Electronic supplementary information for paper

« First phosphinoxide-based extractant with high Am/Cm selectivity »

Solvent extraction procedure

Solvent extraction experiments were carried out as follows. 0.5 mL of nitrobenzene solutions of extractant and 0.5 mL of aqueous phase containing nitric acid and radionuclides were put in 1.5 ml polypropylene vial. First set of samples contained ^{241}Am and ^{152}Eu, second set – ^{241}Am and ^{244}Cm, third and fourth - ^{241}Am and ^{244}Cm separately. The phases were stirred for 15 minutes on a vortex shaker at a temperature of 25.0±0.5 °C. Then samples were centrifuged (5 minutes, 6000 rpm) and aliquots of each phase were taken for determination of radionuclide radioactivity.

Content of ^{241}Am ($E\gamma$ = 59.5 keV) and ^{152}Eu ($E\gamma$ = 121.8 keV) was determined by gamma-spectrometry using high-pure germanium detector GR 3818 (Canberra Ind.) in the first set of experiments. Second set

of samples was analyzed by alpha-spectrometry ($E_\alpha(^{241}Am)$ = 5637 keV, $E_\alpha(^{244}Cm)$ = 5901 keV) using alpha spectrometer Model 7401 with Si detector (Canberra Ind.). Third and fourth sets of samples were analyzed by liquid-scintillation spectrometry (Tri-carb TR 2810, Perkin Elmer).

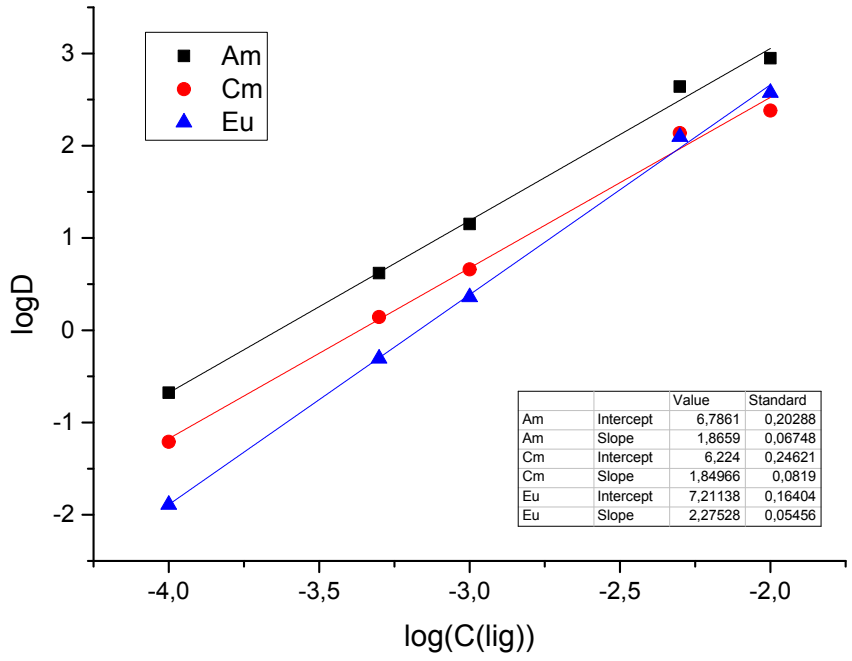
The relative error of each measurement did not exceed 7%. The distribution coefficients (D) of metals were calculated as the ratio of the counting rate in the organic and aqueous phase, the separation factors (SF) were calculated as the ratio of the distribution coefficients.

Table 1. Distribution ratios (D) for Am, Cm and Eu. Organic phase – 0,001 M of *m*-$C_6H_4Ph_2PO$ or 0.01 M of PyPO in nitrobenzene. Aqueous phase – trace amounts of Am, Cm, Eu in nitric acid solutions.

	***m*-$C_6H_4Ph_2PO$**			0.001M **PyPO**		0.01M **PyPO**	
HNO_3, M	D(Am)	D(Cm)	D(Eu)	D(Am)	D(Eu)	D(Am)	D(Eu)
1	-	-	-	-	-	0.001	-
2	-	-	-	0.001	-	0.002	-
3	-	-	-	0.001	-	0.005	0.001
4	0.001	-	-				
5	0.002	-	-				

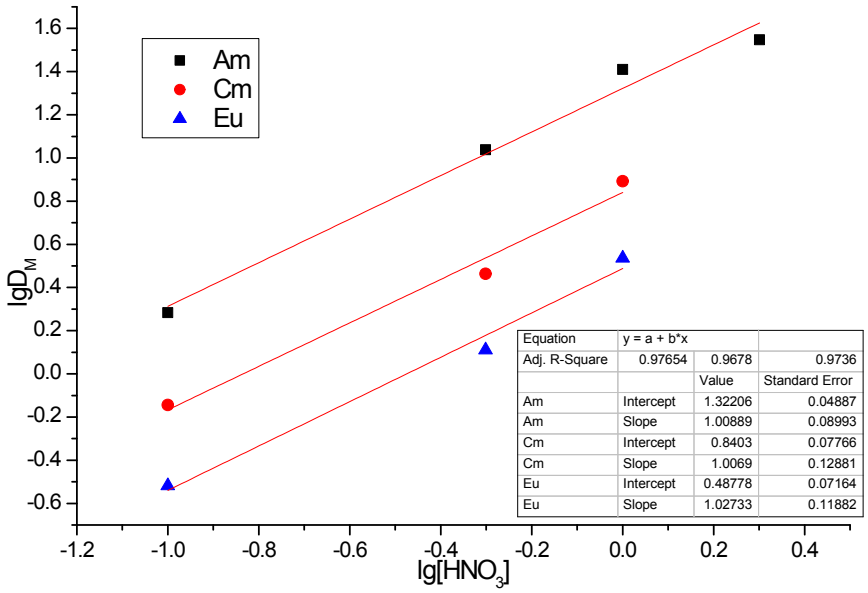
Slope analysis for apparent solvation numbers

Apparent solvation numbers were determined in a range of ligand`s concentration from 10^{-4} to 10^{-2} M.

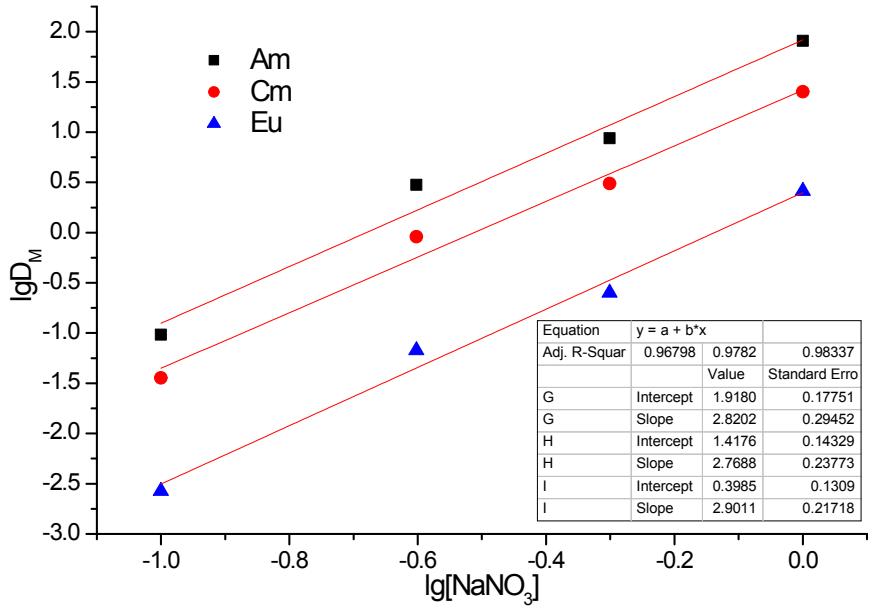


Slope analysis for apparent number of nitrate counterions

Apparent numbers of nitrate groups were determined in a range of nitric acid concentrations below 1M HNO_3.



Equation	y = a + b*x		
Adj. R-Square	0.97654	0.9678	0.9736
		Value	Standard Error
Am	Intercept	1.32206	0.04887
Am	Slope	1.00889	0.08993
Cm	Intercept	0.8403	0.07766
Cm	Slope	1.0069	0.12881
Eu	Intercept	0.48778	0.07164
Eu	Slope	1.02733	0.11882



Equation	y = a + b*x		
Adj. R-Squar	0.96798	0.9782	0.98337
		Value	Standard Erro
G	Intercept	1.9180	0.17751
G	Slope	2.8202	0.29452
H	Intercept	1.4176	0.14329
H	Slope	2.7688	0.23773
I	Intercept	0.3985	0.1309
I	Slope	2.9011	0.21718

Equations for nitric acid extraction and conditional equilibria constants for them:

$$xL + yH^+ + yNO_3^- = L_x(HNO_3)_y$$

$$zL + Me^{3+} + 3NO_3^- = MeL_z(NO_3)_3$$

$$K_{H^+} = \frac{L_x(HNO_3)_y}{[H^+]^y \cdot [L]^x \cdot [NO_3^-]^y} \quad (1)$$

$$K_{Me} = \frac{MeL_z(NO_3)_3}{[Me^{3+}] \cdot [L]^Z \cdot [NO_3^-]^3} \quad (2)$$

Express $[L]^z$ from equation (1):

$$[L]^Z = \left(\frac{L_x(HNO_3)_y}{[H^+]^y \cdot K_{H^+} \cdot [NO_3^-]^y}\right)^{\frac{z}{x}} (3)$$

Present $\frac{MeL_z(NO_3)_3}{[Me^{3+}]}$ as D and substitute $[L]^z$ we can write:

$$K_{Me} = \frac{D}{\left(\frac{L_x(HNO_3)_y}{[H^+]^y K [NO_3^-]^y}\right)^{\frac{z}{x}} \cdot [NO_3^-]^3} (4)$$

$$K_{Me} = \frac{D}{\left(\frac{L_x(HNO_3)_y}{[H^+]^y K}\right)^{\frac{z}{x}} \cdot [NO_3^-]^{(3-yz/x)}} (5)$$

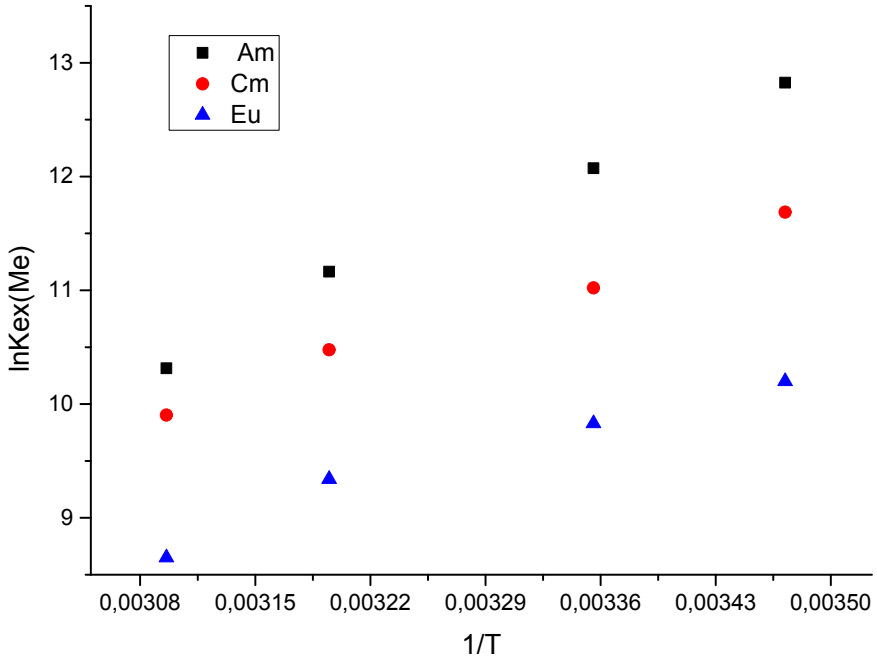
Let's logarithm the expression (5):

$$lgK_{Me} = lg\left(\frac{D}{\left(\frac{L_x(HNO_3)_y}{[H^+]^y K}\right)^z \cdot [NO_3^-]^{(3-yz/x)}}\right)$$

$$lgD = lgK_{Me} + lg\left(\frac{L_x(HNO_3)_y}{[H^+]^y K}\right)^{\frac{z}{x}} + (3 - yz/x)\, lg[NO_3^-]$$

Temperature dependence of lnKex

Before the extraction, the samples were held in an air thermostat for 30 minutes to achieve thermodynamic equilibrium. The extraction was carried out at temperatures of 288, 298, 313 and 323 K.



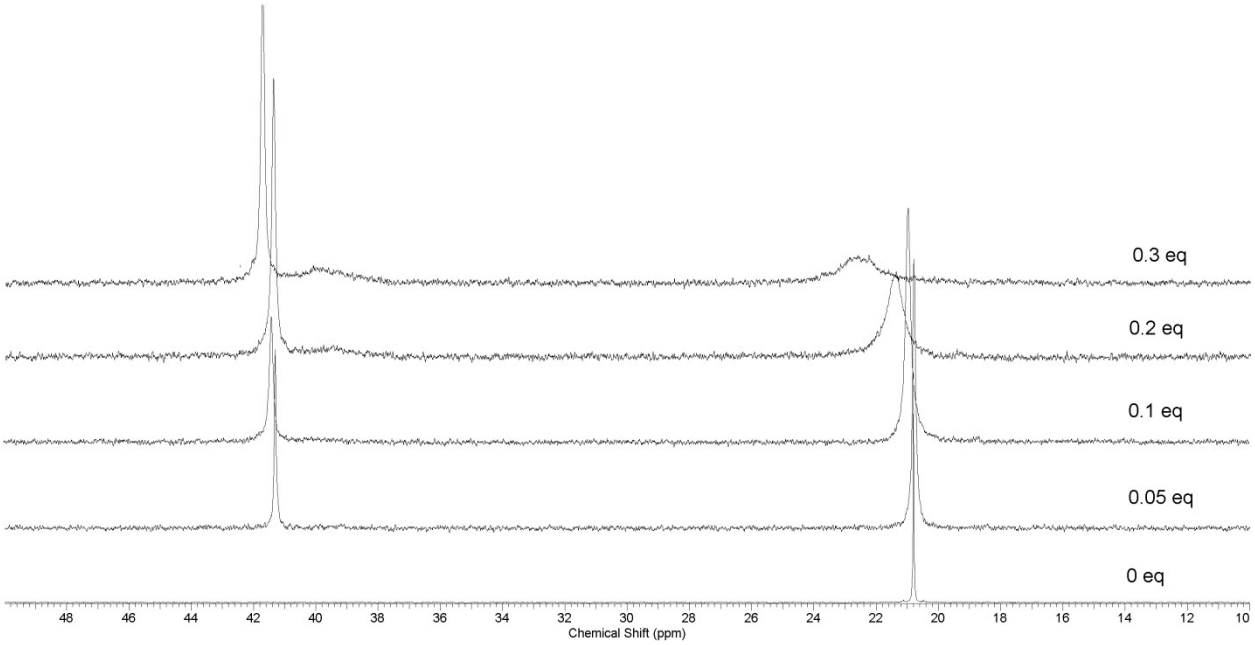
Irradiation procedure

Irradiation of organic phases was performed using “GAMMA-400” installation (Moscow State University) of cesium-137 gamma-source with dose rate of 2.5 Gy·min^{-1}.

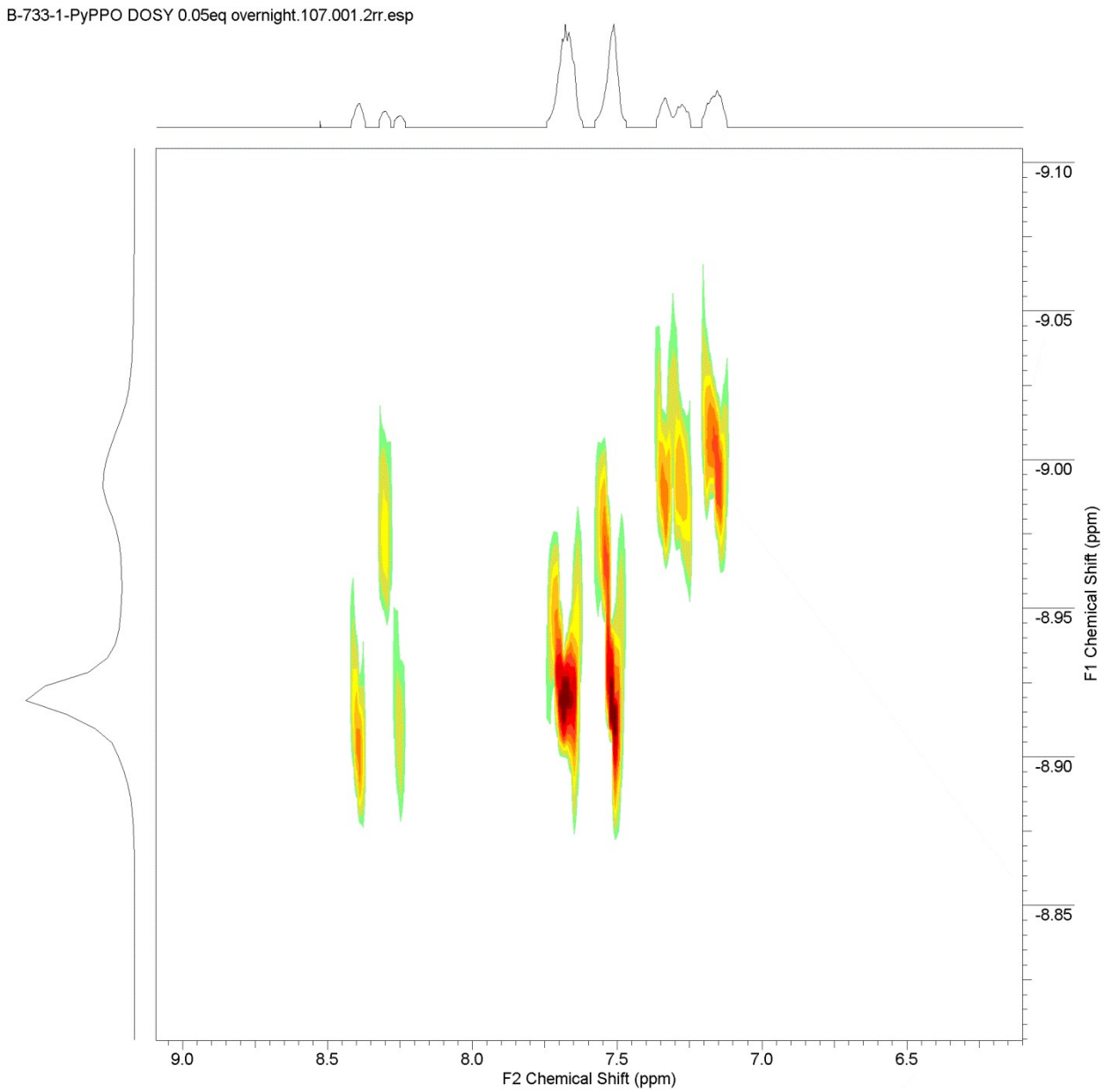
Concentration of **Ph_2PyPO** in nitrobenzene solution ligand was 10^{-3} M. Irradiation was carried out in glass tubes. During irradiation, organic samples were kept in contact with 3 M nitric acid. The volumes of the organic and aqueous phases were 3 mL. Mixed-phase systems were intensively shaken for 15 minutes before the irradiation for saturation and equilibration of the phases. During irradiation, no stirring was performed. Aliquots of organic phases were taken for subsequent solvent extraction experiments after accumulating the certain dose.

NMR Experiments

The NMR spectra were measured on a BRUKER AVANCE-600 MHz NMRspectrometer at 24 °C for solution of weighed amount of approximately 20 mg of **Ph_2PyPO** in acetonitrile-*d3* in 5 mm probe tubes (with the solvent as internal lock). A batch of $La(NO_3)_3{\cdot}6H_2O$ was dissolved in acetonitrile-*d3* for preparation of 0.1M solution of lanthanum salt. An aliquot of the metal salt solution corresponding 0.05, 0.1, 0.2 and 0.3 equivalents were added to NMR-test tube with the solution of the ligand and the corresponding ^1H, ^{31}P NMR spectra were collected as well as DOSY experiment for solution with 0.05 equivalent of lanthanum nitrate.



^{31}P Spectra of **Ph_2PyPO** – $La(NO_3)_3$ system with various ligand-to-metal ratios



2D DOSY Spectrum of 0.05 equivalents of $La(NO_3)_3$ in **Ph_2PyPO** solution. Two peaks at the diffusion axis evidenced formation of a complex.

DFT Modeling

To test the above-mentioned assumption we decided as a first step to perform DFT calculations of metal-to-ligand binding energies in lanthanide complexes with several ligands IV using first-principles DFT (GGA PBE), scalar-relativistic theory29 and large relativistic full-electron basis sets30 (see ESI† for calculation details). All calculations were performed at the MBC-100k Cluster of the Joint Supercomputer Center (JSCC, Moscow) using the PRIRODA program.31

29 R. G. Dyall, J. Chem. Phys., 1994, 100, 2118. 30 D. N. Laikov, Chem. Phys. Lett., 2005, 416, 116.

The relaxed geometries of ligand **Ph_2PyPO** and its complexes (**Ph2PyPO**)$_2$M$(NO_3)_3$ were completely optimized for the gas phase conditions by DFT (GGA PBE functional[1, 2]). The preorganized ligand conformation was optimized with restriction on two O=P-C_{Py}-N_{Py} torsion angles which is assumed equal to zero. We used the scalar relativistic theory and relativistic full-electron basis set[3] consisting of: {2,1}/{6,2} for H; {3,2,1}/{10,7,3} for C, N, and O; {4,3,1}/{15,11,3} for P; {9,8,6,3,1} /{30,29,20,14,6}, for

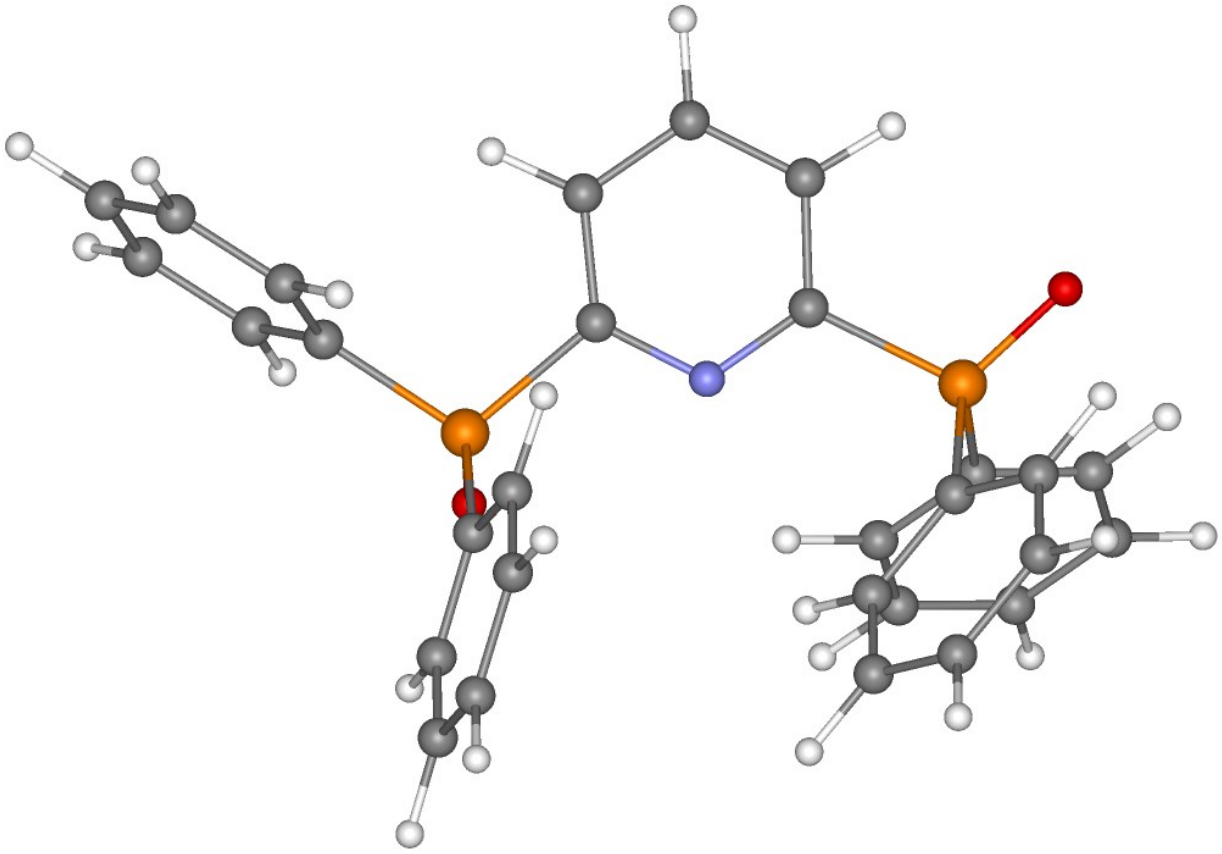
Eu; {10,9,7,4,1}/{34,33,24,18,6}, for Am and Cm. The stationary points were identified by an analysis of Hessians. The statistical formulas for rigid rotator and harmonic oscillator were used for the calculation of the thermodynamic functions (Gibbs energy, G) at 298.15 K. Atomic charges and spin density values were calculated according to Mulliken[4]. All calculations were performed at the MBC-100к Cluster of the Joint Supercomputer Center (JSCC, Moscow) using the PRIRODA code developed by D.N. Laikov.[5]

1. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
2. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396.
3. D. N. Laikov, *Chem. Phys. Lett.*, 2005, **416**, 116-120.
4. R. S. Mulliken, *J. Chem. Phys.*, 1955, **23**, 1833-1840.
5. D. N. Laikov, *Chem. Phys. Lett.*, 1997, **281**, 151-156.

Interatomic distances (A) and angles (°) for complexes of $(Ph_2PyPO)_2M(NO_3)_3$ and $(Ph_2PyPO)_2M(NO_3)_2^+$ compositions where M = Am, Cm and Eu

$(Ph_2PyPO)_2M(NO_3)_3$	Am	Cm	Eu
M-N1/M-N1’	3.017/3.345	2.973/3.339	2.985/3.375
M-O1/M-O1’	2.481/2.486	2.486/2.480	2.475/2.483
M-O2/M-O2’	2.679/2.613	2.601/2.597	2.650/2.637
M-O1N/M-O2N	2.565/2.569	2.706/2.534	2.527/2.540
M-O3N/M-O4N	2.560/2.517	2.556/2.544	2.612/2.577
M-O5N	2.391	2.367	2.417
$M…Py_{plane}$	0.720/1.657	0.684/1.573	0.564/1.672
O1…O2/O1’…O2’*	4.225/4.445	4.199/4.432	4.218/4.451
$O=P\text{-}C_{Py}$*	110.520; 107.737; 109.148; 109.979	110.243; 107.762; 109.007; 109.322	110.644; 107.773; 110.056; 109.386;
$(Ph_2PyPO)_2M(NO_3)_2^+$	Am	Cm	Eu
M-N1/M-N1’	3.012/3.054	3.020/3.037	2.961/2.994
M-O1/M-O1’	2.451/2.450	2.429/2.433	2.429/2.451
M-O2/M-O2’	2.476/2.545	2.453/2.506	2.497/2.485
M-O1N/M-O2N	2.517/2.520	2.477/2.481	2.495/2.476
M-O3N/M-O4N	2.463/2.483	2.545/2.514	2.521/2.2.499
$M…Py_{plane}$	0.769/0.810	0.713/0.807	0.055/0.808
O1…O2/O1’…O2’*	4.315/4.330	4.268/4.296	4.284/4.374
$O=P\text{-}C_{Py}$*	107.687; 108.215; 107.579; 108.013	107.429; 107.837; 107.262; 107.665	107.301; 107.847; 107.434; 108.062

Relaxed geometry of Ph_2PyPO ligand



Cartesian coordinates

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7	1.35816562	-3.47157335	2.49546742	6	-0.13500182	-0.34821433	2.72066760
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6	1.34420848	-3.63229823	4.90102434	6	-1.80372715	-1.26151752	7.23488379
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6	2.67893934	-4.04768181	4.89410591	1	-1.50534129	-0.38467509	7.81074142
1	3.19236374	-4.26847124	5.83094501	6	-2.69716263	-2.18886495	7.78168774
6	3.34249115	-4.17894888	3.67447019	6	-3.08743143	-3.30603075	7.03822517
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15	-1.07645392	-2.92975354	3.50223374	1	-3.78967571	-4.02591801	7.46027708
15	3.51529932	-4.08967543	0.87860870	1	-3.09360147	-2.03543448	8.78607082
6	2.60880685	-5.41628122	-0.01036604	6	-0.24886811	0.84429729	2.00244236
6	3.25957656	-2.52128315	-0.04111328	1	0.72606999	-0.50543255	3.37174273
6	-1.68196428	-2.57696176	5.20307016	1	0.51518977	1.61517870	2.10746503

6	-1.33125567	1.04223430	1.13971841
1	-1.41603267	1.97335529	0.57808286
6	-2.29733801	0.04286557	0.98765785
1	-3.13494682	0.19099058	0.30497009
1	-2.92184091	-1.95030212	1.58160877
6	4.41977501	-1.80474043	-0.36951184
6	1.21165323	-5.55443621	-0.00605474
6	3.40603256	-6.32953691	-0.71731687
6	4.31737328	-0.60419077	-1.07721436
1	5.38862514	-2.20612955	-0.06879411
1	5.22027874	-0.05002270	-1.33702183
6	3.06227493	-0.11786148	-1.45368004
1	2.98403811	0.81836665	-2.00814533
6	1.90600216	-0.83290404	-1.12423718
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6	1.99936128	-2.03605413	-0.42159390
1	1.09559238	-2.58598304	-0.16371450
6	2.80448341	-7.36822557	-1.43143499
1	4.49107170	-6.22151709	-0.68539327
6	0.62053013	-6.59989357	-0.71978956
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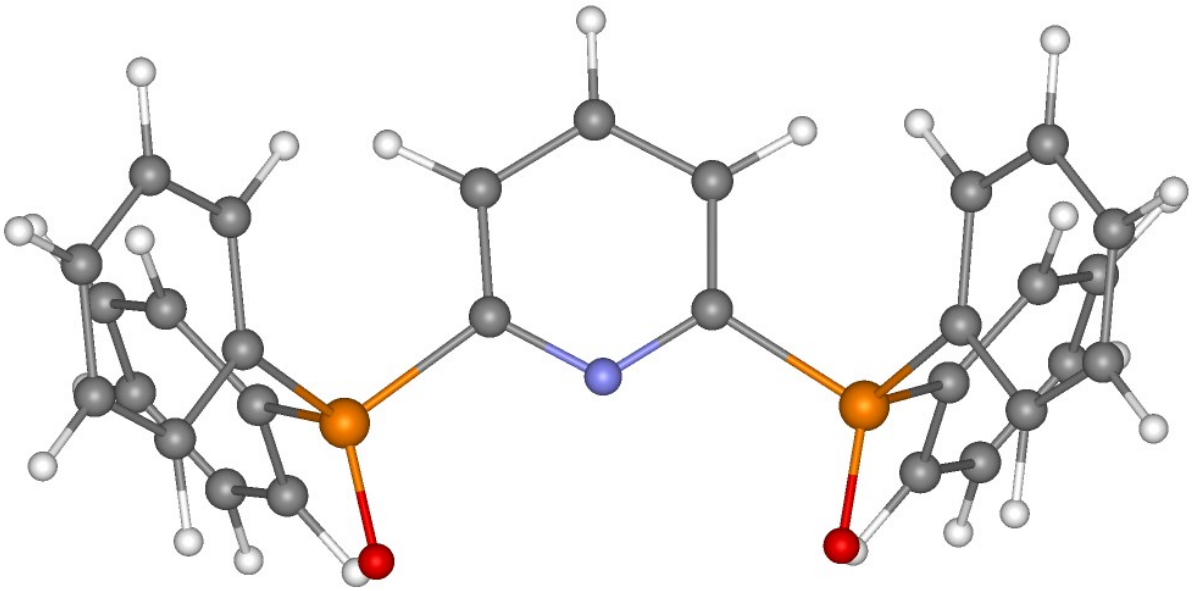
1	-0.46435824	-6.71023798	-0.70842743
6	1.41303051	-7.50264835	-1.43538284
1	0.94531566	-8.31697083	-1.99036896
1	3.42503619	-8.07761097	-1.98049998

Preorganized geometry of Ph_2PyPO ligand



Cartesian coordinates

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1	1.37604690	-0.89567679	2.84119368	1	-5.67159510	-3.47982335	2.65612030
6	1.66994452	-0.59671569	0.71874356	6	-2.54940677	3.85536122	3.37688422
1	2.67569137	-1.01596749	0.71226734	1	-1.53190231	1.98358560	3.10243273
15	-2.69084811	0.87878251	0.43834561	1	-2.03233004	4.07190323	4.31258059
15	1.89372969	-0.29689896	-2.14296961	6	-3.47674108	4.76480770	2.86176777
6	3.40701246	0.76077324	-2.07695079	1	-3.68791890	5.69122982	3.39711547
6	2.44963050	-2.05049706	-2.20796299	6	-4.12164068	4.48986578	1.65260148
6	-3.64059591	-0.48582083	1.22857881	1	-4.83539867	5.20290756	1.23831868
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6	-3.96600795	-0.52721494	2.59157038	6	1.53203547	-2.96803331	-2.74474287
6	-4.06162310	-1.51930630	0.37674254	6	4.25528145	0.93453562	-0.97267336
6	-2.27365470	2.66807103	2.69267702	6	3.67749143	1.45154750	-3.26929021

6	1.87101138	-4.31928015	-2.83476830
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6	4.04306841	-3.84629226	-1.87506032
1	5.02761412	-4.18528938	-1.55011225
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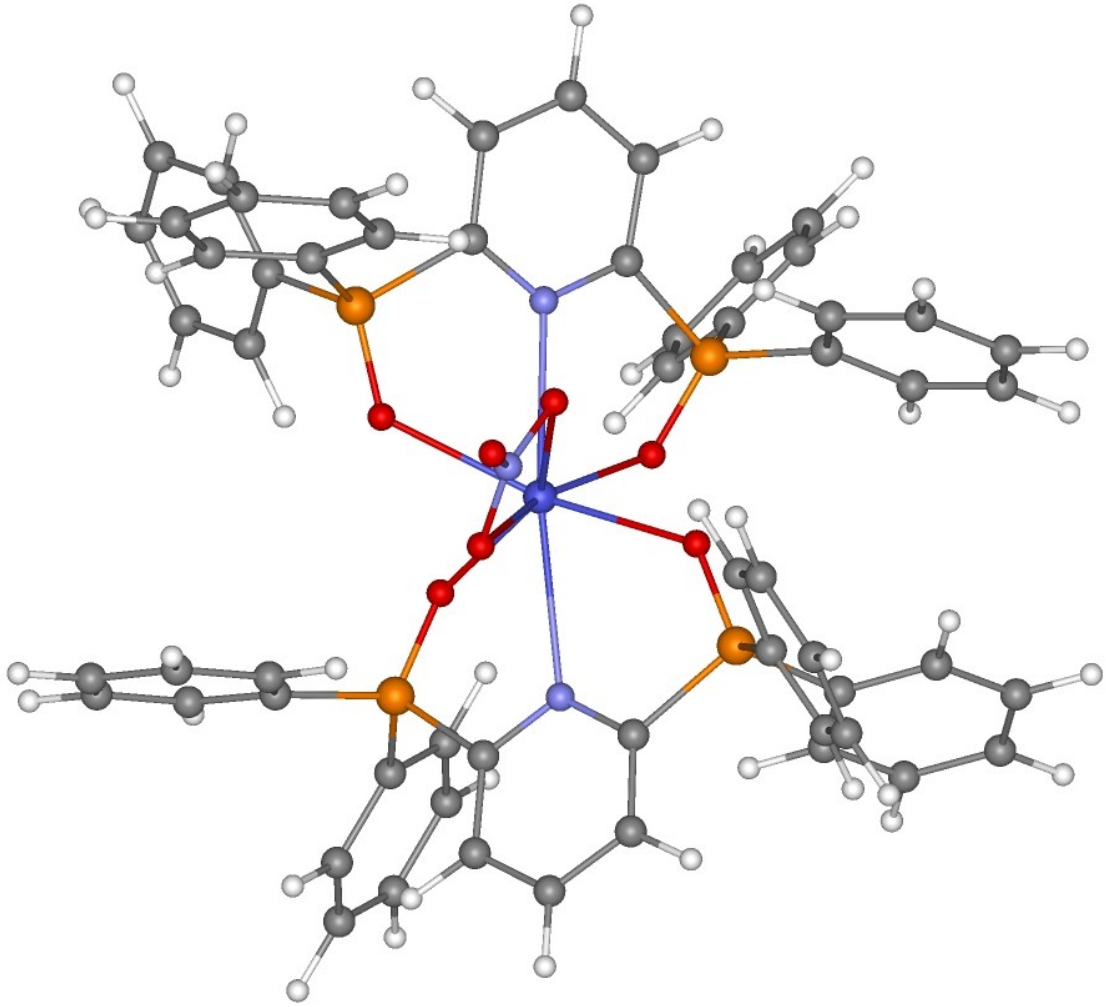
1	6.50804090	3.10676289	-2.32957268
1	4.99201059	2.82290387	-4.28829861

Relaxed geometry of $(Ph_2PyPO)_2Am(NO_3)^{2+}$ complex



Cartesian coordinates

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7	0.61409467	-1.90972281	1.85643935	8	4.23610353	1.46243083	1.01180458
6	0.74702871	-1.65654862	3.17439604	6	2.03475904	-3.88053441	-1.21359158
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6	1.34060431	-4.17097235	2.25200009	6	1.56793547	0.34159869	6.10796881
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6	-3.42050028	-1.17297697	4.93730927
1	-1.91747510	-1.91880858	3.58527207
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1	0.81413794	-0.33347178	6.52236652
1	2.63047290	0.51923072	7.97597933
6	3.52832150	1.72457981	6.41966724
1	4.32022190	2.10623789	7.06841040
6	3.45695233	2.14100337	5.08835030
1	4.18902445	2.84954333	4.69410467
1	2.37975264	1.99420738	3.21851826
6	-2.06454825	-4.32782316	-0.70677567
6	1.99002206	-4.73529768	-2.32952833
6	3.25886083	-3.32829714	-0.79447281
6	-3.04957533	-5.31434536	-0.75620455
1	-2.32421803	-3.27207112	-0.81967628
1	-4.09396696	-5.03198099	-0.90833616
6	-2.70251012	-6.66017199	-0.61470485
1	-3.47676086	-7.42996216	-0.65439153
6	-1.36644793	-7.02763939	-0.42979240
1	-1.09646845	-8.08121490	-0.32912138
6	-0.37231964	-6.05107498	-0.38460556
1	0.67233908	-6.34892607	-0.26263684
6	4.43003559	-3.65483451	-1.47612405
1	3.30525565	-2.63439107	0.05028856
6	3.16890764	-5.05372381	-3.00247502
1	1.03952491	-5.15531445	-2.66713977
1	3.13709593	-5.72583055	-3.86288118
6	4.38673973	-4.51956940	-2.57320094
1	5.30927420	-4.77991486	-3.09767866
1	5.38181877	-3.23237395	-1.14582241
8	-1.80727863	0.80830449	0.03381787
8	1.75793076	0.08153344	-2.00386024
6	0.79424697	2.55238128	-2.61196780
7	-0.08203892	2.18732929	-1.65488923
6	-1.11025226	3.01212049	-1.37399900
6	-1.27032244	4.25379515	-1.99234927
1	-2.11858487	4.89488983	-1.74326098
6	-0.32721955	4.65239239	-2.94038081
1	-0.41382033	5.62315989	-3.43323302
6	0.71142817	3.78112888	-3.27094769
1	1.44529819	4.05171585	-4.03287172
15	-2.32590508	2.24658775	-0.19356816
15	1.98301315	1.18723929	-3.05025887
6	1.49251282	0.63223475	-4.70789099
6	3.64327502	1.89781499	-3.13709664
6	-2.40511298	3.30650973	1.27177334
6	-3.93995357	2.25802541	-1.01247680
6	-3.54911351	3.26869297	2.08875275
6	-1.30211902	4.09465742	1.64092410
6	-4.75236368	3.40511084	-1.03230953
6	-4.33746433	1.09630895	-1.69418621
6	-3.59253597	4.03500462	3.25235820
1	-4.40613461	2.64967561	1.81152463
1	-4.48630667	4.01580906	3.87996030
6	-2.50173354	4.83380556	3.60679173
6	-1.35716403	4.85917759	2.80566716
1	-0.39938530	4.11536741	1.02419996
1	-0.50502872	5.48314238	3.08495259

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6	-5.95605850	3.38390565	-1.73614097
1	-4.45890665	4.30573750	-0.48678964
1	-6.59235430	4.27159929	-1.74902380
6	-6.35174990	2.22712731	-2.41363239
1	-7.29768133	2.21480346	-2.96015429
6	-5.54621983	1.08563483	-2.38953066
1	-5.86269808	0.18181632	-2.91531277
1	-3.70145512	0.20784420	-1.66639340
6	4.57532883	1.37969804	-4.05454922
6	1.76265514	1.38789070	-5.86173296
6	0.77621388	-0.57146269	-4.80208063
6	5.88060713	1.86931336	-4.06396055
1	4.28059578	0.59950817	-4.76034212
1	6.60322285	1.47188151	-4.78010559
6	6.26202774	2.86558580	-3.16156054
1	7.28518534	3.24859190	-3.17493653
6	5.34183168	3.37070990	-2.23904634
1	5.64521742	4.14093685	-1.52652872
6	4.03385782	2.88967657	-2.21937513
1	3.32705140	3.26916885	-1.47677994
6	0.33664337	-1.01490664	-6.05001020
1	0.58018827	-1.15526628	-3.89854431
6	1.31412148	0.93713260	-7.10232830
1	2.33757091	2.31557012	-5.80040455
1	1.52843428	1.51947248	-8.00123024
6	0.60149276	-0.26207832	-7.19631910
1	0.25605842	-0.61301929	-8.17163086
1	-0.21389925	-1.95547140	-6.12856579

Relaxed geometry of $(Ph_2PyPO)_2Cm(NO_3)^{2+}$ complex

Cartesian coordinates

96	0.37196526	0.18731350	0.12163268	1	-0.25019830	-1.07900918	6.45987034
8	-0.00124004	0.73665553	2.41392040	1	-2.37842035	-1.52146387	7.64519835
8	-0.17135392	-1.90674710	-0.87163842	1	-4.55389118	-1.02191138	6.54340458
6	0.84290415	-3.18042564	1.29721642	6	2.25132990	1.95935345	6.64924908
7	0.61123168	-1.95740175	1.80902338	1	0.19461030	1.57427084	6.12081432
6	0.81039435	-1.76264036	3.12721705	1	1.98856091	2.58272147	7.50679731
7	2.87789750	1.36501467	0.99984634	6	3.59291911	1.73140478	6.33231735
6	1.27987349	-2.77177858	3.97061586	1	4.37976265	2.17638516	6.94601393
1	1.43998480	-2.57737303	5.03311110	6	3.93247914	0.94151920	5.23048925
6	1.54454780	-4.02993870	3.42828178	1	4.98149681	0.77548850	4.97570276
1	1.92003965	-4.83756876	4.06032419	1	3.20605493	-0.22571288	3.56853223
6	1.31110370	-4.24530649	2.06999469	6	-2.16961527	-4.23469496	-0.80793232
1	1.49070525	-5.22429085	1.62131274	6	1.85032463	-4.52686882	-2.56062579
15	0.28599393	-0.06936411	3.69474864	6	3.15062833	-3.21954036	-0.96700060
15	0.40703344	-3.29310846	-0.50706232	6	-3.15415359	-5.21935892	-0.88962334
8	2.61485076	0.09417318	1.12125099	1	-2.43470287	-3.17508578	-0.84602982
8	1.92366695	2.06465983	0.45324779	1	-4.20310497	-4.93169165	-0.99158794
8	3.92153001	1.85461605	1.36420083	6	-2.80101562	-6.57014084	-0.84222347
6	1.91839468	-3.74786544	-1.39196718	1	-3.57511687	-7.33842993	-0.90597552
6	-0.82208568	-4.60956335	-0.68589109	6	-1.45968711	-6.94410610	-0.71944839
6	-1.22708559	-0.33272925	4.66246367	1	-1.18547153	-8.00100613	-0.69144195
6	1.58247960	0.58064657	4.77410269	6	-0.46595606	-5.96909189	-0.64241815
6	-2.45294690	-0.04948211	4.03949118	1	0.58214414	-6.27068567	-0.56833023
6	-1.20004320	-0.86767823	5.96198511	6	4.30655956	-3.49274850	-1.69619751
6	1.24257708	1.39089346	5.87244987	1	3.21405339	-2.58876538	-0.07513551
6	2.93391323	0.36630443	4.44657421	6	3.01378918	-4.79344034	-3.28172231
6	-3.64471412	-0.29784217	4.72144794	1	0.89337909	-4.92998600	-2.90106487
1	-2.46266270	0.36771086	3.02876377	1	2.96399093	-5.40805340	-4.18328524
1	-4.60186529	-0.07960454	4.23939371	6	4.23963594	-4.28216505	-2.84765553
6	-3.61834908	-0.82887250	6.01313210	1	5.15010118	-4.50228024	-3.41022086
6	-2.39757609	-1.11236644	6.63261127	1	5.26489496	-3.08945298	-1.36099172

8	-1.88127458	0.95965242	0.13715737
8	1.77104127	0.12687692	-1.81160772
6	0.77801770	2.54259777	-2.58178759
7	-0.13944650	2.20769811	-1.65364933
6	-1.14871109	3.06369209	-1.40844333
6	-1.26585448	4.29666901	-2.05373359
1	-2.09776807	4.96724272	-1.82947159
6	-0.29550791	4.65243149	-2.99054670
1	-0.34970045	5.61378193	-3.50592518
6	0.73876631	3.75788331	-3.26854539
1	1.50607777	4.00384617	-4.00539875
15	-2.37625599	2.38797736	-0.18587150
15	2.00354743	1.18088222	-2.91065025
6	1.57839310	0.52763945	-4.55024481
6	3.65086722	1.92339361	-2.97072887
6	-2.40632701	3.52479339	1.22171104
6	-3.99506283	2.38062978	-0.99499363
6	-3.58467460	3.69650030	1.96965921
6	-1.21354437	4.14648771	1.63223684
6	-4.75265312	3.55503654	-1.14935493
6	-4.45394897	1.16683936	-1.53112435
6	-3.57032180	4.50597811	3.10501575
1	-4.51149893	3.20659232	1.66114283
1	-4.48780775	4.64949131	3.68004394
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1	-0.28683254	5.44330692	3.08202648
1	-2.38436460	5.77928495	4.38463116
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1	-4.41286182	4.50028515	-0.71812052
1	-6.55626917	4.41747332	-1.95686829
6	-6.41987514	2.29880285	-2.37247634
1	-7.37068462	2.26701665	-2.90961933
6	-5.66888237	1.13131213	-2.21529341
1	-6.03262568	0.18751514	-2.62806487
1	-3.85956693	0.25892198	-1.40092862
6	4.61265993	1.43470693	-3.87298965
6	1.85173416	1.23771846	-5.73212957
6	0.90034825	-0.70033437	-4.60382366
6	5.90577555	1.95610178	-3.85269094
1	4.35152149	0.65259296	-4.58958101
1	6.65162659	1.58245611	-4.55775595
6	6.24546862	2.95294547	-2.93455029
1	7.25922918	3.36032915	-2.92459440
6	5.29577255	3.42713475	-2.02527714
1	5.56648540	4.19677639	-1.29911685
6	3.99934912	2.91580057	-2.03599453
1	3.26922894	3.26969671	-1.30284548
6	0.50480515	-1.21464157	-5.83924866
1	0.69419771	-1.24492610	-3.67837572
6	1.44831109	0.71538156	-6.96006680
1	2.39217210	2.18735313	-5.70200682
1	1.66524541	1.26276338	-7.88005257
6	0.77553397	-0.50903416	-7.01377487
1	0.46401283	-0.91517764	-7.97901869
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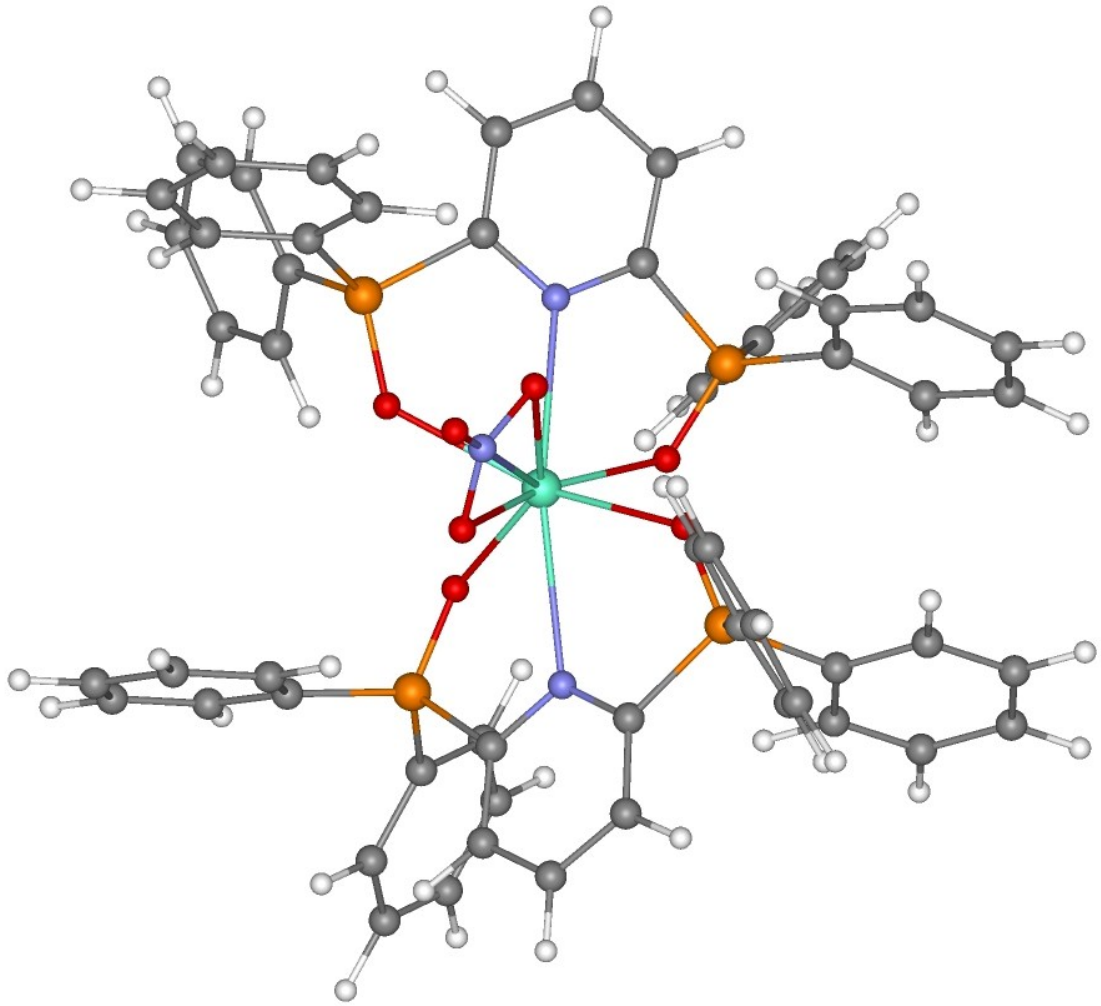
Relaxed geometry of $(Ph_2PyPO)_2Eu(NO_3)^{2+}$ complex



Cartesian coordinates

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8	0.01048408	-1.98993182	-0.87526679	8	2.84197259	-0.22280470	0.76208758
6	0.83700031	-3.16111588	1.42599297	8	2.27665472	1.84665573	0.36294755
7	0.61548239	-1.90372741	1.85472023	8	4.33897018	1.37475240	0.96062356
6	0.72774899	-1.64461088	3.17229462	6	2.04125071	-3.95187140	-1.15493107
7	3.20814943	1.01694775	0.70422071	6	-0.76800078	-4.64495182	-0.55708247
6	1.09520066	-2.62211537	4.09966421	6	-1.24945188	0.07375348	4.49085569
1	1.18440461	-2.37690759	5.15947533	6	1.60147607	0.73359400	4.73901033
6	1.35531712	-3.91491556	3.64441729	6	-1.54679084	1.07065511	5.43595934
1	1.65648723	-4.69806528	4.34355545	6	-2.20864344	-0.90519011	4.17943478
6	1.21483815	-4.19509363	2.28542447	6	1.65085542	0.31652430	6.08134985
1	1.39554691	-5.20106125	1.90136552	6	2.57455969	1.61171877	4.23696852

6	-2.78646779	1.07212341	6.07471800
1	-0.80743015	1.83782375	5.67852163
1	-3.01100802	1.83933198	6.81925869
6	-3.73228049	0.08897898	5.77325583
6	-3.44510055	-0.89533436	4.82345867
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1	-4.18508768	-1.66452622	4.59049702
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1	0.87465960	-0.33403561	6.49352741
1	2.72138119	0.44343105	7.94875574
6	3.65866899	1.62830603	6.40000534
1	4.46402025	1.97760844	7.05040264
6	3.59968376	2.05680060	5.07202244
1	4.35468960	2.74330139	4.68209124
1	2.51257253	1.96085143	3.20344663
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6	1.99553919	-4.79134274	-2.28241897
6	3.27545357	-3.46910906	-0.68342376
6	-3.11043119	-5.16947079	-0.85845834
1	-2.30209804	-3.15758801	-0.89750826
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6	-1.50706673	-6.94878006	-0.48697847
1	-1.28230143	-8.01235962	-0.38053256
6	-0.47650480	-6.01259613	-0.41179180
1	0.55169952	-6.35171032	-0.26104635
6	4.45367432	-3.84832788	-1.32433963
1	3.32407284	-2.78974366	0.17240265
6	3.18126750	-5.16337061	-2.91447258
1	1.03833580	-5.15840626	-2.66051364
1	3.14782906	-5.82382250	-3.78379393
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6	-6.31210947	2.00441027	-2.41748524
1	-7.25199366	1.95974517	-2.97269249
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6	1.75452578	1.46049547	-5.85391760
6	0.81522620	-0.52272141	-4.79588366
6	5.87946320	1.99841630	-4.08892393
1	4.30265236	0.68273932	-4.75210714
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6	6.24439096	3.02027011	-3.20856929
1	7.25899792	3.42471027	-3.23545814
6	5.31816530	3.52467656	-2.29168940
1	5.60854435	4.31674385	-1.59787118
6	4.02112913	3.01576066	-2.25490355
1	3.30949020	3.39729333	-1.51845813
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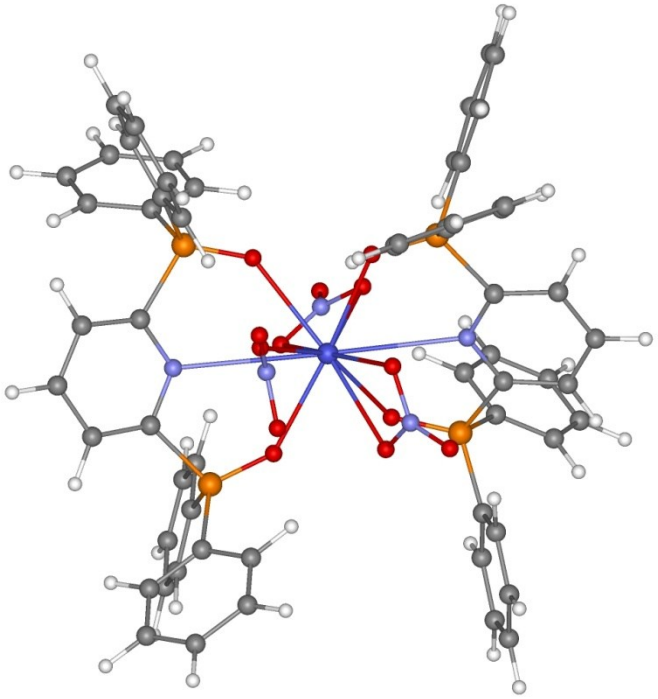
Relaxed geometry of (Ph2PyPO)2Am(NO3)3 complex



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8	-1.19960482	-4.29042224	1.33078298
7	-2.18852663	-2.74798814	-0.89436932
6	0.58736604	-4.40354922	4.59199513
7	2.73873909	-0.85306729	2.34196964
8	-2.73714845	-4.86681527	2.80210436
6	0.55050934	-5.54187276	5.40453862
1	0.29351932	-5.46068036	6.46272787
8	-3.16760646	-2.56637498	-0.16284690
6	0.85677618	-6.77590579	4.83465679
1	0.84214311	-7.68561259	5.43927239
8	-1.03425259	-2.15794491	-0.59017985
6	1.19364822	-6.83109222	3.48229620
1	1.46607791	-7.77983111	3.01702724
8	-2.20649692	-3.44095211	-1.92961989
15	0.38526579	-2.65986634	5.22256098
15	1.60129381	-5.52851239	0.92338540
8	2.64880946	-2.13249618	2.24607397
8	1.70924536	-0.19008985	1.94401984
8	3.73907284	-0.29741512	2.79415590
6	3.36233514	-6.02034843	0.86044694
6	0.59793016	-6.73493108	-0.00509864
6	-1.13079611	-2.62937355	6.24483443
6	1.78870126	-2.47877725	6.39348510
6	-1.21783483	-1.70295336	7.29818629
6	-2.24227170	-3.42633968	5.92568717
6	1.77444984	-3.01695501	7.69068897
6	2.93629477	-1.82051047	5.92584836
6	-2.39287265	-1.59445314	8.04133481
1	-0.36344754	-1.06363871	7.53547272
1	-2.45308574	-0.87134806	8.85847318
6	-3.48837856	-2.40659339	7.73726658

6	-3.41166481	-3.31529569	6.67974533		8	-1.24680457	-0.25459954	2.09627103
1	-2.22526488	-4.10706735	5.07033270		8	1.76174978	-1.54906245	-0.57224054
1	-4.27288586	-3.93746804	6.42439880		6	0.26661162	0.53454630	-1.64727349
1	-4.40874679	-2.32313866	8.32125551		7	-0.19557444	0.60538630	-0.39656516
6	2.89701803	-2.89696483	8.51043879		6	-1.30095273	1.31284667	-0.15194900
1	0.87797138	-3.51333830	8.07168217		6	-1.97926937	2.02091089	-1.14980982
1	2.87776727	-3.31197072	9.52140719		1	-2.89045998	2.57828581	-0.92634767
6	4.03844166	-2.24002193	8.04205163		6	-1.48418073	1.95802480	-2.45357364
1	4.91605856	-2.14463205	8.68677741		1	-1.99914201	2.48017888	-3.26352924
6	4.05466739	-1.70256325	6.75350587		6	-0.35014951	1.18804288	-2.71912817
1	4.94259171	-1.18507269	6.38173421		1	0.02621215	1.07061013	-3.73808602
1	2.95888726	-1.40032406	4.91679087		15	-1.83671428	1.06058031	1.61718771
6	-0.29423900	-6.19636397	-0.94461469		15	1.73021723	-0.60593887	-1.75966005
6	3.84835720	-7.11413158	0.13186208		6	1.57757564	-1.41432011	-3.38994872
6	4.25822885	-5.17372589	1.53916683		6	3.20893155	0.47409923	-1.79962116
6	-1.12500915	-7.04613870	-1.67583659		6	-1.22085636	2.49632514	2.56600045
1	-0.35498561	-5.11498573	-1.09268290		6	-3.65902062	1.04861692	1.61847301
1	-1.82882165	-6.61069555	-2.38900365		6	-2.05289690	3.38934544	3.25636866
6	-1.07003111	-8.42660429	-1.47834044		6	0.17698410	2.63494791	2.64427500
1	-1.72623665	-9.08839749	-2.04961099		6	-4.45710187	2.16138813	1.30017062
6	-0.18116685	-8.96614786	-0.54397952		6	-4.25756955	-0.18872566	1.90033014
1	-0.13716041	-10.04668138	-0.38643072		6	-1.49275165	4.43681471	3.99069370
6	0.65125038	-8.12478347	0.19429423		1	-3.13678744	3.25870865	3.23969338
1	1.34268221	-8.56197208	0.91908796		1	-2.14471548	5.12888305	4.52976073
6	5.62439513	-5.44853378	1.50945230		6	-0.10612458	4.59058174	4.04600734
1	3.88758895	-4.28003738	2.05522123		6	0.72468200	3.68428952	3.38117041
6	5.21955933	-7.38055261	0.10871183		1	0.83469682	1.89545558	2.17279405
1	3.16171416	-7.74640561	-0.43518803		1	1.81133574	3.78324454	3.44480723
1	5.59591931	-8.23218280	-0.46363236		1	0.32957280	5.41082339	4.62268481
6	6.10574765	-6.55500325	0.80283900		6	-5.84621387	2.03467402	1.27245142
1	7.17819731	-6.76568152	0.78206899		1	-4.00153194	3.13108339	1.08039441
1	6.31818864	-4.78703244	2.03452505		1	-6.46594814	2.90115471	1.02810241

6	-6.44131764	0.80162011	1.55587561
1	-7.52979600	0.70447001	1.52883449
6	-5.64845613	-0.30413180	1.86709608
1	-6.10882171	-1.27264819	2.07685174
1	-3.62722527	-1.05308639	2.13043990
6	4.25479130	0.14310457	-0.92730261
6	2.52071881	-1.24652256	-4.41448054
6	0.47684796	-2.27097879	-3.57390164
6	5.40222734	0.93686886	-0.88478327
1	4.15244341	-0.73312980	-0.28164407
1	6.21093187	0.67837517	-0.19688940
6	5.50880254	2.06019916	-1.70711355
1	6.40662799	2.68253379	-1.66958813
6	4.46374441	2.39708008	-2.57249117
1	4.54228665	3.28149193	-3.20979178
6	3.31322534	1.60907588	-2.61808289
1	2.49473672	1.88769728	-3.28760179
6	0.32280058	-2.93519562	-4.79057182
1	-0.25049062	-2.43391719	-2.76672313
6	2.35509235	-1.91898563	-5.62739385
1	3.38670066	-0.59747614	-4.26349784
1	3.09191622	-1.78904311	-6.42423696
6	1.25555626	-2.75927461	-5.81694282
1	1.12890922	-3.28472973	-6.76739524
1	-0.53510535	-3.59830889	-4.92801231

Relaxed geometry of (Ph2PyPO)2Cm(NO3)3 complex

96	0.22221398	-2.14771128	1.46655059	6	1.73263645	-3.01190186	7.65320587
8	0.48079902	-1.68285334	4.01394176	6	2.91861677	-1.82539773	5.89741468
8	1.30949962	-4.11377192	0.40207618	6	-2.40041709	-1.50139034	7.97240210
6	1.14441586	-5.64033747	2.70229030	1	-0.35851285	-1.01830387	7.46979666
8	-1.81697977	-2.84736276	2.79871750	1	-2.44792867	-0.77043003	8.78332615
7	-2.01172853	-4.04795599	2.34982991	6	-3.51165414	-2.29301572	7.67110443
7	0.84418720	-4.44852924	3.24319744	6	-3.45072722	-3.21161962	6.62126350
8	-1.28298068	-4.39456797	1.36287379	1	-2.28104067	-4.04040432	5.01965809
7	-2.18230200	-2.82250285	-0.85513645	1	-4.32390642	-3.81741548	6.36725378
6	0.55408406	-4.39313126	4.55261183	1	-4.43190861	-2.18543458	8.25136948
7	2.79446220	-0.89734316	2.32346416	6	2.84947276	-2.90126729	8.48183537
8	-2.82415247	-4.80549002	2.88203812	1	0.82925969	-3.50170612	8.02634144
6	0.51162356	-5.52950335	5.36675787	1	2.81873775	-3.31640601	9.49243164
1	0.24988173	-5.44593000	6.42350006	6	3.99981570	-2.25329518	8.02272320
8	-3.24152350	-2.67875433	-0.24047072	1	4.87289858	-2.16504931	8.67456818
6	0.81810510	-6.76441383	4.79949236	6	4.03097200	-1.71612251	6.73446131
1	0.79789150	-7.67374754	5.40446234	1	4.92592478	-1.20604300	6.36948967
8	-1.11911535	-2.11178493	-0.48344636	1	2.95464611	-1.40584612	4.88863420
6	1.16119552	-6.82111740	3.44915199	6	-0.35849157	-6.31533146	-0.91672951
1	1.42847109	-7.77148867	2.98478723	6	3.85449457	-7.03140545	0.05770277
8	-2.04038715	-3.57871532	-1.83727598	6	4.21488237	-5.10683823	1.49940538
15	0.36477774	-2.64904809	5.17807913	6	-1.16126764	-7.21968412	-1.61385274
15	1.56327367	-5.53105307	0.88362157	1	-0.49343124	-5.24101543	-1.07336879
8	2.65917563	-2.17555904	2.19548368	1	-1.91149616	-6.83268309	-2.30740952
8	1.78743398	-0.18859468	1.96416616	6	-1.01986313	-8.59298992	-1.41051495
8	3.82578230	-0.39753449	2.77433443	1	-1.65467763	-9.29628181	-1.95586717
6	3.33976102	-5.96814108	0.81206650	6	-0.06977669	-9.07243252	-0.50405526
6	0.59534240	-6.79434633	-0.00617768	1	0.04409375	-10.14728642	-0.34259355
6	-1.15574312	-2.57771516	6.18860102	6	0.73699421	-8.17767525	0.19886883
6	1.76217675	-2.47396946	6.35605240	1	1.48089671	-8.56786728	0.89826083
6	-1.22555137	-1.64097822	7.23442888	6	5.58878756	-5.33887148	1.45354176
6	-2.28209901	-3.35388660	5.87107801	1	3.82486367	-4.23067379	2.03132057

6	5.23288584	-7.25470352	0.01865391
1	3.18341208	-7.67568874	-0.51421046
1	5.63029242	-8.08323479	-0.57305115
6	6.09879971	-6.41581631	0.72231197
1	7.17707396	-6.59270477	0.68943882
1	6.26553965	-4.66538525	1.98563480
8	-1.19118726	-0.22332531	2.13762832
8	1.73589969	-1.55861151	-0.56035286
6	0.28488889	0.55743641	-1.61842835
7	-0.18197371	0.61148757	-0.36897659
6	-1.26975393	1.34060109	-0.11233368
6	-1.92570329	2.08714223	-1.09708261
1	-2.82142973	2.66556573	-0.86449397
6	-1.42967021	2.03654361	-2.40091133
1	-1.92944324	2.58715940	-3.20150542
6	-0.31326607	1.24539638	-2.67909217
1	0.06366804	1.13960326	-3.69919825
15	-1.80723417	1.07713830	1.65533578
15	1.72788763	-0.60745251	-1.74093533
6	1.55874026	-1.40849364	-3.37200141
6	3.22704291	0.44316372	-1.77214181
6	-1.20597577	2.52006698	2.60199404
6	-3.62804651	1.02706313	1.65063286
6	-2.04228592	3.43115830	3.26210856
6	0.19178806	2.64451671	2.70577097
6	-4.45185423	2.12049961	1.33091271
6	-4.19632483	-0.22673552	1.92451227
6	-1.48538649	4.48279095	3.99317694
1	-3.12695789	3.31095409	3.22616076
1	-2.14012027	5.18940544	4.50952864
6	-0.09848647	4.62224102	4.07444143
6	0.73596936	3.69818568	3.43907404
1	0.84909517	1.89177823	2.25441909
1	1.82211721	3.78724885	3.52279735
1	0.33439833	5.44586372	4.64840651
6	-5.83710718	1.95919883	1.29620349
1	-4.02026463	3.10155177	1.11351061
1	-6.47722721	2.81052256	1.05117071
6	-6.40238333	0.71040386	1.57198131
1	-7.48790646	0.58604604	1.53848195
6	-5.58374977	-0.37646094	1.88267100
1	-6.02003527	-1.35765088	2.08480406
1	-3.54728484	-1.07752323	2.15695953
6	4.27556181	0.06758915	-0.92106271
6	2.46175170	-1.19773352	-4.42430973
6	0.48036644	-2.29769635	-3.53013945
6	5.43991756	0.83570766	-0.87210459
1	4.16219521	-0.82185864	-0.29562405
1	6.24999332	0.54321212	-0.19970475
6	5.56128645	1.97720397	-1.66695821
1	6.47249222	2.57939148	-1.62409377
6	4.51383924	2.35845041	-2.51058412
1	4.60364246	3.25754905	-3.12543511
6	3.34584236	1.59684873	-2.56193709
1	2.52493834	1.91191149	-3.21200871
6	0.30806991	-2.95245910	-4.74961519
1	-0.21776915	-2.49664521	-2.70533919
6	2.27751660	-1.86054265	-5.63983870
1	3.31255198	-0.52482295	-4.29244900
1	2.98335600	-1.69791973	-6.45842838
6	1.19985294	-2.73394585	-5.80374002
1	1.05885363	-3.25235868	-6.75602865
1	-0.53163838	-3.64216852	-4.86675787

Relaxed geometry of (Ph2PyPO)2Eu(NO3)3 complex

63	0.23829606	-2.17041041	1.47183658
8	0.48343693	-1.68069793	4.06484926
8	1.38725262	-4.10696263	0.44480791
6	1.19161848	-5.64940084	2.73797540
8	-1.79078921	-2.89411406	2.88547058
7	-1.96692324	-4.05417959	2.36432927
7	0.86748304	-4.46368179	3.27643751
8	-1.23977472	-4.31988112	1.34265379
7	-2.18408744	-2.72040156	-0.90117805
6	0.61109334	-4.40426353	4.59201364
7	2.77072681	-0.89524703	2.34227219
8	-2.75555356	-4.87181758	2.84047791
6	0.62964114	-5.53435201	5.41665524
1	0.39838326	-5.44953380	6.48043680
8	-3.14949071	-2.51201441	-0.15624146
6	0.96532222	-6.76345888	4.85289112
1	0.99921969	-7.66560879	5.46799910
8	-1.01052286	-2.21348203	-0.59659820
6	1.27444207	-6.82172941	3.49430831
1	1.57786430	-7.76390084	3.03472933
8	-2.25743158	-3.37855496	-1.95866711
15	0.38626010	-2.66055392	5.21569956
15	1.58197011	-5.53614937	0.91352090
8	2.65351933	-2.17257100	2.25885707
8	1.75749990	-0.21011152	1.95911485
8	3.79503079	-0.36245248	2.77481587
6	3.33783946	-6.04577292	0.81981569
6	0.55162765	-6.73975780	0.00786886
6	-1.13829425	-2.63348119	6.22627663
6	1.77495627	-2.47147906	6.40467704
6	-1.24622806	-1.67902524	7.25236149
6	-2.23168100	-3.46277750	5.92986641
6	1.73751484	-2.98367675	7.71173977
6	2.93541804	-1.83354725	5.94062883
6	-2.42415542	-1.57387522	7.99129684
1	-0.40575614	-1.01526985	7.47183832
1	-2.50076778	-0.82876151	8.78700771
6	-3.50150490	-2.41813712	7.71060974
6	-3.40400144	-3.35530062	6.68010269
1	-2.20020263	-4.16570691	5.09326975
1	-4.25139308	-4.00286705	6.44226708
1	-4.42407333	-2.33770080	8.29157724
6	2.85001854	-2.85847896	8.54461364
1	0.83088810	-3.46425900	8.08903082
1	2.81271045	-3.25327019	9.56315488
6	4.00406581	-2.22169981	8.07962053
1	4.87355050	-2.12187354	8.73463080
6	4.04343245	-1.70986090	6.78108707
1	4.94151188	-1.20829979	6.41188087
1	2.97504512	-1.43391608	4.92385286
6	-0.31400739	-6.19472796	-0.95217233
6	3.79494229	-7.18162200	0.13887151
6	4.25750590	-5.17417392	1.43158842
6	-1.16054492	-7.03343731	-1.67770206
1	-0.33740619	-5.11428525	-1.11593146
1	-1.84305317	-6.59338091	-2.40853592
6	-1.14838207	-8.41079088	-1.45265817
1	-1.81682578	-9.06444127	-2.01905884
6	-0.28792978	-8.95685413	-0.49594583
1	-0.27924633	-10.03461909	-0.31528891
6	0.56029289	-8.12565385	0.23609255
1	1.22603251	-8.56863631	0.98090340

6	5.62017710	-5.46349805	1.38083098	6	-0.08499451	4.59014446	3.98589468
1	3.90562367	-4.25437162	1.91467807	6	0.73923986	3.65311314	3.35663978
6	5.16290654	-7.46213285	0.09406052	1	0.83631068	1.83597945	2.19054348
1	3.08756568	-7.83818049	-0.37257694	1	1.82648993	3.73412048	3.43485604
1	5.51705990	-8.34675878	-0.44124113	1	0.35649720	5.41616133	4.54983046
6	6.07372278	-6.60924798	0.71991657	6	-5.85852231	1.99646498	1.29468138
1	7.14354428	-6.83082049	0.68220628	1	-4.02001984	3.08551939	1.02137430
1	6.33304841	-4.78329571	1.85399039	1	-6.48434113	2.85212130	1.02867370
8	-1.24479868	-0.27429242	2.08162361	6	-6.44614930	0.77583448	1.64025122
8	1.78174586	-1.53934716	-0.57059184	1	-7.53484501	0.67741036	1.64021582
6	0.26955775	0.52959727	-1.65537394	6	-5.64549014	-0.31595106	1.97980833
7	-0.20136756	0.59712005	-0.40834803	1	-6.10059646	-1.27471849	2.24000619
6	-1.31796122	1.28863984	-0.16960430	1	-3.61637446	-1.05091316	2.23198883
6	-2.00236970	1.98265555	-1.17338584	6	4.25068811	0.21062048	-0.88747213
1	-2.92311074	2.52698988	-0.95726352	6	2.58628421	-1.21804430	-4.39739429
6	-1.49934871	1.92313420	-2.47433285	6	0.53299205	-2.25144257	-3.59602885
1	-2.01837798	2.43468704	-3.28852016	6	5.38168850	1.02689331	-0.83185465
6	-0.35116825	1.17159976	-2.73222187	1	4.15632896	-0.66420729	-0.23906186
1	0.03283730	1.05932301	-3.74886885	1	6.18448999	0.78762760	-0.13024050
15	-1.84004975	1.03694999	1.60545585	6	5.47884346	2.14772963	-1.65868133
15	1.75228371	-0.59062341	-1.75092688	1	6.36374498	2.78767261	-1.61124229
6	1.62752188	-1.39234073	-3.38889924	6	4.44076527	2.45932479	-2.54187512
6	3.21189910	0.51644159	-1.77697876	1	4.51193192	3.34148296	-3.18316359
6	-1.21448345	2.48060547	2.53861115	6	3.30652144	1.64896003	-2.60009070
6	-3.66303911	1.02605014	1.63322442	1	2.49310075	1.90770459	-3.28365482
6	-2.04063495	3.40577506	3.19261733	6	0.39987855	-2.91097456	-4.81757095
6	0.18412925	2.59608318	2.63624573	1	-0.20548780	-2.41840378	-2.80130315
6	-4.46921010	2.12472578	1.28827773	6	2.44289734	-1.88590007	-5.61580768
6	-4.25445686	-0.19858238	1.97836737	1	3.44729794	-0.56658198	-4.22951330
6	-1.47316073	4.46044107	3.91090649	1	3.19246815	-1.75037138	-6.39971113
1	-3.12641326	3.29519121	3.16133842	6	1.34916674	-2.72813532	-5.82752894
1	-2.12083822	5.17728333	4.42208830	1	1.23949572	-3.24959970	-6.78222688

1 -0.45357474 -3.57575834 -4.97336826

Relaxed geometry of $(Ph_2PyPO)_2Eu(NO_3)_2^+$ complex

63	-3.20979612	-1.04140788	-0.48988715	1	-7.85892416	-2.96197476	3.35457313
8	-3.12589841	-0.18579036	1.85202803	1	-8.86058664	-1.08441227	4.65178522
8	-2.37736524	-3.21585379	-1.18427164	6	-1.86358772	0.10779524	6.88507085
6	-2.12313047	-4.19545419	1.37383821	1	-3.59637770	-0.95924443	6.16365881
7	-2.64915228	-2.99848274	1.67175965	1	-2.11436033	-0.05271921	7.93633022
6	-2.74270085	-2.64801192	2.96419307	6	-0.72033513	0.83300473	6.53903139
7	-0.62692253	0.22784586	0.13437015	1	-0.07354242	1.23593365	7.32227438
6	-2.32963630	-3.47878415	4.00934480	6	-0.40425957	1.04633359	5.19489172
1	-2.41838480	-3.15196121	5.04749577	1	0.48955124	1.61354449	4.92399870
6	-1.76456570	-4.71368452	3.69145684	1	-0.98148058	0.69609638	3.13788814
1	-1.40351976	-5.37784832	4.47983046	6	-4.13286111	-5.59114836	-1.89017374
6	-1.64395657	-5.07539741	2.35016682	6	-0.07908344	-6.39739283	-1.24780777
1	-1.16101611	-6.01294354	2.06604904	6	0.68693484	-4.19868414	-0.53015796
15	-3.35560125	-0.90663018	3.17646400	6	-5.08296942	-6.55243459	-2.23621489
15	-2.04819274	-4.51445252	-0.45642787	1	-4.07878829	-4.63933704	-2.42536889
8	-0.82619285	-1.03468352	0.27169962	1	-5.78417082	-6.35015796	-3.04916768
8	-1.60385160	0.89288399	-0.39341363	6	-5.14172870	-7.76163237	-1.54128000
8	0.41056175	0.77241658	0.48163425	1	-5.88802908	-8.51217070	-1.81251107
6	-0.35799888	-5.11196931	-0.76252211	6	-4.25011242	-8.01368421	-0.49480841
6	-3.23598678	-5.84216013	-0.84141699	1	-4.29807308	-8.95875913	0.05112530
6	-5.08702968	-1.01052039	3.72277913	6	-3.29884101	-7.05715889	-0.14057709
6	-2.37537855	-0.19561871	4.53663582	1	-2.61317171	-7.26601917	0.68404150
6	-5.65847494	0.06169675	4.42937193	6	2.00362317	-4.58688258	-0.76981843
6	-5.88655546	-2.09473843	3.32755367	1	0.46533482	-3.18342170	-0.18161016
6	-2.69373163	-0.40720342	5.88825294	6	1.24477783	-6.77494623	-1.48269998
6	-1.22635716	0.53336413	4.19113705	1	-0.89202393	-7.09820603	-1.45141941
6	-7.01196589	0.02986851	4.76215891	1	1.46346146	-7.77558227	-1.86288830
1	-5.04667282	0.92096228	4.71630616	6	2.28328053	-5.87373012	-1.24072783
1	-7.45261771	0.86009232	5.31913464	1	3.31786890	-6.17270980	-1.42666559
6	-7.80105408	-1.06042722	4.38524795	1	2.81654735	-3.87866407	-0.59193349
6	-7.24016013	-2.11644674	3.66377796	8	-5.27348481	0.26042228	0.07159645
1	-5.46372972	-2.91245033	2.73921326	8	-2.22786968	-0.87962222	-2.71038087

6	-3.04998838	1.70905108	-3.12130490
7	-3.83367030	1.39817972	-2.07821060
6	-4.61952689	2.35348342	-1.56273470
6	-4.64258625	3.66241866	-2.05439215
1	-5.28346501	4.41993221	-1.59882904
6	-3.81945387	3.98126249	-3.13397236
1	-3.80655080	4.99489530	-3.54066340
6	-3.01077807	2.98690562	-3.68548290
1	-2.35327145	3.20379156	-4.53007744
15	-5.66514672	1.71279455	-0.16351312
15	-2.09421003	0.23946627	-3.73942510
6	-2.87413323	-0.19636065	-5.32670727
6	-0.39495418	0.80581087	-4.05265094
6	-5.35663123	2.83248490	1.24093092
6	-7.39879643	1.89223891	-0.69242983
6	-6.39128964	3.26348626	2.08528642
6	-4.02259511	3.15829550	1.54289937
6	-8.03255286	3.14019428	-0.81644938
6	-8.08399574	0.71889537	-1.04234755
6	-6.09515414	4.04152877	3.20596845
1	-7.42672653	2.99026172	1.86872300
1	-6.90333223	4.38550469	3.85602678
6	-4.77078867	4.37961216	3.49386630
6	-3.73629863	3.93229446	2.66642993
1	-3.20530052	2.78997784	0.91387437
1	-2.69887044	4.18606736	2.89786119
1	-4.54238317	4.99314715	4.36904313
6	-9.34403937	3.20865016	-1.28554932
1	-7.51290624	4.06015951	-0.53570412
1	-9.83740882	4.17903633	-1.37811698
6	-10.02610637	2.03824278	-1.63118286
1	-11.05400291	2.09599080	-1.99751078
6	-9.39739128	0.79774871	-1.50811122
1	-9.92859035	-0.11808350	-1.77794815
1	-7.58622459	-0.24965565	-0.94969111
6	0.33923442	0.31837458	-5.14621615
6	-2.68865290	0.55457997	-6.49924296
6	-3.75134630	-1.29139462	-5.32166223
6	1.67484245	0.68892613	-5.30554587
1	-0.13065545	-0.35166824	-5.87004415
1	2.24309739	0.31231174	-6.15924980
6	2.28381942	1.53337509	-4.37430468
1	3.33008060	1.82148522	-4.50289977
6	1.56179741	2.00211053	-3.27342769
1	2.04187193	2.64757017	-2.53427402
6	0.22593878	1.63988338	-3.10615811
1	-0.32658098	1.98034865	-2.22522761
6	-4.42851864	-1.63711813	-6.49197138
1	-3.90262240	-1.85573517	-4.39725913
6	-3.37053068	0.20037466	-7.66298982
1	-2.00471611	1.40736888	-6.51211894
1	-3.22160121	0.77967029	-8.57724442
6	-4.23848005	-0.89557201	-7.65979033
1	-4.77006610	-1.17049348	-8.57414414
1	-5.11181679	-2.48990312	-6.48845106
7	-5.67393182	-2.47483111	-1.12111619
8	-5.07499253	-1.74840167	-1.99874532
8	-6.77229665	-2.97198962	-1.32165228
8	-5.03890805	-2.64409008	-0.00965060

Relaxed geometry of $(Ph_2PyPO)_2Am(NO_3)_2^+$ complex

95	-0.04228072	-0.20723144	-0.26563643
8	-0.23666869	0.41348245	2.12354451
8	0.80795604	-2.38048095	-1.01457742
6	1.19611021	-3.45513625	1.48330691
7	0.60869509	-2.30906912	1.85295789
6	0.63403524	-1.97163192	3.14970080
7	-2.48566680	-1.58622968	-1.04057542
6	1.23805591	-2.76415201	4.13058547
1	1.25463501	-2.44263823	5.17432589
6	1.85230496	-3.95338865	3.73746195
1	2.35268256	-4.58829832	4.47202410
6	1.84223694	-4.30473799	2.38731533
1	2.35311045	-5.20488019	2.03738772
15	-0.18617569	-0.33388824	3.45365632
15	1.12427488	-3.71913218	-0.35183276
8	-3.56336906	-2.08150244	-1.31661772
8	-1.83746884	-0.82479198	-1.86583682
8	-1.90294841	-1.77798070	0.10170601
6	2.76196797	-4.36551144	-0.80663218
6	-0.13437082	-4.99021359	-0.68575831
6	-1.83882704	-0.70189579	4.11534703
6	0.81653760	0.50370947	4.71802768
6	-2.93633471	-0.36377242	3.30925768
6	-2.03414285	-1.36017491	5.34117399
6	0.25125551	1.08423086	5.86308864
6	2.19177783	0.65163441	4.45945744
6	-4.22620961	-0.67645918	3.74265423
1	-2.77197176	0.13177659	2.34666417
1	-5.08229059	-0.42058358	3.11338918
6	-4.42269411	-1.32169679	4.96479468
6	-3.32728382	-1.66425724	5.76375778
1	-1.18312484	-1.63490809	5.97040022
1	-3.48165011	-2.17277693	6.71828049
1	-5.43457573	-1.56595212	5.29742778
6	1.06252264	1.78618266	6.75667386
1	-0.82051574	0.99228131	6.05346139
1	0.62229364	2.23379266	7.65085708
6	2.42988074	1.91918266	6.50631921
1	3.06159519	2.46880388	7.20855470
6	2.99224443	1.35731890	5.35588800
1	4.05943047	1.47261938	5.15228940
1	2.63296457	0.23134433	3.54965599
6	-1.01823568	-4.74627861	-1.74701595
6	2.96170409	-5.66783391	-1.28541779
6	3.84820278	-3.47984048	-0.68585327
6	-2.01317487	-5.67677310	-2.04731865
1	-0.92520538	-3.82299371	-2.32518520
1	-2.70709850	-5.47925504	-2.86754070
6	-2.12809883	-6.84727550	-1.29503545
1	-2.91065265	-7.57262395	-1.53011000
6	-1.25053840	-7.09004945	-0.23476858
1	-1.34643840	-8.00205667	0.35895591
6	-0.25539637	-6.16333295	0.07540860
1	0.41464162	-6.35652965	0.91696133
6	5.12762337	-3.90947918	-1.03246391
1	3.68496067	-2.45514497	-0.33434861
6	4.24872559	-6.08774951	-1.62885118
1	2.11447558	-6.34844154	-1.39881904
1	4.40572752	-7.10146316	-2.00485268
6	5.32868514	-5.21230314	-1.49996455
1	6.33393291	-5.54439499	-1.77102444
1	5.97256681	-3.22267029	-0.94085435
8	-2.11715496	1.18571112	0.21786275
8	1.06753525	-0.00327608	-2.44013677

6	0.28644634	2.59182918	-2.88125535
7	-0.54386622	2.29099120	-1.87133738
6	-1.33132399	3.26087723	-1.38624889
6	-1.31697413	4.56915633	-1.87969485
1	-1.96596720	5.33513701	-1.45027413
6	-0.44889497	4.87520890	-2.92700896
1	-0.40634442	5.88762586	-3.33455228
6	0.36766094	3.86856916	-3.44317063
1	1.06288751	4.07465893	-4.25984332
15	-2.43693389	2.65892107	-0.01860971
15	1.25721335	1.11781448	-3.46039374
6	0.55609829	0.69019201	-5.08451065
6	2.97545340	1.67070524	-3.67211222
6	-2.10758596	3.74525675	1.40363796
6	-4.14488564	2.91335693	-0.59545356
6	-3.13444756	4.20239872	2.24449258
6	-0.76416787	4.00440596	1.72943077
6	-4.74746583	4.18074798	-0.66763245
6	-4.83859986	1.77921548	-1.04604468
6	-2.81927248	4.94260770	3.38496819
1	-4.17819479	3.97920671	2.01097767
1	-3.61984875	5.30404605	4.03463686
6	-1.48534600	5.21687519	3.69527480
6	-0.46001842	4.74184342	2.87245920
1	0.04352560	3.60745921	1.10549265
1	0.58453489	4.94086988	3.12398802
1	-1.24253832	5.79954438	4.58737425
6	-6.03792333	4.30675208	-1.18150947
1	-4.21985908	5.06981196	-0.31229736
1	-6.50767571	5.29183844	-1.23236239
6	-6.72916735	3.17550740	-1.62481307
1	-7.74054340	3.27850136	-2.02553228
6	-6.13030856	1.91589539	-1.55643266
1	-6.66817102	1.03084712	-1.90462715
1	-4.36278703	0.79593069	-0.99900291
6	3.76565072	1.20237426	-4.73435374
6	0.81130418	1.43682853	-6.24681362
6	-0.33719352	-0.39150857	-5.12216655
6	5.11180564	1.56203403	-4.80782702
1	3.33149025	0.55509288	-5.49996873
1	5.72411634	1.20111551	-5.63752545
6	5.67490749	2.37549790	-3.82170707
1	6.72953659	2.65511215	-3.88328512
6	4.89611886	2.82400472	-2.75132391
1	5.33960378	3.44464272	-1.96929371
6	3.54932074	2.47328946	-2.66990284
1	2.95086480	2.79860014	-1.81319122
6	-0.96004259	-0.72842450	-6.32473576
1	-0.54579467	-0.95145446	-4.20606999
6	0.18379591	1.09048666	-7.44304198
1	1.50601469	2.28066165	-6.22587201
1	0.38706005	1.66608916	-8.34912124
6	-0.69986180	0.00787562	-7.48233515
1	-1.18916941	-0.26032894	-8.42191889
1	-1.65653013	-1.56993804	-6.35433550
7	2.49138743	1.08877324	0.55787541
8	2.28344817	-0.17854746	0.69676651
8	1.53453183	1.74456233	-0.02764078
8	3.50829735	1.63551205	0.94754538

Relaxed geometry of $(Ph_2PyPO)_2Cm(NO_3)_2^+$ complex

96	-0.10776590	-0.21532680	-0.25226219	1	-3.41195742	-2.08700076	6.82678163
8	-0.24954544	0.39727650	2.11912637	1	-5.39148795	-1.50071759	5.43436964
8	0.62580321	-2.39934462	-1.02162076	6	1.17464104	1.80078438	6.69654879
6	1.13478287	-3.47199227	1.44824847	1	-0.73649543	1.03671070	6.03797189
7	0.57207014	-2.31784655	1.83091546	1	0.75904951	2.27339924	7.58963522
6	0.61269491	-1.99120040	3.13049958	6	2.54018217	1.89951452	6.42161609
7	-2.58800624	-1.56095447	-0.96979034	1	3.19518564	2.44742908	7.10354431
6	1.20950874	-2.80155187	4.10056872	6	3.07103618	1.30582100	5.27230588
1	1.23791627	-2.48954652	5.14688494	1	4.13661557	1.39489325	5.04851852
6	1.80129632	-3.99749118	3.69339350	1	2.65941348	0.15751446	3.49317590
1	2.29648516	-4.64646196	4.41908100	6	-1.18952764	-4.76210954	-1.64443470
6	1.77394902	-4.33831064	2.34123571	6	2.92123945	-5.55145993	-1.45238745
1	2.26638898	-5.24491233	1.98231056	6	3.73787769	-3.37312512	-0.72724852
15	-0.17790053	-0.34334000	3.45201659	6	-2.16995317	-5.71676080	-1.91680546
15	1.02903769	-3.72754958	-0.38715622	1	-1.19697919	-3.79450719	-2.15308186
8	-3.68398858	-2.02072640	-1.24429175	1	-2.95393977	-5.49120171	-2.64331274
8	-1.86678480	-0.92601198	-1.84442434	6	-2.15453648	-6.94602574	-1.25554771
8	-2.06563933	-1.66738467	0.20965159	1	-2.92562484	-7.69034140	-1.46832094
6	2.68282141	-4.29006507	-0.88908496	6	-1.15903283	-7.22561266	-0.31485842
6	-0.18822037	-5.04229957	-0.70299839	1	-1.15095611	-8.18547613	0.20673388
6	-1.81763798	-0.68411758	4.15710054	6	-0.17701112	-6.27645219	-0.03330024
6	0.86731474	0.48841485	4.68531387	1	0.58899509	-6.50321523	0.71250665
6	-2.93026875	-0.35755810	3.36718835	6	5.02625759	-3.73419669	-1.11644824
6	-1.98997246	-1.31366036	5.40145708	1	3.54460020	-2.37629823	-0.31423034
6	0.33374028	1.10139386	5.82880684	6	4.21723210	-5.90210759	-1.83694111
6	2.24080914	0.60199185	4.40189460	1	2.09738897	-6.25389759	-1.59898856
6	-4.21213127	-0.65291160	3.83484147	1	4.40471349	-6.88403794	-2.27770895
1	-2.78461540	0.11361645	2.39001535	6	5.26698361	-4.99755769	-1.66624747
1	-5.07978625	-0.40657468	3.21787603	1	6.27948513	-5.27555065	-1.96937453
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6	-3.27533116	-1.60086411	5.85801300	8	-2.12253759	1.20513370	0.19736046
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6	0.31263123	2.59133846	-2.86241469
7	-0.53978202	2.29849564	-1.86924529
6	-1.32274583	3.27664883	-1.39448986
6	-1.28218426	4.58634404	-1.88254829
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6	0.41875468	3.86776307	-3.42064450
1	1.13170391	4.06778197	-4.22338802
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6	3.01158339	1.65245399	-3.57760170
6	-2.14410469	3.76238281	1.38366191
6	-4.15030982	2.91556074	-0.64315888
6	-3.18838683	4.27015651	2.17210078
6	-0.80628163	3.97838619	1.76175927
6	-4.74085710	4.18388905	-0.77601669
6	-4.85266327	1.76814955	-1.04343920
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1	-4.22861596	4.07977992	1.89791512
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6	-1.56646668	5.24990893	3.67603106
6	-0.52533944	4.72416679	2.90533686
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1	0.51427934	4.88979337	3.19825406
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6	-6.02793602	4.29794363	-1.30053006
1	-4.20688694	5.08405893	-0.46039656
1	-6.48806810	5.28393087	-1.39907448
6	-6.72800622	3.15365309	-1.69402957
1	-7.73677167	3.24732907	-2.10350724
6	-6.14125148	1.89331704	-1.56498918
1	-6.68545801	0.99777612	-1.87418806
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6	0.88534185	1.39917294	-6.19957883
6	-0.24378793	-0.44733038	-5.08364986
6	5.17161066	1.54960968	-4.66710552
1	3.40399750	0.55478509	-5.40859842
1	5.80109491	1.19608525	-5.48706606
6	5.71502919	2.35028685	-3.65973603
1	6.77163294	2.62699499	-3.69480611
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6	3.56476821	2.44366422	-2.55477074
1	2.94844760	2.76587426	-1.70939544
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1	-0.45608799	-1.00770339	-4.16868484
6	0.28737641	1.03209083	-7.40456383
1	1.56092162	2.25826024	-6.17151870
1	0.49423334	1.60660978	-8.31050714
6	-0.57176622	-0.06987996	-7.45261073
1	-1.03813823	-0.35419157	-8.39910023
1	-1.51371708	-1.66193976	-6.33207913
7	2.45355263	1.04942132	0.55945583
8	2.26611172	-0.23088544	0.57465700
8	1.46626032	1.75287176	0.09976930
8	3.48966981	1.56219993	0.95122469