The Strength of Actinide–Element Bonds from the Quantum Theory of Atoms-in-Molecules

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Electronic Supplementary Information

Table S1: Selected bond length (Å), bond angle (degrees) and stretching vibration (cm^{-1}) data for $[AnX_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$ (An = Th–Pu; X = F, Cl, Br, H, Me).

		Th	Pa	U	Np	Pu
X=F	*r*(N–N)	1.259	1.356	1.242	1.231	1.210
	r(An–An)	4.790	4.351	4.680	4.661	4.760
	r(An–N) av.	2.476	2.279	2.421	2.411	2.456
	r(An–F) av.	2.125	2.084	2.075	2.061	2.051
	∠N–An–N	29.4	34.6	29.7	29.6	28.5
	∠An–N–An	150.6	145.4	150.3	150.4	151.5
	σ(N–N)	1515	1087	1566	1582	1696
X=Cl	*r*(N–N)	1.255	1.353	1.278	1.227	1.205
	r(An–An)	4.729	4.313	4.430	4.632	4.753
	r(An–N) av.	2.446	2.260	2.305	2.396	2.452
	r(An–Cl) av.	2.592	2.540	2.518	2.511	2.500
	∠N–An–N	29.7	34.8	32.2	29.7	28.5
	∠An–N–An	150.3	145.2	147.8	150.3	151.5
	σ(N–N)	1523	1098	1307	1602	1718
X=Br	*r*(N–N)	1.255	1.354	1.276	1.228	1.207
	r(An–An)	4.714	4.302	4.430	4.618	4.727
	r(An–N) av.	2.439	2.255	2.305	2.389	2.439
	r(An–Br) av.	2.749	2.697	2.674	2.667	2.659
	∠N–An–N	29.8	34.9	32.1	29.8	28.6
	∠An–N–An	150.2	145.1	147.9	150.2	151.4
	σ(N–N)	1523	1095	1326	1596	1705
X=H	*r*(N–N)	1.257	1.362	1.259	1.267	1.234
	r(An–An)	4.721	4.311	4.553	4.478	4.573
	r(An–N) av.	2.443	2.261	2.362	2.327	2.368
	r(An–H) av.	2.088	2.032	2.027	2.025	2.002
	∠N–An–N	29.8	35.1	30.9	31.6	30.2
	∠An–N–An	150.2	144.9	149.1	148.4	149.8
	σ(N–N)	1504	1092	1456	1382	1564
X=Me	*r*(N–N)	1.257	1.361	1.325	1.240	1.227
	r(An–An)	4.792	4.344	4.382	4.651	4.693
	r(An–N) av.	2.477	2.276	2.289	2.407	2.425
	r(An–C) av.	2.472	2.411	2.390	2.389	2.383
	∠N–An–N	29.4	34.8	33.7	29.8	29.3
	∠An–N–An	150.6	145.2	146.3	150.2	150.7
	σ(N–N)	1513	1087	1159	1548	1605

Table S2: The difference between the QTAIM-calculated actinide atomic partial charge in the AnX_3 fragments and in the full molecules ($\left|\Delta Q_{An}^{QTAIM}\right|$) for $[AnX_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$ (An = Th–Pu; X = F, Cl, Br, OPh, H, Me).

	Th	Pa	U	Np	Pu
X=F	0.58	0.69	0.45	0.38	0.29
X=Cl	0.54	0.57	0.37	0.26	0.18
X=Br	0.54	0.52	0.34	0.24	0.14
X=OPh	0.57	0.67	0.43	0.35	0.25
X=H	0.61	0.70	0.47	0.39	0.30
X=Me	0.61	0.74	0.63	0.47	0.41

Table S3: Optimised An–O bond lengths, and their mean absolute deviations from *ab initio* (CASPT2) results.[1] All triatomics are linear except neutral ThO_2 (bond angle 118.56 degrees).

Method	ThO	PaO	UO	NpO	PuO	AmO	CmO	MAD
CASPT2	1.863	1.818	1.838	1.839	1.820	1.801	1.836	–
B3LYP	1.832	1.803	1.840	1.834	1.827	1.833	1.840	0.014
TPSS	1.839	1.812	1.838	1.831	1.829	1.844	1.839	0.013
TPSSh	1.831	1.801	1.834	1.827	1.821	1.835	1.832	0.015
	ThO^+	PaO^+	UO^+	NpO^+	PuO^+	AmO^+	CmO^+	
CASPT2	1.827	1.804	1.796	1.798	1.789	1.782	1.792	–
B3LYP	1.800	1.776	1.800	1.792	1.791	1.781	1.796	0.010
TPSS	1.807	1.800	1.801	1.796	1.789	1.787	1.800	0.006
TPSSh	1.799	1.794	1.797	1.788	1.781	1.777	1.791	0.009
	ThO^{2+}	PaO^{2+}	UO^{2+}	NpO^{2+}	PuO^{2+}	AmO^{2+}	CmO^{2+}	
CASPT2	1.790	1.733	1.720	1.723	1.731	1.808	1.791	–
B3LYP	1.763	1.738	1.725	1.723	1.722	1.776	1.840	0.018
TPSS	1.768	1.745	1.734	1.735	1.741	1.785	1.794	0.014
TPSSh	1.760	1.735	1.722	1.721	1.723	1.775	1.814	0.014
	ThO_2	PaO_2	UO_2	NpO_2	PuO_2	AmO_2	CmO_2	
CASPT2	1.923	1.816	1.827	1.761	1.744	1.807	1.832	–
B3LYP	1.896	1.805	1.788	1.818	1.746	1.825	1.836	0.023
TPSS	1.898	1.812	1.810	1.800	1.802	1.833	1.841	0.025
TPSSh	1.891	1.801	1.794	1.806	1.806	1.821	1.831	0.029
	ThO_2^+	PaO_2^+	UO_2^+	NpO_2^+	PuO_2^+	AmO_2^+	CmO_2^+	
CASPT2	1.832	1.767	1.745	1.723	1.704	1.721	1.746	–
B3LYP	1.867	1.767	1.752	1.719	1.713	1.715	1.747	0.009
TPSS	1.870	1.775	1.762	1.742	1.725	1.731	1.760	0.018
TPSSh	1.860	1.764	1.750	1.728	1.711	1.714	1.745	0.008
	ThO_2^{2+}	PaO_2^{2+}	UO_2^{2+}	NpO_2^{2+}	PuO_2^{2+}	AmO_2^{2+}	CmO_2^{2+}	
CASPT2	1.903	1.726	1.710	1.700	1.675	1.679	1.674	–
B3LYP	1.849	1.771	1.692	1.675	1.660	1.665	1.687	0.026
TPSS	1.873	1.782	1.706	1.703	1.690	1.683	1.705	0.021
TPSSh	1.886	1.768	1.692	1.688	1.673	1.665	1.686	0.017

Table S4: Ionisation energies (IE*n*, kJ/mol) of actinide atoms, and their mean absolute deviations from experiment.[2]

Method	Th	Pa	U	Np	Pu	Am	Cm	MAD
IE1								
Expt[2]	608.502	568.224	597.632	604.542	581.418	576.382	578.081	
B3LYP[3]	589.000	551.000	562.000	567.000	581.000	580.000	547.000	19.647
B3LYP/PP	605.428	557.493	562.074	567.797	573.693	579.308	532.352	19.139
B3LYP/AE+DKH	653.288	566.374	536.701	558.901	569.942	574.785	567.858	23.146
B3LYP/AE+DKHSO	654.631	481.990	545.856	560.155	571.286	576.201	571.104	31.989
TPSS/PP	587.983	565.515	569.284	539.647	541.608	545.630	488.271	38.170
TPSS/AE+DKH	1039.295	551.582	557.326	532.365	542.801	540.397	562.406	85.325
TPSS/AE+DKHSO	561.143	557.153	923.682	534.194	531.334	541.758	563.993	73.434
TPSSh/PP	586.763	564.923	565.970	537.885	539.862	544.101	511.727	36.079
TPSSh/AE+DKH	575.196	566.730	558.956	525.784	535.223	538.703	529.875	39.038
TPSSh/AE+DKHSO	576.496	564.650	566.387	526.979	536.521	540.094	520.384	39.096
IE2								
Expt[2]	1124.054	1128.878	1128.878	1114.406	1138.527	1157.824	1196.418	
B3LYP/PP	1154.999	1168.386	1125.591	1135.801	1155.658	1172.895	1197.299	16.199
B3LYP/AE+DKH	1090.683	1181.192	1145.335	1255.456	1151.795	1167.244	1196.053	33.541
B3LYP/AE+DKHSO	1085.374	1183.627	1139.635	1258.159	1154.166	1169.717	1171.994	37.537
TPSS/PP	1139.782	1102.417	1075.019	1114.048	1133.728	1150.439	1161.672	21.441
TPSS/AE+DKH	661.488	1145.848	1064.902	1111.545	1129.122	1143.963	1098.296	86.662
TPSS/AE+DKHSO	1110.298	1148.219	704.493	1113.676	1144.080	1146.245	1089.487	75.675
TPSSh/PP	1139.844	1105.928	1079.042	1106.645	1126.194	1142.893	1154.011	24.662
TPSSh/AE+DKH	1145.649	1113.036	1066.929	1126.771	1120.915	1135.861	1147.643	28.524
TPSSh/AE+DKHSO	1140.714	1108.033	1054.957	1129.082	1123.218	1138.256	1150.069	29.124

Table S5: First ionisation energies (kJ/mol) of AnO, and their mean absolute deviations from experiment.[2]

Method	ThO	PaO	UO	NpO	PuO	AmO	CmO	MAD
Expt[2]	637.141	569.264	581.932	588.561	588.561	598.209	617.506	
SO-CASPT2[1]	632.944	605.928	583.736	576.017	595.315	599.174	644.522	12.849
B3LYP/PP	630.239	625.066	593.174	602.127	611.689	626.153	640.033	23.016
B3LYP/PP+ZPE+BSSE	652.605	683.280	486.012	602.780	612.192	626.932	632.937	43.915
B3LYP/AE+DKH	626.765	623.033	606.316	593.127	614.592	623.132	642.399	24.135
B3LYP/AE+DKH+ZPE+BSSE	649.131	681.248	499.154	593.780	615.095	623.911	635.303	40.286
B3LYP/AE+DKHSO	627.060	647.606	555.834	599.008	615.028	624.200	642.625	28.935
B3LYP/AE+DKHSO+ZPE+BSSE	649.426	705.821	448.672	599.661	615.531	624.978	635.529	52.138
TPSS/PP	609.002	584.527	572.916	578.639	586.857	610.640	611.789	11.742
TPSS/PP+ZPE+BSSE	620.721	573.541	604.476	566.525	587.849	611.441	614.938	11.684
TPSS/AE+DKH	599.963	577.153	574.415	572.956	584.543	606.651	613.269	12.126
TPSS/AE+DKH+ZPE+BSSE	611.682	566.166	605.974	560.841	585.535	607.453	616.419	13.382
TPSS/AE+DKHSO	599.833	575.961	578.479	572.612	584.653	608.368	613.166	11.688
TPSS/AE+DKHSO+ZPE+BSSE	611.552	564.974	610.039	560.497	585.645	609.170	616.315	14.445
TPSSh/PP	608.089	586.119	568.381	575.006	582.616	604.563	610.881	13.134
TPSSh/PP+ZPE+BSSE	608.572	597.577	576.054	570.998	582.660	605.445	606.511	14.922
TPSSh/AE+DKH	600.033	583.038	569.559	566.315	584.222	599.954	611.755	13.905
TPSSh/AE+DKH+ZPE+BSSE	600.516	594.496	577.232	562.307	584.265	600.837	607.385	15.694
TPSSh/AE+DKHSO	599.978	618.898	569.440	570.911	587.271	601.666	611.805	18.198
TPSSh/AE+DKHSO+ZPE+BSSE	600.461	630.355	577.113	566.903	587.314	602.548	607.435	19.987

Table S6: Second ionisation energies (kJ/mol) of AnO, and their mean absolute deviations from experiment.[2]

Method	ThO	PaO	UO	NpO	PuO	AmO	CmO	MAD
Expt[2]	1152.035	1167.473	1261.063	1295.798	1385.529	1452.104	1536.047	
SO-CASPT2[1]	1138.527	1138.527	1196.418	1350.795	1350.795	1350.795	1524.468	44.245
B3LYP/PP	1176.968	1201.042	1252.293	1340.629	1408.028	1485.247	1488.292	30.786
B3LYP/PP+ZPE+BSSE	1173.998	1200.626	1204.283	1336.074	1407.691	1483.146	1485.473	36.564
B3LYP/AE+DKH	1173.831	1193.975	1195.552	1319.586	1388.782	1469.860	1474.484	31.453
B3LYP/AE+DKH+ZPE+BSSE	1170.861	1193.560	1147.543	1315.031	1388.446	1467.759	1471.665	37.231
B3LYP/AE+DKHSO	1175.169	1170.807	1282.118	1319.095	1395.414	1476.265	1479.374	23.077
B3LYP/AE+DKHSO+ZPE+BSSE	1172.199	1170.392	1234.108	1314.539	1395.078	1474.163	1476.554	22.840
TPSS/PP	1146.261	1187.227	1240.570	1317.192	1381.874	1451.399	1474.714	19.016
TPSS/PP+ZPE+BSSE	1113.000	1207.990	1216.460	1323.797	1381.308	1449.495	1462.491	33.220
TPSS/AE+DKH	1140.702	1175.818	1276.775	1298.291	1366.022	1437.874	1455.814	21.693
TPSS/AE+DKH+ZPE+BSSE	1107.441	1196.582	1252.666	1304.896	1365.456	1435.970	1443.590	31.409
TPSS/AE+DKHSO	1142.233	1178.363	1277.546	1303.386	1372.584	1444.345	1461.150	20.052
TPSS/AE+DKHSO+ZPE+BSSE	1108.972	1199.127	1253.436	1309.991	1372.017	1442.441	1448.926	29.548
TPSSh/PP	1143.651	1180.735	1244.222	1323.675	1392.751	1463.621	1475.829	20.760
TPSSh/PP+ZPE+BSSE	1153.532	1181.424	1313.407	1340.043	1397.435	1461.556	1473.027	28.059
TPSSh/AE+DKH	1138.319	1169.089	1233.688	1306.530	1365.269	1449.493	1460.067	21.756
TPSSh/AE+DKH+ZPE+BSSE	1148.201	1169.778	1302.873	1322.898	1369.952	1447.428	1457.264	24.869
TPSSh/AE+DKHSO	1139.867	1134.476	1238.783	1306.924	1368.600	1455.996	1465.218	24.317
TPSSh/AE+DKHSO+ZPE+BSSE	1149.748	1135.165	1307.968	1323.291	1373.283	1453.932	1462.415	28.100

Table S7: First ionisation energies (kJ/mol) of AnO_2, and their mean absolute deviations from experiment.[2]

Method	ThO_2	PaO_2	UO_2	NpO_2	PuO_2	AmO_2	CmO_2	MAD
Expt[2]	858.720	569.264	591.262	610.752	678.292	697.589	820.125	
SO-CASPT2[1]	820.125	549.966	599.174	604.963	598.209	652.241	797.934	31.316
B3LYP/PP	821.929	608.142	598.479	666.782	604.881	673.480	797.435	37.018
B3LYP/PP+ZPE+BSSE	820.634	608.630	568.062	671.183	622.024	678.054	801.565	36.492
B3LYP/AE+DKH	819.887	603.095	602.118	659.879	623.047	666.117	777.268	37.460
B3LYP/AE+DKH+ZPE+BSSE	818.592	603.582	571.701	664.280	640.190	670.691	781.397	35.895
B3LYP/AE+DKHSO	820.904	602.894	601.705	663.431	628.135	667.858	779.392	36.456
B3LYP/AE+DKHSO+ZPE+BSSE	819.608	603.382	571.288	667.832	645.278	672.432	783.521	35.008
TPSS/PP	786.698	575.726	575.931	587.083	625.236	635.141	748.955	43.451
TPSS/PP+ZPE+BSSE	781.552	574.002	575.176	590.940	635.263	639.785	752.646	40.874
TPSS/AE+DKH	790.202	566.929	990.458	1039.455	615.418	636.229	745.818	156.756
TPSS/AE+DKH+ZPE+BSSE	785.057	565.204	989.704	1043.313	625.444	640.873	749.508	155.558
TPSS/AE+DKHSO	791.386	566.809	965.880	1010.036	619.287	638.260	748.092	147.722
TPSS/AE+DKHSO+ZPE+BSSE	786.241	565.085	965.126	1013.894	629.313	642.905	751.782	146.524
TPSSh/PP	793.134	570.821	567.699	580.657	621.712	644.093	765.333	40.810
TPSSh/PP+ZPE+BSSE	726.542	501.548	495.648	495.155	539.007	541.718	663.021	123.338
TPSSh/AE+DKH	790.144	567.076	567.892	590.982	615.661	636.391	745.872	44.570
TPSSh/AE+DKH+ZPE+BSSE	789.021	569.607	570.043	595.532	629.313	641.743	752.577	39.836
TPSSh/AE+DKHSO	791.452	567.238	567.618	595.316	619.412	638.634	748.307	42.575
TPSSh/AE+DKHSO+ZPE+BSSE	790.329	569.769	569.769	599.867	633.064	643.987	755.013	37.888

Table S8: Second ionisation energies (kJ/mol) of AnO_2, and their mean absolute deviations from experiment.[2]

Method	ThO_2	PaO_2	UO_2	NpO_2	PuO_2	AmO_2	CmO_2	MAD
Expt[2]	1601.657	1601.657	1408.686	1456.929	1456.929	1514.820	1727.088	
SO-CASPT2[1]	1456.929	1639.286	1385.529	1503.242	1482.980	1570.781	1558.238	71.813
B3LYP/PP	1601.065	1634.044	1466.305	1514.573	1656.836	1627.409	1570.633	88.171
B3LYP/PP+ZPE+BSSE	1599.285	1628.650	1412.031	1515.194	1647.563	1627.946	1561.801	80.003
B3LYP/AE+DKH	1599.566	1630.999	1452.031	1501.688	1635.101	1608.842	1540.622	82.599
B3LYP/AE+DKH+ZPE+BSSE	1597.785	1625.605	1397.757	1502.309	1625.828	1609.378	1531.791	77.555
B3LYP/AE+DKHSO	1600.136	1633.357	1457.240	1507.262	1640.766	1614.265	1543.748	85.533
B3LYP/AE+DKHSO+ZPE+BSSE	1598.356	1627.964	1402.966	1507.883	1631.493	1614.801	1534.916	79.000
TPSS/PP	1560.108	1590.672	1454.374	1520.032	1545.065	1593.780	1520.260	76.464
TPSS/PP+ZPE+BSSE	1541.167	1689.517	1448.727	1519.753	1537.945	1593.863	1510.597	89.681
TPSS/AE+DKH	1577.099	1602.583	1440.973	1537.084	1625.348	1585.655	1510.816	84.779
TPSS/AE+DKH+ZPE+BSSE	1558.158	1701.428	1435.325	1536.805	1618.228	1585.739	1501.154	101.134
TPSS/AE+DKHSO	1578.280	1605.093	1446.386	1543.007	1631.548	1591.248	1514.135	87.799
TPSS/AE+DKHSO+ZPE+BSSE	1559.338	1703.938	1440.738	1542.728	1624.428	1591.332	1504.472	104.154
TPSSh/PP	1558.448	1604.388	1454.562	1529.642	1554.030	1602.180	1539.044	76.719
TPSSh/PP+ZPE+BSSE	1607.789	1656.718	1522.099	1619.104	1649.597	1709.554	1639.244	116.004
TPSSh/AE+DKH	1579.562	1602.356	1440.611	1534.193	1622.108	1584.742	1509.392	83.540
TPSSh/AE+DKH+ZPE+BSSE	1563.433	1582.881	1433.945	1533.603	1621.318	1584.390	1500.574	88.486
TPSSh/AE+DKHSO	1581.028	1604.498	1445.687	1539.742	1627.891	1589.889	1512.305	86.300
TPSSh/AE+DKHSO+ZPE+BSSE	1564.899	1585.024	1439.021	1539.153	1627.101	1589.537	1503.488	90.634

Table S9: Bond energies (D_e or D_0, kJ/mol) of AnO, and their mean absolute deviations from experiment.[2]

Method	ThO	PaO	UO	NpO	PuO	AmO	CmO	MAD
Expt[2]	872.000	801.000	758.000	744.000	658.000	582.000	709.000	
B3LYP[3]	910.000	855.000	784.000	715.000	595.000	494.000	688.000	45.571
B3LYP/PP	915.064	856.905	780.166	714.493	597.824	495.417	687.453	45.564
B3LYP/PP+ZPE+BSSE	924.334	898.907	701.252	704.572	592.773	485.612	678.351	62.669
B3LYP/AE+DKH	906.922	857.787	753.134	715.328	606.864	505.949	689.430	38.858
B3LYP/AE+DKH+ZPE+BSSE	916.192	899.788	674.220	705.407	601.812	496.144	680.327	62.295
B3LYP/AE+DKHSO	909.357	937.995	745.059	706.357	597.799	497.856	689.239	55.577
B3LYP/AE+DKHSO+ZPE+BSSE	918.626	979.997	666.146	696.436	592.748	488.052	680.137	79.015
TPSS/PP	924.561	874.604	827.688	764.023	658.433	566.197	751.099	39.173
TPSS/PP+ZPE+BSSE	907.237	854.671	816.221	747.830	648.842	556.440	743.416	31.442
TPSS/AE+DKH	926.342	876.849	854.706	763.522	670.392	572.865	755.331	44.897
TPSS/AE+DKH+ZPE+BSSE	909.018	856.917	843.239	747.328	660.801	563.108	747.649	34.549
TPSS/AE+DKHSO	954.762	868.583	843.798	754.778	663.158	566.847	756.130	44.909
TPSS/AE+DKHSO+ZPE+BSSE	937.437	848.651	832.331	738.585	653.567	557.090	748.447	37.375
TPSSh/PP	904.835	852.206	807.207	745.651	633.635	534.544	716.839	30.651
TPSSh/PP+ZPE+BSSE	892.202	843.858	800.216	731.521	628.543	525.332	710.213	29.299
TPSSh/AE+DKH	908.667	849.562	814.515	748.100	639.055	542.726	721.271	30.905
TPSSh/AE+DKH+ZPE+BSSE	896.033	841.214	807.524	733.969	633.963	533.514	714.646	28.853
TPSSh/AE+DKHSO	911.175	847.884	813.899	739.606	630.631	536.154	721.599	33.167
TPSSh/AE+DKHSO+ZPE+BSSE	898.541	839.536	806.908	725.475	625.539	526.942	714.974	32.286

Table S10: Bond energies (D_e or D_0, kJ/mol) of AnO^+, and their mean absolute deviations from experiment.[2]

Method	ThO^+	PaO^+	UO^+	NpO^+	PuO^+	AmO^+	CmO^+	MAD
Expt[2]	843.000	800.000	774.000	760.000	651.000	560.000	670.000	
B3LYP[3]	870.000	783.000	750.000	677.000	564.000	444.000	593.000	61.571
B3LYP/PP	890.253	789.332	749.066	680.163	559.829	448.571	579.772	65.074
B3LYP/PP+ZPE+BSSE	877.156	773.119	777.314	669.589	554.274	437.988	577.766	66.533
B3LYP/AE+DKH	933.446	801.127	683.519	681.102	562.214	457.601	614.889	72.464
B3LYP/AE+DKH+ZPE+BSSE	920.349	784.914	711.768	670.528	556.660	447.018	612.883	72.654
B3LYP/AE+DKHSO	936.927	772.379	735.081	667.504	554.057	449.857	617.718	73.190
B3LYP/AE+DKHSO+ZPE+BSSE	923.831	756.166	763.330	656.930	548.502	439.274	615.712	73.702
TPSS/PP	903.543	855.591	824.056	725.031	613.185	501.187	627.581	48.601
TPSS/PP+ZPE+BSSE	874.499	846.645	781.030	720.953	602.602	490.628	616.749	42.177
TPSS/AE+DKH	1365.674	851.279	837.617	722.931	628.650	506.610	704.468	112.121
TPSS/AE+DKH+ZPE+BSSE	1336.630	842.333	794.590	718.852	618.066	496.052	693.636	102.603
TPSS/AE+DKHSO	916.071	849.775	1189.000	716.360	609.839	500.237	706.958	102.767
TPSS/AE+DKHSO+ZPE+BSSE	887.028	840.829	1145.974	712.282	599.256	489.678	696.125	93.249
TPSSh/PP	883.510	831.011	804.795	708.530	590.881	474.082	617.685	50.305
TPSSh/PP+ZPE+BSSE	870.393	811.205	790.132	698.408	585.745	463.988	615.429	47.451
TPSSh/AE+DKH	883.830	833.254	803.911	707.569	590.056	481.475	639.391	46.643
TPSSh/AE+DKH+ZPE+BSSE	870.713	813.448	789.248	697.447	584.920	471.381	637.136	43.789
TPSSh/AE+DKHSO	887.693	793.636	810.846	695.673	579.882	474.582	630.178	49.798
TPSSh/AE+DKHSO+ZPE+BSSE	874.576	773.831	796.182	685.551	574.746	464.487	627.923	52.603

Table S11: Bond energies (D_e or D_0, kJ/mol) of AnO^{2+}, and their mean absolute deviations from experiment.[2]

Method	ThO^{2+}	PaO^{2+}	UO^{2+}	NpO^{2+}	PuO^{2+}	AmO^{2+}	CmO^{2+}	MAD
Expt[2]	829.000	781.000	706.000	524.000	439.000	439.000	342.000	
B3LYP/PP	868.285	756.676	622.364	475.335	307.458	136.219	288.779	97.636
B3LYP/PP+ZPE+BSSE	858.158	740.878	698.622	469.316	302.241	127.737	289.592	90.253
B3LYP/AE+DKH	850.298	788.344	633.302	616.973	325.226	154.984	336.458	85.378
B3LYP/AE+DKH+ZPE+BSSE	840.171	772.546	709.560	610.954	320.009	146.503	337.271	75.194
B3LYP/AE+DKHSO	847.132	785.199	592.598	606.568	312.808	143.309	310.338	95.978
B3LYP/AE+DKHSO+ZPE+BSSE	837.006	769.401	668.856	600.549	307.591	134.828	311.151	85.675
TPSS/PP	897.064	770.782	658.505	521.887	365.038	200.228	314.539	66.869
TPSS/PP+ZPE+BSSE	901.281	741.072	639.589	511.204	355.022	191.573	315.930	78.413
TPSS/AE+DKH	886.460	821.308	625.743	536.184	391.749	212.699	346.950	66.959
TPSS/AE+DKH+ZPE+BSSE	890.677	791.598	606.827	525.501	381.732	204.045	348.342	67.359
TPSS/AE+DKHSO	884.136	819.631	615.947	526.649	381.336	202.137	335.295	69.672
TPSS/AE+DKHSO+ZPE+BSSE	888.353	789.922	597.031	515.967	371.319	193.482	336.686	71.970
TPSSh/PP	879.703	756.204	639.615	491.499	324.324	153.355	295.866	88.691
TPSSh/PP+ZPE+BSSE	856.704	735.709	555.767	465.010	314.505	145.325	296.413	106.568
TPSSh/AE+DKH	891.160	777.201	637.152	527.810	345.702	167.843	326.968	74.015
TPSSh/AE+DKH+ZPE+BSSE	868.162	756.706	553.303	501.320	335.883	159.813	327.515	90.803
TPSSh/AE+DKHSO	888.540	767.193	627.020	517.831	334.500	156.842	315.029	81.732
TPSSh/AE+DKHSO+ZPE+BSSE	865.542	746.698	543.171	491.342	324.681	148.812	315.577	99.609

Table S12: Bond energies (D_e or D_0, kJ/mol) of AnO_2, and their mean absolute deviations from experiment.[2]

Method	ThO_2	PaO_2	UO_2	NpO_2	PuO_2	AmO_2	CmO_2	MAD
Expt[2]	684.000	780.000	750.000	632.000	599.000	509.000	405.000	
B3LYP/PP	662.927	794.151	726.462	653.421	552.752	478.229	423.843	25.149
B3LYP/PP+ZPE+BSSE	630.124	727.175	782.945	642.230	544.078	466.861	413.041	36.425
B3LYP/AE+DKH	657.284	792.388	782.344	671.901	596.602	496.195	439.411	22.995
B3LYP/AE+DKH+ZPE+BSSE	624.481	725.411	838.826	660.710	587.928	484.827	428.609	41.500
B3LYP/AE+DKHSO	658.381	789.874	774.987	669.933	596.447	491.667	437.168	21.495
B3LYP/AE+DKHSO+ZPE+BSSE	625.578	722.898	831.470	658.742	587.773	480.299	426.366	40.719
TPSS/PP	720.731	835.342	759.113	715.031	660.658	535.097	492.615	51.369
TPSS/PP+ZPE+BSSE	712.564	828.563	747.532	710.388	654.794	524.017	480.196	43.427
TPSS/AE+DKH	404.525	478.642	769.541	705.747	150.331	-18.961	-108.966	309.245
TPSS/AE+DKH+ZPE+BSSE	396.357	471.863	757.960	701.103	144.467	-30.040	-121.385	313.257
TPSS/AE+DKHSO	426.791	498.547	765.133	699.686	180.706	12.223	-69.999	287.364
TPSS/AE+DKHSO+ZPE+BSSE	418.624	491.769	753.551	695.042	174.842	1.143	-82.418	291.376
TPSSh/PP	698.483	814.349	725.325	678.890	623.532	501.418	453.327	28.691
TPSSh/PP+ZPE+BSSE	689.647	800.241	712.173	672.877	616.795	490.502	442.866	25.536
TPSSh/AE+DKH	700.134	820.466	747.702	697.672	645.588	519.308	468.383	34.979
TPSSh/AE+DKH+ZPE+BSSE	691.298	806.359	734.549	691.659	638.850	508.392	457.922	28.878
TPSSh/AE+DKHSO	701.770	818.510	741.715	696.681	644.274	514.602	466.809	34.561
TPSSh/AE+DKHSO+ZPE+BSSE	692.934	804.402	728.563	690.668	637.536	503.685	456.348	29.806

Table S13: Bond energies (D_e or D_0, kJ/mol) of AnO_2^+, and their mean absolute deviations from experiment.[2]

Method	ThO_2^+	PaO_2^+	UO_2^+	NpO_2^+	PuO_2^+	AmO_2^+	CmO_2^+	MAD
Expt[2]	462.000	780.000	741.000	610.000	509.000	410.000	202.000	
B3LYP/PP	471.236	811.074	721.157	588.766	559.560	430.902	266.441	31.041
B3LYP/PP+ZPE+BSSE	462.095	801.825	700.895	573.827	534.245	415.739	244.413	24.514
B3LYP/AE+DKH	464.161	812.326	786.542	605.148	588.147	453.210	304.543	44.255
B3LYP/AE+DKH+ZPE+BSSE	455.020	803.077	766.280	590.210	562.833	438.047	282.515	33.932
B3LYP/AE+DKHSO	464.537	834.586	729.116	605.510	583.340	448.009	300.401	40.607
B3LYP/AE+DKHSO+ZPE+BSSE	455.396	825.337	708.854	590.572	558.026	432.845	278.373	35.966
TPSS/PP	543.035	844.143	756.099	706.588	622.279	510.595	355.448	89.169
TPSS/PP+ZPE+BSSE	551.733	828.102	776.831	685.972	607.380	495.673	342.488	82.026
TPSS/AE+DKH	214.285	488.866	353.498	239.247	119.456	-48.538	-241.515	369.814
TPSS/AE+DKH+ZPE+BSSE	222.983	472.825	374.230	218.631	104.558	-63.460	-254.474	376.958
TPSS/AE+DKHSO	235.238	507.699	377.732	262.262	146.073	-17.669	-204.925	343.942
TPSS/AE+DKHSO+ZPE+BSSE	243.935	491.658	398.464	241.646	131.174	-32.591	-217.885	351.085
TPSSh/PP	513.438	829.647	726.007	673.239	584.436	461.888	298.875	57.645
TPSSh/PP+ZPE+BSSE	571.678	896.270	792.579	748.720	660.447	554.229	386.356	128.040
TPSSh/AE+DKH	510.023	836.429	749.369	673.006	614.148	482.872	334.267	69.445
TPSSh/AE+DKH+ZPE+BSSE	502.794	831.248	741.739	658.434	593.803	467.485	312.730	56.319
TPSSh/AE+DKHSO	510.295	870.170	743.537	672.276	612.132	477.633	330.307	71.764
TPSSh/AE+DKHSO+ZPE+BSSE	503.066	864.989	735.907	657.704	591.787	462.247	308.770	60.094

Table S14: Bond energies (D_e or D_0, kJ/mol) of AnO_2^{2+}, and their mean absolute deviations from experiment.[2]

Method	ThO_2^{2+}	PaO_2^{2+}	UO_2^{2+}	NpO_2^{2+}	PuO_2^{2+}	AmO_2^{2+}	CmO_2^{2+}	MAD
Expt[2]	N/A	317.000	529.000	504.000	403.000	256.000	N/A	
B3LYP/PP	47.139	378.072	507.145	414.822	310.752	288.740	184.100	59.419
B3LYP/PP+ZPE+BSSE	36.808	373.801	493.147	394.707	294.374	270.939	168.085	65.103
B3LYP/AE+DKH	38.427	375.303	530.064	423.046	341.829	314.229	238.404	51.944
B3LYP/AE+DKH+ZPE+BSSE	28.096	371.032	516.066	402.931	325.451	296.428	222.389	57.202
B3LYP/AE+DKHSO	39.570	372.035	553.994	417.343	337.989	310.009	236.028	57.141
B3LYP/AE+DKHSO+ZPE+BSSE	29.239	367.764	539.996	397.228	321.611	292.208	220.012	57.226
TPSS/PP	129.188	440.698	542.294	503.748	459.088	368.214	309.902	61.109
TPSS/PP+ZPE+BSSE	123.566	346.576	544.565	490.015	450.744	351.304	294.382	40.435
TPSS/AE+DKH	-222.112	62.101	189.300	0.455	-139.870	-196.319	-296.517	418.667
TPSS/AE+DKH+ZPE+BSSE	-227.734	-32.021	191.570	-13.278	-148.214	-213.229	-312.037	444.834
TPSS/AE+DKHSO	-200.809	80.969	208.892	22.642	-112.892	-164.572	-257.910	394.792
TPSS/AE+DKHSO+ZPE+BSSE	-206.431	-13.154	211.163	8.909	-121.236	-181.482	-273.431	420.960
TPSSh/PP	98.640	405.993	515.667	467.273	423.157	323.329	235.660	45.308
TPSSh/PP+ZPE+BSSE	117.421	420.976	583.887	469.658	408.284	306.231	220.139	49.744
TPSSh/AE+DKH	68.781	403.161	542.446	445.344	357.309	347.622	284.941	59.115
TPSSh/AE+DKH+ZPE+BSSE	87.562	418.144	610.667	447.729	342.437	330.524	269.420	74.834
TPSSh/AE+DKHSO	69.134	400.147	536.633	439.457	352.841	343.740	283.219	58.644
TPSSh/AE+DKHSO+ZPE+BSSE	87.915	415.130	604.854	441.842	337.969	326.642	267.698	74.363

Converged cartesian atomic coordinates of all nitrogen containing systems.

$[Th(OPh)_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Th	-1.040617	0.575588	2.086218
N	0.281352	-0.492777	0.271882
O	-2.182767	2.430925	2.055752
O	-2.472511	-1.001655	2.530123
O	0.549221	0.955885	3.522007
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C	-2.239376	4.804018	2.376136
C	-2.942425	6.008779	2.307487
H	-2.449258	6.935305	2.611659
C	-4.265583	6.035861	1.854889
H	-4.811451	6.980016	1.802980
C	-4.882366	4.841136	1.469496
H	-5.915774	4.848888	1.114236
C	-4.189130	3.630470	1.533921
C	-3.412638	-1.933876	2.842274
C	-4.671818	-1.536591	3.318703
C	-5.631825	-2.500122	3.636069
H	-6.609025	-2.181057	4.006655
C	-5.351166	-3.861728	3.483228
H	-6.104813	-4.611322	3.732551
C	-4.095377	-4.253681	3.008316
H	-3.863673	-5.314396	2.884894
C	-3.127199	-3.299390	2.688236
C	1.513533	1.257339	4.432277
C	1.345518	2.341783	5.307672
C	2.340696	2.645120	6.239506
H	2.200548	3.491005	6.916939
C	3.507558	1.877273	6.310020
H	4.282770	2.118183	7.040124
C	3.671227	0.797292	5.436485
H	4.578064	0.189314	5.482059
C	2.682794	0.483957	4.500910
N	-0.281352	0.492777	-0.271882
Th	1.040617	-0.575588	-2.086218
O	2.182767	-2.430925	-2.055752
O	2.472511	1.001655	-2.530123
O	-0.549221	-0.955885	-3.522007
C	2.860936	-3.606055	-1.988536
C	2.239376	-4.804018	-2.376136
C	2.942425	-6.008779	-2.307487
H	2.449258	-6.935305	-2.611659
C	4.265583	-6.035861	-1.854889
H	4.811451	-6.980016	-1.802980
C	4.882366	-4.841136	-1.469496
H	5.915774	-4.848888	-1.114236
C	4.189130	-3.630470	-1.533921
C	3.412638	1.933876	-2.842274
C	4.671818	1.536591	-3.318703
C	5.631825	2.500122	-3.636069
H	6.609025	2.181057	-4.006655
C	5.351166	3.861728	-3.483228
H	6.104813	4.611322	-3.732551
C	4.095377	4.253681	-3.008316
H	3.863673	5.314396	-2.884894
C	3.127199	3.299390	-2.688236
C	-1.513533	-1.257339	-4.432277
C	-1.345518	-2.341783	-5.307672
C	-2.340696	-2.645120	-6.239506
H	-2.200548	-3.491005	-6.916939
C	-3.507558	-1.877273	-6.310020
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H	-4.578064	-0.189314	-5.482059
C	-2.682794	-0.483957	-4.500910
H	-2.144086	-3.597740	2.317656
H	-4.884315	-0.471556	3.435636
H	4.664873	-2.693691	-1.235254
H	1.206150	-4.775486	-2.729393
H	2.802643	-0.358473	3.816222
H	0.431495	2.936807	5.247458
H	-4.664873	2.693691	1.235254
H	-1.206150	4.775486	2.729393
H	2.144086	3.597740	-2.317656
H	4.884315	0.471556	-3.435636
H	-2.802643	0.358473	-3.816222
H	-0.431495	-2.936807	-5.247458

$[Pa(OPh)_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Pa	-0.914678	0.616054	1.888878
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O	-1.797103	2.539315	1.663054
O	-2.220032	-0.917505	2.581161
O	0.382745	0.906431	3.547295
C	-2.284122	3.804714	1.546459
C	-1.931796	4.784274	2.487175
C	-2.437606	6.079792	2.360025
H	-2.159440	6.838128	3.095844
C	-3.292815	6.409177	1.303269
H	-3.685758	7.423470	1.208688
C	-3.640431	5.428130	0.368825
H	-4.307656	5.674245	-0.460736
C	-3.141406	4.128892	0.484330
C	-2.989557	-1.920883	3.082515
C	-4.299905	-1.653929	3.507143
C	-5.086818	-2.687440	4.019828
H	-6.106325	-2.472134	4.348714
C	-4.580166	-3.987781	4.113660
H	-5.199414	-4.792480	4.515004
C	-3.273389	-4.248337	3.688373
H	-2.866973	-5.260299	3.756279

C	-2.476375	-3.223584	3.173803
C	1.230399	1.100696	4.594079
C	0.896030	0.614164	5.866753
C	1.769599	0.817593	6.937167
H	1.503616	0.436049	7.925891
C	2.974993	1.502479	6.751349
H	3.654483	1.658944	7.591570
C	3.302845	1.984727	5.479927
H	4.242195	2.520391	5.323054
C	2.438166	1.787918	4.401142
N	-0.607061	0.006781	-0.310744
Pa	0.914678	-0.616054	-1.888878
O	1.797103	-2.539315	-1.663054
O	2.220032	0.917505	-2.581161
O	-0.382745	-0.906431	-3.547295
C	2.284122	-3.804714	-1.546459
C	1.931796	-4.784274	-2.487175
C	2.437606	-6.079792	-2.360025
H	2.159440	-6.838128	-3.095844
C	3.292815	-6.409177	-1.303269
H	3.685758	-7.423470	-1.208688
C	3.640431	-5.428130	-0.368825
H	4.307656	-5.674245	0.460736
C	3.141406	-4.128892	-0.484330
C	2.989557	1.920883	-3.082515
C	4.299905	1.653929	-3.507143
C	5.086818	2.687440	-4.019828
H	6.106325	2.472134	-4.348714
C	4.580166	3.987781	-4.113660
H	5.199414	4.792480	-4.515004
C	3.273389	4.248337	-3.688373
H	2.866973	5.260299	-3.756279
C	2.476375	3.223584	-3.173803
C	-1.230399	-1.100696	-4.594079
C	-0.896030	-0.614164	-5.866753
C	-1.769599	-0.817593	-6.937167
H	-1.503616	-0.436049	-7.925891
C	-2.974993	-1.502479	-6.751349
H	-3.654483	-1.658944	-7.591570
C	-3.302845	-1.984727	-5.479927
H	-4.242195	-2.520391	-5.323054
C	-2.438166	-1.787918	-4.401142
H	-1.455534	-3.418481	2.838517
H	-4.686733	-0.635725	3.429313
H	3.405439	-3.355605	0.239922
H	1.263813	-4.517141	-3.308712
H	2.685429	2.158465	3.404246
H	-0.046875	0.080099	6.000767
H	-3.405439	3.355605	-0.239922
H	-1.263813	4.517141	3.308712
H	1.455534	3.418481	-2.838517
H	4.686733	0.635725	-3.429313
H	-2.685429	-2.158465	-3.404246
H	0.046875	-0.080099	-6.000767

$[Np(OPh)_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Np	-1.031677	0.628646	1.995153
N	0.555245	0.015467	0.273112
O	-1.930186	2.527853	1.872696
O	-2.316320	-0.857573	2.753021
O	0.369683	0.858513	3.546656
C	-2.451862	3.781407	1.837816
C	-1.963460	4.771236	2.705465
C	-2.503481	6.058109	2.662828
H	-2.118234	6.823633	3.340683
C	-3.527957	6.370627	1.762765
H	-3.946397	7.378725	1.733377
C	-4.011558	5.380882	0.900793
H	-4.811520	5.613992	0.193928
C	-3.479868	4.090049	0.933261
C	-3.101751	-1.815066	3.309588
C	-4.495034	-1.765603	3.143302
C	-5.297940	-2.753778	3.716449
H	-6.381687	-2.708196	3.583035
C	-4.726016	-3.795100	4.455565
H	-5.358111	-4.565784	4.901285
C	-3.337164	-3.840068	4.619203
H	-2.879580	-4.648410	5.195228
C	-2.523292	-2.857745	4.051482
C	1.187682	1.026319	4.613962
C	0.709780	0.796358	5.914891
C	1.560670	0.969711	7.008322
H	1.180567	0.789480	8.016921
C	2.888266	1.370265	6.820993
H	3.549673	1.504339	7.679452
C	3.360269	1.598336	5.523500
H	4.395493	1.912081	5.364946
C	2.519473	1.429705	4.421583
N	-0.555245	-0.015467	-0.273112
Np	1.031677	-0.628646	-1.995153
O	1.930186	-2.527853	-1.872696
O	2.316320	0.857573	-2.753021
O	-0.369683	-0.858513	-3.546656
C	2.451862	-3.781407	-1.837816
C	1.963460	-4.771236	-2.705465
C	2.503481	-6.058109	-2.662828
H	2.118234	-6.823633	-3.340683
C	3.527957	-6.370627	-1.762765
H	3.946397	-7.378725	-1.733377
C	4.011558	-5.380882	-0.900793
H	4.811520	-5.613992	-0.193928
C	3.479868	-4.090049	-0.933261
C	3.101751	1.815066	-3.309588
C	4.495034	1.765603	-3.143302

C	5.297940	2.753778	-3.716449
H	6.381687	2.708196	-3.583035
C	4.726016	3.795100	-4.455565
H	5.358111	4.565784	-4.901285
C	3.337164	3.840068	-4.619203
H	2.879580	4.648410	-5.195228
C	2.523292	2.857745	-4.051482
C	-1.187682	-1.026319	-4.613962
C	-0.709780	-0.796358	-5.914891
C	-1.560670	-0.969711	-7.008322
H	-1.180567	-0.789480	-8.016921
C	-2.888266	-1.370265	-6.820993
H	-3.549673	-1.504339	-7.679452
C	-3.360269	-1.598336	-5.523500
H	-4.395493	-1.912081	-5.364946
C	-2.519473	-1.429705	-4.421583
H	-1.438396	-2.883298	4.175313
H	-4.931999	-0.948355	2.565212
H	3.850132	-3.310554	-0.264048
H	1.163992	-4.516712	-3.404410
H	2.877848	1.605649	3.404872
H	-0.327589	0.482741	6.051597
H	-3.850132	3.310554	0.264048
H	-1.163992	4.516712	3.404410
H	1.438396	2.883298	-4.175313
H	4.931999	0.948355	-2.565212
H	-2.877848	-1.605649	-3.404872
H	0.327589	-0.482741	-6.051597

$[Pu(OPh)_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Pu	-0.925827	0.694025	2.061728
N	0.437927	-0.301675	0.299514
O	-1.979254	2.514665	2.018296
O	-2.252254	-0.852472	2.568631
O	0.450463	1.016218	3.618737
C	-2.583825	3.718891	2.139940
C	-1.980225	4.743753	2.889275
C	-2.611930	5.982910	3.006857
H	-2.136045	6.774456	3.590798
C	-3.843559	6.215521	2.384868
H	-4.333612	7.186564	2.480115
C	-4.441661	5.193595	1.639362
H	-5.403018	5.365353	1.149143
C	-3.820169	3.950161	1.513243
C	-3.144087	-1.785789	2.977371
C	-4.395240	-1.395937	3.484117
C	-5.309257	-2.365715	3.899552
H	-6.279941	-2.054152	4.292857
C	-4.991268	-3.725675	3.816092
H	-5.709703	-4.480185	4.142701
C	-3.744397	-4.110381	3.311600
H	-3.485009	-5.169624	3.243258
C	-2.821403	-3.150494	2.892833
C	1.253153	1.378901	4.646044
C	0.781007	2.250384	5.642726
C	1.617957	2.618998	6.697317
H	1.242852	3.296110	7.468546
C	2.926065	2.128224	6.772138
H	3.576835	2.419490	7.599052
C	3.392733	1.259764	5.779296
H	4.412269	0.869839	5.829165
C	2.565627	0.882545	4.720112
N	-0.437927	0.301675	-0.299514
Pu	0.925827	-0.694025	-2.061728
O	1.979254	-2.514665	-2.018296
O	2.252254	0.852472	-2.568631
O	-0.450463	-1.016218	-3.618737
C	2.583825	-3.718891	-2.139940
C	1.980225	-4.743753	-2.889275
C	2.611930	-5.982910	-3.006857
H	2.136045	-6.774456	-3.590798
C	3.843559	-6.215521	-2.384868
H	4.333612	-7.186564	-2.480115
C	4.441661	-5.193595	-1.639362
H	5.403018	-5.365353	-1.149143
C	3.820169	-3.950161	-1.513243
C	3.144087	1.785789	-2.977371
C	4.395240	1.395937	-3.484117
C	5.309257	2.365715	-3.899552
H	6.279941	2.054152	-4.292857
C	4.991268	3.725675	-3.816092
H	5.709703	4.480185	-4.142701
C	3.744397	4.110381	-3.311600
H	3.485009	5.169624	-3.243258
C	2.821403	3.150494	-2.892833
C	-1.253153	-1.378901	-4.646044
C	-0.781007	-2.250384	-5.642726
C	-1.617957	-2.618998	-6.697317
H	-1.242852	-3.296110	-7.468546
C	-2.926065	-2.128224	-6.772138
H	-3.576835	-2.419490	-7.599052
C	-3.392733	-1.259764	-5.779296
H	-4.412269	-0.869839	-5.829165
C	-2.565627	-0.882545	-4.720112
H	-1.844706	-3.440295	2.499734
H	-4.634514	-0.332156	3.545237
H	4.276500	-3.145729	-0.932826
H	1.018822	-4.552433	-3.370992
H	2.918369	0.203892	3.940864
H	-0.242311	2.626348	5.577017
H	-4.276500	3.145729	0.932826
H	-1.018822	4.552433	3.370992
H	1.844706	3.440295	-2.499734
H	4.634514	0.332156	-3.545237

H -2.918369 -0.203892 -3.940864
H 0.242311 -2.626348 -5.577017

$[ThF_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Th -1.040320 0.574176 2.079518
N 0.260369 -0.510040 0.260836
F -2.168672 2.373921 2.067443
F -2.452701 -0.954592 2.510650
F 0.526924 0.955435 3.462970
N -0.260369 0.510040 -0.260836
Th 1.040320 -0.574176 -2.079518
F 2.168672 -2.373921 -2.067443
F 2.452701 0.954592 -2.510650
F -0.526924 -0.955435 -3.462970

$[PaF_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pa -0.912077 0.612953 1.877312
N 0.607338 -0.008000 0.301661
F -1.811156 2.484660 1.700027
F -2.217906 -0.849367 2.584484
F 0.362373 0.896269 3.502003
N -0.607338 0.008000 -0.301661
Pa 0.912077 -0.612953 -1.877312
F 1.811156 -2.484660 -1.700027
F 2.217906 0.849367 -2.584484
F -0.362373 -0.896269 -3.502003

$[UF_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
U -0.880208 0.644439 2.070058
N 0.568033 0.004995 0.250645
F -1.788752 2.465322 1.687617
F -2.148726 -0.911155 2.578578
F 0.330007 0.961412 3.736175
N -0.568033 -0.004995 -0.250645
U 0.880208 -0.644439 -2.070058
F 1.788752 -2.465322 -1.687617
F 2.148726 0.911155 -2.578578
F -0.330007 -0.961412 -3.736175

$[NpF_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Np -0.907338 0.629044 2.052533
N 0.563119 0.000558 0.248759
F -1.743646 2.483930 1.697349
F -2.134633 -0.945592 2.582192
F 0.248993 0.922271 3.722651
N -0.563119 -0.000558 -0.248759
Np 0.907338 -0.629044 -2.052533
F 1.743646 -2.483930 -1.697349
F 2.134633 0.945592 -2.582192
F -0.248993 -0.922271 -3.722651

$[PuF_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pu -0.977702 0.751008 2.036041
N 0.285052 -0.441859 0.298990
F -2.101098 2.453176 2.215193
F -2.287088 -0.758832 2.506221
F 0.508241 1.050168 3.419318
N -0.285052 0.441859 -0.298990
Pu 0.977702 -0.751008 -2.036041
F 2.101098 -2.453176 -2.215193
F 2.287088 0.758832 -2.506221
F -0.508241 -1.050168 -3.419318

$[ThCl_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Th -1.029244 0.558629 2.053926
N 0.279563 -0.493904 0.268112
Cl -2.364688 2.777024 1.929332
Cl -2.701494 -1.351578 2.578449
Cl 0.899620 0.966132 3.735783
N -0.279563 0.493904 -0.268112
Th 1.029244 -0.558629 -2.053926
Cl 2.364688 -2.777024 -1.929332
Cl 2.701494 1.351578 -2.578449
Cl -0.899620 -0.966132 -3.735783

$[PaCl_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pa -0.906541 0.585231 1.866866
N 0.570603 0.316793 0.177856
Cl -2.059173 2.819160 1.526465
Cl -2.593453 -1.088863 2.768882
Cl 0.729329 0.792468 3.801450
N -0.570603 -0.316793 -0.177856
Pa 0.906541 -0.585231 -1.866866
Cl 2.059173 -2.819160 -1.526465
Cl 2.593453 1.088863 -2.768882
Cl -0.729329 -0.792468 -3.801450

$[UCl_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
U -0.934164 0.555079 1.930039
N 0.534303 0.306420 0.170262
Cl -2.076761 2.761233 1.532350
Cl -2.602404 -1.129578 2.778991
Cl 0.693886 0.767996 3.839638
N -0.534303 -0.306420 -0.170262
U 0.934164 -0.555079 -1.930039
Cl 2.076761 -2.761233 -1.532350
Cl 2.602404 1.129578 -2.778991
Cl -0.693886 -0.767996 -3.839638

$[NpCl_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Np -0.909250 0.624171 2.036669
N 0.561507 -0.000354 0.247198
Cl -1.948773 2.867284 1.589447
Cl -2.424311 -1.282584 2.655445

Cl 0.575447 0.966592 4.028361
N -0.561507 0.000354 -0.247198
Np 0.909250 -0.624171 -2.036669
Cl 1.948773 -2.867284 -1.589447
Cl 2.424311 1.282584 -2.655445
Cl -0.575447 -0.966592 -4.028361

$[PuCl_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pu -0.939625 0.693877 2.069699
N 0.445474 -0.277796 0.295679
Cl -2.162291 2.869125 1.939329
Cl -2.496378 -1.175381 2.648620
Cl 0.755567 1.044885 3.872266
N -0.445474 0.277796 -0.295679
Pu 0.939625 -0.693877 -2.069699
Cl 2.162291 -2.869125 -1.939329
Cl 2.496378 1.175381 -2.648620
Cl -0.755567 -1.044885 -3.872266

$[ThBr_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Th -1.023387 0.564939 2.046917
N 0.258857 -0.506813 0.264152
Br -2.455981 2.909003 1.899397
Br -2.782178 -1.473733 2.598049
Br 1.036256 0.969954 3.820534
N -0.258857 0.506813 -0.264152
Th 1.023387 -0.564939 -2.046917
Br 2.455981 -2.909003 -1.899397
Br 2.782178 1.473733 -2.598049
Br -1.036256 -0.969954 -3.820534

$[PaBr_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pa -0.898158 0.633598 1.849104
N 0.499843 -0.298661 0.345062
Br -2.178361 3.004110 1.684827
Br -2.639325 -1.269530 2.619525
Br 0.873864 1.050785 3.842244
N -0.499843 0.298661 -0.345062
Pa 0.898158 -0.633598 -1.849104
Br 2.178361 -3.004110 -1.684827
Br 2.639325 1.269530 -2.619525
Br -0.873864 -1.050785 -3.842244

$[UBr_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
U -0.937800 0.633646 1.903970
N 0.468838 -0.284307 0.325906
Br -2.216576 2.976021 1.712083
Br -2.638960 -1.315619 2.570677
Br 0.836069 1.030546 3.867171
N -0.468838 0.284307 -0.325906
U 0.937800 -0.633646 -1.903970
Br 2.216576 -2.976021 -1.712083
Br 2.638960 1.315619 -2.570677
Br -0.836069 -1.030546 -3.867171

$[NpBr_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Np -0.920603 0.624652 2.023208
N 0.560974 0.000129 0.249468
Br -2.034900 3.002625 1.549562
Br -2.535144 -1.397969 2.673563
Br 0.708443 0.970929 4.102511
N -0.560974 -0.000129 -0.249468
Np 0.920603 -0.624652 -2.023208
Br 2.034900 -3.002625 -1.549562
Br 2.535144 1.397969 -2.673563
Br -0.708443 -0.970929 -4.102511

$[PuBr_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pu -0.916667 0.698760 2.063466
N 0.302794 -0.437625 0.284354
Br -2.325657 2.948522 1.955140
Br -2.585963 -1.286155 2.646174
Br 0.986323 1.061060 3.888249
N -0.302794 0.437625 -0.284354
Pu 0.916667 -0.698760 -2.063466
Br 2.325657 -2.948522 -1.955140
Br 2.585963 1.286155 -2.646174
Br -0.986323 -1.061060 -3.888249

$[ThH_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Th -1.096848 0.426168 2.046318
N 0.462475 -0.292908 0.308871
H -1.932196 2.316524 1.769181
H -2.460713 -1.008201 2.729521
H 0.470050 0.796290 3.371353
N -0.462475 0.292908 -0.308871
Th 1.096848 -0.426168 -2.046318
H 1.932196 -2.316524 -1.769181
H 2.460713 1.008201 -2.729521
H -0.470050 -0.796290 -3.371353

$[PaH_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pa -0.999644 0.602219 1.812390
N 0.600527 -0.012486 0.320717
H -1.853673 2.444496 1.711758
H -2.254588 -0.803306 2.576934
H 0.444190 0.816128 3.224268
N -0.600527 0.012486 -0.320717
Pa 0.999644 -0.602219 -1.812390
H 1.853673 -2.444496 -1.711758
H 2.254588 0.803306 -2.576934
H -0.444190 -0.816128 -3.224268

$[UH_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

U -0.791464 0.622642 2.041427
N 0.567335 -0.044876 0.268766
H -1.674188 2.369081 1.535933
H -2.098939 -0.863513 2.444675
H 0.290273 0.968004 3.736021
N -0.567335 0.044876 -0.268766
U 0.791464 -0.622642 -2.041427
H 1.674188 -2.369081 -1.535933
H 2.098939 0.863513 -2.444675
H -0.290273 -0.968004 -3.736021

$[NpH_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Np -0.951716 0.441271 1.978060
N 0.483933 -0.275293 0.302483
H -1.771502 2.258953 1.736189
H -2.375022 -0.805730 2.720203
H 0.355150 0.984916 3.437009
N -0.483933 0.275293 -0.302483
Np 0.951716 -0.441271 -1.978060
H 1.771502 -2.258953 -1.736189
H 2.375022 0.805730 -2.720203
H -0.355150 -0.984916 -3.437009

$[PuH_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pu -0.634765 0.615568 2.108804
N 0.588537 -0.016888 0.183875
H -1.487817 2.271378 1.406379
H -1.845820 -0.957925 2.243899
H 0.110881 1.013327 3.949038
N -0.588537 0.016888 -0.183875
Pu 0.634765 -0.615568 -2.108804
H 1.487817 -2.271378 -1.406379
H 1.845820 0.957925 -2.243899
H -0.110881 -1.013327 -3.949038

$[ThMe_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Th 0.251435 -0.142075 2.378295
N 0.566680 0.268178 -0.042035
C -2.016982 0.095162 3.316814
C 1.323034 -2.125126 3.411630
C 1.234145 1.937624 3.277527
N -0.566680 -0.268178 0.042035
Th -0.251435 0.142075 -2.378295
C 2.016982 -0.095162 -3.316814
C -1.323034 2.125126 -3.411630
C -1.234145 -1.937624 -3.277527
H -2.561704 1.011213 3.015617
H -2.667899 -0.764103 3.055042
H -1.955020 0.116147 4.426346
H 1.996909 2.390808 2.612418
H 0.476675 2.723563 3.473548
H 1.740581 1.740796 4.246828
H 2.175042 -1.853162 4.070433
H 0.614104 -2.700759 4.044393
H 1.728036 -2.849002 2.673061
H 2.667899 0.764103 -3.055042
H 2.561704 -1.011213 -3.015617
H 1.955020 -0.116147 -4.426346
H -0.476675 -2.723563 -3.473548
H -1.996909 -2.390808 -2.612418
H -1.740581 -1.740796 -4.246828
H -0.614104 2.700759 -4.044393
H -2.175042 1.853162 -4.070433
H -1.728036 2.849002 -2.673061

$[PaMe_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
Pa -0.043288 -0.066388 2.170587
N -0.357294 0.579175 0.011899
C -1.909436 -1.241642 3.148206
C 1.916939 -1.069325 3.153934
C 0.085881 2.053531 3.308840
N 0.357294 -0.579175 -0.011899
Pa 0.043288 0.066388 -2.170587
C 1.909436 1.241642 -3.148206
C -1.916939 1.069325 -3.153934
C -0.085881 -2.053531 -3.308840
H -2.630484 -1.653665 2.414971
H -1.544410 -2.097541 3.755169
H -2.486031 -0.587595 3.835324
H -0.165871 2.930318 2.681213
H -0.608360 2.058332 4.175826
H 1.106447 2.218696 3.711214
H 2.802615 -0.403980 3.137659
H 1.709836 -1.310522 4.218207
H 2.208121 -2.015502 2.655803
H -1.709836 1.310522 -4.218207
H -2.802615 0.403980 -3.137659
H -2.208121 2.015502 -2.655803
H 0.608360 -2.058332 -4.175826
H 0.165871 -2.930318 -2.681213
H -1.106447 -2.218696 -3.711214
H 1.544410 2.097541 -3.755169
H 2.630484 1.653665 -2.414971
H 2.486031 0.587595 -3.835324

$[UMe_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$
U -0.010976 -0.193051 2.182381
N -0.332945 0.570938 0.048918
C -1.876986 -1.362028 3.143113
C 1.884792 -1.243989 3.175527
C 0.090838 1.832151 3.436598
N 0.332945 -0.570938 -0.048918
U 0.010976 0.193051 -2.182381
C 1.876986 1.362028 -3.143113

C -1.884792 1.243989 -3.175527
C -0.090838 -1.832151 -3.436598
H -2.585159 -1.715570 2.365215
H -1.555288 -2.253596 3.718753
H -2.453101 -0.717531 3.837822
H -0.479969 2.667632 2.985957
H -0.335469 1.641428 4.443910
H 1.135034 2.174976 3.578486
H 2.709860 -0.524447 3.347358
H 1.583403 -1.645821 4.165692
H 2.290945 -2.087318 2.583247
H -1.583403 1.645821 -4.165692
H -2.709860 0.524447 -3.347358
H -2.290945 2.087318 -2.583247
H 1.555288 2.253596 -3.718753
H 2.585159 1.715570 -2.365215
H 2.453101 0.717531 -3.837822
H 0.335469 -1.641428 -4.443910
H 0.479969 -2.667632 -2.985957
H -1.135034 -2.174976 -3.578486

$[NpMe_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Np 0.001034 0.211481 2.315828
N 0.014102 0.618909 -0.035594
C -1.882753 -1.060582 3.052713
C 1.945513 -1.016344 2.937238
C 0.075739 2.064406 3.833834
N -0.014102 -0.618909 0.035594
Np -0.001034 -0.211481 -2.315828
C 1.882753 1.060582 -3.052713
C -1.945513 1.016344 -2.937238
C -0.075739 -2.064406 -3.833834
H 2.436128 -0.495072 3.786525
H 1.640109 -2.017515 3.308606
H 2.718819 -1.178248 2.162822
H -2.821263 -0.836311 2.506159
H -1.708425 -2.151935 2.966017
H -2.079659 -0.847515 4.124737
H 0.159311 3.004894 3.246893
H -0.871339 2.121222 4.409379
H 0.910854 2.052214 4.559813
H -1.640109 2.017515 -3.308606
H -2.436128 0.495072 -3.786525
H -2.718819 1.178248 -2.162822
H 1.708425 2.151935 -2.966017
H 2.821263 0.836311 -2.506159
H 2.079659 0.847515 -4.124737
H 0.871339 -2.121222 -4.409379
H -0.159311 -3.004894 -3.246893
H -0.910854 -2.052214 -4.559813

$[PuMe_3]_2(\mu\text{-}\eta^2\text{:}\eta^2\text{-}N_2)$

Pu 0.331416 0.317663 2.301236
N 0.274973 0.537613 -0.107592
C -1.844937 0.340331 3.256889
C 1.240925 -1.768504 2.979245
C 1.292463 1.923270 3.800326
N -0.274973 -0.537613 0.107592
Pu -0.331416 -0.317663 -2.301236
C 1.844937 -0.340331 -3.256889
C -1.240925 1.768504 -2.979245
C -1.292463 -1.923270 -3.800326
H -2.604125 0.874805 2.651554
H -2.195048 -0.706041 3.374353
H -1.843482 0.801060 4.264085
H 2.069949 2.476790 3.232059
H 0.529343 2.646834 4.142949
H 1.769436 1.465567 4.686664
H 1.810845 -1.614957 3.920118
H 0.444496 -2.508417 3.192366
H 1.932864 -2.228686 2.246995
H 2.195048 0.706041 -3.374353
H 2.604125 -0.874805 -2.651554
H 1.843482 -0.801060 -4.264085
H -0.529343 -2.646834 -4.142949
H -2.069949 -2.476790 -3.232059
H -1.769436 -1.465567 -4.686664
H -0.444496 2.508417 -3.192366
H -1.810845 1.614957 -3.920118
H -1.932864 2.228686 -2.246995

ThPy

Th	0.000000	0.000000	1.238521
N	0.000000	0.000000	-1.211475
C	0.000000	1.170049	-1.945613
C	0.000000	-1.170049	-1.945613
C	0.000000	1.197860	-3.318961
H	0.000000	2.087561	-1.368093
C	0.000000	-1.197860	-3.318961
H	0.000000	-2.087561	-1.368093
C	0.000000	0.000000	-4.050808
H	0.000000	2.158379	-3.819333
H	0.000000	-2.158379	-3.819333
H	0.000000	0.000000	-5.131945

PaPy

Pa	-1.256935	0.000000	-0.000082
N	1.305279	-0.000004	0.001031
C	2.007931	1.155373	0.000618
C	2.007936	-1.155377	0.000618
C	3.391300	1.195939	-0.000210
H	1.429476	2.071663	0.000886
C	3.391306	-1.195935	-0.000210

H	1.429485	-2.071670	0.000887
C	4.102745	0.000003	-0.000652
H	3.896411	2.152375	-0.000570
H	3.896422	-2.152369	-0.000570
H	5.185036	0.000006	-0.001383

UPy

U	-1.252450	0.000004	-0.000008
N	1.331843	0.001922	0.000105
C	2.028416	1.155486	0.000060
C	2.024962	-1.153426	0.000061
C	3.412960	1.195639	-0.000012
H	1.449666	2.071321	0.000024
C	3.409961	-1.197453	-0.000013
H	1.443421	-2.067636	0.000026
C	4.119048	-0.002062	-0.000057
H	3.920683	2.150414	-0.000082
H	3.915128	-2.153575	-0.000082
H	5.201544	-0.003410	-0.000160

NpPy

Np	0.000000	0.000000	1.240116
N	0.000000	0.000000	-1.334994
C	0.000000	1.155250	-2.029409
C	0.000000	-1.155250	-2.029409
C	0.000000	1.196813	-3.413780
H	0.000000	2.070036	-1.449263
C	0.000000	-1.196813	-3.413780
H	0.000000	-2.070036	-1.449263
C	0.000000	0.000000	-4.120855
H	0.000000	2.152129	-3.920276
H	0.000000	-2.152129	-3.920276
H	0.000000	0.000000	-5.203327

PuPy

Pu	-1.212595	0.000000	-0.000016
N	1.306746	0.000000	0.000210
C	1.997303	1.157400	0.000129
C	1.997303	-1.157400	0.000129
C	3.381117	1.197386	-0.000029
H	1.413428	2.069729	0.000092
C	3.381117	-1.197386	-0.000029
H	1.413428	-2.069729	0.000092
C	4.087311	0.000000	-0.000126
H	3.887623	2.152514	-0.000149
H	3.887623	-2.152514	-0.000149
H	5.169676	0.000000	-0.000314

AmPy

Am	0.000000	0.000000	1.196897
N	0.000000	0.000000	-1.303639
C	0.000000	1.158905	-1.990297
C	0.000000	-1.158905	-1.990297
C	0.000000	1.197991	-3.374132
H	0.000000	2.069606	-1.403818
C	0.000000	-1.197991	-3.374132
H	0.000000	-2.069606	-1.403818
C	0.000000	0.000000	-4.079236
H	0.000000	2.152896	-3.880949
H	0.000000	-2.152896	-3.880949
H	0.000000	0.000000	-5.161625

CmPy

Cm	0.000000	0.000000	1.200807
N	0.000000	0.000000	-1.334427
C	0.000000	1.155743	-2.028090
C	0.000000	-1.155743	-2.028090
C	0.000000	1.196770	-3.412429
H	0.000000	2.069829	-1.446749
C	0.000000	-1.196770	-3.412429
H	0.000000	-2.069829	-1.446749
C	0.000000	0.000000	-4.119495
H	0.000000	2.152088	-3.918913
H	0.000000	-2.152088	-3.918913
H	0.000000	0.000000	-5.201949

ThPz

Th	0.000000	0.000000	1.236858
N	0.000000	0.000000	-1.214322
C	0.000000	1.157559	-1.966432
C	0.000000	-1.157559	-1.966432
C	0.000000	1.133784	-3.337639
H	0.000000	2.095581	-1.425541
C	0.000000	-1.133784	-3.337639
H	0.000000	-2.095581	-1.425541
N	0.000000	0.000000	-4.079796
H	0.000000	2.073738	-3.879252
H	0.000000	-2.073738	-3.879252

PaPz

Pa	1.249096	0.000000	-0.000001
N	-1.296708	-0.000006	0.000002
C	-2.015099	-1.146241	0.000006
C	-2.015091	1.146233	0.000004
C	-3.398996	-1.133100	-0.000006
H	-1.466265	-2.079167	0.000026
C	-3.398987	1.133107	-0.000001
H	-1.466246	2.079153	0.000018
N	-4.113407	0.000006	-0.000005
H	-3.947678	-2.067509	0.000005
H	-3.947658	2.067521	0.000003

UPz

U	-1.297093	0.000000	-0.000090
N	1.446575	-0.000020	0.001482
C	2.146011	1.142717	0.000702
C	2.146021	-1.142749	0.000716
C	3.535430	1.134486	-0.000261
H	1.588398	2.070422	0.000284
C	3.535463	-1.134459	-0.000275
H	1.588454	-2.070480	0.000337
N	4.239168	0.000018	-0.000846
H	4.088941	2.065848	-0.001014
H	4.089023	-2.065793	-0.001071

NpPz

Np	-1.236876	0.000000	0.000099
N	1.342540	0.000000	-0.001174
C	2.044317	1.144733	-0.000856
C	2.044317	-1.144733	-0.000856
C	3.433095	1.134331	0.000314
H	1.490450	2.074345	-0.001525
C	3.433095	-1.134331	0.000314
H	1.490450	-2.074345	-0.001525
N	4.135891	0.000000	0.001025
H	3.985314	2.066087	0.000679
H	3.985314	-2.066087	0.000679

PuPz

Pu	-0.000544	-1.218273	0.000000
N	0.001298	1.332318	0.000000
C	0.001236	2.031932	1.145918
C	0.001236	2.031932	-1.145918
C	0.001236	3.420800	1.134651
H	0.000931	1.477508	2.075211
C	0.001236	3.420800	-1.134651
H	0.000931	1.477508	-2.075211
N	0.001221	4.122544	0.000000
H	0.001004	3.972933	2.066339
H	0.001004	3.972933	-2.066339

AmPz

Am	-0.000316	-1.205667	0.000000
N	0.000694	1.335273	0.000000
C	0.000712	2.032035	1.146791
C	0.000712	2.032035	-1.146791
C	0.000712	3.421538	1.135044
H	0.000528	1.476764	2.075662
C	0.000712	3.421538	-1.135044
H	0.000528	1.476764	-2.075662
N	0.000800	4.121174	0.000000
H	0.000716	3.973417	2.066851
H	0.000716	3.973417	-2.066851

CmPz

Cm	0.000234	-1.208521	0.000000
N	-0.000544	1.367152	0.000000
C	-0.000545	2.067658	1.144930
C	-0.000545	2.067658	-1.144930
C	-0.000545	3.456574	1.134575
H	-0.000603	1.512525	2.073776
C	-0.000545	3.456574	-1.134575
H	-0.000603	1.512525	-2.073776
N	-0.000487	4.159075	0.000000
H	-0.000489	4.009288	2.066080
H	-0.000489	4.009288	-2.066080

ThTz

Th	0.000000	0.000000	1.230003
N	0.000000	0.000000	-1.239511
C	0.000000	1.154135	-2.004150
C	0.000000	-1.154135	-2.004150
N	0.000000	1.195427	-3.309821
H	0.000000	2.092522	-1.460708
N	0.000000	-1.195427	-3.309821
H	0.000000	-2.092522	-1.460708
C	0.000000	0.000000	-3.947698
H	0.000000	0.000000	-5.028759

PaTz

Pa	-1.247046	0.000000	-0.000011
N	1.326938	-0.000002	0.000204
C	2.061456	-1.136054	0.000059
C	2.061454	1.136053	0.000059
N	3.382022	-1.188344	-0.000052
H	1.519473	-2.074062	0.000069
N	3.382020	1.188345	-0.000052
H	1.519468	2.074059	0.000070
C	3.997815	0.000002	-0.000049
H	5.081070	0.000003	-0.000233

UTz

Th	0.000000	0.000000	1.230003
N	0.000000	0.000000	-1.239511
C	0.000000	1.154135	-2.004150
C	0.000000	-1.154135	-2.004150
N	0.000000	1.195427	-3.309821
H	0.000000	2.092522	-1.460708
N	0.000000	-1.195427	-3.309821
H	0.000000	-2.092522	-1.460708
C	0.000000	0.000000	-3.947698
H	0.000000	0.000000	-5.028759

NpTz

Np	1.271743	0.000000	0.000031
N	-1.453005	-0.000026	-0.000109
C	-2.171926	-1.132260	-0.000336
C	-2.171891	1.132245	-0.000334
N	-3.497347	-1.188207	0.000025
H	-1.625042	-2.067407	-0.000923
N	-3.497308	1.188230	0.000024
H	-1.624986	2.067380	-0.000927
C	-4.105923	0.000018	0.000365
H	-5.189980	0.000034	0.001217

PuTz

Pu	1.214413	0.000000	0.000398
N	-1.354108	-0.000002	-0.005375
C	-2.074990	-1.135084	-0.003191
C	-2.074988	1.135082	-0.003191
N	-3.398357	-1.187887	0.001276
H	-1.531025	-2.071581	-0.004741
N	-3.398354	1.187889	0.001276
H	-1.531020	2.071577	-0.004743
C	-4.007625	0.000002	0.003665
H	-5.091464	0.000003	0.008152

AmTz

Am	1.201901	0.000004	0.000000
N	-1.356305	0.000179	0.000000
C	-2.075604	1.136138	0.000002
C	-2.075262	-1.136052	0.000000
N	-3.398942	1.187908	-0.000003
H	-1.530512	2.072065	0.000022
N	-3.398578	-1.188046	0.000006
H	-1.530005	-2.071838	-0.000007
C	-4.007751	-0.000172	-0.000006
H	-5.091621	-0.000330	-0.000001

CmTz

Cm	-1.250305	0.000001	0.000003
N	1.495783	-0.000135	-0.000035
C	2.213231	1.131811	-0.000026
C	2.213436	-1.131955	-0.000026
N	3.539135	1.188427	0.000008
H	1.665817	2.066604	-0.000014
N	3.539359	-1.188287	0.000008
H	1.666232	-2.066867	-0.000013
C	4.147597	0.000130	0.000027
H	5.231718	0.000247	0.000058

$ThPy_3$

Th	0.000000	0.000000	0.000000
N	0.000000	2.605312	0.000000
N	-2.256267	-1.302656	0.000000
N	2.256267	-1.302656	0.000000
C	0.000000	3.309596	1.158926
C	0.000000	3.309596	-1.158926
C	0.000000	4.690894	1.197220
C	0.000000	4.690894	-1.197220
C	0.000000	5.406114	0.000000
H	0.000000	2.730507	2.074554
H	0.000000	2.730507	-2.074554
H	0.000000	5.195647	2.154086
H	0.000000	5.195647	-2.154086
H	0.000000	6.488153	0.000000
C	-2.866194	-1.654798	1.158926
C	-2.866194	-1.654798	-1.158926
C	-4.062433	-2.345447	1.197220
C	-4.062433	-2.345447	-1.197220
C	-4.681832	-2.703057	0.000000
H	-2.364688	-1.365253	2.074554
H	-2.364688	-1.365253	-2.074554
H	-4.499562	-2.597824	2.154086
H	-4.499562	-2.597824	-2.154086
H	-5.618906	-3.244077	0.000000
C	2.866194	-1.654798	1.158926
C	2.866194	-1.654798	-1.158926
C	4.062433	-2.345447	1.197220
C	4.062433	-2.345447	-1.197220
C	4.681832	-2.703057	0.000000
H	2.364688	-1.365253	2.074554
H	2.364688	-1.365253	-2.074554
H	4.499562	-2.597824	2.154086
H	4.499562	-2.597824	-2.154086
H	5.618906	-3.244077	0.000000

$PaPy_3$

Pa	0.000000	0.000000	0.000000
N	0.000000	2.651452	0.000000
N	-2.296225	-1.325726	0.000000
N	2.296225	-1.325726	0.000000
C	0.000000	3.345044	1.154459
C	0.000000	3.345044	-1.154459
C	0.000000	4.729937	1.196872
C	0.000000	4.729937	-1.196872
C	0.000000	5.438676	0.000000
H	0.000000	2.761997	2.067590
H	0.000000	2.761997	-2.067590
H	0.000000	5.236999	2.152225
H	0.000000	5.236999	-2.152225
H	0.000000	6.521163	0.000000
C	-2.896893	-1.672522	1.154459
C	-2.896893	-1.672522	-1.154459
C	-4.096245	-2.364968	1.196872

C	-4.096245	-2.364968	-1.196872
C	-4.710032	-2.719338	0.000000
H	-2.391959	-1.380998	2.067590
H	-2.391959	-1.380998	-2.067590
H	-4.535374	-2.618500	2.152225
H	-4.535374	-2.618500	-2.152225
H	-5.647493	-3.260582	0.000000
C	2.896893	-1.672522	1.154459
C	2.896893	-1.672522	-1.154459
C	4.096245	-2.364968	1.196872
C	4.096245	-2.364968	-1.196872
C	4.710032	-2.719338	0.000000
H	2.391959	-1.380998	2.067590
H	2.391959	-1.380998	-2.067590
H	4.535374	-2.618500	2.152225
H	4.535374	-2.618500	-2.152225
H	5.647493	-3.260582	0.000000

UPy_3

U	0.000000	0.000000	0.000000
N	0.000000	2.653525	0.000000
N	-2.298020	-1.326762	0.000000
N	2.298020	-1.326762	0.000000
C	0.000000	3.343895	1.153835
C	0.000000	3.343895	-1.153835
C	0.000000	4.729447	1.197078
C	0.000000	4.729447	-1.197078
C	0.000000	5.436616	0.000000
H	0.000000	2.759561	2.066109
H	0.000000	2.759561	-2.066109
H	0.000000	5.237105	2.152023
H	0.000000	5.237105	-2.152023
H	0.000000	6.519220	0.000000
C	-2.895898	-1.671947	1.153835
C	-2.895898	-1.671947	-1.153835
C	-4.095821	-2.364724	1.197078
C	-4.095821	-2.364724	-1.197078
C	-4.708248	-2.718308	0.000000
H	-2.389850	-1.379781	2.066109
H	-2.389850	-1.379781	-2.066109
H	-4.535466	-2.618553	2.152023
H	-4.535466	-2.618553	-2.152023
H	-5.645810	-3.259610	0.000000
C	2.895898	-1.671947	1.153835
C	2.895898	-1.671947	-1.153835
C	4.095821	-2.364724	1.197078
C	4.095821	-2.364724	-1.197078
C	4.708248	-2.718308	0.000000
H	2.389850	-1.379781	2.066109
H	2.389850	-1.379781	-2.066109
H	4.535466	-2.618553	2.152023
H	4.535466	-2.618553	-2.152023
H	5.645810	-3.259610	0.000000

$NpPy_3$

Np	0.000000	0.000000	0.000000
N	0.000000	2.607754	0.000000
N	-2.258381	-1.303877	0.000000
N	2.258381	-1.303877	0.000000
C	0.000000	3.299933	1.154288
C	0.000000	3.299933	-1.154288
C	0.000000	4.685056	1.196684
C	0.000000	4.685056	-1.196684
C	0.000000	5.392344	0.000000
H	0.000000	2.718602	2.068247
H	0.000000	2.718602	-2.068247
H	0.000000	5.191942	2.151925
H	0.000000	5.191942	-2.151925
H	0.000000	6.474859	0.000000
C	-2.857826	-1.649966	1.154288
C	-2.857826	-1.649966	-1.154288
C	-4.057378	-2.342528	1.196684
C	-4.057378	-2.342528	-1.196684
C	-4.669907	-2.696172	0.000000
H	-2.354379	-1.359301	2.068247
H	-2.354379	-1.359301	-2.068247
H	-4.496353	-2.595971	2.151925
H	-4.496353	-2.595971	-2.151925
H	-5.607393	-3.237430	0.000000
C	2.857826	-1.649966	1.154288
C	2.857826	-1.649966	-1.154288
C	4.057378	-2.342528	1.196684
C	4.057378	-2.342528	-1.196684
C	4.669907	-2.696172	0.000000
H	2.354379	-1.359301	2.068247
H	2.354379	-1.359301	-2.068247
H	4.496353	-2.595971	2.151925
H	4.496353	-2.595971	-2.151925
H	5.607393	-3.237430	0.000000

$PuPy_3$

Pu	0.000000	0.000000	0.000000
N	0.000000	2.589840	0.000000
N	-2.242867	-1.294920	0.000000
N	2.242867	-1.294920	0.000000
C	0.000000	3.282187	1.154743
C	0.000000	3.282187	-1.154743
C	0.000000	4.667115	1.196584
C	0.000000	4.667115	-1.196584
C	0.000000	5.374425	0.000000

H	0.000000	2.701673	2.069046
H	0.000000	2.701673	-2.069046
H	0.000000	5.173643	2.151964
H	0.000000	5.173643	-2.151964
H	0.000000	6.456927	0.000000
C	-2.842457	-1.641093	1.154743
C	-2.842457	-1.641093	-1.154743
C	-4.041841	-2.333558	1.196584
C	-4.041841	-2.333558	-1.196584
C	-4.654388	-2.687212	0.000000
H	-2.339717	-1.350836	2.069046
H	-2.339717	-1.350836	-2.069046
H	-4.480507	-2.586822	2.151964
H	-4.480507	-2.586822	-2.151964
H	-5.591862	-3.228463	0.000000
C	2.842457	-1.641093	1.154743
C	2.842457	-1.641093	-1.154743
C	4.041841	-2.333558	1.196584
C	4.041841	-2.333558	-1.196584
C	4.654388	-2.687212	0.000000
H	2.339717	-1.350836	2.069046
H	2.339717	-1.350836	-2.069046
H	4.480507	-2.586822	2.151964
H	4.480507	-2.586822	-2.151964
H	5.591862	-3.228463	0.000000

$AmPy_3$

Am	0.000000	0.000000	0.000000
N	0.000000	2.581365	0.000000
N	-2.235527	-1.290682	0.000000
N	2.235527	-1.290682	0.000000
C	0.000000	3.272476	1.155086
C	0.000000	3.272476	-1.155086
C	0.000000	4.657482	1.196776
C	0.000000	4.657482	-1.196776
C	0.000000	5.364533	0.000000
H	0.000000	2.691246	2.068938
H	0.000000	2.691246	-2.068938
H	0.000000	5.164231	2.152044
H	0.000000	5.164231	-2.152044
H	0.000000	6.447044	0.000000
C	-2.834047	-1.636238	1.155086
C	-2.834047	-1.636238	-1.155086
C	-4.033498	-2.328741	1.196776
C	-4.033498	-2.328741	-1.196776
C	-4.645822	-2.682266	0.000000
H	-2.330687	-1.345623	2.068938
H	-2.330687	-1.345623	-2.068938
H	-4.472355	-2.582116	2.152044
H	-4.472355	-2.582116	-2.152044
H	-5.583304	-3.223522	0.000000
C	2.834047	-1.636238	1.155086
C	2.834047	-1.636238	-1.155086
C	4.033498	-2.328741	1.196776
C	4.033498	-2.328741	-1.196776
C	4.645822	-2.682266	0.000000
H	2.330687	-1.345623	2.068938
H	2.330687	-1.345623	-2.068938
H	4.472355	-2.582116	2.152044
H	4.472355	-2.582116	-2.152044
H	5.583304	-3.223522	0.000000

$CmPy_3$

Cm	0.000000	0.000000	0.000000
N	0.000000	2.587145	0.000000
N	-2.240534	-1.293573	0.000000
N	2.240534	-1.293573	0.000000
C	0.000000	3.277373	1.154732
C	0.000000	3.277373	-1.154732
C	0.000000	4.662571	1.196995
C	0.000000	4.662571	-1.196995
C	0.000000	5.369509	0.000000
H	0.000000	2.694566	2.067650
H	0.000000	2.694566	-2.067650
H	0.000000	5.169973	2.151979
H	0.000000	5.169973	-2.151979
H	0.000000	6.452012	0.000000
C	-2.838288	-1.638686	1.154732
C	-2.838288	-1.638686	-1.154732
C	-4.037905	-2.331285	1.196995
C	-4.037905	-2.331285	-1.196995
C	-4.650131	-2.684754	0.000000
H	-2.333563	-1.347283	2.067650
H	-2.333563	-1.347283	-2.067650
H	-4.477328	-2.584987	2.151979
H	-4.477328	-2.584987	-2.151979
H	-5.587607	-3.226006	0.000000
C	2.838288	-1.638686	1.154732
C	2.838288	-1.638686	-1.154732
C	4.037905	-2.331285	1.196995
C	4.037905	-2.331285	-1.196995
C	4.650131	-2.684754	0.000000
H	2.333563	-1.347283	2.067650
H	2.333563	-1.347283	-2.067650
H	4.477328	-2.584987	2.151979
H	4.477328	-2.584987	-2.151979
H	5.587607	-3.226006	0.000000

$ThPz_3$

Th	0.000000	0.000000	0.000000

N	0.000000	2.618952	0.000000
N	-2.268079	-1.309476	0.000000
N	2.268079	-1.309476	0.000000
C	0.000000	3.331820	1.148805
C	0.000000	3.331820	-1.148805
C	0.000000	4.715095	1.134969
C	0.000000	4.715095	-1.134969
N	0.000000	5.429898	0.000000
H	0.000000	2.778275	2.078967
H	0.000000	2.778275	-2.078967
H	0.000000	5.264917	2.068700
H	0.000000	5.264917	-2.068700
C	-2.885441	-1.665910	1.148805
C	-2.885441	-1.665910	-1.148805
C	-4.083392	-2.357547	1.134969
C	-4.083392	-2.357547	-1.134969
N	-4.702430	-2.714949	0.000000
H	-2.406057	-1.389138	2.078967
H	-2.406057	-1.389138	-2.078967
H	-4.559552	-2.632458	2.068700
H	-4.559552	-2.632458	-2.068700
C	2.885441	-1.665910	1.148805
C	2.885441	-1.665910	-1.148805
C	4.083392	-2.357547	1.134969
C	4.083392	-2.357547	-1.134969
N	4.702430	-2.714949	0.000000
H	2.406057	-1.389138	2.078967
H	2.406057	-1.389138	-2.078967
H	4.559552	-2.632458	2.068700
H	4.559552	-2.632458	-2.068700

$PaPz_3$

Pa	0.000000	0.000000	0.000000
N	0.000000	2.679458	0.000000
N	-2.320478	-1.339729	0.000000
N	2.320478	-1.339729	0.000000
C	0.000000	3.381929	1.144720
C	0.000000	3.381929	-1.144720
C	0.000000	4.769714	1.134668
C	0.000000	4.769714	-1.134668
N	0.000000	5.475897	0.000000
H	0.000000	2.825059	2.072991
H	0.000000	2.825059	-2.072991
H	0.000000	5.322497	2.066479
H	0.000000	5.322497	-2.066479
C	-2.928836	-1.690964	1.144720
C	-2.928836	-1.690964	-1.144720
C	-4.130693	-2.384857	1.134668
C	-4.130693	-2.384857	-1.134668
N	-4.742266	-2.737948	0.000000
H	-2.446573	-1.412530	2.072991
H	-2.446573	-1.412530	-2.072991
H	-4.609418	-2.661249	2.066479
H	-4.609418	-2.661249	-2.066479
C	2.928836	-1.690964	1.144720
C	2.928836	-1.690964	-1.144720
C	4.130693	-2.384857	1.134668
C	4.130693	-2.384857	-1.134668
N	4.742266	-2.737948	0.000000
H	2.446573	-1.412530	2.072991
H	2.446573	-1.412530	-2.072991
H	4.609418	-2.661249	2.066479
H	4.609418	-2.661249	-2.066479

UPz_3

U	0.000000	0.000000	0.000000
N	0.000000	2.723807	0.000000
N	-2.358886	-1.361904	0.000000
N	2.358886	-1.361904	0.000000
C	-0.000002	3.421481	1.143326
C	0.000002	3.421481	-1.143326
C	-0.000002	4.810966	1.134867
C	0.000002	4.810966	-1.134867
N	0.000000	5.514111	0.000000
H	-0.000003	2.863071	2.070675
H	0.000003	2.863071	-2.070675
H	-0.000003	5.365084	2.065846
H	0.000003	5.365084	-2.065846
C	-2.963089	-1.710742	1.143326
C	-2.963091	-1.710739	-1.143326
C	-4.166418	-2.405484	1.134867
C	-4.166419	-2.405481	-1.134867
N	-4.775360	-2.757055	0.000000
H	-2.479491	-1.431538	2.070675
H	-2.479494	-1.431533	-2.070675
H	-4.646298	-2.682545	2.065846
H	-4.646301	-2.682539	-2.065846
C	2.963091	-1.710739	1.143326
C	2.963089	-1.710742	-1.143326
C	4.166419	-2.405481	1.134867
C	4.166418	-2.405484	-1.134867
N	4.775360	-2.757055	0.000000
H	2.479494	-1.431533	2.070675
H	2.479491	-1.431538	-2.070675
H	4.646301	-2.682539	2.065846
H	4.646298	-2.682545	-2.065846

$NpPz_3$

Np	0.000000	0.000000	0.000000
N	0.000000	2.638445	0.000000

N	-2.284960	-1.319222	0.000000
N	2.284960	-1.319222	0.000000
C	0.000000	3.336165	1.144743
C	0.000000	3.336165	-1.144743
C	0.000000	4.725365	1.135062
C	0.000000	4.725365	-1.135062
N	0.000000	5.427619	0.000000
H	0.000000	2.777828	2.072002
H	0.000000	2.777828	-2.072002
H	0.000000	5.279156	2.066044
H	0.000000	5.279156	-2.066044
C	-2.889204	-1.668083	1.144743
C	-2.889204	-1.668083	-1.144743
C	-4.092286	-2.362682	1.135062
C	-4.092286	-2.362682	-1.135062
N	-4.700456	-2.713810	0.000000
H	-2.405669	-1.388914	2.072002
H	-2.405669	-1.388914	-2.072002
H	-4.571883	-2.639578	2.066044
H	-4.571883	-2.639578	-2.066044
C	2.889204	-1.668083	1.144743
C	2.889204	-1.668083	-1.144743
C	4.092286	-2.362682	1.135062
C	4.092286	-2.362682	-1.135062
N	4.700456	-2.713810	0.000000
H	2.405669	-1.388914	2.072002
H	2.405669	-1.388914	-2.072002
H	4.571883	-2.639578	2.066044
H	4.571883	-2.639578	-2.066044

$PuPz_3$

Pu	0.000000	0.000000	0.000000
N	0.000000	2.620597	0.000000
N	-2.269504	-1.310299	0.000000
N	2.269504	-1.310299	0.000000
C	0.000000	3.318141	1.145166
C	0.000000	3.318141	-1.145166
C	0.000000	4.707349	1.135056
C	0.000000	4.707349	-1.135056
N	0.000000	5.409250	0.000000
H	0.000000	2.760185	2.072525
H	0.000000	2.760185	-2.072525
H	0.000000	5.260925	2.066106
H	0.000000	5.260925	-2.066106
C	-2.873595	-1.659071	1.145166
C	-2.873595	-1.659071	-1.145166
C	-4.076684	-2.353675	1.135056
C	-4.076684	-2.353675	-1.135056
N	-4.684548	-2.704625	0.000000
H	-2.390390	-1.380092	2.072525
H	-2.390390	-1.380093	-2.072525
H	-4.556094	-2.630462	2.066106
H	-4.556094	-2.630462	-2.066106
C	2.873595	-1.659071	1.145166
C	2.873595	-1.659071	-1.145166
C	4.076684	-2.353675	1.135056
C	4.076684	-2.353675	-1.135056
N	4.684548	-2.704625	0.000000
H	2.390390	-1.380093	2.072525
H	2.390390	-1.380092	-2.072525
H	4.556094	-2.630462	2.066106
H	4.556094	-2.630462	-2.066106

$AmPz_3$

Am	0.000000	0.000000	0.000000
N	0.000000	2.617109	0.000000
N	-2.266482	-1.308554	0.000000
N	2.266482	-1.308554	0.000000
C	0.000000	3.313256	1.145355
C	0.000000	3.313256	-1.145355
C	0.000000	4.702710	1.135213
C	0.000000	4.702710	-1.135213
N	0.000000	5.404120	0.000000
H	0.000000	2.755108	2.072565
H	0.000000	2.755108	-2.072565
H	0.000000	5.256444	2.066189
H	0.000000	5.256444	-2.066189
C	-2.869364	-1.656628	1.145355
C	-2.869364	-1.656628	-1.145355
C	-4.072667	-2.351355	1.135213
C	-4.072667	-2.351355	-1.135213
N	-4.680105	-2.702060	0.000000
H	-2.385994	-1.377554	2.072565
H	-2.385994	-1.377554	-2.072565
H	-4.552214	-2.628222	2.066189
H	-4.552214	-2.628222	-2.066189
C	2.869364	-1.656628	1.145355
C	2.869364	-1.656628	-1.145355
C	4.072667	-2.351355	1.135213
C	4.072667	-2.351355	-1.135213
N	4.680105	-2.702060	0.000000
H	2.385994	-1.377554	2.072565
H	2.385994	-1.377554	-2.072565
H	4.552214	-2.628222	2.066189
H	4.552214	-2.628222	-2.066189

$CmPz_3$

Cm	0.000000	0.000000	0.000000
N	0.000000	2.625142	0.000000
N	-2.273440	-1.312571	0.000000

N	2.273440	-1.312571	0.000000
C	0.000000	3.321838	1.144839
C	0.000000	3.321838	-1.144839
C	0.000000	4.711151	1.135143
C	0.000000	4.711151	-1.135143
N	0.000000	5.413256	0.000000
H	0.000000	2.763540	2.071968
H	0.000000	2.763540	-2.071968
H	0.000000	5.265161	2.066007
H	0.000000	5.265161	-2.066007
C	-2.876796	-1.660919	1.144839
C	-2.876796	-1.660919	-1.144839
C	-4.079977	-2.355576	1.135143
C	-4.079977	-2.355576	-1.135143
N	-4.688017	-2.706628	0.000000
H	-2.393296	-1.381770	2.071968
H	-2.393296	-1.381770	-2.071968
H	-4.559763	-2.632581	2.066007
H	-4.559763	-2.632581	-2.066007
C	2.876796	-1.660919	1.144839
C	2.876796	-1.660919	-1.144839
C	4.079977	-2.355576	1.135143
C	4.079977	-2.355576	-1.135143
N	4.688017	-2.706628	0.000000
H	2.393296	-1.381770	2.071968
H	2.393296	-1.381770	-2.071968
H	4.559763	-2.632581	2.066007
H	4.559763	-2.632581	-2.066007

$ThTz_3$

Th	0.000000	0.000000	0.000000
N	0.000000	2.690653	0.000000
N	-2.330174	-1.345326	0.000000
N	2.330174	-1.345326	0.000000
C	0.000000	3.420228	1.138118
C	0.000000	3.420228	-1.138118
N	0.000000	4.739780	1.190606
N	0.000000	4.739780	-1.190606
C	0.000000	5.356662	0.000000
H	0.000000	2.873818	2.073893
H	0.000000	2.873818	-2.073893
H	0.000000	6.439705	0.000000
C	-2.962004	-1.710114	1.138118
C	-2.962004	-1.710114	-1.138118
N	-4.104770	-2.369890	1.190606
N	-4.104770	-2.369890	-1.190606
C	-4.639005	-2.678331	0.000000
H	-2.488799	-1.436909	2.073893
H	-2.488799	-1.436909	-2.073893
H	-5.576948	-3.219852	0.000000
C	2.962004	-1.710114	1.138118
C	2.962004	-1.710114	-1.138118
N	4.104770	-2.369890	1.190606
N	4.104770	-2.369890	-1.190606
C	4.639005	-2.678331	0.000000
H	2.488799	-1.436909	2.073893
H	2.488799	-1.436909	-2.073893
H	5.576948	-3.219852	0.000000

$PaTz_3$

Pa	0.000000	0.000000	0.000000
N	0.000000	2.752794	0.000000
N	-2.383989	-1.376397	0.000000
N	2.383989	-1.376397	0.000000
C	0.000000	3.473348	1.132341
C	0.000000	3.473348	-1.132341
N	0.000000	4.798471	1.188591
N	0.000000	4.798471	-1.188591
C	0.000000	5.408373	0.000000
H	0.000000	2.926925	2.068008
H	0.000000	2.926925	-2.068008
H	0.000000	6.492306	0.000000
C	-3.008008	-1.736674	1.132341
C	-3.008008	-1.736674	-1.132341
N	-4.155598	-2.399235	1.188591
N	-4.155598	-2.399235	-1.188591
C	-4.683788	-2.704187	0.000000
H	-2.534792	-1.463463	2.068008
H	-2.534792	-1.463463	-2.068008
H	-5.622502	-3.246153	0.000000
C	3.008008	-1.736674	1.132341
C	3.008008	-1.736674	-1.132341
N	4.155598	-2.399235	1.188591
N	4.155598	-2.399235	-1.188591
C	4.683788	-2.704187	0.000000
H	2.534792	-1.463463	2.068008
H	2.534792	-1.463463	-2.068008
H	5.622502	-3.246153	0.000000

UTz_3

U	0.000000	0.000000	0.000000
N	0.000000	2.783273	0.000000
N	-2.410385	-1.391636	0.000000
N	2.410385	-1.391636	0.000000
C	0.000000	3.501010	1.131209
C	0.000000	3.501010	-1.131209
N	0.000000	4.827265	1.188479
N	0.000000	4.827265	-1.188479
C	0.000000	5.435613	0.000000
H	0.000000	2.954171	2.066607

H	0.000000	2.954171	-2.066607
H	0.000000	6.519742	0.000000
C	-3.031964	-1.750505	1.131209
C	-3.031964	-1.750505	-1.131209
N	-4.180534	-2.413633	1.188479
N	-4.180534	-2.413633	-1.188479
C	-4.707379	-2.717806	0.000000
H	-2.558387	-1.477085	2.066607
H	-2.558387	-1.477085	-2.066607
H	-5.646262	-3.259871	0.000000
C	3.031964	-1.750505	1.131209
C	3.031964	-1.750505	-1.131209
N	4.180534	-2.413633	1.188479
N	4.180534	-2.413633	-1.188479
C	4.707379	-2.717806	0.000000
H	2.558387	-1.477085	2.066607
H	2.558387	-1.477085	-2.066607
H	5.646262	-3.259871	0.000000

$NpTz_3$

Np	0.000000	0.000000	0.000000
N	0.000000	2.703875	0.000000
N	-2.341625	-1.351938	0.000000
N	2.341625	-1.351938	0.000000
C	0.000000	3.421739	1.132728
C	0.000000	3.421739	-1.132728
N	0.000000	4.747055	1.188459
N	0.000000	4.747055	-1.188459
C	0.000000	5.355537	0.000000
H	0.000000	2.874533	2.067857
H	0.000000	2.874533	-2.067857
H	0.000000	6.439567	0.000000
C	-2.963313	-1.710870	1.132728
C	-2.963313	-1.710870	-1.132728
N	-4.111070	-2.373527	1.188459
N	-4.111070	-2.373527	-1.188459
C	-4.638031	-2.677769	0.000000
H	-2.489418	-1.437266	2.067857
H	-2.489418	-1.437266	-2.067857
H	-5.576829	-3.219784	0.000000
C	2.963313	-1.710870	1.132728
C	2.963313	-1.710870	-1.132728
N	4.111070	-2.373527	1.188459
N	4.111070	-2.373527	-1.188459
C	4.638031	-2.677769	0.000000
H	2.489418	-1.437266	2.067857
H	2.489418	-1.437266	-2.067857
H	5.576829	-3.219784	0.000000

$PuTz_3$

Pu	0.000000	0.000000	0.000000
N	0.000000	2.648172	0.000000
N	-2.293384	-1.324086	0.000000
N	2.293384	-1.324086	0.000000
C	0.000000	3.365851	1.134019
C	0.000000	3.365851	-1.134019
N	0.000000	4.690517	1.188570
N	0.000000	4.690517	-1.188570
C	0.000000	5.298957	0.000000
H	0.000000	2.818151	2.068816
H	0.000000	2.818151	-2.068816
H	0.000000	6.382922	0.000000
C	-2.914913	-1.682926	1.134019
C	-2.914913	-1.682926	-1.134019
N	-4.062107	-2.345258	1.188570
N	-4.062107	-2.345258	-1.188570
C	-4.589032	-2.649479	0.000000
H	-2.440590	-1.409075	2.068816
H	-2.440590	-1.409075	-2.068816
H	-5.527772	-3.191461	0.000000
C	2.914913	-1.682926	1.134019
C	2.914913	-1.682926	-1.134019
N	4.062107	-2.345258	1.188570
N	4.062107	-2.345258	-1.188570
C	4.589032	-2.649479	0.000000
H	2.440590	-1.409075	2.068816
H	2.440590	-1.409075	-2.068816
H	5.527772	-3.191461	0.000000

$CmTz_3$

Cm	0.000000	0.000000	0.000000
N	0.000000	2.672194	0.000000
N	-2.314188	-1.336097	0.000000
N	2.314188	-1.336097	0.000000
C	0.000011	3.389571	1.132955
C	-0.000011	3.389571	-1.132955
N	0.000011	4.714842	1.188520
N	-0.000011	4.714842	-1.188520
C	0.000000	5.323232	0.000000
H	0.000019	2.842268	2.067917
H	-0.000019	2.842268	-2.067917
H	0.000000	6.407266	0.000000
C	-2.935460	-1.694776	1.132955
C	-2.935449	-1.694795	-1.132955
N	-4.083179	-2.357412	1.188520
N	-4.083168	-2.357430	-1.188520
C	-4.610054	-2.661616	0.000000
H	-2.461486	-1.421117	2.067917
H	-2.461466	-1.421151	-2.067917
H	-5.548855	-3.203633	0.000000

C	2.935449	-1.694795	1.132955
C	2.935460	-1.694776	-1.132955
N	4.083168	-2.357430	1.188520
N	4.083179	-2.357412	-1.188520

C	4.610054	-2.661616	0.000000
H	2.461466	-1.421151	2.067917
H	2.461486	-1.421117	-2.067917
H	5.548855	-3.203633	0.000000

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