26784300	-0.00661500
H	-1.75195200	-5.34432400	0.13995000
H	0.76571700	-5.79311100	-0.01864800
C	-1.01001900	-3.21657900	-0.02726500
N	0.27910000	-2.79933700	-0.14216600
N	1.46436800	2.28349100	0.26112000
N	-1.14657800	1.68631300	0.00529700
C	-3.10969200	3.65689900	-0.07586300
H	-3.87801700	4.42331200	-0.11565200
N	1.07963300	-3.80442500	-0.14480800
N	0.32195800	-4.88909400	-0.03493300
C	1.33752700	4.47564700	0.23894900
C	-0.98809500	-4.59093800	0.04083400
C	-4.84720200	1.88902100	-0.11653200
H	-5.61961600	2.65127200	-0.15097400
C	-5.17335100	0.57332500	-0.11144500
H	-6.21215200	0.25924500	-0.14317200
N	2.62614700	2.85446500	0.38960900
H	3.45069400	2.27231300	0.49963500
N	2.62170600	4.16589900	0.38612800
Am	0.78357400	-0.21969900	0.02323300
N	0.50440700	0.14448000	-2.86432400
O	0.43051500	0.28670500	-4.05050500
O	1.05656700	1.00678600	-2.10672900
O	0.03176100	-0.86799900	-2.26398900
N	3.71142500	-0.63122000	-0.28855900
O	2.85346100	-1.31649500	-0.90735600
O	3.23325600	0.20513000	0.55819200
O	4.89096100	-0.73844000	-0.46850800
N	0.41807400	-0.43633000	2.93003300
O	0.26559500	-0.54635500	4.11254600

O	0.51268400	0.68524800	2.34975600
O	0.49062800	-1.44783500	2.15644100

AmR₄PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.68863100	0.49997800	0.01006600
C	-1.66214800	2.55666200	-0.08056800
C	-2.89856300	3.22521900	-0.11917300
H	-2.94927900	4.30583800	-0.19843200
C	-2.56499000	-0.94094400	0.04235200
C	-3.73939700	-1.72386700	0.07788600
C	-3.57895800	-3.12026300	0.13348800
C	-2.32087300	-3.65858400	0.16957200
H	-4.45581700	-3.76032600	0.16032100
H	-2.18090900	-4.73158000	0.23593600
N	-1.33509500	-1.48122200	0.04291100
C	-3.97849000	1.08078600	-0.01619800
C	-0.38796600	3.25772200	-0.17678700
H	-0.84218000	5.32686600	0.04369600
C	-1.20636700	-2.79778600	0.12681000
H	0.18321300	-5.57419200	0.15723200
H	2.69982000	-5.12978800	0.35548700
C	0.15298900	-3.31646300	0.20615100
N	1.22155100	-2.47948000	0.30550300
N	0.76539900	2.65740200	-0.35796600
N	-1.57046500	1.23825700	0.00341700
C	-4.05082800	2.48292500	-0.07433900
H	-5.02140400	2.96913200	-0.09891700
N	2.31521900	-3.15002500	0.37222100
N	1.97460500	-4.43185700	0.31966000
C	0.64308700	-4.60173900	0.21773600
C	-5.13882300	0.25135000	0.01140800
H	-6.11704000	0.72196000	-0.00637600
C	-5.02227900	-1.09882400	0.05985900
H	-5.90676100	-1.72823600	0.08451600
N	1.74657600	3.58219400	-0.41345600
H	1.67901200	5.69720000	-0.26260500
C	1.17344600	4.74398000	-0.26843900
N	-0.17051700	4.59707600	-0.12166500
Am	0.87697800	0.08719700	-0.02584800
N	3.75927100	0.29449400	-0.02778000
O	3.09941900	-0.02450500	1.01317600
O	4.95326800	0.38056000	-0.02868600
O	3.05848300	0.51162200	-1.06662900

N	0.18085400	-0.52232500	-2.84220600
O	-0.10681800	-0.78883800	-3.97774700
O	-0.14748600	0.57329000	-2.29694800
O	0.82191700	-1.32728800	-2.09920800
N	0.23906300	0.51500000	2.83809900
O	-0.02681400	0.70305000	3.99478100
O	0.58993500	1.45787800	2.06297400
O	0.17384400	-0.63052900	2.30261300

AmR₄PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.58438300	-0.97611500	-0.01573500
C	-1.20150900	-2.80883400	0.08101600
C	-2.28793900	-3.70073000	0.05712300
H	-2.10012800	-4.76676300	0.10114000
C	-2.73329100	0.46090300	-0.01735400
C	-4.03401800	1.01133200	-0.06429500
C	-4.14050600	2.41350600	-0.08510200
C	-3.00739300	3.18117800	-0.08413400
H	-5.12265000	2.87575500	-0.11806000
H	-3.07064100	4.26252500	-0.12909600
N	-1.62683900	1.22579400	0.01883100
C	-3.74052800	-1.78866400	-0.03799700
C	0.16805300	-3.29008300	0.22941300
C	-1.75226600	2.54433600	-0.03925800
H	-0.90166600	5.52982600	0.07897900
H	1.65137700	5.56828200	-0.15691600
C	-0.51535000	3.31183800	-0.09490300
N	0.68650900	2.69204800	-0.24504500
N	1.20280300	-2.42424600	0.36890300
N	-1.34483200	-1.49390100	0.01805500
C	-3.55384900	-3.18387700	-0.01382100
H	-4.41931900	-3.83948600	-0.03734400
N	1.63777000	3.55604200	-0.27899900
N	1.06764500	4.74758700	-0.15509600
C	-0.27113100	4.66407000	-0.03818600
C	-5.03495800	-1.19094700	-0.07949000
H	-5.90631900	-1.83846500	-0.09955600
C	-5.17620100	0.15764600	-0.09332800
H	-6.16266800	0.61011000	-0.12717900
H	2.39264600	-5.31743200	0.53953300
C	2.25030800	-3.20044000	0.51383500
H	3.26698200	-2.86426800	0.65303000
N	1.84349300	-4.47755200	0.46451800
N	0.51893100	-4.55913900	0.28528200

Am	0.84109100	0.09324600	0.01187600
N	0.36925000	0.53302400	2.89629300
O	0.18669000	0.73249600	4.06561600
O	0.07010700	-0.56231700	2.33564000
O	0.86835800	1.41668700	2.12865500
N	3.75579600	0.22633200	-0.26126300
O	3.19102700	-0.42080700	0.68486800
O	4.94680700	0.23243900	-0.40004200
O	2.97207100	0.84566300	-1.03599200
N	0.36778500	-0.41839800	-2.85269100
O	0.20660600	-0.62712600	-4.02298500
O	0.93657400	-1.25854000	-2.08548700
O	-0.02695000	0.64621200	-2.28914800

AmR₄PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.61308100	0.84560200	-0.03517000
C	1.32098600	2.74545000	0.07217700
C	2.45449200	3.57693100	0.06329000
H	2.35683800	4.65525900	0.12559400
C	2.68669300	-0.59855700	-0.04443900
C	3.95689500	-1.21381200	-0.09444600
C	3.99057200	-2.61984700	-0.12424700
C	2.81882700	-3.32698600	-0.12795500
H	4.94698700	-3.13296700	-0.15929700
H	2.82609500	-4.40990100	-0.17777400
N	1.54251800	-1.30342300	-0.01210200
C	3.81148900	1.59736500	-0.04832400
C	-0.03278400	3.26307700	0.22959900
C	1.59771800	-2.62650700	-0.07820300
H	0.59353500	-5.56609600	-0.01280000
H	-1.96016200	-5.46629200	-0.21594200
C	0.32202800	-3.32717500	-0.13384900
N	-0.84768300	-2.64263900	-0.25574500
N	-1.09117600	2.49608700	0.42302800
N	1.40482000	1.42557600	-0.00336900
C	3.69466900	2.99753800	-0.01074300
H	4.59063100	3.61073400	-0.02259500
N	-1.84253500	-3.45487500	-0.29585900
N	-1.33416000	-4.67734500	-0.20402400
C	0.00798800	-4.66607900	-0.10237300
C	5.07357800	0.93445600	-0.09206000
H	5.97795500	1.53497300	-0.10506200
C	5.14218300	-0.41952300	-0.11605300
H	6.10366700	-0.92271700	-0.15177100

C	-2.11328400	3.36785200	0.56226900
H	-3.12989100	3.05073900	0.73633400
N	-0.43250800	4.54505900	0.26149700
H	0.09910800	5.38853200	0.12916800
N	-1.75350100	4.63154800	0.46996100
Am	-0.86603300	-0.04063400	0.02900600
N	-0.24104700	-0.57139100	2.87205500
O	0.01820800	-0.81073400	4.01931100
O	0.12718300	0.49728200	2.29890400
O	-0.89279500	-1.38153800	2.14106400
N	-3.76996100	-0.06846000	-0.21200600
O	-3.16889300	0.50350100	0.75936600
O	-4.96261700	-0.05245200	-0.31858800
O	-3.01406100	-0.64431500	-1.04964800
N	-0.33513400	0.46828300	-2.83206900
O	-0.13397500	0.68150000	-3.99594000
O	-0.82947800	1.34682800	-2.05722600
O	-0.05605200	-0.64002500	-2.28447000

AmR₅PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.70511000	0.81385200	-0.04317000
C	-1.45383600	2.74825500	-0.00414300
C	-2.60840400	3.55038900	0.00500200
H	-2.52014600	4.63035000	0.03191700
C	-2.75373400	-0.63135200	-0.05578900
C	-4.01301300	-1.27328100	-0.08550900
C	-4.02121400	-2.67893500	-0.12599400
C	-2.83709200	-3.36623500	-0.15642200
H	-4.96903900	-3.20849400	-0.14638400
H	-2.82040500	-4.44858200	-0.21140900
N	-1.59732100	-1.31697900	-0.04869600
C	-3.91917400	1.53854400	-0.03584200
C	-0.12052700	3.33414600	0.04751000
H	-0.13480600	5.59623800	0.05597100
C	-1.63155100	-2.64300400	-0.12245000
H	-0.52320300	-5.56867900	-0.08143200
C	-0.34209600	-3.31735600	-0.19318300
N	0.76633500	-2.58703600	-0.29960800
N	0.93238600	2.52160300	0.10261700
N	-1.50571200	1.42094100	-0.04076700
C	-3.83520600	2.94191000	-0.01573100
H	-4.74632700	3.53268000	-0.01112500
N	1.70231800	4.59497400	0.15677900

N	1.38193800	-4.71342600	-0.24198500
C	0.37575600	4.64614100	0.08098100
C	0.05597900	-4.66209700	-0.16299700
C	-5.16885300	0.85075200	-0.05098400
H	-6.08379600	1.43521000	-0.04373700
C	-5.21412400	-0.50363800	-0.07760800
H	-6.16602200	-1.02547700	-0.09450000
N	1.96716600	3.31344700	0.16264500
H	2.89750800	2.91750000	0.24330800
N	1.73980700	-3.45721000	-0.32047200
H	2.70098500	-3.13538700	-0.34949200
N	0.33718000	-0.32742600	2.90748700
N	0.82887700	0.33277800	-2.86880700
N	3.75617000	-0.13578500	0.23049700
O	-0.09954600	-0.30344500	-2.27068700
O	0.84092900	0.48042100	-4.05640200
O	1.73451100	0.80140700	-2.11148500
O	0.74225800	-1.28525300	2.17248100
O	0.14364800	0.77275300	2.30282400
O	0.14550800	-0.45869600	4.08223900
O	3.03908000	-1.10841900	-0.16683100
O	3.09957200	0.87368900	0.63068500
O	4.95038000	-0.17497200	0.22792800
Am	0.78509200	-0.03278900	0.02022100

AmR₅PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.42561300	-1.33093400	0.00603300
C	0.80075200	-2.95763100	-0.11271000
C	1.76528700	-3.98252400	-0.09229600
H	1.45589200	-5.01998900	-0.14558100
C	2.77231600	0.07332000	0.01458000
C	4.13682700	0.44416400	0.07509300
C	4.43094700	1.81752900	0.11124700
C	3.41130700	2.73424000	0.10883000
H	5.46562800	2.14314700	0.16023900
H	3.62930000	3.79451200	0.17755500
N	1.78454100	0.98043800	-0.03004200
C	3.46340500	-2.28918100	0.02518600
C	-0.61675200	-3.24873000	-0.27118700
H	-1.07272000	-5.46360600	-0.34406900
C	2.08680700	2.26891000	0.04121300
H	1.71502000	5.12889400	-0.18111700
C	0.94044600	3.16553300	0.10063700
N	-0.29316000	2.75838300	0.28899700

N	-1.46951300	-2.23322400	-0.38146400
N	1.12810300	-1.67243600	-0.03262800
C	3.08980200	-3.64485600	-0.01068500
H	3.85687100	-4.41315900	0.01167100
N	-2.64807400	-4.09900700	-0.54871800
C	-1.37088300	-4.42719800	-0.37954000
C	4.82710700	-1.87250000	0.07742800
H	5.60174100	-2.63311900	0.09621000
C	5.15302300	-0.55668700	0.10370100
H	6.19168100	-0.24389700	0.14745200
N	-2.63676100	-2.78887200	-0.53868500
H	-3.45417700	-2.19542400	-0.64471900
N	-1.11801300	3.82682700	0.30471200
N	0.93616000	4.51934600	0.00103300
C	-0.36933400	4.87893100	0.12972400
H	-0.71957300	5.89874100	0.08958700
Am	-0.82717100	0.23819200	0.00192400
N	-0.38852900	-0.42498000	2.83357100
O	-0.22632700	-0.69624100	3.98966000
O	0.21981400	0.53358400	2.26605800
O	-1.17153000	-1.08742500	2.08222000
N	-3.72918000	0.63193500	0.29977800
O	-2.87749300	1.26928300	0.97416900
O	-3.23945700	-0.14808000	-0.59678100
O	-4.90958000	0.72873700	0.46895200
N	-0.28796800	0.60434300	-2.87923600
O	-0.04719900	0.77624100	-4.04167000
O	-0.64796400	1.55522300	-2.11340100
O	-0.18923100	-0.52856000	-2.32105700

AmR₅PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.63837400	1.01153000	-0.06257300
C	1.25488800	2.85115100	-0.02418100
C	2.35028100	3.73311400	-0.02708500
H	2.18582700	4.80422400	-0.00287900
C	2.78774800	-0.42520800	-0.06415200
C	4.08715900	-0.98165900	-0.08183700
C	4.19366700	-2.38478100	-0.10412900
C	3.06070800	-3.15289400	-0.13381000
H	5.17656800	-2.84643200	-0.11066300
H	3.09604900	-4.23496600	-0.17167000
N	1.68023600	-1.18831800	-0.06008900
C	3.79915200	1.81885700	-0.06167300
C	-0.11525200	3.34016800	0.04896900

H	-0.26522900	5.59703700	0.01793800
C	1.81382300	-2.50499400	-0.11973000
C	0.57182300	-3.26521700	-0.20664300
N	-0.62866400	-2.64137500	-0.31808800
N	-1.10399400	2.45437900	0.14684300
N	1.39899900	1.53107200	-0.05958300
C	3.61695100	3.21297600	-0.05168900
H	4.48416500	3.86661100	-0.05440100
N	-2.02147900	4.46757200	0.18577400
C	-0.70448000	4.61316500	0.07367200
C	5.09289800	1.21808700	-0.06985300
H	5.96563400	1.86405600	-0.06820000
C	5.23186100	-0.13042600	-0.08038900
H	6.21772400	-0.58509800	-0.08916900
N	-2.19138200	3.17038000	0.22065000
H	-3.08635400	2.70486300	0.33283300
C	-1.49478000	-3.62792500	-0.37284000
H	-2.56663600	-3.52205300	-0.44566700
N	-0.82459000	-4.78592200	-0.30781100
H	-1.18697200	-5.72480800	-0.32059400
N	0.49435100	-4.58022300	-0.20093600
Am	-0.80398600	-0.10332000	0.02661200
N	-0.87142100	0.29548800	-2.87152300
O	-0.90247200	0.44490800	-4.05948700
O	0.07055400	-0.33305000	-2.28897600
O	-1.77089700	0.75544900	-2.10160800
N	-3.76747900	-0.31861700	0.25828900
O	-3.02904900	-1.25118800	-0.17792900
O	-3.13949400	0.69542000	0.70248600
O	-4.96227800	-0.38528700	0.25776900
N	-0.25262000	-0.39935900	2.90639000
O	-0.01972800	-0.53213600	4.07435100
O	-0.61994000	-1.37261900	2.17149200
O	-0.14353900	0.71610300	2.31097500

AmR₅PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.59846300	1.09033300	-0.06292900
C	-1.16070900	2.88512300	-0.00886700
C	-2.23009700	3.79952100	-0.01738300
H	-2.03382500	4.86514500	0.01079000
C	-2.79102100	-0.34255600	-0.06781800
C	-4.10794100	-0.85998400	-0.10068100
C	-4.25231300	-2.25730900	-0.13032600
C	-3.13920500	-3.05687600	-0.14907000

H	-5.24632000	-2.69338000	-0.15411800
H	-3.24082600	-4.13527800	-0.20244300
N	-1.70889300	-1.13577800	-0.05024400
C	-3.73497600	1.93012800	-0.06988700
C	0.22218200	3.33297900	0.07376000
H	0.43486900	5.58525500	0.06646800
C	-1.87235900	-2.44951300	-0.11252900
H	-1.18541200	-5.27214100	-0.05042400
C	-0.63668100	-3.21782800	-0.19017000
N	0.56084600	-2.67510500	-0.32862800
N	1.18531700	2.41865500	0.16634600
N	-1.34489600	1.57027400	-0.04901000
C	-3.51163000	3.31863200	-0.05414300
H	-4.35845600	3.99833400	-0.06247600
N	2.15795100	4.40544100	0.22935600
C	0.84626900	4.58890900	0.11357100
C	-5.04613800	1.36734600	-0.09195200
H	-5.89906100	2.03922500	-0.09662200
C	-5.22732000	0.02395300	-0.10838600
H	-6.22639200	-0.40023500	-0.12870200
N	2.29118200	3.10337000	0.25176000
H	3.17208900	2.61043400	0.36272500
N	-0.49256600	-4.55237300	-0.16711000
C	1.40148100	-3.73400900	-0.37623600
H	2.47018300	-3.62682700	-0.47490600
N	0.79675700	-4.89913100	-0.28277000
Am	0.82704200	-0.13817200	0.02794200
N	0.17403400	-0.40995300	2.89136600
O	-0.12115300	-0.53724000	4.04595500
O	0.49004600	-1.40211900	2.15745400
O	0.18416800	0.71674700	2.30893200
N	3.77524800	-0.40917100	0.22024300
O	3.17014000	0.60719600	0.69749100
O	3.01297500	-1.31828100	-0.22235900
O	4.96762100	-0.49267600	0.19829600
N	0.81472300	0.30032100	-2.86424400
O	0.80861000	0.47110600	-4.04924900
O	-0.11732600	-0.32574200	-2.26208500
O	1.74363800	0.73436900	-2.11517600

AmR₆PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.63092200	0.72441400	-0.00012200
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C	1.42704200	2.68501000	-0.00003900
C	2.60433300	3.45542500	-0.00009900
H	2.56445700	4.53926200	-0.00008800
C	2.63121000	-0.72341300	-0.00013400
C	3.86686200	-1.40941700	-0.00020300
C	3.81836400	-2.81385200	-0.00021400
C	2.60570500	-3.45443700	-0.00015800
H	4.74267500	-3.38356100	-0.00026800
H	2.56626000	-4.53828900	-0.00017200
N	1.45244400	-1.35935200	-0.00007900
C	3.86630000	1.41090800	-0.00018200
C	0.09941400	3.28690800	0.00004300
H	0.42342000	5.39560600	-0.00002500
C	1.42810900	-2.68448800	-0.00008700
H	0.42553800	-5.39547400	-0.00008300
C	0.10071500	-3.28690400	-0.00003600
N	-1.02083900	-2.60493000	-0.00001300
N	-1.02187700	2.60450100	0.00011700
N	1.45190200	1.35988300	-0.00005300
C	3.81724700	2.81532300	-0.00016900
H	4.74133300	3.38539700	-0.00021600
N	-0.23532500	0.00001600	-2.87964400
N	-0.23545600	-0.00012800	2.87976100
N	-3.76349300	-0.00061200	0.00015100
O	-0.38176200	1.07006600	2.21593700
O	0.03435000	-0.00010700	4.05027000
O	-0.38150500	-1.07034300	2.21591600
O	-0.38167000	-1.07023400	-2.21591900
O	-0.38199300	1.07017600	-2.21585000
O	0.03389700	0.00009400	-4.05028700
O	-3.08145300	-0.00070400	1.07429300
O	-3.08153600	-0.00031700	-1.07404400
O	-4.96079000	-0.00076200	0.00019700
N	-2.06392800	-3.45844500	0.00006800
N	-0.20642700	4.61201900	0.00004100
N	-0.20461200	-4.61213300	-0.00005000
N	-2.06529700	3.45761100	0.00018100
C	-1.56424700	4.66195600	0.00017900
H	-2.13318600	5.57882700	0.00023000
C	-1.56241300	-4.66259700	0.00002100
H	-2.13099700	-5.57968800	0.00004700
C	5.09201300	0.67916500	-0.00025200
H	6.02722900	1.23068000	-0.00029900
C	5.09228400	-0.67718500	-0.00026200

H	6.02772000	-1.22832600	-0.00031600
Am	-0.87292200	-0.00018200	0.00004200

AmR₆PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.74550300	0.28414800	0.00117600
C	-1.89757000	2.42064800	-0.03661300
C	-3.18497100	2.98282300	-0.09539200
H	-3.32427300	4.05633600	-0.16428800
C	-2.50117900	-1.14014400	0.00956600
C	-3.60109100	-2.02539700	-0.00462100
C	-3.32166500	-3.40516600	0.02661700
C	-2.02312500	-3.83469400	0.09587600
H	-4.14057200	-4.11818100	0.00925400
H	-1.76448200	-4.88559800	0.14485500
N	-1.22978900	-1.57050000	0.04080800
C	-4.07909100	0.75316600	-0.05158800
C	-0.68668200	3.22744200	-0.10798000
H	-1.30844700	5.24509600	0.17148100
H	1.17550600	5.82718400	-0.11635100
C	-0.99760100	-2.87240600	0.11019800
H	2.75085900	-5.13575800	0.59805500
C	0.40175700	-3.25977500	0.25607200
N	1.37993300	-2.32737000	0.37204800
N	0.51110300	2.72713400	-0.30277900
N	-1.69256900	1.11393000	0.03643300
C	-4.27061500	2.14468900	-0.08856500
H	-5.27845800	2.54652100	-0.13088000
N	1.41419200	3.73007600	-0.32709800
C	0.74874300	4.83674900	-0.15109000
N	-0.57925300	4.57777500	-0.01347400
C	-4.93181100	-1.51058800	-0.04750800
H	-5.75960700	-2.21313700	-0.06127900
C	-5.16304000	-0.17434500	-0.07225100
H	-6.17755500	0.21062900	-0.10914300
C	2.47437400	-3.03242600	0.52938100
H	3.46809100	-2.63078900	0.66087800
N	2.14940600	-4.33405200	0.50750900
N	0.83251100	-4.50277400	0.33626500
Am	0.85772400	0.16499900	-0.00817400
N	0.31437800	0.57110700	2.87623700
O	0.08248600	0.75697400	4.03973200
O	0.19149900	-0.56378200	2.32901500
O	0.68869800	1.50863400	2.10263900
N	3.75151300	0.46582300	-0.27700400

O	3.22255800	-0.16026000	0.70513700
O	2.93450600	0.98882700	-1.08687200
O	4.94016300	0.53586900	-0.41459400
N	0.28931600	-0.47818200	-2.83468600
O	0.07499300	-0.74149800	-3.98563000
O	1.00759400	-1.21667900	-2.09114500
O	-0.19695200	0.54737100	-2.26897700

AmR₆PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.70391800	0.45302700	-0.02285200
C	1.72303700	2.53132200	-0.06824700
C	2.97337000	3.17156300	-0.13563500
H	3.04600800	4.25129200	-0.20908700
C	2.55047500	-0.98517800	-0.00631000
C	3.70596900	-1.79912800	-0.01251100
C	3.51174900	-3.19058800	0.03439600
C	2.24062500	-3.69929900	0.10879200
H	4.37168900	-3.85338900	0.02818600
H	2.08429700	-4.77040600	0.17583500
N	1.31178100	-1.49458400	0.02425800
C	4.00511700	1.00276200	-0.08224300
C	0.46328900	3.25976200	-0.13318500
H	0.95891300	5.31830900	0.10477400
H	-1.56059000	5.73542600	-0.14853000
C	1.15341200	-2.80721700	0.10740500
C	-0.22856900	-3.24727700	0.25795800
N	-1.24734700	-2.42144000	0.41951000
N	-0.70316400	2.68165700	-0.30117000
N	1.60167800	1.21435500	0.01210300
C	4.10937700	2.40337300	-0.12814900
H	5.08975300	2.86758500	-0.17563100
N	-1.66802800	3.62402600	-0.32555800
C	-1.07187600	4.77380900	-0.17598300
N	0.27159400	4.60204700	-0.05596700
C	5.00211400	-1.20298800	-0.06143800
H	5.87305000	-1.85116200	-0.06977800
C	5.14591300	0.14489700	-0.09824000
H	6.13372500	0.59343800	-0.14007800
C	-2.31487100	-3.23430300	0.56766100
H	-3.31517500	-2.86077200	0.72407000
N	-0.69602500	-4.50560000	0.31453200
H	-0.20830800	-5.37919600	0.21207300
N	-2.02125500	-4.51753400	0.50909700

Am	-0.88467800	0.10170100	0.00732100
N	-0.24366500	-0.51684200	-2.81566500
O	0.01373900	-0.77680100	-3.95916700
O	-0.87686200	-1.32033400	-2.06297700
O	0.11285900	0.56977400	-2.26842300
N	-3.77358200	0.27723000	-0.25306500
O	-2.98319200	0.76250900	-1.11509000
O	-3.20844200	-0.27471300	0.75291200
O	-4.96437000	0.32057700	-0.36631200
N	-0.22085900	0.58478300	2.85791900
O	0.06955000	0.80539000	4.00217800
O	0.00124200	-0.53187700	2.30227100
O	-0.75766600	1.46340100	2.11362800

AmR₇PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.72185000	-0.72136700	-0.12012200
C	1.53309100	-2.68007400	-0.23977500
C	2.70402500	-3.45736300	-0.23043300
H	2.62469000	-4.53647900	-0.28426600
C	2.72198400	0.72131300	-0.11992100
C	3.95528400	1.41028800	-0.10316400
C	3.91250300	2.81636900	-0.14998200
C	2.70466400	3.45734900	-0.22941100
H	4.83965200	3.38160400	-0.13386800
H	2.62553200	4.53649900	-0.28290400
N	1.53961500	1.35807300	-0.16817400
C	3.95501400	-1.41057400	-0.10354900
C	0.21500800	-3.29722000	-0.34063800
C	1.53360000	2.68027200	-0.23894700
C	0.21555600	3.29755500	-0.33946400
N	-0.90906000	2.53822700	-0.36615300
N	-0.90963100	-2.53792400	-0.36779200
N	1.53934800	-1.35789800	-0.16854900
C	3.91197600	-2.81663500	-0.15076400
H	4.83902300	-3.38204100	-0.13479000
C	-1.88297500	-3.41645700	-0.44881900
H	-2.93785000	-3.18887800	-0.45997600
C	-1.88246200	3.41669900	-0.44713300
H	-2.93732800	3.18906600	-0.45803200
C	5.17886000	-0.67856400	-0.05590400
H	6.11355300	-1.23048500	-0.02931100
C	5.17899100	0.67803500	-0.05572100
H	6.11379100	1.22976700	-0.02897900

N	-0.00956300	-4.59372500	-0.40959700
N	-0.00905600	4.59403900	-0.40857200
N	-1.34642100	4.64424100	-0.47831500
H	-1.81294400	5.53436200	-0.53317400
N	-1.34689600	-4.64398700	-0.47967700
H	-1.81338300	-5.53412900	-0.53450600
N	-1.32728700	0.00135200	-2.77699200
N	0.05961400	-0.00155600	2.90676200
N	-3.63881000	0.00007400	0.89729700
O	-0.15323800	1.07325400	2.26189400
O	0.44265700	-0.00229800	4.04281300
O	-0.15528700	-1.07557700	2.26119900
O	-2.27171800	0.00230200	-1.93092600
O	-0.15280100	-0.00011700	-2.28918900
O	-1.52536000	0.00180000	-3.96193400
O	-2.96493400	1.06903000	0.78163300
O	-2.96549100	-1.06903200	0.77965700
O	-4.81973900	0.00018800	1.10110900
Am	-0.80718100	0.00000100	0.12095300

AmR₇PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.64819400	0.84567700	0.00828500
C	1.37136100	2.75269300	0.06055000
C	2.50754100	3.58106400	0.05403400
H	2.37959900	4.65638900	0.08521900
C	2.71663200	-0.59720700	0.01958500
C	3.98394000	-1.22600700	0.00623600
C	4.00634700	-2.63119400	-0.00851100
C	2.82812500	-3.33145200	-0.03968300
H	4.95867500	-3.15270100	-0.01567300
H	2.83558600	-4.41482600	-0.08890600
N	1.56966700	-1.29328700	0.03018600
C	3.84906200	1.58895000	0.00797200
C	0.02850900	3.31090900	0.17266900
C	1.61812300	-2.61611000	-0.02809600
C	0.31998200	-3.26759500	-0.14815800
N	-0.80928200	-2.61378300	-0.35652800
N	-1.05490600	2.50367700	0.28790000
N	1.43873900	1.43070500	0.01022500
C	3.74343800	2.99280000	0.01676300
H	4.64518000	3.59780200	0.00825400
C	-2.06073900	3.33791100	0.40613100
H	-3.09710200	3.06002100	0.52546800
C	-1.74429500	-3.58578800	-0.44183500

H	-2.78904200	-3.37549200	-0.60881100
C	5.10743000	0.91570300	0.00210800
H	6.01482400	1.51201600	-0.00114400
C	5.17362500	-0.43881500	0.00058300
H	6.13370900	-0.94558800	-0.00677500
N	-0.25203200	4.59795300	0.21601100
N	-1.58252500	4.59024200	0.36328300
H	-2.08596500	5.45947300	0.42514500
N	-1.26285400	-4.80363400	-0.30363700
N	0.04615900	-4.58195900	-0.12061300
H	0.65837300	-5.36332700	0.04153200
Am	-0.85117800	-0.05048100	-0.01538200
N	-0.41082700	-0.48365000	2.87384200
O	-0.23416700	-0.67543600	4.04471200
O	-0.14002300	0.62058300	2.31437000
O	-0.87370900	-1.38334500	2.10120600
N	-0.40579900	0.48106200	-2.87881300
O	-0.23673400	0.70212100	-4.04499100
O	-1.17390500	1.19082000	-2.15603200
O	0.17917100	-0.46922600	-2.27337400
N	-3.79997600	-0.15401100	-0.00682700
O	-3.15069000	0.67118100	0.71154800
O	-4.99737000	-0.18035300	-0.02933800
O	-3.08634600	-0.94391000	-0.69810000

AmR₈PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.65905100	0.72196100	0.00437900
C	-1.46624300	2.68550800	-0.05372100
C	-2.64230700	3.45633100	-0.06221500
H	-2.59960600	4.53884400	-0.11163800
C	-2.65846400	-0.72407000	-0.00595400
C	-3.89406700	-1.41073900	0.00413800
C	-3.84982400	-2.81572700	0.02188800
C	-2.63949700	-3.45840200	0.06099800
H	-4.77598400	-3.38231600	0.02465800
H	-2.59590800	-4.54086300	0.11081100
N	-1.48016000	-1.36320300	-0.01125600
C	-3.89521500	1.40761900	-0.00610300
C	-0.13865800	3.27281300	-0.18352300
H	-0.37904900	5.38839300	-0.06194000
C	-1.46406700	-2.68660800	0.05282200
H	-0.37437000	-5.38841300	0.05837700
C	-0.13609400	-3.27283500	0.18357000
N	0.96051700	-2.56063700	0.37289600

N	0.95883300	2.56136900	-0.37047700
N	-1.48126500	1.36206500	0.01011600
C	-3.85211600	2.81264600	-0.02369000
H	-4.77873900	3.37847800	-0.02668100
N	0.30043500	0.54873400	2.84060000
N	0.30336200	-0.54776600	-2.83994200
N	3.80331000	0.00103300	-0.00119400
O	-0.07938200	0.52036800	-2.27433500
O	0.06373100	-0.79045900	-3.99006600
O	0.94605000	-1.35349400	-2.09519200
O	0.94769300	1.35229800	2.09755400
O	-0.08565700	-0.51750000	2.27357900
O	0.05954000	0.79167400	3.99040400
O	3.12078200	-0.73524000	0.77963300
O	3.11961500	0.73695000	-0.78127900
O	5.00007800	0.00125200	-0.00184400
N	0.19608800	4.57385900	-0.19434300
N	0.19981400	-4.57357700	0.19304700
C	1.93723000	3.48528300	-0.48534100
H	2.97046100	3.22257200	-0.65017600
C	1.93963800	-3.48384200	0.48751300
H	2.97247400	-3.22039900	0.65366200
N	1.51318900	4.72835800	-0.38336000
N	1.51682200	-4.72715800	0.38350300
C	-5.12068900	0.67594600	-0.00424800
H	-6.05590200	1.22732800	-0.00860100
C	-5.12013700	-0.68006800	0.00185000
H	-6.05490100	-1.23221300	0.00590900
Am	0.87739700	0.00026700	0.00070200

EuR₁PhR₁(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.65806900	0.75431100	-0.00430200
C	-1.44905500	2.71431300	0.01559900
C	-2.62308300	3.48900600	0.05046200
H	-2.55766100	4.57037100	0.07921400
C	-2.67186700	-0.69040400	-0.03446000
C	-3.91610200	-1.36108500	-0.05654000
C	-3.89132400	-2.76524600	-0.12787400
C	-2.69189100	-3.42090200	-0.19502500
H	-4.82662200	-3.31711800	-0.14446300
H	-2.64943900	-4.50058900	-0.27691300
N	-1.49788400	-1.34653100	-0.05809700
C	-3.88875200	1.44969300	0.02948900
C	-0.12845500	3.33259100	0.03843300

C	0.28894000	4.67694300	0.02403900
H	-0.31165900	5.57151200	-0.02600500
C	1.66537400	4.60993100	0.08522200
H	2.42023900	5.38077100	0.10197200
H	2.89084100	2.84899800	0.21651600
C	-1.50098900	-2.67157800	-0.16316800
C	0.17353000	-4.67777000	-0.24177400
C	1.54899400	-4.65749500	-0.33067800
H	-0.45440200	-5.55080200	-0.15896900
H	2.83617000	-2.94307100	-0.41485200
H	2.27845700	-5.45249800	-0.34345200
C	-0.19913800	-3.32032300	-0.26069400
N	0.87842000	-2.54732200	-0.36685400
N	0.92615800	2.52507500	0.10206400
N	-1.47326200	1.38691600	-0.02128300
C	-3.83603300	2.85457900	0.05457200
H	-4.76009300	3.42466000	0.08059800
N	1.98997600	3.30626400	0.12666600
N	1.91471000	-3.36609800	-0.40421500
N	0.53898000	-0.39623800	2.87306500
N	0.93888400	0.40206800	-2.82463400
N	3.78754000	-0.05569500	0.28950800
O	1.86444000	0.79403700	-2.05178400
O	0.97214800	0.57516700	-4.01015800
O	-0.03192400	-0.18770300	-2.25110300
O	0.05124600	0.60869300	2.26709400
O	1.14620000	-1.23123300	2.13387000
O	0.42763200	-0.54734900	4.05732400
O	3.08769700	0.92614500	0.68456300
O	3.11879600	-1.02886700	-0.16453800
O	4.98396200	-0.06079500	0.34289800
C	-5.13490300	-0.62162800	-0.01474700
H	-6.07393900	-1.16675900	-0.02315600
C	-5.12168600	0.73310300	0.02983200
H	-6.04996200	1.29561900	0.06052300
Eu	0.83299900	-0.01386000	0.02190200

EuR₁PhR₂(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.70393000	0.50512000	-0.10560200
C	-1.65493100	2.55086800	-0.24174500
C	-2.89242900	3.22681900	-0.23842100
H	-2.92171500	4.30849100	-0.30408500
C	-2.59753800	-0.93465900	-0.09993700

C	-3.77977400	-1.70999700	-0.09152000
C	-3.63204100	-3.10809800	-0.12614900
C	-2.37868900	-3.65748700	-0.16800900
H	-4.51505500	-3.74050800	-0.12123100
H	-2.24058400	-4.73214400	-0.19439100
N	-1.37308600	-1.48270600	-0.12807300
C	-3.98699000	1.09548000	-0.10175200
C	-0.39839000	3.26850500	-0.37902100
C	-0.14318900	4.61291900	-0.48499900
H	-0.78129200	5.48160500	-0.48222500
H	1.74039700	5.56649000	-0.68761500
C	-1.25918800	-2.80402200	-0.16247300
C	0.61199800	-4.63813100	-0.23323700
C	1.98016300	-4.47825600	-0.15318700
H	0.07555900	-5.56947400	-0.32475900
H	3.07291200	-2.64468300	0.10545500
H	2.78666700	-5.19514000	-0.15600100
C	0.10153600	-3.32811300	-0.16821300
N	1.09714700	-2.45195900	-0.06339500
N	0.78502200	2.57612600	-0.43355300
N	-1.57100000	1.22986800	-0.14675200
C	-4.04786800	2.50061500	-0.15433000
H	-5.01447000	2.99589700	-0.14469000
N	2.21303200	-3.15844200	-0.05836200
C	-5.05544700	-1.07400200	-0.05992400
H	-5.94625800	-1.69471500	-0.04036800
C	-5.15512300	0.27871700	-0.06347500
H	-6.12739400	0.76203800	-0.04730500
C	1.73566600	3.46566100	-0.56064600
H	2.79091500	3.24388300	-0.59503400
N	1.21499000	4.71298100	-0.60149700
N	3.74296200	0.22483700	0.73591200
O	4.93633700	0.25820600	0.85205800
O	3.05447300	1.23762400	0.43481900
O	3.07219700	-0.84156400	0.91268400
N	1.32103500	-0.20363900	-2.71697800
O	2.25738200	-0.31111100	-1.86814900
O	0.17334300	0.04144300	-2.23063400
O	1.50495700	-0.32369600	-3.89649100
N	0.06802800	0.35473300	2.87535800
O	-0.27944500	0.47347500	4.01783100
O	0.44333800	1.34485900	2.17350300
O	0.08041400	-0.76770100	2.28231300
Eu	0.86010200	0.08066300	0.10930200

EuR₁PhR₃(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.68612600	-0.49024600	-0.12188600
C	-1.63130800	-2.52933500	-0.25088400
C	-2.86210800	-3.21312700	-0.23594000
H	-2.90072300	-4.29593700	-0.28693700
C	-2.57819800	0.94882800	-0.12338600
C	-3.75812800	1.72458700	-0.12425000
C	-3.60511500	3.12170600	-0.17986600
C	-2.34903200	3.66424900	-0.24049900
H	-4.48473100	3.75873400	-0.18064400
H	-2.20753100	4.73761100	-0.29057500
N	-1.35148100	1.48823300	-0.15621300
C	-3.96854600	-1.08514600	-0.10970400
C	-0.35410500	-3.20594000	-0.38555100
H	-0.85339400	-5.25833400	-0.52582800
C	1.19554800	-4.74788900	-0.64364300
H	1.61515600	-5.73376200	-0.76214400
H	2.81242700	-3.23178300	-0.60010600
C	-1.23141100	2.80759200	-0.22410500
C	0.64805900	4.62648300	-0.36600100
C	2.01657000	4.45973200	-0.31455200
H	0.11503500	5.55932100	-0.46185100
H	3.10480000	2.62805000	-0.03965700
H	2.82706500	5.17122000	-0.34949100
C	0.13171600	3.32142100	-0.26457300
N	1.12444300	2.44012100	-0.16675000
N	0.80060200	-2.56677600	-0.41878700
N	-1.55434900	-1.20760400	-0.16878700
C	-4.02242100	-2.48920100	-0.15311600
H	-4.98555200	-2.99053400	-0.13502000
N	2.24391800	3.14050500	-0.20034600
C	-5.03379000	1.08659000	-0.08275600
H	-5.92486200	1.70701100	-0.06683400
C	-5.13593500	-0.26634700	-0.07311400
H	-6.10915100	-0.74714100	-0.04897400
C	1.77078000	-3.50773900	-0.57439400
N	-0.15117800	-4.53914200	-0.52143400
N	1.40881500	0.04580300	-2.69985900
O	1.61719900	0.08766200	-3.88213300
O	2.34525700	0.01986000	-1.84616400
O	0.23070000	0.02558200	-2.22319000
N	-0.05887700	-0.24224400	2.88022700
O	0.20539600	-1.27847900	2.19674300

O	0.14451500	0.86685200	2.29602900
O	-0.47946100	-0.30599700	4.00358500
N	3.68928600	-0.23461100	0.89464100
O	3.04784500	0.86650400	0.85442600
O	4.87299700	-0.27688100	1.07213200
O	2.97494100	-1.25976600	0.73749900
Eu	0.87268900	-0.07769000	0.13947800

EuR₁PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.69274500	0.36726800	0.00297100
C	-1.80546300	2.48673500	-0.05414400
C	-3.07778800	3.07363900	0.07765200
H	-3.18466000	4.15230100	0.10602400
C	-2.48297900	-1.06042000	-0.07101600
C	-3.60596100	-1.91774700	-0.05821100
C	-3.36404500	-3.29615300	-0.19974600
C	-2.08165200	-3.74899400	-0.35992500
H	-4.19958100	-3.99001700	-0.19417700
H	-1.87557300	-4.80467500	-0.49217900
N	-1.22543900	-1.51950300	-0.17924300
C	-4.01112500	0.86205900	0.12398300
C	-0.59909300	3.29444700	-0.18481300
C	-0.39516800	4.65243300	-0.25839200
H	-1.05116000	5.50657400	-0.22863700
H	1.49990500	5.59646500	-0.48175700
C	-1.02213600	-2.82213500	-0.34394900
C	0.95741300	-4.51806000	-0.59631200
C	2.31144900	-4.26433000	-0.65791100
H	0.48292000	-5.48663100	-0.60283400
H	3.29822400	-2.36601300	-0.52217400
H	3.16199300	-4.92513300	-0.72288600
C	0.36525000	-3.24426200	-0.50288600
N	1.30240400	-2.29988000	-0.52495300
N	0.62075000	2.69887900	-0.28045800
N	-1.62472100	1.17632100	-0.07846900
C	-4.17382400	2.25814300	0.17095900
H	-5.16991300	2.67839000	0.27353400
N	2.45986300	-2.92864400	-0.61547800
C	-4.91918900	-1.37877600	0.08391800
H	-5.76167800	-2.06339300	0.11002500
C	-5.11469600	-0.04014200	0.17784700
H	-6.11571400	0.36714800	0.28297800
N	1.54691500	3.58517900	-0.40668500
N	0.94139000	4.76254600	-0.39526000

N	0.22314600	-0.40231400	2.81415700
O	-0.02028400	-0.59058200	3.97431700
O	0.92472500	-1.20025700	2.12607700
O	-0.22073200	0.61263200	2.18823600
N	3.55556000	0.41165900	1.08825400
O	4.66268500	0.50670900	1.53550000
O	2.63495800	1.23840700	1.34377900
O	3.21802400	-0.53911800	0.31216400
N	1.10936400	0.45735100	-2.81795900
O	-0.00158700	0.18526500	-2.26712300
O	2.09825400	0.54894300	-2.02940100
O	1.21495300	0.61677900	-4.00364500
Eu	0.86878000	0.13478400	0.04294200

EuR₁PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.67614400	-0.61646300	-0.09766000
C	-1.55711300	-2.62245300	-0.26113600
C	-2.76356500	-3.34371400	-0.29970000
H	-2.74842600	-4.42319700	-0.39637600
C	-2.62092200	0.82651800	-0.05864900
C	-3.83093200	1.55616600	-0.04239300
C	-3.73734700	2.95916800	-0.04220400
C	-2.50595500	3.55713500	-0.06654600
H	-4.64391200	3.55693300	-0.02808000
H	-2.40961100	4.63653400	-0.07143600
N	-1.41762500	1.42244700	-0.06791100
C	-3.93690500	-1.25539900	-0.12694500
C	-0.26849400	-3.29153300	-0.37438900
C	0.12985800	-4.63595300	-0.41402600
H	-0.44916800	-5.54591600	-0.38690400
H	2.77321400	-3.10134000	-0.45228900
C	-1.35413600	2.74884400	-0.07789000
C	0.44086800	4.65966700	-0.11683400
C	1.81597900	4.55276200	-0.07729400
H	-0.13360300	5.57159700	-0.15926200
H	2.99038800	2.76068800	0.07179900
H	2.59269100	5.30178100	-0.07477900
C	-0.01576000	3.32882800	-0.08784000
N	1.01655500	2.49102900	-0.04055100
N	0.83894800	-2.55456100	-0.43321600
N	-1.51976800	-1.30062300	-0.13537400
C	-3.94684100	-2.65853300	-0.21725800
H	-4.89510700	-3.18740000	-0.23808600

N	2.10381100	3.24074700	-0.03647600
C	-5.08286900	0.87225900	-0.04032800
H	-5.99558600	1.45989000	-0.01461800
C	-5.13474800	-0.48191200	-0.08170900
H	-6.08903600	-0.99961800	-0.09079400
N	1.81276300	-3.42257100	-0.49382600
N	1.45657600	-4.68194100	-0.48297300
N	0.20144300	-0.38050000	2.88413200
O	-0.07685800	-0.53098400	4.03988600
O	0.65728000	-1.32369800	2.16502900
O	0.05551200	0.73291400	2.28892700
N	3.73730900	-0.18070600	0.58267600
O	3.07513100	0.87811600	0.81275100
O	3.02754600	-1.18747200	0.29032400
O	4.93142900	-0.22391300	0.64167300
N	1.21564400	0.31500900	-2.74336900
O	0.08291400	0.06972300	-2.21682200
O	2.18837400	0.36980100	-1.93338000
O	1.34736700	0.48263600	-3.92336300
Eu	0.83887600	-0.02758000	0.09818500

EuR₁PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.71274700	-0.35244000	0.06168200
C	1.78816100	-2.44868200	0.17996700
C	3.04861400	-3.06427800	0.08917100
H	3.14811400	-4.14446600	0.09824900
C	2.52048700	1.07930900	0.08216700
C	3.65444300	1.91995400	0.05712300
C	3.42628700	3.30519500	0.14628500
C	2.14578300	3.77507700	0.26973800
H	4.26859200	3.99057400	0.12914000
H	1.94877300	4.83694000	0.35962400
N	1.26635900	1.54970800	0.15331400
C	4.02577400	-0.87319900	-0.02119000
C	0.54978400	-3.20239300	0.32120800
H	1.11352200	-5.25394900	0.41390900
C	-0.94121600	-4.74214700	0.56939600
H	-1.39870800	-5.71290400	0.68259800
C	1.07586000	2.85899200	0.26937900
C	-0.88525200	4.57772100	0.50063800
C	-2.24305600	4.33954000	0.54640800
H	-0.39870300	5.53988500	0.53013700
H	-3.25109600	2.45291000	0.37781900

H	-3.08612400	5.00953000	0.61478200
C	-0.30839700	3.29812900	0.39610700
N	-1.25737800	2.36447900	0.39215400
N	-0.63638000	-2.64301900	0.38876000
N	1.63133300	-1.13510200	0.15559000
C	4.16285300	-2.27120500	-0.01619600
H	5.15143800	-2.71440700	-0.08848000
N	-2.40730600	3.00726900	0.48252100
C	4.96191400	1.35623000	-0.04504100
H	5.81463600	2.02759400	-0.08212600
C	5.14222500	0.01249400	-0.08930100
H	6.13962300	-0.40975200	-0.16449200
N	-1.57399400	-3.60436300	0.54544500
N	0.39892500	-4.54673000	0.43123000
N	-1.30420600	-0.30644400	2.76654900
O	-1.44357000	-0.40630000	3.95482300
O	-2.27352500	-0.34663700	1.95716200
O	-0.15575400	-0.14904300	2.23545500
N	-3.60781600	-0.35912500	-1.07057200
O	-3.16227400	0.70091000	-0.51510100
O	-4.74405200	-0.45069700	-1.43821200
O	-2.75858900	-1.27975600	-1.19977500
N	-0.10332400	-0.01981400	-2.85962100
O	-0.67675100	0.94547100	-2.26369400
O	0.20388100	0.03588000	-4.01845800
O	0.13032200	-1.04037100	-2.14444800
Eu	-0.89322400	-0.11516500	-0.07961900

EuR₁PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.68929600	-0.51377300	-0.11595400
C	-1.63264800	-2.54521700	-0.25507200
C	-2.85178700	-3.24354400	-0.26025300
H	-2.84358400	-4.32467300	-0.32935900
C	-2.59073700	0.92504600	-0.10188600
C	-3.77647700	1.69259300	-0.09561900
C	-3.63544100	3.09128100	-0.13047500
C	-2.38401000	3.64584800	-0.17877500
H	-4.52071900	3.72038600	-0.12499100
H	-2.25147000	4.72095200	-0.21233000
N	-1.36793700	1.47676900	-0.12599700
C	-3.96582600	-1.11991300	-0.11773400
C	-0.35798900	-3.24181100	-0.37766800
H	1.52501000	-5.59602500	-0.63280300

H	2.79319500	-3.32817900	-0.54839300
C	-1.25998500	2.79844900	-0.17314500
C	0.60221800	4.63781400	-0.28101500
C	1.97253900	4.48369900	-0.23553400
H	0.05984300	5.56699500	-0.35768000
H	3.08062300	2.65834300	-0.00470700
H	2.77570200	5.20393500	-0.25869300
C	0.09862700	3.32633900	-0.20401800
N	1.10041700	2.45337900	-0.12504900
N	0.81091200	-2.55233200	-0.41608000
N	-1.55127400	-1.22690800	-0.16107300
C	-4.01521800	-2.52502200	-0.17838100
H	-4.97767100	-3.02807100	-0.17440500
N	2.21349900	3.16510100	-0.14711500
C	-5.04723700	1.04458700	-0.06793700
H	-5.94292100	1.65824900	-0.04787200
C	-5.13912000	-0.30878900	-0.07701700
H	-6.10874800	-0.79712100	-0.06421600
N	-0.21516500	-4.54809400	-0.46615300
C	1.72648000	-3.48884800	-0.52321900
N	1.11512300	-4.67981700	-0.55940100
N	0.03654800	-0.29822800	2.88633300
O	-0.33138100	-0.39695200	4.02442000
O	0.33641000	-1.31104600	2.18076200
O	0.14767100	0.82541000	2.30489400
N	3.71307500	-0.23602500	0.78236100
O	3.00777900	-1.26286200	0.59453000
O	3.05565900	0.85463300	0.82694000
O	4.90308600	-0.27040300	0.91370200
N	1.35696200	0.10008400	-2.72352100
O	1.54822800	0.16389100	-3.90741800
O	0.18743900	0.02806100	-2.23137000
O	2.30519700	0.09873500	-1.88194600
Eu	0.86222800	-0.06064200	0.12367300

EuR₁PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.70021000	-0.39067200	-0.12435800
C	1.73069600	-2.46746800	-0.28513500
C	2.98209800	-3.10651300	-0.28989200
H	3.05861000	-4.18526600	-0.37189400
C	2.53571800	1.04377900	-0.10365400
C	3.68695100	1.86114400	-0.09300000
C	3.48514800	3.25292500	-0.12043900

C	2.21046300	3.75155200	-0.15962000
H	4.34178900	3.92039000	-0.11335800
H	2.03079500	4.82007100	-0.18276400
N	1.29061000	1.53979800	-0.12353700
C	4.00470300	-0.93872300	-0.12656000
C	0.47468600	-3.18906200	-0.44008400
H	0.95554200	-5.26488500	-0.48974300
H	-2.64196100	-3.46807700	-0.75391700
C	1.12348800	2.85591700	-0.15485100
C	-0.81886800	4.61498200	-0.21469800
C	-2.17924100	4.40058300	-0.13141300
H	-0.32102800	5.56772600	-0.30356400
H	-3.19821300	2.52565500	0.12317300
H	-3.01348800	5.08494800	-0.12936400
C	-0.25654500	3.32600900	-0.15706300
N	-1.21648300	2.41020000	-0.05308100
N	-0.70227000	-2.59475400	-0.53481900
N	1.59856000	-1.15341300	-0.17700600
C	4.11401300	-2.33781600	-0.19532700
H	5.09635100	-2.80032600	-0.19190700
N	-2.35895300	3.07179100	-0.04092300
C	4.98572900	1.26993000	-0.06632800
H	5.85257000	1.92354500	-0.04235300
C	5.14100900	-0.07752000	-0.07986100
H	6.13181500	-0.52100800	-0.06712000
N	-1.01281500	-4.80598300	-0.68882000
N	0.28725000	-4.51480800	-0.53752200
C	-1.57669800	-3.61673000	-0.67747200
N	0.06536200	-0.44413400	2.83621400
O	0.49244900	-0.58153900	3.94897000
O	-0.01269300	0.69347700	2.27564900
O	-0.33100200	-1.42509700	2.13448800
N	-1.39865200	0.20176500	-2.69462500
O	-1.59383900	0.34165700	-3.87004000
O	-2.34029300	0.12398200	-1.85117400
O	-0.22434300	0.12296500	-2.20982300
N	-3.68482300	-0.40832400	0.84193300
O	-4.86466200	-0.51840700	1.01080300
O	-3.08062300	0.70832600	0.95821800
O	-2.93745100	-1.37914000	0.53933500
Eu	-0.87760300	-0.10986400	0.12309900

EuR₂PhR₂(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.60817400	-0.73652800	0.02295300
C	1.40206200	-2.69917400	-0.05196000
C	2.58301400	-3.47035500	-0.02957600
H	2.52570300	-4.55210500	-0.07098500
C	2.61873200	0.70718200	0.00986800
C	3.86105500	1.38075800	0.01839300
C	3.83220100	2.78836900	0.01562100
C	2.63256000	3.44204700	0.03752500
H	4.76638300	3.34253500	0.01270300
H	2.59015300	4.52498600	0.06324000
N	1.44210200	1.36130700	-0.00105800
C	3.84055400	-1.42788800	0.03318800
C	0.09684800	-3.32053500	-0.19658300
C	-0.27237800	-4.64305600	-0.18908900
H	0.28105800	-5.55722100	-0.04742100
H	-2.21684900	-5.44863600	-0.44387400
H	-3.04617100	-3.04346000	-0.68994700
C	1.44063100	2.68792100	0.04355700
C	-0.21355800	4.65398700	0.15520700
H	0.35513500	5.56443600	0.05637300
H	-3.01730500	3.07822500	0.55642700
H	-2.15464400	5.47788300	0.37453500
C	0.13977200	3.32685100	0.14604100
N	-0.98106300	2.55584300	0.30703000
N	-1.00893800	-2.53951300	-0.40935700
N	1.42205500	-1.37347500	0.00954200
C	3.79128300	-2.83488500	0.02518600
H	4.71707900	-3.40271300	0.04162100
N	-0.57604600	-0.50934400	2.83065100
N	-0.57229600	0.52520000	-2.85303600
N	-3.80307900	0.01001000	0.08974700
O	0.06192600	-0.40494800	-2.27018700
O	-0.46555700	0.73812000	-4.03024900
O	-1.32156600	1.22319200	-2.10342800
O	-1.14214200	-1.32709000	2.03970100
O	-0.11241500	0.53607600	2.28726200
O	-0.48143000	-0.72085400	4.00928700
O	-3.10242300	0.79194700	0.79868800
O	-3.14569300	-0.77299100	-0.65930800
O	-5.00344900	0.01034100	0.12324100
C	-2.02542300	-3.35188600	-0.52431300
C	-1.99063000	3.37731700	0.41194000
N	-1.62223700	-4.63866500	-0.39917700

N	-1.56913800	4.66157900	0.32467900
C	5.07134700	-0.71057800	0.04242400
H	6.00089500	-1.27190700	0.05299600
C	5.08130300	0.64571700	0.03352900
H	6.01895300	1.19345700	0.03913600
Eu	-0.87655900	0.00384100	-0.01303900

EuR₂PhR₃(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.60939100	-0.83994300	-0.12489200
C	-1.32551000	-2.74185700	-0.26533500
C	-2.47432400	-3.56080500	-0.24760300
H	-2.37403300	-4.63891400	-0.30339800
C	-2.67046400	0.60235600	-0.12561900
C	-3.93295700	1.23907700	-0.10098600
C	-3.94091300	2.64439300	-0.15085200
C	-2.75810900	3.32924800	-0.24307200
H	-4.88692700	3.17718900	-0.12590800
H	-2.76074500	4.41294900	-0.29186800
N	-1.51699600	1.28155800	-0.18578200
C	-3.81396900	-1.57496400	-0.10119000
C	0.01204100	-3.29690900	-0.38699800
C	0.44239400	-4.59310100	-0.52623200
H	-0.07710100	-5.53631600	-0.57658500
H	2.43967600	-5.28641000	-0.69918300
H	3.17400800	-2.84907000	-0.49694300
C	-1.55030600	2.60423100	-0.26333500
H	-0.68186900	5.30500500	-0.56826000
H	2.91942900	3.16376400	-0.49960200
H	1.80663900	5.70176400	-0.73147200
C	-0.24980600	3.23988800	-0.38225300
N	0.88422400	2.56574100	-0.37271300
N	1.09564400	-2.45654100	-0.37949000
N	-1.40023800	-1.42052400	-0.18374500
C	-3.70806200	-2.97800900	-0.15363900
H	-4.60811600	-3.58550000	-0.13061000
C	2.15709200	-3.20892300	-0.50440600
C	1.88707900	3.47402300	-0.51039100
N	1.80524300	-4.51185300	-0.60136400
C	-5.06699500	-0.89621600	-0.04346700
H	-5.97734900	-1.48738600	-0.00975700
C	-5.12549200	0.45980400	-0.04321100
H	-6.08233500	0.97197900	-0.00912300
N	-0.00250700	4.56536700	-0.52807100
C	1.35359000	4.73074200	-0.61279400

N	-0.08828400	-0.01736400	2.86435600
O	-0.52428900	-0.04476700	3.98254100
O	0.22830400	-1.07201600	2.23364100
O	0.08150100	1.06928200	2.22974400
N	3.63904500	0.15721700	1.08712500
O	4.80226800	0.20727900	1.37683700
O	3.02904900	-0.93996800	0.90634900
O	2.92639700	1.19322200	0.93901900
N	1.48556400	0.05133300	-2.67658800
O	1.72358900	0.04146500	-3.85503500
O	2.40193900	0.06817700	-1.80064800
O	0.29787700	0.04279200	-2.22845800
Eu	0.89378400	0.04483300	0.15432300

EuR₂PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.41469200	1.12958400	-0.01203800
C	0.90634200	2.87095000	0.08975400
C	1.94817500	3.82175500	0.06186700
H	1.71906000	4.88030300	0.10861000
C	2.65583600	-0.29489200	-0.01157100
C	3.98889800	-0.76347300	-0.05201700
C	4.18279900	-2.15663900	-0.07097900
C	3.09999900	-2.99308100	-0.07884200
H	5.19231000	-2.55618900	-0.09771200
H	3.22947100	-4.06844700	-0.12612600
N	1.59936800	-1.12776700	0.01856600
C	3.51941100	2.00896000	-0.03253700
C	-0.48287500	3.26740600	0.25061300
C	-1.06285600	4.51085600	0.30978600
H	-0.66600100	5.50914200	0.21999600
H	-3.10923800	4.97782800	0.60716400
H	-3.53519100	2.45841800	0.74189600
C	1.80714600	-2.43535000	-0.04310100
C	0.45703600	-4.64116600	-0.04664600
H	1.13417300	-5.46617800	0.10086800
H	-1.40611300	-5.65777200	-0.19770200
C	0.62167500	-3.27767700	-0.11750900
N	-0.60892500	-2.73059100	-0.30636800
N	-1.44787800	2.30944600	0.42305600
N	1.14354800	1.56683800	0.01941600
C	3.24291700	3.38965800	-0.01118100
H	4.06399100	4.10026100	-0.03491000

C	-2.58118500	2.93743000	0.58083600
N	-2.39259600	4.27754900	0.51905800
N	-0.87126600	-4.80463500	-0.19452600
C	4.84851900	1.49542200	-0.06836800
H	5.67688000	2.19739000	-0.08673200
C	5.07595300	0.15829700	-0.07779900
H	6.08889800	-0.23172900	-0.10651200
N	-1.50665000	-3.64890800	-0.35035400
N	-0.38469400	-0.63478600	2.83795300
O	-0.18976000	-0.84792700	4.00457200
O	-0.12537000	0.47906000	2.29710100
O	-0.85719900	-1.51964600	2.05934200
N	-3.73603700	-0.52839600	-0.24391400
O	-4.92469000	-0.63346100	-0.36869200
O	-3.21565400	0.10601700	0.73401300
O	-2.91399100	-1.02290100	-1.06379300
N	-0.47648100	0.44127600	-2.80981500
O	-0.33145300	0.66982100	-3.98022200
O	-1.12998000	1.21299900	-2.04423500
O	0.02316500	-0.58075200	-2.25094900
Eu	-0.89130800	-0.14376400	0.00573000

EuR₂PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.66287500	0.67640100	-0.08375300
C	-1.49116800	2.65675900	-0.16769700
C	-2.68458400	3.40692600	-0.13419500
H	-2.64703600	4.48998400	-0.16280600
C	-2.64474500	-0.76719200	-0.11833500
C	-3.87148700	-1.47027200	-0.13400100
C	-3.80922700	-2.87228600	-0.22410100
C	-2.59179000	-3.49456500	-0.30459200
H	-4.72875700	-3.44990800	-0.23862100
H	-2.51987100	-4.57292300	-0.38854400
N	-1.45520700	-1.38811000	-0.16378300
C	-3.90713200	1.34314000	-0.05391900
C	-0.19025700	3.29588500	-0.28104800
C	0.15988000	4.61979400	-0.37439800
H	-0.41575000	5.53114300	-0.37719000
H	2.10803900	5.43989800	-0.55185900
H	2.99213000	3.04649700	-0.46446100
C	-1.42444700	-2.71028200	-0.26933100
C	0.37070300	-4.63293300	-0.40371100
H	-0.15929000	-5.57147800	-0.45208700
H	2.92438800	-2.96043400	-0.21069600

C	-0.10031200	-3.31317200	-0.33704600
N	0.96808200	-2.52027800	-0.29603200
N	0.94279800	2.52392900	-0.32587400
N	-1.48865200	1.33073200	-0.11801200
C	-3.88227800	2.75058400	-0.06559500
H	-4.81649400	3.30361200	-0.03441300
C	1.95541500	3.34385400	-0.43729000
N	1.52356600	4.62463700	-0.47448300
C	-5.12219900	0.59692800	-0.03253600
H	-6.06338000	1.13721800	0.00518900
C	-5.10588000	-0.75879800	-0.07398300
H	-6.03299700	-1.32395600	-0.07077900
N	1.98891600	-3.33343900	-0.33162400
N	1.70032700	-4.60853300	-0.39154600
N	1.34143700	0.07188200	-2.71976500
O	1.52782300	0.13497700	-3.90393700
O	2.29194500	0.08877400	-1.88003900
O	0.17558000	-0.01423100	-2.22161800
N	0.07782500	0.00925500	2.89084800
O	-0.27132900	0.00117500	4.03724600
O	0.26652600	1.08615800	2.24446700
O	0.28077700	-1.06000900	2.23419500
N	3.71032700	-0.04715900	0.81383700
O	3.01885500	-1.10496700	0.67763800
O	4.89987600	-0.07083100	0.95440900
O	3.04115700	1.02517000	0.79274400
Eu	0.86282000	0.02500900	0.13101000

EuR₂PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.68648800	0.37846800	-0.08738100
C	-1.77942000	2.48301400	-0.17605900
C	-3.04486900	3.08841300	-0.07730900
H	-3.15182100	4.16796600	-0.06435000
C	-2.48065300	-1.05015000	-0.12176600
C	-3.60436000	-1.90188300	-0.08262200
C	-3.36163100	-3.28580900	-0.17774100
C	-2.08074700	-3.74126200	-0.33226600
H	-4.19580700	-3.98051600	-0.14409400
H	-1.87836300	-4.80172700	-0.43137000
N	-1.22240400	-1.50803000	-0.22544600
C	-4.00314500	0.88687300	0.00893200
C	-0.54036700	3.24302600	-0.27810100
H	-1.10731600	5.28818100	-0.45343200
H	1.41538600	5.75565100	-0.58037500

C	-1.01882700	-2.81302300	-0.35893600
C	0.92745600	-4.46128200	-0.71793600
H	0.51726400	-5.45811100	-0.72510300
H	3.44241000	-2.42071500	-0.86251400
H	2.97667300	-4.92752700	-1.00333900
C	0.36160700	-3.22050200	-0.56024500
N	1.34262300	-2.26384400	-0.62637600
N	0.64942400	2.68803100	-0.26715400
N	-1.61300300	1.17187500	-0.17575100
C	-4.15204400	2.28426300	0.01801100
H	-5.14413600	2.71796200	0.09991600
C	2.47332000	-2.89237100	-0.80919800
N	2.26509900	-4.22770200	-0.87661200
C	-5.10991800	-0.00984700	0.08301900
H	-6.11096100	0.40164700	0.16906500
C	-4.91586500	-1.35209300	0.03618600
H	-5.76131500	-2.03212600	0.08232800
N	1.59078500	3.65111000	-0.38954900
C	0.95617900	4.78509400	-0.47234600
N	-0.38918900	4.58603300	-0.40437500
N	-0.02739600	-0.43286000	2.78606100
O	0.73294300	-1.21529500	2.13844600
O	-0.39401000	0.61110700	2.16645100
O	-0.38684400	-0.67144900	3.90749000
N	3.46058900	0.41023200	1.37489700
O	4.52741400	0.51210300	1.91295200
O	2.53026500	1.25323000	1.53027200
O	3.18235300	-0.56212700	0.60409800
N	1.38347500	0.48135500	-2.73942800
O	1.55563000	0.61773400	-3.92179000
O	2.33271600	0.48206400	-1.90655500
O	0.22030800	0.32267500	-2.24562700
Eu	0.90270500	0.12809500	0.09314400

EuR₂PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.62358500	0.81627500	-0.10270100
C	1.35922400	2.73476200	-0.21027200
C	2.51563200	3.54186500	-0.18276200
H	2.42607000	4.62162900	-0.22132100
C	2.67308800	-0.62545800	-0.12270800
C	3.92827800	-1.27556000	-0.11336300
C	3.92924500	-2.68148300	-0.18511400
C	2.74234600	-3.35830300	-0.27980200
H	4.87367600	-3.21767400	-0.17602300

H	2.69684200	-4.43829300	-0.35291000
N	1.51229100	-1.29794300	-0.18351300
C	3.83497900	1.54044400	-0.07179600
C	0.02771200	3.30836200	-0.31832000
C	-0.38670900	4.61200600	-0.43175000
H	0.14479800	5.54919000	-0.46606400
H	-2.37536700	5.33442300	-0.58548200
H	-3.14103500	2.90370300	-0.42742400
C	1.54785200	-2.61715200	-0.27772200
H	-2.90568500	-3.24634600	-0.48567900
H	-1.71815700	-5.55685700	-0.62604600
C	0.24836900	-3.26983400	-0.38942100
N	-0.89618400	-2.54128900	-0.39292300
N	-1.06716600	2.48227000	-0.32320200
N	1.41951400	1.41131000	-0.15030700
C	3.74346800	2.94481300	-0.10219000
H	4.64995900	3.54237900	-0.07287700
C	-2.11959300	3.25065400	-0.43048400
C	-1.84498100	-3.44454100	-0.48917300
N	-1.75094700	4.54988200	-0.50386200
N	-1.27592600	-4.65593800	-0.55229900
C	5.08169900	0.84950400	-0.02888200
H	5.99746600	1.43198200	0.00994300
C	5.12776100	-0.50655200	-0.04947400
H	6.07999300	-1.02783300	-0.02753900
N	0.06024100	-4.57035800	-0.48776400
N	-1.44202300	0.01746900	-2.69929100
O	-1.66487900	0.05133700	-3.87987600
O	-0.26054600	0.00786600	-2.23500700
O	-2.36989500	-0.01089100	-1.83526900
N	-3.67066900	-0.16186000	0.97898800
O	-4.84623600	-0.20869700	1.21502400
O	-2.96966100	-1.20023700	0.79483300
O	-3.03525800	0.93195200	0.89553700
N	0.00284600	-0.08078500	2.87509400
O	-0.21088200	-1.14097400	2.20891900
O	-0.21948500	1.00479800	2.25521300
O	0.39204900	-0.10385400	4.00943900
Eu	-0.88390200	-0.02436200	0.13952500

EuR₂PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.57889900	0.95970800	0.09676500
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C	-1.22596600	2.81546200	0.13461800
C	-2.34265400	3.67675300	0.09123700
H	-2.20091200	4.75163100	0.08661200
C	-2.69782900	-0.47900900	0.13214300
C	-3.98548600	-1.06727300	0.12640600
C	-4.05277100	-2.46872300	0.20322300
C	-2.89820100	-3.20132600	0.30156300
H	-5.02053300	-2.96109800	0.19678200
H	-2.94132900	-4.28215000	0.38120100
N	-1.57330100	-1.20643400	0.19343500
C	-3.75525300	1.73831900	0.05035400
C	0.13476300	3.32373300	0.17694500
C	0.62083700	4.60559600	0.24659000
H	0.14086800	5.56958700	0.29459100
H	2.64961200	5.22444600	0.28913700
H	3.27968800	2.75512200	0.13963900
C	-1.66681600	-2.52321100	0.29687200
H	-0.82654300	-5.29636100	0.52113600
H	2.73889800	-3.42211500	0.65564800
C	-0.39050500	-3.21193500	0.43184100
N	0.77557000	-2.59270800	0.48501500
N	1.18429400	2.44170800	0.14085600
N	-1.34966300	1.49579200	0.13249000
C	-3.59838000	3.13733000	0.04457900
H	-4.47590700	3.77599200	0.00497000
C	2.27902200	3.15544200	0.18283700
C	1.67541300	-3.59489900	0.61348900
N	1.98182800	4.47289000	0.25077100
C	-5.03422900	1.10758200	0.01978900
H	-5.92057500	1.73332500	-0.02741500
C	-5.14759000	-0.24387100	0.05698500
H	-6.12377400	-0.71868300	0.04092800
N	1.13723300	-4.79532800	0.65458400
N	-0.17258600	-4.53263000	0.53791300
N	3.68354700	-0.36515000	-0.94094200
O	3.00073700	-1.33180200	-0.49291300
O	3.04053200	0.72156300	-1.08296800
O	4.84753900	-0.46414900	-1.21036300
N	1.39775700	0.22314900	2.71626500
O	1.57912800	0.39118300	3.89064600
O	0.24175600	-0.00176500	2.23575600
O	2.33961100	0.26031300	1.86969300
N	-0.04767300	-0.34716900	-2.82178200
O	-0.47199600	-0.46313100	-3.93900900

O	0.32259100	-1.34723300	-2.13057600
O	0.05298200	0.77905400	-2.24740700
Eu	0.91977300	-0.08601400	-0.10164700

EuR₃PhR₃(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.56729000	-0.72221900	0.00863500
C	1.36652900	-2.68495700	-0.04382400
C	2.54775000	-3.45385400	-0.04336200
H	2.50785500	-4.53680600	-0.08917700
C	2.56710300	0.72286700	-0.00874300
C	3.80323200	1.40806100	-0.00345000
C	3.75633600	2.81389500	0.00567900
C	2.54686700	3.45449900	0.04319500
H	4.68217600	3.38148400	0.00393900
H	2.50669500	4.53744200	0.08897400
N	1.38707800	1.35972500	-0.01708200
C	3.80359600	-1.40709300	0.00317700
C	0.04671900	-3.27427400	-0.17546600
H	0.37555300	-5.36259800	-0.01710700
H	-2.09783900	-5.67274100	-0.41009200
H	-3.07760000	-3.08077200	-0.67614400
C	1.36584700	2.68529500	0.04383500
H	0.37409000	5.36265600	0.01659500
H	-3.07830200	3.07996500	0.67664600
H	-2.09926600	5.67219100	0.41030800
C	0.04589300	3.27427600	0.17553200
N	-1.04325400	2.55846900	0.37437700
N	-1.04263500	-2.55874200	-0.37416900
N	1.38743100	-1.35938300	0.01711900
C	3.75705800	-2.81294000	-0.00596800
H	4.68304300	-3.38029200	-0.00435700
N	-0.44344800	-0.53215600	2.82408900
N	-0.44413500	0.53201600	-2.82405600
N	-3.82174800	-0.00042700	-0.00006400
O	-0.00938000	-0.51425900	-2.25821700
O	-0.25788300	0.76022700	-3.98879000
O	-1.07998100	1.33184200	-2.07058200
O	-1.07945500	-1.33201100	2.07078000
O	-0.00899300	0.51420000	2.25816800
O	-0.25698300	-0.76030500	3.98880100
O	-3.14089300	0.69853900	0.81141800
O	-3.14068400	-0.69933700	-0.81141200
O	-5.02087800	-0.00061800	-0.00005000
C	-2.07350500	-3.43319400	-0.49985400

C	-2.07433800	3.43265500	0.50015600
C	-1.60422400	-4.71492600	-0.37507400
C	-1.60540800	4.71450300	0.37525000
N	-0.25731900	-4.59742200	-0.17311800
N	-0.25853100	4.59733300	0.17290500
C	5.02893800	-0.67773800	0.00114800
C	5.02876300	0.67902200	-0.00157100
H	5.96372500	-1.23017000	0.00042500
H	5.96340700	1.23169600	-0.00097000
Eu	-0.92433700	-0.00011800	0.00006700

EuR₃PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.46505900	0.98969900	-0.01424000
C	-1.04945400	2.80753200	0.04692200
C	-2.13781300	3.70293300	0.02676900
H	-1.97895700	4.77533500	0.06048700
C	-2.62610900	-0.44692200	-0.00433900
C	-3.93059600	-0.98764600	-0.03018500
C	-4.04392000	-2.38991800	-0.03937800
C	-2.91441500	-3.16245800	-0.04816900
H	-5.02841600	-2.84806600	-0.05524100
H	-2.98458800	-4.24374900	-0.08302300
N	-1.52323300	-1.21549200	0.02206200
C	-3.61636700	1.80958000	-0.03104400
C	0.32820500	3.24964500	0.17455800
H	0.21749600	5.36617200	0.09663100
H	2.71309800	5.40477700	0.45853400
H	3.42119500	2.71838500	0.63609400
C	-1.65326500	-2.53395000	-0.02522300
H	-0.83729300	-5.52674000	0.07021700
H	1.71306400	-5.59550700	-0.18037700
C	-0.42365300	-3.31187500	-0.09178800
N	0.78456000	-2.70559200	-0.24529700
N	1.34091100	2.42069100	0.33438900
N	-1.22201800	1.49227700	-0.00094200
C	-3.41089100	3.20115100	-0.02260400
H	-4.26689500	3.86921500	-0.04031400
C	2.45771000	3.17744000	0.47654600
C	2.12278100	4.50468600	0.39814500
N	0.76938300	4.53370300	0.20928000
C	-4.91550300	1.22258200	-0.05106100
C	-5.06680600	-0.12554300	-0.05117400
H	-5.78245100	1.87622000	-0.06588000
H	-6.05706000	-0.57055900	-0.06840700

N	1.72361700	-3.58007400	-0.29002400
C	-0.19681400	-4.66794000	-0.04474100
N	1.13961500	-4.76785200	-0.16956300
N	0.43212700	0.32943000	-2.82290500
O	0.26520500	0.51122900	-3.99788800
O	0.92528900	1.22023800	-2.06321700
O	0.12028300	-0.75381900	-2.24888400
N	3.77776000	-0.31941200	-0.16576100
O	3.19817600	0.20578800	0.84071400
O	3.00712800	-0.76793000	-1.06381400
O	4.97348400	-0.37418700	-0.25308700
N	0.39157200	-0.49448100	2.84394900
O	0.19428800	-0.68789800	4.01264200
O	0.22696300	0.63310700	2.29956900
O	0.77389400	-1.42177100	2.06159700
Eu	0.91023600	-0.09253800	0.00714200

EuR₃PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.68353800	0.54447500	-0.08689500
C	1.60039100	2.57109400	-0.17994300
C	2.82162300	3.27188500	-0.15064000
H	2.84547100	4.35581300	-0.18303900
C	2.59966200	-0.89754200	-0.11327300
C	3.79300400	-1.65395900	-0.12287700
C	3.66631100	-3.05228100	-0.20381700
C	2.42091100	-3.61759500	-0.28212900
H	4.55773700	-3.67241800	-0.21294500
H	2.29957400	-4.69211500	-0.35844100
N	1.38322800	-1.46029500	-0.15778700
C	3.95719900	1.15762500	-0.06005500
C	0.31404200	3.23574400	-0.29713300
H	0.78638200	5.29856700	-0.37540500
H	-1.68761000	5.74958700	-0.59070900
H	-2.85333100	3.22682600	-0.50477400
C	1.29041000	-2.78005900	-0.25473300
H	-0.11819000	-5.57601900	-0.42926200
H	-3.06427800	-2.80917300	-0.20205800
C	-0.06161000	-3.31710100	-0.32160900
N	-1.08847700	-2.47026900	-0.28501500
N	-0.83303000	2.58417200	-0.34762600
N	1.54227500	1.24699000	-0.12440900
C	3.99163000	2.56298200	-0.07899200
H	4.94768500	3.07715000	-0.05053500
C	-1.81544400	3.51668500	-0.47159600

C	-1.25577400	4.76568300	-0.50372900
N	0.09386000	4.57011400	-0.39156200
C	5.13754100	0.35713100	-0.03311600
C	5.05825100	-0.99667500	-0.06584300
H	6.10262400	0.85336100	0.00227700
H	5.95911100	-1.60278800	-0.05763200
N	-1.92588500	-4.51872400	-0.37527100
N	-2.14883700	-3.23033400	-0.32018000
C	-0.59921000	-4.61127100	-0.38483600
N	-1.33516700	0.08140200	-2.72363000
O	-1.51027400	0.11455500	-3.91017900
O	-0.17186900	0.02389300	-2.21275500
O	-2.29290900	0.10064200	-1.89278000
N	-3.71194100	0.12739100	0.83884500
O	-3.06689400	-0.96183700	0.70204100
O	-2.99864400	1.16917400	0.79050200
O	-4.89738500	0.15329700	1.00367100
N	-0.04745700	0.04482200	2.87527500
O	0.33186500	0.02869100	4.01211600
O	-0.31739800	-1.01796100	2.23311300
O	-0.20217300	1.12508900	2.22509600
Eu	-0.88705700	0.07522300	0.12861500

EuR₃PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.35990300	-1.17699100	0.00205900
C	-0.80407700	-2.86984100	-0.10507600
C	-1.81657500	-3.85071800	-0.09556100
H	-1.57184000	-4.90568300	-0.15584000
C	-2.63670500	0.24207800	0.01102900
C	-3.97954500	0.68139700	0.06529300
C	-4.19925000	2.06914600	0.10545000
C	-3.13056900	2.92848500	0.11527900
H	-5.21488900	2.45082300	0.14847100
H	-3.29124900	3.99880500	0.18746800
N	-1.60091000	1.09159000	-0.02388100
C	-3.44169400	-2.08493200	0.01279600
C	0.60321400	-3.19172500	-0.26070600
H	0.67802700	-5.30918900	-0.18756800
H	3.16149900	-5.13023700	-0.59001000
H	3.63223100	-2.39059600	-0.75555300
C	-1.83094300	2.39367400	0.05481800
H	-1.29124200	5.23150000	-0.14248200
H	1.18289100	5.85163200	0.14665100

C	-0.63591600	3.22232500	0.13024000
N	0.56867800	2.74015200	0.32378700
N	1.53781700	-2.27673400	-0.43111900
N	-1.08116500	-1.57436100	-0.02498000
C	-3.12584400	-3.45535300	-0.02315100
H	-3.92456700	-4.19094700	-0.01074200
C	2.71404500	-2.93342600	-0.59217200
C	2.49620900	-4.28505000	-0.51731200
C	0.77195900	4.85438800	0.17843900
N	1.15330000	-4.43198000	-0.31019800
C	-4.78305200	-1.60090100	0.05627000
C	-5.04325400	-0.26963100	0.08387200
H	-5.59551700	-2.32123100	0.06788100
H	-6.06593900	0.09292900	0.12152200
N	1.45480300	3.75723500	0.35138000
N	-0.55158200	4.57521300	0.03994700
N	0.38960100	-0.47527500	2.78755300
O	0.17450200	-0.73833100	3.94057800
O	1.09022300	-1.22175700	2.04112800
O	-0.08244400	0.56061500	2.22990400
N	3.74503500	0.62720200	0.26000100
O	2.91553700	1.01227400	1.13207400
O	3.23276500	0.05997600	-0.76360700
O	4.92858900	0.77077800	0.37873700
N	0.29460700	0.62948700	-2.82750100
O	0.02452800	0.82792700	-3.98231000
O	0.15121800	-0.50259500	-2.28119700
O	0.73053600	1.54744600	-2.06794200
Eu	0.93360500	0.18121100	-0.00306400

EuR₃PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.61923700	0.63485900	0.02132600
C	1.48526100	2.63691400	-0.03060300
C	2.69030600	3.36701700	-0.03023700
H	2.68569900	4.45048700	-0.07998900
C	2.57490400	-0.80838900	0.00442800
C	3.78725800	-1.53416600	0.00584000
C	3.70223300	-2.93944500	0.00760600
C	2.47518500	-3.54562900	0.03927400
H	4.61303600	-3.53086600	-0.00084200
H	2.36212600	-4.62275700	0.06650500
N	1.37412300	-1.41093900	-0.00015200
C	3.87722900	1.28038000	0.01711700
C	0.18738600	3.27425300	-0.15953200

H	0.59075300	5.34194300	0.06522300
H	-1.86840100	5.75438900	-0.32899800
H	-2.94261400	3.20936900	-0.66154400
C	1.32726700	-2.73351400	0.04742700
H	-3.12956300	-3.09604100	0.54019400
H	-2.09599300	-5.48353200	0.40567200
C	-0.00693400	-3.31027800	0.16085500
N	-1.09580900	-2.51489100	0.29318700
N	-0.92644800	2.60402200	-0.38124900
N	1.45991300	1.31125900	0.02919000
C	3.87772200	2.68650600	0.00752700
H	4.82211600	3.22267600	0.00801400
C	-1.92542600	3.51963000	-0.48250500
C	-2.09131900	-3.36078900	0.40947800
C	-1.40988600	4.77872200	-0.32141800
N	-0.06845000	4.60632800	-0.12105900
C	5.07858200	0.51238800	0.01429300
C	5.03528400	-0.84327300	0.00894300
H	6.03032800	1.03509800	0.01417700
H	5.95175200	-1.42554300	0.00735900
N	-0.27228800	-4.60146200	0.19219500
N	-1.60189900	-4.60875800	0.34937000
N	-0.54311100	-0.48493600	-2.84342100
O	-0.41183600	-0.70025800	-4.01662100
O	-1.30962800	-1.17982200	-2.10728700
O	0.08112600	0.44444100	-2.24798300
N	-3.82112300	0.08647100	0.01804100
O	-3.12974700	0.87399700	-0.69470800
O	-3.15055100	-0.70993400	0.74457600
O	-5.02034400	0.09057500	0.00602300
N	-0.55078000	0.48704400	2.83039800
O	-0.42058900	0.67501400	4.00906400
O	-0.17788600	-0.58375100	2.26619800
O	-1.06406900	1.35625200	2.05835800
Eu	-0.91390000	0.04766000	-0.01684400

EuR₃PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.57406700	0.74923900	0.00757400
C	-1.35805100	2.70157400	0.04740000
C	-2.53285100	3.48027200	0.05718800
H	-2.48380700	4.56301300	0.09721500
C	-2.58922100	-0.69606100	0.01972000
C	-3.83188800	-1.37168900	0.01975600

C	-3.80083200	-2.77696300	0.00213300
C	-2.59697800	-3.43014300	-0.04728900
H	-4.73240000	-3.33474400	0.00618400
H	-2.56239600	-4.51281500	-0.10050100
N	-1.41643100	-1.34560100	0.01647700
C	-3.80444000	1.44406700	0.02327800
C	-0.03194900	3.28125500	0.15165400
H	-0.35054000	5.37541200	0.04790600
H	2.13550000	5.66063200	0.36784300
H	3.10369700	3.05884500	0.56366900
C	-1.41464800	-2.66879800	-0.04881300
H	-0.34752900	-5.37883400	-0.01020700
H	3.00440800	-3.24919800	-0.70545400
C	-0.09533500	-3.26873900	-0.19307500
N	1.00121900	-2.56851700	-0.41654500
N	1.05784300	2.55530600	0.30567300
N	-1.38889900	1.37552000	-0.00903100
C	-3.74757300	2.84937000	0.03295500
H	-4.66899900	3.42394000	0.03882600
C	2.09805300	3.42019500	0.41755400
C	1.97168100	-3.50175400	-0.52348500
C	1.63412600	4.70701200	0.32892100
N	0.28168200	4.60233400	0.16231300
N	0.22951200	-4.57253800	-0.17887400
C	-5.03636100	0.72526500	0.03238100
C	-5.05096900	-0.63097600	0.02987800
H	-5.96567400	1.28682600	0.04153300
H	-5.99094200	-1.17417000	0.03362500
N	1.54277900	-4.74000200	-0.38547700
N	0.46304900	-0.52289400	2.80666400
O	0.28211000	-0.74406900	3.97271400
O	1.01216900	-1.36936600	2.03369200
O	0.10989600	0.56133700	2.25622000
N	3.82428000	-0.07587200	0.09838500
O	3.13173400	0.69129200	0.83601800
O	3.15313400	-0.81323100	-0.68723200
O	5.02128800	-0.10092700	0.13963900
N	0.50104100	0.51366400	-2.83965900
O	0.33009300	0.73295400	-4.00748700
O	-0.08109100	-0.43788400	-2.23509500
O	1.26549100	1.22499700	-2.11979700
Eu	0.93580000	-0.00489300	-0.01517300

EuR₄PhR₄(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.56133300	0.72402800	-0.00012500
C	1.35400800	2.68475800	-0.00028700
C	2.53363200	3.45502800	-0.00030300
H	2.48045500	4.53789100	-0.00034300
C	2.56187100	-0.72187200	0.00007500
C	3.79637900	-1.40762900	0.00013600
C	3.74733300	-2.81372800	0.00027000
C	2.53620300	-3.45288300	0.00030400
H	4.67244500	-3.38258400	0.00032400
H	2.48382000	-4.53578500	0.00037000
N	1.38032700	-1.35914700	0.00019700
C	3.79532700	1.41070700	-0.00015200
C	0.03769200	3.31124300	-0.00020200
H	0.19351200	5.56423600	-0.00001600
H	-2.35885600	5.32595000	0.00018000
C	1.35600800	-2.68349400	0.00025300
H	0.19775400	-5.56381100	0.00003000
H	-2.35479900	-5.32755500	-0.00023700
C	0.04014800	-3.31094700	0.00017300
N	-1.09861900	-2.56570400	0.00006500
N	-1.10046800	2.56510200	-0.00010600
N	1.37929900	1.36042600	-0.00026100
C	3.74522900	2.81676700	-0.00026500
H	4.66992300	3.38630100	-0.00029100
N	-0.35646500	-0.00060600	-2.86263300
N	-0.35630000	-0.00089300	2.86255800
N	-3.78503400	-0.00098300	0.00019600
O	-0.47820400	1.06889700	2.19549400
O	-0.13313100	-0.00108200	4.04312300
O	-0.47771300	-1.07048800	2.19504400
O	-0.47945000	1.06911200	-2.19557800
O	-0.47670900	-1.07027100	-2.19509100
O	-0.13337600	-0.00055100	-4.04321200
O	-3.10519600	-0.00553200	-1.07350100
O	-3.10503600	0.00400400	1.07378700
O	-4.98400700	-0.00132500	0.00028600
N	-2.13812300	3.32135300	0.00005400
N	-2.13566400	-3.32277000	-0.00009400
N	-1.69195100	4.57138800	0.00004000
N	-1.68849300	-4.57246600	-0.00008500
C	-0.34708300	4.63228200	-0.00006100
C	-0.34358800	-4.63229000	0.00005500
C	5.02086600	0.68041000	-0.00006000
H	5.95577800	1.23270100	-0.00009600

C	5.02136700	-0.67641500	0.00006400
H	5.95668700	-1.22801600	0.00012100
Eu	-0.92498500	-0.00027100	-0.00002600

EuR₄PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.42066900	1.18785300	-0.01738300
C	-0.88588500	2.89965500	0.10972300
C	-1.90170800	3.87297100	0.09158400
H	-1.64660600	4.92467500	0.15278900
C	-2.69207100	-0.23215400	-0.02736200
C	-4.03524200	-0.66878500	-0.08626100
C	-4.26406400	-2.05613600	-0.11310600
C	-3.20255200	-2.91927300	-0.10288300
H	-5.28263000	-2.43018000	-0.15668200
H	-3.35757700	-3.99111100	-0.15153700
N	-1.65628900	-1.09068000	0.01696200
C	-3.50707000	2.09268600	-0.03670100
C	0.51358300	3.26704000	0.26759700
H	0.86118000	5.50257200	0.24365100
C	-1.89807000	-2.39323200	-0.04381900
H	-1.30691500	-5.44284300	0.11185600
H	1.23650300	-5.69588900	-0.10029900
C	-0.73352400	-3.26652700	-0.08050300
N	0.51604100	-2.75033500	-0.22465200
N	1.41355600	2.29866000	0.41300200
N	-1.14267300	1.59921400	0.02344500
C	-3.20574700	3.46598000	0.00452700
H	-4.01296900	4.19210700	-0.01620500
N	1.39204500	-3.69120100	-0.24124700
N	0.72300600	-4.82949000	-0.11158000
C	1.20962900	4.48430100	0.32144600
C	-0.60507500	-4.63417000	-0.00809300
C	-4.84704100	1.60841800	-0.09259200
H	-5.65971100	2.32819700	-0.11271600
C	-5.10184300	0.27731200	-0.11858500
H	-6.12226900	-0.09094400	-0.16306600
N	2.55401300	2.91653600	0.53484500
H	3.40321000	2.36930600	0.63141400
N	2.50270800	4.22508200	0.49004400
N	0.55674500	0.36165700	-2.80301000
O	0.45522600	0.57586900	-3.97820600
O	1.22125100	1.11970000	-2.02910100
O	-0.00016900	-0.62934600	-2.24041800

N	3.74128600	-0.49018900	-0.32889800
O	2.90109700	-1.18547200	-0.95808500
O	3.23838700	0.31460700	0.53288200
O	4.92222700	-0.56016300	-0.51000800
N	0.50512800	-0.61035200	2.85732300
O	0.35835200	-0.79643500	4.03305200
O	0.08683100	0.43552800	2.27509200
O	1.08237900	-1.45459300	2.10337200
Eu	0.88076600	-0.18589500	0.01496800

EuR₄PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.60655200	0.43127600	-0.00175100
C	-1.63323500	2.51333700	-0.07308100
C	-2.88737100	3.14879600	-0.11004500
H	-2.96635700	4.22849700	-0.17801200
C	-2.44231900	-1.00494400	0.02182900
C	-3.59282600	-1.82232000	0.04660300
C	-3.38929000	-3.21363300	0.09224700
C	-2.11492500	-3.71243400	0.12900700
H	-4.24564100	-3.88120400	0.11080400
H	-1.94187300	-4.78107600	0.18743300
N	-1.19642100	-1.50526600	0.02399500
C	-3.91134500	0.97651600	-0.02831500
C	-0.37759200	3.24769400	-0.15450100
H	-0.88937300	5.30686900	0.03987700
C	-1.02683000	-2.81756000	0.09789500
H	0.45090300	-5.54849800	0.10982500
H	2.95106700	-5.02381100	0.32088100
C	0.34759200	-3.29325000	0.17818800
N	1.38748100	-2.42240900	0.28846400
N	0.79315500	2.67608700	-0.31221700
N	-1.50747100	1.19700900	0.00027400
C	-4.02034500	2.37670400	-0.07579600
H	-5.00311200	2.83782700	-0.09932100
N	2.50186800	-3.05718400	0.35271600
N	2.20360800	-4.34976300	0.28771800
C	0.87879100	-4.56219700	0.18023300
C	-5.04741400	0.11376000	-0.01085500
H	-6.03873500	0.55617100	-0.02855100
C	-4.89274500	-1.23321100	0.02805400
H	-5.75939500	-1.88723200	0.04470400
N	1.75075100	3.62512900	-0.35643900
H	1.62673000	5.73893300	-0.22064600

C	1.14584100	4.77302900	-0.22855600
N	-0.19595300	4.59298400	-0.10328200
N	3.76366800	0.41889700	-0.04003200
O	3.12504200	0.05271300	0.99778100
O	4.95394700	0.54303200	-0.05012600
O	3.04504900	0.63941700	-1.06404200
N	0.33540000	-0.43602900	-2.82229800
O	0.09106400	-0.66436700	-3.97713100
O	0.00711600	0.65171700	-2.26246300
O	0.92768500	-1.27277600	-2.07757500
N	0.30560800	0.47593600	2.82243200
O	0.04475900	0.62522800	3.98682800
O	0.60901900	1.44792700	2.06739300
O	0.28295500	-0.65916100	2.26258100
Eu	0.94530600	0.11915200	-0.01411500

EuR₄PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.48800200	-0.97387900	-0.01649900
C	-1.09988800	-2.80117100	0.08182000
C	-2.18349900	-3.69662000	0.05507900
H	-1.99186800	-4.76196500	0.09966300
C	-2.63990900	0.46221700	-0.01363400
C	-3.94175100	1.00997400	-0.05720200
C	-4.05111800	2.41198700	-0.07275600
C	-2.91911800	3.18100100	-0.07221600
H	-5.03413200	2.87263300	-0.10240600
H	-2.98339200	4.26238200	-0.11508700
N	-1.53400600	1.22779700	0.02382500
C	-3.64186400	-1.78950000	-0.03974900
C	0.27025800	-3.27646600	0.23888600
C	-1.66259400	2.54616000	-0.03242800
H	-0.81119900	5.53159200	0.11138300
H	1.73920400	5.57019700	-0.15583000
C	-0.42780300	3.31540100	-0.09338100
N	0.77043800	2.69540900	-0.26533700
N	1.29667200	-2.40419400	0.39218800
N	-1.24671200	-1.48680600	0.01631000
C	-3.45101500	-3.18420100	-0.01792200
H	-4.31434100	-3.84258300	-0.04332600
N	1.72176900	3.55859200	-0.30069300
N	1.15448300	4.75030900	-0.15610500
C	-0.18278600	4.66693100	-0.02415700
C	-4.93764400	-1.19470500	-0.07894000
H	-5.80757900	-1.84411400	-0.10029900

C	-5.08189600	0.15367000	-0.08814700
H	-6.06942700	0.60400600	-0.11967900
H	2.50439300	-5.29114400	0.55727900
C	2.34744800	-3.17427700	0.54111000
H	3.36113100	-2.83325300	0.68908700
N	1.95032000	-4.45459100	0.48192800
N	0.62797800	-4.54409100	0.29111800
N	0.47560300	0.55762300	2.85121300
O	0.31398000	0.75705100	4.02429400
O	0.13488900	-0.52512700	2.29091900
O	0.99289900	1.42636200	2.08211100
N	3.77288600	0.26586100	-0.26049500
O	3.21434600	-0.38603000	0.68435700
O	4.96373500	0.28437500	-0.39923000
O	2.98222300	0.87587000	-1.03337600
N	0.47408100	-0.42633200	-2.81183000
O	0.32825200	-0.63180300	-3.98530900
O	1.05742000	-1.25416100	-2.04544000
O	0.04744600	0.62477400	-2.24690600
Eu	0.91155800	0.09913600	0.00815600

EuR₄PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.53342300	0.79516500	-0.02798400
C	1.27371500	2.71578000	0.07454500
C	2.42128000	3.52794700	0.06128300
H	2.34122700	4.60792300	0.12000100
C	2.58094100	-0.64961500	-0.02987800
C	3.83955000	-1.28818200	-0.07549300
C	3.84704400	-2.69480500	-0.09763200
C	2.66191600	-3.37906200	-0.10069000
H	4.79360900	-3.22614800	-0.12875400
H	2.64785600	-4.46207800	-0.14706300
N	1.42318700	-1.33129900	0.00486200
C	3.74462400	1.52579700	-0.04391600
C	-0.07047900	3.25508200	0.23602500
C	1.45395800	-2.65533000	-0.05732300
H	0.38651000	-5.57297100	0.04334300
H	-2.16154100	-5.41936600	-0.19987900
C	0.16582500	-3.33086500	-0.11903800
N	-0.98525300	-2.62180000	-0.26957700
N	-1.13835200	2.50295900	0.43052600
N	1.33487200	1.39447400	0.00110100
C	3.65160700	2.92795300	-0.01225100
H	4.55766200	3.52607700	-0.02748100

N	-1.99711700	-3.41189500	-0.31099200
N	-1.51793900	-4.64478400	-0.19163400
C	-0.17753400	-4.66200100	-0.07062600
C	4.99453500	0.84002000	-0.08407600
H	5.90962800	1.42401800	-0.09995800
C	5.03877400	-0.51520600	-0.10070500
H	5.99113200	-1.03570100	-0.13336200
C	-2.14621200	3.38906000	0.57569300
H	-3.16687200	3.08709700	0.75247500
N	-0.45019600	4.54344100	0.27334000
H	0.09339400	5.37952900	0.14292000
N	-1.76895500	4.64840900	0.48657500
N	-0.39228200	-0.55748900	2.83669400
O	-0.17304000	-0.78986300	3.99431500
O	0.00934400	0.50011000	2.26725500
O	-1.03310800	-1.36280700	2.09367100
N	-3.79086300	-0.02617600	-0.22116500
O	-3.18493600	0.54112200	0.74830700
O	-4.98303000	0.00323600	-0.33016300
O	-3.03965100	-0.61253200	-1.05366500
N	-0.41484500	0.48008600	-2.79555800
O	-0.22114000	0.68307900	-3.96303900
O	-0.91166000	1.36040200	-2.02746300
O	-0.12493300	-0.62109200	-2.23984300
Eu	-0.93792000	-0.02481800	0.02041200

EuR₅PhR₅(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.66281500	0.72276900	0.00046200
C	-1.47509200	2.69585000	0.04958600
C	-2.65533000	3.45993200	0.07223900
H	-2.60129500	4.54157800	0.11643700
C	-2.66295000	-0.72256700	0.00041100
C	-3.90018200	-1.40649900	-0.01851400
C	-3.86215100	-2.81205500	-0.04488100
C	-2.65594600	-3.45973700	-0.07136800
H	-4.79208700	-3.37267500	-0.05703000
H	-2.60209900	-4.54139300	-0.11557000
N	-1.48372600	-1.36838800	0.01209300
C	-3.89992800	1.40691700	0.01924600
C	-0.16220500	3.32113100	0.12165300
H	-0.23760600	5.58020100	0.03457400
C	-1.47558300	-2.69585700	-0.04864900
H	-0.23849100	-5.58041900	-0.03428400
C	-0.16280400	-3.32135000	-0.12096100

N	0.90838300	-2.53994100	-0.23241900
N	0.90890300	2.53958100	0.23277000
N	-1.48347000	1.36837900	-0.01110500
C	-3.86164700	2.81246800	0.04565000
H	-4.79148300	3.37325400	0.05772000
N	1.62325400	4.63429600	0.21054600
N	1.62243200	-4.63474800	-0.21093300
C	0.29753500	4.64648600	0.11131200
C	0.29674800	-4.64676900	-0.11112800
C	-5.12602500	0.67796800	0.01145100
H	-6.05991500	1.23156600	0.02227900
C	-5.12614900	-0.67733000	-0.01087700
H	-6.06013900	-1.23075600	-0.02183100
N	1.92039100	3.36096900	0.27682100
H	2.86189700	2.99059600	0.34905700
N	1.91974000	-3.36146700	-0.27709200
H	2.86123200	-2.99120200	-0.35009200
N	0.74655400	-0.35692700	2.85985500
N	0.74304900	0.35790300	-2.85941000
N	3.78017300	-0.00030500	-0.00192000
O	0.10409300	-0.56510200	-2.25967300
O	0.71053300	0.49000200	-4.04889400
O	1.40940600	1.13052800	-2.10393300
O	1.41138500	-1.13058100	2.10410300
O	0.10712700	0.56582800	2.26020800
O	0.71582100	-0.48782500	4.04951600
O	3.09357900	-0.95450600	-0.48142800
O	3.09450300	0.95399900	0.47857800
O	4.97535500	-0.00043800	-0.00285100
Eu	0.83830100	-0.00031100	0.00008700

EuR₅PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.35872900	-1.32248000	-0.01419000
C	-0.73355900	-2.94564600	0.11057300
C	-1.69667000	-3.97215000	0.09153100
H	-1.38474500	-5.00864500	0.14892600
C	-2.70600000	0.08052400	-0.02721400
C	-4.07086800	0.45024700	-0.08910600
C	-4.36641600	1.82315500	-0.12714400
C	-3.34707600	2.73961700	-0.12520000
H	-5.40131500	2.14802100	-0.17660700
H	-3.56428700	3.79996100	-0.19459600
N	-1.71706500	0.98687400	0.01632900
C	-3.39576100	-2.28167000	-0.03224300

C	0.68330400	-3.23323000	0.26596300
H	1.16034400	-5.44517600	0.28638800
C	-2.02224700	2.27493500	-0.05726900
H	-1.64873000	5.13728200	0.16228400
C	-0.87782900	3.17131300	-0.11622500
N	0.35355700	2.75932200	-0.30255100
N	1.52551400	-2.21154100	0.39146900
N	-1.06031200	-1.66029200	0.02675400
C	-3.02128800	-3.63702400	0.00759800
H	-3.78762100	-4.40611300	-0.01323000
N	2.72373800	-4.06912300	0.50771500
C	1.44854600	-4.40687700	0.34316100
C	-4.75958700	-1.86655500	-0.08708100
H	-5.53350200	-2.62792300	-0.10481700
C	-5.08637800	-0.55103800	-0.11658400
H	-6.12513000	-0.23880700	-0.16186400
N	2.69855100	-2.75883800	0.52637300
H	3.51153000	-2.15775800	0.62480800
N	1.18117100	3.82505900	-0.31770800
N	-0.87122100	4.52529000	-0.01723600
C	0.43572200	4.87982800	-0.14459100
H	0.78952100	5.89846100	-0.10514800
N	0.62711200	-0.37965300	-2.80229900
O	0.52258000	-0.60691700	-3.97476300
O	-0.04254200	0.53755400	-2.22840200
O	1.39803900	-1.03914100	-2.04401100
N	3.73661800	0.69890300	-0.26307000
O	2.87990700	1.38299300	-0.87812500
O	3.25308900	-0.14767600	0.57303100
O	4.91655300	0.81050900	-0.42995900
N	0.44189600	0.65892100	2.85419300
O	0.24199800	0.81043300	4.02752900
O	0.78257500	1.61300700	2.09191600
O	0.31486300	-0.46914300	2.28466300
Eu	0.88285000	0.25278700	0.00836800

EuR₅PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.61362600	0.86283200	-0.09819800
C	1.32859600	2.76544800	-0.21492500
C	2.46910300	3.58856900	-0.23605300
H	2.36151900	4.66531000	-0.30017400
C	2.68154200	-0.57928400	-0.08480700
C	3.94585000	-1.21026700	-0.06897200
C	3.96824900	-2.61723200	-0.10017200

C	2.79143400	-3.31478800	-0.16938400
H	4.92078800	-3.13846100	-0.08255700
H	2.76270500	-4.39686900	-0.21396900
N	1.53067400	-1.27138800	-0.12126400
C	3.81598000	1.60548700	-0.10387700
C	-0.01626900	3.32276000	-0.27339800
H	-0.03940800	5.58358300	-0.34075900
C	1.58597800	-2.59273000	-0.18370800
C	0.29769300	-3.26943300	-0.28781800
N	-0.85887300	-2.56096900	-0.34413500
N	-1.05591800	2.49106100	-0.25347500
N	1.40375800	1.44314000	-0.13317700
C	3.70724600	3.00583600	-0.16862200
H	4.60676600	3.61421500	-0.17409400
N	-1.86285400	4.55258300	-0.30852700
C	-0.53484800	4.62553400	-0.31440700
C	5.07295300	0.93188200	-0.05871400
H	5.98123900	1.52682100	-0.04825900
C	5.13565500	-0.42284200	-0.03996100
H	6.09475300	-0.93102700	-0.01375800
N	-2.10549500	3.26735100	-0.27637700
H	-3.02799400	2.85860100	-0.17182300
C	-1.79153000	-3.48305500	-0.42377800
H	-2.85517800	-3.30278000	-0.45395000
N	-1.20162900	-4.68555900	-0.42645400
H	-1.62774300	-5.59617400	-0.47421700
N	0.13104200	-4.57511300	-0.33882800
N	-1.29752400	-0.04890800	-2.74231400
O	-1.46173100	-0.07416700	-3.93036800
O	-0.13973100	0.00651400	-2.21932700
O	-2.26333400	-0.07748000	-1.92037900
N	-3.72884400	-0.11279900	0.74721000
O	-3.02307700	-1.16009400	0.68874400
O	-3.07005000	0.97328500	0.67245500
O	-4.91979000	-0.13413800	0.86729600
N	-0.12108300	-0.09057000	2.88137100
O	0.21545100	-0.10561100	4.03063500
O	-0.29596800	-1.15462300	2.20870400
O	-0.32454400	0.99103600	2.24522700
Eu	-0.87580300	-0.05039800	0.11590800

EuR₅PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.54828600	-1.04772800	0.06601300
C	-1.14240900	-2.86425800	0.02941600
C	-2.22588800	-3.76196400	0.03057500
H	-2.04631400	-4.83068000	0.00555200
C	-2.71298800	0.38775400	0.07134500
C	-4.02068300	0.92893400	0.09416100
C	-4.14060500	2.32820200	0.13087000
C	-3.01324200	3.10633300	0.16953600
H	-5.12669000	2.78231500	0.14532400
H	-3.09494400	4.18608800	0.22877200
N	-1.61455600	1.15994500	0.06853900
C	-3.69945600	-1.86750200	0.06271700
C	0.23568200	-3.32608700	-0.04479200
H	0.43999400	-5.57764600	0.02996500
C	-1.75743200	2.47600600	0.14301900
H	-1.02138100	5.28808100	0.16327000
C	-0.51025600	3.22030600	0.24304000
N	0.67539600	2.65060500	0.36660900
N	1.20078400	-2.41715700	-0.16493300
N	-1.30402900	-1.54753600	0.06598800
C	-3.49971000	-3.25968400	0.05293000
H	-4.35802600	-3.92487800	0.05398600
N	2.16726300	-4.40832100	-0.16967200
C	0.85470800	-4.58463100	-0.04836100
C	-5.00015200	-1.28099800	0.07065600
H	-5.86559300	-1.93669500	0.06565200
C	-5.15614800	0.06561100	0.08710300
H	-6.14722300	0.50848000	0.09777500
N	2.30404800	-3.10820400	-0.23052600
H	3.18572400	-2.61943200	-0.35337000
N	-0.34199100	4.55220100	0.25557600
C	1.53606200	3.69191100	0.44147200
H	2.60271900	3.56276600	0.53219600
N	0.95353700	4.87065600	0.38057000
N	0.28741600	0.46630900	-2.84837600
O	0.01792900	0.59971900	-4.00823100
O	0.70384800	1.42689600	-2.12932800
O	0.16682700	-0.64561500	-2.24536200
N	3.79399800	0.37786300	-0.32705200
O	3.14431700	-0.64159500	-0.73974000
O	3.07329200	1.31894400	0.10303100
O	4.98878500	0.42493300	-0.35390700
N	1.04346500	-0.30448800	2.80313300
O	1.08858200	-0.46751600	3.98950500

O	0.06991900	0.29563900	2.23933000
O	1.95018400	-0.71707700	2.02078600
Eu	0.89602800	0.13477200	-0.04722200

EuR₆PhR₆(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.54339200	0.72409000	-0.00009600
C	1.32960200	2.67366900	-0.00003000
C	2.50178400	3.45181400	-0.00007100
H	2.45500700	4.53550400	-0.00005500
C	2.54392100	-0.72230000	-0.00011500
C	3.77698900	-1.41129300	-0.00016500
C	3.72126800	-2.81571000	-0.00017700
C	2.50429800	-3.45005600	-0.00014000
H	4.64215500	-3.39097000	-0.00021300
H	2.45831300	-4.53378000	-0.00014600
N	1.36293100	-1.34912800	-0.00008500
C	3.77595700	1.41398200	-0.00013900
C	-0.00668100	3.25424800	0.00003100
H	0.27045900	5.36749600	-0.00009500
C	1.33155000	-2.67276400	-0.00009300
H	0.27436800	-5.36735600	-0.00015900
C	-0.00431100	-3.25431200	-0.00005400
N	-1.11113800	-2.54829800	0.00000200
N	-1.11299500	2.54742800	0.00012800
N	1.36194500	1.35005500	-0.00004100
C	3.71921600	2.81835500	-0.00012400
H	4.63968600	3.39428300	-0.00015300
N	-0.27500700	-0.00007300	-2.85582900
N	-0.27433600	-0.00018200	2.85578700
N	-3.81949400	-0.00121200	0.00014200
O	-0.44013200	1.06989300	2.19956600
O	0.02869500	-0.00010200	4.02004300
O	-0.43952500	-1.07034300	2.19955300
O	-0.43982000	-1.07025400	-2.19952800
O	-0.44033900	1.06998000	-2.19946200
O	0.02825800	0.00003400	-4.02002400
O	-3.13702200	-0.00136200	1.07393500
O	-3.13708500	-0.00052600	-1.07368900
O	-5.01614100	-0.00137800	0.00017800
N	-2.17318500	-3.37719000	0.00004300
N	-0.34292200	4.57087900	0.00000000
N	-0.33959300	-4.57118600	-0.00009700
N	-2.17564400	3.37554800	0.00017100
C	-1.70193300	4.59056900	0.00009900

H	-2.29141500	5.49427200	0.00010700
C	-1.69859100	-4.59186600	-0.00002900
H	-2.28741400	-5.49599900	-0.00003000
C	5.00124800	0.68035100	-0.00019200
H	5.93731300	1.23050600	-0.00022200
C	5.00174400	-0.67676600	-0.00020300
H	5.93821100	-1.22623500	-0.00024200
Eu	-0.98146700	-0.00037800	0.00006500

EuR₆PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.65845400	0.19818000	0.00163000
C	-1.88940400	2.36363300	-0.03223800
C	-3.19716600	2.87821900	-0.08273400
H	-3.37514100	3.94622600	-0.14766300
C	-2.36149300	-1.21543400	0.00304400
C	-3.42704700	-2.14150300	-0.01246200
C	-3.09538700	-3.50975400	0.01265700
C	-1.78138100	-3.88910500	0.08178500
H	-3.88651500	-4.25340300	-0.00760600
H	-1.48228400	-4.92932700	0.12875800
N	-1.07464000	-1.59605400	0.03145400
C	-4.00853700	0.61742200	-0.04463800
C	-0.70962900	3.21372300	-0.10967800
H	-1.39840600	5.20726600	0.18973100
H	1.06153900	5.87541100	-0.11808800
C	-0.79337700	-2.88810900	0.10107800
H	3.04056600	-4.99711400	0.61279400
C	0.61859500	-3.21967100	0.25765200
N	1.55348600	-2.24714800	0.39247800
N	0.50139200	2.75524900	-0.32012800
N	-1.63578400	1.06515000	0.03705400
C	-4.25142600	2.00117900	-0.07438600
H	-5.27346900	2.36612700	-0.11083800
N	1.36913300	3.78875000	-0.34615700
C	0.66834100	4.87124300	-0.15571100
N	-0.64860600	4.56665700	-0.00665900
C	-4.77608300	-1.67688600	-0.04976000
H	-5.57707200	-2.40982200	-0.06483100
C	-5.05709400	-0.34995200	-0.06671700
H	-6.08537200	-0.00290400	-0.09874800
C	2.67455600	-2.90633200	0.55653100
H	3.64923500	-2.46478700	0.70123700
N	2.40652000	-4.22110600	0.52126600

N	1.10014200	-4.44452900	0.33365600
N	0.39383600	0.61750500	2.83294200
O	0.18061100	0.79796300	4.00149900
O	0.24922600	-0.51226700	2.28124300
O	0.76878500	1.55336100	2.06120600
N	3.74615000	0.63549800	-0.27306100
O	3.24418500	-0.00991600	0.70907200
O	2.90704400	1.11877200	-1.08316200
O	4.93046500	0.75771100	-0.41037100
N	0.42680300	-0.44751700	-2.80086000
O	0.24478900	-0.70676500	-3.95879300
O	1.16089300	-1.16192300	-2.05224400
O	-0.11164700	0.55140300	-2.23548900
Eu	0.92115800	0.20900500	-0.01140700

EuR₆PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.64544400	0.25529700	-0.00220800
C	1.82230700	2.40161800	-0.00658800
C	3.12019100	2.94388300	-0.04794000
H	3.27572200	4.01646300	-0.08825100
C	2.38066300	-1.16653100	-0.00530300
C	3.46844000	-2.06808600	-0.03120900
C	3.16365200	-3.44050500	-0.02402700
C	1.85543700	-3.84659400	0.02473800
H	3.96747400	-4.16995400	-0.04852000
H	1.61323300	-4.90345400	0.04483300
N	1.10412900	-1.57348400	0.01930800
C	3.98510800	0.70355800	-0.03990300
C	0.62849300	3.23441100	-0.04020700
H	1.31058000	5.24358800	0.18005700
H	-1.16753900	5.87951900	0.00635600
C	0.84066300	-2.87254700	0.05225200
C	-0.57146100	-3.21475400	0.16073800
N	-1.53713600	-2.32091700	0.25746300
N	-0.58777000	2.76236800	-0.17547700
N	1.60155200	1.09507200	0.03362100
C	4.19524200	2.09311600	-0.05502100
H	5.20801700	2.48328400	-0.08554500
N	-1.46550100	3.78562300	-0.17075700
C	-0.76639300	4.87867400	-0.03612000
N	0.55884200	4.58947100	0.04604400
C	4.80689900	-1.57358900	-0.06222100
H	5.62483400	-2.28720600	-0.08282900

C	5.05548600	-0.24020600	-0.06726700
H	6.07555300	0.13062600	-0.09359900
C	-2.65851300	-3.05694300	0.39228400
H	-3.63654800	-2.61649400	0.50990700
N	-1.12190900	-4.44025200	0.23470000
H	-0.68919200	-5.34712700	0.19323900
N	-2.44994000	-4.35905200	0.38127300
N	-0.39161800	-0.24287900	-2.82654400
O	-0.18792200	-0.40971000	-3.99782900
O	-0.92458200	-1.13251300	-2.09565900
O	-0.07878400	0.82926900	-2.22791600
N	-3.75186800	0.59174000	-0.24774500
O	-2.92672400	1.01828200	-1.10686100
O	-3.23098800	-0.00658000	0.75377600
O	-4.93666800	0.72652000	-0.36105000
N	-0.39545100	0.40178300	2.86548400
O	-0.16681600	0.49865400	4.04032900
O	-0.48781400	-0.71542700	2.27847300
O	-0.55223600	1.41710100	2.11897600
Eu	-0.92722400	0.18341000	0.00083900

EuR₇PhR₇(NO₃)₃ (PBE0/6-311G*-RECP)

C	2.64951700	-0.72098600	-0.09992900
C	1.45872400	-2.67553000	-0.22008200
C	2.62816400	-3.45546700	-0.20996800
H	2.54705500	-4.53449500	-0.26380200
C	2.64938600	0.72148500	-0.09983400
C	3.88204700	1.41147500	-0.08213400
C	3.83692700	2.81752000	-0.12928500
C	2.62752600	3.45597700	-0.20948700
H	4.76291100	3.38469700	-0.11263300
H	2.54621700	4.53499700	-0.26316300
N	1.46629700	1.35446400	-0.14888400
C	3.88230700	-1.41075100	-0.08233200
C	0.13811000	-3.28677400	-0.32093400
C	1.45823300	2.67582000	-0.21972900
C	0.13749700	3.28681900	-0.32050100
N	-0.98265700	2.52090500	-0.34367600
N	-0.98220300	-2.52109100	-0.34407300
N	1.46654200	-1.35418100	-0.14904000
C	3.83744700	-2.81679700	-0.12968300
H	4.76353600	-3.38380600	-0.11311900
C	-1.96026000	-3.39449000	-0.42563000
H	-3.01383100	-3.16112100	-0.43216900

C	-1.96089600	3.39410200	-0.42518500
H	-3.01441900	3.16051900	-0.43177000
C	5.10586200	-0.67794600	-0.03377500
H	6.04092300	-1.22928800	-0.00640100
C	5.10573700	0.67889000	-0.03367700
H	6.04069700	1.23040000	-0.00622100
N	-0.09318200	-4.58182900	-0.39304500
N	-0.09406500	4.58183000	-0.39253000
N	-1.43202100	4.62438500	-0.46040200
H	-1.90367600	5.51159100	-0.51751400
N	-1.43112800	-4.62466000	-0.46091900
H	-1.90259800	-5.51196100	-0.51807600
N	-1.38544200	0.00047900	-2.72947000
N	-0.05925800	-0.00051300	2.87085700
N	-3.70472300	-0.00038400	0.90122300
O	-0.26651700	1.07274200	2.22306700
O	0.30998700	-0.00068300	4.01104200
O	-0.26697500	-1.07357800	2.22289500
O	-2.33455200	0.00041100	-1.88824200
O	-0.21548200	0.00016700	-2.23344600
O	-1.57687200	0.00080000	-3.91502100
O	-3.03236900	1.06752700	0.78053900
O	-3.03243900	-1.06822900	0.77965900
O	-4.88451200	-0.00043100	1.11498600
Eu	-0.90006400	-0.00011500	0.12228100

EuR₇PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.60805200	0.87369200	0.11589300
C	-1.29658600	2.74821800	0.20485900
C	-2.41475000	3.60061500	0.18885000
H	-2.26509400	4.67305200	0.22506400
C	-2.69990000	-0.56709400	0.11949400
C	-3.97596200	-1.17749000	0.10587500
C	-4.01612600	-2.58168000	0.14408000
C	-2.84581600	-3.29401000	0.20566000
H	-4.97385900	-3.09308800	0.13115000
H	-2.86715600	-4.37779900	0.24371800
N	-1.56155000	-1.27099100	0.15764100
C	-3.79530700	1.63811600	0.09576400
C	0.06065100	3.27461800	0.28869700
C	-1.62802900	-2.59111800	0.21209000
C	-0.33332500	-3.25577400	0.28552300
N	0.82297100	-2.61460200	0.27960300
N	1.12888000	2.43854300	0.31601700

N	-1.38785400	1.42908000	0.15542600
C	-3.66265300	3.03908600	0.12548000
H	-4.55124200	3.66303900	0.10619100
C	2.16199200	3.24749100	0.38582000
H	3.19805000	2.94581800	0.39208100
C	1.74773400	-3.60006800	0.35568300
H	2.80821800	-3.40472500	0.34576300
C	-5.06351000	0.98360400	0.05827200
H	-5.96150300	1.59353100	0.03183300
C	-5.15178700	-0.37019200	0.06385800
H	-6.12028000	-0.86042000	0.04218200
N	0.37522100	4.55267400	0.34631600
N	1.71315300	4.50935000	0.40855100
H	2.24168400	5.36470400	0.45345900
N	1.23499300	-4.81035900	0.41737000
N	-0.08407400	-4.57208300	0.37080700
H	-0.72386700	-5.34766100	0.39519300
N	0.00106100	0.04868200	-2.84176800
O	-0.42256300	0.09175400	-3.96317000
O	0.34758000	1.08838000	-2.20377400
O	0.12756500	-1.04684900	-2.20700700
N	1.37120000	-0.00900100	2.72819900
O	1.53265900	0.04071100	3.91536600
O	2.32865900	0.08759200	1.90390500
O	0.21957400	-0.16015500	2.20705900
N	3.74106800	-0.22459900	-0.86857200
O	3.13344100	0.88495500	-0.81434300
O	4.91628600	-0.31188700	-1.08452900
O	3.00577700	-1.24361600	-0.67758600
Eu	0.94200400	-0.07537300	-0.11105600

EuR₈PhR₈(NO₃)₃ (PBE0/6-311G*-RECP)

C	-2.57009400	-0.72820500	-0.01097700
C	-1.37290500	-2.68771200	0.04170900
C	-2.54689800	-3.46190100	0.04526300
H	-2.50032700	-4.54437800	0.09172100
C	-2.57343100	0.71731900	0.00647600
C	-3.81112300	1.40050800	-0.00181700
C	-3.77137100	2.80561300	-0.01280600
C	-2.56280900	3.45119900	-0.04829100
H	-4.69919800	3.36948700	-0.01344900
H	-2.52120900	4.53394100	-0.09324800
N	-1.39628400	1.35857900	0.01652900
C	-3.80461300	-1.41709700	-0.00445800

C	-0.04530600	-3.27230100	0.17417600
H	-0.27572400	-5.38876700	0.03420600
C	-1.38526600	2.68244700	-0.04321500
H	-0.30101100	5.38922600	-0.04493900
C	-0.05987000	3.27297500	-0.17133000
N	1.03602700	2.56156500	-0.36012600
N	1.04627700	-2.55672400	0.37242400
N	-1.38998500	-1.36399600	-0.01907500
C	-3.75839000	-2.82198900	0.00714900
H	-4.68359900	-3.39014600	0.00668100
N	0.44677600	-0.52190400	-2.81363000
N	0.44085000	0.52608400	2.81718300
N	3.83498900	0.00594100	-0.00815600
O	-0.00536100	-0.50958100	2.23807900
O	0.24126700	0.75212200	3.97832200
O	1.10287700	1.31660700	2.07515300
O	1.08812300	-1.32369500	-2.06515100
O	0.01890600	0.52449300	-2.24047600
O	0.24945200	-0.74777200	-3.97520200
O	3.14762100	0.75745300	-0.76791400
O	3.15441400	-0.74740900	0.75606900
O	5.03159900	0.00741000	-0.01185500
N	0.29448800	-4.57248300	0.17652600
N	0.27389100	4.57476100	-0.17850500
C	2.02817700	-3.47671300	0.48451100
H	3.05936400	-3.21043400	0.65560500
C	2.01411500	3.48546800	-0.47246900
H	3.04718500	3.22326200	-0.63837400
N	1.61129800	-4.72168700	0.37108400
N	1.59090100	4.72907400	-0.36749200
C	-5.03209900	-0.68910100	-0.00415600
H	-5.96567000	-1.24328600	-0.00306500
C	-5.03523500	0.66684300	-0.00406500
H	-5.97135600	1.21669700	-0.00649100
Eu	0.94886400	0.00172700	0.00243800