Supplementary Materials: Comparative Study of Complexes of Rare Earths and Actinides with 2,6-Bis(1,2,4-triazin-3-yl)pyridine

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Content:

Table S1. Crystallographic details of the measured $[M(BTP)_3](CF_3SO_3)_3$ complexes

Identification code	$[Y(BTP)_3](CF_3SO_3)_3$ *EtOH	$[Pu(BTP)_3](CF_3SO_3)_3$ *EtOH	$[ScBTP)_3](CF_3SO_3)_3$
Empirical formula	$C_{74}H_{96}F_9N_{21}O_{10}S_3Y$	$C_{74}H_{96}F_9N_{21}O_{10}S_3Pu$	$C_{36}H_{46.5}F_{4.5}N_{10.5}O_{4.5}S_{1.5}Sc_{0.5}$
Formula weight	1795.79	1948.89	854.40
Temperature	100(2) K	173(2) K	173(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	C2/c
Unit cell dimensions	a = 13.136(7) Å, α= 91.675(8)°.	a = 13.238(3) Å, α= 91.813(4)°.	a = 29.545(9) Å, α= 90°.
	b = 13.313(7) Å, β= 101.968(8)°.	b = 13.314(3) Å, β= 101.908(3)°.	b = 17.305(5) Å, β= 109.663(5)°.
	c = 25.935(13) Å, γ = 110.575(7)°.	c = 26.027(6) Å, γ = 110.169(4)°.	c = 17.648(5) Å, γ = 90°.
Volume	4128(4) $Å^3$	4186.8(18) $Å^3$	8497(4) $Å^3$
Z	2	2	8
Density (calculated)	1.443 Mg/m^3	1.546 Mg/m^3	1.336 Mg/m^3
Absorption coefficient	0.872 mm^{-1}	0.951 mm^{-1}	0.245 mm^{-1}
F(000)	1866	1980	3576
Crystal size	0.08 x 0.05 x 0.05 mm^3	0.23 x 0.02 x 0.02 mm^3	0.15 x 0.2 x 0.3 mm^3
θ range for data collection	1.644 to 25.474°.	1.609 to 28.714°.	1.386 to 28.357°.
Index ranges	-15<=h<=15, -15<=k<=15, -31<=l<=31	-17<=h<=17, -17<=k<=17, -34<=l<=34	-38<=h<=39, -22<=k<=23, -23<=l<=23
Reflections collected	28454	25495	57337
Independent reflections	13515 [$R_{(int)}$ = 0.1194]	14921 [$R_{(int)}$ = 0.1954]	10437 [$R_{(int)}$ = 0.1107]
Completeness	90.3 % (θ = 25.0°)	81.4 % (θ = 25.0°)	100.0 % (θ = 25.0°)
Refinement method	Full-matrix least-squares on F^2		
Data/restraints/parameters	13515 / 6 / 1063	14921 / 684 / 1063	10437 / 64 / 554
Goodness-of-fit on F^2	1.091	1.012	1.234
Final R indices [I>2sigma(I)]	R1 = 0.1094, wR2 = 0.2892	R1 = 0.1557, wR2 = 0.3534	R1 = 0.1191, wR2 = 0.3351
R indices (all data)	R1 = 0.1898, wR2 = 0.3312	R1 = 0.2714, wR2 = 0.3889	R1 = 0.2170, wR2 = 0.3737
Extinction coefficient	n/a	n/a	n/a
Largest diff. peak and hole	1.293 and -1.331 e.$Å^{-3}$	2.649 and -3.250 e.	1.934 and -1.021 e.$Å^{-3}$

Table S2. Selected bond lengths [Å] for $[M(BTP)_3](CF_3SO_3)$.

Bond[a]	Length
Y(1)-N(8)	2.480(8)
Y(1)-N(1)	2.485(8)
Y(1)-N(9)	2.500(8)
Y(1)-N(12)	2.503(8)
Y(1)-N(15)	2.504(8)
Y(1)-N(16)	2.517(9)
Y(1)-N(5)	2.520(7)
Y(1)-N(19)	2.521(9)
Y(1)-N(2)	2.541(8)
Pu(1)-N(5)	2.44(2)
Pu(1)-N(12)	2.512(19)
Pu(1)-N(16)	2.523(19)
Pu(1)-N(9)	2.558(19)
Pu(1)-N(1)	2.562(19)
Pu(1)-N(15)	2.570(18)
Pu(1)-N(19)	2.573(16)
Pu(1)-N(8)	2.590(16)
Pu(1)-N(2)	2.613(15)
Sc(1)-N(8)	2.371(4)
Sc(1)-N(8)#1	2.371(4)
Sc(1)-N(4)	2.369(6)
Sc(1)-N(1)#1	2.403(4)
Sc(1)-N(1)	2.403(4)
Sc(1)-N(5)#1	2.421(4)
Sc(1)-N(5)	2.421(4)
Sc(1)-N(9)#1	2.420(4)
Sc(1)-N(9)	2.420(4)

[a]For the numbering of atoms see Figure S1. N(1), N(8) and N(15) correspond to the pyridine nitrogens.

Table S3. IR spectral data and proposed assignment for $M(BTP)_3(CF_3SO_3)$ (M=Pu, Am, Y, Sc) complexes

No.	Pu	Am	Y	Sc	Character
	3093 w		3098 sh	3100 sh	$\nu(CH_{Py})$
	3083 sh	3084 w	3083 w	3084 w	$\nu(CH_{Py})$
	3062 w	3065 sh	3035 w	3039 w	$\nu(CH_{Py})$
	2965 s	2966 s	2965 s	2966 s	$\nu_{as}(CH_3)$
	2933 s	2935 s	2935 s	2935 s	$\nu_{as}(CH_2)$
	2874 s	2875 s	2875 s	2874 s	$\nu_s(CH_2)$
	1603 m	1603 m	1606 m	1610 m	ν(Aza), ν(Py), ν(M-N)
	1580 w	1580 w	1583 w	1585 w	ν(Aza), ν(Py), ν(M-N)
	1550 s	1548 s	1548 s	1554 s	ν(Aza)
	1532 s	1533 s	1534 sh	1538 s	ν(Aza), ν(Py), ν(M-N)
			1475 sh	1486 s	$\delta_{as}(CH_3)$
	1465 s	1467 s	1466 s	1466 s	$\delta_{as}(CH_3)$
	1452 sh	1456 sh	1458 sh	1457 sh	$\delta_{as}(CH_3)$
	1387 s	1388 s	1390 s	1394 s	$\beta(CH_2)$, ν(Aza), ν(Py), ν(M-N)
	1354 w	1356 sh		1356 w	$\delta_s(CH_3)$
	1340 w	1340 w	1340 w	1341 w	$\delta_s(CH_3)$
	1310 w	1309 sh	1311 sh	1313 sh	$\gamma(CH_2)$
	1270 sbr	1272 sbr	1270 sbr	1270 sbr	ν(CS), $\nu_{as}(SO_3)$, $\nu_{as}(CF_3)$
	1223 s	1223 s	1223 m	1222 s	$\nu_{as}(CF_3)$
	1154 s	1153 sh	1165 sh	1165 sh	ν(Aza), $\beta(CH)_{Py}$
	1146 s	1148 s	1148 s	1145 s	ν(Aza), $\gamma(CH_2)$
	1088 m	1089 m	1190 m	1089 m	$\nu(C_{Aza}\text{-}CH_2)$
	1061 w	1065 w	1067 w	1063 w	$\beta(CH)_{Py}$
	1052 w	1051 sh			$\beta(CH)_{Py}$
	1031 s	1031 s	1031 s	1031 s	$\nu_s(SO_3)$
	1014 m	1015 m	1017 w	1018 m	β(Aza), $\nu(CC)_{propyl}$, ν(M-N)
	995 w	995 w	993 w	996 w	β(Aza), $\nu(CC)_{propyl}$
	905 m	903 w	902 w	903 w	β(Aza)
	880 w	879 w	876 w	883 w	β(Aza)
	840 m	841 m	843 w	842 w	$\gamma(CH)_{Py}$
	821 w	822 w	824 w	823 w	$\delta(CH_3)$, $\delta(CH_2)$, $\gamma(CH)_{Py}$
	811 sh			815 w	β(Aza), β(Py)
			800 sh	795 sh	$\delta(CH_2)$
	786 m	785 w	784 w	786 w	τ(Aza)
	750 s	751 s	751 m	753 m	$\delta(CH_3)$, $\delta(CH_2)$, $\gamma(CH)_{Py}$
			745 sh	748 m	β(Aza), $\delta(CH_2)$
	696 w	696 sh		699 w	β(Aza), β(Py)
	690 sh	688 w	690 w	690 sh	τ(Aza), τ(Py)
	651 m	651 m	652 m	653 m	β(Aza), ν(M-N)
	636 s	637 s	637 s	636 s	$\delta_s(SO_3,CF_3)$
	597 w	597 w	597 vw	599 w	τ(Aza), τ(Py)
	571 m	572 m	572 m	572 m	$\delta_{as}(SO_3,CF_3)$
	516 s	517 s	517 s	517 s	$\delta_{as}(SO_3,CF_3)$

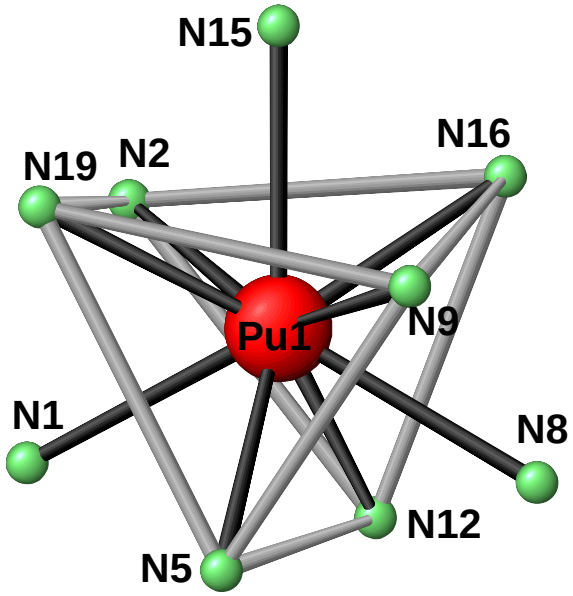
	463 w		470 w	477 w	τ(Aza), γ(N-M)
				444 m	τ(Aza), τ(Py)
	425 m	425 m		437 sh	τ(Aza), τ(Py), γ(N-M)
				426 sh	τ(Py)
				394 vw	τ(Aza)
				374 w	β(C_{Aza}-C_{CH2}-C_{CH3})
				336 w	β(Aza-Py)
	308 w	306 w		308 m	τ(Aza)
				272 m	τ(CH_3)
	213 w	210 w		208 w	τ(CH_3)
	148 m	148 m			β(Aza-C_{CH2})

[a]The meaning of vibrational symbols is the following: ν, stretch; β, bend; δ, deformation, γ, out-of-plane bend; tw, twist, τ, torsion. The notations mean: s, symmetric; as, asymmetric, Py, pyridine; Aza, triazine. The assignment is based on the DFT calculations on $La(BTP)_3(CF_3SO_3)_3$ reported in Ref. [Kovács, 2015 #922].

Table S4. Molecular data computed with the B3LYP xc functional

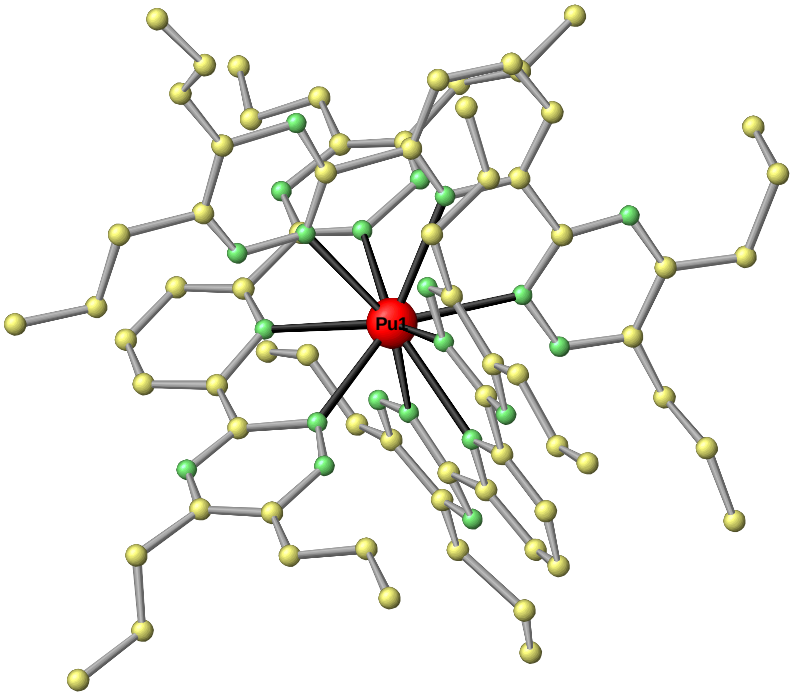
	Parameters	**Sc**	**La**	**Lu**	**U**	**Am**
Geometry	M-N_1	2.417	2.751	2.533	2.637(2)	2.636(11)
	M-N_2	2.460	2.705	2.546	2.619(4)	2.632(9)
	N_1-C	1.345	1.349	1.346	1.349(-)	1.348(1)
	N_2-N_3	1.333	1.337	1.336	1.337(-)	1.336(-)
	N_2-C	1.342	1.342	1.343	1.344(-)	1.343(1)
NBO	n(M)	+1.73	+2.16	+2.05	+1.61	+1.78
	n(N_1)	-0.52	-0.54	-0.55	-0.50	-0.51
	n(N_2)	-0.34	-0.38	-0.37	-0.33	-0.34
	s	0.24	0.16	0.22	0.23	0.25
	d	0.96	0.56	0.70	0.96	0.82
	f	0.01	0.01	0.01	2.99	6.08
	N_1(LP) → M	166	97	123	337	200
	N_2(LP) → M	185	106	137	370	232
	N_2-N_3 → M	28	24	33	39	22
	M → Py	-	-	-	5	2
	M → Aza	-	-	-	19	4
QTAIM	q(M)	+2.07	+2.26	+2.17	+2.30	+2.10
	q_{N1}	-1.33	-1.32	-1.33	-1.32	-1.31
	q_{N2}	-0.77	-0.78	-0.78	-0.78	-0.77
	$\rho(M,N_1)$	0.041	0.036	0.040	0.044	0.041
	$\rho(M,N_2)$	0.036	0.038	0.039	0.046	0.041
	$\nabla^2 \rho(M,N_1)$	0.123	0.095	0.131	0.135	0.131
	$\nabla^2 \rho(M,N_2)$	0.110	0.106	0.127	0.136	0.135
	Δ(M)	1.05	1.09	1.02	1.68	1.33
	DI(M,N_1)	0.22	0.21	0.21	0.30	0.26
	DI(M,N_2)	0.19	0.22	0.20	0.30	0.25

Fig S1. View to the coordination polyeder of $[Pu(BTP)_3](CF_3SO_3)$
(N1, N8 and N15 represent the pyridine nitrogens)



Note: The structure data of $Pu(BTP)_3(CF_3SO_3)$ do not allow the determination of the solid state structure at a high or satisfying level; however, the cell parameters can easily be determined as well as the connectivity. The coordination environment of the Pu atom in $Pu(BTP)_3(CF_3SO_3)$ is, however, identical to the one of its isostructural lanthanide homologues and can be described as tricapped prismatic.

Fig S2. View to the molecular solid state structure of the cation of $[Pu(BTP)_3]^{+3}$



Cartesian coordinates of the M062X computed $[M(BTP')_3]^{3+}$ structures

$[Sc(BTP')_3]^{3+}$

Sc	-0.00085	-0.00053	-0.00031
N	-0.22063	2.38052	0.00092
N	1.38001	1.08026	-1.66917
N	2.10533	0.37693	-2.52694
N	2.13519	3.12321	-2.60456
N	-1.55778	0.80649	1.66654
N	-2.13911	-0.01918	2.52492
N	-2.66765	2.67585	2.61134
N	-1.95302	-1.3844	-0.01318
N	0.06318	-1.74559	1.67491
N	1.06051	-1.83129	2.54361
N	-1.00811	-3.63852	2.61714
N	-1.61532	0.64909	-1.68126
N	-1.35883	1.62566	-2.53980
N	-3.74833	0.27275	-2.64391
N	2.17458	-0.99996	0.01085
N	0.25915	-1.72407	-1.67583
N	-0.7062	-1.98882	-2.54437
N	1.66317	-3.37819	-2.63011
N	1.46518	0.9301	1.68370
N	1.03042	1.83844	2.54526
N	3.62849	0.94994	2.65198
C	-1.07949	2.99403	0.82146
C	-1.25335	4.37617	0.85205
H	-1.97346	4.80796	1.53743
C	-0.47683	5.15786	0.00319
H	-0.57648	6.23822	0.00414
C	0.4297	4.53274	-0.84655
H	1.05922	5.09049	-1.53017
C	0.51154	3.1421	-0.81849
C	1.39948	2.41103	-1.74466
C	2.83392	1.02018	-3.42034
C	2.86494	2.42817	-3.45197
C	-1.81815	2.11137	1.74666
C	-2.96813	0.47881	3.42357
C	-3.25489	1.8576	3.45947
C	-2.97094	-1.13597	-0.84349
C	-4.13236	-1.90476	-0.88090
H	-4.92311	-1.64275	-1.57432
C	-4.22722	-2.99865	-0.02694
H	-5.1118	-3.62685	-0.03246
C	-3.17062	-3.2742	0.83461
H	-3.19057	-4.11043	1.52382
C	-2.06137	-2.43128	0.81128
C	-0.93669	-2.6241	1.74870
C	1.03591	-2.79449	3.44596
C	-0.01412	-3.73319	3.47545
C	-2.77456	-0.00303	-1.77014
C	-2.2688	1.9292	-3.44685
C	-3.50193	1.24957	-3.49178
C	3.12888	-0.5697	0.84250
C	4.41276	-1.10976	0.87790
C	4.70891	-2.1641	0.02015
C	3.72157	-2.62809	-0.84280
C	2.47521	-2.00579	-0.81695
C	1.40522	-2.40028	-1.75526
C	-0.5036	-2.92468	-3.45316
C	0.70295	-3.65088	-3.48885
C	2.72472	0.50299	1.77362

C	1.86609	2.30049	3.45684
C	3.2034	1.86023	3.50314
H	5.69474	-2.6173	0.02390
H	3.89633	-3.44347	-1.53512
H	5.14107	-0.70855	1.57314
H	1.86336	-2.82743	4.14622
H	-0.033	-4.54807	4.19477
H	-4.27148	1.50792	-4.21488
H	-2.02002	2.7266	-4.13851
H	0.87234	-4.44309	-4.21371
H	-1.31094	-3.10675	-4.15397
H	3.90984	2.25285	4.23015
H	1.47251	3.03475	4.15113
H	-3.95672	2.2777	4.17553
H	-3.41682	-0.22524	4.11577
H	3.40678	0.41147	-4.11135
H	3.48153	2.9713	-4.16384

[Y(BTP‘)$_3$]$^{3+}$

Y	0.00018	-0.00012	0.00110
N	-0.4008	2.48264	0.00308
N	1.29691	1.30325	-1.73363
N	2.08818	0.67165	-2.59207
N	1.74926	3.39828	-2.74004
N	-1.64157	0.82585	1.73522
N	-2.19442	-0.02506	2.59099
N	-2.73089	2.66938	2.74592
N	-1.95083	-1.58804	-0.00638
N	0.09606	-1.83335	1.73509
N	1.10534	-1.88557	2.59571
N	-0.95643	-3.70244	2.73744
N	-1.7697	0.47171	-1.74038
N	-1.61311	1.4732	-2.59725
N	-3.80785	-0.17907	-2.75483
N	2.35295	-0.89395	0.00318
N	0.48513	-1.76893	-1.73609
N	-0.45916	-2.13792	-2.59288
N	2.07231	-3.20553	-2.74763
N	1.53406	0.99992	1.74132
N	1.07035	1.89922	2.60045
N	3.67279	1.0195	2.75702
C	-1.24688	3.04313	0.87687
C	-1.5049	4.41253	0.91279
H	-2.20433	4.80599	1.64095
C	-0.84458	5.2338	0.00504
H	-1.01761	6.30483	0.00562
C	0.04014	4.6631	-0.90366
H	0.57901	5.25761	-1.63190
C	0.22598	3.28205	-0.86962
C	1.14195	2.62425	-1.83324
C	2.70581	1.38101	-3.51869
C	2.53948	2.77826	-3.59192
C	-1.91043	2.12824	1.83801
C	-3.0044	0.4513	3.51845
C	-3.28654	1.82982	3.59503
C	-2.95341	-1.44428	-0.88248
C	-4.05673	-2.29535	-0.92069
H	-4.83876	-2.12456	-1.65107
C	-4.11167	-3.34786	-0.01307
H	-4.95297	-4.03298	-0.01583
C	-3.07329	-3.50987	0.89788

H	-3.06707	-4.31258	1.62571
C	-2.01638	-2.60168	0.86639
C	-0.89644	-2.71905	1.83205
C	1.09552	-2.82699	3.52138
C	0.04494	-3.7634	3.59083
C	-2.83734	-0.32108	-1.84468
C	-2.53234	1.65623	-3.52716
C	-3.66086	0.81598	-3.60507
C	3.25987	-0.44424	0.87994
C	4.57536	-0.90385	0.91513
C	4.9588	-1.88143	0.00309
C	4.02375	-2.35952	-0.90879
C	2.73402	-1.83209	-0.87334
C	1.70664	-2.29471	-1.83825
C	-0.15491	-3.02586	-3.52144
C	1.13878	-3.57892	-3.59842
C	2.7965	0.58229	1.84530
C	1.88498	2.35881	3.53233
C	3.22023	1.91551	3.60967
H	5.97343	-2.26571	0.00292
H	4.27052	-3.12017	-1.63999
H	5.2644	-0.49728	1.64590
H	1.93167	-2.84193	4.21184
H	0.03179	-4.55138	4.33959
H	-4.43111	0.96402	-4.35779
H	-2.37519	2.48078	-4.21390
H	1.39851	-4.31946	-4.35067
H	-0.94653	-3.3054	-4.20800
H	3.90498	2.29646	4.36319
H	1.47614	3.0897	4.22137
H	-3.96143	2.23316	4.34586
H	-3.4377	-0.26811	4.20464
H	3.34323	0.83653	-4.20672
H	3.05193	3.37527	-4.34198

[U(BTP‘)$_3$]$^{3+}$

U	-0.00214	-0.00634	-0.01724
N	-2.48351	-0.87656	-0.06896
N	-0.67323	-1.8353	1.73441
N	0.23565	-2.2437	2.61251
N	-2.36092	-3.15914	2.72998
N	-1.60575	1.03126	-1.79641
N	-1.11212	1.92806	-2.64325
N	-3.70199	1.01906	-2.89199
N	0.45816	2.57055	0.02363
N	1.7367	0.91919	-1.72311
N	2.3033	0.0741	-2.57899
N	2.78379	2.78377	-2.73358
N	-1.28381	1.41033	1.75647
N	-2.10968	0.79419	2.59600
N	-1.63783	3.49919	2.81212
N	2.01767	-1.69359	0.04532
N	1.83627	0.3767	1.79650
N	1.67758	1.3788	2.65510
N	3.7852	-0.37693	2.90802
N	0.01741	-1.92357	-1.77098
N	-0.97952	-1.96489	-2.64842
N	1.12028	-3.74798	-2.79248
C	-3.35736	-0.41762	-0.97825
C	-4.68117	-0.8494	-1.04224
H	-5.3402	-0.44113	-1.79939

C	-5.11399	-1.79762	-0.12207
H	-6.13768	-2.1563	-0.14251
C	-4.21713	-2.27962	0.82539
H	-4.50556	-3.01832	1.56387
C	-2.91159	-1.79078	0.81534
C	-1.92676	-2.28548	1.81466
C	-0.13895	-3.1011	3.54455
C	-1.46496	-3.57405	3.60268
C	-2.85963	0.59771	-1.94271
C	-1.89746	2.37349	-3.60720
C	-3.22405	1.91552	-3.73162
C	-0.13866	3.36764	0.92298
C	0.0826	4.74336	0.98196
H	-0.43118	5.33424	1.73113
C	0.96191	5.3144	0.06919
H	1.15685	6.38143	0.08601
C	1.59083	4.49741	-0.86398
H	2.28829	4.89129	-1.59367
C	1.31074	3.13198	-0.84891
C	1.97477	2.22912	-1.82263
C	3.10518	0.56796	-3.50353
C	3.3569	1.95309	-3.57967
C	-1.06912	2.72266	1.88325
C	-2.69862	1.51224	3.53466
C	-2.45903	2.89584	3.64710
C	2.1133	-2.68853	-0.85139
C	3.16605	-3.6016	-0.86134
C	4.16357	-3.47432	0.10018
C	4.0759	-2.44646	1.03218
C	2.98538	-1.57955	0.96768
C	2.8602	-0.46759	1.94524
C	2.55607	1.5111	3.63128
C	3.6386	0.61836	3.75855
C	1.0272	-2.79164	-1.86068
C	-0.93773	-2.88681	-3.59173
C	0.13443	-3.80039	-3.66472
H	4.99836	-4.16709	0.12178
H	4.82569	-2.30191	1.80104
H	3.18558	-4.38496	-1.61001
H	3.5572	-0.13989	-4.18949
H	4.02481	2.36888	-4.32995
H	-2.93964	3.49682	4.41503
H	-3.369	0.98559	4.20518
H	4.37437	0.72578	4.55162
H	2.40375	2.33656	4.31797
H	0.17504	-4.56636	-4.43542
H	-1.7617	-2.90485	-4.29651
H	-3.88304	2.28428	-4.51352
H	-1.47287	3.10503	-4.28585
H	0.62003	-3.41974	4.25055
H	-1.78253	-4.28678	4.35971

$[Np(BTP')_3]^{3+}$

Np	-0.005262	0.000356	0.002371
N	1.650586	-2.030012	-0.146252
N	1.962985	-0.088682	1.737367
N	2.062783	0.874479	2.646658
N	3.751265	-1.301924	2.700293
N	-0.388907	-1.700046	-1.921436
N	-1.391451	-1.487011	-2.766139
N	0.282317	-3.654326	-3.070395

N	-2.599992	-0.428341	0.003542
N	-1.466205	1.424589	-1.632378
N	-0.852097	2.277642	-2.442983
N	-3.559394	1.813466	-2.662891
N	-0.928429	-1.811015	1.644566
N	-0.071309	-2.418863	2.455748
N	-2.783142	-2.857585	2.673096
N	0.918835	2.450217	0.140705
N	-0.904193	1.497140	1.923511
N	-1.789246	0.981050	2.768829
N	-0.889393	3.569190	3.062302
N	1.820645	0.702841	-1.747899
N	2.221904	-0.180984	-2.654666
N	3.141045	2.415158	-2.707405
C	1.516534	-2.949729	-1.113251
C	2.359452	-4.053646	-1.230663
H	2.200020	-4.765166	-2.032095
C	3.386648	-4.204502	-0.305658
H	4.061405	-5.051843	-0.366988
C	3.539319	-3.252798	0.696341
H	4.326204	-3.321118	1.438127
C	2.647889	-2.181213	0.737087
C	2.789746	-1.135095	1.784410
C	2.993989	0.762182	3.576197
C	3.858620	-0.350101	3.604619
C	0.410392	-2.755286	-2.087319
C	-1.564595	-2.342716	-3.756545
C	-0.709003	-3.451218	-3.913696
C	-3.153013	-1.310693	0.849624
C	-4.522115	-1.570446	0.886501
H	-4.908969	-2.294168	1.594107
C	-5.351095	-0.885521	0.005027
H	-6.421321	-1.063653	0.005638
C	-4.789201	0.031357	-0.876520
H	-5.390150	0.591870	-1.582797
C	-3.409509	0.228544	-0.840900
C	-2.775295	1.207503	-1.764120
C	-1.574501	2.900547	-3.356871
C	-2.959845	2.669230	-3.465945
C	-2.237054	-2.030425	1.774254
C	-0.553667	-3.241591	3.369720
C	-1.939302	-3.471621	3.477634
C	1.814796	2.905257	-0.747039
C	2.322889	4.203336	-0.711856
C	1.880781	5.061911	0.288283
C	0.956184	4.598128	1.217614
C	0.504407	3.284058	1.105951
C	-0.481947	2.752670	2.083410
C	-2.226632	1.742657	3.754692
C	-1.766298	3.065977	3.906734
C	2.277972	1.955633	-1.793398
C	3.074291	0.217103	-3.581279
C	3.545018	1.544811	-3.609847
H	2.254187	6.078974	0.344516
H	0.582308	5.225532	2.017990
H	3.046306	4.514177	-1.456197
H	-1.050775	3.593094	-4.006610
H	-3.565912	3.184200	-4.207171
H	-2.346295	-4.154229	4.219382
H	0.165475	-3.726531	4.020647
H	-2.119273	3.701311	4.715238
H	-2.950520	1.300680	4.430551

H	4.247475	1.883533	-4.367290
H	3.389721	-0.524395	-4.307055
H	-0.842538	-4.162143	-4.725285
H	-2.390379	-2.149049	-4.432305
H	3.057063	1.563041	4.304746
H	4.629968	-0.451997	4.363980

$[Pu(BTP')_3]^{3+}$

Pu	0.01763	-0.0024	0.00508
N	-1.52911	-2.10133	0.04412
N	-1.88003	-0.12649	-1.80164
N	-2.01246	0.85585	-2.68549
N	-3.61223	-1.38092	-2.81566
N	0.45562	-1.74176	1.86515
N	1.42581	-1.50355	2.73995
N	-0.15179	-3.75449	2.94611
N	2.62636	-0.26606	0.03204
N	1.34962	1.46257	1.69965
N	0.66983	2.25162	2.52306
N	3.39804	1.95598	2.77401
N	1.06474	-1.70813	-1.66772
N	0.25985	-2.34818	-2.50745
N	2.99686	-2.59764	-2.70218
N	-1.07282	2.36556	-0.07703
N	0.8498	1.60375	-1.83955
N	1.77764	1.17053	-2.68460
N	0.69716	3.69369	-2.93361
N	-1.86596	0.5107	1.75314
N	-2.21675	-0.42185	2.63130
N	-3.34382	2.08871	2.71642
C	-1.3719	-3.04841	0.98115
C	-2.16134	-4.19533	1.04144
H	-1.98365	-4.92658	1.82102
C	-3.16053	-4.36216	0.08906
H	-3.79491	-5.24206	0.10565
C	-3.33667	-3.3843	-0.88306
H	-4.10316	-3.46462	-1.64467
C	-2.49725	-2.27066	-0.86755
C	-2.66665	-1.20067	-1.88573
C	-2.9315	0.73401	-3.62613
C	-3.75015	-0.41011	-3.69515
C	-0.29839	-2.83475	1.98550
C	1.61323	-2.37572	3.71354
C	0.80886	-3.52813	3.81868
C	3.24484	-1.08556	-0.83056
C	4.62857	-1.25428	-0.85496
H	5.07181	-1.93041	-1.57638
C	5.39901	-0.54257	0.05812
H	6.4785	-0.65037	0.06820
C	4.76761	0.30938	0.95776
H	5.3222	0.88645	1.68815
C	3.37862	0.41726	0.90709
C	2.66811	1.32607	1.84622
C	1.33707	2.89264	3.46549
C	2.73296	2.74767	3.59065
C	2.38699	-1.83563	-1.78678
C	0.80633	-3.10979	-3.43785
C	2.20555	-3.24295	-3.53481
C	-2.01541	2.72994	0.80367
C	-2.61539	3.98894	0.79363
C	-2.21659	4.90662	-0.17140

C	-1.24205	4.53798	-1.09203
C	-0.70056	3.25665	-1.00820
C	0.33739	2.82661	-1.98008
C	2.16816	1.98258	-3.64975
C	1.61815	3.27375	-3.77669
C	-2.42576	1.72012	1.81504
C	-3.12021	-0.11543	3.54463
C	-3.69732	1.16876	3.59041
H	-2.66061	5.89586	-0.20700
H	-0.89719	5.21451	-1.86494
H	-3.37353	4.22464	1.53100
H	0.7599	3.53062	4.12577
H	3.29349	3.27905	4.35573
H	2.66573	-3.87432	-4.29075
H	0.12809	-3.62221	-4.11135
H	1.93633	3.95233	-4.56430
H	2.92647	1.60825	-4.32856
H	-4.44158	1.43298	4.33751
H	-3.3908	-0.89693	4.24632
H	0.95809	-4.25528	4.61297
H	2.4107	-2.16161	4.41661
H	-3.02082	1.55262	-4.33192
H	-4.50933	-0.52265	-4.46508

$[Am(BTP')_3]^{3+}$

Am	-0.00016	0.00755	-0.00745
N	0.12806	2.60762	-0.01726
N	1.54294	1.09073	-1.75820
N	2.16276	0.29717	-2.62273
N	2.3548	3.03824	-2.82340
N	-1.43106	1.265	1.73919
N	-2.133	0.55203	2.61105
N	-2.03367	3.29967	2.78326
N	-2.31478	-1.19369	0.06456
N	-0.31118	-1.87644	1.75647
N	0.68476	-2.12493	2.59919
N	-1.73172	-3.42754	2.83998
N	-1.78974	0.80308	-1.70844
N	-1.45098	1.7422	-2.58264
N	-3.9186	0.51827	-2.69468
N	2.18543	-1.40547	-0.05490
N	0.12252	-1.91998	-1.73667
N	-0.89513	-2.08482	-2.57435
N	1.38334	-3.62093	-2.79112
N	1.85913	0.65152	1.70575
N	1.6236	1.62307	2.57908
N	3.94807	0.14825	2.69413
C	-0.5567	3.33954	0.87065
C	-0.51116	4.73289	0.90371
H	-1.08991	5.26969	1.64625
C	0.28661	5.39133	-0.02568
H	0.34934	6.47438	-0.02848
C	1.00443	4.64131	-0.95096
H	1.64187	5.10428	-1.69511
C	0.89188	3.25256	-0.90986
C	1.63526	2.41529	-1.88307
C	2.87553	0.85726	-3.58200
C	2.98493	2.25935	-3.67861
C	-1.38457	2.59376	1.85058
C	-2.78454	1.19498	3.56238
C	-2.74395	2.60144	3.64533

C	-3.28671	-0.85248	-0.79626
C	-4.54275	-1.45773	-0.79441
H	-5.28787	-1.13747	-1.51322
C	-4.79729	-2.45987	0.13555
H	-5.76414	-2.9516	0.16326
C	-3.79497	-2.8229	1.02864
H	-3.94047	-3.59675	1.77293
C	-2.5708	-2.16061	0.95643
C	-1.47728	-2.50734	1.90214
C	0.48611	-3.01422	3.55495
C	-0.74479	-3.68917	3.67252
C	-2.98045	0.21378	-1.78939
C	-2.33097	2.0754	-3.50972
C	-3.59651	1.45788	-3.56104
C	3.18238	-1.15746	0.80783
C	4.36694	-1.89402	0.82441
C	4.51889	-2.93148	-0.08822
C	3.48899	-3.19983	-0.98322
C	2.34263	-2.40986	-0.93019
C	1.22156	-2.66228	-1.87156
C	-0.78583	-3.00682	-3.51315
C	0.37342	-3.80168	-3.61749
C	2.98333	-0.05686	1.78930
C	2.53428	1.86338	3.50594
C	3.72745	1.11674	3.55989
H	5.42656	-3.52562	-0.09973
H	3.55456	-3.99911	-1.71187
H	5.13726	-1.64692	1.54530
H	1.31239	-3.19811	4.23274
H	-0.9126	-4.43595	4.44454
H	-4.33446	1.73809	-4.30883
H	-2.03225	2.84271	-4.21549
H	0.46554	-4.57745	-4.37349
H	-1.62762	-3.12199	-4.18699
H	4.49098	1.31662	4.30764
H	2.31821	2.65887	4.21076
H	-3.29051	3.14309	4.41342
H	-3.34968	0.59033	4.26316
H	3.37133	0.1892	-4.27764
H	3.58586	2.73159	-4.45173

$[Cm(BTP‘)_3]^{3+}$

Cm	-0.001032	-0.000239	0.000692
N	2.569144	-0.361597	0.002884
N	0.948201	-1.638099	-1.771581
N	0.119241	-2.216378	-2.632546
N	2.839249	-2.611555	-2.807350
N	1.359240	1.314755	1.772836
N	0.720313	2.101562	2.630508
N	3.443561	1.732577	2.810774
N	-0.969680	2.409932	-0.006380
N	-1.818654	0.532522	1.765485
N	-2.183581	-0.414806	2.620929
N	-3.231051	2.126658	2.794726
N	0.943382	1.632187	-1.775618
N	1.858525	1.195595	-2.632558
N	0.853601	3.752934	-2.819464
N	-1.594965	-2.050400	0.003997
N	-1.892144	-0.011714	-1.769457
N	-1.982086	0.999348	-2.625155
N	-3.687029	-1.156936	-2.800199

N	0.454684	-1.828813	1.778493
N	1.451592	-1.660711	2.639067
N	-0.217670	-3.843604	2.819542
C	3.349702	0.254587	0.901631
C	4.733890	0.092304	0.939846
H	5.313509	0.617660	1.689515
C	5.328379	-0.746996	0.004143
H	6.402742	-0.897342	0.004870
C	4.527577	-1.391165	-0.932354
H	4.941701	-2.055198	-1.681673
C	3.151890	-1.167747	-0.895553
C	2.262316	-1.839682	-1.878981
C	0.632897	-2.986143	-3.574777
C	2.023734	-3.191797	-3.663821
C	2.677921	1.146967	1.882672
C	1.424621	2.703216	3.571773
C	2.818089	2.517616	3.663869
C	-0.558291	3.314049	-0.906447
C	-1.047483	4.618806	-0.947091
H	-0.674566	5.306047	-1.697192
C	-2.007081	4.995611	-0.014091
H	-2.410805	6.002652	-0.016960
C	-2.442597	4.064506	0.922472
H	-3.189334	4.307155	1.669281
C	-1.894361	2.783136	0.889288
C	-2.335680	1.757607	1.871343
C	-3.062606	-0.107204	3.557146
C	-3.601084	1.191695	3.645937
C	0.467407	2.873053	-1.887974
C	2.274657	2.019406	-3.576907
C	1.763549	3.328680	-3.672255
C	-1.450058	-3.032521	0.904654
C	-2.279430	-4.152334	0.943796
C	-3.303311	-4.251241	0.008230
C	-3.463766	-3.236649	-0.929044
C	-2.584783	-2.155012	-0.893639
C	-2.725569	-1.047722	-1.876028
C	-2.911252	0.944855	-3.561971
C	-3.785427	-0.156462	-3.651626
C	-0.344523	-2.890894	1.888336
C	1.622157	-2.567442	3.583767
C	0.771097	-3.686264	3.675560
H	-3.967988	-5.108683	0.009615
H	-4.246037	-3.265180	-1.678301
H	-2.111683	-4.915659	1.694252
H	-3.344929	-0.899129	4.242178
H	-4.328765	1.455271	4.409597
H	2.102636	4.017304	-4.442184
H	3.022726	1.638737	-4.263607
H	-4.556443	-0.210255	-4.416275
H	-2.964865	1.784164	-4.246634
H	0.905486	-4.442220	4.445242
H	2.443346	-2.406815	4.273690
H	3.408958	3.011147	4.431433
H	0.878971	3.340749	4.258796
H	-0.065661	-3.446818	-4.264648
H	2.457488	-3.827754	-4.431405