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Unexpected chalcogen bonds in tetravalent sulfur compounds

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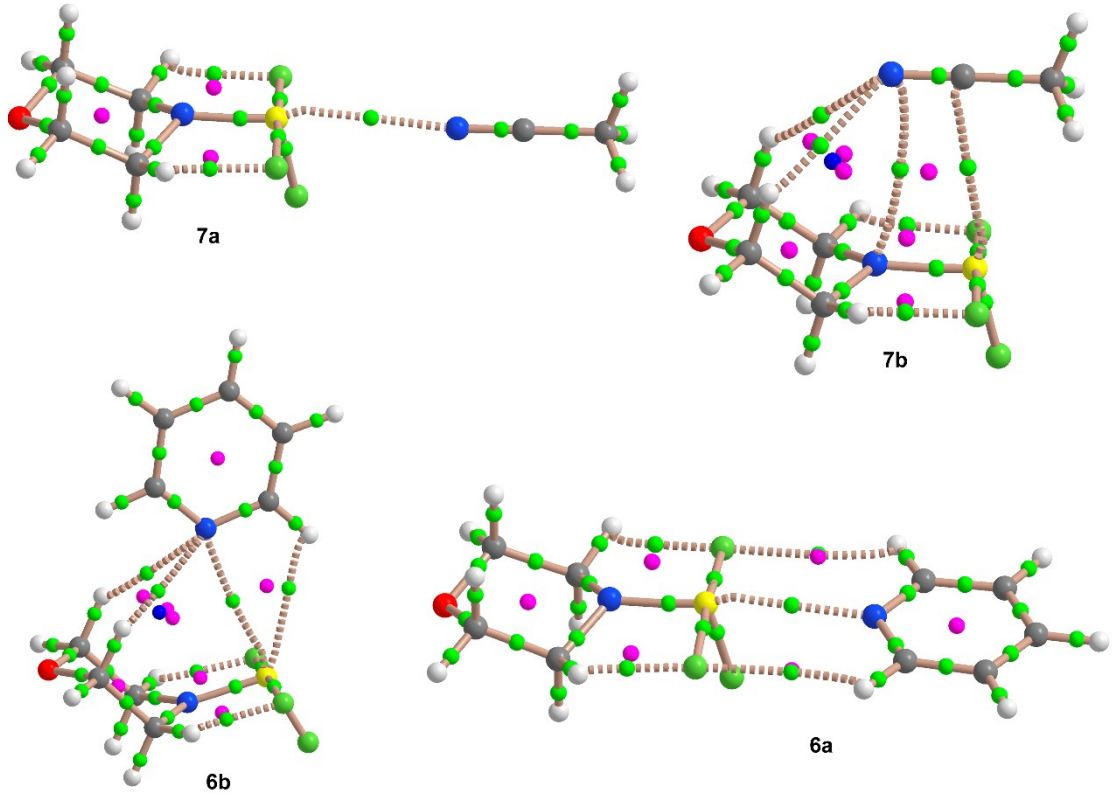

Figure S1. Distribution of bond, ring and cage critical points (green, pink and blue spheres, respectively) and bond paths for types a and b of complexes **6**, and **7** at the MP2/def2-TZVP.

Cartesian Coordinates

Complex **4a** (1 + OH_2)

S	1.5721608	-0.3978638	0.0000000
F	1.6290437	-0.3068020	-1.6879962
F	1.6290437	-0.3068020	1.6879962
F	2.1787831	1.0939664	0.0000000
H	4.6207108	0.2856254	-0.7594895
H	4.6207108	0.2856254	0.7594895
O	4.9305249	-0.2196430	0.0000000
C	-2.2198108	-0.2827886	-1.1451392
C	-0.7934294	0.2252016	-1.2058390
C	-0.7934294	0.2252016	1.2058390
C	-2.2198108	-0.2827886	1.1451392
H	-0.3239078	-0.1649353	-2.1008766
H	-2.2160849	-1.3815715	-1.1665677
H	-2.7655892	0.0860330	-2.0144079
H	-0.3239078	-0.1649353	2.1008766
H	-0.7864279	1.3201502	1.2504331
H	-2.2160849	-1.3815715	1.1665677
H	-2.7655892	0.0860330	2.0144079
H	-0.7864279	1.3201502	-1.2504331
O	-2.9085773	0.1761887	0.0000000
N	-0.0619007	-0.2144739	0.0000000

Complex **4b** (1 + OH_2)

S	1.8710822	1.0392073	0.0000000
F	1.8943574	1.1281811	-1.6934890
F	1.8943574	1.1281811	1.6934890
F	1.9793491	2.6365592	0.0000000

H	2.4286853	-2.1911939	-0.7613223
H	2.4286853	-2.1911939	0.7613223
O	1.8405388	-2.2488617	0.0000000
C	-1.4665362	-0.5595165	-1.1498242
C	-0.5695137	0.6621987	-1.2014559
C	-0.5695137	0.6621987	1.2014559
C	-1.4665362	-0.5595165	1.1498242
H	0.0294557	0.6324312	-2.1025469
H	-0.8462908	-1.4652310	-1.1706523
H	-2.1314329	-0.5561928	-2.0147966
H	0.0294557	0.6324312	2.1025469
H	-1.1788776	1.5729638	1.2124809
H	-0.8462908	-1.4652310	1.1706523
H	-2.1314329	-0.5561928	2.0147966
H	-1.1788776	1.5729638	-1.2124809
O	-2.2925663	-0.5636766	0.0000000
N	0.2819020	0.6894904	0.0000000

Complex **5a** (1 + NH_3)

S	1.3473953	-0.2879620	0.0000000
F	1.3931778	-0.2007255	-1.6937829
F	1.3931778	-0.2007255	1.6937829
F	1.8248962	1.2379212	0.0000000
C	-2.4664457	-0.2578891	-1.1449261
C	-1.0401367	0.2500798	-1.2020756
C	-1.0401367	0.2500798	1.2020756
C	-2.4664457	-0.2578891	1.1449261
H	-0.5713220	-0.1392239	-2.0982738
H	-2.4617578	-1.3568053	-1.1673779
H	-3.0122328	0.1113987	-2.0141662
H	-0.5713220	-0.1392239	2.0982738

H	-1.0351107	1.3456531	1.2490826
H	-2.4617578	-1.3568053	1.1673779
H	-3.0122328	0.1113987	2.0141662
H	-1.0351107	1.3456531	-1.2490826
O	-3.1588567	0.1978553	0.0000000
N	-0.3095019	-0.1953052	0.0000000
N	4.4052495	-0.2038099	0.0000000
H	5.0591168	-0.9777645	0.0000000
H	4.6096782	0.3620447	0.8155823
H	4.6096782	0.3620447	-0.8155823

Complex **5b** (1 + NH_3)

S	1.7310528	1.2075797	0.0000000
F	1.7540450	1.2997233	-1.6925037
F	1.7540450	1.2997233	1.6925037
F	1.8684293	2.8024990	0.0000000
C	-1.5213986	-0.4738099	-1.1519603
C	-0.7109748	0.8072442	-1.2004006
C	-0.7109748	0.8072442	1.2004006
C	-1.5213986	-0.4738099	1.1519603
H	-0.1144098	0.8289355	-2.1031213
H	-0.8378516	-1.3321372	-1.1735147
H	-2.1874356	-0.5154353	-2.0151879
H	-0.1144098	0.8289355	2.1031213
H	-1.3813511	1.6739547	1.1991716
H	-0.8378516	-1.3321372	1.1735147
H	-2.1874356	-0.5154353	2.0151879
H	-1.3813511	1.6739547	-1.1991716
O	-2.3441016	-0.5359645	0.0000000
N	0.1378562	0.8873701	0.0000000
N	1.8880375	-2.1203996	0.0000000

H	1.8622840	-3.1342373	0.0000000
H	2.4275974	-1.8418989	0.8126244
H	2.4275974	-1.8418989	-0.8126244

Complex **6a** (1 + Py)

S	-0.2229471	-0.2135142	0.0000000
F	-0.1713850	-0.1302490	-1.6989718
F	-0.1713850	-0.1302490	1.6989718
F	0.1776339	1.3287530	0.0000000
C	-4.0394214	-0.2833016	-1.1452731
C	-2.6225965	0.2505596	-1.2018282
C	-2.6225965	0.2505596	1.2018282
C	-4.0394214	-0.2833016	1.1452731
H	-2.1459753	-0.1304772	-2.0978566
H	-4.0146851	-1.3819575	-1.1679106
H	-4.5920663	0.0762727	-2.0143034
H	-2.1459753	-0.1304772	2.0978566
H	-2.6372580	1.3461674	1.2489550
H	-4.0146851	-1.3819575	1.1679106
H	-4.5920663	0.0762727	2.0143034
H	-2.6372580	1.3461674	-1.2489550
O	-4.7399537	0.1595720	0.0000000
N	-1.8852780	-0.1840196	0.0000000
C	3.3767996	-0.1129956	1.1452588
C	4.7649674	-0.0220848	1.1955908
C	5.4748849	0.0242050	0.0000000
C	4.7649674	-0.0220848	-1.1955908
C	3.3767996	-0.1129956	-1.1452588
N	2.6854986	-0.1590649	0.0000000
H	6.5565386	0.0953768	0.0000000
H	2.7853675	-0.1494528	2.0555376

H	5.2730645	0.0118646	2.1518368
H	5.2730645	0.0118646	-2.1518368
H	2.7853675	-0.1494528	-2.0555376

Complex **6b** (1 + Py)

S	-0.7257023	2.3093668	0.0000000
F	-0.7767758	2.3963205	-1.6905659
F	-0.7767758	2.3963205	1.6905659
F	-1.5897724	3.6566250	0.0000000
C	-1.8755278	-1.0350695	-1.1631202
C	-2.3265063	0.4123126	-1.1953289
C	-2.3265063	0.4123126	1.1953289
C	-1.8755278	-1.0350695	1.1631202
H	-1.9868458	0.8924489	-2.1036739
H	-0.7801583	-1.0644028	-1.2153051
H	-2.2934031	-1.5738112	-2.0152603
H	-1.9868458	0.8924489	2.1036739
H	-3.4198522	0.4634173	1.1580123
H	-0.7801583	-1.0644028	1.2153051
H	-2.2934031	-1.5738112	2.0152603
H	-3.4198522	0.4634173	-1.1580123
O	-2.3337589	-1.7081394	0.0000000
N	-1.8200089	1.1043335	0.0000000
C	1.8369819	-1.4098319	0.0000000
C	3.1541546	-1.8592349	0.0000000
C	4.1794769	-0.9195228	0.0000000
C	3.8386754	0.4287011	0.0000000
C	2.4918248	0.7805123	0.0000000
N	1.4934348	-0.1139027	0.0000000
H	5.2178288	-1.2303621	0.0000000
H	1.0170476	-2.1234634	0.0000000

H	3.3646701	-2.9219302	0.0000000
H	4.5991331	1.2002108	0.0000000
H	2.1941533	1.8242064	0.0000000

Complex **7a** (1 + $NCCH_3$)

S	0.4690369	-0.1271803	0.0000000
F	0.5033759	-0.0445002	-1.6909840
F	0.5033759	-0.0445002	1.6909840
F	0.8678273	1.4145365	0.0000000
C	-3.3378760	-0.3475912	-1.1448697
C	-1.9491539	0.2555589	-1.2019229
C	-1.9491539	0.2555589	1.2019229
C	-3.3378760	-0.3475912	1.1448697
H	-1.4555518	-0.1006506	-2.0984222
H	-3.2587568	-1.4436905	-1.1676237
H	-3.9072313	-0.0158453	-2.0141331
H	-1.4555518	-0.1006506	2.0984222
H	-2.0180334	1.3489344	1.2483156
H	-3.2587568	-1.4436905	1.1676237
H	-3.9072313	-0.0158453	2.0141331
H	-2.0180334	1.3489344	-1.2483156
O	-4.0600628	0.0596548	0.0000000
N	-1.1899039	-0.1398870	0.0000000
C	6.2872160	-0.0908758	0.0000000
H	6.6490805	-1.1182493	0.0000000
H	6.6648974	0.4169198	-0.8864877
H	6.6648974	0.4169198	0.8864877
C	4.8307966	-0.0752230	0.0000000
N	3.6626691	-0.0610467	0.0000000

Complex **7b** (1 + $NCCH_3$)

S	0.7437381	1.6905456	0.0000000
F	0.7364170	1.7832981	-1.6909421
F	0.7364170	1.7832981	1.6909421
F	0.1722384	3.1859398	0.0000000
C	-1.8298507	-1.0407561	-1.1455995
C	-1.3392246	0.3926238	-1.2070533
C	-1.3392246	0.3926238	1.2070533
C	-1.8298507	-1.0407561	1.1455995
H	-0.7434849	0.5232840	-2.1018107
H	-0.9692789	-1.7213523	-1.1573210
H	-2.4586065	-1.2368746	-2.0153765
H	-0.7434849	0.5232840	2.1018107
H	-2.1911977	1.0810064	1.2438413
H	-0.9692789	-1.7213523	1.1573210
H	-2.4586065	-1.2368746	2.0153765
H	-2.1911977	1.0810064	-1.2438413
O	-2.6253131	-1.2818612	0.0000000
N	-0.5437081	0.6919534	0.0000000
C	3.7046742	-0.3454794	0.0000000
H	3.6893910	0.2884746	-0.8859419
H	3.6893910	0.2884746	0.8859419
H	4.6172625	-0.9405930	0.0000000
C	2.5401280	-1.2204484	0.0000000
N	1.6026504	-1.9194648	0.0000000

Complex **8a** (1 + Cl^-)

S	2.1976515	-0.3554437	0.0000000
F	2.1852403	-0.2600688	-1.7093746
F	2.1852403	-0.2600688	1.7093746
F	2.3764401	1.2272732	0.0000000
C	-1.7073017	-0.1959160	-1.1478891

C	-0.2432458	0.1926969	-1.1815655
C	-0.2432458	0.1926969	1.1815655
C	-1.7073017	-0.1959160	1.1478891
H	0.1973694	-0.2152370	-2.0864337
H	-1.7879434	-1.2924707	-1.1817275
H	-2.2227939	0.2252947	-2.0138839
H	0.1973694	-0.2152370	2.0864337
H	-0.1563340	1.2891983	1.2223662
H	-1.7879434	-1.2924707	1.1817275
H	-2.2227939	0.2252947	2.0138839
H	-0.1563340	1.2891983	-1.2223662
O	-2.3807539	0.2947403	0.0000000
N	0.4350670	-0.3430043	0.0000000
Cl	4.8416135	-0.3105603	0.0000000

Complex **8b** (1 + Cl^-)

S	2.1015570	0.6814587	0.0000000
F	2.1257340	0.8206008	-1.7068275
F	2.1257340	0.8206008	1.7068275
F	2.4049762	2.2940595	0.0000000
C	-1.1304356	-0.8223644	-1.1503718
C	-0.3652047	0.4871263	-1.1976788
C	-0.3652047	0.4871263	1.1976788
C	-1.1304356	-0.8223644	1.1503718
H	0.2394705	0.5283279	-2.0942091
H	-0.4157992	-1.6529183	-1.1460756
H	-1.7904500	-0.8848859	-2.0196924
H	0.2394705	0.5283279	2.0942091
H	-1.0750259	1.3252410	1.2095502
H	-0.4157992	-1.6529183	1.1460756
H	-1.7904500	-0.8848859	2.0196924

H	-1.0750259	1.3252410	-1.2095502
O	-1.9704519	-0.8866890	0.0000000
N	0.4669499	0.6493906	0.0000000
Cl	1.8203906	-2.3404746	0.0000000

Complex **9a** (2 + OH_2)

S	1.5255449	0.3974649	0.0000000
F	1.5869354	0.2891752	1.6856636
F	1.5869354	0.2891752	-1.6856636
F	2.0310318	-1.1094474	0.0000000
C	-0.2560360	0.1839900	0.0000000
C	-0.9521980	0.1340118	1.2129406
C	-0.9521980	0.1340118	-1.2129406
C	-2.3368790	0.0000353	1.2013530
H	-0.4245260	0.1862110	2.1521130
C	-2.3368790	0.0000353	-1.2013530
H	-0.4245260	0.1862110	-2.1521130
C	-3.0356972	-0.0664104	0.0000000
H	-2.8686860	-0.0448838	2.1446378
H	-2.8686860	-0.0448838	-2.1446378
H	-4.1150070	-0.1656764	0.0000000
H	4.5792646	-0.3166644	0.7617093
H	4.5792646	-0.3166644	-0.7617093
O	4.6823413	0.2643090	0.0000000

Complex **9b** (2 + OH_2)

S	-0.8516574	-2.0154298	0.0000000
F	-0.9506938	-2.0404872	1.6927901
F	-0.9506938	-2.0404872	-1.6927901
F	-2.4359699	-2.0203077	0.0000000
C	-0.5064933	-0.2531180	0.0000000

C	-0.3528850	0.4270036	1.2112964
C	-0.3528850	0.4270036	-1.2112964
C	-0.0796468	1.7910126	1.2005518
H	-0.4582864	-0.0919140	2.1505728
C	-0.0796468	1.7910126	-1.2005518
H	-0.4582864	-0.0919140	-2.1505728
C	0.0624652	2.4794067	0.0000000
H	0.0319500	2.3122632	2.1443108
H	0.0319500	2.3122632	-2.1443108
H	0.2807516	3.5411036	0.0000000
H	2.4613944	-2.3416720	0.7634382
H	2.4613944	-2.3416720	-0.7634382
O	2.1472389	-1.8440672	0.0000000

Complex **10a** (2 + NH_3)

S	1.2605792	0.2295180	0.0000000
F	1.3119049	0.1276795	1.6907276
F	1.3119049	0.1276795	-1.6907276
F	1.6795354	-1.2942051	0.0000000
C	-0.5336505	0.0810369	0.0000000
C	-1.2332673	0.0573302	1.2115303
C	-1.2332673	0.0573302	-1.2115303
C	-2.6224526	-0.0219962	1.2009391
H	-0.7028670	0.0863193	2.1503447
C	-2.6224526	-0.0219962	-1.2009391
H	-0.7028670	0.0863193	-2.1503447
C	-3.3241200	-0.0603321	0.0000000
H	-3.1554120	-0.0472475	2.1444776
H	-3.1554120	-0.0472475	-2.1444776
H	-4.4065491	-0.1175008	0.0000000
N	4.2523509	0.2010920	0.0000000

H	4.5877228	-0.7552922	0.0000000
H	4.6441597	0.6557564	0.8165988
H	4.6441597	0.6557564	-0.8165988

Complex **10b** (2 + NH_3)

S	-1.9803248	-0.9462035	0.0000000
F	-1.9973945	-1.0426394	-1.6970507
F	-1.9973945	-1.0426394	1.6970507
F	-1.9733634	-2.5335567	0.0000000
C	-0.2068976	-0.6243460	0.0000000
C	0.4775153	-0.4871731	-1.2105777
C	0.4775153	-0.4871731	1.2105777
C	1.8462229	-0.2342703	-1.2003378
H	-0.0444348	-0.5848933	-2.1492830
C	1.8462229	-0.2342703	1.2003378
H	-0.0444348	-0.5848933	2.1492830
C	2.5378429	-0.1029766	0.0000000
H	2.3696839	-0.1359108	-2.1445377
H	2.3696839	-0.1359108	2.1445377
H	3.6032268	0.0967177	0.0000000
N	-1.8096279	1.9893807	0.0000000
H	-2.2958528	2.3450010	0.8162497
H	-2.2958528	2.3450010	-0.8162497
H	-0.8823360	2.4007561	0.0000000

Complex **11a** (2 + Py)

S	-0.4446599	0.1141508	0.0000000
F	-0.3896242	0.0116618	1.6954261
F	-0.3896242	0.0116618	-1.6954261
F	-0.1330094	-1.4328482	0.0000000
C	-2.2448985	0.0703734	0.0000000

C	-2.9436558	0.0887259	1.2118396
C	-2.9436558	0.0887259	-1.2118396
C	-4.3351593	0.0936007	1.2012390
H	-2.4114246	0.0854814	2.1503019
C	-4.3351593	0.0936007	-1.2012390
H	-2.4114246	0.0854814	-2.1503019
C	-5.0375969	0.0977232	0.0000000
H	-4.8690904	0.1002250	2.1445671
H	-4.8690904	0.1002250	-2.1445671
H	-6.1215032	0.1061153	0.0000000
C	3.0815774	-0.0147874	-1.1460519
C	4.4712108	0.0478323	-1.1957759
C	5.1816397	0.0798650	0.0000000
C	4.4712108	0.0478323	1.1957759
C	3.0815774	-0.0147874	1.1460519
N	2.3905963	-0.0465248	0.0000000
H	6.2645243	0.1285074	0.0000000
H	2.4884018	-0.0419636	-2.0553852
H	4.9802181	0.0705429	-2.1518457
H	4.9802181	0.0705429	2.1518457
H	2.4884018	-0.0419636	2.0553852

Complex **11b** (2 + Py)

S	-2.3080530	1.0057984	0.0000000
F	-2.3714376	1.0797292	1.6974534
F	-2.3714376	1.0797292	-1.6974534
F	-3.1165791	2.3746274	0.0000000
C	-0.6209713	1.6417842	0.0000000
C	0.0396984	1.8675259	1.2104851
C	0.0396984	1.8675259	-1.2104851
C	1.3508862	2.3361849	1.2003125

H	-0.4591115	1.6834791	2.1489946
C	1.3508862	2.3361849	-1.2003125
H	-0.4591115	1.6834791	-2.1489946
C	2.0151090	2.5713962	0.0000000
H	1.8526576	2.5132477	2.1449545
H	1.8526576	2.5132477	-2.1449545
H	3.0369977	2.9331817	0.0000000
C	-1.4152290	-2.3757229	0.0000000
C	-0.8426567	-3.6440722	0.0000000
C	0.5444753	-3.7498872	0.0000000
C	1.3004801	-2.5817315	0.0000000
C	0.6400125	-1.3569175	0.0000000
N	-0.6947512	-1.2478828	0.0000000
H	1.0257489	-4.7210923	0.0000000
H	-2.4941653	-2.2492348	0.0000000
H	-1.4731997	-4.5248984	0.0000000
H	2.3833858	-2.6139230	0.0000000
H	1.1940094	-0.4217588	0.0000000

Complex **12a** (2 + $NCCH_3$)

S	0.5643476	0.8677907	0.0000000
F	0.6431686	0.7722115	1.6828302
F	0.6431686	0.7722115	-1.6828302
F	1.3873577	-0.4944315	0.0000000
C	-1.1320608	0.2799411	0.0000000
C	-1.8021409	0.0839621	1.2129647
C	-1.8021409	0.0839621	-1.2129647
C	-3.1266852	-0.3412838	1.2013441
H	-1.2979884	0.2482123	2.1521118
C	-3.1266852	-0.3412838	-1.2013441
H	-1.2979884	0.2482123	-2.1521118

C	-3.7954116	-0.5549562	0.0000000
H	-3.6370289	-0.4974911	2.1446385
H	-3.6370289	-0.4974911	-2.1446385
H	-4.8290813	-0.8810400	0.0000000
C	4.5328973	-0.4273140	0.0000000
H	4.1569113	-0.9381617	-0.8854437
H	5.6215722	-0.4631774	0.0000000
H	4.1569113	-0.9381617	0.8854437
C	4.0774898	0.9558521	0.0000000
N	3.7004161	2.0624367	0.0000000

Complex **12b** (2 + $NCCH_3$)

S	-2.6391545	-0.4749688	0.0000000
F	-2.6839268	-0.5709761	-1.6862343
F	-2.6839268	-0.5709761	1.6862343
F	-3.1803204	-1.9640125	0.0000000
C	-0.8579711	-0.7594402	0.0000000
C	-0.1664971	-0.8614740	-1.2116227
C	-0.1664971	-0.8614740	1.2116227
C	1.2028885	-1.1142487	-1.2012584
H	-0.6898426	-0.7679665	-2.1503643
C	1.2028885	-1.1142487	1.2012584
H	-0.6898426	-0.7679665	2.1503643
C	1.8942482	-1.2459692	0.0000000
H	1.7273227	-1.2088880	-2.1453952
H	1.7273227	-1.2088880	2.1453952
H	2.9591378	-1.4493945	0.0000000
C	1.0023206	2.4836608	0.0000000
H	1.3860554	2.9864618	-0.8873535
H	1.3439610	1.4480935	0.0000000
H	1.3860554	2.9864618	0.8873535

C	-0.4523521	2.5134548	0.0000000
N	-1.6218698	2.5227592	0.0000000

Complex **13a** (2 + Cl^-)

S	2.2196318	0.1990387	0.0000000
F	2.2095597	0.0834674	1.7073612
F	2.2095597	0.0834674	-1.7073612
F	2.4280934	-1.3735490	0.0000000
C	0.3694953	0.0725182	0.0000000
C	-0.3444800	0.0801465	1.2039655
C	-0.3444800	0.0801465	-1.2039655
C	-1.7376753	0.0695500	1.1990248
H	0.1925796	0.0795452	2.1411202
C	-1.7376753	0.0695500	-1.1990248
H	0.1925796	0.0795452	-2.1411202
C	-2.4454607	0.0675965	0.0000000
H	-2.2705644	0.0681382	2.1446440
H	-2.2705644	0.0681382	-2.1446440
H	-3.5303977	0.0632861	0.0000000
Cl	4.8597990	0.2094150	0.0000000

Complex **13b** (2 + Cl^-)

S	-2.2999633	0.6384785	0.0000000
F	-2.2818100	0.7336953	1.7420039
F	-2.2818100	0.7336953	-1.7420039
F	-1.8889542	2.2671277	0.0000000
C	-0.5470823	0.1542707	0.0000000
C	0.1368064	-0.0110928	1.2056907
C	0.1368064	-0.0110928	-1.2056907
C	1.4902174	-0.3364005	1.1975517
H	-0.3919215	0.0987383	2.1390841

C	1.4902174	-0.3364005	-1.1975517
H	-0.3919215	0.0987383	-2.1390841
C	2.1807771	-0.5004475	0.0000000
H	2.0041660	-0.4675986	2.1444909
H	2.0041660	-0.4675986	-2.1444909
H	3.2347442	-0.7579811	0.0000000
Cl	-2.5944381	-1.8361316	0.0000000

Complex **14a** (3 + OH_2)

S	2.5105178	0.2261274	0.0000000
F	2.5164860	0.1201917	1.6686491
F	2.5164860	0.1201917	-1.6686491
F	2.9247618	-1.2882879	0.0000000
H	5.8560559	-0.0679067	0.7638011
H	5.8560559	-0.0679067	-0.7638011
O	5.4141647	0.3190053	0.0000000
C	-1.2977504	0.0564793	0.7196585
C	-1.2977504	0.0564793	-0.7196585
C	-2.5201963	0.0248144	-1.4317447
C	-3.6905488	-0.0051313	-0.7117716
C	-3.6905488	-0.0051313	0.7117716
C	-2.5201963	0.0248144	1.4317447
C	0.0242914	0.0937205	1.1438780
C	0.0242914	0.0937205	-1.1438780
H	-2.5324636	0.0233675	-2.5164769
H	-4.6392014	-0.0295440	-1.2364966
H	-4.6392014	-0.0295440	1.2364966
H	-2.5324636	0.0233675	2.5164769
H	0.4533508	0.1034059	2.1274254
H	0.4533508	0.1034059	-2.1274254
N	0.8105085	0.1043600	0.0000000

Complex **14b** (3 + OH_2)

S	-0.5274015	-3.2349663	0.0000000
F	-0.6319535	-3.2259460	1.6624568
F	-0.6319535	-3.2259460	-1.6624568
F	-2.0598617	-3.5792121	0.0000000
H	2.2286186	-0.8922870	0.7560758
H	2.2286186	-0.8922870	-0.7560758
O	2.5476698	-1.4013581	0.0000000
C	-0.2682858	0.5581801	0.7197358
C	-0.2682858	0.5581801	-0.7197358
C	-0.1290912	1.7730531	-1.4330064
C	0.0109518	2.9346162	-0.7118716
C	0.0109518	2.9346162	0.7118716
C	-0.1290912	1.7730531	1.4330064
C	-0.4217568	-0.7567215	1.1431484
C	-0.4217568	-0.7567215	-1.1431484
H	-0.1339531	1.7861356	-2.5176503
H	0.1210399	3.8773566	-1.2360041
H	0.1210399	3.8773566	1.2360041
H	-0.1339531	1.7861356	2.5176503
H	-0.4884810	-1.1793368	2.1276449
H	-0.4884810	-1.1793368	-2.1276449
N	-0.5345847	-1.5345644	0.0000000

Complex **15a** (3 + NH_3)

S	2.2781778	0.1966654	0.0000000
F	2.2845665	0.0926000	1.6718203
F	2.2845665	0.0926000	-1.6718203
F	2.6690788	-1.3222051	0.0000000
C	-1.5369758	0.0169680	0.7195598

C	-1.5369758	0.0169680	-0.7195598
C	-2.7590013	-0.0156146	-1.4314138
C	-3.9300512	-0.0463066	-0.7114694
C	-3.9300512	-0.0463066	0.7114694
C	-2.7590013	-0.0156146	1.4314138
C	-0.2133703	0.0541436	1.1428583
C	-0.2133703	0.0541436	-1.1428583
H	-2.7713597	-0.0174583	-2.5161994
H	-4.8786120	-0.0716726	-1.2364042
H	-4.8786120	-0.0716726	1.2364042
H	-2.7713597	-0.0174583	2.5161994
H	0.2166566	0.0612527	2.1261227
H	0.2166566	0.0612527	-2.1261227
N	0.5711623	0.0646204	0.0000000
N	5.1333815	0.2205291	0.0000000
H	5.5359157	-0.7102058	0.0000000
H	5.4942891	0.7013858	0.8165239
H	5.4942891	0.7013858	-0.8165239

Complex **15b** (3 + NH_3)

S	-0.5401431	-3.0145892	0.0000000
F	-0.6377486	-3.0030914	1.6718575
F	-0.6377486	-3.0030914	-1.6718575
F	-2.0770216	-3.3624645	0.0000000
C	-0.4355401	0.7921778	0.7195414
C	-0.4355401	0.7921778	-0.7195414
C	-0.3541658	2.0118163	-1.4317860
C	-0.2700329	3.1801601	-0.7115254
C	-0.2700329	3.1801601	0.7115254
C	-0.3541658	2.0118163	1.4317860
C	-0.5276274	-0.5294639	1.1417724

C	-0.5276274	-0.5294639	-1.1417724
H	-0.3592141	2.0248372	-2.5165891
H	-0.2054380	4.1268752	-1.2363690
H	-0.2054380	4.1268752	1.2363690
H	-0.3592141	2.0248372	2.5165891
H	-0.5684141	-0.9558970	2.1256895
H	-0.5684141	-0.9558970	-2.1256895
N	-0.6022921	-1.3096837	0.0000000
N	2.2401328	-2.0471551	0.0000000
H	3.0420091	-2.6683822	0.0000000
H	2.3268385	-1.4462769	0.8136569
H	2.3268385	-1.4462769	-0.8136569

Complex **16a** (3 + Py)

S	0.7300819	0.0535901	0.0000000
F	0.7448981	-0.0500376	1.6781259
F	0.7448981	-0.0500376	-1.6781259
F	1.0277439	-1.4852835	0.0000000
C	-3.0931425	0.0341081	0.7196408
C	-3.0931425	0.0341081	-0.7196408
C	-4.3150992	0.0555123	-1.4310255
C	-5.4869565	0.0767778	-0.7111783
C	-5.4869565	0.0767778	0.7111783
C	-4.3150992	0.0555123	1.4310255
C	-1.7679026	0.0120666	1.1423612
C	-1.7679026	0.0120666	-1.1423612
H	-4.3276526	0.0542843	-2.5158591
H	-6.4355608	0.0935265	-1.2364343
H	-6.4355608	0.0935265	1.2364343
H	-4.3276526	0.0542843	2.5158591
H	-1.3357664	-0.0007543	2.1249566

H	-1.3357664	-0.0007543	-2.1249566
N	-0.9859391	-0.0129385	0.0000000
C	4.0962610	0.0171517	-1.1482561
C	5.4830908	0.1177002	-1.1962458
C	6.1915857	0.1690575	0.0000000
C	5.4830908	0.1177002	1.1962458
C	4.0962610	0.0171517	1.1482561
N	3.4095985	-0.0335832	0.0000000
H	7.2725819	0.2474282	0.0000000
H	3.5034622	-0.0265145	-2.0569956
H	5.9914093	0.1542971	-2.1520529
H	5.9914093	0.1542971	2.1520529
H	3.5034622	-0.0265145	2.0569956

Complex **16b** (3 + Py)

S	-2.7139913	-1.0692736	0.0000000
F	-2.7709676	-1.0017942	1.6747955
F	-2.7709676	-1.0017942	-1.6747955
F	-4.1238182	-0.3559075	0.0000000
C	-0.3640591	1.9428840	0.7192066
C	-0.3640591	1.9428840	-0.7192066
C	0.4112177	2.8863059	-1.4312315
C	1.1585757	3.7900166	-0.7109450
C	1.1585757	3.7900166	0.7109450
C	0.4112177	2.8863059	1.4312315
C	-1.1986143	0.9106447	1.1413686
C	-1.1986143	0.9106447	-1.1413686
H	0.4152030	2.8986225	-2.5161145
H	1.7606729	4.5231408	-1.2363504
H	1.7606729	4.5231408	1.2363504
H	0.4152030	2.8986225	2.5161145

H	-1.4708914	0.5789161	2.1249792
H	-1.4708914	0.5789161	-2.1249792
N	-1.7059692	0.3170828	0.0000000
C	-0.1966164	-3.4737096	0.0000000
C	0.9983940	-4.1863884	0.0000000
C	2.1959795	-3.4785736	0.0000000
C	2.1478889	-2.0878460	0.0000000
C	0.9066481	-1.4593334	0.0000000
N	-0.2496274	-2.1368665	0.0000000
H	3.1464855	-3.9995080	0.0000000
H	-1.1537736	-3.9880968	0.0000000
H	0.9853054	-5.2695039	0.0000000
H	3.0537382	-1.4937522	0.0000000
H	0.8270826	-0.3757960	0.0000000

Complex **17a** (3 + $NCCH_3$)

S	1.3510273	0.0107731	0.0000000
F	1.3437597	-0.0926321	1.6667345
F	1.3437597	-0.0926321	-1.6667345
F	1.7198195	-1.5138464	0.0000000
C	-2.4635717	0.0052319	0.7195244
C	-2.4635717	0.0052319	-0.7195244
C	-3.6856829	0.0444228	-1.4319781
C	-4.8556681	0.0864680	-0.7118213
C	-4.8556681	0.0864680	0.7118213
C	-3.6856829	0.0444228	1.4319781
C	-1.1410413	-0.0085972	1.1437501
C	-1.1410413	-0.0085972	-1.1437501
H	-3.6973506	0.0385939	-2.5166798
H	-5.8045795	0.1192073	-1.2356514
H	-5.8045795	0.1192073	1.2356514

H	-3.6973506	0.0385939	2.5166798
H	-0.7125966	-0.0076713	2.1274469
H	-0.7125966	-0.0076713	-2.1274469
N	-0.3548644	-0.0350835	0.0000000
C	7.0469661	0.1794254	0.0000000
H	7.4021399	-0.3441309	0.8867180
H	7.4505933	1.1910710	0.0000000
H	7.4021399	-0.3441309	-0.8867180
C	5.5914801	0.2245618	0.0000000
N	4.4241603	0.2613139	0.0000000

Complex **17b** (3 + $NCCH_3$)

S	-2.4811642	-2.5185443	0.0000000
F	-2.5717960	-2.4599856	1.6636402
F	-2.5717960	-2.4599856	-1.6636402
F	-3.9964730	-2.0962019	0.0000000
C	-0.4602355	0.6983254	0.7203099
C	-0.4602355	0.6983254	-0.7203099
C	0.2631160	1.6837079	-1.4323547
C	0.9701511	2.6189962	-0.7119442
C	0.9701511	2.6189962	0.7119442
C	0.2631160	1.6837079	1.4323547
C	-1.2259266	-0.3805840	1.1428432
C	-1.2259266	-0.3805840	-1.1428432
H	0.2636911	1.6989966	-2.5172996
H	1.5350586	3.3816308	-1.2367779
H	1.5350586	3.3816308	1.2367779
H	0.2636911	1.6989966	2.5172996
H	-1.4622176	-0.7377563	2.1266665
H	-1.4622176	-0.7377563	-2.1266665
N	-1.6897584	-1.0112076	0.0000000

C	2.6107285	-0.8834754	0.0000000
H	3.2340848	-0.9937979	0.8872847
H	3.2340848	-0.9937979	-0.8872847
H	2.1624537	0.1109922	0.0000000
C	1.5675141	-1.8993300	0.0000000
N	0.7348475	-2.7212992	0.0000000

Complex **18a** (3 + Cl^-)

S	3.2946447	0.2686624	0.0000000
F	3.2452646	0.1393485	1.6996132
F	3.2452646	0.1393485	-1.6996132
F	3.4135107	-1.3111921	0.0000000
C	-0.7192039	0.0401200	0.7230397
C	-0.7192039	0.0401200	-0.7230397
C	-1.9400043	0.0258358	-1.4242787
C	-3.1233637	0.0135432	-0.7080440
C	-3.1233637	0.0135432	0.7080440
C	-1.9400043	0.0258358	1.4242787
C	0.6237471	0.0531117	1.1273903
C	0.6237471	0.0531117	-1.1273903
H	-1.9547481	0.0241463	-2.5108249
H	-4.0704539	0.0026330	-1.2387003
H	-4.0704539	0.0026330	1.2387003
H	-1.9547481	0.0241463	2.5108249
H	1.0707072	0.0501716	2.1064447
H	1.0707072	0.0501716	-2.1064447
N	1.3932426	0.0483858	0.0000000
Cl	5.6347121	0.2963235	0.0000000

Complex **18b** (3 + Cl^-)

S	-0.2374290	-3.3221142	0.0000000

F	-0.3033905	-3.2485468	1.7112126
F	-0.3033905	-3.2485468	-1.7112126
F	-1.9092038	-3.1866570	0.0000000
C	0.0028599	0.5451367	0.7207031
C	0.0028599	0.5451367	-0.7207031
C	0.0775499	1.7624497	-1.4253962
C	0.1504183	2.9416496	-0.7087575
C	0.1504183	2.9416496	0.7087575
C	0.0775499	1.7624497	1.4253962
C	-0.0779764	-0.7878181	1.1333005
C	-0.0779764	-0.7878181	-1.1333005
H	0.0800003	1.7753988	-2.5116126
H	0.2107807	3.8871093	-1.2387558
H	0.2107807	3.8871093	1.2387558
H	0.0800003	1.7753988	2.5116126
H	-0.0804699	-1.2273977	2.1115595
H	-0.0804699	-1.2273977	-2.1115595
N	-0.1321378	-1.5527718	0.0000000
Cl	2.1592259	-3.2344200	0.0000000