Electronic Supplementary Information (ESI) for:

Selective Separation of Americium from Europium Using 2,9-Bis(triazine)-1,10-phenanthrolines in Ionic Liquids: A New Twist on an Old Story

Neil J. Williams[ab], Jérémy Dehaudt[a], Vyacheslav S. Bryanstev[b], Huimin Luo[c]*, Carter W. Abney[b]*, and Sheng Dai [ab]*

[a] Department of Chemistry, University of Tennessee, Knoxville, TN 37916, USA
[b] Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA. E-mail: abneycw@ornl.gov; dais@ornl.gov
[c] Energy and Transportation Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA. E-mail: luoh@ornl.gov

Section S1. Materials and Synthetic Methods.

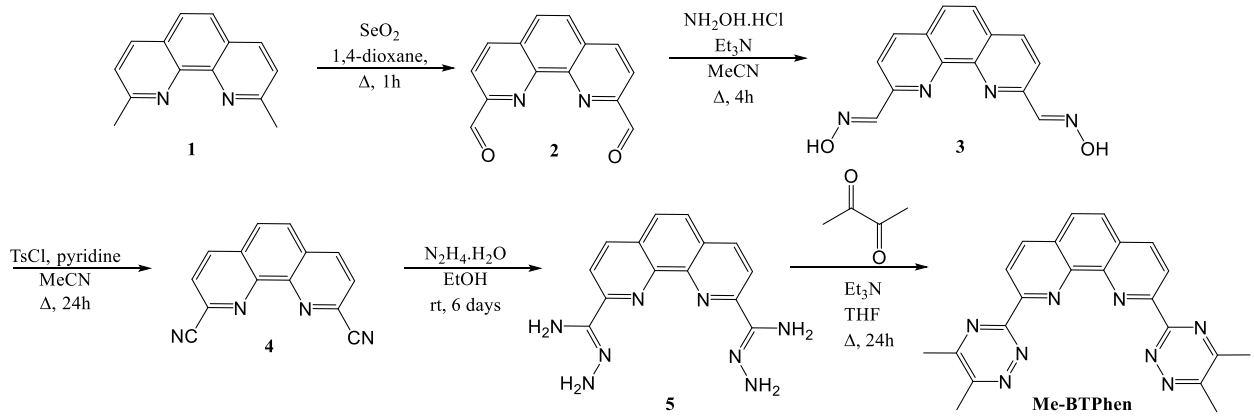
Materials

All reagents were obtained from Aldrich in their purest form and used without further purification. The solvent trifluoromethylphenyl sulfone (FS-13) was obtained from Marshallton Research Laboratories and used as received. The 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)-sulfonyl]amide ([C_4mim][NTf_2]) ionic liquid was obtained from Sigma-Aldrich. Europium-152/154 was obtained from Isotope Products (presently owned by Eckert & Ziegler) and americium-241was produced at Oak Ridge National Laboratory.

Synthetic Methods

^{1}H and ^{13}C NMR spectra were recorded using a Varian VNMRS 500 MHz spectrometer. The chemical shifts at 25°C (given in parts per million) were referenced to the residual protonated solvent. The mass peaks for protonated molecules were determined using DART (direct analysis in real time) at the Mass Spectrometry Center located in the Department of Chemistry at the University of Tennessee. The DART analyses were performed using a JEOL AccuTOF-D time-of-flight mass spectrometer with a DART ionization source from JEOL USA, Inc. (Peabody, MA).

Me-BTPhen was prepared according to a literature procedure[1] with a slight modification for the last step (Scheme 1). Neocuproine **1** was oxidized using selenium dioxide. The resulting dialdehyde **2** was treated with hydroxylamine hydrochloride. The dioxime **3** was then converted to the dinitrile 4. The latter was reacted with hydrazine hydrate to give the dicarbohydrazonamide **5**. Me-BTPhen was obtained by reaction of **5** with diacetyl in presence of triethylamine. Synthetic details for the last step and NMR spectra of Me-BTPhen are given below.



Scheme 1: synthetic route for the preparation of Me-BTPhen

To a suspension of 1,10-phenanthroline-2,9-dicarbohydrazonamide **5** (800 mg, 2.72 mmol) in THF (50 mL) was added diacetyl (0.5 mL, 5.75 mmol, 2.1 eq) and Et_3N (5 mL). The mixture was refluxed for 24h. After cooling, the solvent was removed under vacuum and the residue was washed with Et_2O. The crude product was purified by silica gel column chromatography (CH_2Cl_2/MeOH, 100:0 to 70:30 v/v) to give the desired compound as a yellow powder (660 mg, 62%). ^1H NMR (500 MHz, $CDCl_3$): δ 2.81 (s, 6H), 2.84 (s, 6H), 7.94 (s, 2H), 8.47 (dd, 2H, *J* = 8.4 Hz, 0.5 Hz), 8.99 (dd, 2H, *J* = 8.4 Hz, 0.5 Hz). ^{13}C NMR (126 MHz, $CDCl_3$): δ 19.7, 21.6, 123.0, 127.7, 130.1, 137.5, 146.4, 152.9, 157.5, 160.0, 161.3. HRMS: *m/z*: 395.1741 [M + H^+]. $C_{22}H_{19}N_8^+$ requires 395.1732.

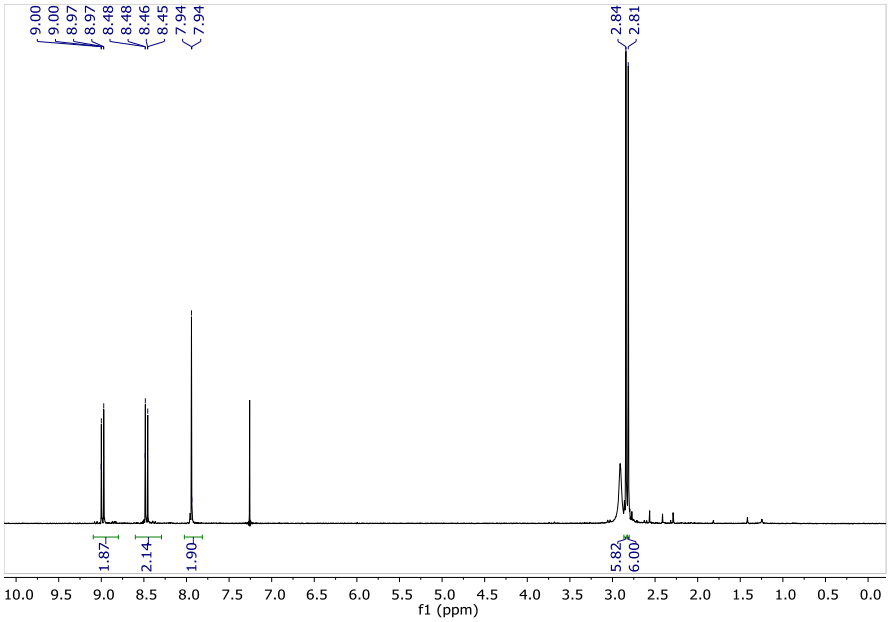


Figure S1 ^{1}H NMR of Me-BTPhen in $CDCl_3$

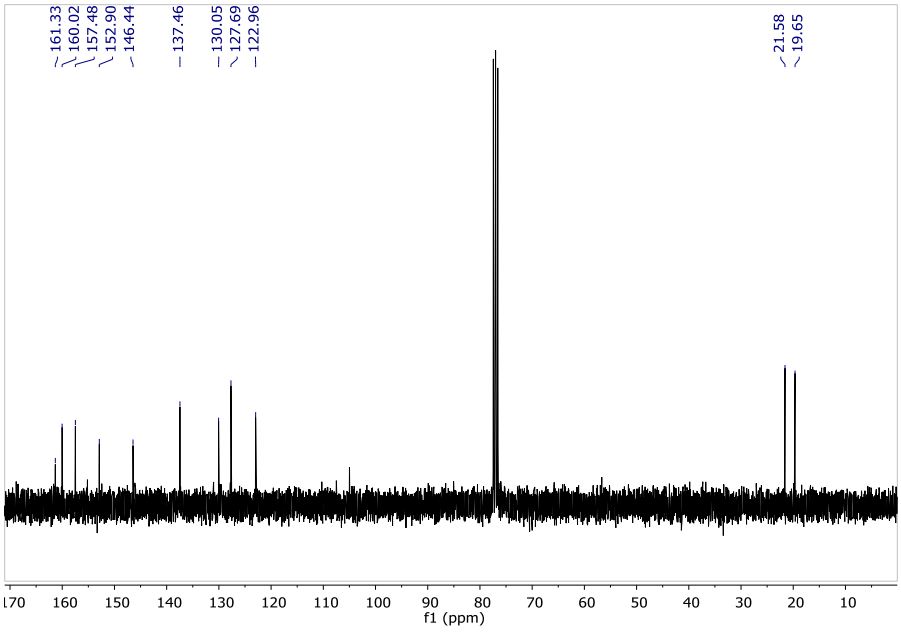


Figure S2 ^{13}C NMR of Me-BTPhen in $CDCl_3$

Section S2. Determination of distribution ratios.

The distribution ratio (D_M) for extraction of trivalent metal ions (M^{3+}) is defined by

$$D_M = \frac{C_{M,org}}{C_{M,aq}}$$

In this equation, $C_{m,aq}$ and $C_{m,org}$ represent the counts per a minute for the isotopes of $^{152/154}$Eu or ^{241}Am in either the organic or aqueous phases, respectively. A volume ratio is needed in the calculation of distribution ratios to account for the difference in volume between the two immiscible phases. In all of our experiments, the volume ratio was close to 1:1 v/v. Separation factors SF for the metal ions *M* and *M'* are defined from:

$$SF_{M/M'} = D_M / D_{M'}$$

Eu/Am measurements.

The distribution ratios for extraction using radiotracer techniques were calculated by measuring the amount of radioactivity of both aqueous and organic phases at equilibrium. Counting efficiency (^{241}Am or ^{152,154}Eu gamma ray absorption in solid scintillators) is identical for both phases; hence, the distribution ratio is defined by the ratio of specific radioactivity *S* (Bq/mL) of element *M* in the IL vs. aqueous phases.

$$D_M = \frac{C_{IL,f}}{C_{IL,f}} \propto \frac{S_{org,f}}{S_{aq,f}}$$

An equal volume of both IL (containing 4 mM complexant) and aqueous phases, 0.4 mL of each were used, respectively. Each sample was individually spiked with a 10 μL solution containing 1.85×10^6 Bq/mL (50 μCi/mL) of each radiotracer respectively. The solutions were mixed using a rotating wheel set at 60 rpm for 3 h at 25±0.2 °C. (Initial studies were performed at 1, 3, and 24 h, with samples contacted for 3 and 24 h observed to have the same *D* values. Due to this observation it was assumed that the samples achieved equilibrium by the 3 h time point. Samples contacted/mixed for 1 h had lower *D* values than those at 3 h. For the sake of brevity and consistency, all samples were contacted for 3 h). After 3 h the samples were centrifuged at 3,000 rpm for 5 min at 25 °C to ensure the phases separated from each other. Then a 100 μL aliquots were subsampled from each phase and placed into polypropylene tubes that were sealed with a cap. These tubes were then placed in a Canberra Gamma Analyst germanium spectrometer to determine the amounts of ^{241}Am and ^{152,154}Eu present in each sample. Prior to testing these samples, a quality assurance calibration was performed. The organic and aqueous samples were counted for a period of 30 min to ensure an accurate measurement. Additional blank samples (no isotopes present in solution) were run to ensure no background subtraction was necessary. Once the data was collected the total counts for each isotope in the samples was normalized to give the average counts per minute.

Slope Analysis

To determine the stoichiometry of the metal–ligand complex a slope analysis experiment was conducted. This experiment made use of the $^{152/154}$Eu radiotracer employing similar techniques to those discussed in the above section discussing use of Eu and Am radiotracers. In this experiment the concentration of the Me-BTPhen was varied in [C_4mim][NTf_2]; the concentrations were as follows: 1.0, 3.0, 10.0, and 30.0 mM. The IL solutions were then contacted with 0.1 M HNO_3 which had been spiked with a 10 µL solution containing 50 µCi/mL of the Eu radiotracer.

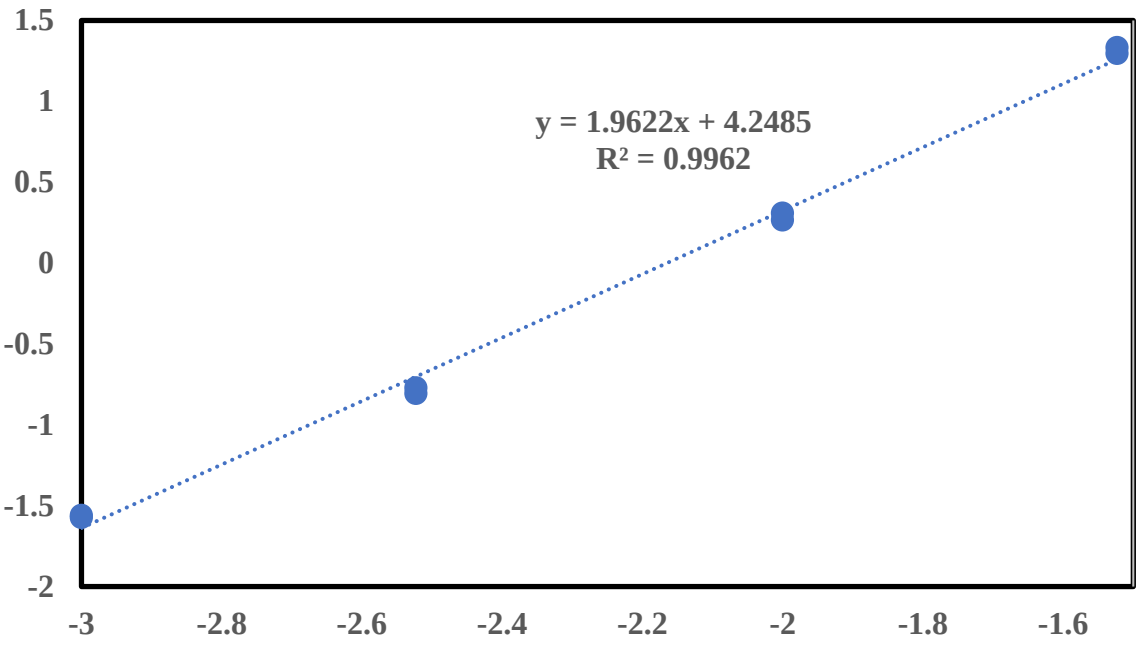


Figure S3. Slope Analysis of Me-BTPhen with Eu extracted from 0.1 M HNO_3. The y-axis represents the logD_{Eu} and the x-axis is the log[Me-BTPhen].

From Figure S3 above, the trend line associated with the D_{Eu} for Me-BTPhen has a slope of two indicating that the ligand-metal complex is likely 2-to-1 during the extraction process. These results correlate with the solutions structural data presented and discussed in the manuscript. Additionally the 2-to-1 structure has been shown to exist in crystal structures in the previous reported examples in the literature.[2]

Quantification of Extracted Nitrate

The amount of nitrate extracted was determined by Ion Chromatography (IC) using conductivity detection. The IC used was a Dionex ICS-5000+ Reagent-Free High-Pressure IC

system, the detector was a conductivity detector, the columns used were a Thermo Scientific Dionex IonPac AS11-HC Hydroxide-Selective Anion-Exchange Column (4 x 250 mm) with a IonPac AG11-HC Guard Column (4 x 50 mm). The program used to run the instrument and process the data is Chromeleon version 6.2. The eluent used in the IC for the samples was 30 mM KOH, using a flow rate of 1.5 mL/min with the conductivity set at 112 mA. A calibration curve was made by dilution a purchased 1000 ppm nitrate standard purchased from Inorganic Ventures.

Section S3. Computational Methods

DFT calculations were performed on a series of Eu-Me-BTPhen and Am-Me-BTPhen complexes using the Gaussian 09,[3] Revision D01, software package at the B3LYP[4, 5] level of theory. A standard 6-311+G** basis sets were used for all light atoms. F-elements were modelled using the large-core (LC) relativistic effective core potential (RECP) and the associated (7s6p5d2f) /[5s4p3d2f][6, 7] basis sets. Since LC RECP calculations include the 4f electrons in the core, they were performed on a pseudo singlet state configuration. Solvent corrections we included as single-point energies using a generic ionic liquid implicit solvation model, SMD-GIL,[8] with generic values of solvent descriptors. Cartesian coordinates of all the ligand-metal ion complexes accompanied by their electronic energies obtained at the B3LYP/LC(7s6p5d2f)/[5s4p3d2f]/6-311+G** level are given in Section S5.

Comparison of the relative stability of 2:1 ligand-metal ion complexes with monodentate and chelate coordination of NTf_2^- indicated that the chelate form with Eu^{3+} and Am^{3+} was 0.13−2.3 kcal/mol more stable than the monodentate form in the gas phase, but it was 5.4−5.7 kcal/mol less stable in the presence of implicit solvent. With the NO_3^- anion, we could locate only the Eu(III) and Am(III) complexes in the chelate mode, whereas the complex in the monodentate mode were not a stationary point on the potential energy surface, which converged to the chelating species during the geometry optimization. Eu/Am-ligand bond distances for the DFT optimized 2:1 ligand-metal ion complexes are listed in Table S1

Table S1. Eu/Am-Ligand Bond Distances in Å for Geometrically Optimized Molecules as Determined by DFT Calculations

	No Anion	**OH^-**	**H_2O**	**NTf_2^- (mono)**	**NO_3^- (chelate)**	**NTf_2^- (chelate)**
$O_{Anion-1}$	---	2.126/2.194	2.570/2.692	2.436/2.492	2.537/2.584	2.551/2.602
$O_{Anion-2}$	---	---	---	---	2.539/2.587	2.568/2.614
N_{Phen-1}	2.563/2.634	2.637/2.696	2.571/2.635	2.582/2.645	2.633/2.698	2.630/2.667
N_{Phen-2}	2.564/2.634	2.638/2.697	2.594/2.636	2.591/2.655	2.637/2.699	2.667/2.691
N_{Phen-3}	2.564/2.634	2.640/2.706	2.595/2.661	2.593/2.659	2.637/2.718	2.605/2.714
N_{Phen-4}	2.564/2.635	2.646/2.711	2.611/2.662	2.599/2.664	2.663/2.719	2.659/2.721
$N_{Azide-1}$	2.587/2.635	2.703/2.738	2.611/2.656	2.636/2.680	2.652/2.695	2.658/2.700
$N_{Azide-2}$	2.587/2.636	2.706/2.748	2.646/2.657	2.640/2.686	2.652/2.695	2.684/2.726
$N_{Azide-3}$	2.588/2.636	2.712/2.752	2.657/2.702	2.656/2.700	2.684/2.729	2.705/2.737
$N_{Azide-4}$	2.588/2.637	2.714/2.758	2.657/2.703	2.656/2.701	2.685/2.730	2.713/2.746
Average	*2.576/2.635*	*2.614/2.667*	*2.599/2.667*	*2.599/2.654*	*2.635/2.685*	*2.644/2.692*
Coord. #	*8*	*9*	*9*	*9*	*10*	*10*

Section S4. X-ray Absorption Fine Structure Spectroscopy

Data Collection and Processing

XAFS samples were prepared by mixing 2 mL of a 15 mM Me-BTPhen dissolved in $[C_4mim][NTf_2]$ with an equal volume of an aqueous solution of 15 mM $Eu(NO_3)_3$. The samples were mixed, then centrifuged to separate the two phases, then the top aqueous layer was removed by pipette and a fresh solution of $Eu(NO_3)_3$ was added to the IL solution and the process was repeated once more. The sample was contacted twice to ensure complete loading of the Me-BTPhen. After the second contact, 1.5 mL of Eu-loaded ionic liquid solution was pipetted into a screw-cap sample vial.

X-ray absorption data were collected at beamline 11-2 at Stanford Synchrotron Radiation Lightsource. Samples were inserted into a plexiglass sample box which was purged with He throughout the duration of the experiment. Spectra were collected at ambient temperature and pressures at the europium L_3-edge (6.977 keV) with fluorescence detection afforded by a Canberra 100-pixel Ge solid-state monolith detector. Sollar slits were used to decrease noise from x-ray scattering. Signal intensity was investigated both with and without use of a Cr-filter, with superior signal afforded when the filter was not used. A $Eu(NO_3)_3$ reference sample was measured simultaneously for energy calibration and data alignment. Samples were positioned on the beam to maximize fluorescence signal. The beam dimensions were 2 × 5 mm for all scans. Data were collected over four regions: -230 to -30 eV (10 eV step size, dwell time of 0.25 seconds), -30 to -5 eV (5 eV step size, dwell time of 0.5 seconds), -5 to 30 eV (1 eV step size), 3 $Å^{-1}$ to 13 $Å^{-1}$ (0.05 $Å^{-1}$ step size), with dwell time increasing as a function of k from 2 seconds at 3 $Å^{-1}$ to 16 seconds at 13 $Å^{-1}$.

Data were not collected further in k-space due to the occurrence of the Eu L_{II}-edge (7.617 keV, 12.95 $Å^{-1}$). Nine scans were collected.

The data were reformatted using SixPack[9] then processed and analyzed using the Athena and Artemis programs of the IFEFFIT package based on FEFF 6.[10, 11] Reference foil data were aligned to the first zero-crossing of the second derivative of the normalized μ(E) data, which was subsequently calibrated to the literature E_0 for the europium L_{III}-edge (6.977 keV). Any contributions from the Eu L_{II}-pre-edge were removed by truncating all data sets at 7.578 keV. Spectra were averaged in μ(E) prior to normalization. The background was removed and the data were assigned an Rbkg value of 1.1, less than one-half the value of the half-path length for the nearest scattering element, prior to normalizing to obtain a unit edge step.

Principal Component Analysis

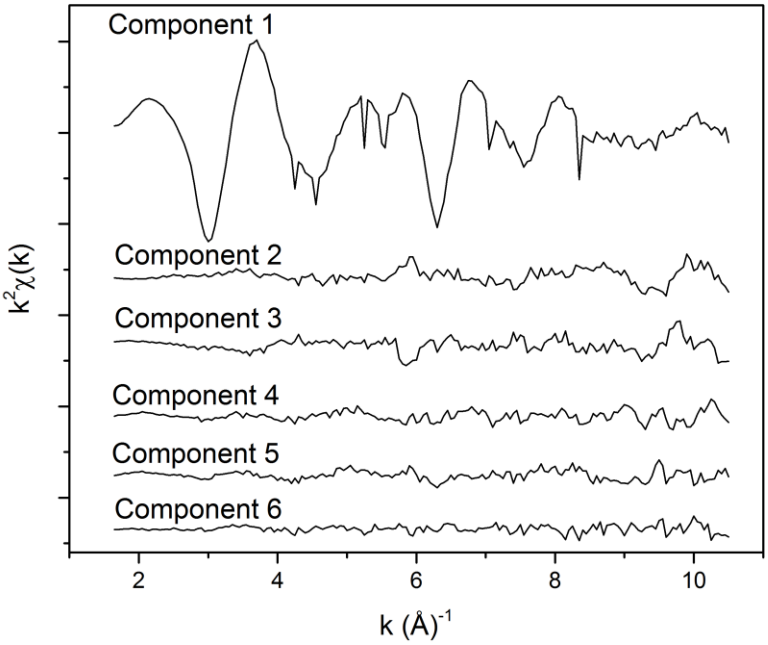


Figure S4. The first six principal components derived from nine Eu L_{III}-edge k^2-weighted EXAFS spectra of a Eu solution with 7.5 mM Me-BTPhen in an ionic liquid solvent. Components 7-9 (not shown) are similar to components 2 – 6. These data reveal only one mathematical component in the EXAFS spectra, indicating an adequate fit should be achievable from a single appropriate structure model.

EXAFS Analysis

The processed data set was initially qualitatively compared against scattering paths generated from DFT-derived potential structure models, as displayed in Figure S5. Inspection of the simulated direct scattering paths reveals all models display reasonable scattering paths for the majority of features, but that with the exception of $[Eu(Me\text{-}BTPhen)_2(OH)]^{2+}$, none are immediately capable of adequately fitting the shoulder observed at 1.5 Å. Of the remaining structure models, Eu-bound H_2O and monodentate-bound NTf_2^- both possess a single scattering

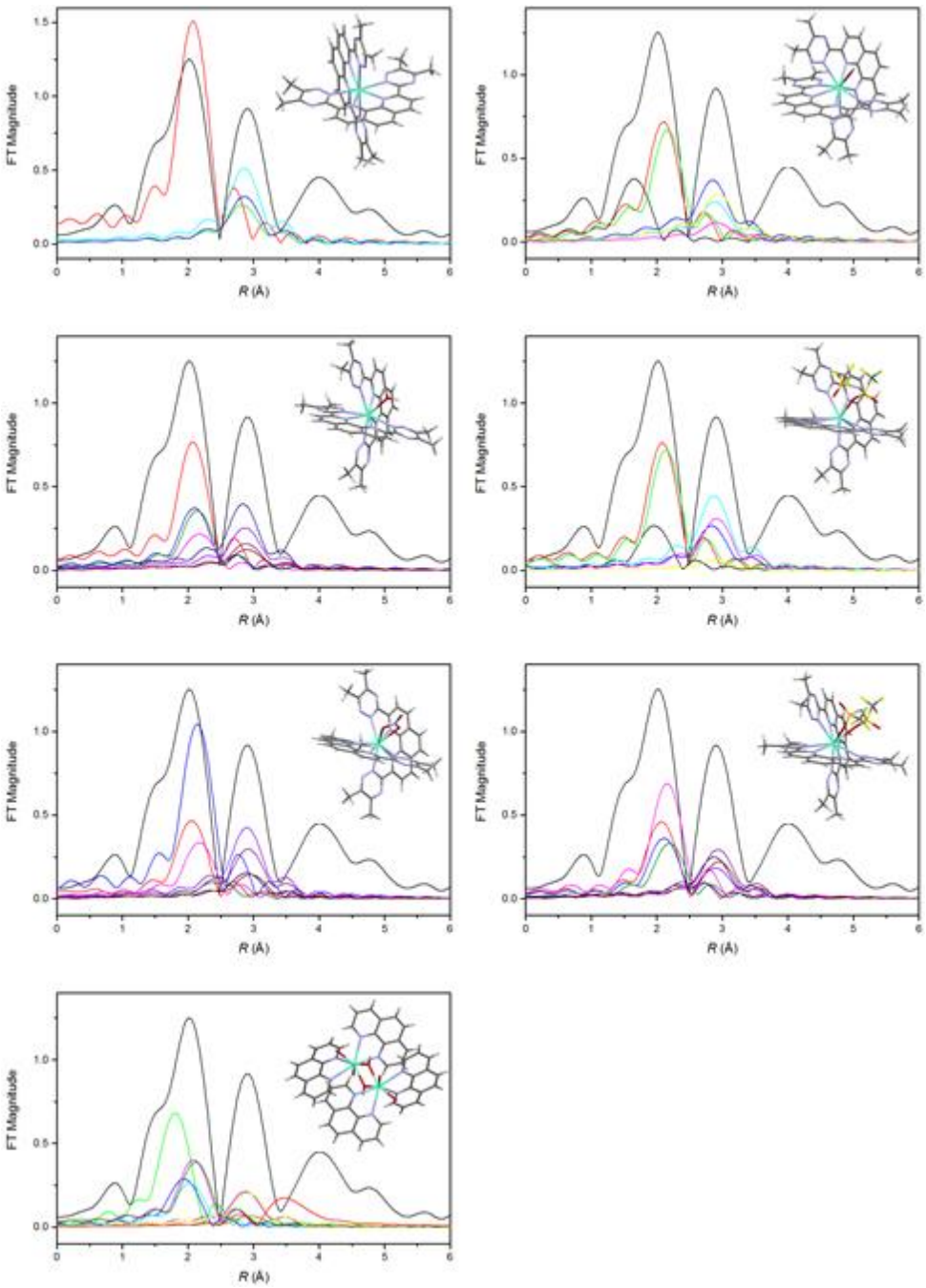


Figure S5. Single scattering paths for potential structure models compared against experimental EXAFS data, ordered by increasing coordination number and first-shell bond length. Representative DFT-calculated structures are provided in the upper corner of their corresponding spectrum. Top row, left to right: No anion, OH^-; second row, left to right: H_2O, NTf_2 (monodentate); third row, left to right: NO_3 (chelate), NTf_2 (chelate);bottom row: Eu2(Phen)2(OH)2 dimer.

path capable of shifting to fit this shoulder without inducing physically unreasonable distortions in the Me-BTPhen coordinating ligands. Accordingly, structure models generated from

chelating NO_3^- and NTf_2^- were discarded. Notably, both of these discarded models also would require a first coordination shell of 10 atoms. The final model was intended to interrogate whether the large feature at 4 Å could be attributed to formation of dimeric Eu species. A search of the CCDC database reveal that while no 4:2 Me-BTPhen:M complexes had been reported, several related 4:2 phenanthroline (Phen):Eu complexes were known. However, inspection of the Eu-Eu scattering path (3.73 Å) for this complex (plotted in red in Figure S5) was not located in a position that would beneficially contribute to a fit of the experimental spectrum. Additionally, as BTPhen possesses more *N*-donor atoms than Phen it would completely or (near completely) fill the Eu first coordination sphere, discouraging the prospects of forming a dimeric species.

The EXAFS data was initially fit with k-weighting of 1,2, and 3, then finalized with k^2-weighting in R-space. Structural parameters that were determined by the fits were the change in R_{eff} (ΔR_i), the relative mean square displacement of the scattering element (σ^2_i), the passive electron reduction factor (S_0^2), and the energy shift of the photoelectron, (ΔE_0). The data range used for fitting was 1.15 – 3.4 Å in R-space and 3 – 10.3 $Å^{-1}$ in k-space, affording 10 independent points, with the range identified to minimize truncation effects in k-space and avoid spectral contributions from the artifact of the Fourier transform at approximately 0.8 Å in R-space. The number of variables was not permitted to exceed 2/3 the number of independent points in keeping with the Nyquist criterion.[12, 13] Preliminary models were constructed from all first and second shell single scattering paths, as well as all multiple scattering paths providing at least 15% of the contribution of the most intense single scattering peak and with half-path length les s than 3.7 Å. We asserted any changes in half path length would be attributable to translation of the Me-BTPhen with respect to Eu, rather than distortion of bond lengths within the rigid and electronically delocalized ligand. Therefore, scattering path lengths were fitted with only two parameters (one for translation of the phenanthroline portion, the second for translation of the triazine), while different mean square relative deviation parameters (σ^2) were afforded for each of the first two shells of coordinating atoms (Figure S6).

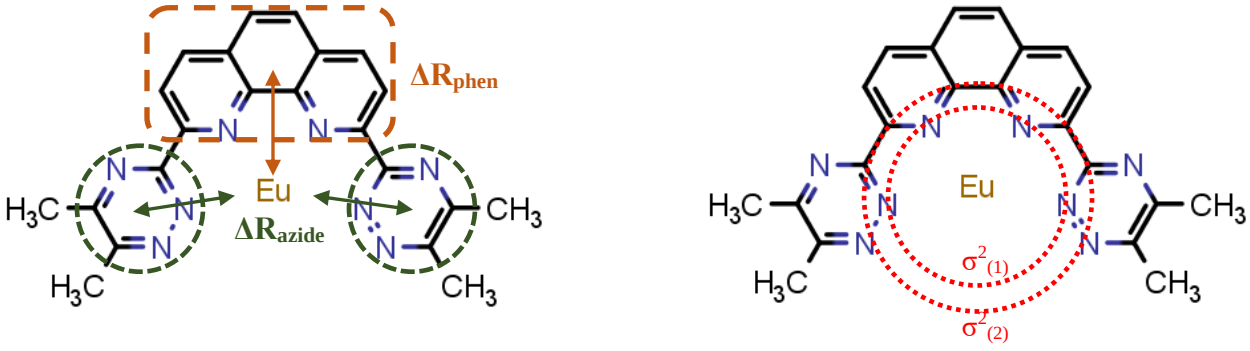


Figure S6. Assignment of ΔR and σ^2 parameters for the Me-BTPhen ligands.

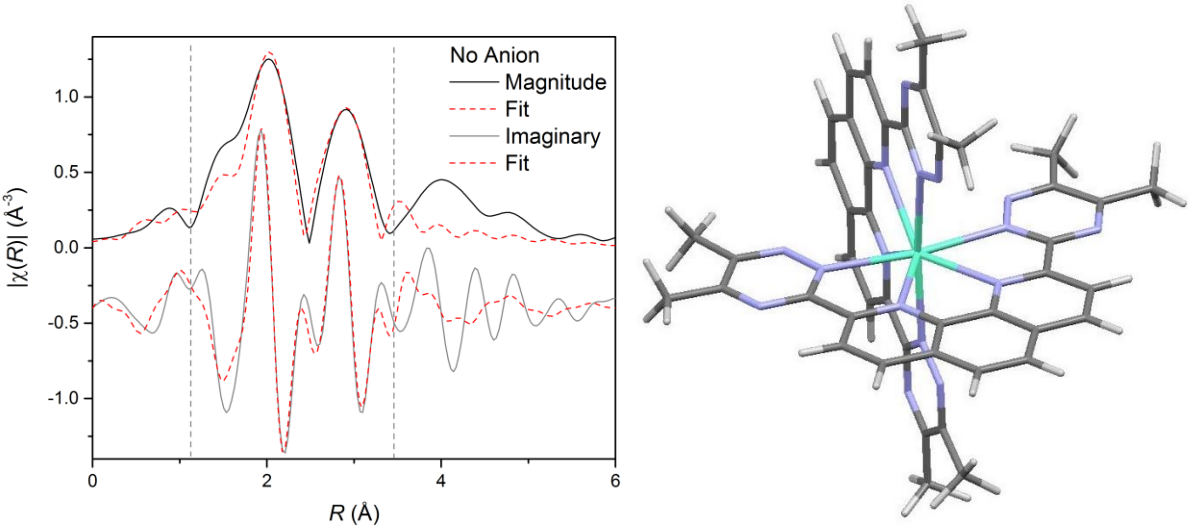


Figure S7. (Left) Rejected XAFS fit from structure model $[Eu(Me\text{-}BTPhen)_2]^{3+}$. (Right) DFT-optimized structure model used for preparation of the structure model.

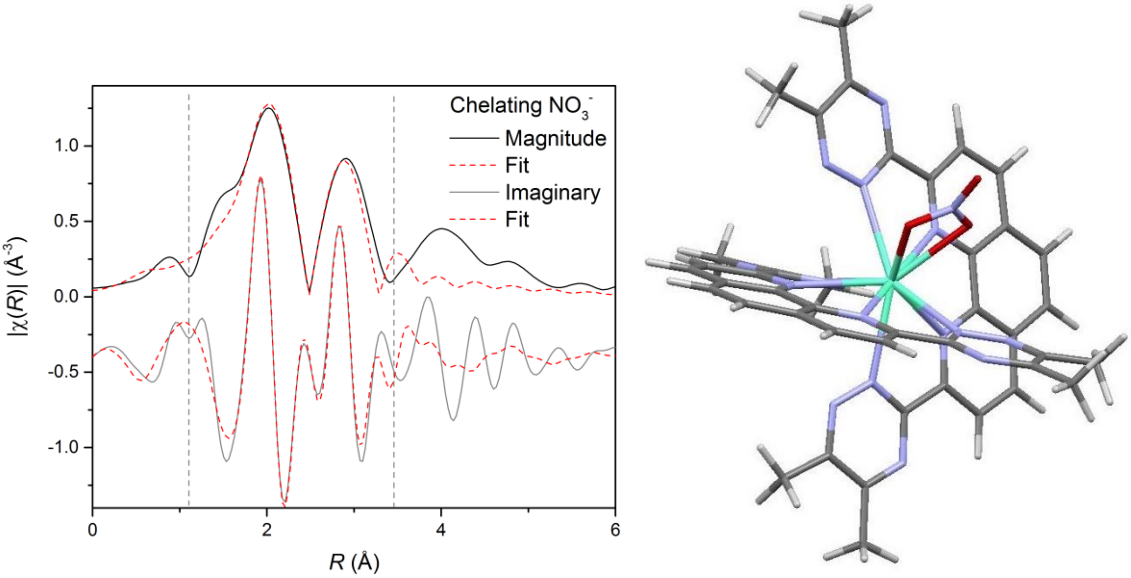


Figure S8. (Left) Rejected XAFS fit from structure model $[Eu(Me\text{-}BTPhen)_2NO_3]^{2+}$. (Right) DFT-optimized structure model used for preparation of the structure model.

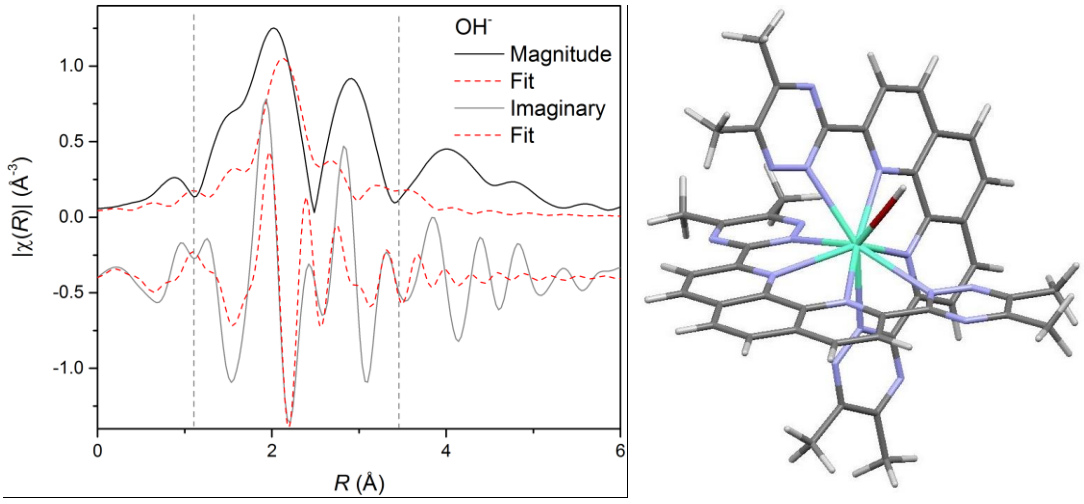


Figure S9. (Left) Rejected XAFS fit from structure model $[Eu(Me\text{-}BTPhen)_2OH]^{2+}$. (Right) DFT-optimized structure model used for preparation of the structure model.

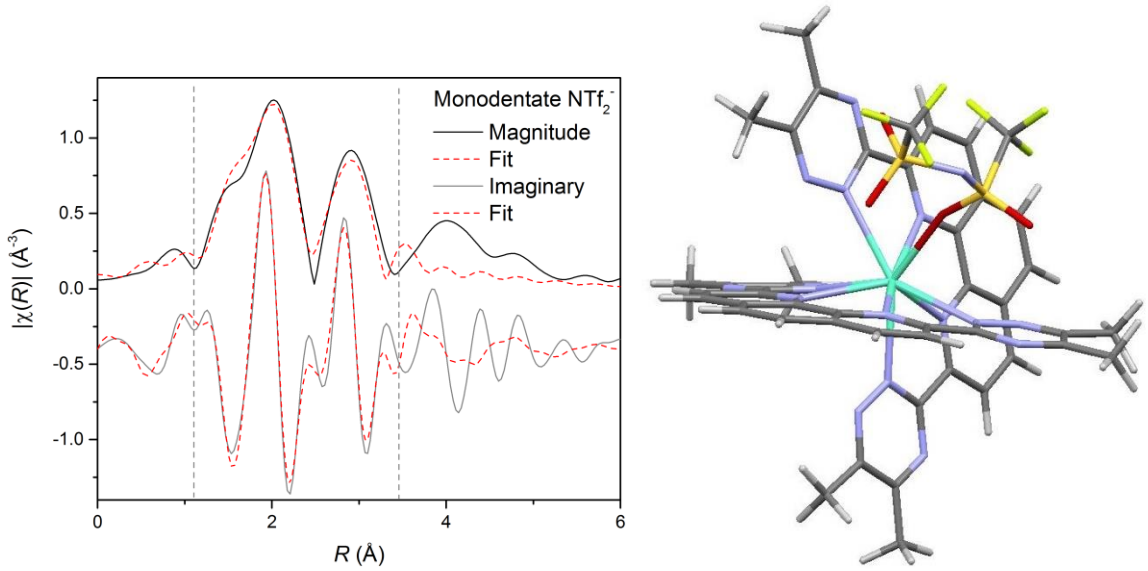


Figure S10. (Left) Rejected XAFS fit from structure model $[Eu(Me\text{-}BTPhen)_2NTf_2]^{2+}$. (Right) DFT-optimized structure model used for preparation of the structure model.

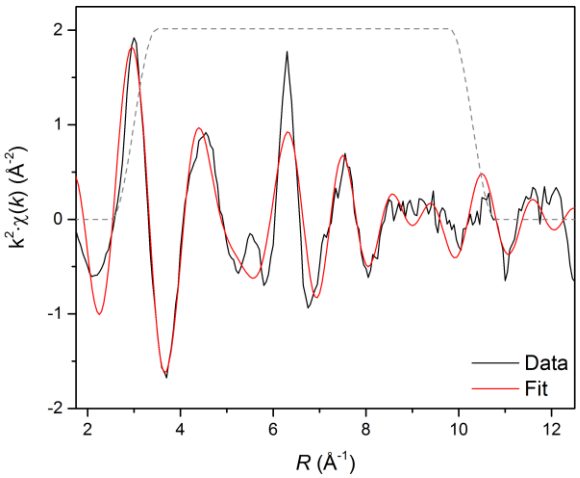


Figure S11. k^2-weighted $\chi(k)$ EXAFS data and fit for $[Eu(Me\text{-}BTPhen)_2(H_2O)]^{3+}$.

Section S5. Cartesian coordinates and electronic energies of ligand-metal ion complexes obtained at the B3LYP/LC(7s6p5d2f)/[5s4p3d2f]/6-311+G level.**

$[Eu(Me\text{-}BTPhen)_2]^{3+}$; E(RB3LYP) = -2609.82409307 A.U.

Eu	7.9366	12.8739	1.0053
N	11.1662	13.4254	-0.0923
N	9.9680	14.0239	-0.1119
N	10.8378	15.8637	-1.3138
N	7.5136	15.1480	-0.1005
N	5.5238	13.7303	1.1453
N	6.2309	11.3628	2.2308
N	6.6310	10.1961	2.7532
N	4.0132	11.0015	2.9636
N	6.3052	12.4989	-2.0155
N	7.2223	11.8693	-1.2696
N	7.4409	10.1511	-2.8775
N	9.0638	10.6801	0.3039
N	9.6501	11.9411	2.6676
N	8.3223	14.2376	3.1706
N	7.6387	15.3712	3.3752
N	9.4534	14.4746	5.2322
C	6.5360	10.7532	-3.6352
C	5.9456	11.9797	-3.1812
C	7.7574	10.7301	-1.7139
C	8.7714	10.0721	-0.8507
C	9.3805	8.8704	-1.2501
H	9.1032	8.4247	-2.1950
C	10.3183	8.2946	-0.4201
H	10.8048	7.3676	-0.7027
C	10.6489	8.9118	0.8034
C	9.9829	10.1222	1.1258

C	11.6160	8.3638	1.7089
H	12.1120	7.4382	1.4411
C	11.9072	8.9893	2.8801
H	12.6392	8.5703	3.5607
C	10.2922	10.7871	2.3716
C	11.2550	10.2137	3.2418
C	11.5280	10.8929	4.4464
H	12.2573	10.4869	5.1386
C	10.8685	12.0672	4.7388
H	11.0532	12.6136	5.6530
C	9.9303	12.5633	3.8178
C	9.1974	13.8260	4.0907
C	7.8436	16.0637	4.4871
C	8.7911	15.5993	5.4596
C	12.0336	15.2935	-1.3100
C	12.2008	14.0199	-0.6702
C	9.8383	15.2088	-0.7125
C	8.4901	15.8317	-0.7068
C	8.2759	17.0800	-1.3154
H	9.1039	17.5864	-1.7912
C	7.0096	17.6234	-1.2865
H	6.8155	18.5854	-1.7476
C	5.9592	16.9271	-0.6551
C	6.2665	15.6727	-0.0677
C	4.6213	17.4384	-0.5917
H	4.4103	18.3990	-1.0470
C	3.6350	16.7356	0.0254
H	2.6253	17.1271	0.0698
C	5.2177	14.9255	0.5887
C	3.9059	15.4640	0.6298
C	2.9115	14.7036	1.2779
H	1.8962	15.0805	1.3301
C	3.2331	13.4874	1.8409
H	2.4959	12.8785	2.3452
C	4.5596	13.0317	1.7540
C	4.9527	11.7286	2.3486
C	5.7506	9.4259	3.3773
C	4.3818	9.8425	3.4888
C	13.5193	13.3153	-0.6248
H	13.4231	12.3733	-0.0881
H	13.8889	13.1122	-1.6344
H	14.2757	13.9310	-0.1291
C	13.1667	15.9999	-1.9741
H	12.8280	16.9433	-2.3970
H	13.9742	16.1940	-1.2606
H	13.5963	15.3818	-2.7693

C	6.2417	8.1326	3.9458
H	7.3049	8.0145	3.7450
H	6.0783	8.0934	5.0270
H	5.7022	7.2847	3.5134
C	3.3552	9.0093	4.1785
H	2.3898	9.5109	4.1648
H	3.2597	8.0325	3.6925
H	3.6460	8.8132	5.2156
C	4.9193	12.7180	-3.9806
H	4.6037	13.6138	-3.4490
H	5.3180	13.0073	-4.9576
H	4.0434	12.0902	-4.1698
C	6.1631	10.1306	-4.9379
H	6.7265	9.2130	-5.0936
H	5.0920	9.9049	-4.9668
H	6.3582	10.8189	-5.7668
C	7.0577	17.3226	4.6742
H	6.4068	17.4891	3.8179
H	6.4461	17.2711	5.5799
H	7.7211	18.1849	4.7891
C	9.0573	16.3445	6.7234
H	9.8013	15.8219	7.3208
H	9.4147	17.3569	6.5082
H	8.1388	16.4571	7.3088

$[Am(Me\text{-}BTPhen)_2]^{3+}$; E(RB3LYP) = -2608.30226125 A.U.

Am	7.9375	12.8758	1.0084
N	11.1607	13.5193	-0.1624
N	9.9554	14.1048	-0.1620
N	10.7873	15.9647	-1.3565
N	7.4752	15.2116	-0.1175
N	5.4676	13.7828	1.1360
N	6.1366	11.3899	2.2311
N	6.5131	10.2164	2.7569
N	3.9075	11.0663	2.9413
N	6.3448	12.3933	-2.0550
N	7.2618	11.7828	-1.2925
N	7.5131	10.0456	-2.8725
N	9.1144	10.6223	0.3175
N	9.7048	11.8973	2.6983
N	8.3832	14.2079	3.2390
N	7.7073	15.3430	3.4637
N	9.5363	14.4129	5.2900

C	6.6093	10.6270	-3.6466
C	6.0013	11.8541	-3.2161
C	7.8134	10.6443	-1.7138
C	8.8280	10.0052	-0.8344
C	9.4433	8.8039	-1.2260
H	9.1698	8.3518	-2.1689
C	10.3811	8.2377	-0.3910
H	10.8729	7.3113	-0.6662
C	10.7059	8.8635	0.8293
C	10.0347	10.0741	1.1465
C	11.6744	8.3173	1.7334
H	12.1711	7.3921	1.4650
C	11.9652	8.9443	2.9028
H	12.6982	8.5285	3.5844
C	10.3445	10.7427	2.3942
C	11.3105	10.1674	3.2619
C	11.5888	10.8420	4.4677
H	12.3204	10.4321	5.1550
C	10.9318	12.0150	4.7666
H	11.1201	12.5582	5.6819
C	9.9906	12.5146	3.8505
C	9.2649	13.7792	4.1428
C	7.9274	16.0203	4.5815
C	8.8830	15.5378	5.5381
C	11.9894	15.4095	-1.3723
C	12.1805	14.1310	-0.7478
C	9.8022	15.2920	-0.7495
C	8.4464	15.9020	-0.7259
C	8.2266	17.1530	-1.3273
H	9.0511	17.6637	-1.8044
C	6.9598	17.6922	-1.2896
H	6.7598	18.6558	-1.7447
C	5.9146	16.9896	-0.6573
C	6.2251	15.7317	-0.0757
C	4.5788	17.5047	-0.5916
H	4.3709	18.4676	-1.0435
C	3.5921	16.8021	0.0231
H	2.5828	17.1941	0.0703
C	5.1727	14.9826	0.5807
C	3.8623	15.5282	0.6217
C	2.8609	14.7735	1.2649
H	1.8484	15.1584	1.3150
C	3.1718	13.5540	1.8246
H	2.4291	12.9486	2.3249
C	4.4955	13.0897	1.7398
C	4.8654	11.7786	2.3360

C	5.6142	9.4612	3.3718
C	4.2511	9.9012	3.4690
C	13.5077	13.4418	-0.7274
H	13.4283	12.4899	-0.2055
H	13.8694	13.2605	-1.7439
H	14.2614	14.0586	-0.2288
C	13.1060	16.1360	-2.0427
H	12.7522	17.0814	-2.4486
H	13.9218	16.3288	-1.3381
H	13.5302	15.5325	-2.8520
C	6.0777	8.1600	3.9456
H	7.1418	8.0261	3.7594
H	5.8983	8.1220	5.0242
H	5.5316	7.3209	3.5043
C	3.2038	9.0844	4.1472
H	2.2464	9.6008	4.1223
H	3.0989	8.1088	3.6608
H	3.4798	8.8849	5.1877
C	4.9750	12.5701	-4.0354
H	4.6453	13.4701	-3.5195
H	5.3800	12.8496	-5.0127
H	4.1074	11.9305	-4.2235
C	6.2550	9.9820	-4.9437
H	6.8307	9.0692	-5.0818
H	5.1870	9.7429	-4.9784
H	6.4489	10.6611	-5.7804
C	7.1509	17.2811	4.7927
H	6.4910	17.4613	3.9459
H	6.5496	17.2219	5.7049
H	7.8205	18.1383	4.9102
C	9.1662	16.2661	6.8081
H	9.9144	15.7329	7.3910
H	9.5256	17.2796	6.6016
H	8.2546	16.3751	7.4048

$[Eu(Me\text{-}BTPhen)_2(NO_3)]^{2+}$ chelate; E(RB3LYP) = -2890.57968384 A.U.

Eu	8.1641	12.8991	0.4133
O	8.2836	13.7758	-1.9644
O	9.6976	12.2153	-1.4909
O	9.6731	13.0764	-3.4996
N	11.4990	13.9379	0.4684
N	10.2906	14.4803	0.3105
N	11.2394	16.5082	-0.4496
N	7.8095	15.5119	0.0378
N	5.7440	13.8859	0.7629

N	6.4133	11.5291	1.9177
N	6.7879	10.4355	2.5832
N	4.1410	11.1248	2.4392
N	5.6915	11.9543	-1.8660
N	6.7109	11.3925	-1.2145
N	6.5940	9.4657	-2.5799
N	8.7612	10.3148	0.1729
N	9.7484	11.8182	2.2235
N	8.4039	14.0969	2.8042
N	7.6463	15.1466	3.1261
N	9.7299	14.4011	4.7402
N	9.2396	13.0250	-2.3737
C	5.6036	10.0188	-3.2609
C	5.1295	11.3120	-2.8809
C	7.1260	10.1782	-1.5769
C	8.2593	9.5876	-0.8222
C	8.7722	8.3255	-1.1771
H	8.3228	7.7833	-1.9969
C	9.8446	7.8255	-0.4741
H	10.2684	6.8604	-0.7280
C	10.3976	8.5745	0.5839
C	9.8083	9.8328	0.8682
C	11.5026	8.1099	1.3695
H	11.9464	7.1518	1.1247
C	11.9787	8.8460	2.4083
H	12.8056	8.4828	3.0076
C	10.3275	10.6269	1.9608
C	11.3949	10.1117	2.7417
C	11.8251	10.8823	3.8394
H	12.6409	10.5260	4.4586
C	11.1897	12.0674	4.1336
H	11.4678	12.6678	4.9880
C	10.1447	12.5015	3.2976
C	9.3926	13.7382	3.6245
C	7.8986	15.8242	4.2388
C	9.0033	15.4578	5.0653
C	12.4460	15.9790	-0.3293
C	12.5785	14.6411	0.1547
C	10.1920	15.7338	-0.1336
C	8.8292	16.2986	-0.2971
C	8.6525	17.5995	-0.8055
H	9.5208	18.1901	-1.0609
C	7.3723	18.0755	-0.9754
H	7.2022	19.0695	-1.3733
C	6.2732	17.2636	-0.6304
C	6.5538	15.9702	-0.1210

C	4.9142	17.6987	-0.7638
H	4.7229	18.6852	-1.1700
C	3.8845	16.8995	-0.3779
H	2.8594	17.2399	-0.4679
C	5.4578	15.1103	0.2705
C	4.1284	15.5956	0.1646
C	3.0941	14.7570	0.6239
H	2.0639	15.0888	0.5567
C	3.4005	13.5354	1.1795
H	2.6380	12.8806	1.5764
C	4.7482	13.1353	1.2348
C	5.1207	11.8563	1.8888
C	5.8736	9.6860	3.1862
C	4.4906	10.0258	3.0873
C	13.9079	13.9740	0.3257
H	13.7680	12.9649	0.7096
H	14.4383	13.9154	-0.6295
H	14.5474	14.5343	1.0141
C	13.6321	16.8066	-0.7064
H	13.3131	17.8014	-1.0111
H	14.3337	16.8906	0.1290
H	14.1783	16.3389	-1.5320
C	6.3573	8.4887	3.9454
H	7.4425	8.4257	3.8855
H	6.0640	8.5465	4.9978
H	5.9258	7.5666	3.5447
C	3.4184	9.1805	3.6964
H	2.4407	9.6158	3.4989
H	3.4476	8.1634	3.2931
H	3.5601	9.0939	4.7782
C	4.0054	11.9988	-3.5925
H	3.8033	12.9600	-3.1232
H	4.2580	12.1684	-4.6436
H	3.0954	11.3920	-3.5750
C	5.0138	9.2635	-4.4078
H	5.5103	8.3013	-4.5173
H	3.9415	9.1019	-4.2605
H	5.1228	9.8305	-5.3378
C	6.9943	16.9726	4.5657
H	6.2211	17.0641	3.8046
H	6.5170	16.8313	5.5399
H	7.5530	17.9119	4.6181
C	9.3675	16.2280	6.2938
H	10.2503	15.7945	6.7598
H	9.5650	17.2771	6.0529
H	8.5433	16.2207	7.0142

$[Am(Me\text{-}BTPhen)_2(NO_3)]^{2+}$ chelate; E(RB3LYP) = -2889.06067191 A.U.

Am	8.1607	12.8999	0.4219
O	8.2915	13.7857	-2.0023
O	9.7036	12.2139	-1.5378
O	9.6708	13.0806	-3.5431
N	11.5040	14.0210	0.4544
N	10.2884	14.5491	0.3007
N	11.2069	16.5792	-0.4856
N	7.7823	15.5638	0.0340
N	5.6961	13.9376	0.7776
N	6.3279	11.5509	1.9286
N	6.6786	10.4404	2.5795
N	4.0459	11.1815	2.4266
N	5.6947	11.8608	-1.8753
N	6.7215	11.3184	-1.2187
N	6.6507	9.3909	-2.5835
N	8.7943	10.2665	0.1857
N	9.7794	11.7710	2.2637
N	8.4573	14.0747	2.8679
N	7.7212	15.1377	3.1972
N	9.8013	14.3470	4.7946
N	9.2425	13.0291	-2.4149
C	5.6533	9.9243	-3.2701
C	5.1511	11.2079	-2.8936
C	7.1636	10.1134	-1.5774
C	8.3037	9.5395	-0.8161
C	8.8294	8.2839	-1.1750
H	8.3899	7.7424	-2.0004
C	9.9005	7.7892	-0.4675
H	10.3342	6.8290	-0.7233
C	10.4403	8.5361	0.5983
C	9.8415	9.7900	0.8872
C	11.5442	8.0690	1.3832
H	11.9911	7.1138	1.1323
C	12.0155	8.7998	2.4269
H	12.8426	8.4367	3.0261
C	10.3564	10.5801	1.9889
C	11.4268	10.0612	2.7652
C	11.8611	10.8247	3.8660
H	12.6785	10.4630	4.4799
C	11.2308	12.0098	4.1683
H	11.5152	12.6060	5.0234
C	10.1836	12.4503	3.3383
C	9.4464	13.6953	3.6772

C	7.9939	15.8070	4.3100
C	9.0954	15.4146	5.1290
C	12.4204	16.0650	-0.3698
C	12.5729	14.7331	0.1251
C	10.1702	15.7962	-0.1546
C	8.7999	16.3490	-0.3135
C	8.6196	17.6461	-0.8301
H	9.4857	18.2350	-1.0961
C	7.3385	18.1202	-0.9934
H	7.1648	19.1114	-1.3970
C	6.2420	17.3113	-0.6348
C	6.5236	16.0196	-0.1185
C	4.8854	17.7527	-0.7661
H	4.6982	18.7382	-1.1766
C	3.8539	16.9598	-0.3746
H	2.8296	17.3026	-0.4637
C	5.4226	15.1646	0.2812
C	4.0951	15.6576	0.1717
C	3.0536	14.8273	0.6292
H	2.0264	15.1677	0.5587
C	3.3479	13.6030	1.1838
H	2.5787	12.9533	1.5758
C	4.6923	13.1926	1.2431
C	5.0425	11.9019	1.8911
C	5.7462	9.6986	3.1637
C	4.3708	10.0679	3.0626
C	13.9113	14.0829	0.2906
H	13.7864	13.0756	0.6842
H	14.4342	14.0224	-0.6686
H	14.5499	14.6565	0.9688
C	13.5938	16.9028	-0.7639
H	13.2610	17.8917	-1.0731
H	14.3021	17.0008	0.0642
H	14.1374	16.4349	-1.5912
C	6.2019	8.4793	3.9049
H	7.2862	8.3971	3.8506
H	5.9028	8.5243	4.9563
H	5.7559	7.5727	3.4852
C	3.2791	9.2369	3.6567
H	2.3111	9.6932	3.4590
H	3.2909	8.2238	3.2428
H	3.4133	9.1362	4.7384
C	4.0178	11.8727	-3.6114
H	3.7967	12.8311	-3.1449
H	4.2714	12.0443	-4.6618
H	3.1186	11.2499	-3.5958

C	5.0852	9.1574	-4.4204
H	5.5991	8.2038	-4.5248
H	4.0148	8.9776	-4.2810
H	5.1917	9.7249	-5.3503
C	7.1154	16.9729	4.6452
H	6.3389	17.0810	3.8897
H	6.6423	16.8397	5.6226
H	7.6933	17.9007	4.6948
C	9.4782	16.1705	6.3608
H	10.3572	15.7208	6.8186
H	9.6891	17.2184	6.1264
H	8.6581	16.1694	7.0860

$[Eu(Me\text{-}BTPhen)_2(NTf_2)]^{2+}$ chelate; E(RB3LYP) = -4437.69912506 A.U.

Eu	8.1891	12.9165	0.3557
O	8.0396	13.7438	-2.0524
O	10.1765	12.2150	-1.1108
N	11.5167	14.1364	0.8340
N	10.3142	14.5985	0.4867
N	11.2684	16.5968	-0.3480
N	7.8440	15.5367	-0.0041
N	5.7924	13.9208	0.7586
N	6.4726	11.5716	1.9210
N	6.8528	10.4803	2.5863
N	4.2138	11.2045	2.5232
N	5.4508	12.0284	-1.7406
N	6.5173	11.4495	-1.1832
N	6.3141	9.5788	-2.6192
N	8.6227	10.3114	0.0455
N	9.7027	11.7258	2.1095
N	8.4286	14.0152	2.7646
N	7.7065	15.0800	3.1130
N	9.7710	14.2298	4.7005
C	5.2983	10.1664	-3.2276
C	4.8330	11.4295	-2.7474
C	6.8972	10.2476	-1.6153
C	8.0480	9.6108	-0.9285
C	8.4878	8.3266	-1.3045
H	7.9837	7.8109	-2.1096
C	9.5564	7.7723	-0.6385
H	9.9244	6.7889	-0.9091
C	10.1750	8.4854	0.4094
C	9.6596	9.7696	0.7152
C	11.2720	7.9588	1.1664
H	11.6646	6.9838	0.9014

C	11.8012	8.6570	2.2061
H	12.6200	8.2463	2.7856
C	10.2312	10.5193	1.8108
C	11.2794	9.9407	2.5714
C	11.7451	10.6637	3.6877
H	12.5491	10.2582	4.2919
C	11.1542	11.8610	4.0217
H	11.4555	12.4236	4.8938
C	10.1247	12.3597	3.2028
C	9.4115	13.6071	3.5697
C	7.9863	15.7244	4.2392
C	9.0791	15.3010	5.0537
C	12.4733	16.1210	-0.0858
C	12.5960	14.8572	0.5698
C	10.2230	15.8139	-0.0502
C	8.8606	16.3370	-0.3150
C	8.6785	17.6269	-0.8501
H	9.5459	18.2244	-1.0922
C	7.3966	18.0844	-1.0530
H	7.2225	19.0704	-1.4691
C	6.2998	17.2696	-0.7047
C	6.5855	15.9852	-0.1780
C	4.9390	17.6966	-0.8435
H	4.7426	18.6750	-1.2667
C	3.9140	16.9024	-0.4351
H	2.8874	17.2386	-0.5242
C	5.4962	15.1309	0.2372
C	4.1654	15.6125	0.1361
C	3.1387	14.7877	0.6356
H	2.1075	15.1180	0.5769
C	3.4553	13.5826	1.2199
H	2.7002	12.9387	1.6475
C	4.8037	13.1831	1.2625
C	5.1837	11.9146	1.9294
C	5.9493	9.7497	3.2273
C	4.5692	10.1089	3.1737
C	13.9214	14.2835	0.9626
H	13.7770	13.3344	1.4761
H	14.5412	14.1129	0.0770
H	14.4736	14.9653	1.6157
C	13.6663	16.9267	-0.4836
H	13.3516	17.8708	-0.9240
H	14.3148	17.1239	0.3750
H	14.2659	16.3745	-1.2149
C	6.4414	8.5519	3.9806
H	7.5239	8.4768	3.8921

H 6.1768 8.6182 5.0401
H 5.9899 7.6320 3.5968
C 3.5068 9.2886 3.8321
H 2.5288 9.7336 3.6591
H 3.5098 8.2644 3.4463
H 3.6829 9.2191 4.9102
C 3.6634 12.1354 -3.3572
H 3.4673 13.0616 -2.8196
H 3.8676 12.3749 -4.4051
H 2.7657 11.5109 -3.3370
C 4.6747 9.4863 -4.4017
H 5.1521 8.5238 -4.5748
H 3.6015 9.3377 -4.2496
H 4.7864 10.1060 -5.2975
C 7.1223 16.8952 4.5946
H 6.3478 17.0268 3.8408
H 6.6469 16.7508 5.5693
H 7.7117 17.8147 4.6609
C 9.4680 16.0269 6.3015
H 10.3405 15.5576 6.7519
H 9.6917 17.0768 6.0889
H 8.6463 16.0210 7.0249
N 9.7887 12.6813 -3.6116
S 10.8295 12.6214 -2.3897
O 11.7849 13.7188 -2.3088
S 8.3565 13.3655 -3.4634
O 7.3419 12.6465 -4.2139
C 11.8024 11.0919 -2.9224
F 10.9886 10.0418 -3.0197
F 12.4014 11.3112 -4.0782
F 12.7132 10.8516 -1.9760
C 8.5372 15.0413 -4.3208
F 9.4963 15.7474 -3.7180
F 8.8411 14.8660 -5.5946
F 7.3798 15.6993 -4.2156

$[Am(Me\text{-}BTPhen)_2(NTf_2)]^{2+}$ chelate; E(RB3LYP) = -4436.18276125 A.U.

Am 8.1811 12.9193 0.3768
O 8.0660 13.7550 -2.0846
O 10.2141 12.2051 -1.1022
N 11.4982 14.2369 0.8350
N 10.2881 14.6765 0.4838
N 11.2100 16.6652 -0.4039
N 7.7932 15.5853 -0.0058
N 5.7327 13.9612 0.7802

N	6.3926	11.5928	1.9494
N	6.7575	10.4934	2.6108
N	4.1268	11.2480	2.5337
N	5.4652	11.9853	-1.7623
N	6.5249	11.4067	-1.1913
N	6.3506	9.5413	-2.6355
N	8.6270	10.2601	0.0670
N	9.7217	11.6644	2.1559
N	8.4870	13.9824	2.8397
N	7.7932	15.0630	3.1982
N	9.8609	14.1634	4.7551
C	5.3424	10.1281	-3.2573
C	4.8646	11.3880	-2.7801
C	6.9166	10.2078	-1.6199
C	8.0605	9.5688	-0.9194
C	8.5018	8.2874	-1.3026
H	8.0048	7.7790	-2.1165
C	9.5633	7.7266	-0.6315
H	9.9325	6.7449	-0.9064
C	10.1755	8.4309	0.4256
C	9.6602	9.7141	0.7405
C	11.2688	7.8924	1.1790
H	11.6562	6.9175	0.9062
C	11.8019	8.5806	2.2224
H	12.6198	8.1633	2.7984
C	10.2366	10.4545	1.8439
C	11.2871	9.8647	2.5946
C	11.7691	10.5787	3.7096
H	12.5751	10.1629	4.3041
C	11.1953	11.7813	4.0528
H	11.5126	12.3387	4.9225
C	10.1625	12.2924	3.2458
C	9.4737	13.5517	3.6269
C	8.1030	15.6989	4.3211
C	9.1962	15.2477	5.1206
C	12.4226	16.2091	-0.1412
C	12.5664	14.9651	0.5473
C	10.1758	15.8784	-0.0776
C	8.8043	16.3844	-0.3394
C	8.6124	17.6636	-0.8958
H	9.4748	18.2608	-1.1554
C	7.3269	18.1115	-1.0952
H	7.1446	19.0897	-1.5259
C	6.2365	17.2978	-0.7260
C	6.5299	16.0221	-0.1800
C	4.8751	17.7209	-0.8678

H	4.6765	18.6934	-1.3032
C	3.8529	16.9293	-0.4491
H	2.8251	17.2607	-0.5416
C	5.4410	15.1682	0.2470
C	4.1089	15.6466	0.1352
C	3.0799	14.8245	0.6342
H	2.0492	15.1547	0.5672
C	3.3921	13.6219	1.2249
H	2.6339	12.9794	1.6485
C	4.7405	13.2232	1.2783
C	5.1081	11.9500	1.9481
C	5.8417	9.7694	3.2414
C	4.4662	10.1460	3.1819
C	13.9013	14.4198	0.9478
H	13.7723	13.4841	1.4892
H	14.5178	14.2318	0.0635
H	14.4485	15.1270	1.5777
C	13.6024	17.0166	-0.5733
H	13.2722	17.9366	-1.0516
H	14.2471	17.2608	0.2764
H	14.2115	16.4446	-1.2809
C	6.3150	8.5608	3.9892
H	7.3969	8.4728	3.9048
H	6.0466	8.6238	5.0480
H	5.8537	7.6492	3.5975
C	3.3909	9.3364	3.8326
H	2.4191	9.7938	3.6566
H	3.3833	8.3135	3.4435
H	3.5611	9.2614	4.9113
C	3.7017	12.0917	-3.4049
H	3.4931	13.0142	-2.8657
H	3.9213	12.3373	-4.4483
H	2.8065	11.4632	-3.4017
C	4.7398	9.4506	-4.4438
H	5.2234	8.4905	-4.6134
H	3.6650	9.2974	-4.3090
H	4.8632	10.0744	-5.3352
C	7.2719	16.8894	4.6889
H	6.4928	17.0415	3.9437
H	6.8034	16.7540	5.6683
H	7.8841	17.7941	4.7511
C	9.6152	15.9596	6.3667
H	10.4813	15.4685	6.8061
H	9.8611	17.0048	6.1555
H	8.8013	15.9700	7.0987
N	9.8228	12.6513	-3.6072

S	10.8621	12.6145	-2.3829
O	11.8007	13.7269	-2.3045
S	8.3966	13.3538	-3.4858
O	7.3846	12.6315	-4.2370
C	11.8559	11.0954	-2.9077
F	11.0570	10.0330	-2.9950
F	12.4489	11.3144	-4.0668
F	12.7722	10.8758	-1.9618
C	8.6020	15.0154	-4.3651
F	9.5511	15.7270	-3.7531
F	8.9321	14.8198	-5.6296
F	7.4454	15.6789	-4.2943

$[Eu(Me\text{-}BTPhen)_2(NTf_2)]^{2+}$ monodentate; E(RB3LYP) = -4437.69891049 A.U.

Eu	8.0596	12.9884	0.5936
O	6.6917	15.1228	-2.9830
O	8.9378	13.0325	-1.6780
N	11.4190	14.0275	0.6574
N	10.2048	14.5505	0.4805
N	11.1318	16.5666	-0.3383
N	7.7140	15.5036	0.0751
N	5.6818	13.9255	0.9581
N	6.3970	11.5707	2.0762
N	6.7996	10.4501	2.6777
N	4.1547	11.1700	2.7124
N	5.3973	12.1112	-1.5528
N	6.5200	11.5852	-1.0597
N	6.4899	9.8631	-2.6805
N	8.7746	10.5563	0.0188
N	9.7382	11.8530	2.2106
N	8.3868	14.0629	2.9780
N	7.6532	15.1117	3.3531
N	9.7239	14.2325	4.9210
C	5.4146	10.4075	-3.2256
C	4.8358	11.5657	-2.6222
C	7.0178	10.4831	-1.6192
C	8.2365	9.8964	-1.0065
C	8.7719	8.6869	-1.4892
H	8.3000	8.2027	-2.3325
C	9.8851	8.1601	-0.8744
H	10.3229	7.2339	-1.2295
C	10.4532	8.8201	0.2352
C	9.8474	10.0318	0.6480
C	11.5828	8.3093	0.9546
H	12.0448	7.3912	0.6104

C	12.0585	8.9505	2.0556
H	12.9041	8.5506	2.6032
C	10.3550	10.7185	1.8144
C	11.4461	10.1578	2.5263
C	11.8648	10.8240	3.6957
H	12.6962	10.4294	4.2692
C	11.2037	11.9576	4.1129
H	11.4808	12.4802	5.0175
C	10.1363	12.4446	3.3367
C	9.3794	13.6467	3.7663
C	7.9269	15.7273	4.4965
C	9.0151	15.2815	5.3076
C	12.3427	16.0560	-0.1997
C	12.4881	14.7271	0.3049
C	10.0963	15.7789	-0.0274
C	8.7275	16.3038	-0.2581
C	8.5323	17.5887	-0.7959
H	9.3937	18.1842	-1.0628
C	7.2454	18.0442	-0.9747
H	7.0635	19.0239	-1.4020
C	6.1567	17.2391	-0.5864
C	6.4517	15.9610	-0.0549
C	4.7933	17.6657	-0.6964
H	4.5878	18.6370	-1.1313
C	3.7765	16.8792	-0.2537
H	2.7484	17.2142	-0.3275
C	5.3734	15.1220	0.4136
C	4.0400	15.5990	0.3335
C	3.0274	14.7781	0.8672
H	1.9944	15.1053	0.8261
C	3.3565	13.5768	1.4554
H	2.6091	12.9332	1.8970
C	4.7056	13.1817	1.4791
C	5.1055	11.9050	2.1192
C	5.9126	9.6853	3.3012
C	4.5315	10.0504	3.3085
C	13.8236	14.0701	0.4603
H	13.7004	13.0709	0.8748
H	14.3241	13.9895	-0.5093
H	14.4807	14.6506	1.1144
C	13.5199	16.8907	-0.5850
H	13.1944	17.8915	-0.8619
H	14.2472	16.9543	0.2293
H	14.0355	16.4382	-1.4388
C	6.4222	8.4476	3.9734
H	7.5014	8.3754	3.8485

H	6.1889	8.4567	5.0422
H	5.9562	7.5513	3.5533
C	3.4910	9.2067	3.9716
H	2.5080	9.6562	3.8452
H	3.4823	8.1964	3.5510
H	3.7015	9.1004	5.0406
C	3.6053	12.2191	-3.1637
H	3.3311	13.0685	-2.5407
H	3.7888	12.5759	-4.1813
H	2.7671	11.5178	-3.2083
C	4.8506	9.7950	-4.4640
H	5.3829	8.8770	-4.7056
H	3.7835	9.5821	-4.3555
H	4.9544	10.4959	-5.2993
C	7.0607	16.8879	4.8770
H	6.2932	17.0416	4.1204
H	6.5769	16.7166	5.8432
H	7.6507	17.8042	4.9742
C	9.3816	15.9622	6.5866
H	10.2483	15.4795	7.0339
H	9.6058	17.0195	6.4147
H	8.5480	15.9293	7.2955
N	8.9885	14.3761	-3.8734
S	9.7839	13.5281	-2.8215
O	11.0432	14.1626	-2.4593
S	7.3601	14.3446	-4.0289
O	6.8125	13.0267	-4.3596
C	10.3106	11.9155	-3.6634
F	9.2433	11.1988	-4.0155
F	11.0394	12.1894	-4.7327
F	11.0418	11.1990	-2.7956
C	7.2730	15.3784	-5.6106
F	7.7782	16.5891	-5.3994
F	7.9285	14.7782	-6.5933
F	5.9824	15.4871	-5.9331

$[Am(Me\text{-}BTPhen)_2(NTf_2)]^{2+}$ monodentate; E(RB3LYP) = -4436.17912977 A.U.

Am	8.0526	12.9923	0.6070
O	6.7198	15.0178	-2.9248
O	8.9991	12.9982	-1.6978
N	11.4153	14.1263	0.6629
N	10.1945	14.6328	0.4788
N	11.0945	16.6392	-0.3886
N	7.6812	15.5660	0.0727
N	5.6255	13.9829	0.9578

N	6.3014	11.6139	2.1056
N	6.6796	10.4899	2.7172
N	4.0438	11.2438	2.6992
N	5.3974	12.0275	-1.5567
N	6.5267	11.5161	-1.0618
N	6.5360	9.8072	-2.6948
N	8.7963	10.5004	0.0306
N	9.7787	11.7974	2.2389
N	8.4479	14.0205	3.0505
N	7.7295	15.0724	3.4465
N	9.8172	14.1582	4.9714
C	5.4570	10.3396	-3.2440
C	4.8517	11.4808	-2.6332
C	7.0458	10.4257	-1.6232
C	8.2684	9.8481	-1.0054
C	8.8164	8.6499	-1.5016
H	8.3523	8.1717	-2.3524
C	9.9315	8.1263	-0.8888
H	10.3789	7.2079	-1.2523
C	10.4918	8.7795	0.2284
C	9.8757	9.9825	0.6553
C	11.6272	8.2669	0.9363
H	12.0914	7.3544	0.5802
C	12.1060	8.9006	2.0393
H	12.9570	8.5014	2.5789
C	10.3896	10.6646	1.8255
C	11.4912	10.1015	2.5217
C	11.9238	10.7594	3.6903
H	12.7625	10.3604	4.2500
C	11.2696	11.8905	4.1230
H	11.5592	12.4076	5.0267
C	10.1930	12.3828	3.3632
C	9.4496	13.5871	3.8159
C	8.0267	15.6738	4.5913
C	9.1236	15.2088	5.3802
C	12.3113	16.1436	-0.2477
C	12.4749	14.8301	0.2915
C	10.0685	15.8493	-0.0504
C	8.6925	16.3622	-0.2776
C	8.4943	17.6380	-0.8357
H	9.3540	18.2304	-1.1144
C	7.2067	18.0878	-1.0182
H	7.0214	19.0608	-1.4591
C	6.1202	17.2853	-0.6191
C	6.4160	16.0148	-0.0671
C	4.7586	17.7124	-0.7440

H	4.5580	18.6790	-1.1913
C	3.7388	16.9311	-0.3014
H	2.7110	17.2642	-0.3869
C	5.3312	15.1785	0.4011
C	3.9986	15.6571	0.2995
C	2.9759	14.8435	0.8246
H	1.9451	15.1749	0.7665
C	3.2913	13.6446	1.4235
H	2.5351	13.0062	1.8573
C	4.6384	13.2448	1.4682
C	5.0149	11.9655	2.1214
C	5.7714	9.7380	3.3254
C	4.3953	10.1214	3.3053
C	13.8189	14.1945	0.4604
H	13.7098	13.2069	0.9055
H	14.3162	14.0906	-0.5088
H	14.4717	14.8025	1.0935
C	13.4767	16.9787	-0.6665
H	13.1385	17.9675	-0.9701
H	14.2092	17.0741	0.1400
H	13.9908	16.5066	-1.5106
C	6.2523	8.4956	4.0098
H	7.3322	8.4078	3.9026
H	6.0019	8.5116	5.0747
H	5.7804	7.6046	3.5849
C	3.3318	9.2934	3.9517
H	2.3578	9.7575	3.8101
H	3.3144	8.2835	3.5302
H	3.5240	9.1834	5.0237
C	3.6116	12.1152	-3.1756
H	3.3170	12.9525	-2.5455
H	3.7932	12.4854	-4.1887
H	2.7876	11.3980	-3.2319
C	4.9157	9.7325	-4.4951
H	5.4631	8.8243	-4.7399
H	3.8504	9.5047	-4.4018
H	5.0208	10.4437	-5.3216
C	7.1778	16.8388	4.9967
H	6.4024	17.0090	4.2517
H	6.7044	16.6610	5.9669
H	7.7786	17.7477	5.0969
C	9.5152	15.8719	6.6611
H	10.3819	15.3744	7.0918
H	9.7500	16.9282	6.4969
H	8.6907	15.8417	7.3806
N	9.0046	14.3346	-3.8975

S	9.8281	13.5126	-2.8443
O	11.0716	14.1804	-2.4871
S	7.3743	14.2808	-4.0100
O	6.8368	12.9646	-4.3631
C	10.3874	11.9122	-3.6871
F	9.3328	11.1752	-4.0359
F	11.1078	12.1997	-4.7587
F	11.1344	11.2108	-2.8209
C	7.2282	15.3568	-5.5586
F	7.7175	16.5705	-5.3255
F	7.8672	14.7975	-6.5752
F	5.9275	15.4520	-5.8440

$[Eu(Me\text{-}BTPhen)_2(H_2O)]^{3+}$; E(RB3LYP) = -2686.29318346 A.U.

Eu	0.0026	0.0549	-0.1952
O	0.9287	0.1924	-2.6696
N	3.3995	1.0149	-0.3593
N	2.1796	1.5393	-0.5354
N	3.1109	3.6017	-1.2227
N	-0.3193	2.5438	-0.8531
N	-2.3733	0.9991	0.0704
N	-1.6879	-1.3545	1.2097
N	-1.2945	-2.4737	1.8279
N	-3.9289	-1.7083	1.8758
N	-2.4301	-0.7611	-2.6240
N	-1.3686	-1.3081	-2.0173
N	-1.5382	-3.2481	-3.3594
N	0.7681	-2.3668	-0.7271
N	1.6608	-0.9993	1.4621
N	0.3144	1.2561	2.1015
N	-0.4244	2.3259	2.4171
N	1.5634	1.4605	4.0988
C	-2.6016	-2.7376	-3.9608
C	-3.0596	-1.4332	-3.5797
C	-0.9512	-2.5160	-2.4033
C	0.2386	-3.0856	-1.7210
C	0.7499	-4.3379	-2.1066
H	0.2830	-4.8732	-2.9214
C	1.8360	-4.8494	-1.4299
H	2.2582	-5.8072	-1.7131
C	2.3857	-4.1369	-0.3447
C	1.7990	-2.8857	-0.0225
C	3.4752	-4.6382	0.4406
H	3.9235	-5.5851	0.1627
C	3.9250	-3.9525	1.5249

H	4.7379	-4.3447	2.1251
C	2.2743	-2.1588	1.1333
C	3.3222	-2.7108	1.9132
C	3.7085	-2.0063	3.0716
H	4.5071	-2.3933	3.6947
C	3.0523	-0.8458	3.4183
H	3.3011	-0.2957	4.3150
C	2.0240	-0.3726	2.5840
C	1.2645	0.8505	2.9453
C	-0.1996	2.9622	3.5590
C	0.8476	2.5229	4.4334
C	4.3274	3.1139	-1.0341
C	4.4744	1.7568	-0.5947
C	2.0703	2.7970	-0.9697
C	0.7035	3.3390	-1.1791
C	0.5220	4.6417	-1.6777
H	1.3875	5.2389	-1.9280
C	-0.7607	5.1216	-1.8320
H	-0.9305	6.1175	-2.2257
C	-1.8587	4.3242	-1.4502
C	-1.5787	3.0270	-0.9481
C	-3.2147	4.7830	-1.5266
H	-3.4079	5.7680	-1.9353
C	-4.2378	4.0092	-1.0761
H	-5.2595	4.3683	-1.1205
C	-2.6660	2.2063	-0.4643
C	-3.9889	2.7147	-0.5119
C	-5.0118	1.9128	0.0341
H	-6.0376	2.2639	0.0160
C	-4.6986	0.7014	0.6104
H	-5.4517	0.0739	1.0661
C	-3.3577	0.2776	0.6123
C	-2.9729	-1.0003	1.2621
C	-2.1857	-3.2089	2.4796
C	-3.5655	-2.8214	2.4942
C	5.8132	1.1220	-0.3878
H	5.6933	0.0838	-0.0835
H	6.4103	1.1573	-1.3038
H	6.3831	1.6537	0.3803
C	5.5031	3.9948	-1.2943
H	5.1728	4.9838	-1.6052
H	6.1253	4.0870	-0.3982
H	6.1425	3.5684	-2.0743
C	-1.6925	-4.4385	3.1751
H	-0.6166	-4.5378	3.0429
H	-1.9158	-4.3984	4.2455

H	-2.1830	-5.3348	2.7837
C	-4.6096	-3.6318	3.1867
H	-5.5891	-3.1758	3.0577
H	-4.6324	-4.6547	2.7975
H	-4.3899	-3.7108	4.2566
C	-4.2381	-0.7774	-4.2271
H	-4.4046	0.2073	-3.7941
H	-4.0842	-0.6694	-5.3050
H	-5.1414	-1.3809	-4.0971
C	-3.2814	-3.5380	-5.0205
H	-2.7717	-4.4890	-5.1612
H	-4.3266	-3.7263	-4.7535
H	-3.2965	-2.9935	-5.9702
C	-1.0671	4.1387	3.8783
H	-1.7973	4.2925	3.0857
H	-1.5971	3.9884	4.8236
H	-0.4697	5.0482	3.9925
C	1.1585	3.2245	5.7130
H	1.9976	2.7448	6.2128
H	1.3984	4.2772	5.5327
H	0.2903	3.2133	6.3804
H	1.8324	0.3988	-2.9352
H	0.4334	0.0436	-3.4833

$[Am(Me\text{-}BTPhen)_2(H_2O)]^{3+}$; E(RB3LYP) = -2684.77367393 A.U.

Am	0.0052	0.0551	-0.2012
O	0.9493	0.1953	-2.7184
N	3.4058	1.1108	-0.3916
N	2.1785	1.6204	-0.5628
N	3.0791	3.7041	-1.2214
N	-0.3447	2.6107	-0.8558
N	-2.4202	1.0517	0.0581
N	-1.7719	-1.3209	1.2167
N	-1.4012	-2.4424	1.8452
N	-4.0253	-1.6411	1.8517
N	-2.4090	-0.8496	-2.6624
N	-1.3462	-1.3839	-2.0458
N	-1.5111	-3.3480	-3.3505
N	0.7909	-2.4347	-0.7196
N	1.7067	-1.0543	1.4783
N	0.3769	1.2174	2.1575
N	-0.3515	2.2877	2.4954
N	1.6585	1.3928	4.1350
C	-2.5743	-2.8503	-3.9625
C	-3.0368	-1.5405	-3.6053

C	-0.9262	-2.5977	-2.4063
C	0.2643	-3.1572	-1.7130
C	0.7792	-4.4087	-2.0969
H	0.3134	-4.9474	-2.9099
C	1.8678	-4.9138	-1.4208
H	2.2939	-5.8703	-1.7022
C	2.4177	-4.1961	-0.3395
C	1.8275	-2.9457	-0.0158
C	3.5141	-4.6963	0.4358
H	3.9607	-5.6427	0.1537
C	3.9721	-4.0095	1.5150
H	4.7909	-4.3990	2.1089
C	2.3126	-2.2158	1.1381
C	3.3705	-2.7688	1.9062
C	3.7724	-2.0671	3.0606
H	4.5784	-2.4572	3.6721
C	3.1237	-0.9064	3.4178
H	3.3851	-0.3586	4.3122
C	2.0858	-0.4301	2.5972
C	1.3375	0.7958	2.9799
C	-0.1054	2.9101	3.6403
C	0.9542	2.4556	4.4920
C	4.3022	3.2315	-1.0391
C	4.4697	1.8713	-0.6160
C	2.0493	2.8814	-0.9788
C	0.6747	3.4105	-1.1829
C	0.4883	4.7116	-1.6842
H	1.3512	5.3128	-1.9334
C	-0.7960	5.1834	-1.8432
H	-0.9708	6.1774	-2.2395
C	-1.8908	4.3803	-1.4652
C	-1.6081	3.0846	-0.9576
C	-3.2459	4.8375	-1.5556
H	-3.4360	5.8215	-1.9680
C	-4.2713	4.0628	-1.1141
H	-5.2935	4.4187	-1.1686
C	-2.7009	2.2607	-0.4818
C	-4.0241	2.7702	-0.5462
C	-5.0556	1.9719	-0.0121
H	-6.0798	2.3263	-0.0443
C	-4.7538	0.7608	0.5692
H	-5.5144	0.1364	1.0162
C	-3.4142	0.3335	0.5884
C	-3.0512	-0.9479	1.2484
C	-2.3111	-3.1624	2.4877
C	-3.6856	-2.7558	2.4801

C	5.8176	1.2540	-0.4155
H	5.7127	0.2095	-0.1270
H	6.4160	1.3121	-1.3294
H	6.3777	1.7825	0.3620
C	5.4650	4.1324	-1.2890
H	5.1201	5.1222	-1.5808
H	6.0910	4.2167	-0.3949
H	6.1055	3.7285	-2.0801
C	-1.8443	-4.3950	3.1959
H	-0.7678	-4.5084	3.0803
H	-2.0831	-4.3472	4.2626
H	-2.3401	-5.2868	2.8009
C	-4.7503	-3.5489	3.1613
H	-5.7218	-3.0812	3.0151
H	-4.7804	-4.5737	2.7778
H	-4.5476	-3.6243	4.2349
C	-4.2170	-0.8997	-4.2646
H	-4.3856	0.0925	-3.8499
H	-4.0634	-0.8115	-5.3443
H	-5.1189	-1.5029	-4.1231
C	-3.2503	-3.6709	-5.0093
H	-2.7385	-4.6233	-5.1316
H	-4.2957	-3.8563	-4.7414
H	-3.2641	-3.1436	-5.9687
C	-0.9619	4.0870	3.9866
H	-1.7063	4.2504	3.2094
H	-1.4742	3.9304	4.9405
H	-0.3588	4.9933	4.0972
C	1.2898	3.1420	5.7736
H	2.1407	2.6589	6.2498
H	1.5216	4.1980	5.6025
H	0.4359	3.1180	6.4590
H	1.8374	0.4587	-2.9861
H	0.4719	-0.0116	-3.5303

$[Eu(Me\text{-}BTPhen)_2(OH)]^{2+}$; E(RB3LYP) = -2686.03084884 A.U.

Eu	0.0500	0.0537	-0.2710
O	0.8345	0.1556	-2.2441
N	3.4089	1.2540	-0.0015
N	2.1902	1.7232	-0.2545
N	3.0934	3.6136	-1.3527
N	-0.3237	2.6142	-0.7831
N	-2.3829	1.0345	0.0771
N	-1.7156	-1.3213	1.2613
N	-1.3483	-2.4337	1.8973

N	-3.9800	-1.6745	1.8496
N	-2.5876	-0.9532	-2.4408
N	-1.5147	-1.4784	-1.8551
N	-1.4660	-3.2494	-3.4224
N	0.7193	-2.4669	-0.6624
N	1.6799	-1.0636	1.4789
N	0.3294	1.1914	2.1685
N	-0.3983	2.2529	2.5152
N	1.6622	1.4073	4.1112
C	-2.5250	-2.7342	-4.0277
C	-3.1066	-1.5388	-3.5150
C	-0.9865	-2.5960	-2.3558
C	0.2111	-3.1592	-1.6797
C	0.7595	-4.3831	-2.1111
H	0.3106	-4.8967	-2.9494
C	1.8554	-4.8895	-1.4506
H	2.3005	-5.8283	-1.7609
C	2.3965	-4.1906	-0.3524
C	1.7820	-2.9627	0.0029
C	3.5088	-4.6798	0.4071
H	3.9712	-5.6133	0.1074
C	3.9655	-3.9995	1.4918
H	4.7962	-4.3830	2.0730
C	2.2820	-2.2258	1.1459
C	3.3550	-2.7687	1.8992
C	3.7635	-2.0603	3.0468
H	4.5800	-2.4416	3.6499
C	3.1099	-0.9039	3.4054
H	3.3766	-0.3494	4.2937
C	2.0643	-0.4337	2.5885
C	1.3155	0.7915	2.9715
C	-0.1259	2.8966	3.6444
C	0.9579	2.4694	4.4679
C	4.3143	3.1512	-1.1310
C	4.4758	1.9272	-0.4202
C	2.0657	2.8777	-0.9102
C	0.6924	3.3895	-1.1558
C	0.5023	4.6558	-1.7433
H	1.3654	5.2365	-2.0358
C	-0.7813	5.1168	-1.9273
H	-0.9587	6.0869	-2.3779
C	-1.8747	4.3297	-1.5128
C	-1.5849	3.0645	-0.9411
C	-3.2343	4.7662	-1.6319
H	-3.4317	5.7311	-2.0847
C	-4.2562	3.9974	-1.1707

H	-5.2816	4.3405	-1.2472
C	-2.6747	2.2340	-0.4705
C	-4.0032	2.7239	-0.5645
C	-5.0290	1.9192	-0.0305
H	-6.0579	2.2579	-0.0811
C	-4.7161	0.7208	0.5686
H	-5.4722	0.0894	1.0126
C	-3.3701	0.3091	0.6011
C	-3.0007	-0.9670	1.2673
C	-2.2631	-3.1708	2.5164
C	-3.6365	-2.7868	2.4787
C	5.8208	1.3446	-0.1117
H	5.7028	0.4237	0.4569
H	6.3719	1.1231	-1.0307
H	6.4318	2.0441	0.4663
C	5.4813	3.9396	-1.6351
H	5.1333	4.8274	-2.1598
H	6.1326	4.2440	-0.8097
H	6.0929	3.3381	-2.3146
C	-1.7880	-4.3990	3.2304
H	-0.7073	-4.4886	3.1327
H	-2.0456	-4.3609	4.2930
H	-2.2565	-5.2991	2.8210
C	-4.7080	-3.6012	3.1312
H	-5.6796	-3.1377	2.9715
H	-4.7243	-4.6189	2.7292
H	-4.5266	-3.6904	4.2069
C	-4.3052	-0.8928	-4.1389
H	-4.5709	0.0061	-3.5850
H	-4.1063	-0.6202	-5.1797
H	-5.1624	-1.5726	-4.1450
C	-3.0727	-3.4326	-5.2318
H	-2.4944	-4.3313	-5.4379
H	-4.1216	-3.7061	-5.0825
H	-3.0386	-2.7778	-6.1083
C	-0.9903	4.0690	3.9933
H	-1.7555	4.2044	3.2306
H	-1.4778	3.9238	4.9620
H	-0.3991	4.9866	4.0686
C	1.3263	3.1830	5.7295
H	2.1922	2.7095	6.1883
H	1.5533	4.2350	5.5313
H	0.4937	3.1692	6.4401
H	1.1761	0.1881	-3.1361

$[Am(Me\text{-}BTPhen)_2(OH)]^{2+}$; E(RB3LYP) = -2684.50792474 A.U.

Am	0.0473	0.0548	-0.2601
O	0.8563	0.1609	-2.2965
N	3.3949	1.3466	0.0043
N	2.1711	1.7993	-0.2558
N	3.0517	3.6825	-1.3814
N	-0.3613	2.6660	-0.7940
N	-2.4393	1.0820	0.0719
N	-1.8081	-1.2896	1.2754
N	-1.4631	-2.4079	1.9141
N	-4.0837	-1.6138	1.8304
N	-2.5793	-1.0403	-2.4375
N	-1.4985	-1.5502	-1.8518
N	-1.4141	-3.3121	-3.4255
N	0.7540	-2.5184	-0.6501
N	1.7272	-1.1145	1.5095
N	0.3959	1.1553	2.2382
N	-0.3156	2.2222	2.6022
N	1.7603	1.3435	4.1600
C	-2.4781	-2.8111	-4.0334
C	-3.0844	-1.6296	-3.5159
C	-0.9498	-2.6566	-2.3531
C	0.2525	-3.2084	-1.6730
C	0.8096	-4.4257	-2.1114
H	0.3656	-4.9372	-2.9532
C	1.9077	-4.9278	-1.4524
H	2.3601	-5.8616	-1.7670
C	2.4436	-4.2310	-0.3507
C	1.8216	-3.0083	0.0137
C	3.5610	-4.7217	0.3995
H	4.0245	-5.6517	0.0907
C	4.0210	-4.0464	1.4848
H	4.8566	-4.4288	2.0595
C	2.3257	-2.2751	1.1607
C	3.4081	-2.8202	1.9010
C	3.8294	-2.1182	3.0475
H	4.6529	-2.5035	3.6387
C	3.1817	-0.9633	3.4193
H	3.4600	-0.4128	4.3064
C	2.1266	-0.4890	2.6172
C	1.3908	0.7396	3.0206
C	-0.0192	2.8553	3.7310
C	1.0718	2.4095	4.5353
C	4.2774	3.2357	-1.1557
C	4.4538	2.0250	-0.4252
C	2.0319	2.9425	-0.9265
C	0.6527	3.4406	-1.1758

C	0.4594	4.6991	-1.7784
H	1.3207	5.2790	-2.0772
C	-0.8251	5.1532	-1.9681
H	-1.0060	6.1175	-2.4297
C	-1.9163	4.3669	-1.5469
C	-1.6254	3.1079	-0.9598
C	-3.2744	4.8031	-1.6787
H	-3.4680	5.7637	-2.1419
C	-4.2985	4.0385	-1.2177
H	-5.3238	4.3792	-1.3039
C	-2.7201	2.2797	-0.4881
C	-4.0479	2.7706	-0.5997
C	-5.0818	1.9724	-0.0722
H	-6.1088	2.3143	-0.1367
C	-4.7800	0.7764	0.5361
H	-5.5433	0.1493	0.9736
C	-3.4357	0.3610	0.5865
C	-3.0875	-0.9185	1.2612
C	-2.3958	-3.1341	2.5188
C	-3.7632	-2.7306	2.4637
C	5.8055	1.4629	-0.1084
H	5.6983	0.5481	0.4723
H	6.3598	1.2363	-1.0241
H	6.4074	2.1773	0.4609
C	5.4353	4.0272	-1.6759
H	5.0772	4.9044	-2.2114
H	6.0878	4.3485	-0.8579
H	6.0487	3.4213	-2.3499
C	-1.9469	-4.3703	3.2357
H	-0.8664	-4.4744	3.1512
H	-2.2171	-4.3308	4.2952
H	-2.4227	-5.2629	2.8185
C	-4.8539	-3.5299	3.1029
H	-5.8172	-3.0537	2.9303
H	-4.8786	-4.5479	2.7019
H	-4.6876	-3.6201	4.1811
C	-4.2929	-1.0027	-4.1401
H	-4.5823	-0.1171	-3.5767
H	-4.0926	-0.7123	-5.1757
H	-5.1346	-1.7013	-4.1612
C	-3.0070	-3.5106	-5.2452
H	-2.4058	-4.3920	-5.4602
H	-4.0485	-3.8129	-5.0990
H	-2.9900	-2.8460	-6.1147
C	-0.8651	4.0349	4.1003
H	-1.6380	4.1852	3.3482

H	-1.3423	3.8874	5.0737
H	-0.2622	4.9449	4.1756
C	1.4649	3.1088	5.7976
H	2.3316	2.6222	6.2410
H	1.7009	4.1597	5.6046
H	0.6417	3.0983	6.5190
H	1.1999	0.1925	-3.1881

Section S6 References

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