Supplementary Information

Effects of Removing Boron from Subphthalocyanines: A Theoretical Perspective

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1. TD-DFT calculations

Table S1.1. Selected transition properties of **B-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	497	0.3488	H --> L (68%)
S2	497	0.3488	H --> L+1 (68%)
S10	266	0.1622	H-6 --> L (48%)

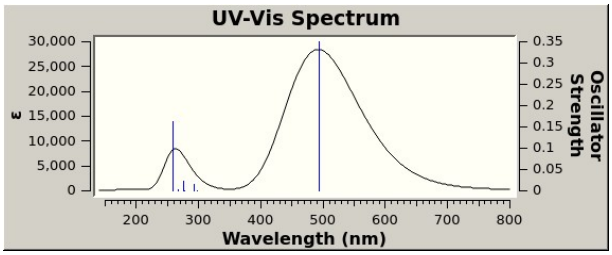

Figure S1.1. Calculated spectra of **B-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.2. Selected transition properties of **Al-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	514	0.2912	H --> L (67%)
S2	514	0.2912	H --> L+1 (67%)
S4	303	0.0182	H --> L+4 (52%)
S5	303	0.0182	H --> L+5 (52%)
S10	275	0.0203	H-8 --> L+1 (30%) H-9 --> L+2 (30%) H-5 --> L+2 (29%) H-4 --> L (29%)

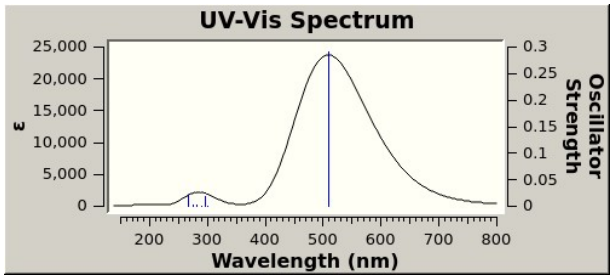

Figure S1.2. Calculated spectra of **Al-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.3. Selected transition properties of **Ga-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S_1	513	0.2915	H --> L (69%)
S_2	513	0.2915	H --> L+1 (69%)
S_4	303	0.0168	H-2 --> L (31%) H-1 --> L+1 (31%) H --> L+3 (47%) H --> L+4 (19%)
S_5	303	0.0168	H-2 --> L+1 (31%) H-1 --> L (31%) H --> L+3 (47%) H --> L+4 (19%)
S_{10}	275	0.0155	H-9 --> L (17%) H-9 --> L+1 (27%) H-8 --> L (27%) H-8 --> L+1 (17%) H-5 --> L+1 (28%) H-4 --> L (28%)

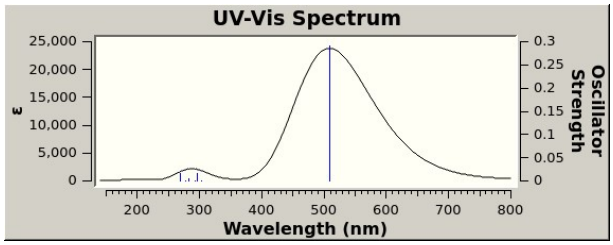

Figure S1.3. Calculated spectra of **Ga-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.4. Selected transition properties of **In-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)

state			
S1	518	0.2784	H --> L (69%)
S2	518	0.2784	H --> L+1 (69%)
S5	307	0.0159	H-2 --> L (28%) H-1 --> (28%) H --> L+3 (53%)
S6	307	0.0159	H-2 --> L+1 (28%) H-1 --> L (28%) H --> L+4 (53%)

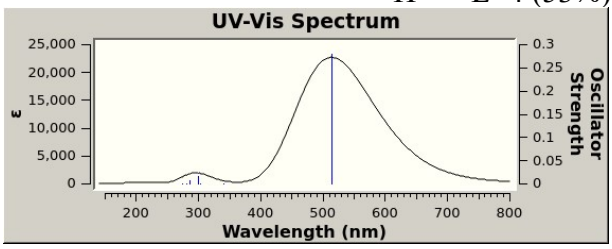

Figure S1.4. Calculated spectra of **In-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.5. Selected transition properties of **C-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	526	0.3038	H --> L (69%)
S2	526	0.3038	H --> L+1 (69%)
S4	313	0.0577	H-5 --> L+1 (28%)
S9	278	0.0835	H-4 --> L (28%) H-3 --> L+1 (30%) H-2 --> L (30%) H-1 --> L+1 (34%)
S5	313	0.0577	H-5 --> L (28%) H-4 --> L+1 (28%) H-3 --> L (30%) H-2 --> L+1 (30%) H-1 --> L (34%)
S8	290	0.1803	H-5 --> L (28%) H-4 --> L+1 (28%) H-1 --> L (50%) H --> L+4 (20%)
S9	290	0.18	H-5 --> L+1 (28%) H-4 --> L (28%) H-1 --> L+1 (50%) H --> L+3 (20%)

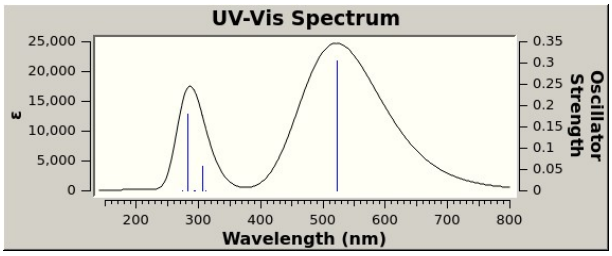

Figure S1.5. Calculated spectra of **C-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.6. Selected transition properties of **Sc-TdCl** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	529	0.2451	H --> L (67%)
S2	529	0.2451	H --> L+1 (67%)
S4	397	0.0409	H --> L+2 (68%)
S5	397	0.0408	H --> L+3 (68%)

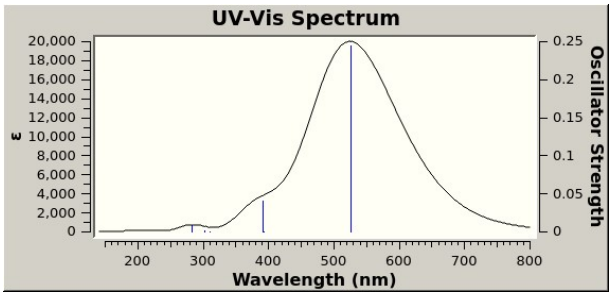

Figure S1.6. Calculated spectra of **Sc-TdCl** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.7. Selected transition properties of P-Td=O calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	546	0.254	H --> L (69%)
S2	546	0.254	H --> L+1 (69%)
S7	299	0.2365	H-1 --> L (52%)
S8	299	0.2364	H-1 --> L+1 (52%)
S10	288	0.4577	H-3 --> L+1 (40%) H-2 --> L (40%) H-1 --> L (22%)

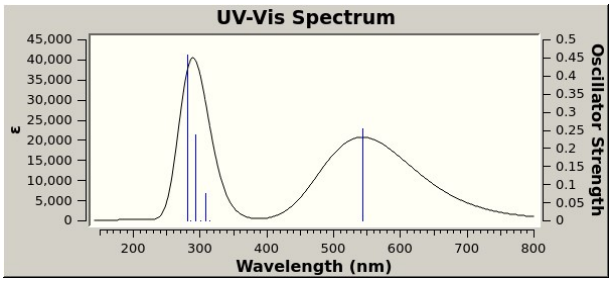

Figure S1.7. Calculated spectra of **P-Td=O** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.8. Selected transition properties of **P-Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	563	0.2251	H --> L (59%) H --> L+1 (35%)
S2	563	0.2251	H --> L (35%) H --> L+1 (59%)
S9	300	0.0278	H-6 --> L (38%)
S10	300	0.0276	H-6 --> L+1 (28%)

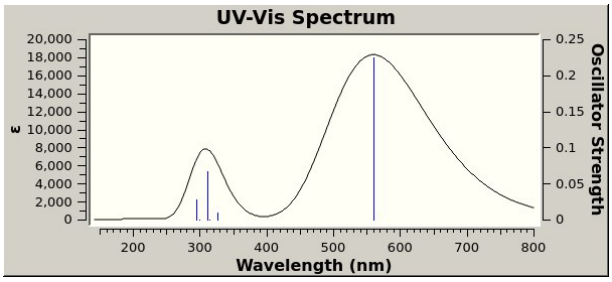

Figure S1.8. Calculated spectra of **P-Td** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.9. Selected transition properties of **H_2-Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	514	0.3055	H --> L (67%)
S2	500	0.3290	H --> L+1 (67%)
S4	307	0.0566	H --> L+2 (64%)
S9	278	0.0835	H-3 --> L+1 (28%)

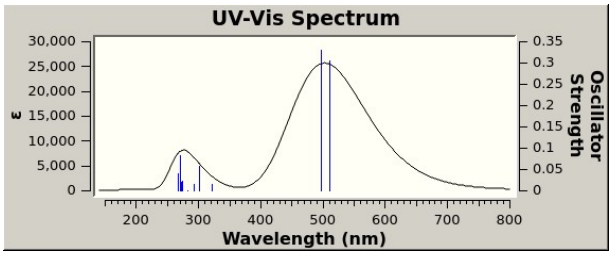

Figure S1.9. Calculated spectra of **H_2-Td** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.10. Selected transition properties of **H^--Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S1	496	0.3982	H --> L (68%)
S2	485	0.3352	H --> L+1 (68%)
S8	297	0.1484	H-5 --> L (13%) H-4 --> L+1 (23%) H-3 --> L (20%) H-2 --> L (57%) H-1 --> L+1 (11%) H --> L+1 (10%)
S9	295	0.1606	H-4 --> L (26%) H-2 --> L+1 (55%)

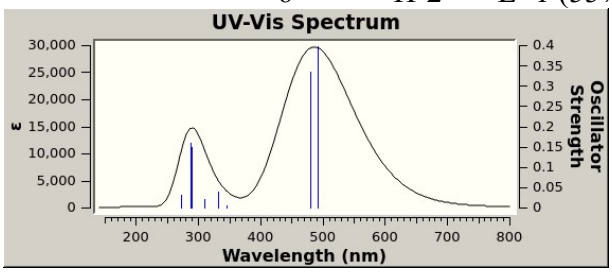

Figure S1.10. Calculated spectra of **H^--Td** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.11. Selected transition properties of **2^--Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S7	451	0.0723	H -11--> L (37%) H-10 --> L (33%) H-7 --> L (46%)
S8	451	0.0723	H -11--> L (33%) H-10 --> L (37%)

S10	364	0.2818	H-8 --> L (46%) H -11--> L (29%) H-10 --> L (34%) H-8 --> L (49%)

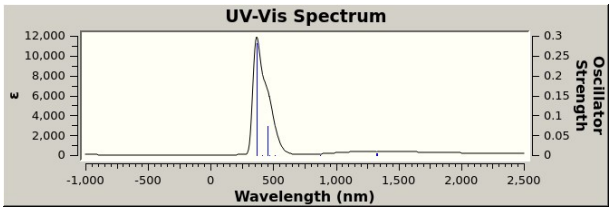

Figure S1.11. Calculated spectra of **2¯-Td** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.12. Selected transition properties of **Si-Oc** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S3	507	0.4299	H --> L+2 (62%) H-1 --> L (26%) H --> L+3 (16%)
S4	508	0.4299	H --> L+3 (62%) H-1 --> L+1 (26%) H --> L+2 (16%)
S5	457	0.0714	H-1 --> L (64%) H --> L+2 (27%)
S6	457	0.0715	H-1 --> L+1 (64%) H --> L+3 (27%)

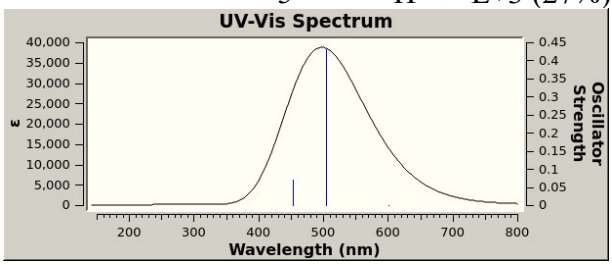

Figure S1.12. Calculated spectra of **Si-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.13. Selected transition properties of **Ge-Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S3	505	0.4566	H-1 --> L (34%) H --> L+2 (60%)
S4	505	0.4565	H-1 --> L+1 (34%) H --> L+3 (60%)
S5	450	0.0374	H-1 --> L (61%) H --> L+2 (35%)

S6	450	0.0375	H-1 --> L+1 (61%) H --> L+3 (35%)

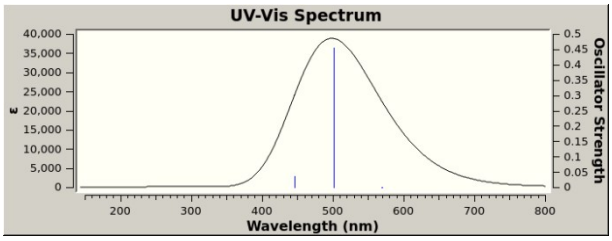

Figure S1.13. Calculated spectra of **Ge-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.14. Selected transition properties of **Sn-Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S3	508	0.4729	H-1 --> L (41%) H --> L+2 (55%)
S4	508	0.4299	H-1 --> L+1 (41%) H --> L+3 (55%)
S5	435	0.0125	H-1 --> L (56%) H --> L+2 (42%)
S6	435	0.0125	H-1 --> L+1 (56%) H --> L+3 (42%)

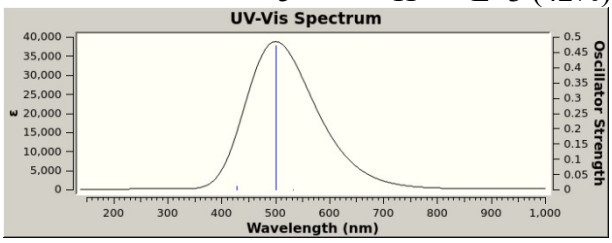

Figure S1.14. Calculated spectra of **Sn-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.15. Selected transition properties of **Pb-Td** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S3	509	0.4681	H-1 --> L (41%) H --> L+2 (54%)
S4	509	0.4681	H-1 --> L+1 (42%) H --> L+3 (54%)

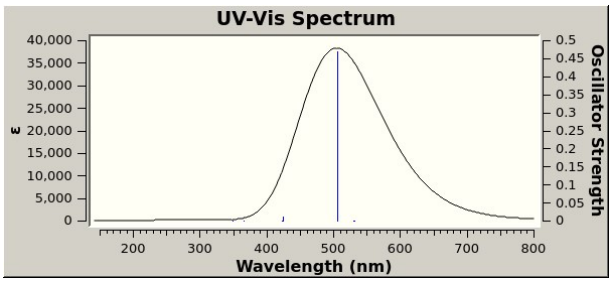

Figure S1.15. Calculated spectra of **Pb-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.16. Selected transition properties of **Ti-Oc** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S3	866	0.0187	H-1 --> L (68%) H-1 --> L+6 (18%)
S4	864	0.0188	H-1 --> L+1 (68%) H --> L+5 (18%)

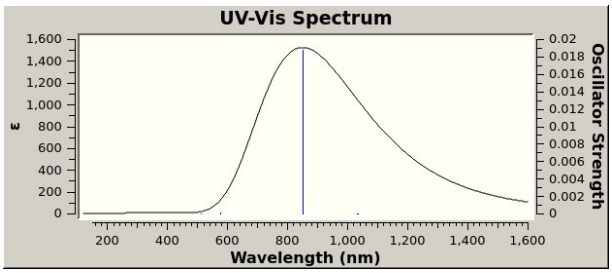

Figure S1. 16. Calculated spectra of **Ti-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

Table S1.17. Selected transition properties of **Zn-Oc** calculated at CAM-B3LYP/cc-pVTZ level of theory. [a]Oscillator strength. [b]MOs involved in the transitions (H and L denoting HOMO and LUMO)

Excited state	Energy (nm)	*f*[a]	Orbitals[b] (coefficient)
S2	508	0.285	H --> L+1 (68%)
S3	508	0.2922	H --> L+2 (68%)
S7	310	0.0174	H --> L+5 (60%)
S8	310	0.0119	H --> L+6 (56%)
S9	296	0.0263	H-6 --> L+2 (19%) H-2 --> L+2 (36%) H-1 --> L+1 (37%)
S10	296	0.019	H --> L+6 (41%) H-6 --> L+1 (21%)

H-2 --> L+1 (41%)
H-1 --> L+2 (35%)
H --> L+6 (35%)

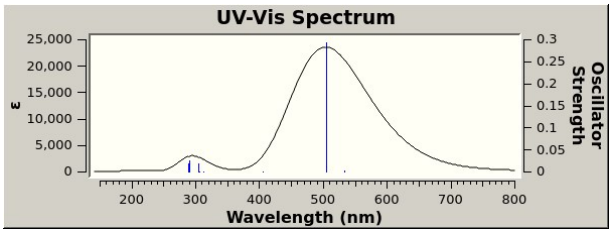

Figure S1.17. Calculated spectra of **Zn-Oc** calculated at CAM-B3LYP/6-31+G(d,p) level of theory.

2. Cartesian coordinates

B-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.086132	-1.665681	0.190288
C	-2.267192	-0.343076	0.324145
C	-0.836421	-2.135000	0.324307
N	0.203999	-1.348141	0.743588
N	-1.269535	0.497391	0.743312
C	1.430691	-1.791941	0.324429
N	2.485605	-0.973876	0.190514
C	2.267218	0.343085	0.324304
N	1.065478	0.850721	0.743283
C	-1.430733	1.791808	0.323916
N	-0.399421	2.639413	0.189902
C	0.836500	2.134901	0.323927
C	-3.309358	0.527740	-0.202905
C	-2.787115	1.860639	-0.203053
C	-0.217857	-3.344044	-0.202757
C	1.197585	-3.129850	-0.202705
C	2.111778	2.601933	-0.203096
C	3.005031	1.483242	-0.202868
C	-4.572499	0.260298	-0.735587
C	-5.314178	1.325812	-1.237732
C	-4.800537	2.636751	-1.237871
C	-3.532389	2.914892	-0.735883
C	-0.758260	-4.516501	-0.735768

C	0.116644	-5.475540	-1.238103
C	1.508766	-5.264871	-1.238065
C	2.060719	-4.089919	-0.735685
C	2.511741	3.829477	-0.735960
C	3.805385	3.938988	-1.238002
C	4.683916	2.838733	-1.237808
C	4.290739	1.601506	-0.735566
H	-6.305615	1.144594	-1.641462
H	-4.959654	-0.753082	-0.749777
H	-5.405002	3.443175	-1.641711
H	-3.128051	3.921537	-0.750305
H	1.827642	4.671398	-0.750436
H	4.144161	4.888128	-1.641918
H	5.684566	2.958956	-1.641578
H	4.960403	0.748055	-0.749744
H	3.131900	-3.918468	-0.750003
H	2.161395	-6.032745	-1.642083
H	-0.279543	-6.402128	-1.642151
H	-1.832210	-4.669657	-0.750145
Cl	-0.000049	0.000389	3.219354
B	-0.000035	0.000089	1.340480

Al-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.472375	-2.585269	0.246719
C	-0.793771	-2.168827	0.416226
C	1.509505	-1.748024	0.416035
N	1.420813	-0.507208	1.013294
N	-1.149668	-0.976948	1.013708
C	2.275196	0.397066	0.416226
N	2.002714	1.701830	0.247026
C	0.759023	2.181275	0.416446
N	-0.271171	1.484039	1.013766
C	-2.268753	-0.433259	0.416778
N	-2.475333	0.883552	0.247607
C	-1.481545	1.771853	0.416764
C	-1.958876	-2.601159	-0.348622
C	-2.883507	-1.513078	-0.348404
C	2.752144	-1.740385	-0.348984
C	3.232122	-0.395588	-0.348877
C	-1.273580	2.996894	-0.348348
C	0.131034	3.253632	-0.348453
C	-2.211082	-3.748033	-1.106372
C	-3.402704	-3.815372	-1.821338
C	-4.315004	-2.741765	-1.821158
C	-4.056151	-1.576762	-1.105995
C	3.393659	-2.723888	-1.106805
C	4.531967	-2.365340	-1.821928
C	5.005533	-1.038451	-1.821812
C	4.351394	-0.040340	-1.106559
C	-2.140854	3.788649	-1.106014
C	-1.603500	4.854197	-1.821234

C	-0.217591	5.107527	-1.821333
C	0.662054	4.300972	-1.106222
H	-3.632732	-4.706558	-2.397462
H	-1.493601	-4.561608	-1.126213
H	-5.231747	-2.824866	-2.397107
H	-4.743356	-0.737449	-1.125465
H	-3.204182	3.574117	-1.125572
H	-2.260399	5.498918	-2.397311
H	0.168677	5.942906	-2.397510
H	1.732523	4.476426	-1.125969
H	4.697228	0.987810	-1.126121
H	5.892320	-0.791900	-2.397890
H	5.062286	-3.117544	-2.398119
H	3.010407	-3.738680	-1.126564
Cl	0.001294	-0.000620	4.165875
Al	0.000167	-0.000136	2.062037

Ga-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.332053	-2.609827	0.098770
C	-1.413206	-1.827420	0.260023
C	0.910628	-2.123132	0.259902
N	1.209561	-0.919854	0.855925
N	-1.401392	-0.587653	0.856140
C	2.289332	-0.310046	0.260292
N	2.426267	1.017538	0.099506
C	1.383413	1.850304	0.260757
N	0.191819	1.507492	0.856686
C	-2.294106	0.273113	0.260574
N	-2.094280	1.592700	0.099835
C	-0.876110	2.137789	0.260998
C	-2.650619	-1.885548	-0.511683
C	-3.202865	-0.568439	-0.511554
C	2.093949	-2.489143	-0.512087
C	2.958346	-1.352243	-0.511973
C	-0.307981	3.238459	-0.510925
C	1.108786	3.058213	-0.511087
C	-3.231215	-2.899217	-1.278184
C	-4.382538	-2.601084	-2.000313
C	-4.927222	-1.301930	-2.000259
C	-4.332800	-0.271899	-1.278024
C	2.402151	-3.615749	-1.278844
C	3.591219	-3.615136	-2.001365
C	4.443729	-2.493668	-2.001401
C	4.126284	-1.347801	-1.278806
C	-0.895761	4.247902	-1.277520
C	-0.062125	5.095694	-2.000153
C	1.335324	4.917906	-2.000359
C	1.930359	3.888377	-1.277919
H	-4.866969	-3.379075	-2.582633

H	-2.792436	-3.891264	-1.298884
H	-5.821689	-1.102039	-2.582504
H	-4.732787	0.736415	-1.298550
H	-1.974299	4.363860	-1.298009
H	-0.493843	5.904025	-2.582613
H	1.955506	5.592419	-2.582978
H	3.003569	3.730594	-1.298745
H	4.765883	-0.471674	-1.299431
H	5.359530	-2.523865	-2.584012
H	3.865323	-4.489498	-2.583943
H	1.729009	-4.466374	-1.299498
Cl	0.001209	-0.001691	4.098707
Ga	0.000044	-0.000302	1.955652

In-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.617839	0.121832	-0.062103
C	2.043809	-1.082395	0.100758
C	1.934419	1.267510	0.100829
N	0.714886	1.383043	0.734903
N	0.840315	-1.310720	0.734895
C	-0.084440	2.311110	0.100553
N	-1.414323	2.206166	-0.062564
C	-2.064865	1.041508	0.100393
N	-1.555247	-0.072379	0.734576
C	0.130550	-2.308926	0.100451
N	-1.203309	-2.327891	-0.062706
C	-1.959237	-1.228703	0.100267
C	2.295055	-2.257997	-0.730442
C	1.094096	-3.027913	-0.730582
C	2.075469	2.461399	-0.730287
C	0.808242	3.116530	-0.730391
C	-3.102963	-0.858372	-0.730867
C	-3.169282	0.566649	-0.730736
C	3.371166	-2.618687	-1.546122
C	3.255471	-3.772149	-2.316686
C	2.069278	-4.532598	-2.316807
C	0.972727	-4.156271	-1.546374
C	3.113468	2.920433	-1.545936
C	2.891256	4.058260	-2.316395
C	1.639646	4.705408	-2.316404
C	0.582737	4.228882	-1.546017
C	-3.953352	-1.609833	-1.546704
C	-4.894491	-0.932791	-2.317092
C	-4.959991	0.474704	-2.316956
C	-4.085771	1.236059	-1.546437
H	4.088802	-4.088548	-2.937177
H	4.271343	-2.013080	-1.567368
H	2.008996	-5.421868	-2.937390
H	0.046622	-4.721429	-1.567801

H	-3.878954	-2.692209	-1.568137
H	-5.585189	-1.496185	-2.937640
H	-5.700024	0.971645	-2.937406
H	-4.112193	2.320672	-1.567649
H	-0.391809	4.705682	-1.567397
H	1.497127	5.585332	-2.936870
H	3.691640	4.450672	-2.936844
H	4.065944	2.400942	-1.567250
Cl	-0.000544	-0.000204	4.350152
In	-0.000248	-0.000192	2.055209

C-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.281498	2.685053	0.089093
C	1.341162	1.877310	0.181279
C	-0.922639	2.114654	0.181321
N	-1.059437	0.769320	0.476552
N	1.195961	0.532856	0.476467
C	-2.296434	0.222798	0.181729
N	-2.466145	-1.098762	0.089726
C	-1.370044	-1.856326	0.181649
N	-0.136513	-1.302106	0.476637
C	2.292699	-0.258340	0.181616
N	2.184614	-1.586363	0.089605
C	0.955235	-2.100124	0.181585
C	2.733885	2.005411	-0.187784
C	3.319344	0.691396	-0.187529
C	-2.258500	2.528801	-0.187804
C	-3.103771	1.364797	-0.187476
C	0.369841	-3.370272	-0.187644
C	-1.060845	-3.220269	-0.187586
C	3.484556	3.118215	-0.579270
C	4.811461	2.915082	-0.942976
C	5.385151	1.627518	-0.942682
C	4.648790	0.505236	-0.578714
C	-2.762031	3.773083	-0.579369
C	-4.102215	3.849567	-0.943069
C	-4.930491	2.709000	-0.942679
C	-4.442922	1.458411	-0.578640
C	0.958259	-4.576765	-0.579132
C	0.118926	-5.624295	-0.943046
C	-1.282973	-5.477309	-0.942984
C	-1.886746	-4.278471	-0.579009
H	5.419709	3.764331	-1.236113
H	3.041313	4.107791	-0.589773
H	6.423374	1.511742	-1.235609
H	5.088143	-0.486078	-0.588818
H	2.036879	-4.687713	-0.589508
H	0.550301	-6.575649	-1.236234
H	-1.902320	-6.318493	-1.236136

H	-2.964922	-4.163280	-0.589301
H	-5.078336	0.579785	-0.588697
H	-5.970155	2.811068	-1.235595
H	-4.521090	4.806489	-1.236262
H	-2.123169	4.649199	-0.589933
Cl	0.000121	0.000333	2.838880
C	0.000027	0.000087	0.968956

Sc-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.154797	2.358824	0.085285
C	1.920888	1.269372	0.257302
C	-0.175551	2.295760	0.257211
N	-0.830245	1.234865	0.849230
N	1.484456	0.101637	0.849308
C	-2.059746	1.028799	0.257238
N	-2.620148	-0.179413	0.085404
C	-1.900334	-1.299969	0.257462
N	-0.654230	-1.336428	0.849464
C	2.075936	-0.995837	0.257500
N	1.465465	-2.179544	0.085686
C	0.138931	-2.298283	0.257603
C	3.126230	0.929277	-0.492550
C	3.223690	-0.494779	-0.492430
C	-1.183379	3.039046	-0.492852
C	-2.367881	2.242553	-0.492826
C	-0.758182	-3.172120	-0.492325
C	-2.040193	-2.544515	-0.492431
C	4.023064	1.703489	-1.233796
C	5.033159	1.050336	-1.933392
C	5.129358	-0.355206	-1.933255
C	4.217639	-1.139741	-1.233534
C	-1.121846	4.222111	-1.234307
C	-2.257133	4.619166	-1.934155
C	-3.426235	3.833026	-1.934120
C	-3.486771	2.631853	-1.234238
C	-0.535967	-4.335925	-1.233492
C	-1.606534	-4.884145	-1.933260
C	-2.871871	-4.264692	-1.933377
C	-3.095591	-3.082855	-1.233702
H	5.757230	1.631382	-2.496571
H	3.930402	2.784296	-1.253643
H	5.925864	-0.832290	-2.496310
H	4.273077	-2.223099	-1.253149
H	0.446370	-4.796089	-1.253134
H	-1.465262	-5.801753	-2.496378
H	-3.683177	-4.715961	-2.496583
H	-4.061533	-2.589207	-1.253502
H	-4.376410	2.011147	-1.253937
H	-4.291475	4.169385	-2.497400

H	-2.242250	5.547351	-2.497460
H	-0.211389	4.811858	-1.254052
Sc	-0.000171	0.000346	2.243364
Cl	-0.000507	0.000929	4.603247

Cr(2)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.272142	1.300052	0.066847
C	2.306525	-0.023027	0.261234
C	1.139587	1.996707	0.237730
N	0.000040	1.469073	0.820114
N	1.264391	-0.750363	0.817227
C	-1.139476	1.996771	0.237728
N	-2.272070	1.300179	0.066843
C	-2.306527	-0.022898	0.261231
N	-1.264433	-0.750291	0.817224
C	1.164224	-2.003537	0.235329
N	-0.000074	-2.633341	0.034762
C	-1.164336	-2.003472	0.235328
C	3.150336	-0.995019	-0.425713
C	2.431450	-2.228903	-0.451494
C	0.714916	3.180118	-0.493492
C	-0.714737	3.180159	-0.493493
C	-2.431576	-2.228768	-0.451494
C	-3.150393	-0.994844	-0.425713
C	4.372937	-0.870077	-1.089597
C	4.882425	-1.986265	-1.747194
C	4.173498	-3.202257	-1.773417
C	2.938770	-3.331300	-1.143247
C	1.425617	4.152239	-1.204919
C	0.705120	5.130389	-1.880908
C	-0.704828	5.130429	-1.880909
C	-1.425382	4.152320	-1.204920
C	-2.938958	-3.331138	-1.143244
C	-4.173680	-3.202027	-1.773412
C	-4.882540	-1.985996	-1.747189
C	-4.372989	-0.869836	-1.089595
H	5.839618	-1.918480	-2.255161
H	4.906099	0.074778	-1.086139
H	4.596819	-4.052056	-2.300314
H	2.381459	-4.261384	-1.179976
H	-2.381698	-4.261253	-1.179972
H	-4.597049	-4.051804	-2.300306
H	-5.839730	-1.918159	-2.255154
H	-4.906098	0.075050	-1.086138
H	-2.510072	4.138356	-1.220370
H	-1.234595	5.906105	-2.425540
H	1.234931	5.906035	-2.425539
H	2.510306	4.138213	-1.220368
Cr	-0.000002	-0.002597	1.929687

Cl	0.000010	0.170656	4.115857

Cr(4)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.642301	-2.069921	0.050835
C	0.326987	-2.273008	0.214071
C	2.139313	-0.834860	0.213083
N	1.432218	0.212476	0.759258
N	-0.531755	-1.346413	0.760633
C	1.804834	1.419964	0.213050
N	0.970666	2.457539	0.050734
C	-0.346945	2.270022	0.213903
N	-0.899717	1.134050	0.760494
C	-1.793371	-1.435554	0.216604
N	-2.614551	-0.387878	0.055199
C	-2.132869	0.853044	0.216491
C	-0.515790	-3.245065	-0.472529
C	-1.843797	-2.720423	-0.471024
C	3.276315	-0.235786	-0.475473
C	3.066743	1.176728	-0.475555
C	-2.554179	2.067984	-0.471089
C	-1.435685	2.955563	-0.472652
C	-0.219353	-4.429472	-1.151910
C	-1.258895	-5.096291	-1.793296
C	-2.569019	-4.578769	-1.791804
C	-2.870975	-3.382045	-1.148936
C	4.361731	-0.794120	-1.155691
C	5.246045	0.066095	-1.799407
C	5.039301	1.459581	-1.799492
C	3.943311	2.026068	-1.155870
C	-3.729270	2.402924	-1.148831
C	-3.787840	3.635829	-1.791594
C	-2.684396	4.511404	-1.793159
C	-1.495949	4.175061	-1.151933
H	-1.058147	-6.029510	-2.310720
H	0.795080	-4.813561	-1.170855
H	-3.354362	-5.122503	-2.308055
H	-3.874132	-2.969294	-1.165529
H	-4.569387	1.716708	-1.165389
H	-4.697285	3.928166	-2.307709
H	-2.763280	5.462759	-2.310482
H	-0.636740	4.837147	-1.170925
H	3.768851	3.096684	-1.173562
H	5.746382	2.100238	-2.317680
H	6.108672	-0.341735	-2.317555
H	4.505594	-1.869277	-1.173287
Cr	0.000912	0.000207	1.986037
Cl	0.012662	0.001824	4.209707

Fe(2)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.031003	-2.638951	0.042042
C	-1.180596	-1.973931	0.213623
C	1.133884	-2.000838	0.212785
N	1.244857	-0.738095	0.755163
N	-1.261861	-0.709035	0.756325
C	2.299630	-0.034949	0.212908
N	2.300608	1.293267	0.042153
C	1.165562	1.982803	0.213668
N	0.016734	1.447259	0.756355
C	-2.300261	0.018473	0.214512
N	-2.270562	1.346332	0.043745
C	-1.119714	2.009396	0.214528
C	-2.455240	-2.198208	-0.456881
C	-3.154831	-0.953176	-0.456460
C	2.402528	-2.254702	-0.458562
C	3.130920	-1.026282	-0.458557
C	-0.677110	3.225372	-0.456378
C	0.750907	3.208759	-0.456880
C	-2.984529	-3.311348	-1.114437
C	-4.220945	-3.178562	-1.739440
C	-4.910791	-1.950775	-1.739101
C	-4.381009	-0.825984	-1.113675
C	2.905264	-3.379821	-1.116563
C	4.144004	-3.275823	-1.742415
C	4.862246	-2.064440	-1.742489
C	4.359229	-0.927639	-1.116657
C	-1.376918	4.240241	-1.113590
C	-0.644133	5.244729	-1.738914
C	0.764087	5.228363	-1.739367
C	1.473711	4.207087	-1.114549
H	-4.661205	-4.034092	-2.242514
H	-2.441673	-4.250466	-1.130422
H	-5.870614	-1.881612	-2.241893
H	-4.900880	0.126067	-1.128996
H	-2.461657	4.239684	-1.128872
H	-1.165244	6.053761	-2.241660
H	1.303564	6.025061	-2.242442
H	2.558134	4.181283	-1.130552
H	4.901103	0.012054	-1.132290
H	5.823081	-2.017634	-2.245925
H	4.563883	-4.141360	-2.245797
H	2.340717	-4.306072	-1.132157
Fe	0.000493	-0.000352	1.821049
Cl	0.005365	-0.003260	3.981359

Fe(6)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.797085	2.502406	0.077893
C	0.508819	2.248378	0.251301
C	-1.715581	1.540081	0.251611
N	-1.460210	0.319309	0.841728
N	1.006519	1.105180	0.841906
C	-2.201849	-0.683592	0.251925
N	-1.768888	-1.941486	0.078472
C	-0.476096	-2.255601	0.251716
N	0.453357	-1.424291	0.842069
C	2.191548	0.715665	0.252254
N	2.565711	-0.561025	0.079094
C	1.692772	-1.564964	0.252322
C	1.617396	2.835358	-0.493593
C	2.673233	1.873676	-0.492975
C	-2.959525	1.377929	-0.493191
C	-3.264626	-0.017237	-0.492935
C	1.647107	-2.818325	-0.492892
C	0.286274	-3.251655	-0.493302
C	1.733071	4.018171	-1.229082
C	2.916625	4.246800	-1.923715
C	3.958427	3.297897	-1.923117
C	3.840583	2.098590	-1.227871
C	-3.738033	2.276133	-1.228424
C	-4.835864	1.778289	-1.923030
C	-5.136941	0.401647	-1.922729
C	-4.347075	-0.508744	-1.227848
C	2.613994	-3.509874	-1.227908
C	2.220472	-4.648870	-1.923179
C	0.877730	-5.076431	-1.923607
C	-0.102317	-4.374811	-1.228754
H	3.040216	5.169153	-2.483145
H	0.919241	4.735307	-1.248081
H	4.865620	3.506558	-2.482075
H	4.630410	1.355077	-1.245893
H	3.642038	-3.163814	-1.246064
H	2.957733	-5.217061	-2.482267
H	0.605054	-5.966180	-2.483042
H	-1.141161	-4.686924	-1.247586
H	-4.561357	-1.572091	-1.246130
H	-5.997769	0.047342	-2.481672
H	-5.470269	2.459354	-2.482184
H	-3.488902	3.331853	-1.247103
Fe	-0.000123	0.000186	2.048846
Cl	0.000333	0.000287	4.230544

Ru(2)-TdCl

Atom	Coordinates (Angstroms)

	X	Y	Z
N	2.327788	-1.238532	-0.121262
C	1.210903	-1.956409	0.048608
C	2.298367	0.089284	0.045286
N	1.244018	0.777758	0.607779
N	0.051244	-1.466048	0.611379
C	1.087194	2.027005	0.044880
N	-0.093517	2.635057	-0.122149
C	-1.228134	1.945551	0.047825
N	-1.295391	0.688428	0.610960
C	-1.072641	-2.036577	0.051697
N	-2.237544	-1.398742	-0.115182
C	-2.300531	-0.072086	0.051327
C	0.824055	-3.177226	-0.647751
C	-0.602958	-3.227236	-0.646001
C	3.092872	1.091182	-0.654634
C	2.335994	2.302000	-0.655010
C	-3.165240	0.871589	-0.646362
C	-2.495112	2.132471	-0.648496
C	1.569377	-4.138911	-1.335149
C	0.882416	-5.160588	-1.984940
C	-0.525578	-5.209899	-1.983273
C	-1.280796	-4.238748	-1.331734
C	4.306109	1.009656	-1.343266
C	4.767922	2.149032	-1.996341
C	4.021169	3.343718	-1.996693
C	2.794449	3.428039	-1.344012
C	-4.371647	0.705237	-1.331720
C	-4.913999	1.809473	-1.983232
C	-4.252859	3.053578	-1.985281
C	-3.033273	3.223646	-1.335935
H	1.439370	-5.931160	-2.509564
H	2.652915	-4.085482	-1.353752
H	-1.028484	-6.017622	-2.506605
H	-2.365457	-4.261327	-1.347652
H	-4.867137	-0.259911	-1.347315
H	-5.860594	1.711165	-2.506206
H	-4.701768	3.891754	-2.509825
H	-2.510626	4.174300	-1.354735
H	2.206425	4.339731	-1.361402
H	4.408794	4.211178	-2.522494
H	5.717645	2.117206	-2.521904
H	4.867967	0.081602	-1.360170
Ru	0.002249	0.001674	1.884145
Cl	0.016320	0.010987	4.197637

Ru(6)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.416286	-2.187776	-0.229515
C	0.076196	-2.240771	-0.125389

C	2.029415	-1.020253	0.029401
N	1.467108	0.041944	0.675981
N	-0.698277	-1.317032	0.508183
C	1.947167	1.204626	0.149444
N	1.246123	2.345224	0.021977
C	-0.093143	2.285998	0.131512
N	-0.792093	1.240100	0.656769
C	-1.889935	-1.198617	-0.140712
N	-2.596928	-0.060798	-0.261925
C	-1.978291	1.104064	-0.003838
C	-0.803603	-3.051439	-0.993234
C	-2.056536	-2.387662	-1.002636
C	3.234347	-0.530716	-0.672719
C	3.180513	0.884146	-0.598770
C	-2.240703	2.370411	-0.719483
C	-1.040563	3.120745	-0.636128
C	-0.579380	-4.167662	-1.789380
C	-1.645726	-4.644903	-2.563106
C	-2.883572	-3.989161	-2.572343
C	-3.096645	-2.834109	-1.808201
C	4.227026	-1.171586	-1.403537
C	5.201235	-0.376905	-2.022123
C	5.147935	1.021046	-1.949160
C	4.118726	1.670998	-1.255187
C	-3.318933	2.826424	-1.467590
C	-3.200182	4.073851	-2.094593
C	-2.014331	4.815059	-2.012383
C	-0.907636	4.333686	-1.300441
H	-1.508427	-5.532523	-3.173382
H	0.390661	-4.653696	-1.804551
H	-3.687904	-4.377942	-3.189642
H	-4.043359	-2.304675	-1.837671
H	-4.223657	2.233957	-1.556262
H	-4.037472	4.469209	-2.661834
H	-1.949449	5.774359	-2.517041
H	0.023631	4.889293	-1.261920
H	4.055210	2.753790	-1.224181
H	5.912258	1.610166	-2.447044
H	6.006057	-0.851342	-2.575564
H	4.245675	-2.253413	-1.485455
Cl	-0.405376	-0.598337	4.539927
Ru	-0.069719	-0.104562	2.269979

Os(2)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.514576	2.582235	-0.333018
C	1.525574	1.722783	-0.160199
C	-0.748734	2.174840	-0.164457
N	-1.104487	0.968026	0.410507
N	1.390526	0.471965	0.414580

C	-2.254502	0.457039	-0.163905
N	-2.492784	-0.848801	-0.332139
C	-1.508094	-1.738338	-0.159495
N	-0.285639	-1.440303	0.414944
C	2.260570	-0.439788	-0.155390
N	1.982711	-1.737895	-0.323419
C	0.732175	-2.183381	-0.155155
C	2.799528	1.701928	-0.865010
C	3.258908	0.350233	-0.862134
C	-1.931300	2.641619	-0.874350
C	-2.872277	1.568007	-0.874162
C	0.079723	-3.276776	-0.861591
C	-1.320527	-2.998562	-0.864321
C	3.500394	2.690391	-1.561355
C	4.672232	2.325618	-2.218394
C	5.125547	0.991693	-2.215594
C	4.417791	-0.009098	-1.555688
C	-2.198569	3.822176	-1.572887
C	-3.418250	3.932136	-2.234938
C	-4.346797	2.872627	-2.234834
C	-4.077742	1.678000	-1.572621
C	0.587815	-4.378481	-1.555314
C	-0.311606	-5.211147	-2.215374
C	-1.693440	-4.936565	-2.218090
C	-2.208642	-3.822816	-1.560767
H	5.245046	3.079581	-2.750080
H	3.136098	3.712244	-1.581369
H	6.039837	0.740864	-2.745148
H	4.751669	-1.041366	-1.571336
H	1.654943	-4.574142	-1.571079
H	0.056863	-6.084552	-2.745151
H	-2.365843	-5.603140	-2.749899
H	-3.269441	-3.595637	-1.580658
H	-4.780620	0.851597	-1.590253
H	-5.285437	2.989574	-2.768261
H	-3.657347	4.847254	-2.768474
H	-1.471480	4.627355	-1.590815
Os	-0.002536	0.002514	1.703949
Cl	-0.018503	0.016935	4.000491

Os(6)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.446001	1.250760	0.007101
C	2.322860	-0.081990	0.095255
C	1.278243	1.954395	-0.027039
N	0.096232	1.507515	0.444137
N	1.225697	-0.782975	0.541291
C	-0.959256	2.075453	-0.249384
N	-2.095695	1.382296	-0.569709
C	-2.191540	0.092095	-0.384722

N	-1.347104	-0.754053	0.388949
C	1.148586	-2.040031	-0.083311
N	-0.027924	-2.613599	-0.449439
C	-1.158584	-1.959631	-0.328218
C	3.199934	-1.077351	-0.534800
C	2.454107	-2.288089	-0.655130
C	0.997447	3.139894	-0.844554
C	-0.423667	3.209107	-0.980705
C	-2.356519	-2.100927	-1.171554
C	-3.000586	-0.837102	-1.198281
C	4.473865	-0.961672	-1.080553
C	5.024742	-2.079446	-1.715357
C	4.292233	-3.272190	-1.838143
C	2.997470	-3.385494	-1.329292
C	1.826277	4.038932	-1.508412
C	1.229470	5.036391	-2.286185
C	-0.166965	5.103689	-2.426774
C	-1.006064	4.184115	-1.794083
C	-2.823107	-3.155390	-1.946615
C	-3.972506	-2.945635	-2.720617
C	-4.608673	-1.699261	-2.745810
C	-4.115366	-0.621370	-1.997919
H	6.026792	-2.022829	-2.129261
H	5.018186	-0.025519	-1.010244
H	4.740728	-4.120497	-2.346867
H	2.425423	-4.300028	-1.446033
H	-2.310628	-4.111644	-1.945877
H	-4.370384	-3.760646	-3.317658
H	-5.491873	-1.562448	-3.362389
H	-4.585114	0.355760	-2.037254
H	-2.082823	4.225904	-1.922235
H	-0.600903	5.883183	-3.046222
H	1.852916	5.762796	-2.798576
H	2.905321	3.961996	-1.420919
Cl	-1.111375	0.538607	3.817504
Os	-0.177488	-0.149249	1.813985

Co(3)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.522361	-0.681465	0.096076
C	1.588056	-1.632272	0.269210
C	2.193911	0.610543	0.268558
N	1.069895	1.065737	0.900206
N	0.387907	-1.459614	0.901292
C	0.619589	2.190995	0.267444
N	-0.670953	2.524698	0.093889
C	-1.625573	1.594322	0.266816
N	-1.457816	0.393704	0.899253
C	-0.567792	-2.205312	0.268687
N	-1.850790	-1.843931	0.094891

C	-2.207250	-0.559361	0.267262
C	1.496159	-2.868179	-0.532622
C	0.126069	-3.232298	-0.533068
C	2.736720	1.724439	-0.533609
C	1.736184	2.728808	-0.534408
C	-3.231178	0.138184	-0.535191
C	-2.861586	1.506837	-0.535375
C	2.423944	-3.575253	-1.286410
C	1.971388	-4.688278	-2.006369
C	0.617974	-5.047816	-2.006977
C	-0.327878	-4.306380	-1.287512
C	3.894353	1.868073	-1.287382
C	4.063756	3.057440	-2.007586
C	3.075436	4.049505	-2.008423
C	1.884847	3.885245	-1.289033
C	-4.306986	-0.311811	-1.289555
C	-5.044354	0.636594	-2.009852
C	-4.679289	1.988512	-2.010005
C	-3.564709	2.436999	-1.289893
H	2.679438	-5.276936	-2.581537
H	3.465942	-3.274174	-1.309603
H	0.295900	-5.910120	-2.582629
H	-1.381894	-4.562155	-1.311537
H	-4.567077	-1.364783	-1.312982
H	-5.907821	0.317672	-2.585511
H	-5.264871	2.698616	-2.585783
H	-3.259451	3.477771	-1.313629
H	1.102984	4.636945	-1.313231
H	3.231344	4.956605	-2.584213
H	4.971929	3.209414	-2.582736
H	4.643145	1.083385	-1.310297
Co	-0.000736	0.000901	2.119364
Cl	-0.003804	0.003079	4.323729

Co(5)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.082400	-1.578037	0.100525
C	0.859118	-2.108115	0.272031
C	2.262001	-0.256923	0.271343
N	1.394350	0.587512	0.906221
N	-0.188297	-1.501110	0.907206
C	1.395995	1.798179	0.271157
N	0.325047	2.592389	0.100267
C	-0.908804	2.087446	0.272114
N	-1.205867	0.913837	0.907256
C	-1.353625	-1.830558	0.272748
N	-2.408065	-1.014551	0.101974
C	-2.255654	0.309952	0.272961
C	0.310426	-3.215959	-0.534255
C	-1.096044	-3.039332	-0.534156

C	3.179820	0.570624	-0.535664
C	2.629320	1.876891	-0.535862
C	-2.940784	1.338522	-0.533993
C	-2.084916	2.468488	-0.534175
C	0.905385	-4.215792	-1.292909
C	0.068405	-5.074272	-2.016836
C	-1.321195	-4.899606	-2.016965
C	-1.919814	-3.860797	-1.292993
C	4.303019	0.268018	-1.294627
C	4.903027	1.305798	-2.018916
C	4.359123	2.596402	-2.019159
C	3.197239	2.891935	-1.295072
C	-4.103999	1.322594	-1.292848
C	-4.429313	2.476383	-2.017118
C	-3.583740	3.592844	-2.017231
C	-2.384880	3.592425	-1.293120
H	0.503726	-5.883059	-2.595649
H	1.984267	-4.327227	-1.316440
H	-1.943029	-5.575547	-2.595835
H	-2.992736	-3.701910	-1.316518
H	-4.739603	0.443723	-1.316293
H	-5.347330	2.503310	-2.596070
H	-3.858419	4.469111	-2.596346
H	-1.711012	4.442306	-1.316930
H	2.754057	3.881878	-1.318799
H	4.841556	3.377709	-2.598366
H	5.799253	1.105264	-2.597907
H	4.702087	-0.740526	-1.317999
Co	0.000649	0.000352	2.125145
Cl	0.003059	0.001429	4.329492

Rh(3)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.486533	-0.003242	-0.375810
C	1.850352	-1.160484	-0.137835
C	1.853211	1.155645	-0.138223
N	0.721270	1.314821	0.607735
N	0.718148	-1.316731	0.608371
C	-0.058182	2.288870	0.076848
N	-1.405018	2.288899	0.093070
C	-2.024748	1.126242	0.341805
N	-1.450380	0.001909	0.875305
C	-0.063761	-2.288914	0.077718
N	-1.410596	-2.285547	0.093958
C	-2.027434	-1.121243	0.342249
C	1.999016	-2.381360	-0.957637
C	0.780937	-3.095670	-0.824421
C	2.004975	2.375980	-0.958269
C	0.788647	3.093321	-0.825327
C	-3.313344	-0.704826	-0.246164

C	-3.311661	0.712693	-0.246420
C	2.994330	-2.819743	-1.821111
C	2.775654	-4.016018	-2.518177
C	1.572854	-4.721054	-2.386924
C	0.547081	-4.254564	-1.553417
C	3.001490	2.811720	-1.821704
C	2.785862	4.008383	-2.519034
C	1.584781	4.716419	-2.388071
C	0.557764	4.252653	-1.554601
C	-4.350763	-1.419521	-0.832263
C	-5.417310	-0.694229	-1.379177
C	-5.415636	0.706761	-1.379428
C	-4.347355	1.429685	-0.832765
H	3.548134	-4.398438	-3.178522
H	3.911833	-2.253848	-1.944017
H	1.429620	-5.639849	-2.947571
H	-0.398230	-4.781170	-1.473463
H	-4.331960	-2.504001	-0.859283
H	-6.255161	-1.226169	-1.819657
H	-6.252211	1.240544	-1.820104
H	-4.325941	2.514106	-0.860165
H	-0.386256	4.781604	-1.474857
H	1.443909	5.635446	-2.948938
H	3.559356	4.388780	-3.179360
H	3.917611	2.243535	-1.944348
Rh	0.142535	0.000196	2.108986
Cl	1.853232	-0.000859	3.713036

Rh(5)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.609784	-0.232590	-0.147221
C	1.845066	-1.324751	0.020229
C	2.050171	0.977606	0.019891
N	0.855606	1.217826	0.632979
N	0.626797	-1.349724	0.633148
C	0.224792	2.260004	0.019397
N	-1.103392	2.376222	-0.148199
C	-1.871745	1.286617	0.019380
N	-1.482337	0.132194	0.632654
C	-0.178334	-2.264321	0.020166
N	-1.506176	-2.143879	-0.147295
C	-2.069706	-0.935490	0.019854
C	1.975970	-2.571670	-0.761510
C	0.689917	-3.168982	-0.761386
C	2.399481	2.181531	-0.762190
C	1.239202	2.996651	-0.762483
C	-3.215123	-0.425582	-0.761844
C	-3.089185	0.986822	-0.762355
C	3.018898	-3.118804	-1.498522
C	2.771932	-4.305935	-2.200593

C	1.501421	-4.896146	-2.200344
C	0.435137	-4.319023	-1.498100
C	3.522714	2.535578	-1.499250
C	3.489312	3.747333	-2.201899
C	2.342988	4.552632	-2.202167
C	1.191519	4.173234	-1.499786
C	-4.210664	-1.055419	-1.498354
C	-5.115207	-0.248164	-2.200717
C	-4.990768	1.147208	-2.201275
C	-3.957622	1.782255	-1.499486
H	3.575836	-4.772140	-2.762258
H	3.992821	-2.641038	-1.522411
H	1.338995	-5.811254	-2.761834
H	-0.558178	-4.755052	-1.521717
H	-4.284059	-2.137744	-1.521692
H	-5.921067	-0.711392	-2.762042
H	-5.702012	1.745263	-2.763002
H	-3.838445	2.860480	-1.523614
H	0.290822	4.777825	-1.523698
H	2.344762	5.481785	-2.764083
H	4.362967	4.063996	-2.763618
H	4.396964	1.893325	-1.522783
Cl	0.000215	0.001711	4.522511
Rh	-0.000134	0.000387	2.190170

Ir(3)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.260289	-1.327619	-0.287757
C	-2.274224	0.001333	-0.146638
C	-1.131072	-2.032758	-0.115748
N	-0.002424	-1.522045	0.456603
N	-1.249264	0.774579	0.388665
C	1.125081	-2.036487	-0.114653
N	2.256768	-1.335056	-0.285552
C	2.274814	-0.006136	-0.144423
N	1.251792	0.770341	0.389805
C	-1.151892	2.002845	-0.238749
N	0.004814	2.643442	-0.443111
C	1.159167	1.999001	-0.237603
C	-3.110514	0.941365	-0.881931
C	-2.410817	2.184708	-0.942739
C	-0.718476	-3.229454	-0.852086
C	0.709248	-3.231813	-0.851399
C	2.419420	2.176809	-0.940248
C	3.114972	0.931180	-0.878784
C	-4.318182	0.770450	-1.565566
C	-4.832581	1.853548	-2.271065
C	-4.142104	3.081278	-2.330358
C	-2.921417	3.253774	-1.685864
C	-1.431315	-4.193275	-1.567274

C	-0.710849	-5.175340	-2.244647
C	0.696529	-5.177662	-2.243976
C	1.419585	-4.197980	-1.565912
C	2.934299	3.244243	-1.682767
C	4.155092	3.067791	-2.325987
C	4.841478	1.837801	-2.266048
C	4.322790	0.756349	-1.561160
H	-5.779632	1.752174	-2.792614
H	-4.834542	-0.183299	-1.536904
H	-4.569792	3.903363	-2.896445
H	-2.376494	4.189896	-1.748374
H	2.392510	4.182149	-1.745789
H	4.586067	3.888504	-2.891573
H	5.788737	1.733354	-2.786612
H	4.835988	-0.199091	-1.532026
H	2.504475	-4.183746	-1.584453
H	1.226311	-5.953796	-2.788316
H	-1.242670	-5.949721	-2.789496
H	-2.516133	-4.175455	-1.586855
Ir	-0.000514	0.152747	1.750074
Cl	-0.005837	-0.218868	4.019233

Ir(5)-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.439052	-0.956605	-0.387089
C	-2.244393	0.361816	-0.219114
C	-1.400063	-1.790887	-0.217812
N	-0.222289	-1.472325	0.396186
N	-1.164091	0.928910	0.394257
C	0.808729	-2.124486	-0.218078
N	2.047703	-1.634204	-0.387639
C	2.251027	-0.317094	-0.219677
N	1.386454	0.543669	0.393909
C	-0.851102	2.107687	-0.220157
N	0.391054	2.590110	-0.389416
C	1.435365	1.762337	-0.220455
C	-2.916794	1.419403	-0.999265
C	-2.032034	2.528092	-0.999908
C	-1.174071	-3.024088	-0.997037
C	0.228432	-3.235919	-0.997209
C	2.687689	1.815347	-1.000350
C	3.205633	0.494844	-0.999873
C	-4.094805	1.444031	-1.735574
C	-4.403778	2.616453	-2.437719
C	-3.529971	3.711429	-2.438341
C	-2.317822	3.670767	-1.736853
C	-2.021225	-3.843146	-1.733243
C	-1.450783	-4.913397	-2.434762
C	-0.065571	-5.122619	-2.434940
C	0.795697	-4.268625	-1.733599

C	3.298094	2.822768	-1.737216
C	4.468172	2.503783	-2.438791
C	4.979681	1.199605	-2.438359
C	4.338334	0.170612	-1.736304
H	-5.331516	2.674764	-2.998920
H	-4.753495	0.582114	-1.758728
H	-3.792981	4.602719	-3.000012
H	-1.623547	4.504259	-1.760947
H	2.880885	3.824102	-1.761153
H	4.982625	3.277739	-3.000374
H	5.883247	0.981434	-2.999621
H	4.713169	-0.847360	-1.759569
H	1.871474	-4.408050	-1.757375
H	0.347461	-5.955377	-2.996158
H	-2.091484	-5.586994	-2.995846
H	-3.090198	-3.658624	-1.756750
Cl	0.001660	0.008976	4.272016
Ir	0.000143	-0.000941	1.946072

Ni-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.935894	1.771348	0.053902
C	-0.678579	2.204302	0.232973
C	-2.255754	0.480568	0.232534
N	-1.414707	-0.447269	0.800613
N	0.320040	1.448903	0.801356
C	-1.569535	-1.689826	0.232277
N	-0.565895	-2.562198	0.053479
C	0.711836	-2.193784	0.232586
N	1.094700	-1.001691	0.801107
C	1.544146	1.713413	0.233434
N	2.502105	0.791068	0.054695
C	2.248386	-0.514345	0.233248
C	-0.005998	3.283759	-0.484457
C	1.388996	2.975638	-0.484254
C	-3.271223	-0.284936	-0.485230
C	-2.840578	-1.647110	-0.485304
C	2.847102	-1.636283	-0.484473
C	1.882825	-2.690392	-0.484737
C	-0.489494	4.390270	-1.186750
C	0.427262	5.197799	-1.853414
C	1.802583	4.894050	-1.853186
C	2.293756	3.775549	-1.186322
C	-4.416233	0.098613	-1.187495
C	-5.139261	-0.886057	-1.854317
C	-4.714710	-2.229013	-1.854353
C	-3.557036	-2.619138	-1.187585
C	4.047323	-1.770594	-1.186439
C	4.288592	-2.968191	-1.853173
C	3.337928	-4.007428	-1.853456

C	2.123456	-3.873732	-1.186985
H	0.078054	6.075026	-2.389542
H	-1.551846	4.609690	-1.203820
H	2.488930	5.542603	-2.389105
H	3.349703	3.527114	-1.203012
H	4.768514	-0.960264	-1.203024
H	5.223116	-3.104280	-2.388945
H	3.556631	-4.925965	-2.389518
H	1.380384	-4.664033	-1.204089
H	-3.215891	-3.648877	-1.204486
H	-5.299779	-2.970091	-2.390454
H	-6.044017	-0.615958	-2.390384
H	-4.729071	1.137302	-1.204309
Ni	-0.000291	-0.000208	1.907902
Cl	-0.001987	-0.000961	4.041921

Cu-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.217063	1.437419	-0.001839
C	-1.036635	2.046024	0.163787
C	-2.290653	0.111228	0.162831
N	-1.301365	-0.664502	0.714072
N	0.075284	1.459399	0.715212
C	-1.253221	-1.920702	0.162743
N	-0.135842	-2.638757	-0.002094
C	1.049354	-2.039469	0.163468
N	1.226228	-0.794852	0.714996
C	1.241734	1.928435	0.164033
N	2.353412	1.201653	-0.001115
C	2.290176	-0.125032	0.163885
C	-0.547822	3.245619	-0.507138
C	0.879263	3.171975	-0.506943
C	-3.186092	-0.824463	-0.508494
C	-2.536238	-2.097158	-0.508654
C	3.084941	-1.147840	-0.507077
C	2.307706	-2.346968	-0.507422
C	-1.206958	4.291961	-1.157477
C	-0.433454	5.266674	-1.779972
C	0.974073	5.193989	-1.779839
C	1.642870	4.144774	-1.157201
C	-4.410326	-0.649677	-1.158865
C	-4.984363	-1.753498	-1.781668
C	-4.343415	-3.008736	-1.781845
C	-3.112608	-3.191161	-1.159216
C	4.320783	-1.099750	-1.157191
C	4.778575	-2.256753	-1.779760
C	4.012037	-3.439480	-1.780032
C	2.768805	-3.494444	-1.157748
H	-0.920734	6.097229	-2.281570
H	-2.290767	4.335897	-1.171399

H	1.544440	5.969958	-2.281253
H	2.725442	4.076812	-1.170843
H	4.900570	-0.182999	-1.170721
H	5.741662	-2.249788	-2.281034
H	4.399124	-4.321237	-2.281562
H	2.168869	-4.398130	-1.171743
H	-2.608697	-4.151709	-1.173054
H	-4.818939	-3.846032	-2.283518
H	-5.941484	-1.647588	-2.283232
H	-4.892870	0.321783	-1.172497
Cl	-0.003214	-0.001954	4.043371
Cu	-0.000266	-0.000233	1.902940

Fe(3)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.750061	0.000564	1.423874
C	1.305159	1.183601	0.965149
C	1.305708	-1.182730	0.965193
N	0.573443	-1.370831	-0.190305
N	0.572850	1.371287	-0.190394
C	-0.380569	-2.335058	-0.006109
N	-1.604042	-2.288348	-0.562361
C	-2.057306	-1.137620	-1.083370
N	-1.296314	-0.000276	-1.274028
C	-0.381676	2.335013	-0.006264
N	-1.605120	2.287679	-0.562497
C	-2.057841	1.136697	-1.083454
C	1.067824	2.366490	1.796285
C	0.004875	3.094202	1.181953
C	1.068993	-2.365681	1.796391
C	0.006393	-3.093970	1.182126
C	-3.454764	0.711856	-1.140566
C	-3.454423	-0.713429	-1.140498
C	1.592109	2.779399	3.023005
C	1.081867	3.937249	3.605698
C	0.033672	4.654742	2.999503
C	-0.527116	4.229448	1.797470
C	1.593517	-2.778269	3.023130
C	1.083861	-3.936320	3.605905
C	0.035998	-4.654382	2.999774
C	-0.525017	-4.229454	1.797734
C	-4.656212	1.421783	-1.091828
C	-5.848994	0.702348	-1.079934
C	-5.848656	-0.705072	-1.079853
C	-4.655528	-1.423934	-1.091668
H	1.490494	4.288356	4.548942
H	2.378314	2.206308	3.504042
H	-0.349459	5.548049	3.484337
H	-1.356226	4.762787	1.343481

H	-4.651728	2.506659	-1.064490
H	-6.796123	1.233763	-1.061248
H	-6.795530	-1.236940	-1.061107
H	-4.650527	-2.508804	-1.064223
H	-1.353867	-4.763230	1.343780
H	-0.346672	-5.547842	3.484689
H	1.492668	-4.287170	4.549166
H	2.379446	-2.204746	3.504102
C	3.089607	-1.159870	-2.256881
C	4.393525	-1.200343	-2.734066
C	5.058300	0.000429	-2.982467
C	4.392608	1.201160	-2.736461
C	3.088721	1.160583	-2.259130
N	2.438078	0.000358	-2.024007
H	6.078046	0.000440	-3.354325
H	2.537607	-2.064361	-2.025027
H	4.875270	-2.157192	-2.901430
H	4.873579	2.158063	-2.905720
H	2.536108	2.065142	-2.028958
Fe	0.528004	0.000172	-1.478406

Fe(5)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.300424	-2.550389	-0.659830
C	0.814871	-1.646288	-1.513597
C	-0.414108	-2.161657	0.411754
N	-0.917153	-0.897512	0.607507
N	0.447632	-0.323603	-1.568964
C	-0.870819	-0.555750	1.936606
N	-0.618637	0.682965	2.398999
C	-0.124040	1.627519	1.578305
N	-0.081721	1.526240	0.210652
C	1.532317	0.465726	-1.860292
N	1.742295	1.696110	-1.356105
C	1.045492	2.129460	-0.290035
C	2.114663	-1.752146	-2.175119
C	2.567836	-0.417283	-2.394983
C	-0.400187	-2.814784	1.722317
C	-0.684172	-1.800743	2.684613
C	1.567774	2.990954	0.772823
C	0.833184	2.670693	1.952618
C	2.936665	-2.839941	-2.480522
C	4.184791	-2.588102	-3.043504
C	4.632091	-1.270346	-3.260816
C	3.840418	-0.177217	-2.919503
C	-0.067156	-4.108030	2.131386
C	-0.062217	-4.390289	3.495381
C	-0.342133	-3.389533	4.444994
C	-0.632918	-2.085461	4.051007
C	2.636816	3.887901	0.823760
C	2.937444	4.490622	2.043118
C	2.212684	4.174300	3.207505
C	1.172018	3.248643	3.177832
H	4.830901	-3.419313	-3.311147
H	2.601705	-3.853139	-2.282635
H	5.615673	-1.107519	-3.692140
H	4.194663	0.839557	-3.056016
H	3.213663	4.105173	-0.069564
H	3.750382	5.208743	2.101406
H	2.477674	4.654199	4.145329
H	0.631516	2.979539	4.079729
H	-0.817512	-1.304246	4.781549
H	-0.320158	-3.638734	5.502096
H	0.171647	-5.395214	3.835111

H	0.179966	-4.868728	1.397699
C	-4.084932	-0.010513	-0.780978
C	-5.442914	0.117466	-1.040662
C	-5.855722	0.945212	-2.084576
C	-4.888730	1.617443	-2.831750
C	-3.548974	1.441913	-2.508741
N	-3.143663	0.642852	-1.498719
H	-6.910224	1.063274	-2.312585
H	-3.715806	-0.647115	0.016932
H	-6.158593	-0.426038	-0.434142
H	-5.161994	2.270524	-3.652932
H	-2.767024	1.948832	-3.065276
Fe	-1.214653	0.359805	-0.861994

Ru(3)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.040175	-2.460069	0.892601
C	0.754759	-2.263606	-0.167932
C	-0.762522	-1.442358	1.389366
N	-0.974802	-0.237063	0.753509
N	0.721819	-1.145283	-0.966058
C	-0.997323	0.811633	1.651043
N	-0.509883	2.041970	1.421398
C	0.287469	2.268786	0.367931
N	0.464981	1.392315	-0.672859
C	1.971136	-0.836819	-1.440041
N	2.421058	0.410473	-1.654835
C	1.739484	1.460286	-1.165201
C	2.028204	-2.928849	-0.439262
C	2.795580	-2.030003	-1.238473
C	-1.063004	-1.205953	2.797223
C	-1.210650	0.204647	2.961023
C	2.315897	2.708999	-0.660209
C	1.397832	3.220109	0.305111
C	2.582587	-4.128540	0.013146
C	3.886054	-4.438485	-0.369042
C	4.643374	-3.551334	-1.157545
C	4.114724	-2.333881	-1.581825
C	-1.104042	-2.057955	3.904930
C	-1.332543	-1.499035	5.159367
C	-1.477977	-0.106871	5.321070
C	-1.398243	0.756475	4.231781
C	3.541494	3.341231	-0.879151
C	3.823187	4.501849	-0.160748
C	2.917439	5.006126	0.791538
C	1.708721	4.361527	1.047401
H	4.331051	-5.375711	-0.047182
H	2.005784	-4.797460	0.643920
H	5.660150	-3.818936	-1.430680
H	4.705489	-1.635300	-2.165775
H	4.250452	2.934363	-1.593228
H	4.761187	5.022977	-0.330025
H	3.171361	5.908016	1.341223
H	1.020869	4.731894	1.800908
H	-1.479033	1.831585	4.356401
H	-1.644405	0.297967	6.315247
H	-1.389466	-2.144007	6.031574
H	-0.961171	-3.126615	3.780629
C	-3.984295	-0.129178	-0.816796
C	-5.332171	-0.109655	-1.140828
C	-5.718963	0.061240	-2.473209
C	-4.716743	0.211747	-3.436188

C	-3.388767	0.188368	-3.040693
N	-3.002383	0.017438	-1.747405
H	-6.767133	0.078095	-2.752596
H	-3.645939	-0.263586	0.204095
H	-6.067483	-0.229819	-0.352310
H	-4.957564	0.349376	-4.484966
H	-2.588719	0.309152	-3.766372
Ru	-0.956680	-0.010306	-1.190410

Ru(5)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.149352	-2.297553	1.152297
C	0.576849	-2.288269	0.000792
C	-0.788698	-1.222462	1.564720
N	-1.115909	-0.068224	0.828777
N	0.565135	-1.237295	-0.910864
C	-0.839688	1.041399	1.649757
N	-0.252580	2.173672	1.321744
C	0.471616	2.288881	0.174324
N	0.507388	1.313909	-0.817084
C	1.800741	-1.058177	-1.451154
N	2.316524	0.117080	-1.882395
C	1.749734	1.232398	-1.362897
C	1.790664	-3.046371	-0.246710
C	2.565815	-2.282436	-1.171131
C	-0.976709	-0.854935	2.986448
C	-1.008491	0.559473	3.039625
C	2.460989	2.462477	-0.983781
C	1.651346	3.117029	-0.006522
C	2.304541	-4.228178	0.293348
C	3.566763	-4.653560	-0.125510
C	4.326252	-3.900400	-1.036823
C	3.838897	-2.694228	-1.550942
C	-1.001681	-1.613523	4.148170
C	-1.106612	-0.938804	5.374548
C	-1.137966	0.457838	5.427078
C	-1.065465	1.226767	4.254984
C	3.715537	2.957853	-1.323387
C	4.148806	4.139726	-0.713327
C	3.355487	4.785000	0.250384
C	2.112161	4.273579	0.627681
H	3.975124	-5.580427	0.267530
H	1.731282	-4.798697	1.017133
H	5.308813	-4.254354	-1.334587
H	4.432776	-2.088651	-2.228368
H	4.336664	2.433900	-2.043113
H	5.115579	4.558295	-0.977019
H	3.722271	5.694800	0.717354
H	1.513224	4.759799	1.391134
H	-1.051074	2.311216	4.291974
H	-1.206411	0.955824	6.389888
H	-1.151079	-1.510246	6.297128
H	-0.938746	-2.695956	4.103683
C	-4.062809	-0.020131	-0.709995
C	-5.415485	-0.011726	-1.012456
C	-5.824322	0.040761	-2.348647
C	-4.837011	0.084004	-3.337572
C	-3.502437	0.073596	-2.964349
N	-3.095020	0.021388	-1.666596
H	-6.877007	0.048102	-2.611022
H	-3.702259	-0.061094	0.311602
H	-6.138574	-0.046517	-0.204296
H	-5.094603	0.126092	-4.390634
H	-2.713200	0.107491	-3.710433

Ru	-1.043387	0.007139	-1.139751

Os(3)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.069109	2.272271	1.358543
C	-0.606954	2.290548	0.204100
C	0.637900	1.140272	1.798159
N	0.821532	-0.001521	1.036191

N	-0.580328	1.273799	-0.729188
C	0.636068	-1.143671	1.796855
N	0.065918	-2.274541	1.355882
C	-0.609801	-2.290441	0.201220
N	-0.581334	-1.272788	-0.731060
C	-1.791736	1.162793	-1.372131
N	-2.318209	0.002291	-1.792534
C	-1.792890	-1.159254	-1.373848
C	-1.769055	3.112051	-0.117063
C	-2.514861	2.403298	-1.105888
C	0.747017	0.711056	3.186231
C	0.745814	-0.716234	3.185424
C	-2.517583	-2.399177	-1.109216
C	-1.772901	-3.110051	-0.121119
C	-2.258975	4.302748	0.425691
C	-3.471316	4.794749	-0.051653
C	-4.207441	4.095153	-1.027426
C	-3.748320	2.887586	-1.548230
C	0.734781	1.421308	4.390112
C	0.761567	0.700400	5.580866
C	0.760406	-0.708455	5.580051
C	0.732418	-1.427905	4.388445
C	-3.751654	-2.881279	-1.552270
C	-4.212453	-4.088827	-1.032928
C	-3.477395	-4.790541	-0.057861
C	-2.264474	-4.300708	0.420223
H	-3.862453	5.729293	0.339954
H	-1.701953	4.825432	1.196591
H	-5.153915	4.502093	-1.371469
H	-4.326312	2.332756	-2.280263
H	-4.328783	-2.324813	-2.283740
H	-5.159421	-4.494112	-1.377567
H	-3.869844	-5.725015	0.332596
H	-1.708244	-4.825001	1.190601
H	0.702297	-2.512661	4.384194
H	0.771448	-1.240155	6.527082
H	0.773478	1.230970	6.528520
H	0.706465	2.506116	4.387177
C	3.948065	-0.000538	-0.480556
C	5.278160	-0.001091	-0.835155
C	5.657098	-0.000777	-2.189133
C	4.628846	0.000416	-3.146590
C	3.311583	0.001014	-2.747409
N	2.922149	0.000172	-1.414403
H	6.700199	-0.001257	-2.483156
H	3.628427	-0.000676	0.554172
H	6.024421	-0.001757	-0.046941
H	4.852153	0.000975	-4.208768
H	2.503734	0.002128	-3.474856
Os	0.970855	-0.000378	-0.910941

Os(5)-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.040000	2.198607	1.451050
C	-0.605030	2.286361	0.256784
C	0.624485	1.084590	1.834824
N	0.950397	-0.033245	1.038074
N	-0.575163	1.279671	-0.714123
C	0.614994	-1.188474	1.774623
N	0.021499	-2.275999	1.333128
C	-0.625111	-2.294657	0.136335
N	-0.586316	-1.238833	-0.780184
C	-1.782178	1.185561	-1.345306

N	-2.300649	0.058228	-1.884700
C	-1.792465	-1.100765	-1.404857
C	-1.767378	3.102973	-0.031264
C	-2.509257	2.422545	-1.044806
C	0.735972	0.618436	3.232926
C	0.730260	-0.797694	3.195519
C	-2.531296	-2.344376	-1.168387
C	-1.795336	-3.083961	-0.192612
C	-2.270531	4.274583	0.540530
C	-3.484957	4.774038	0.066358
C	-4.210568	4.104113	-0.933395
C	-3.737192	2.908515	-1.482950
C	0.729378	1.300091	4.441573
C	0.760694	0.545634	5.624742
C	0.755080	-0.851722	5.587789
C	0.717945	-1.542259	4.366350
C	-3.764246	-2.795018	-1.629817
C	-4.248737	-4.013018	-1.142853
C	-3.528904	-4.741250	-0.180315
C	-2.309398	-4.278966	0.317812
H	-3.882650	5.694428	0.484403
H	-1.724624	4.781072	1.329934
H	-5.156790	4.514585	-1.272891
H	-4.307178	2.366560	-2.230955
H	-4.329465	-2.209310	-2.347858
H	-5.199139	-4.396084	-1.502137
H	-3.935217	-5.678338	0.189569
H	-1.767857	-4.831219	1.079033
H	0.677981	-2.626087	4.332494
H	0.767096	-1.411800	6.518155
H	0.777027	1.055634	6.583413
H	0.698239	2.384482	4.465164
C	3.953674	0.003642	-0.477326
C	5.285913	0.012703	-0.822683
C	5.674893	0.047349	-2.173824
C	4.652659	0.071575	-3.137721
C	3.332669	0.061069	-2.747960
N	2.933244	0.027565	-1.417926
H	6.720015	0.055013	-2.460603
H	3.623925	-0.022583	0.553799
H	6.026816	-0.007397	-0.029509
H	4.883112	0.098480	-4.198121
H	2.529139	0.079006	-3.479548
Os	0.981346	0.018578	-0.920422

Co-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.091582	1.106840	-2.373576
C	-0.527423	1.776215	-1.290734
C	0.290076	-0.180246	-2.293929
N	0.037293	-1.011361	-1.229238
N	-0.893651	1.193429	-0.101110
C	1.091050	-1.864716	-1.013602
N	1.513985	-2.272193	0.196912
C	1.102962	-1.655716	1.319961
N	0.050679	-0.776635	1.391051
C	-0.516154	1.978069	0.962328
N	-0.068757	1.511249	2.142384
C	0.313317	0.230155	2.288622
C	-0.255870	3.184439	-0.998909
C	-0.248734	3.311764	0.422190
C	1.392405	-0.786840	-3.042699
C	1.897868	-1.848502	-2.235209
C	1.423611	-0.234735	3.122131

C	1.921938	-1.423435	2.511132
C	0.078790	4.271203	-1.810088
C	0.374955	5.487015	-1.198902
C	0.381957	5.612666	0.203327
C	0.092965	4.525154	1.023854
C	2.025918	-0.441452	-4.238245
C	3.132373	-1.186127	-4.640065
C	3.631141	-2.233722	-3.843264
C	3.034109	-2.559114	-2.627563
C	2.068676	0.317088	4.230878
C	3.179770	-0.345262	4.747575
C	3.671533	-1.518200	4.144672
C	3.062706	-2.053969	3.012180
H	0.615415	6.351384	-1.811267
H	0.103849	4.162628	-2.889694
H	0.627690	6.571928	0.649847
H	0.128828	4.610281	2.105256
H	1.705657	1.238755	4.674337
H	3.683020	0.053314	5.623820
H	4.546355	-2.005665	4.565379
H	3.457885	-2.940349	2.526287
H	3.434901	-3.345384	-1.995837
H	4.502138	-2.789003	-4.179359
H	3.626513	-0.950080	-5.578169
H	1.657724	0.387084	-4.834790
C	-3.620201	-2.533565	0.226025
C	-4.961107	-2.894839	0.261364
C	-5.930671	-1.894380	0.190160
C	-5.519901	-0.566172	0.085946
C	-4.159696	-0.284286	0.056542
N	-3.218539	-1.249480	0.125356
H	-6.986129	-2.146109	0.215418
H	-2.834090	-3.280015	0.278624
H	-5.233507	-3.941076	0.343049
H	-6.237624	0.244358	0.027756
H	-3.790530	0.733083	-0.023874
Co	-1.292010	-0.651816	0.066174

Rh-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.427676	0.184152	-2.647486
C	-0.352330	-1.025630	-2.068209
C	-0.295159	1.299504	-1.910181
N	0.168156	1.334326	-0.620890
N	0.103856	-1.257204	-0.796702
C	-0.468287	2.301267	0.112081
N	-0.774248	2.196332	1.416626
C	-0.701699	1.007017	2.037061
N	-0.093653	-0.108252	1.521273
C	-0.580675	-2.283016	-0.199685
N	-0.885383	-2.341301	1.108000
C	-0.757089	-1.251787	1.883638
C	-1.118140	-2.213228	-2.453839
C	-1.262501	-3.005737	-1.275819
C	-1.001697	2.563880	-2.128730
C	-1.111222	3.195356	-0.853601
C	-1.624069	-0.886915	3.006137
C	-1.589068	0.536416	3.102857
C	-1.753852	-2.583704	-3.641302
C	-2.494734	-3.763552	-3.654009
C	-2.637213	-4.545529	-2.491629
C	-2.041929	-4.164960	-1.290827

C	-1.615015	3.122358	-3.252767
C	-2.297850	4.327489	-3.102736
C	-2.405972	4.950544	-1.844534
C	-1.833587	4.382250	-0.708518
C	-2.473293	-1.633803	3.826171
C	-3.250008	-0.956915	4.764004
C	-3.215415	0.447579	4.859488
C	-2.403375	1.206218	4.019217
H	-2.979767	-4.082933	-4.572148
H	-1.666628	-1.963182	-4.527619
H	-3.229879	-5.455108	-2.532342
H	-2.174580	-4.749481	-0.385843
H	-2.519756	-2.713975	3.729872
H	-3.901329	-1.518824	5.427528
H	-3.840599	0.945803	5.595112
H	-2.396495	2.290452	4.070064
H	-1.940655	4.844283	0.267866
H	-2.953812	5.884823	-1.759450
H	-2.763991	4.791557	-3.967372
H	-1.555218	2.624327	-4.215375
C	4.385622	1.059730	0.289584
C	5.775000	1.085673	0.338212
C	6.471770	-0.121852	0.384071
C	5.747252	-1.313877	0.378069
C	4.358898	-1.257494	0.328248
N	3.680587	-0.091276	0.285878
H	7.556523	-0.133783	0.422477
H	3.804684	1.975476	0.250302
H	6.293420	2.038239	0.338807
H	6.243611	-2.277586	0.410456
H	3.757505	-2.160754	0.319552
Rh	1.491985	-0.058232	0.189923

Ir-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.245034	0.029590	2.121503
C	-0.880981	-1.144524	1.581001
C	-0.887523	1.189115	1.544324
N	-0.380209	1.307188	0.276061
N	-0.368816	-1.299599	0.317567
C	0.555849	2.304700	0.203192
N	1.645567	2.265517	-0.581259
C	2.027211	1.121937	-1.166732
N	1.253970	-0.018652	-1.255787
C	0.570874	-2.294822	0.277430
N	1.660792	-2.276338	-0.507937
C	2.035367	-1.150535	-1.130901
C	-0.524910	-2.358176	2.318464
C	0.392561	-3.081353	1.498018
C	-0.534660	2.425813	2.244207
C	0.377008	3.127920	1.399303
C	3.410644	-0.726275	-1.376666
C	3.405501	0.699574	-1.399142
C	-0.824634	-2.801604	3.608963
C	-0.238270	-3.984313	4.054031
C	0.666177	-4.698019	3.244188
C	1.004681	-4.244689	1.971221
C	-0.832612	2.906968	3.521563
C	-0.250560	4.105434	3.928545
C	0.648146	4.798345	3.094581
C	0.985108	4.307933	1.835043
C	4.612470	-1.434354	-1.458934
C	5.794206	-0.712734	-1.606679
C	5.789128	0.695793	-1.628950

C	4.602237	1.413257	-1.503953
H	-0.473396	-4.359642	5.045974
H	-1.499276	-2.233916	4.242005
H	1.113444	-5.611787	3.624996
H	1.723388	-4.776551	1.355866
H	4.615068	-2.518602	-1.411908
H	6.738440	-1.242035	-1.697210
H	6.729551	1.228733	-1.736270
H	4.597055	2.498436	-1.491186
H	1.699617	4.824027	1.201628
H	1.092185	5.725363	3.446003
H	-0.484478	4.509684	4.909352
H	-1.502439	2.355588	4.173859
C	-3.511499	1.133185	-1.600937
C	-4.895644	1.166796	-1.692456
C	-5.598388	-0.030208	-1.840008
C	-4.877869	-1.224458	-1.884456
C	-3.493934	-1.185131	-1.785837
N	-2.806768	-0.024863	-1.643045
H	-6.680681	-0.031768	-1.921045
H	-2.922845	2.035978	-1.488693
H	-5.408210	2.121544	-1.651039
H	-5.375923	-2.181173	-1.996874
H	-2.891796	-2.085362	-1.819104
Ir	-0.734290	-0.027167	-1.316450

Zn-Tdpy

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-0.026544	1.300283	-2.274655
C	-0.286215	-0.021006	-2.303132
C	0.347152	1.922124	-1.139730
N	0.805686	1.300665	-0.005939
N	0.071502	-0.923075	-1.334848
C	0.343525	1.935350	1.118957
N	-0.033716	1.326845	2.259963
C	-0.293422	0.005967	2.303046
N	0.067410	-0.907382	1.346567
C	-0.902366	-1.871998	-1.164823
N	-1.261301	-2.419291	0.012599
C	-0.905958	-1.858300	1.184598
C	-1.363284	-0.645860	-3.075640
C	-1.752486	-1.814258	-2.356852
C	-0.097463	3.256865	-0.732056
C	-0.099763	3.265216	0.694269
C	-1.759739	-1.786679	2.373271
C	-1.372845	-0.609901	3.079495
C	-2.070905	-0.242012	-4.209723
C	-3.130825	-1.033877	-4.645134
C	-3.515100	-2.187272	-3.935478
C	-2.847447	-2.573037	-2.775528
C	-0.588783	4.350609	-1.448605
C	-1.032820	5.462427	-0.737311
C	-1.035077	5.470673	0.670712
C	-0.593348	4.367263	1.396392
C	-2.855952	-2.540592	2.797412
C	-3.527210	-2.141315	3.950693
C	-3.145199	-0.979644	4.647960
C	-2.083989	-0.192834	4.206565
H	-3.678821	-0.753093	-5.540060
H	-1.793630	0.666711	-4.734419
H	-4.353404	-2.777632	-4.294298
H	-3.162449	-3.441913	-2.206476

H	-3.169145	-3.416109	2.237618
H	-4.366584	-2.727505	4.313821
H	-3.695973	-0.688439	5.537836
H	-1.808383	0.722008	4.721413
H	-0.626501	4.356189	2.481196
H	-1.398969	6.348816	1.196540
H	-1.395012	6.334344	-1.274550
H	-0.618457	4.326845	-2.533306
C	4.188602	0.110322	0.005552
C	5.568525	-0.052165	0.007487
C	6.093315	-1.343954	0.014060
C	5.217614	-2.429460	0.018462
C	3.849460	-2.186411	0.016158
N	3.342143	-0.938659	0.009846
H	7.167033	-1.502814	0.015713
H	3.726910	1.092786	0.000442
H	6.212407	0.819932	0.003869
H	5.582167	-3.450359	0.023589
H	3.130826	-2.999294	0.019382
Zn	1.380125	-0.530121	0.005683

P-Td=O

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.388903	2.266395	0.302844
C	2.042525	1.113937	0.461149
C	0.065328	2.325618	0.461259
N	-0.683328	1.258683	0.973692
N	1.431828	-0.037498	0.973736
C	-1.985918	1.211880	0.461377
N	-2.657202	0.069614	0.303145
C	-2.046675	-1.106227	0.461417
N	-0.748330	-1.221197	0.973797
C	1.981376	-1.219328	0.461162
N	1.268294	-2.335955	0.302815
C	-0.056552	-2.325800	0.461206
C	3.265827	0.632961	-0.141973
C	3.228157	-0.803082	-0.142017
C	-0.918617	3.197192	-0.141937
C	-2.181073	2.511722	-0.141826
C	-1.084747	-3.144666	-0.141990
C	-2.309603	-2.394079	-0.141802
C	4.312135	1.317544	-0.769664
C	5.322392	0.566037	-1.358415
C	5.285380	-0.844019	-1.358486
C	4.237098	-1.541548	-0.769784
C	-0.783645	4.440114	-0.769883
C	-1.911882	4.998986	-1.358751
C	-3.151483	4.325929	-1.358593
C	-3.297114	3.075377	-0.769600
C	-1.015035	-4.392966	-0.769909
C	-2.170999	-4.892030	-1.358718
C	-3.373693	-4.155037	-1.358492
C	-3.453648	-2.898566	-0.769513
H	6.156902	1.072369	-1.832105
H	4.333025	2.401539	-0.782996
H	6.092200	-1.393384	-1.832196
H	4.201130	-2.625147	-0.783143
H	-0.086709	-4.953050	-0.783385
H	-2.149752	-5.867824	-1.832571
H	-4.252890	-4.579039	-1.832193
H	-4.374090	-2.325620	-0.782738
H	-4.246280	2.551387	-0.782889
H	-4.007265	4.795330	-1.832368
H	-1.839574	5.972299	-1.832666

H	0.172749	4.950788	-0.783383
O	0.000106	0.000051	3.303210
P	0.000089	-0.000003	1.838629

Mn(2)-Td=O

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.355613	2.254698	0.237341
C	-0.027879	2.300876	0.413846
C	-2.028409	1.109503	0.420269
N	-1.466703	-0.024111	0.968723
N	0.711451	1.275760	0.971700
C	-1.990314	-1.176271	0.420648
N	-1.279719	-2.298410	0.237822
C	0.048813	-2.301103	0.414663
N	0.753931	-1.251672	0.971835
C	1.967875	1.194206	0.410770
N	2.632260	0.043653	0.234797
C	2.006948	-1.128574	0.411170
C	0.929521	3.146495	-0.289550
C	2.180287	2.456067	-0.287092
C	-3.238075	0.660982	-0.262341
C	-3.214109	-0.768370	-0.262334
C	2.261337	-2.383270	-0.285676
C	1.034072	-3.114776	-0.288137
C	0.785290	4.352253	-0.980889
C	1.898594	4.874459	-1.632149
C	3.132215	4.194379	-1.628540
C	3.280990	2.975916	-0.973488
C	-4.245075	1.354192	-0.938375
C	-5.236490	0.616770	-1.579295
C	-5.212853	-0.791057	-1.579342
C	-4.197260	-1.494887	-0.938491
C	3.378814	-2.866677	-0.971578
C	3.270623	-4.089602	-1.626304
C	2.060205	-4.810114	-1.629986
C	0.930051	-4.324844	-0.979128
H	1.816145	5.820462	-2.158722
H	-0.171281	4.863733	-1.000118
H	3.978391	4.627694	-2.153090
H	4.223502	2.438802	-0.987576
H	4.303032	-2.298658	-0.985649
H	4.130812	-4.494816	-2.150520
H	2.009235	-5.758511	-2.156241
H	-0.009031	-4.867765	-0.998404
H	-4.165054	-2.579207	-0.955583
H	-5.998766	-1.335067	-2.094456
H	-6.040181	1.134138	-2.094421
H	-4.249206	2.438983	-0.955405
P	0.185742	0.011528	3.629772

Mn	0.002647	-0.000029	2.085779

Mn(4)-Td=O

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.348494	1.178425	0.229927
C	2.291856	-0.147606	0.416768
C	1.241669	1.921081	0.380061
N	0.075468	1.456053	0.934756
N	1.217635	-0.806316	0.977528
C	-1.036834	2.038716	0.380502
N	-2.214650	1.414526	0.231349
C	-2.295290	0.089749	0.418472
N	-1.294725	-0.676335	0.978867
C	1.052248	-2.062161	0.437457
N	-0.138255	-2.659121	0.280357
C	-1.260617	-1.942379	0.438554
C	3.074483	-1.170341	-0.267492
C	2.298227	-2.369007	-0.254640
C	0.876675	3.133671	-0.347734
C	-0.549120	3.207398	-0.347284
C	-2.531977	-2.118866	-0.253000
C	-3.180123	-0.846399	-0.265292
C	4.288526	-1.116422	-0.957540
C	4.732722	-2.269918	-1.596417
C	3.967078	-3.452564	-1.583524
C	2.739310	-3.509492	-0.931380
C	1.636658	4.062439	-1.061863
C	0.966857	5.078778	-1.737891
C	-0.439013	5.151515	-1.737407
C	-1.209672	4.209685	-1.060910
C	-3.089079	-3.207583	-0.929389
C	-4.304935	-3.024009	-1.580557
C	-4.944234	-1.768573	-1.592836
C	-4.382632	-0.667202	-0.954348
H	5.683360	-2.259481	-2.120949
H	4.864591	-0.197552	-0.985297
H	4.341364	-4.332111	-2.098579
H	2.136578	-4.411518	-0.939730
H	-2.582852	-4.167095	-0.938190
H	-4.768561	-3.860131	-2.095266
H	-5.889125	-1.659874	-2.116594
H	-4.860608	0.306315	-0.981757
H	-2.293685	4.249228	-1.078483
H	-0.929074	5.953975	-2.280413
H	1.536752	5.826432	-2.281207
H	2.718958	3.989978	-1.080047
O	0.043079	0.628406	3.657480
Mn	0.003328	0.034436	2.169333

V-Td=O

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.213865	1.409217	0.318294
C	2.290299	0.078806	0.464804
C	1.057338	2.066293	0.506386
N	-0.058600	1.502310	1.088425
N	1.298050	-0.710949	1.020133
C	-1.216391	1.976440	0.507612
N	-2.317721	1.230347	0.320372
C	-2.289629	-0.102053	0.466603
N	-1.238085	-0.811671	1.021209
C	1.239087	-1.942651	0.407262
N	0.103697	-2.631310	0.217058
C	-1.082531	-2.034523	0.407736
C	3.148371	-0.828890	-0.291379
C	2.490696	-2.095270	-0.326314
C	0.586993	3.238829	-0.224307
C	-0.840717	3.182354	-0.223589
C	-2.318443	-2.284839	-0.325559
C	-3.073765	-1.074124	-0.289848
C	4.328608	-0.621030	-1.009827
C	4.862507	-1.691369	-1.721225
C	4.214302	-2.941539	-1.754361
C	3.016739	-3.149956	-1.077015
C	1.258544	4.226160	-0.950782
C	0.499865	5.170434	-1.635336
C	-0.907865	5.114749	-1.634617
C	-1.588892	4.113503	-0.949348
C	-2.760024	-3.377251	-1.076774
C	-3.970329	-3.263311	-1.753919
C	-4.714896	-2.068032	-1.720051
C	-4.266804	-0.959403	-1.008091
H	5.792156	-1.561408	-2.267049
H	4.812280	0.350068	-1.002885
H	4.655391	-3.752796	-2.325575
H	2.501241	-4.103550	-1.121163
H	-2.171124	-4.287319	-1.121507
H	-4.346278	-4.106436	-2.325572
H	-5.651943	-2.011342	-2.265753
H	-4.825404	-0.029387	-1.000570
H	-2.671990	4.052961	-0.968407
H	-1.468530	5.863798	-2.185630
H	0.999046	5.961388	-2.186922
H	2.343022	4.251341	-0.970954
O	0.024494	-0.481584	3.818808
V	0.002146	-0.047401	2.285422

P-Td

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.730908	-2.564393	0.464379
C	-0.560252	-2.246906	0.602605
C	1.660662	-1.613834	0.602350
N	1.382856	-0.347123	1.107773
N	-0.992083	-1.024221	1.108356
C	2.226012	0.638314	0.602602
N	1.855366	1.915302	0.464793
C	0.567304	2.245171	0.602945
N	-0.390811	1.371313	1.108553
C	-2.227930	-0.631272	0.603025
N	-2.586299	0.649183	0.465149
C	-1.665689	1.608587	0.603106
C	-1.732869	-2.819341	-0.024742
C	-2.763074	-1.821280	-0.024462
C	2.958915	-1.482078	-0.024833
C	3.308177	-0.090846	-0.024649
C	-1.575337	2.910214	-0.024441
C	-0.195923	3.303477	-0.024570
C	-1.926350	-4.043101	-0.674339
C	-3.155929	-4.270676	-1.281588
C	-4.169021	-3.289197	-1.281288
C	-3.980289	-2.053203	-0.673756
C	3.768561	-2.420057	-0.674218
C	4.933444	-1.965326	-1.281367
C	5.276911	-0.597225	-1.281173
C	4.464900	0.353650	-0.673833
C	-2.538649	3.689372	-0.673991
C	-2.121232	4.867879	-1.281663
C	-0.764735	5.254623	-1.281811
C	0.211533	4.473471	-0.674275
H	-3.341397	-5.220804	-1.771638
H	-1.140376	-4.789903	-0.691242
H	-5.112944	-3.504522	-1.771118
H	-4.751583	-1.291241	-0.690241
H	-3.578341	3.381942	-0.690626
H	-2.851514	5.503336	-1.771739
H	-0.479453	6.179607	-1.772024
H	1.257025	4.760553	-0.691114
H	4.718661	1.407730	-0.690392
H	6.192584	-0.282652	-1.770945
H	5.591993	-2.674984	-1.771254
H	3.494373	-3.469006	-0.691019
P	0.000438	-0.000199	2.088434

H_2-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	0.193398	2.635186	-0.392287
C	-1.002761	2.047539	-0.629708
C	1.310410	1.909521	-0.583604
N	1.263414	0.662977	-1.137766
N	-1.131075	0.826348	-1.218247
C	2.281995	-0.164594	-0.760156
N	2.173418	-1.497541	-0.686422
C	0.991423	-2.101708	-0.881337
N	-0.124945	-1.528161	-1.474015
C	-2.268127	0.204701	-0.819634
N	-2.396471	-1.133747	-0.736574
C	-1.322305	-1.919116	-0.898682
C	-2.305020	2.383931	-0.033040
C	-3.110874	1.213803	-0.156592
C	2.655387	2.020198	-0.023211
C	3.264870	0.725787	-0.141987
C	-0.977369	-3.112999	-0.148542
C	0.451606	-3.224889	-0.137593
C	-2.784845	3.509144	0.633473
C	-4.083372	3.469480	1.145097
C	-4.876946	2.317481	1.022834
C	-4.393756	1.173397	0.384968
C	3.331351	3.064005	0.611768
C	4.611307	2.821691	1.103754
C	5.208545	1.552592	0.987914
C	4.540810	0.494732	0.376535
C	-1.762509	-3.991095	0.609335
C	-1.125750	-4.992446	1.329541
C	0.281748	-5.102330	1.340892
C	1.078325	-4.213127	0.632703
H	-4.486211	4.341331	1.652081
H	-2.162063	4.390645	0.746674
H	-5.880668	2.316446	1.437487
H	-4.996895	0.274353	0.309127
H	-2.842072	-3.884577	0.621435
H	-1.717163	-5.699216	1.903723
H	0.746859	-5.892075	1.923137
H	2.160938	-4.276881	0.662265
H	4.993938	-0.488366	0.300985
H	6.206230	1.396935	1.387286
H	5.158496	3.623366	1.590584
H	2.863649	4.037650	0.715122
H	-0.100689	-0.830846	-2.196837
H	0.246621	0.421614	-1.324270

H_1^--TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z

N	-1.325150	-2.310038	-0.560710
C	0.017120	-2.296508	-0.755182
C	-1.991401	-1.151682	-0.716050
N	-1.433310	-0.000230	-1.202291
N	0.668853	-1.255704	-1.314055
C	-1.991665	1.151121	-0.716106
N	-1.325701	2.309654	-0.560810
C	0.016579	2.296509	-0.755258
N	0.668623	1.255921	-1.314161
C	1.927974	-1.159807	-0.837051
N	2.609049	0.000327	-0.699124
C	1.927730	1.160312	-0.837077
C	1.011518	-3.153018	-0.081756
C	2.238887	-2.423951	-0.136041
C	-3.241483	-0.719091	-0.098729
C	-3.241652	0.718265	-0.098774
C	2.238292	2.424523	-0.136036
C	1.010731	3.153274	-0.081793
C	0.943053	-4.372349	0.590338
C	2.106085	-4.882041	1.173493
C	3.313156	-4.165309	1.120386
C	3.383281	-2.923888	0.482812
C	-4.285231	-1.421657	0.511712
C	-5.329403	-0.705490	1.089761
C	-5.329570	0.704241	1.089716
C	-4.285569	1.420620	0.511622
C	3.382530	2.924741	0.482881
C	3.312056	4.166132	1.120474
C	2.104798	4.882554	1.173538
C	0.941923	4.372574	0.590322
H	2.076985	-5.842761	1.682432
H	0.001515	-4.910524	0.654978
H	4.201932	-4.580707	1.589864
H	4.307035	-2.352501	0.466139
H	4.306431	2.353590	0.466242
H	4.200704	4.581749	1.590001
H	2.075428	5.843255	1.682496
H	0.000242	4.910504	0.654936
H	-4.270837	2.506435	0.529750
H	-6.155208	1.237040	1.555202
H	-6.154914	-1.238457	1.555280
H	-4.270242	-2.507467	0.529904
H	-0.434067	-0.000117	-1.522380

2⁻-TdCl

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.093273	1.601684	-0.694428
C	-2.247621	0.263502	-0.862807

C	-0.842023	2.100599	-0.862999
N	0.186439	1.431365	-1.426509
N	-1.332806	-0.554268	-1.426263
C	1.352044	1.814780	-0.863021
N	2.433753	1.012003	-0.694488
C	2.240165	-0.321076	-0.862860
N	1.146349	-0.877185	-1.426264
C	-1.398163	-1.779529	-0.862696
N	-0.340469	-2.613680	-0.694114
C	0.895609	-2.078287	-0.862668
C	-3.211910	-0.559468	-0.102842
C	-2.661708	-1.882767	-0.102764
C	-0.299704	3.246411	-0.102922
C	1.121415	3.061316	-0.102997
C	2.090514	-2.501762	-0.102694
C	2.961418	-1.363619	-0.102879
C	-4.396440	-0.293346	0.584012
C	-5.063424	-1.343804	1.226250
C	-4.523601	-2.642172	1.226321
C	-3.308437	-2.910178	0.584167
C	-0.866197	4.319948	0.584313
C	-0.026598	5.238179	1.226755
C	1.367751	5.056627	1.226596
C	1.944081	3.954005	0.584056
C	2.452371	-3.660506	0.584384
C	3.695658	-3.712775	1.226503
C	4.550193	-2.596108	1.226237
C	4.174624	-1.409863	0.583918
H	-6.006616	-1.154360	1.738629
H	-4.790182	0.720384	0.613913
H	-5.054481	-3.444418	1.738767
H	-2.867409	-3.904244	0.614186
H	1.771330	-4.508356	0.614534
H	4.003240	-4.624223	1.739034
H	5.510463	-2.654648	1.738569
H	4.814971	-0.530864	0.613718
H	3.018880	3.788202	0.613936
H	2.003350	5.778661	1.739153
H	-0.455988	6.098870	1.739460
H	-1.947609	4.434913	0.614382

Si-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-1.907450	-2.526495	0.652581
C	-1.733881	-1.598495	1.603761
C	-1.738248	-2.172161	-0.628790
N	-1.168825	-0.982810	-1.026702

N	-1.164098	-0.365150	1.376876
C	-1.704414	-0.549086	-2.219319
N	-1.839751	0.742477	-2.550593
C	-1.666409	1.670809	-1.599655
N	-1.128653	1.406492	-0.359443
C	-1.695464	0.590274	2.214896
N	-1.830795	1.881676	1.883069
C	-1.661980	2.236443	0.601770
C	-2.428668	-1.503154	2.880312
C	-2.404551	-0.129708	3.263826
C	-2.437985	-2.703333	-1.790535
C	-2.416754	-1.684822	-2.788638
C	-2.333223	3.314753	-0.111019
C	-2.336033	2.959822	-1.492371
C	-3.140450	-2.440131	3.634014
C	-3.787235	-2.002364	4.785689
C	-3.763426	-0.645617	5.164532
C	-3.092299	0.304022	4.400274
C	-3.151643	-3.886907	-1.996534
C	-3.803230	-4.057890	-3.214127
C	-3.782285	-3.051757	-4.200084
C	-3.109277	-1.851935	-3.990757
C	-3.005938	4.456719	0.331675
C	-3.640313	5.254410	-0.615743
C	-3.643092	4.903800	-1.980249
C	-3.011542	3.747569	-2.428171
H	-4.327223	-2.715604	5.401232
H	-3.177883	-3.479567	3.325269
H	-4.285497	-0.337168	6.065362
H	-3.093112	1.353666	4.674871
H	-3.023431	4.709894	1.386547
H	-4.149729	6.159814	-0.299626
H	-4.154599	5.545169	-2.691722
H	-3.033280	3.460860	-3.474346
H	-3.112283	-1.064596	-4.737243
H	-4.308083	-3.215208	-5.136039
H	-4.344795	-4.979012	-3.407595
H	-3.186834	-4.648768	-1.224857
N	1.831720	-1.882011	-1.883208
C	1.695956	-0.590529	-2.214829
C	1.662705	-2.236987	-0.601912
N	1.128545	-1.407674	0.359299
N	1.163949	0.364490	-1.376987
C	1.666770	-1.671470	1.599371
N	1.839954	-0.743090	2.550387
C	1.704199	0.548426	2.219020
N	1.168507	0.981873	1.026423
C	1.732799	1.598199	-1.603833
N	1.905832	2.526403	-0.652621
C	1.736874	2.171783	0.628766
C	2.404962	0.129842	-3.263595
C	2.428032	1.503323	-2.880173
C	2.334708	-3.314907	0.110799
C	2.337265	-2.960000	1.492149
C	2.436282	2.703263	1.790568

C	2.415816	1.684542	2.788476
C	3.093390	-0.303509	-4.399795
C	3.764113	0.646532	-5.163867
C	3.786879	2.003354	-4.785096
C	3.139437	2.440753	-3.633692
C	3.008327	-4.456349	-0.331920
C	3.643274	-5.253554	0.615496
C	3.645807	-4.902941	1.980033
C	3.013427	-3.747207	2.427960
C	3.149111	3.887326	1.996815
C	3.800604	4.058514	3.214404
C	3.780424	3.052146	4.200176
C	3.108282	1.851905	3.990626
H	4.286713	0.338444	-6.064512
H	3.094993	-1.353180	-4.674283
H	4.326612	2.716875	-5.400535
H	3.176064	3.480218	-3.324935
H	3.183730	4.649355	1.225277
H	4.341526	4.979969	3.408096
H	4.306165	3.215835	5.136122
H	3.111856	1.064389	4.736924
H	3.034990	-3.460412	3.474116
H	4.157840	-5.543964	2.691442
H	4.153392	-6.158588	0.299453
H	3.026031	-4.709445	-1.386806
Si	-0.000166	-0.000324	-0.000003

Ge-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.947221	2.612911	-0.343607
C	1.786074	2.115907	0.892381
C	1.786353	1.813111	-1.409000
N	1.214641	0.564221	-1.364078
N	1.214408	0.897847	1.171872
C	1.783735	-0.288122	-2.279760
N	1.942371	-1.607329	-2.092332
C	1.781493	-2.129785	-0.866799
N	1.212900	-1.464573	0.192746
C	1.783339	0.311386	2.276987

N	1.942032	-1.011399	2.437124
C	1.781341	-1.833037	1.388405
C	2.531757	2.496139	2.085783
C	2.529979	1.364306	2.954304
C	2.532289	1.871723	-2.660004
C	2.530560	0.553776	-3.206248
C	2.525028	-3.058106	1.122040
C	2.525158	-3.244231	-0.292490
C	3.267873	3.638693	2.408736
C	3.961319	3.655939	3.614964
C	3.959550	2.538505	4.472460
C	3.264325	1.379183	4.142631
C	3.268631	2.891831	-3.267265
C	3.962370	2.596484	-4.436728
C	3.960655	1.295296	-4.976049
C	3.265198	0.260763	-4.357788
C	3.258139	-3.910620	1.951117
C	3.950470	-4.965160	1.363952
C	3.950613	-5.148912	-0.032544
C	3.258423	-4.282180	-0.872661
H	4.521047	4.542123	3.898770
H	3.288548	4.487523	1.733340
H	4.517942	2.582239	5.402757
H	3.282322	0.507116	4.787824
H	3.277402	-3.750287	3.023975
H	4.507859	-5.655175	1.990340
H	4.508109	-5.977462	-0.459003
H	3.277919	-4.404850	-1.950471
H	3.283261	-0.748508	-4.755464
H	4.519302	1.096892	-5.885837
H	4.522301	3.379075	-4.939913
H	3.289292	3.886445	-2.834348
N	-1.942511	1.011510	-2.437201
C	-1.783812	-0.311306	-2.276966
C	-1.781813	1.833103	-1.388408
N	-1.213740	1.464323	-0.192740
N	-1.215083	-0.897609	-1.171763
C	-1.781895	2.129787	0.866817
N	-1.942751	1.607342	2.092391
C	-1.784116	0.288085	2.279704
N	-1.215254	-0.564123	1.363838
C	-1.786121	-2.115969	-0.892468
N	-1.947117	-2.613088	0.343551
C	-1.786422	-1.813224	1.408963
C	-2.530149	-1.364391	-2.954387
C	-2.531647	-2.496318	-2.085952
C	-2.525085	3.058450	-1.122021
C	-2.525162	3.244538	0.292533
C	-2.532173	-1.871944	2.660087
C	-2.530645	-0.553967	3.206299
C	-3.264389	-1.379381	-4.142772
C	-3.959241	-2.538877	-4.472763
C	-3.960740	-3.656390	-3.615368
C	-3.267391	-3.639055	-2.409087
C	-3.257844	3.911285	-1.951064

C	-3.949750	4.966108	-1.363882
C	-3.949835	5.149821	0.032608
C	-3.258013	4.282767	0.872707
C	-3.268190	-2.892179	3.267533
C	-3.961785	-2.596937	4.437105
C	-3.960255	-1.295728	4.976387
C	-3.265133	-0.261077	4.357966
H	-4.517549	-2.582702	-5.403105
H	-3.282578	-0.507257	-4.787883
H	-4.520184	-4.542709	-3.899309
H	-3.287858	-4.487960	-1.733778
H	-3.288705	-3.886816	2.834663
H	-4.521461	-3.379623	4.940423
H	-4.518785	-1.097426	5.886269
H	-3.283318	0.748210	4.755601
H	-3.277474	4.405413	1.950522
H	-4.506994	5.978590	0.459083
H	-4.506839	5.656372	-1.990261
H	-3.277161	3.750998	-3.023929
Ge	-0.000144	-0.000031	0.000036

Sn-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	-2.179148	1.156923	2.360083
C	-2.015436	1.924581	1.270938
C	-2.015477	-0.174220	2.299764
N	-1.409120	-0.846020	1.259586
N	-1.409075	1.513909	0.102769
C	-2.015285	-2.063120	1.031198
N	-2.178837	-2.622562	-0.178191
C	-2.015290	-1.904648	-1.300783
N	-1.409231	-0.667774	-1.362378
C	-2.015284	2.078963	-0.999129
N	-2.179070	1.465620	-2.182053
C	-2.015538	0.138519	-2.302177
C	-2.805017	3.103239	0.925748
C	-2.804970	3.200016	-0.497663
C	-2.805035	-1.169089	3.019970
C	-2.804992	-2.353434	2.224471

C	-2.805060	-0.749826	-3.150319
C	-2.804959	-2.030923	-2.522383
C	-3.584489	3.969483	1.697541
C	-4.319963	4.953131	1.042645
C	-4.319964	5.048681	-0.363224
C	-3.584461	4.162700	-1.145174
C	-3.584403	-1.089790	4.177538
C	-4.319698	-2.210085	4.553912
C	-4.319692	-3.379797	3.768183
C	-3.584345	-3.455012	2.588780
C	-3.584318	-0.514709	-4.286590
C	-4.319430	-1.573852	-4.811191
C	-4.319365	-2.839134	-4.190967
C	-3.584158	-3.073168	-3.032489
H	-4.912378	5.655072	1.622241
H	-3.605057	3.874042	2.778273
H	-4.912362	5.822597	-0.842523
H	-3.604933	4.214409	-2.228884
H	-3.604833	0.468906	-4.744405
H	-4.911577	-1.423035	-5.709092
H	-4.911413	-3.641329	-4.621748
H	-3.604461	-4.037586	-2.535493
H	-3.604783	-4.343259	1.965793
H	-4.911938	-4.232804	4.086356
H	-4.911967	-2.182065	5.463880
H	-3.604898	-0.177156	4.764222
N	2.179022	-1.465625	2.182039
C	2.015252	-2.078962	0.999107
C	2.015497	-0.138523	2.302161
N	1.409215	0.667776	1.362356
N	1.409069	-1.513901	-0.102798
C	2.015281	1.904646	1.300780
N	2.178852	2.622565	0.178196
C	2.015318	2.063129	-1.031200
N	1.409149	0.846033	-1.259604
C	2.015449	-1.924575	-1.270959
N	2.179185	-1.156912	-2.360095
C	2.015522	0.174231	-2.299778
C	2.804941	-3.200019	0.497654
C	2.805016	-3.103239	-0.925757
C	2.805006	0.749814	3.150329
C	2.804926	2.030913	2.522399
C	2.805099	1.169098	-3.01996
C	2.805049	2.353441	-2.224454
C	3.584411	-4.162711	1.145178
C	4.319921	-5.048697	0.36324
C	4.319948	-4.953144	-1.042628
C	3.584495	-3.969488	-1.697536
C	3.584234	0.514687	4.286616
C	4.31934	1.573823	4.81124
C	4.319296	2.839107	4.191023
C	3.584118	3.073151	3.032528
C	3.584491	1.0898	-4.177513
C	4.319802	2.210091	-4.553867
C	4.319788	3.3798	-3.768132

C	3.584419	3.455014	-2.588744
H	4.912303	-5.822619	0.842549
H	3.604861	-4.214422	2.228888
H	4.912369	-5.655089	-1.622215
H	3.605085	-3.874046	-2.778268
H	3.604991	0.17717	-4.764203
H	4.912089	2.182071	-5.463823
H	4.912047	4.232804	-4.086288
H	3.604851	4.343258	-1.965752
H	3.604438	4.037571	2.535537
H	4.911339	3.641297	4.621821
H	4.911466	1.422998	5.709154
H	3.604734	-0.468932	4.744426
Sn	0	0.000011	-0.000035

Pb-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.259899	0.300904	2.610510
C	2.096306	-0.933974	2.110026
C	2.098998	1.390609	1.842925
N	1.490307	1.402818	0.606830
N	1.488731	-1.224673	0.907902
C	2.101361	2.295903	-0.247179
N	2.264685	2.110050	-1.566733
C	2.101077	0.901024	-2.126860
N	1.489637	-0.174632	-1.519656
C	2.095646	-2.291397	0.281058
N	2.258664	-2.412479	-1.046048
C	2.097663	-1.361959	-1.866335
C	2.894768	-2.109175	2.452095
C	2.894351	-2.959458	1.306278
C	2.903134	2.608915	1.907862
C	2.904602	3.176020	0.598494
C	2.900632	-1.071184	-3.052085
C	2.902871	0.346352	-3.215192
C	3.681594	-2.416675	3.565473
C	4.423382	-3.594430	3.542606
C	4.422964	-4.434022	2.411231
C	3.680775	-4.114460	1.277706

C	3.693572	3.157837	2.921396
C	4.440884	4.295636	2.630466
C	4.442381	4.855608	1.337605
C	3.696590	4.290185	0.307171
C	3.689919	-1.882473	-3.872025
C	4.436651	-1.274555	-4.877281
C	4.438774	0.125132	-5.038385
C	3.694228	0.947769	-4.197785
H	5.020950	-3.868773	4.407052
H	3.702582	-1.752257	4.423171
H	5.020249	-5.341068	2.423069
H	3.701208	-4.742868	0.393273
H	3.708974	-2.957517	-3.725556
H	5.036236	-1.886635	-5.544719
H	5.039975	0.567791	-5.827199
H	3.716583	2.027913	-4.299385
H	3.718387	4.700618	-0.697122
H	5.044012	5.738490	1.142218
H	5.041398	4.756521	3.409300
H	3.713108	2.705943	3.907776
N	-2.259195	2.407504	1.057662
C	-2.098780	2.294722	-0.270438
C	-2.095256	1.352566	1.871808
N	-1.487179	0.167853	1.516728
N	-1.489483	1.234088	-0.905706
C	-2.094731	-0.911441	2.120829
N	-2.258172	-2.118416	1.555766
C	-2.097479	-2.296205	0.234800
N	-1.490473	-1.397088	-0.614776
C	-2.101722	0.946840	-2.106554
N	-2.265048	-0.286345	-2.612069
C	-2.101085	-1.379584	-1.849937
C	-2.903667	2.965167	-1.289053
C	-2.905529	2.120807	-2.439293
C	-2.894674	1.054964	3.058145
C	-2.894103	-0.363345	3.214315
C	-2.902184	-2.59963	-1.920474
C	-2.899892	-3.174	-0.614333
C	-3.694649	4.116858	-1.251135
C	-4.442729	4.439328	-2.379856
C	-4.444529	3.605593	-3.51568
C	-3.698286	2.430987	-3.547822
C	-3.682655	1.860981	3.884509
C	-4.425332	1.246898	4.889015
C	-4.424707	-0.153576	5.043241
C	-3.681425	-0.970892	4.196355
C	-3.692783	-3.145022	-2.935753
C	-4.43653	-4.286465	-2.649862
C	-4.434309	-4.853605	-1.360149
C	-3.688286	-4.291888	-0.327804
H	-5.043691	5.344004	-2.384535
H	-3.713984	4.740445	-0.363276
H	-5.046829	3.882115	-4.376138
H	-3.720325	1.770835	-4.408777
H	-3.71528	-2.687643	-3.91954

H	-5.037163	-4.74465	-3.430198
H	-5.03324	-5.739178	-1.168679
H	-3.707346	-4.707861	0.674266
H	-3.701804	-2.051566	4.29262
H	-5.02278	-0.601037	5.831724
H	-5.023831	1.854686	5.561329
H	-3.703839	2.936703	3.743396
Pb	0.000037	0.002978	-0.003924

Ti-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.101667	-2.604266	-0.281184
C	1.927258	-1.833977	-1.365778
C	1.944199	-2.087758	0.946824
N	1.373693	-0.858057	1.200942
N	1.354050	-0.580691	-1.338524
C	1.969016	-0.257910	2.290150
N	2.149271	1.066130	2.411058
C	1.974602	1.869095	1.350424
N	1.386119	1.470634	0.168079
C	1.934248	0.242525	-2.280422
N	2.114497	1.561844	-2.117703
C	1.957188	2.117481	-0.906649
C	2.652681	-1.932441	-2.627680
C	2.656333	-0.626410	-3.203339
C	2.685890	-2.456275	2.147607
C	2.701676	-1.305393	2.992261
C	2.696439	3.251469	-0.363693
C	2.706560	3.095671	1.055477
C	3.370019	-2.974016	-3.222562
C	4.049313	-2.711102	-4.408091
C	4.052846	-1.421651	-4.976487
C	3.377159	-0.366097	-4.372133
C	3.408199	-3.601966	2.493090
C	4.105008	-3.601556	3.697309
C	4.120575	-2.465464	4.531093
C	3.439701	-1.304302	4.179336
C	3.419518	4.281904	-0.971193
C	4.111602	5.169924	-0.153763

C	4.121531	5.016157	1.247068
C	3.439563	3.970910	1.861948
H	4.593464	-3.510082	-4.902839
H	3.386916	-3.959126	-2.768224
H	4.599655	-1.250341	-5.898925
H	3.399566	0.633812	-4.792645
H	3.431007	4.382166	-2.051454
H	4.660823	5.993295	-0.600587
H	4.678186	5.723831	1.854161
H	3.466360	3.834357	2.937950
H	3.470858	-0.419226	4.806090
H	4.680874	-2.497786	5.460745
H	4.653637	-4.488581	3.999680
H	3.415512	-4.465558	1.836363
N	-2.124769	-1.598691	2.089697
C	-1.968675	-0.280528	2.284530
C	-1.939144	-2.125342	0.869955
N	-1.357044	-1.450834	-0.182502
N	-1.391426	0.571318	1.366756
C	-1.922102	-1.831668	-1.380023
N	-2.091320	-1.006984	-2.424432
C	-1.935752	0.316168	-2.268177
N	-1.374249	0.902307	-1.153518
C	-1.982687	1.816452	1.414708
N	-2.152598	2.608811	0.345738
C	-1.967303	2.117931	-0.889006
C	-2.714804	0.557134	3.216610
C	-2.722882	1.875942	2.670019
C	-2.655551	-3.257299	0.292173
C	-2.645648	-3.072157	-1.123142
C	-2.691538	2.499660	-2.096332
C	-2.671484	1.366506	-2.963914
C	-3.445493	0.261155	4.370834
C	-4.143144	1.293452	4.990012
C	-4.151061	2.595341	4.450451
C	-3.461477	2.894118	3.279595
C	-3.376082	-4.307839	0.867133
C	-4.045427	-5.186506	0.020950
C	-4.035728	-5.003688	-1.376220
C	-3.356483	-3.938087	-1.958698
C	-3.424817	3.640793	-2.433303
C	-4.096874	3.654228	-3.651590
C	-4.077107	2.535471	-4.508146
C	-3.384823	1.378063	-4.165714
H	-4.698391	1.094007	5.901696
H	-3.458559	-0.747972	4.769124
H	-4.712281	3.375450	4.956125
H	-3.486754	3.888883	2.847217
H	-3.459412	4.490573	-1.759628
H	-4.653367	4.538625	-3.947249
H	-4.618718	2.577953	-5.448416
H	-3.388982	0.505555	-4.810588
H	-3.368699	-3.779326	-3.031919
H	-4.574913	-5.704642	-2.006458
H	-4.591916	-6.025027	0.442238

H	-3.403264	-4.430387	1.944815
Ti	0.001497	0.020918	0.025039

V-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.053043	-2.300538	1.272393
C	1.891475	-2.286792	-0.058418
C	1.877103	-1.173645	1.977580
N	1.303544	-0.029118	1.466632
N	1.325518	-1.243229	-0.757975
C	1.876888	1.093882	2.023557
N	2.052711	2.248342	1.364394
C	1.891221	2.288208	0.034112
N	1.325800	1.273408	-0.706938
C	1.892221	-1.119623	-2.006170
N	2.064605	0.053614	-2.632873
C	1.892163	1.200521	-1.959182
C	2.605071	-3.100250	-1.036910
C	2.610008	-2.365136	-2.260100
C	2.592466	-0.778184	3.183394
C	2.592427	0.650008	3.212321
C	2.609389	2.455607	-2.162745
C	2.604338	3.140776	-0.910903
C	3.308865	-4.302423	-0.926098
C	3.980519	-4.776930	-2.048828
C	3.986539	-4.050504	-3.255694
C	3.321204	-2.832952	-3.367753
C	3.302066	-1.509056	4.141194
C	3.971033	-0.808590	5.139134
C	3.971047	0.601215	5.167663
C	3.302076	1.341507	4.198898
C	3.320269	2.967951	-3.250696
C	3.985198	4.180258	-3.089733
C	3.979103	4.857382	-1.854555
C	3.307766	4.337713	-0.751781
H	4.516271	-5.719918	-1.994496
H	3.323170	-4.846287	0.012615
H	4.526146	-4.446922	-4.110647
H	3.344473	-2.259517	-4.288520

H	3.343659	2.432087	-4.193821
H	4.524577	4.610985	-3.928070
H	4.514542	5.797591	-1.762255
H	3.322095	4.843246	0.208119
H	3.320712	2.426289	4.203729
H	4.510365	1.115034	5.957823
H	4.510353	-1.353979	5.907841
H	3.320736	-2.593144	4.102083
N	-2.064513	-0.054362	2.632837
C	-1.892470	1.119144	2.006551
C	-1.891800	-1.200983	1.958739
N	-1.325472	-1.273323	0.706446
N	-1.325879	1.243284	0.758356
C	-1.890625	-2.288032	-0.034865
N	-2.052144	-2.247778	-1.365135
C	-1.876669	-1.093062	-2.023923
N	-1.303647	0.029956	-1.466659
C	-1.892155	2.286945	0.059117
N	-2.053794	2.301066	-1.271668
C	-1.877558	1.174471	-1.977254
C	-2.610519	2.364409	2.260904
C	-2.605823	3.099920	1.037941
C	-2.608701	-2.456327	2.161941
C	-2.603531	-3.141089	0.909886
C	-2.592812	0.779168	-3.183172
C	-2.592331	-0.649017	-3.212547
C	-3.321736	2.831731	3.368755
C	-3.987336	4.049175	3.257128
C	-3.981554	4.775990	2.050492
C	-3.309874	4.301987	0.927569
C	-3.319400	-2.969193	3.249758
C	-3.984026	-4.181627	3.088440
C	-3.977814	-4.858348	1.853051
C	-3.306661	-4.338145	0.750406
C	-3.302645	1.510122	-4.140742
C	-3.971394	0.809765	-5.138901
C	-3.970967	-0.600032	-5.167877
C	-3.301763	-1.340421	-4.199347
H	-4.526968	4.445204	4.112246
H	-3.344814	2.258005	4.289345
H	-4.517508	5.718882	1.996497
H	-3.324352	4.846154	-0.010966
H	-3.321647	2.594192	-4.101292
H	-4.510885	1.355230	-5.907434
H	-4.510124	-1.113770	-5.958199
H	-3.320058	-2.425207	-4.204523
H	-3.320910	-4.843374	-0.209655
H	-4.513011	-5.798666	1.760467
H	-4.523250	-4.612758	3.926669
H	-3.342888	-2.433636	4.193054
V	-0.000036	0.000437	-0.000057

Mn-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	1.973781	-2.628267	0.149242
C	1.809624	-2.034745	-1.040855
C	1.809079	-1.904228	1.264638
N	1.253452	-0.646970	1.292732
N	1.253953	-0.788802	-1.210878
C	1.800947	0.126401	2.288917
N	1.957674	1.454832	2.208750
C	1.793842	2.057722	1.023350
N	1.246950	1.449250	-0.081371
C	1.802235	-0.132460	-2.287363
N	1.958953	1.196487	-2.357239
C	1.794383	1.929224	-1.247493
C	2.510531	-2.339459	-2.283082
C	2.505891	-1.145954	-3.065129
C	2.509165	-2.066980	2.533703
C	2.504089	-0.792966	3.176314
C	2.487687	3.162423	-0.892661
C	2.487457	3.242980	0.532010
C	3.208496	-3.470333	-2.714546
C	3.862795	-3.409976	-3.941406
C	3.858263	-2.231669	-4.713469
C	3.199294	-1.086287	-4.276687
C	3.206953	-3.141979	3.090246
C	3.860646	-2.943643	4.302770
C	3.855647	-1.685840	4.937184
C	3.196815	-0.597071	4.373826
C	3.176142	4.106541	-1.658689
C	3.825229	5.143643	-0.995271
C	3.824953	5.223182	0.411171
C	3.175626	4.267434	1.187022
H	4.393127	-4.283233	-4.309337
H	3.230738	-4.368199	-2.105904
H	4.385188	-2.217516	-5.662863
H	3.214574	-0.169649	-4.856895
H	3.195261	4.028481	-2.740651
H	4.348077	5.902694	-1.569442
H	4.347538	6.042171	0.896312
H	3.194275	4.311843	2.270894
H	3.211637	0.379102	4.847076
H	4.382081	-1.564806	5.879213
H	4.390855	-3.769789	4.767060

H	3.229556	-4.102692	2.586640
N	-1.958359	-1.197145	2.357329
C	-1.802162	0.132124	2.287083
C	-1.792817	-1.929362	1.247045
N	-1.245378	-1.448846	0.081450
N	-1.253804	0.788577	1.211209
C	-1.791702	-2.057148	-1.023383
N	-1.956098	-1.454268	-2.209035
C	-1.800068	-0.125470	-2.288361
N	-1.252648	0.647757	-1.292512
C	-1.809037	2.034399	1.041438
N	-1.973145	2.628896	-0.148520
C	-1.808233	1.904723	-1.264090
C	-2.507135	1.144966	3.064669
C	-2.511417	2.338722	2.283031
C	-2.486306	-3.162382	0.891891
C	-2.485701	-3.242494	-0.532807
C	-2.509546	2.067534	-2.532602
C	-2.504485	0.793549	-3.175273
C	-3.201825	1.084545	4.275462
C	-3.861611	2.22954	4.711943
C	-3.865796	3.408145	3.940251
C	-3.210318	3.469185	2.71409
C	-3.175339	-4.10648	1.657507
C	-3.824427	-5.143169	0.993565
C	-3.823816	-5.222263	-0.41297
C	-3.174123	-4.266485	-1.188376
C	-3.208243	3.142276	-3.088488
C	-3.862816	2.943713	-4.300491
C	-3.857865	1.685915	-4.934951
C	-3.19819	0.597368	-4.372162
H	-4.389543	2.214958	5.660774
H	-3.2175	0.167637	4.855238
H	-4.396868	4.281022	4.308028
H	-3.232373	4.367155	2.105588
H	-3.230915	4.102923	-2.584752
H	-4.393729	3.769638	-4.76438
H	-4.385057	1.564764	-5.876544
H	-3.21317	-0.378841	-4.845342
H	-3.192593	-4.310412	-2.272267
H	-4.346548	-6.041028	-0.898343
H	-4.347668	-5.902358	1.567207
H	-3.194807	-4.028622	2.739473
Mn	0.000947	0.000392	0.00016

Tc-Oc

Atom	Coordinates (Angstroms)		
	X	Y	Z
N	2.158722	-2.631811	0.044167
C	1.994780	-2.001541	-1.128552
C	1.994821	-1.962536	1.195077
N	1.413335	-0.718377	1.294507
N	1.413310	-0.761411	-1.269629
C	1.994500	0.024114	2.298009
N	2.157934	1.354910	2.257511
C	1.994012	2.016895	1.102390
N	1.413145	1.480482	-0.024897
C	1.994297	-0.053042	-2.297608
N	2.157657	1.278379	-2.301879
C	1.993822	1.978782	-1.169628
C	2.734343	-2.248706	-2.361597
C	2.734060	-1.024360	-3.096134
C	2.734591	-2.168141	2.435596
C	2.734353	-0.919837	3.128616
C	2.732731	3.170677	-0.767353
C	2.732875	3.194627	0.660248
C	3.466221	-3.350089	-2.814549
C	4.156389	-3.231063	-4.017397
C	4.156131	-2.022379	-4.742515
C	3.465685	-0.905327	-4.281221
C	3.466681	-3.253637	2.925085
C	4.157064	-3.094282	4.123133
C	4.156833	-1.861949	4.807287
C	3.466206	-0.761055	4.308896
C	3.463768	4.114091	-1.494932
C	4.153522	5.096744	-0.790662
C	4.153661	5.120397	0.618634
C	3.464058	4.161926	1.355620
H	4.712424	-4.080645	-4.402921
H	3.486225	-4.270577	-2.240264
H	4.711956	-1.962454	-5.673676
H	3.485225	0.034631	-4.823072
H	3.483485	4.076970	-2.579245
H	4.708898	5.855752	-1.333852
H	4.709135	5.897212	1.135934
H	3.483982	4.161224	2.440566
H	3.485864	0.196583	4.818842
H	4.712886	-1.770750	5.735768
H	4.713286	-3.930397	4.536804
H	3.486677	-4.192866	2.381989
N	-2.157638	-1.278405	2.301858
C	-1.994350	0.053027	2.297623
C	-1.993741	-1.978771	1.169597
N	-1.413070	-1.480413	0.024887
N	-1.413384	0.761451	1.269672
C	-1.993877	-2.016835	-1.102422

N	-2.157810	-1.354836	-2.257531
C	-1.994449	-0.024029	-2.297998
N	-1.413350	0.718473	-1.294466
C	-1.994925	2.001554	1.128609
N	-2.158878	2.631834	-0.044101
C	-1.994913	1.962599	-1.195023
C	-2.734186	1.024284	3.096154
C	-2.734521	2.248649	2.361646
C	-2.732569	-3.170705	0.767279
C	-2.732683	-3.194622	-0.660321
C	-2.734662	2.168187	-2.435554
C	-2.734337	0.919897	-3.1286
C	-3.465824	0.905185	4.281226
C	-4.156341	2.022188	4.742534
C	-4.156651	3.23089	4.017444
C	-3.466467	3.349981	2.814612
C	-3.463559	-4.11418	1.494822
C	-4.153238	-5.096862	0.790517
C	-4.153348	-5.120483	-0.618778
C	-3.463791	-4.16195	-1.35573
C	-3.466801	3.253653	-2.925039
C	-4.157148	3.094284	-4.123106
C	-4.156831	1.861965	-4.807285
C	-3.466153	0.761099	-4.308901
H	-4.712178	1.96221	5.673683
H	-3.485323	-0.034787	4.823055
H	-4.712739	4.080433	4.402977
H	-3.486511	4.270482	2.240349
H	-3.486862	4.192869	-2.381924
H	-4.713407	3.930376	-4.536772
H	-4.712857	1.770754	-5.735782
H	-3.485745	-0.196529	-4.818869
H	-3.483693	-4.161226	-2.440675
H	-4.708762	-5.89732	-1.136109
H	-4.708577	-5.855917	1.33368
H	-3.483301	-4.077085	2.579137
Tc	-0.000003	0.000076	0.000028

Re-Oc

Atom	Coordinates (Angstroms)

	X	Y	Z
N	-2.161817	-2.630696	-0.082121
C	-1.999000	-2.017880	1.099899
C	-1.999102	-1.945297	-1.223600
N	-1.412924	-0.699908	-1.305535
N	-1.412852	-0.780015	1.259330
C	-1.998986	0.057277	-2.297787
N	-2.161359	1.387407	-2.237525
C	-1.998211	2.033219	-1.073264
N	-1.412385	1.481115	0.046263
C	-1.998843	-0.086234	2.296937
N	-2.161246	1.245060	2.319793
C	-1.998174	1.962269	1.198088
C	-2.742800	-2.280574	2.326089
C	-2.742701	-1.067264	3.077965
C	-2.742994	-2.130957	-2.463741
C	-2.742954	-0.873089	-3.138435
C	-2.741056	3.156152	0.812653
C	-2.741035	3.200737	-0.614043
C	-3.479455	-3.386533	2.759874
C	-4.173785	-3.283524	3.961782
C	-4.173689	-2.085466	4.704213
C	-3.479248	-0.963404	4.261484
C	-3.479681	-3.207692	-2.965646
C	-4.174115	-3.029866	-4.158720
C	-4.174086	-1.787806	-4.824932
C	-3.479605	-0.695563	-4.313100
C	-3.476686	4.085517	1.553675
C	-4.169948	5.075740	0.863649
C	-4.169918	5.119770	-0.545106
C	-3.476634	4.174568	-1.295599
H	-4.733263	-4.137303	4.332773
H	-3.499488	-4.298362	2.171971
H	-4.733110	-2.037632	5.633916
H	-3.499140	-0.031099	4.816350
H	-3.496633	4.032275	2.637295
H	-4.728488	5.824540	1.417651
H	-4.728449	5.901697	-1.051289
H	-3.496568	4.189088	-2.380430
H	-3.499506	0.269542	-4.808723
H	-4.733559	-1.682052	-5.749807
H	-4.733609	-3.858834	-4.582237
H	-3.499653	-4.154439	-2.435804
N	2.161229	-1.245076	-2.319778
C	1.998894	0.086229	-2.296951
C	1.998095	-1.962257	-1.198070
N	1.412315	-1.481050	-0.046262
N	1.412922	0.780062	-1.259370
C	1.998076	-2.033173	1.073287
N	2.161230	-1.387354	2.237539
C	1.998928	-0.057214	2.297781
N	1.412939	0.699992	1.305501
C	1.999151	2.017897	-1.099941
N	2.161981	2.630710	0.082074
C	1.999196	1.945346	1.223562

C	2.742831	1.067200	-3.077977
C	2.742992	2.280521	-2.326119
C	2.740895	-3.156184	-0.812598
C	2.740836	-3.200749	0.614098
C	2.743066	2.130977	2.463719
C	2.742927	0.873120	3.138434
C	3.479392	0.963276	-4.261481
C	4.173912	2.085287	-4.704214
C	4.174071	3.283356	-3.961801
C	3.479727	3.386426	-2.759907
C	3.476476	-4.085609	-1.553589
C	4.169656	-5.075870	-0.863532
C	4.169590	-5.119880	0.545221
C	3.476351	-4.174619	1.295686
C	3.479807	3.207674	2.965626
C	4.174196	3.029825	4.158723
C	4.174069	1.787776	4.824956
C	3.479533	0.695568	4.313123
H	4.733345	2.037402	-5.633907
H	3.499235	0.030961	-4.816332
H	4.733609	4.137095	-4.332793
H	3.499806	4.298265	-2.172019
H	3.499853	4.154413	2.435771
H	4.733729	3.858765	4.582241
H	4.733507	1.682001	5.749849
H	3.499360	-0.269530	4.808762
H	3.496259	-4.189126	2.380517
H	4.728054	-5.901836	1.051432
H	4.728157	-5.824715	-1.417513
H	3.496452	-4.032386	-2.637210
Re	0.000002	0.000072	-0.000027