

Supporting information for manuscript

**“Like-like” tetrel bonding interactions between Sn centres: a
combined *ab initio* and CSD study**

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1. Table S1

Type I refcodes			
AFAJAU	AFAJEU	AGEBUJ	BAVSIC
BELKEK	CUGRAX	FIWFEW	GUJCIZ
HUCGUH	KAJVEX	NENWIN	OFIYEH
OFIYIL	OFIYAD	OFIYOR	OFIYUX
OFIZIM	OFIZUY	OMDTSN	OMIVAI
OMIVEM	SOQREW	TAXHOQ	TUBKAC
VAPMEE	VAYVEY	VAYVIC	XEXSUP
YERBED	YIJLUY	WIBPOP	GAYRAC
SANHIZ			
Type II refcodes			
BAMWOE	CUMGUO	DMSNCL	DMSNCL01
DMSNCL01	DMSNCL03	DORZER	DPPRSN
FEDYES	FEDIW	FUXGIO	GUXTUP01
ICULAW	IHOROM	JERTIK	JERTIK01
JERTOK	KEJLOA	KEJLUG	MELPAU
MOVJUC	MOVKEN	MOVKIR	MXSNOX
OLAGIT	QUVROK	SEFDUE	SIHQIJ
SISKEM	TAKHOQ	UYOBIU	UZAJEM
VOLDUX	VURFUJ	WIDCAN	YICPAD
YICPOR	YICPUX	YICQAE	LEMHET
LEMHIX	YICQAE01	REGGAM	GAYRAC
SANHIZ			
Type III refcodes			
DINWEE	FILJOZ	OFIXIK	OFIXOQ
OFIXUW	OFIZEI	PIGSII	

2. Figures S1 to S4

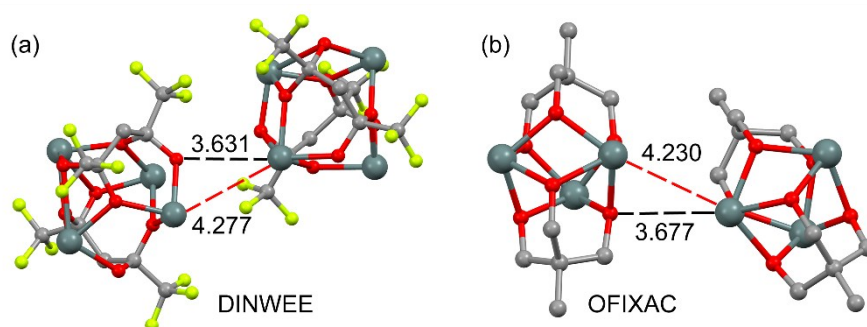


Fig S1. (a) X-ray structure of refcode DINWEE. (b) X-ray structure of refcode OFIXAC.

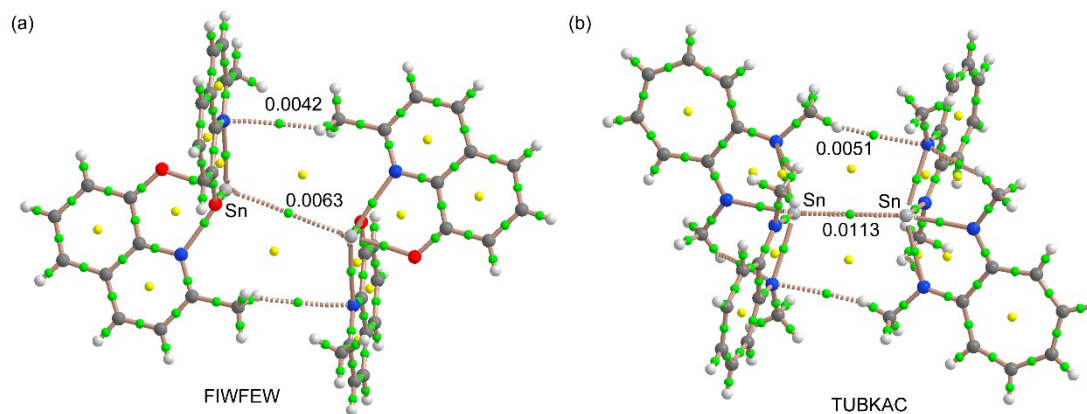


Fig S2. Distribution of bond and ring critical points (green and yellow spheres, respectively) and bond paths for X-ray structures FIWFEW (a) and TUBKAC (b). The values of $\rho(r)$ at the bond CPs are given in atomic units.

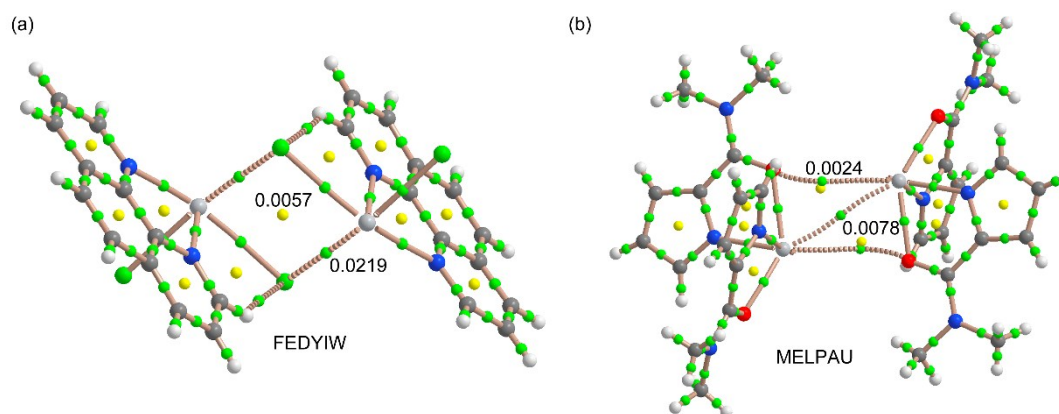


Fig S3. Distribution of bond and ring critical points (green and yellow spheres, respectively) and bond paths for X-ray structures FEDYIW (a) and MELPAU (b). The values of $\rho(r)$ at the bond CPs are given in atomic units.

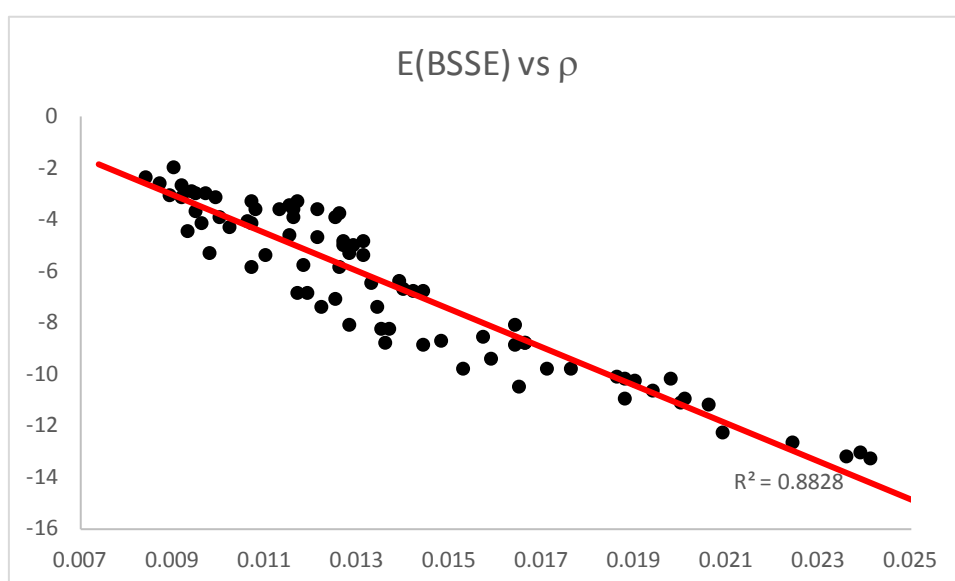


Fig. S4. Linear regression plot of interaction energy (kcal/mol) vs $\rho(r)$ in a.u. for complexes 19-99.

3. Cartesian coordinates

Complex 19 (X=H, Y=H)

C	6.6337556	-0.0438710	0.0000000
C	5.9318013	-0.0370377	1.2040549
C	4.5363775	-0.0189337	1.1964699
C	3.8061118	-0.0076874	0.0000000
C	4.5363775	-0.0189337	-1.1964699
C	5.9318013	-0.0370377	-1.2040549
H	6.4708409	-0.0466333	2.1465128
H	4.0098452	-0.0218433	2.1483045
H	4.0098452	-0.0218433	-2.1483045
H	6.4708409	-0.0466333	-2.1465128
Sn	1.6351942	0.0529075	0.0000000
H	1.2603788	-0.7402854	1.4374695
H	1.2783035	1.6995457	0.0000000
H	1.2603788	-0.7402854	-1.4374695
H	7.7187213	-0.0594109	0.0000000
Sn	-2.0189715	0.0031248	0.0000000
C	-3.4625522	-0.0034702	1.5275416
C	-4.8272324	-0.0336971	1.2539259
H	-5.5100755	-0.0589737	2.1142222
C	-5.4539220	-0.0451243	0.0000000
H	-6.5417413	-0.0854282	0.0000000
C	-4.8272324	-0.0336971	-1.2539259
H	-5.5100755	-0.0589737	-2.1142222
C	-3.4625522	-0.0034702	-1.5275416
C	-3.0616876	0.0381727	-2.9867131
H	-3.7020178	-0.6096064	-3.6003898
H	-3.1487487	1.0529244	-3.3946090
H	-2.0256555	-0.2776444	-3.1370743

C	-3.0616876	0.0381727	2.9867131
H	-3.1487487	1.0529244	3.3946090
H	-3.7020178	-0.6096064	3.6003898
H	-2.0256555	-0.2776444	3.1370743

Complex 20 (X=H, Y=F)

C	6.5668286	-0.0405218	0.0000000
C	5.8967444	-0.0351485	1.2116470
C	4.5006135	-0.0210540	1.1949979
C	3.7684661	-0.0135209	0.0000000
C	4.5006135	-0.0210540	-1.1949979
C	5.8967444	-0.0351485	-1.2116470
H	6.4611710	-0.0431653	2.1373684
H	3.9782431	-0.0235213	2.1487160
H	3.9782431	-0.0235213	-2.1487160
H	6.4611710	-0.0431653	-2.1373684
Sn	1.5918220	0.0387705	0.0000000
H	1.2415529	-0.7587573	1.4415944
H	1.2508118	1.6874116	0.0000000
H	1.2415529	-0.7587573	-1.4415944
F	7.9223551	-0.0566629	0.0000000
Sn	-2.0086115	0.0208992	0.0000000
C	-3.4488760	0.0025574	1.5285377
C	-4.8131726	-0.0370575	1.2540995
H	-5.4959824	-0.0670003	2.1141228
C	-5.4392928	-0.0528073	0.0000000
H	-6.5268011	-0.0996201	0.0000000
C	-4.8131726	-0.0370575	-1.2540995
H	-5.4959824	-0.0670003	-2.1141228
C	-3.4488760	0.0025574	-1.5285377
C	-3.0478666	0.0469714	-2.9874819

H -3.6840206 -0.6045867 -3.6013643
H -3.1412085 1.0612564 -3.3949798
H -2.0099873 -0.2624684 -3.1377918
C -3.0478666 0.0469714 2.9874819
H -3.1412085 1.0612564 3.3949798
H -3.6840206 -0.6045867 3.6013643
H -2.0099873 -0.2624684 3.1377918

Complex 21 ($X=H$, $Y=CF_3$)

C 5.8031056 0.0177595 0.0000000
C 5.1082004 0.0111516 1.2085207
C 3.7144848 0.0078417 1.1943889
C 2.9810096 0.0070200 0.0000000
C 3.7144848 0.0078417 -1.1943889
C 5.1082004 0.0111516 -1.2085207
H 5.6519202 0.0151450 2.1467595
H 3.1907301 -0.0010606 2.1475839
H 3.1907301 -0.0010606 -2.1475839
H 5.6519202 0.0151450 -2.1467595
Sn 0.7904197 0.0439131 0.0000000
H 0.4889895 -0.7570257 1.4513186
H 0.4811261 1.6991394 0.0000000
H 0.4889895 -0.7570257 -1.4513186
C 7.2951291 -0.0352804 0.0000000
F 7.7587222 -1.3044457 0.0000000
F 7.8315908 0.5603616 1.0804409
F 7.8315908 0.5603616 -1.0804409
Sn -2.7106365 -0.0011863 0.0000000
C -4.1444333 -0.0160795 1.5303378
C -5.5083977 -0.0571947 1.2543971
H -6.1914145 -0.0852045 2.1140026

C	-6.1337206	-0.0748625	0.0000000
H	-7.2211035	-0.1216867	0.0000000
C	-5.5083977	-0.0571947	-1.2543971
H	-6.1914145	-0.0852045	-2.1140026
C	-4.1444333	-0.0160795	-1.5303378
C	-3.7429273	0.0364833	-2.9885676
H	-4.3746897	-0.6162745	-3.6053207
H	-3.8429991	1.0520964	-3.3908254
H	-2.7030800	-0.2654255	-3.1400697
C	-3.7429273	0.0364833	2.9885676
H	-3.8429991	1.0520964	3.3908254
H	-4.3746897	-0.6162745	3.6053207
H	-2.7030800	-0.2654255	3.1400697

Complex 22 (X=H, Y=CN)

C	6.2275282	-0.0194016	0.0000000
C	5.5290305	-0.0188455	1.2131186
C	4.1365824	-0.0109408	1.1951945
C	3.4031575	-0.0040297	0.0000000
C	4.1365824	-0.0109408	-1.1951945
C	5.5290305	-0.0188455	-1.2131186
H	6.0795536	-0.0251182	2.1480957
H	3.6110340	-0.0186803	2.1476358
H	3.6110340	-0.0186803	-2.1476358
H	6.0795536	-0.0251182	-2.1480957
Sn	1.2040933	0.0517177	0.0000000
H	0.9267907	-0.7480671	1.4579605
H	0.9374920	1.7153199	0.0000000
H	0.9267907	-0.7480671	-1.4579605
C	7.6579159	-0.0249457	0.0000000
N	8.8312702	-0.0277154	0.0000000

Sn	-2.2307776	0.0201893	0.0000000
C	-3.6589643	-0.0066935	1.5323285
C	-5.0223225	-0.0547599	1.2547127
H	-5.7054322	-0.0887704	2.1136883
C	-5.6468350	-0.0745586	0.0000000
H	-6.7338212	-0.1278951	0.0000000
C	-5.0223225	-0.0547599	-1.2547127
H	-5.7054322	-0.0887704	-2.1136883
C	-3.6589643	-0.0066935	-1.5323285
C	-3.2572192	0.0405804	-2.9905735
H	-3.8887382	-0.6154724	-3.6038430
H	-3.3579301	1.0541427	-3.3975945
H	-2.2173963	-0.2617154	-3.1408967
C	-3.2572192	0.0405804	2.9905735
H	-3.3579301	1.0541427	3.3975945
H	-3.8887382	-0.6154724	3.6038430
H	-2.2173963	-0.2617154	3.1408967

Complex 23 ($X=H$, $Y=P(CN)_2$)

C	5.4651521	-0.3933191	0.0000000
C	4.7697341	-0.3554236	1.2118136
C	3.3781719	-0.2585762	1.1934502
C	2.6447939	-0.2096298	0.0000000
C	3.3781719	-0.2585762	-1.1934502
C	4.7697341	-0.3554236	-1.2118136
H	5.3039193	-0.3835248	2.1576278
H	2.8560292	-0.2260653	2.1476247
H	2.8560292	-0.2260653	-2.1476247
H	5.3039193	-0.3835248	-2.1576278
Sn	0.4438224	-0.0437716	0.0000000
P	7.2516733	-0.7304530	0.0000000

C	7.7842684	0.3339526	1.3289196
N	8.1727033	0.9121428	2.2759944
C	7.7842684	0.3339526	-1.3289196
N	8.1727033	0.9121428	-2.2759944
H	0.1556603	-0.8315269	1.4633700
H	0.2714386	1.6322859	0.0000000
H	0.1556603	-0.8315269	-1.4633700
Sn	-2.9450826	0.0509121	0.0000000
C	-4.3703016	0.0673059	1.5331099
C	-5.7344404	0.0708731	1.2547387
H	-6.4182678	0.0586943	2.1136002
C	-6.3589182	0.0772906	0.0000000
H	-7.4471739	0.0666330	0.0000000
C	-5.7344404	0.0708731	-1.2547387
H	-6.4182678	0.0586943	-2.1136002
C	-4.3703016	0.0673059	-1.5331099
C	-3.9672704	0.0884446	-2.9914519
H	-4.6284466	-0.5421851	-3.5999578
H	-4.0220688	1.1028912	-3.4046446
H	-2.9425435	-0.2619768	-3.1403276
C	-3.9672704	0.0884446	2.9914519
H	-4.0220688	1.1028912	3.4046446
H	-4.6284466	-0.5421851	3.5999578
H	-2.9425435	-0.2619768	3.1403276

Complex 24 (X=H, Y=SO₂CN)

C	5.4349780	0.2938373	0.0000000
C	4.7594307	0.2495725	1.2208430
C	3.3684388	0.1756077	1.1965064
C	2.6369122	0.1396895	0.0000000
C	3.3684388	0.1756077	-1.1965064

C	4.7594307	0.2495725	-1.2208430
H	5.3156673	0.2888918	2.1507724
H	2.8411327	0.1421224	2.1476268
H	2.8411327	0.1421224	-2.1476268
H	5.3156673	0.2888918	-2.1507724
Sn	0.4141398	0.1146564	0.0000000
S	7.1667112	0.3780519	0.0000000
O	7.6505319	0.8818272	1.2532185
O	7.6505319	0.8818272	-1.2532185
C	7.5840250	-1.3348047	0.0000000
N	7.8912738	-2.4694954	0.0000000
H	0.2334865	-0.6909608	1.4729580
H	0.1706085	1.7838041	0.0000000
H	0.2334865	-0.6909608	-1.4729580
Sn	-2.8802258	-0.0030217	0.0000000
C	-4.2958138	-0.0566350	1.5354415
C	-5.6576466	-0.1296814	1.2552672
H	-6.3403640	-0.1751812	2.1135383
C	-6.2804494	-0.1611336	0.0000000
H	-7.3662246	-0.2337550	0.0000000
C	-5.6576466	-0.1296814	-1.2552672
H	-6.3403640	-0.1751812	-2.1135383
C	-4.2958138	-0.0566350	-1.5354415
C	-3.8922468	-0.0004264	-2.9923640
H	-4.5094530	-0.6684236	-3.6067232
H	-4.0124582	1.0113045	-3.3979638
H	-2.8465799	-0.2819322	-3.1411438
C	-3.8922468	-0.0004264	2.9923640
H	-4.0124582	1.0113045	3.3979638
H	-4.5094530	-0.6684236	3.6067232
H	-2.8465799	-0.2819322	3.1411438

Complex 25 (X=H, Y=tBu)

C	4.2464519	0.0413754	0.0000000
C	3.5157671	0.0210183	1.1947352
C	2.1208103	-0.0018138	1.1898060
C	1.3826768	-0.0083769	0.0000000
C	2.1208103	-0.0018138	-1.1898060
C	3.5157671	0.0210183	-1.1947352
H	4.0306956	0.0251530	2.1491995
H	1.6028898	-0.0182986	2.1466968
H	1.6028898	-0.0182986	-2.1466968
H	4.0306956	0.0251530	-2.1491995
Sn	-0.7871807	0.0310878	0.0000000
H	-1.1563702	-0.7663769	1.4368485
H	-1.1492217	1.6756100	0.0000000
H	-1.1563702	-0.7663769	-1.4368485
C	5.7685910	0.0064019	0.0000000
C	6.3469493	0.7002960	1.2350612
H	6.0898223	0.1783039	2.1578569
H	7.4382990	0.7229008	1.1668005
H	5.9853481	1.7287205	1.3124927
C	6.3469493	0.7002960	-1.2350612
H	7.4382990	0.7229008	-1.1668005
H	6.0898223	0.1783039	-2.1578569
H	5.9853481	1.7287205	-1.3124927
C	6.2174618	-1.4597911	0.0000000
H	5.8354346	-1.9774280	-0.8834078
H	7.3104133	-1.5309099	0.0000000
H	5.8354346	-1.9774280	0.8834078
Sn	-4.4380481	0.0203128	0.0000000
C	-5.8813662	-0.0023331	1.5275505
C	-7.2456359	-0.0484532	1.2539566

H	-7.9280730	-0.0825108	2.1142803
C	-7.8720437	-0.0673479	0.0000000
H	-8.9593263	-0.1206503	0.0000000
C	-7.2456359	-0.0484532	-1.2539566
H	-7.9280730	-0.0825108	-2.1142803
C	-5.8813662	-0.0023331	-1.5275505
C	-5.4807012	0.0432816	-2.9866267
H	-6.1141032	-0.6114555	-3.6000903
H	-5.5782497	1.0569005	-3.3950362
H	-4.4414039	-0.2617604	-3.1365597
C	-5.4807012	0.0432816	2.9866267
H	-5.5782497	1.0569005	3.3950362
H	-6.1141032	-0.6114555	3.6000903
H	-4.4414039	-0.2617604	3.1365597

Complex 26 ($X=H$, $Y=NH_2$)

C	6.1434366	-0.0365657	0.0000000
C	5.4290747	-0.0454752	1.1999659
C	4.0354166	-0.0465504	1.1916352
C	3.2986297	-0.0453673	0.0000000
C	4.0354166	-0.0465504	-1.1916352
C	5.4290747	-0.0454752	-1.1999659
H	5.9698566	-0.0506433	2.1433821
H	3.5169751	-0.0553323	2.1478961
H	3.5169751	-0.0553323	-2.1478961
H	5.9698566	-0.0506433	-2.1433821
Sn	1.1345415	0.0165598	0.0000000
H	0.7463085	-0.7733841	1.4361654
H	0.7684944	1.6614434	0.0000000
H	0.7463085	-0.7733841	-1.4361654
N	7.5514265	-0.0954939	0.0000000

H	7.9538507	0.3252465	-0.8275420
H	7.9538507	0.3252465	0.8275420
Sn	-2.5317582	-0.0062381	0.0000000
C	-3.9759388	-0.0180070	1.5273637
C	-5.3405486	-0.0514171	1.2541065
H	-6.0233945	-0.0797295	2.1143792
C	-5.9671696	-0.0637501	0.0000000
H	-7.0548944	-0.1064819	0.0000000
C	-5.3405486	-0.0514171	-1.2541065
H	-6.0233945	-0.0797295	-2.1143792
C	-3.9759388	-0.0180070	-1.5273637
C	-3.5734651	0.0211477	-2.9862171
H	-4.2128775	-0.6277756	-3.5997117
H	-3.6593706	1.0351250	-3.3964321
H	-2.5372405	-0.2952579	-3.1343267
C	-3.5734651	0.0211477	2.9862171
H	-3.6593706	1.0351250	3.3964321
H	-4.2128775	-0.6277756	3.5997117
H	-2.5372405	-0.2952579	3.1343267

Complex 27 (X=H, Y=NMe₂)

C	4.9200149	-0.1679153	0.0000000
C	4.1873523	-0.1632034	1.1992468
C	2.7936514	-0.1710894	1.1866852
C	2.0516728	-0.1725866	0.0000000
C	2.7936514	-0.1710894	-1.1866852
C	4.1873523	-0.1632034	-1.1992468
H	4.6952738	-0.1591685	2.1551053
H	2.2803170	-0.1752898	2.1459438
H	2.2803170	-0.1752898	-2.1459438
H	4.6952738	-0.1591685	-2.1551053

Sn	-0.1094406	-0.1130402	0.0000000
N	6.3244178	-0.2053939	0.0000000
C	6.9728580	0.2544950	-1.2120675
H	8.0524557	0.2048037	-1.0706101
H	6.7227821	-0.3925122	-2.0525082
H	6.6983387	1.2869285	-1.4782360
C	6.9728580	0.2544950	1.2120675
H	6.6983387	1.2869285	1.4782360
H	6.7227821	-0.3925122	2.0525082
H	8.0524557	0.2048037	1.0706101
H	-0.5099106	-0.9053899	1.4314483
H	-0.4847309	1.5291067	0.0000000
H	-0.5099106	-0.9053899	-1.4314483
Sn	-3.8390413	-0.0826343	0.0000000
C	-5.2858754	-0.0447080	1.5266368
C	-6.6510732	-0.0375006	1.2536949
H	-7.3343520	-0.0438828	2.1141292
C	-7.2783111	-0.0326158	0.0000000
H	-8.3669227	-0.0441952	0.0000000
C	-6.6510732	-0.0375006	-1.2536949
H	-7.3343520	-0.0438828	-2.1141292
C	-5.2858754	-0.0447080	-1.5266368
C	-4.8849643	-0.0129873	-2.9862555
H	-5.5361976	-0.6513033	-3.5984889
H	-4.9550513	1.0020786	-3.3970593
H	-3.8544341	-0.3466333	-3.1359867
C	-4.8849643	-0.0129873	2.9862555
H	-4.9550513	1.0020786	3.3970593
H	-5.5361976	-0.6513033	3.5984889
H	-3.8544341	-0.3466333	3.1359867

Complex 28 (X=F, Y=H)

C	6.6421044	-0.0565994	0.0000000
C	5.9403999	-0.0483248	1.2042610
C	4.5452273	-0.0273693	1.1968210
C	3.8158827	-0.0146211	0.0000000
C	4.5452273	-0.0273693	-1.1968210
C	5.9403999	-0.0483248	-1.2042610
H	6.4793931	-0.0590964	2.1467151
H	4.0181843	-0.0292752	2.1483580
H	4.0181843	-0.0292752	-2.1483580
H	6.4793931	-0.0590964	-2.1467151
Sn	1.6487604	0.0494101	0.0000000
H	1.2664071	-0.7425263	1.4364694
H	1.2867630	1.6945650	0.0000000
H	1.2664071	-0.7425263	-1.4364694
H	7.7269226	-0.0742655	0.0000000
Sn	-2.0026355	0.0085423	0.0000000
C	-3.4515513	0.0036008	1.5240204
C	-4.8181402	-0.0233702	1.2582457
H	-5.5271130	-0.0494653	2.0930863
C	-5.4110785	-0.0339772	0.0000000
C	-4.8181402	-0.0233702	-1.2582457
H	-5.5271130	-0.0494653	-2.0930863
C	-3.4515513	0.0036008	-1.5240204
C	-3.0546744	0.0446481	-2.9841010
H	-3.6957627	-0.6028701	-3.5968284
H	-3.1413483	1.0595072	-3.3916972
H	-2.0190101	-0.2722027	-3.1339716
C	-3.0546744	0.0446481	2.9841010
H	-3.1413483	1.0595072	3.3916972
H	-3.6957627	-0.6028701	3.5968284

H	-2.0190101	-0.2722027	3.1339716
F	-6.7907424	-0.0795658	0.0000000

Complex 29 ($X=F$, $Y=F$)

C	6.5750646	-0.0400500	0.0000000
C	5.9051643	-0.0347489	1.2118079
C	4.5094069	-0.0209620	1.1954889
C	3.7784270	-0.0130194	0.0000000
C	4.5094069	-0.0209620	-1.1954889
C	5.9051643	-0.0347489	-1.2118079
H	6.4694549	-0.0430232	2.1375289
H	3.9863483	-0.0243454	2.1488272
H	3.9863483	-0.0243454	-2.1488272
H	6.4694549	-0.0430232	-2.1375289
Sn	1.6061842	0.0403183	0.0000000
H	1.2481496	-0.7574056	1.4395927
H	1.2573638	1.6874870	0.0000000
H	1.2481496	-0.7574056	-1.4395927
F	7.9301528	-0.0556801	0.0000000
Sn	-1.9919079	0.0195595	0.0000000
C	-3.4376949	0.0026964	1.5249257
C	-4.8036974	-0.0359258	1.2584009
H	-5.5124509	-0.0681266	2.0930298
C	-5.3961629	-0.0517220	0.0000000
C	-4.8036974	-0.0359258	-1.2584009
H	-5.5124509	-0.0681266	-2.0930298
C	-3.4376949	0.0026964	-1.5249257
C	-3.0410277	0.0474670	-2.9846585
H	-3.6768760	-0.6048890	-3.5976761
H	-3.1357169	1.0617353	-3.3918509
H	-2.0030173	-0.2613414	-3.1341704

C	-3.0410277	0.0474670	2.9846585
H	-3.1357169	1.0617353	3.3918509
H	-3.6768760	-0.6048890	3.5976761
H	-2.0030173	-0.2613414	3.1341704
F	-6.7752072	-0.1091551	0.0000000

Complex 30 ($X = F$, $Y = CF_3$)

C	5.8105303	0.0120940	0.0000000
C	5.1163139	0.0056591	1.2087685
C	3.7227289	0.0041830	1.1949180
C	2.9907759	0.0043944	0.0000000
C	3.7227289	0.0041830	-1.1949180
C	5.1163139	0.0056591	-1.2087685
H	5.6602227	0.0090779	2.1467315
H	3.1978574	-0.0038040	2.1473816
H	3.1978574	-0.0038040	-2.1473816
H	5.6602227	0.0090779	-2.1467315
Sn	0.8054998	0.0442062	0.0000000
H	0.4937344	-0.7564496	1.4492225
H	0.4890856	1.6980621	0.0000000
H	0.4937344	-0.7564496	-1.4492225
C	7.3024814	-0.0420211	0.0000000
F	7.7635902	-1.3118369	0.0000000
F	7.8392123	0.5529919	1.0804803
F	7.8392123	0.5529919	-1.0804803
Sn	-2.6947374	0.0023311	0.0000000
C	-4.1341719	-0.0112688	1.5266706
C	-5.4997907	-0.0502356	1.2586956
H	-6.2087930	-0.0800003	2.0929604
C	-6.0917362	-0.0671920	0.0000000
C	-5.4997907	-0.0502356	-1.2586956

H	-6.2087930	-0.0800003	-2.0929604
C	-4.1341719	-0.0112688	-1.5266706
C	-3.7368124	0.0405051	-2.9857176
H	-4.3691231	-0.6124624	-3.6014273
H	-3.8368731	1.0560063	-3.3882289
H	-2.6972347	-0.2621738	-3.1362236
C	-3.7368124	0.0405051	2.9857176
H	-3.8368731	1.0560063	3.3882289
H	-4.3691231	-0.6124624	3.6014273
H	-2.6972347	-0.2621738	3.1362236
F	-7.4700307	-0.1240951	0.0000000

Complex 31 ($X = F$, $Y = CN$)

C	6.2612933	-0.0333112	0.0000000
C	5.5632382	-0.0297718	1.2132571
C	4.1709259	-0.0184753	1.1958229
C	3.4386514	-0.0099215	0.0000000
C	4.1709259	-0.0184753	-1.1958229
C	5.5632382	-0.0297718	-1.2132571
H	6.1142296	-0.0367657	2.1478987
H	3.6449895	-0.0237206	2.1478336
H	3.6449895	-0.0237206	-2.1478336
H	6.1142296	-0.0367657	-2.1478987
Sn	1.2470716	0.0445074	0.0000000
H	0.9454932	-0.7542187	1.4525168
H	0.9534032	1.7026322	0.0000000
H	0.9454932	-0.7542187	-1.4525168
C	7.6916494	-0.0431679	0.0000000
N	8.8649134	-0.0501671	0.0000000
Sn	-2.2320060	0.0113097	0.0000000
C	-3.6696224	-0.0013927	1.5272345

C	-5.0355424	-0.0345470	1.2590178
H	-5.7452316	-0.0611107	2.0929475
C	-5.6272206	-0.0480365	0.0000000
C	-5.0355424	-0.0345470	-1.2590178
H	-5.7452316	-0.0611107	-2.0929475
C	-3.6696224	-0.0013927	-1.5272345
C	-3.2725238	0.0424060	-2.9867920
H	-3.8742575	-0.6488833	-3.5908517
H	-3.4170005	1.0450045	-3.4076788
H	-2.2207578	-0.2175107	-3.1317971
C	-3.2725238	0.0424060	2.9867920
H	-3.4170005	1.0450045	3.4076788
H	-3.8742575	-0.6488833	3.5908517
H	-2.2207578	-0.2175107	3.1317971
F	-7.0056363	-0.0958728	0.0000000

Complex 32 ($X = F$, $Y = P(CN)_2$)

C	5.4745443	-0.3650106	0.0000000
C	4.7792171	-0.3304285	1.2120561
C	3.3874201	-0.2410810	1.1939730
C	2.6552229	-0.1961339	0.0000000
C	3.3874201	-0.2410810	-1.1939730
C	4.7792171	-0.3304285	-1.2120561
H	5.3133235	-0.3561539	2.1579929
H	2.8644446	-0.2113723	2.1477440
H	2.8644446	-0.2113723	-2.1477440
H	5.3133235	-0.3561539	-2.1579929
Sn	0.4603459	-0.0418071	0.0000000
H	0.1652119	-0.8299381	1.4613292
H	0.2682866	1.6318090	0.0000000
H	0.1652119	-0.8299381	-1.4613292

P	7.2630172	-0.6933764	0.0000000
C	7.7897113	0.3738488	1.3288767
N	8.1752207	0.9543966	2.2755839
C	7.7897113	0.3738488	-1.3288767
N	8.1752207	0.9543966	-2.2755839
Sn	-2.9299504	0.0337132	0.0000000
C	-4.3609186	0.0444033	1.5293619
C	-5.7265553	0.0417810	1.2590676
H	-6.4365971	0.0252129	2.0925065
C	-6.3180739	0.0438291	0.0000000
C	-5.7265553	0.0417810	-1.2590676
H	-6.4365971	0.0252129	-2.0925065
C	-4.3609186	0.0444033	-1.5293619
C	-3.9617977	0.0686758	-2.9884375
H	-4.6191027	-0.5659545	-3.5967079
H	-4.0231820	1.0830751	-3.4007843
H	-2.9349692	-0.2755174	-3.1364633
C	-3.9617977	0.0686758	2.9884375
H	-4.0231820	1.0830751	3.4007843
H	-4.6191027	-0.5659545	3.5967079
H	-2.9349692	-0.2755174	3.1364633
F	-7.6962460	0.0250811	0.0000000

Complex 33 ($X = F$, $Y = SO_2CN$)

C	5.4799358	0.2703577	0.0000000
C	4.8040398	0.2352866	1.2208496
C	3.4123827	0.1767145	1.1972360
C	2.6817725	0.1469231	0.0000000
C	3.4123827	0.1767145	-1.1972360
C	4.8040398	0.2352866	-1.2208496
H	5.3601910	0.2680679	2.1511202

H	2.8848258	0.1488261	2.1481097
H	2.8848258	0.1488261	-2.1481097
H	5.3601910	0.2680679	-2.1511202
Sn	0.4696413	0.1207645	0.0000000
H	0.2556639	-0.6882170	1.4639488
H	0.1878454	1.7819649	0.0000000
H	0.2556639	-0.6882170	-1.4639488
S	7.2141427	0.3234179	0.0000000
O	7.7061652	0.8182639	1.2533404
O	7.7061652	0.8182639	-1.2533404
C	7.5962623	-1.3972230	0.0000000
N	7.8789283	-2.5382535	0.0000000
Sn	-2.8900553	-0.0017580	0.0000000
C	-4.3174952	-0.0381603	1.5305229
C	-5.6818835	-0.0966358	1.2593387
H	-6.3913471	-0.1363536	2.0924561
C	-6.2724654	-0.1211844	0.0000000
C	-5.6818835	-0.0966358	-1.2593387
H	-6.3913471	-0.1363536	-2.0924561
C	-4.3174952	-0.0381603	-1.5305229
C	-3.9212266	0.0146466	-2.9897141
H	-4.5223582	-0.6743980	-3.5965154
H	-4.0684504	1.0191800	-3.4044730
H	-2.8692756	-0.2420352	-3.1379105
C	-3.9212266	0.0146466	2.9897141
H	-4.0684504	1.0191800	3.4044730
H	-4.5223582	-0.6743980	3.5965154
H	-2.8692756	-0.2420352	3.1379105
F	-7.6484711	-0.1953810	0.0000000

Complex 34 (X= F, Y=tBu)

C	4.2817705	0.0436058	0.0000000
C	3.5508319	0.0317584	1.1945916
C	2.1558065	0.0214280	1.1901570
C	1.4181515	0.0188628	0.0000000
C	2.1558065	0.0214280	-1.1901570
C	3.5508319	0.0317584	-1.1945916
H	4.0656403	0.0324226	2.1489775
H	1.6383419	0.0104698	2.1471169
H	1.6383419	0.0104698	-2.1471169
H	4.0656403	0.0324226	-2.1489775
Sn	-0.7470008	0.0440648	0.0000000
H	-1.1319308	-0.7571360	1.4304700
H	-1.1492779	1.6791148	0.0000000
H	-1.1319308	-0.7571360	-1.4304700
C	5.8032502	-0.0113763	0.0000000
C	6.3903320	0.6741601	1.2355161
H	6.1268045	0.1540668	2.1576745
H	7.4818172	0.6835358	1.1672800
H	6.0416012	1.7069146	1.3141225
C	6.3903320	0.6741601	-1.2355161
H	7.4818172	0.6835358	-1.1672800
H	6.1268045	0.1540668	-2.1576745
H	6.0416012	1.7069146	-1.3141225
C	6.2322572	-1.4835742	0.0000000
H	5.8442926	-1.9964486	-0.8835757
H	7.3241203	-1.5688036	0.0000000
H	5.8442926	-1.9964486	0.8835757
Sn	-4.4598888	-0.0001496	0.0000000
C	-5.9116534	0.0001320	1.5233013
C	-7.2786990	-0.0196404	1.2582055
H	-7.9881770	-0.0386646	2.0930163

C	-7.8716076	-0.0272603	0.0000000
C	-7.2786990	-0.0196404	-1.2582055
H	-7.9881770	-0.0386646	-2.0930163
C	-5.9116534	0.0001320	-1.5233013
C	-5.5189208	0.0346077	-2.9849437
H	-6.0945927	-0.6902407	-3.5755174
H	-5.7031404	1.0231620	-3.4242688
H	-4.4581201	-0.1878961	-3.1277455
C	-5.5189208	0.0346077	2.9849437
H	-5.7031404	1.0231620	3.4242688
H	-6.0945927	-0.6902407	3.5755174
H	-4.4581201	-0.1878961	3.1277455
F	-9.2522425	-0.0597469	0.0000000

Complex 35 (X= F, Y=NH₂)

C	6.1992207	-0.0429459	0.0000000
C	5.4845130	-0.0490142	1.1998686
C	4.0908743	-0.0488939	1.1919686
C	3.3542840	-0.0485198	0.0000000
C	4.0908743	-0.0488939	-1.1919686
C	5.4845130	-0.0490142	-1.1998686
H	6.0255731	-0.0548985	2.1430262
H	3.5732171	-0.0558506	2.1484023
H	3.5732171	-0.0558506	-2.1484023
H	6.0255731	-0.0548985	-2.1430262
Sn	1.1948413	-0.0014426	0.0000000
H	0.7862698	-0.7954160	1.4280923
H	0.7969000	1.6353258	0.0000000
H	0.7862698	-0.7954160	-1.4280923
N	7.6059469	-0.1099530	0.0000000
H	8.0129765	0.3049547	-0.8281307

H	8.0129765	0.3049547	0.8281307
Sn	-2.5535111	-0.0127345	0.0000000
C	-4.0068009	-0.0133840	1.5231254
C	-5.3738158	-0.0342195	1.2582530
H	-6.0832920	-0.0548830	2.0930606
C	-5.9666207	-0.0419573	0.0000000
C	-5.3738158	-0.0342195	-1.2582530
H	-6.0832920	-0.0548830	-2.0930606
C	-4.0068009	-0.0133840	-1.5231254
C	-3.6134755	0.0258871	-2.9844455
H	-4.2099121	-0.6743019	-3.5842192
H	-3.7686125	1.0245587	-3.4116230
H	-2.5593571	-0.2245501	-3.1302296
C	-3.6134755	0.0258871	2.9844455
H	-3.7686125	1.0245587	3.4116230
H	-4.2099121	-0.6743019	3.5842192
H	-2.5593571	-0.2245501	3.1302296
F	-7.3473771	-0.0777500	0.0000000

Complex 36 ($X = F$, $Y = NMe_2$)

C	4.9405293	-0.1579210	0.0000000
C	4.2078335	-0.1471502	1.1993300
C	2.8142194	-0.1478313	1.1869940
C	2.0727049	-0.1470543	0.0000000
C	2.8142194	-0.1478313	-1.1869940
C	4.2078335	-0.1471502	-1.1993300
H	4.7157208	-0.1455478	2.1551916
H	2.3009766	-0.1487653	2.1461874
H	2.3009766	-0.1487653	-2.1461874
H	4.7157208	-0.1455478	-2.1551916
Sn	-0.0852140	-0.0978776	0.0000000

H	-0.4938767	-0.8921961	1.4280233
H	-0.4864821	1.5383088	0.0000000
H	-0.4938767	-0.8921961	-1.4280233
N	6.3436525	-0.2075821	0.0000000
C	6.9979706	0.2410156	1.2130353
H	6.7421252	-0.4066505	2.0513209
H	8.0767935	0.1807262	1.0703522
H	6.7344904	1.2750919	1.4834769
C	6.9979706	0.2410156	-1.2130353
H	6.7421252	-0.4066505	-2.0513209
H	6.7344904	1.2750919	-1.4834769
H	8.0767935	0.1807262	-1.0703522
Sn	-3.8419062	-0.1065766	0.0000000
C	-5.2942378	-0.0539586	1.5229562
C	-6.6611465	-0.0202092	1.2583418
H	-7.3712513	-0.0098973	2.0929106
C	-7.2537195	-0.0043370	0.0000000
C	-6.6611465	-0.0202092	-1.2583418
H	-7.3712513	-0.0098973	-2.0929106
C	-5.2942378	-0.0539586	-1.5229562
C	-4.8999544	-0.0411856	-2.9846975
H	-5.4701941	-0.7789692	-3.5644088
H	-5.0889386	0.9388060	-3.4410422
H	-3.8378880	-0.2611879	-3.1219170
C	-4.8999544	-0.0411856	2.9846975
H	-5.0889386	0.9388060	3.4410422
H	-5.4701941	-0.7789692	3.5644088
H	-3.8378880	-0.2611879	3.1219170
F	-8.6348500	0.0188584	0.0000000

Complex 37 ($X=CF_3$, $Y=H$)

C	7.3436824	-0.0721938	0.0000000
C	6.6420404	-0.0644473	1.2040792
C	5.2468368	-0.0454135	1.1974153
C	4.5182454	-0.0341973	0.0000000
C	5.2468368	-0.0454135	-1.1974153
C	6.6420404	-0.0644473	-1.2040792
H	7.1808475	-0.0741899	2.1464983
H	4.7207730	-0.0467291	2.1491439
H	4.7207730	-0.0467291	-2.1491439
H	7.1808475	-0.0741899	-2.1464983
Sn	2.3575180	0.0285636	0.0000000
H	1.9409266	-0.7626938	1.4270548
H	1.9672125	1.6667672	0.0000000
H	1.9409266	-0.7626938	-1.4270548
H	8.4285013	-0.0885846	0.0000000
Sn	-1.3960663	0.0356355	0.0000000
C	-2.8511669	0.0426776	1.5175961
C	-4.2154287	0.0302382	1.2555427
H	-4.8883029	0.0082372	2.1181523
C	-4.8450064	0.0373311	0.0000000
C	-4.2154287	0.0302382	-1.2555427
H	-4.8883029	0.0082372	-2.1181523
C	-2.8511669	0.0426776	-1.5175961
C	-2.4508957	0.0710615	-2.9774980
H	-3.1162325	-0.5499001	-3.5907683
H	-2.4999164	1.0897753	-3.3798733
H	-1.4277961	-0.2827471	-3.1285128
C	-2.4508957	0.0710615	2.9774980
H	-2.4999164	1.0897753	3.3798733
H	-3.1162325	-0.5499001	3.5907683
H	-1.4277961	-0.2827471	3.1285128

C	-6.3304608	-0.0651734	0.0000000
F	-6.7780711	-1.3538789	0.0000000
F	-6.9144628	0.5069962	1.0780384
F	-6.9144628	0.5069962	-1.0780384

Complex 38 ($X=CF_3$, $Y=F$)

C	7.2715713	-0.0286923	0.0000000
C	6.6015421	-0.0241679	1.2116364
C	5.2058268	-0.0110908	1.1960134
C	4.4752792	-0.0030777	0.0000000
C	5.2058268	-0.0110908	-1.1960134
C	6.6015421	-0.0241679	-1.2116364
H	7.1658405	-0.0322911	2.1371506
H	4.6839415	-0.0144497	2.1495648
H	4.6839415	-0.0144497	-2.1495648
H	7.1658405	-0.0322911	-2.1371506
Sn	2.3097139	0.0505894	0.0000000
H	1.9141317	-0.7448322	1.4303649
H	1.9265784	1.6900159	0.0000000
H	1.9141317	-0.7448322	-1.4303649
F	8.6258158	-0.0425595	0.0000000
Sn	-1.3830287	0.0397551	0.0000000
C	-2.8350109	0.0289668	1.5192205
C	-4.1989029	0.0032334	1.2560372
H	-4.8722542	-0.0265566	2.1181264
C	-4.8275293	0.0045785	0.0000000
C	-4.1989029	0.0032334	-1.2560372
H	-4.8722542	-0.0265566	-2.1181264
C	-2.8350109	0.0289668	-1.5192205
C	-2.4356036	0.0585275	-2.9794189
H	-3.0928592	-0.5730969	-3.5905463

H	-2.4983253	1.0753453	-3.3845708
H	-1.4080391	-0.2820923	-3.1301248
C	-2.4356036	0.0585275	2.9794189
H	-2.4983253	1.0753453	3.3845708
H	-3.0928592	-0.5730969	3.5905463
H	-1.4080391	-0.2820923	3.1301248
C	-6.3118048	-0.1156054	0.0000000
F	-6.9020167	0.4498112	1.0779146
F	-6.9020167	0.4498112	-1.0779146
F	-6.7431369	-1.4096482	0.0000000

Complex 39 ($X=CF_3$, $Y=CF_3$)

C	6.5189987	-0.0062353	0.0000000
C	5.8248948	-0.0091348	1.2086734
C	4.4315118	-0.0028143	1.1957937
C	3.7005351	0.0021080	0.0000000
C	4.4315118	-0.0028143	-1.1957937
C	5.8248948	-0.0091348	-1.2086734
H	6.3689860	-0.0091026	2.1465064
H	3.9075077	-0.0078752	2.1484162
H	3.9075077	-0.0078752	-2.1484162
H	6.3689860	-0.0091026	-2.1465064
Sn	1.5253796	0.0546856	0.0000000
H	1.1645098	-0.7415610	1.4386967
H	1.1782778	1.7016987	0.0000000
H	1.1645098	-0.7415610	-1.4386967
C	8.0113673	-0.0669944	0.0000000
F	8.4651234	-1.3388368	0.0000000
F	8.5495153	0.5257658	1.0804845
F	8.5495153	0.5257658	-1.0804845
Sn	-2.0941921	0.0366298	0.0000000

C	-3.5423560	0.0323090	1.5195272
C	-4.9062103	0.0091833	1.2557352
H	-5.5793309	-0.0174241	2.1177437
C	-5.5349612	0.0112987	0.0000000
C	-4.9062103	0.0091833	-1.2557352
H	-5.5793309	-0.0174241	-2.1177437
C	-3.5423560	0.0323090	-1.5195272
C	-3.1416238	0.0647681	-2.9789467
H	-3.8030394	-0.5595630	-3.5927502
H	-3.1971830	1.0838030	-3.3793700
H	-2.1164596	-0.2827472	-3.1303171
C	-3.1416238	0.0647681	2.9789467
H	-3.1971830	1.0838030	3.3793700
H	-3.8030394	-0.5595630	3.5927502
H	-2.1164596	-0.2827472	3.1303171
C	-7.0204688	-0.1023744	0.0000000
F	-7.4562391	-1.3942554	0.0000000
F	-7.6076328	0.4655309	-1.0779688
F	-7.6076328	0.4655309	1.0779688

Complex 40 ($X=CF_3$, $Y=CN$)

C	6.9474952	-0.0596382	0.0000000
C	6.2496253	-0.0520433	1.2132204
C	4.8575828	-0.0339450	1.1966288
C	4.1266651	-0.0220278	0.0000000
C	4.8575828	-0.0339450	-1.1966288
C	6.2496253	-0.0520433	-1.2132204
H	6.8002431	-0.0617579	2.1479084
H	4.3320300	-0.0366605	2.1485505
H	4.3320300	-0.0366605	-2.1485505
H	6.8002431	-0.0617579	-2.1479084

Sn	1.9452163	0.0427534	0.0000000
H	1.6032137	-0.7528928	1.4440527
H	1.6248592	1.6951899	0.0000000
H	1.6032137	-0.7528928	-1.4440527
C	8.3778228	-0.0802269	0.0000000
N	9.5509601	-0.0975541	0.0000000
Sn	-1.6166044	0.0439716	0.0000000
C	-3.0611003	0.0432768	1.5207352
C	-4.4247103	0.0203551	1.2559160
H	-5.0978739	-0.0049749	2.1177538
C	-5.0529638	0.0214708	0.0000000
C	-4.4247103	0.0203551	-1.2559160
H	-5.0978739	-0.0049749	-2.1177538
C	-3.0611003	0.0432768	-1.5207352
C	-2.6596007	0.0801647	-2.9796454
H	-3.3296164	-0.5302916	-3.5978785
H	-2.7007094	1.1026224	-3.3729002
H	-1.6394345	-0.2806625	-3.1332841
C	-2.6596007	0.0801647	2.9796454
H	-2.7007094	1.1026224	3.3729002
H	-3.3296164	-0.5302916	3.5978785
H	-1.6394345	-0.2806625	3.1332841
C	-6.5386800	-0.0933182	0.0000000
F	-7.1256649	0.4742180	1.0779977
F	-7.1256649	0.4742180	-1.0779977
F	-6.9727392	-1.3854375	0.0000000

Complex 41 ($X=CF_3$, $Y=P(CN)_2$)

C	6.1900561	-0.3676764	0.0000000
C	5.4945504	-0.3343284	1.2117818
C	4.1025010	-0.2499479	1.1949897

C	3.3708706	-0.2086731	0.0000000
C	4.1025010	-0.2499479	-1.1949897
C	5.4945504	-0.3343284	-1.2117818
H	6.0286238	-0.3565254	2.1577344
H	3.5810032	-0.2197686	2.1490871
H	3.5810032	-0.2197686	-2.1490871
H	6.0286238	-0.3565254	-2.1577344
Sn	1.1870539	-0.0633696	0.0000000
H	0.8351472	-0.8501673	1.4467052
H	0.9409539	1.6012735	0.0000000
H	0.8351472	-0.8501673	-1.4467052
P	7.9812276	-0.6873538	0.0000000
C	8.4981094	0.3834341	1.3291381
N	8.8750385	0.9685612	2.2767517
C	8.4981094	0.3834341	-1.3291381
N	8.8750385	0.9685612	-2.2767517
Sn	-2.3306703	0.0374850	0.0000000
C	-3.7715788	0.0594717	1.5224333
C	-5.1350947	0.0659291	1.2561670
H	-5.8093067	0.0526686	2.1174061
C	-5.7623068	0.0812186	0.0000000
C	-5.1350947	0.0659291	-1.2561670
H	-5.8093067	0.0526686	-2.1174061
C	-3.7715788	0.0594717	-1.5224333
C	-3.3720630	0.0791782	-2.9822092
H	-4.0484266	-0.5324924	-3.5921802
H	-3.4066146	1.0976742	-3.3859275
H	-2.3553110	-0.2913125	-3.1348805
C	-3.3720630	0.0791782	2.9822092
H	-3.4066146	1.0976742	3.3859275
H	-4.0484266	-0.5324924	3.5921802

H	-2.3553110	-0.2913125	3.1348805
C	-7.2502839	-0.0030384	0.0000000
F	-7.7087091	-1.2864206	0.0000000
F	-7.8256740	0.5759027	1.0779813
F	-7.8256740	0.5759027	-1.0779813

Complex 42 ($X=CF_3$, $Y=SO_2CN$)

C	6.1516822	0.2447872	0.0000000
C	5.4760467	0.2151623	1.2207293
C	4.0842614	0.1678520	1.1981496
C	3.3552760	0.1447963	0.0000000
C	4.0842614	0.1678520	-1.1981496
C	5.4760467	0.2151623	-1.2207293
H	6.0325085	0.2427806	2.1507265
H	3.5563144	0.1441330	2.1486223
H	3.5563144	0.1441330	-2.1486223
H	6.0325085	0.2427806	-2.1507265
Sn	1.1545230	0.1343481	0.0000000
H	0.8995301	-0.6716631	1.4574019
H	0.8477276	1.7900905	0.0000000
H	0.8995301	-0.6716631	-1.4574019
S	7.8872015	0.2855962	0.0000000
O	8.3809939	0.7772995	1.2536307
O	8.3809939	0.7772995	-1.2536307
C	8.2535990	-1.4377543	0.0000000
N	8.5238795	-2.5818942	0.0000000
Sn	-2.2659716	0.0371605	0.0000000
C	-3.7004014	0.0163265	1.5235857
C	-5.0632927	-0.0239256	1.2565154
H	-5.7367144	-0.0568097	2.1177158
C	-5.6901097	-0.0304447	0.0000000

C	-5.0632927	-0.0239256	-1.2565154
H	-5.7367144	-0.0568097	-2.1177158
C	-3.7004014	0.0163265	-1.5235857
C	-3.2983110	0.0593940	-2.9819063
H	-3.9468118	-0.5762029	-3.5973574
H	-3.3735797	1.0780974	-3.3796046
H	-2.2666309	-0.2678539	-3.1330055
C	-3.2983110	0.0593940	2.9819063
H	-3.3735797	1.0780974	3.3796046
H	-3.9468118	-0.5762029	3.5973574
H	-2.2666309	-0.2678539	3.1330055
C	-7.1758234	-0.1570409	0.0000000
F	-7.5982786	-1.4520731	0.0000000
F	-7.7657656	0.4066241	1.0777428
F	-7.7657656	0.4066241	-1.0777428

Complex 43 ($X = CF_3$, $Y = tBu$)

C	4.9344512	0.0303722	0.0000000
C	4.2035015	0.0197984	1.1945770
C	2.8085478	0.0112879	1.1906866
C	2.0720714	0.0097276	0.0000000
C	2.8085478	0.0112879	-1.1906866
C	4.2035015	0.0197984	-1.1945770
H	4.7189605	0.0206298	2.1485433
H	2.2904312	0.0011461	2.1471304
H	2.2904312	0.0011461	-2.1471304
H	4.7189605	0.0206298	-2.1485433
Sn	-0.0871651	0.0488650	0.0000000
H	-0.4972440	-0.7472505	1.4263777
H	-0.4912415	1.6836930	0.0000000
H	-0.4972440	-0.7472505	-1.4263777

C	6.4559255	-0.0278672	0.0000000
C	7.0448007	0.6560782	1.2357062
H	6.7800665	0.1366384	2.1578739
H	8.1362969	0.6624791	1.1675372
H	6.6989881	1.6898072	1.3148039
C	7.0448007	0.6560782	-1.2357062
H	8.1362969	0.6624791	-1.1675372
H	6.7800665	0.1366384	-2.1578739
H	6.6989881	1.6898072	-1.3148039
C	6.8808455	-1.5014487	0.0000000
H	6.4915738	-2.0135763	-0.8834903
H	7.9723783	-1.5896247	0.0000000
H	6.4915738	-2.0135763	0.8834903
Sn	-3.8462327	0.0430385	0.0000000
C	-5.3020430	0.0461893	1.5173858
C	-6.6662783	0.0269688	1.2555066
H	-7.3390587	0.0020506	2.1181412
C	-7.2959169	0.0303649	0.0000000
C	-6.6662783	0.0269688	-1.2555066
H	-7.3390587	0.0020506	-2.1181412
C	-5.3020430	0.0461893	-1.5173858
C	-4.9018001	0.0804424	-2.9771424
H	-5.5692546	-0.5346352	-3.5940472
H	-4.9469718	1.1015527	-3.3740228
H	-3.8800159	-0.2763640	-3.1296299
C	-4.9018001	0.0804424	2.9771424
H	-4.9469718	1.1015527	3.3740228
H	-5.5692546	-0.5346352	3.5940472
H	-3.8800159	-0.2763640	3.1296299
C	-8.7804315	-0.0839089	0.0000000
F	-9.2171948	-1.3764067	0.0000000

F -9.3692452 0.4833546 1.0780219
F -9.3692452 0.4833546 -1.0780219

Complex 44 ($X=CF_3$, $Y=NH_2$)

C 6.8762238 -0.0598690 0.0000000
C 6.1613494 -0.0647151 1.1999585
C 4.7679689 -0.0585553 1.1925135
C 4.0326005 -0.0539054 0.0000000
C 4.7679689 -0.0585553 -1.1925135
C 6.1613494 -0.0647151 -1.1999585
H 6.7016684 -0.0739240 2.1434045
H 4.2500580 -0.0642771 2.1486991
H 4.2500580 -0.0642771 -2.1486991
H 6.7016684 -0.0739240 -2.1434045
Sn 1.8793107 0.0016560 0.0000000
H 1.4513312 -0.7898742 1.4239247
H 1.4678538 1.6354381 0.0000000
H 1.4513312 -0.7898742 -1.4239247
N 8.2819735 -0.1298822 0.0000000
H 8.6917413 0.2813080 -0.8285046
H 8.6917413 0.2813080 0.8285046
Sn -1.9191343 0.0119947 0.0000000
C -3.3768131 0.0238669 1.5167408
C -4.7412674 0.0122853 1.2554687
H -5.4140888 -0.0084407 2.1183015
C -5.3712071 0.0190090 0.0000000
C -4.7412674 0.0122853 -1.2554687
H -5.4140888 -0.0084407 -2.1183015
C -3.3768131 0.0238669 -1.5167408
C -2.9761405 0.0564516 -2.9765310
H -3.6429342 -0.5599691 -3.5929257

H	-3.0215560	1.0770677	-3.3747503
H	-1.9540952	-0.3001539	-3.1282425
C	-2.9761405	0.0564516	2.9765310
H	-3.0215560	1.0770677	3.3747503
H	-3.6429342	-0.5599691	3.5929257
H	-1.9540952	-0.3001539	3.1282425
C	-6.8563038	-0.0850047	0.0000000
F	-7.3029391	-1.3742852	0.0000000
F	-7.4414110	0.4863543	1.0780843
F	-7.4414110	0.4863543	-1.0780843

Complex 45 ($X=CF_3$, $Y=NMe_2$)

C	5.6170631	-0.1610145	0.0000000
C	4.8843088	-0.1493944	1.1994052
C	3.4909075	-0.1478079	1.1875583
C	2.7503632	-0.1456373	0.0000000
C	3.4909075	-0.1478079	-1.1875583
C	4.8843088	-0.1493944	-1.1994052
H	5.3922287	-0.1484055	2.1551531
H	2.9778418	-0.1474856	2.1466585
H	2.9778418	-0.1474856	-2.1466585
H	5.3922287	-0.1484055	-2.1551531
Sn	0.5981222	-0.0904620	0.0000000
H	0.1660932	-0.8817306	1.4229886
H	0.1832971	1.5425815	0.0000000
H	0.1660932	-0.8817306	-1.4229886
N	7.0190638	-0.2110226	0.0000000
C	7.6747856	0.2329806	1.2140443
H	7.4192372	-0.4176674	2.0501611
H	8.7534034	0.1726538	1.0703579
H	7.4119848	1.2661359	1.4882734

C 7.6747856 0.2329806 -1.2140443
H 7.4192372 -0.4176674 -2.0501611
H 7.4119848 1.2661359 -1.4882734
H 8.7534034 0.1726538 -1.0703579
Sn -3.2150302 -0.0740745 0.0000000
C -4.6727559 -0.0283805 1.5167918
C -6.0370677 -0.0123140 1.2552684
H -6.7098373 -0.0192069 2.1182638
C -6.6670236 0.0066494 0.0000000
C -6.0370677 -0.0123140 -1.2552684
H -6.7098373 -0.0192069 -2.1182638
C -4.6727559 -0.0283805 -1.5167918
C -4.2719873 -0.0001969 -2.9766012
H -4.9768779 -0.5649183 -3.6002730
H -4.2540476 1.0267550 -3.3603157
H -3.2739096 -0.4167119 -3.1353986
C -4.2719873 -0.0001969 2.9766012
H -4.2540476 1.0267550 3.3603157
H -4.9768779 -0.5649183 3.6002730
H -3.2739096 -0.4167119 3.1353986
C -8.1536772 -0.0697703 0.0000000
F -8.6245894 -1.3504996 0.0000000
F -8.7281020 0.5123194 1.0781206
F -8.7281020 0.5123194 -1.0781206

Complex 46 (X= CN, Y=H)

C 6.9545258 -0.0632594 0.0000000
C 6.2532041 -0.0542657 1.2042037
C 4.8581159 -0.0335414 1.1978491
C 4.1303954 -0.0216571 0.0000000
C 4.8581159 -0.0335414 -1.1978491

C	6.2532041	-0.0542657	-1.2042037
H	6.7920871	-0.0643893	2.1464840
H	4.3318075	-0.0342833	2.1493421
H	4.3318075	-0.0342833	-2.1493421
H	6.7920871	-0.0643893	-2.1464840
Sn	1.9731430	0.0378372	0.0000000
H	1.5496038	-0.7541675	1.4249162
H	1.5682869	1.6727247	0.0000000
H	1.5496038	-0.7541675	-1.4249162
H	8.0392937	-0.0816574	0.0000000
Sn	-1.8095327	0.0399013	0.0000000
C	-3.2623606	0.0234406	1.5242326
C	-4.6239201	-0.0175773	1.2630017
H	-5.3117505	-0.0491504	2.1161009
C	-5.2499854	-0.0351138	0.0000000
C	-4.6239201	-0.0175773	-1.2630017
H	-5.3117505	-0.0491504	-2.1161009
C	-3.2623606	0.0234406	-1.5242326
C	-2.8587002	0.0665113	-2.9823786
H	-3.5195855	-0.5517631	-3.6024890
H	-2.9117638	1.0889342	-3.3738172
H	-1.8335303	-0.2805888	-3.1336866
C	-2.8587002	0.0665113	2.9823786
H	-2.9117638	1.0889342	3.3738172
H	-3.5195855	-0.5517631	3.6024890
H	-1.8335303	-0.2805888	3.1336866
C	-6.6787727	-0.0916439	0.0000000
N	-7.8537686	-0.1354504	0.0000000

Complex 47 (X= CN, Y=F)

C	6.8904712	-0.0375616	0.0000000
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C	6.2203871	-0.0327370	1.2117186
C	4.8248703	-0.0181443	1.1965007
C	4.0954522	-0.0086053	0.0000000
C	4.8248703	-0.0181443	-1.1965007
C	6.2203871	-0.0327370	-1.2117186
H	6.7843166	-0.0414605	2.1374299
H	4.3026904	-0.0216468	2.1498517
H	4.3026904	-0.0216468	-2.1498517
H	6.7843166	-0.0414605	-2.1374299
Sn	1.9348864	0.0530750	0.0000000
H	1.5251857	-0.7382784	1.4286735
H	1.5482465	1.6919887	0.0000000
H	1.5251857	-0.7382784	-1.4286735
F	8.2441877	-0.0520834	0.0000000
Sn	-1.8015162	0.0396855	0.0000000
C	-3.2516330	0.0122659	1.5252201
C	-4.6127707	-0.0397849	1.2633187
H	-5.3009083	-0.0764446	2.1159535
C	-5.2380756	-0.0625534	0.0000000
C	-4.6127707	-0.0397849	-1.2633187
H	-5.3009083	-0.0764446	-2.1159535
C	-3.2516330	0.0122659	-1.5252201
C	-2.8469110	0.0595103	-2.9830397
H	-3.5021926	-0.5633374	-3.6045656
H	-2.9070928	1.0817896	-3.3738962
H	-1.8188820	-0.2796110	-3.1333303
C	-2.8469110	0.0595103	2.9830397
H	-2.9070928	1.0817896	3.3738962
H	-3.5021926	-0.5633374	3.6045656
H	-1.8188820	-0.2796110	3.1333303
C	-6.6664985	-0.1286888	0.0000000

N -7.8412730 -0.1794986 0.0000000

Complex 48 (X= CN, Y=CF₃)

C 6.1286486 0.0029246 0.0000000

C 5.4347217 0.0028068 1.2087051

C 4.0414587 0.0116485 1.1962286

C 3.3113267 0.0162572 0.0000000

C 4.0414587 0.0116485 -1.1962286

C 5.4347217 0.0028068 -1.2087051

H 5.9790111 0.0026508 2.1463774

H 3.5173254 0.0091583 2.1486074

H 3.5173254 0.0091583 -2.1486074

H 5.9790111 0.0026508 -2.1463774

Sn 1.1404642 0.0558489 0.0000000

H 0.7692368 -0.7429935 1.4346752

H 0.7647749 1.6963216 0.0000000

H 0.7692368 -0.7429935 -1.4346752

C 7.6210917 -0.0625377 0.0000000

F 8.0703051 -1.3357262 0.0000000

F 8.1604644 0.5286369 1.0804895

F 8.1604644 0.5286369 -1.0804895

Sn -2.5167515 0.0255911 0.0000000

C -3.9629046 0.0038715 1.5263037

C -5.3236753 -0.0515260 1.2632180

H -6.0114484 -0.0858768 2.1158858

C -5.9485694 -0.0784769 0.0000000

C -5.3236753 -0.0515260 -1.2632180

H -6.0114484 -0.0858768 -2.1158858

C -3.9629046 0.0038715 -1.5263037

C -3.5592171 0.0668249 -2.9835239

H -4.2322778 -0.5259687 -3.6152701

H	-3.5937509	1.0978901	-3.3534787
H	-2.5406376	-0.2956475	-3.1433939
C	-3.5592171	0.0668249	2.9835239
H	-3.5937509	1.0978901	3.3534787
H	-4.2322778	-0.5259687	3.6152701
H	-2.5406376	-0.2956475	3.1433939
C	-7.3767802	-0.1524111	0.0000000
N	-8.5511224	-0.2107425	0.0000000

Complex 49 (X= CN, Y=CN)

C	6.5659940	-0.0431653	0.0000000
C	5.8682209	-0.0349480	1.2132409
C	4.4762919	-0.0171717	1.1970550
C	3.7460263	-0.0070408	0.0000000
C	4.4762919	-0.0171717	-1.1970550
C	5.8682209	-0.0349480	-1.2132409
H	6.4186974	-0.0452668	2.1479806
H	3.9510339	-0.0190258	2.1489639
H	3.9510339	-0.0190258	-2.1489639
H	6.4186974	-0.0452668	-2.1479806
Sn	1.5695338	0.0480434	0.0000000
H	1.2104476	-0.7506324	1.4377532
H	1.2269450	1.6956939	0.0000000
H	1.2104476	-0.7506324	-1.4377532
C	7.9963285	-0.0648158	0.0000000
N	9.1694493	-0.0818822	0.0000000
Sn	-2.0358885	0.0416773	0.0000000
C	-3.4790376	0.0175512	1.5272423
C	-4.8398035	-0.0355842	1.2634781
H	-5.5279959	-0.0719958	2.1156939
C	-5.4641754	-0.0599048	0.0000000

C -4.8398035 -0.0355842 -1.2634781
H -5.5279959 -0.0719958 -2.1156939
C -3.4790376 0.0175512 -1.5272423
C -3.0743002 0.0711850 -2.9844687
H -3.7415366 -0.5330244 -3.6113888
H -3.1166108 1.0982856 -3.3644147
H -2.0527338 -0.2847478 -3.1395165
C -3.0743002 0.0711850 2.9844687
H -3.1166108 1.0982856 3.3644147
H -3.7415366 -0.5330244 3.6113888
H -2.0527338 -0.2847478 3.1395165
C -6.8925894 -0.1308573 0.0000000
N -8.0669700 -0.1869981 0.0000000

Complex 50 ($X=CN$, $Y=P(CN)_2$)

C 5.8052863 -0.3712354 0.0000000
C 5.1094938 -0.3373629 1.2115542
C 3.7177611 -0.2510134 1.1953434
C 2.9871914 -0.2082066 0.0000000
C 3.7177611 -0.2510134 -1.1953434
C 5.1094938 -0.3373629 -1.2115542
H 5.6432313 -0.3610736 2.1575071
H 3.1961801 -0.2208608 2.1491461
H 3.1961801 -0.2208608 -2.1491461
H 5.6432313 -0.3610736 -2.1575071
Sn 0.8108765 -0.0568336 0.0000000
H 0.4355240 -0.8413787 1.4415712
H 0.5497767 1.6053237 0.0000000
H 0.4355240 -0.8413787 -1.4415712
P 7.5966654 -0.6926952 0.0000000
C 8.1131235 0.3771056 1.3298914

N	8.4893898	0.9600659	2.2788948
C	8.1131235	0.3771056	-1.3298914
N	8.4893898	0.9600659	-2.2788948
Sn	-2.7617340	0.0577382	0.0000000
C	-4.2030647	0.0563159	1.5276840
C	-5.5644837	0.0283204	1.2634864
H	-6.2532108	0.0041909	2.1156218
C	-6.1888941	0.0159934	0.0000000
C	-5.5644837	0.0283204	-1.2634864
H	-6.2532108	0.0041909	-2.1156218
C	-4.2030647	0.0563159	-1.5276840
C	-3.7975357	0.0995113	-2.9848527
H	-4.4810548	-0.4873113	-3.6106317
H	-3.8130660	1.1272439	-3.3650005
H	-2.7858820	-0.2834162	-3.1402865
C	-3.7975357	0.0995113	2.9848527
H	-3.8130660	1.1272439	3.3650005
H	-4.4810548	-0.4873113	3.6106317
H	-2.7858820	-0.2834162	3.1402865
C	-7.6184200	-0.0283067	0.0000000
N	-8.7935601	-0.0624516	0.0000000

Complex 51 ($X=CN$, $Y=SO_2CN$)

C	5.7815659	0.2661314	0.0000000
C	5.1060894	0.2346334	1.2206581
C	3.7144052	0.1820770	1.1987728
C	2.9860944	0.1552438	0.0000000
C	3.7144052	0.1820770	-1.1987728
C	5.1060894	0.2346334	-1.2206581
H	5.6627528	0.2635919	2.1505954
H	3.1871572	0.1566638	2.1493932

H	3.1871572	0.1566638	-2.1493932
H	5.6627528	0.2635919	-2.1505954
Sn	0.7930479	0.1318053	0.0000000
H	0.5083352	-0.6764512	1.4491416
H	0.4493027	1.7791276	0.0000000
H	0.5083352	-0.6764512	-1.4491416
S	7.5182138	0.3082901	0.0000000
O	8.0105553	0.8004765	1.2538432
O	8.0105553	0.8004765	-1.2538432
C	7.8832799	-1.4149473	0.0000000
N	8.1521872	-2.5593004	0.0000000
Sn	-2.6999093	0.0257986	0.0000000
C	-4.1350422	-0.0164345	1.5293141
C	-5.4947710	-0.0853170	1.2637535
H	-6.1826252	-0.1292794	2.1156072
C	-6.1178259	-0.1166462	0.0000000
C	-5.4947710	-0.0853170	-1.2637535
H	-6.1826252	-0.1292794	-2.1156072
C	-4.1350422	-0.0164345	-1.5293141
C	-3.7314634	0.0390943	-2.9865323
H	-4.3778148	-0.5931272	-3.6073035
H	-3.8096647	1.0607978	-3.3750319
H	-2.6987013	-0.2837020	-3.1389738
C	-3.7314634	0.0390943	2.9865323
H	-3.8096647	1.0607978	3.3750319
H	-4.3778148	-0.5931272	3.6073035
H	-2.6987013	-0.2837020	3.1389738
C	-7.5454872	-0.2052201	0.0000000
N	-8.7188943	-0.2763293	0.0000000

Complex 52 (X= CN, Y=tBu)

C	4.5428397	0.0355951	0.0000000
C	3.8120134	0.0239260	1.1945346
C	2.4171586	0.0159992	1.1909883
C	1.6810812	0.0157798	0.0000000
C	2.4171586	0.0159992	-1.1909883
C	3.8120134	0.0239260	-1.1945346
H	4.3271424	0.0235190	2.1486072
H	1.8999087	0.0056827	2.1477334
H	1.8999087	0.0056827	-2.1477334
H	4.3271424	0.0235190	-2.1486072
Sn	-0.4749071	0.0535399	0.0000000
H	-0.8956076	-0.7417434	1.4238881
H	-0.8950380	1.6845762	0.0000000
H	-0.8956076	-0.7417434	-1.4238881
C	6.0643562	-0.0176127	0.0000000
C	6.6506397	0.6688406	1.2354186
H	6.3889666	0.1482257	2.1578115
H	7.7419924	0.6799415	1.1661658
H	6.3004133	1.7010798	1.3143681
C	6.6506397	0.6688406	-1.2354186
H	7.7419924	0.6799415	-1.1661658
H	6.3889666	0.1482257	-2.1578115
H	6.3004133	1.7010798	-1.3143681
C	6.4950470	-1.4892968	0.0000000
H	6.1081110	-2.0028875	-0.8836329
H	7.5869649	-1.5724431	0.0000000
H	6.1081110	-2.0028875	0.8836329
Sn	-4.2693147	0.0351359	0.0000000
C	-5.7223119	0.0185796	1.5241506
C	-7.0836457	-0.0293482	1.2629873
H	-7.7713802	-0.0621449	2.1160806

C	-7.7095325	-0.0518065	0.0000000
C	-7.0836457	-0.0293482	-1.2629873
H	-7.7713802	-0.0621449	-2.1160806
C	-5.7223119	0.0185796	-1.5241506
C	-5.3178915	0.0704866	-2.9818409
H	-5.9832670	-0.5371059	-3.6078638
H	-5.3626454	1.0966228	-3.3646365
H	-4.2951557	-0.2829202	-3.1355836
C	-5.3178915	0.0704866	2.9818409
H	-5.3626454	1.0966228	3.3646365
H	-5.9832670	-0.5371059	3.6078638
H	-4.2951557	-0.2829202	3.1355836
C	-9.1377899	-0.1176818	0.0000000
N	-10.3125886	-0.1692932	0.0000000

Complex 53 ($X=CN$, $Y=NH_2$)

C	6.4785502	-0.0493162	0.0000000
C	5.7636372	-0.0532205	1.2000600
C	4.3703643	-0.0482201	1.1927687
C	3.6354890	-0.0450006	0.0000000
C	4.3703643	-0.0482201	-1.1927687
C	5.7636372	-0.0532205	-1.2000600
H	6.3036068	-0.0615683	2.1437002
H	3.8525636	-0.0536957	2.1489058
H	3.8525636	-0.0536957	-2.1489058
H	6.3036068	-0.0615683	-2.1437002
Sn	1.4849071	0.0047782	0.0000000
H	1.0493527	-0.7877817	1.4215571
H	1.0599202	1.6354271	0.0000000
H	1.0493527	-0.7877817	-1.4215571
N	7.8835699	-0.1211864	0.0000000

H	8.2949265	0.2875982	-0.8288411
H	8.2949265	0.2875982	0.8288411
Sn	-2.3406634	0.0118300	0.0000000
C	-3.7950954	0.0017215	1.5244169
C	-5.1567452	-0.0387366	1.2633136
H	-5.8452742	-0.0680046	2.1160859
C	-5.7825745	-0.0572526	0.0000000
C	-5.1567452	-0.0387366	-1.2633136
H	-5.8452742	-0.0680046	-2.1160859
C	-3.7950954	0.0017215	-1.5244169
C	-3.3903475	0.0506943	-2.9824497
H	-4.0519554	-0.5626261	-3.6070242
H	-3.4402388	1.0753753	-3.3689400
H	-2.3656074	-0.2977735	-3.1344488
C	-3.3903475	0.0506943	2.9824497
H	-3.4402388	1.0753753	3.3689400
H	-4.0519554	-0.5626261	3.6070242
H	-2.3656074	-0.2977735	3.1344488
C	-7.2111767	-0.1124062	0.0000000
N	-8.3863965	-0.1543978	0.0000000

Complex 54 ($X=CN$, $Y=NMe_2$)

C	5.2162050	-0.1585091	0.0000000
C	4.4834601	-0.1457643	1.1994940
C	3.0901723	-0.1426348	1.1878686
C	2.3501428	-0.1399708	0.0000000
C	3.0901723	-0.1426348	-1.1878686
C	4.4834601	-0.1457643	-1.1994940
H	4.9914438	-0.1454971	2.1552176
H	2.5771938	-0.1413364	2.1469124
H	2.5771938	-0.1413364	-2.1469124

H	4.9914438	-0.1454971	-2.1552176
Sn	0.2009821	-0.0828162	0.0000000
H	-0.2423628	-0.8729326	1.4202640
H	-0.2231415	1.5480034	0.0000000
H	-0.2423628	-0.8729326	-1.4202640
N	6.6173348	-0.2106348	0.0000000
C	7.2749399	0.2286904	1.2147679
H	7.0185695	-0.4233626	2.0496223
H	8.3532520	0.1661867	1.0701211
H	7.0146780	1.2616592	1.4918005
C	7.2749399	0.2286904	-1.2147679
H	7.0185695	-0.4233626	-2.0496223
H	7.0146780	1.2616592	-1.4918005
H	8.3532520	0.1661867	-1.0701211
Sn	-3.6438613	-0.0636412	0.0000000
C	-5.0993848	-0.0411177	1.5237586
C	-6.4615142	-0.0536245	1.2628496
H	-7.1495008	-0.0705214	2.1163211
C	-7.0882464	-0.0592455	0.0000000
C	-6.4615142	-0.0536245	-1.2628496
H	-7.1495008	-0.0705214	-2.1163211
C	-5.0993848	-0.0411177	-1.5237586
C	-4.6939305	0.0007328	-2.9815187
H	-5.4019346	-0.5495150	-3.6140488
H	-4.6653429	1.0323142	-3.3508810
H	-3.6989597	-0.4222209	-3.1421010
C	-4.6939305	0.0007328	2.9815187
H	-4.6653429	1.0323142	3.3508810
H	-5.4019346	-0.5495150	3.6140488
H	-3.6989597	-0.4222209	3.1421010
C	-8.5175719	-0.0875942	0.0000000

N -9.6934016 -0.1077034 0.0000000

Complex 55 ($X= P(CN)_2$, $Y=H$)

C 7.6359225 0.1065467 0.0000000

C 6.9347996 0.0903911 1.2041639

C 5.5399242 0.0619757 1.1981289

C 4.8126674 0.0487681 0.0000000

C 5.5399242 0.0619757 -1.1981289

C 6.9347996 0.0903911 -1.2041639

H 7.4739248 0.0981043 2.1462111

H 5.0142973 0.0425088 2.1497089

H 5.0142973 0.0425088 -2.1497089

H 7.4739248 0.0981043 -2.1462111

Sn 2.6576393 0.0278708 0.0000000

H 2.2529125 -0.7796651 1.4219036

H 2.1771623 1.6422335 0.0000000

H 2.2529125 -0.7796651 -1.4219036

H 8.7205998 0.1277013 0.0000000

Sn -1.1497104 -0.1224384 0.0000000

C -2.6046171 -0.1869883 1.5240607

C -3.9676278 -0.2701893 1.2628954

H -4.6392744 -0.3182901 2.1301174

C -4.5844574 -0.2898449 0.0000000

C -3.9676278 -0.2701893 -1.2628954

H -4.6392744 -0.3182901 -2.1301174

C -2.6046171 -0.1869883 -1.5240607

C -2.2049658 -0.1242258 -2.9822496

H -2.8505963 -0.7544679 -3.6066950

H -2.2852560 0.8989989 -3.3664822

H -1.1712242 -0.4439933 -3.1355878

C -2.2049658 -0.1242258 2.9822496

H	-2.2852560	0.8989989	3.3664822
H	-2.8505963	-0.7544679	3.6066950
H	-1.1712242	-0.4439933	3.1355878
C	-6.9877431	0.3515805	1.3139748
N	-7.4637229	0.9078578	2.2344627
C	-6.9877431	0.3515805	-1.3139748
N	-7.4637229	0.9078578	-2.2344627
P	-6.3514854	-0.6880316	0.0000000

Complex 56 ($X = P(CN)_2$, $Y = F$)

C	7.5969406	0.0819381	0.0000000
C	6.9268499	0.0686134	1.2115119
C	5.5315079	0.0441502	1.1966668
C	4.8021883	0.0327962	0.0000000
C	5.5315079	0.0441502	-1.1966668
C	6.9268499	0.0686134	-1.2115119
H	7.4913821	0.0753681	2.1367798
H	5.0102045	0.0266523	2.1500667
H	5.0102045	0.0266523	-2.1500667
H	7.4913821	0.0753681	-2.1367798
Sn	2.6442650	0.0194452	0.0000000
H	2.2456238	-0.7874830	1.4229933
H	2.1783529	1.6372584	0.0000000
H	2.2456238	-0.7874830	-1.4229933
F	8.9500319	0.1041848	0.0000000
Sn	-1.1566086	-0.1203182	0.0000000
C	-2.6115378	-0.1792235	1.5236656
C	-3.9749245	-0.2578402	1.2626099
H	-4.6462505	-0.3035003	2.1301667
C	-4.5922158	-0.2756299	0.0000000
C	-3.9749245	-0.2578402	-1.2626099

H -4.6462505 -0.3035003 -2.1301667
C -2.6115378 -0.1792235 -1.5236656
C -2.2123622 -0.1171719 -2.9818922
H -2.8607813 -0.7447905 -3.6059798
H -2.2894460 0.9065347 -3.3653701
H -1.1798632 -0.4404556 -3.1359988
C -2.2123622 -0.1171719 2.9818922
H -2.2894460 0.9065347 3.3653701
H -2.8607813 -0.7447905 3.6059798
H -1.1798632 -0.4404556 3.1359988
C -6.9935240 0.3728827 1.3141136
N -7.4679655 0.9306732 2.2344650
C -6.9935240 0.3728827 -1.3141136
N -7.4679655 0.9306732 -2.2344650
P -6.3607805 -0.6684937 0.0000000

Complex 57 ($X = P(CN)_2$, $Y = CF_3$)

C 6.8113665 0.0728355 0.0000000
C 6.1178475 0.0513867 1.2086618
C 4.7249277 0.0203484 1.1965416
C 3.9954585 0.0057457 0.0000000
C 4.7249277 0.0203484 -1.1965416
C 6.1178475 0.0513867 -1.2086618
H 6.6617636 0.0660727 2.1463588
H 4.2012665 0.0019359 2.1489129
H 4.2012665 0.0019359 -2.1489129
H 6.6617636 0.0660727 -2.1463588
Sn 1.8279846 -0.0029291 0.0000000
H 1.4592037 -0.8097016 1.4308481
H 1.4036166 1.6257399 0.0000000
H 1.4592037 -0.8097016 -1.4308481

C	8.3054461	0.0541901	0.0000000
F	8.7936077	-1.2043644	0.0000000
F	8.8255319	0.6619644	1.0805040
F	8.8255319	0.6619644	-1.0805040
Sn	-1.8553446	-0.1179997	0.0000000
C	-3.3049362	-0.1721648	1.5251237
C	-4.6679791	-0.2507391	1.2628042
H	-5.3392419	-0.2949285	2.1302271
C	-5.2847064	-0.2698850	0.0000000
C	-4.6679791	-0.2507391	-1.2628042
H	-5.3392419	-0.2949285	-2.1302271
C	-3.3049362	-0.1721648	-1.5251237
C	-2.9044859	-0.1040291	-2.9824086
H	-3.5715405	-0.7039885	-3.6138634
H	-2.9511498	0.9263627	-3.3522965
H	-1.8819335	-0.4552803	-3.1415109
C	-2.9044859	-0.1040291	2.9824086
H	-2.9511498	0.9263627	3.3522965
H	-3.5715405	-0.7039885	3.6138634
H	-1.8819335	-0.4552803	3.1415109
C	-7.6844942	0.3776194	1.3146319
N	-8.1567055	0.9352714	2.2362082
C	-7.6844942	0.3776194	-1.3146319
N	-8.1567055	0.9352714	-2.2362082
P	-7.0535773	-0.6635925	0.0000000

Complex 58 ($X = P(CN)_2$, $Y = CN$)

C	7.2517067	0.0671567	0.0000000
C	6.5541129	0.0526303	1.2131843
C	5.1623580	0.0277315	1.1974474
C	4.4328781	0.0164066	0.0000000

C	5.1623580	0.0277315	-1.1974474
C	6.5541129	0.0526303	-1.2131843
H	7.1043724	0.0602309	2.1479353
H	4.6375727	0.0099737	2.1493430
H	4.6375727	0.0099737	-2.1493430
H	7.1043724	0.0602309	-2.1479353
Sn	2.2604145	0.0043034	0.0000000
H	1.9106514	-0.8044054	1.4345066
H	1.8488653	1.6359741	0.0000000
H	1.9106514	-0.8044054	-1.4345066
C	8.6820461	0.0930404	0.0000000
N	9.8550423	0.1150338	0.0000000
Sn	-1.3797069	-0.1179684	0.0000000
C	-2.8262599	-0.1726400	1.5260680
C	-4.1889320	-0.2539583	1.2628812
H	-4.8603105	-0.2979365	2.1300116
C	-4.8052950	-0.2756783	0.0000000
C	-4.1889320	-0.2539583	-1.2628812
H	-4.8603105	-0.2979365	-2.1300116
C	-2.8262599	-0.1726400	-1.5260680
C	-2.4260044	-0.1022769	-2.9832360
H	-3.0859979	-0.7108986	-3.6136898
H	-2.4845929	0.9269330	-3.3547202
H	-1.3995846	-0.4424191	-3.1414934
C	-2.4260044	-0.1022769	2.9832360
H	-2.4845929	0.9269330	3.3547202
H	-3.0859979	-0.7108986	3.6136898
H	-1.3995846	-0.4424191	3.1414934
C	-7.2063581	0.3605807	1.3154077
N	-7.6776683	0.9161026	2.2387147
C	-7.2063581	0.3605807	-1.3154077

N -7.6776683 0.9161026 -2.2387147
P -6.5726687 -0.6775641 0.0000000

Complex 59 ($X=P(CN)_2$, $Y=P(CN)_2$)

C 6.4716336 -0.4669845 0.0000000
C 5.7773845 -0.4115726 1.2115885
C 4.3892771 -0.2804437 1.1958410
C 3.6615342 -0.2127635 0.0000000
C 4.3892771 -0.2804437 -1.1958410
C 5.7773845 -0.4115726 -1.2115885
H 6.3099469 -0.4526293 2.1575627
H 3.8689181 -0.2341751 2.1495740
H 3.8689181 -0.2341751 -2.1495740
H 6.3099469 -0.4526293 -2.1575627
Sn 1.4967255 0.0107922 0.0000000
H 1.0791974 -0.7563155 1.4388549
H 1.2710101 1.6782196 0.0000000
H 1.0791974 -0.7563155 -1.4388549
P 8.2540274 -0.8377410 0.0000000
C 8.7967163 0.2194231 1.3294166
N 9.1854808 0.7956922 2.2774432
C 8.7967163 0.2194231 -1.3294166
N 9.1854808 0.7956922 -2.2774432
Sn -2.1043965 0.2370804 0.0000000
C -3.5491967 0.2850664 1.5267351
C -4.9141819 0.3030414 1.2631269
H -5.5874622 0.2975264 2.1297922
C -5.5303025 0.2972901 0.0000000
C -4.9141819 0.3030414 -1.2631269
H -5.5874622 0.2975264 -2.1297922
C -3.5491967 0.2850664 -1.5267351

C	-3.1473643	0.3024435	-2.9855304
H	-3.8287949	-0.2998628	-3.5982309
H	-3.1694667	1.3230826	-3.3845196
H	-2.1342981	-0.0784640	-3.1356022
C	-3.1473643	0.3024435	2.9855304
H	-3.1694667	1.3230826	3.3845196
H	-3.8287949	-0.2998628	3.5982309
H	-2.1342981	-0.0784640	3.1356022
P	-7.3244002	0.5579693	0.0000000
C	-7.8741505	-0.5268421	1.3152791
N	-8.2999215	-1.1179017	2.2386833
C	-7.8741505	-0.5268421	-1.3152791
N	-8.2999215	-1.1179017	-2.2386833

Complex 60 ($X=P(CN)_2$, $Y=SO_2CN$)

C	6.4657289	0.1493782	0.0000000
C	5.7894135	0.1494168	1.2204502
C	4.3967919	0.1590447	1.1990153
C	3.6686060	0.1632381	0.0000000
C	4.3967919	0.1590447	-1.1990153
C	5.7894135	0.1494168	-1.2204502
H	6.3461692	0.1543882	2.1506822
H	3.8691750	0.1582917	2.1495505
H	3.8691750	0.1582917	-2.1495505
H	6.3461692	0.1543882	-2.1506822
Sn	1.4819463	0.2199948	0.0000000
H	1.1470737	-0.5775297	1.4438712
H	1.1745850	1.8745221	0.0000000
H	1.1470737	-0.5775297	-1.4438712
S	8.2033874	0.1139259	0.0000000
O	8.7162251	0.5842973	1.2538187

O 8.7162251 0.5842973 -1.2538187
C 8.4896577 -1.6237584 0.0000000
N 8.7041725 -2.7795736 0.0000000
Sn -2.0549029 0.2381676 0.0000000
C -3.4956483 0.2494893 1.5277367
C -4.8604708 0.2298011 1.2632496
H -5.5335324 0.2068355 2.1296654
C -5.4759270 0.2067153 0.0000000
C -4.8604708 0.2298011 -1.2632496
H -5.5335324 0.2068355 -2.1296654
C -3.4956483 0.2494893 -1.5277367
C -3.0932166 0.2790969 -2.9860121
H -3.7329244 -0.3718859 -3.5935912
H -3.1807390 1.2924221 -3.3946389
H -2.0576547 -0.0376252 -3.1308885
C -3.0932166 0.2790969 2.9860121
H -3.1807390 1.2924221 3.3946389
H -3.7329244 -0.3718859 3.5935912
H -2.0576547 -0.0376252 3.1308885
P -7.2773323 0.4175663 0.0000000
C -7.7957756 -0.6817913 1.3153826
N -8.2048475 -1.2843396 2.2389504
C -7.7957756 -0.6817913 -1.3153826
N -8.2048475 -1.2843396 -2.2389504

Complex 61 ($X = P(CN)_2$, $Y = tBu$)

C 5.2051251 0.1007161 0.0000000
C 4.4754003 0.0679838 1.1947332
C 3.0815845 0.0186658 1.1915544
C 2.3469361 -0.0037565 0.0000000
C 3.0815845 0.0186658 -1.1915544

C	4.4754003	0.0679838	-1.1947332
H	4.9906450	0.0835531	2.1485242
H	2.5646190	-0.0062798	2.1481693
H	2.5646190	-0.0062798	-2.1481693
H	4.9906450	0.0835531	-2.1485242
Sn	0.1945353	-0.0325418	0.0000000
H	-0.2114316	-0.8405271	1.4212195
H	-0.2872439	1.5814094	0.0000000
H	-0.2114316	-0.8405271	-1.4212195
C	6.7272727	0.0919118	0.0000000
C	7.2923456	0.7948054	1.2360232
H	7.0433065	0.2674919	2.1581153
H	8.3830447	0.8355909	1.1695543
H	6.9138395	1.8171121	1.3140009
C	7.2923456	0.7948054	-1.2360232
H	8.3830447	0.8355909	-1.1695543
H	7.0433065	0.2674919	-2.1581153
H	6.9138395	1.8171121	-1.3140009
C	7.1997860	-1.3668898	0.0000000
H	6.8276600	-1.8914362	-0.8835379
H	8.2935575	-1.4188997	0.0000000
H	6.8276600	-1.8914362	0.8835379
Sn	-3.6233361	-0.1733482	0.0000000
C	-5.0799493	-0.2151181	1.5237457
C	-6.4438512	-0.2839221	1.2628078
H	-7.1156273	-0.3221919	2.1304871
C	-7.0609181	-0.2989836	0.0000000
C	-6.4438512	-0.2839221	-1.2628078
H	-7.1156273	-0.3221919	-2.1304871
C	-5.0799493	-0.2151181	-1.5237457
C	-4.6812518	-0.1480813	-2.9819756

H	-5.3418953	-0.7583523	-3.6105620
H	-4.7402605	0.8802327	-3.3563763
H	-3.6548122	-0.4880662	-3.1408835
C	-4.6812518	-0.1480813	2.9819756
H	-4.7402605	0.8802327	3.3563763
H	-5.3418953	-0.7583523	3.6105620
H	-3.6548122	-0.4880662	3.1408835
P	-8.8312971	-0.6808148	0.0000000
C	-9.4574945	0.3644893	1.3144174
N	-9.9280801	0.9246488	2.2353785
C	-9.4574945	0.3644893	-1.3144174
N	-9.9280801	0.9246488	-2.2353785

Complex 62 ($X=P(CN)_2$, $Y=NH_2$)

C	7.1498612	0.0832384	0.0000000
C	6.4356958	0.0533268	1.2001325
C	5.0432545	0.0102868	1.1932020
C	4.3095240	-0.0112283	0.0000000
C	5.0432545	0.0102868	-1.1932020
C	6.4356958	0.0533268	-1.2001325
H	6.9761332	0.0636718	2.1433650
H	4.5258753	-0.0139172	2.1493090
H	4.5258753	-0.0139172	-2.1493090
H	6.9761332	0.0636718	-2.1433650
Sn	2.1616248	-0.0340530	0.0000000
H	1.7463766	-0.8418221	1.4192570
H	1.6713917	1.5781211	0.0000000
H	1.7463766	-0.8418221	-1.4192570
N	8.5562222	0.0629739	0.0000000
H	8.9525582	0.4861872	-0.8288769
H	8.9525582	0.4861872	0.8288769

Sn	-1.6617400	-0.1517828	0.0000000
C	-3.1183727	-0.2041875	1.5232521
C	-4.4818230	-0.2808048	1.2627989
H	-5.1532780	-0.3246774	2.1304188
C	-5.0989764	-0.2984395	0.0000000
C	-4.4818230	-0.2808048	-1.2627989
H	-5.1532780	-0.3246774	-2.1304188
C	-3.1183727	-0.2041875	-1.5232521
C	-2.7178499	-0.1384209	-2.9809285
H	-3.3732284	-0.7544809	-3.6094260
H	-2.7822564	0.8884730	-3.3582277
H	-1.6889009	-0.4725523	-3.1362547
C	-2.7178499	-0.1384209	2.9809285
H	-2.7822564	0.8884730	3.3582277
H	-3.3732284	-0.7544809	3.6094260
H	-1.6889009	-0.4725523	3.1362547
C	-7.5000555	0.3510027	1.3139709
N	-7.9746439	0.9088938	2.2342191
C	-7.5000555	0.3510027	-1.3139709
N	-7.9746439	0.9088938	-2.2342191
P	-6.8668774	-0.6907876	0.0000000

Complex 63 ($X = P(CN)_2$, $Y = NMe_2$)

C	5.9028311	-0.0600996	0.0000000
C	5.1701311	-0.0833966	1.1994585
C	3.7783092	-0.1450563	1.1881507
C	3.0394956	-0.1756142	0.0000000
C	3.7783092	-0.1450563	-1.1881507
C	5.1701311	-0.0833966	-1.1994585
H	5.6772370	-0.0588556	2.1552220
H	3.2657215	-0.1679449	2.1470695

H	3.2657215	-0.1679449	-2.1470695
H	5.6772370	-0.0588556	-2.1552220
Sn	0.8928201	-0.2003327	0.0000000
H	0.4677580	-1.0062738	1.4175415
H	0.4014364	1.4115941	0.0000000
H	0.4677580	-1.0062738	-1.4175415
N	7.3047472	-0.0426284	0.0000000
C	7.9398754	0.4321438	1.2136297
H	7.7127389	-0.2266736	2.0514153
H	9.0201210	0.4183076	1.0701901
H	7.6325395	1.4538155	1.4842663
C	7.9398754	0.4321438	-1.2136297
H	9.0201210	0.4183076	-1.0701901
H	7.7127389	-0.2266736	-2.0514153
H	7.6325395	1.4538155	-1.4842663
Sn	-2.9794983	-0.2882038	0.0000000
C	-4.4392866	-0.2886419	1.5223902
C	-5.8046725	-0.3199301	1.2624695
H	-6.4767618	-0.3404729	2.1305070
C	-6.4226631	-0.3183245	0.0000000
C	-5.8046725	-0.3199301	-1.2624695
H	-6.4767618	-0.3404729	-2.1305070
C	-4.4392866	-0.2886419	-1.5223902
C	-4.0367827	-0.2324634	-2.9796326
H	-4.7317014	-0.7965157	-3.6145273
H	-4.0338270	0.8009899	-3.3442002
H	-3.0318258	-0.6307953	-3.1406750
C	-4.0367827	-0.2324634	2.9796326
H	-4.0338270	0.8009899	3.3442002
H	-4.7317014	-0.7965157	3.6145273
H	-3.0318258	-0.6307953	3.1406750

C	-8.8077201	0.3950149	1.3135636
N	-9.2713315	0.9648113	2.2321084
C	-8.8077201	0.3950149	-1.3135636
N	-9.2713315	0.9648113	-2.2321084
P	-8.2002133	-0.6625167	0.0000000

Complex 64 ($X=SO_2CN$, $Y=H$)

C	7.5593910	-0.3975219	0.0000000
C	6.8612209	-0.3339775	1.2043259
C	5.4725417	-0.2024847	1.1986347
C	4.7498252	-0.1316630	0.0000000
C	5.4725417	-0.2024847	-1.1986347
C	6.8612209	-0.3339775	-1.2043259
H	7.3973694	-0.3886850	2.1464861
H	4.9476176	-0.1627999	2.1498781
H	4.9476176	-0.1627999	-2.1498781
H	7.3973694	-0.3886850	-2.1464861
Sn	2.6122413	0.1030570	0.0000000
H	2.0988612	-0.6460984	1.4189329
H	2.3177251	1.7622984	0.0000000
H	2.0988612	-0.6460984	-1.4189329
H	8.6393123	-0.5003721	0.0000000
Sn	-1.2189870	0.3823826	0.0000000
C	-2.6697064	0.3642163	1.5294139
C	-4.0271844	0.3067071	1.2712708
H	-4.7131795	0.2749917	2.1212970
C	-4.6400351	0.2951042	0.0000000
C	-4.0271844	0.3067071	-1.2712708
H	-4.7131795	0.2749917	-2.1212970
C	-2.6697064	0.3642163	-1.5294139
C	-2.2551388	0.4162620	-2.9833840

H	-3.0460283	0.0381792	-3.6423680
H	-2.0356539	1.4437960	-3.2922475
H	-1.3507057	-0.1686301	-3.1701784
C	-2.2551388	0.4162620	2.9833840
H	-2.0356539	1.4437960	3.2922475
H	-3.0460283	0.0381792	3.6423680
H	-1.3507057	-0.1686301	3.1701784
S	-6.3403273	0.1013326	0.0000000
C	-6.5252359	-1.6654731	0.0000000
N	-6.6396307	-2.8364561	0.0000000
O	-6.9371534	0.5021791	-1.2480805
O	-6.9371534	0.5021791	1.2480805

Complex 65 ($X=SO_2CN$, $Y=F$)

C	7.5238299	-0.3323442	0.0000000
C	6.8560032	-0.2768670	1.2116412
C	5.4658282	-0.1567260	1.1972284
C	4.7403844	-0.0919486	0.0000000
C	5.4658282	-0.1567260	-1.1972284
C	6.8560032	-0.2768670	-1.2116412
H	7.4179140	-0.3288968	2.1370413
H	4.9454857	-0.1207379	2.1505297
H	4.9454857	-0.1207379	-2.1505297
H	7.4179140	-0.3288968	-2.1370413
Sn	2.5983194	0.1257046	0.0000000
H	2.0997097	-0.6291649	1.4202983
H	2.2976569	1.7830665	0.0000000
H	2.0997097	-0.6291649	-1.4202983
F	8.8714380	-0.4490418	0.0000000
Sn	-1.2295581	0.3722696	0.0000000
C	-2.6795407	0.3426180	1.5293883

C	-4.0366155	0.2736061	1.2710759
H	-4.7222028	0.2358603	2.1212056
C	-4.6492767	0.2568160	0.0000000
C	-4.0366155	0.2736061	-1.2710759
H	-4.7222028	0.2358603	-2.1212056
C	-2.6795407	0.3426180	-1.5293883
C	-2.2656600	0.3983495	-2.9833323
H	-3.0536847	0.0141297	-3.6421660
H	-2.0546426	1.4277156	-3.2920430
H	-1.3565906	-0.1792428	-3.1702741
C	-2.2656600	0.3983495	2.9833323
H	-2.0546426	1.4277156	3.2920430
H	-3.0536847	0.0141297	3.6421660
H	-1.3565906	-0.1792428	3.1702741
S	-6.3486173	0.0498945	0.0000000
C	-6.5177521	-1.7183014	0.0000000
N	-6.6222306	-2.8901913	0.0000000
O	-6.9481009	0.4463944	-1.2481723
O	-6.9481009	0.4463944	1.2481723

Complex 66 ($X=SO_2CN$, $Y=CF_3$)

C	6.7712900	-0.1521701	0.0000000
C	6.0788287	-0.1138399	1.2087205
C	4.6884553	-0.0267557	1.1972511
C	3.9615574	0.0193229	0.0000000
C	4.6884553	-0.0267557	-1.1972511
C	6.0788287	-0.1138399	-1.2087205
H	6.6217809	-0.1458927	2.1464318
H	4.1653888	-0.0006216	2.1496169
H	4.1653888	-0.0006216	-2.1496169
H	6.6217809	-0.1458927	-2.1464318

Sn	1.8066862	0.1840582	0.0000000
H	1.3545628	-0.5882936	1.4257406
H	1.4907109	1.8378222	0.0000000
H	1.3545628	-0.5882936	-1.4257406
C	8.2583797	-0.3007393	0.0000000
F	8.6342275	-1.5967642	0.0000000
F	8.8283735	0.2596282	1.0806683
F	8.8283735	0.2596282	-1.0806683
Sn	-1.9412904	0.3447794	0.0000000
C	-3.3874495	0.3132202	1.5302124
C	-4.7440538	0.2345942	1.2711271
H	-5.4298892	0.1946535	2.1208243
C	-5.3556236	0.2110278	0.0000000
C	-4.7440538	0.2345942	-1.2711271
H	-5.4298892	0.1946535	-2.1208243
C	-3.3874495	0.3132202	-1.5302124
C	-2.9736145	0.3807831	-2.9834589
H	-3.7566502	-0.0087637	-3.6449651
H	-2.7747781	1.4144135	-3.2858398
H	-2.0577680	-0.1850528	-3.1729841
C	-2.9736145	0.3807831	2.9834589
H	-2.7747781	1.4144135	3.2858398
H	-3.7566502	-0.0087637	3.6449651
H	-2.0577680	-0.1850528	3.1729841
S	-7.0537690	-0.0141700	0.0000000
C	-7.1987432	-1.7839802	0.0000000
N	-7.2859111	-2.9572388	0.0000000
O	-7.6569439	0.3759533	-1.2481208
O	-7.6569439	0.3759533	1.2481208

Complex 67 ($X=SO_2CN$, $Y=CN$)

C	7.2151368	-0.1735733	0.0000000
C	6.5181409	-0.1454326	1.2132589
C	5.1275351	-0.0865130	1.1980501
C	4.3998522	-0.0536402	0.0000000
C	5.1275351	-0.0865130	-1.1980501
C	6.5181409	-0.1454326	-1.2132589
H	7.0676851	-0.1711479	2.1480466
H	4.6026088	-0.0732355	2.1497432
H	4.6026088	-0.0732355	-2.1497432
H	7.0676851	-0.1711479	-2.1480466
Sn	2.2368671	0.0632363	0.0000000
H	1.8191613	-0.7191730	1.4305046
H	1.8993050	1.7125117	0.0000000
H	1.8191613	-0.7191730	-1.4305046
C	8.6444023	-0.2356718	0.0000000
N	9.8164672	-0.2865925	0.0000000
Sn	-1.4560505	0.1663103	0.0000000
C	-2.8976579	0.2324826	1.5311997
C	-4.2560866	0.2597128	1.2712531
H	-4.9430131	0.2708107	2.1209038
C	-4.8669121	0.2867255	0.0000000
C	-4.2560866	0.2597128	-1.2712531
H	-4.9430131	0.2708107	-2.1209038
C	-2.8976579	0.2324826	-1.5311997
C	-2.4792981	0.2562153	-2.9844033
H	-3.2992586	-0.0499171	-3.6449189
H	-2.1728023	1.2626938	-3.2879217
H	-1.6283288	-0.4031700	-3.1738501
C	-2.4792981	0.2562153	2.9844033
H	-2.1728023	1.2626938	3.2879217

H	-3.2992586	-0.0499171	3.6449189
H	-1.6283288	-0.4031700	3.1738501
S	-6.5785241	0.2069780	0.0000000
C	-6.8743966	-1.5435634	0.0000000
N	-7.0633704	-2.7047498	0.0000000
O	-7.1450744	0.6476885	-1.2483007
O	-7.1450744	0.6476885	1.2483007

Complex 68 ($X=SO_2CN$, $Y=P(CN)_2$)

C	6.4635235	-0.4252248	0.0000000
C	5.7679578	-0.3857144	1.2114675
C	4.3773562	-0.2855533	1.1964043
C	3.6492746	-0.2336797	0.0000000
C	4.3773562	-0.2855533	-1.1964043
C	5.7679578	-0.3857144	-1.2114675
H	6.3010709	-0.4144793	2.1575292
H	3.8562641	-0.2505929	2.1500130
H	3.8562641	-0.2505929	-2.1500130
H	6.3010709	-0.4144793	-2.1575292
Sn	1.4873996	-0.0515649	0.0000000
H	1.0575686	-0.8241597	1.4321788
H	1.2089408	1.6080218	0.0000000
H	1.0575686	-0.8241597	-1.4321788
P	8.2553662	-0.7518905	0.0000000
C	8.7715333	0.3185999	1.3289594
N	9.1474960	0.9052306	2.2758103
C	8.7715333	0.3185999	-1.3289594
N	9.1474960	0.9052306	-2.2758103
Sn	-2.1777761	0.1514468	0.0000000
C	-3.6169804	0.2367144	1.5316622
C	-4.9750405	0.2791330	1.2711940

H	-5.6618455	0.2983074	2.1207537
C	-5.5852626	0.3124213	0.0000000
C	-4.9750405	0.2791330	-1.2711940
H	-5.6618455	0.2983074	-2.1207537
C	-3.6169804	0.2367144	-1.5316622
C	-3.1991455	0.2589101	-2.9850326
H	-4.0206107	-0.0444327	-3.6449060
H	-2.8898713	1.2645036	-3.2887884
H	-2.3505257	-0.4032795	-3.1751388
C	-3.1991455	0.2589101	2.9850326
H	-2.8898713	1.2645036	3.2887884
H	-4.0206107	-0.0444327	3.6449060
H	-2.3505257	-0.4032795	3.1751388
S	-7.2980205	0.2494305	0.0000000
C	-7.6084369	-1.4983584	0.0000000
N	-7.8053252	-2.6582078	0.0000000
O	-7.8600691	0.6956156	-1.2482704
O	-7.8600691	0.6956156	1.2482704

Complex 69 ($X=SO_2CN$, $Y=SO_2CN$)

C	6.4431854	0.1394902	0.0000000
C	5.7672141	0.1467762	1.2204117
C	4.3749342	0.1726908	1.1997841
C	3.6482172	0.1867680	0.0000000
C	4.3749342	0.1726908	-1.1997841
C	5.7672141	0.1467762	-1.2204117
H	6.3242125	0.1457706	2.1504836
H	3.8479117	0.1780188	2.1503812
H	3.8479117	0.1780188	-2.1503812
H	6.3242125	0.1457706	-2.1504836
Sn	1.4716977	0.2772372	0.0000000

H	1.0953382	-0.5127176	1.4373028
H	1.1603391	1.9304862	0.0000000
H	1.0953382	-0.5127176	-1.4373028
S	8.1815451	0.0867127	0.0000000
O	8.6977189	0.5524563	1.2540111
O	8.6977189	0.5524563	-1.2540111
C	8.4480954	-1.6535286	0.0000000
N	8.6477745	-2.8119895	0.0000000
Sn	-2.1344897	0.3540871	0.0000000
C	-3.5707657	0.2931102	1.5329053
C	-4.9259228	0.1949291	1.2712823
H	-5.6112126	0.1405644	2.1205116
C	-5.5353389	0.1659346	0.0000000
C	-4.9259228	0.1949291	-1.2712823
H	-5.6112126	0.1405644	-2.1205116
C	-3.5707657	0.2931102	-1.5329053
C	-3.1594309	0.3572347	-2.9867507
H	-3.9264738	-0.0741206	-3.6405695
H	-3.0044714	1.3936333	-3.3047154
H	-2.2215902	-0.1734429	-3.1693056
C	-3.1594309	0.3572347	2.9867507
H	-3.0044714	1.3936333	3.3047154
H	-3.9264738	-0.0741206	3.6405695
H	-2.2215902	-0.1734429	3.1693056
S	-7.2337535	-0.0729418	0.0000000
C	-7.3603475	-1.8430095	0.0000000
N	-7.4366912	-3.0169416	0.0000000
O	-7.8375791	0.3139443	-1.2483817
O	-7.8375791	0.3139443	1.2483817

Complex 70 ($X=SO_2CN$, $Y=tBu$)

C	5.1734155	-0.0458834	0.0000000
C	4.4432071	-0.0216390	1.1947510
C	3.0497860	0.0371532	1.1919710
C	2.3164280	0.0718540	0.0000000
C	3.0497860	0.0371532	-1.1919710
C	4.4432071	-0.0216390	-1.1947510
H	4.9576870	-0.0467727	2.1487244
H	2.5323637	0.0517502	2.1484282
H	2.5323637	0.0517502	-2.1484282
H	4.9576870	-0.0467727	-2.1487244
Sn	0.1718183	0.1991663	0.0000000
H	-0.3051065	-0.5744577	1.4185124
H	-0.2110460	1.8404767	0.0000000
H	-0.3051065	-0.5744577	-1.4185124
C	6.6904766	-0.1726618	0.0000000
C	7.0490128	-1.6637492	0.0000000
H	6.6382174	-2.1585418	-0.8836429
H	8.1356260	-1.7986867	0.0000000
H	6.6382174	-2.1585418	0.8836429
C	7.3086219	0.4845324	1.2360000
H	8.3991802	0.4428934	1.1674635
H	7.0089794	1.5325937	1.3153757
H	7.0219602	-0.0230882	2.1582691
C	7.3086219	0.4845324	-1.2360000
H	7.0219602	-0.0230882	-2.1582691
H	7.0089794	1.5325937	-1.3153757
H	8.3991802	0.4428934	-1.1674635
Sn	-3.6902868	0.3088724	0.0000000
C	-5.1420002	0.3184352	1.5288939
C	-6.5003660	0.2855058	1.2712007

H	-7.1865103	0.2658297	2.1215752
C	-7.1135609	0.2851391	0.0000000
C	-6.5003660	0.2855058	-1.2712007
H	-7.1865103	0.2658297	-2.1215752
C	-5.1420002	0.3184352	-1.5288939
C	-4.7257338	0.3633230	-2.9824996
H	-5.5252203	0.0066990	-3.6430714
H	-4.4804511	1.3856659	-3.2890755
H	-3.8358626	-0.2431972	-3.1700570
C	-4.7257338	0.3633230	2.9824996
H	-4.4804511	1.3856659	3.2890755
H	-5.5252203	0.0066990	3.6430714
H	-3.8358626	-0.2431972	3.1700570
S	-8.8172683	0.1261675	0.0000000
C	-9.0374855	-1.6368087	0.0000000
N	-9.1732194	-2.8054883	0.0000000
O	-9.4057073	0.5391160	-1.2482000
O	-9.4057073	0.5391160	1.2482000

Complex 71 ($X = SO_2CN$, $Y = NH_2$)

C	7.1181237	-0.2592757	0.0000000
C	6.4041431	-0.2234246	1.2002465
C	5.0138415	-0.1375032	1.1936432
C	4.2819510	-0.0905634	0.0000000
C	5.0138415	-0.1375032	-1.1936432
C	6.4041431	-0.2234246	-1.2002465
H	6.9429407	-0.2648636	2.1435130
H	4.4965927	-0.1140918	2.1496187
H	4.4965927	-0.1140918	-2.1496187
H	6.9429407	-0.2648636	-2.1435130
Sn	2.1448509	0.0780362	0.0000000

H	1.6407994	-0.6842025	1.4158287
H	1.7819121	1.7247060	0.0000000
H	1.6407994	-0.6842025	-1.4158287
N	8.5155516	-0.4090077	0.0000000
H	8.9510146	-0.0274971	-0.8293158
H	8.9510146	-0.0274971	0.8293158
Sn	-1.7492576	0.2695055	0.0000000
C	-3.2023462	0.2945508	1.5286713
C	-4.5609115	0.2772540	1.2711717
H	-5.2471839	0.2661965	2.1215720
C	-5.1745426	0.2841447	0.0000000
C	-4.5609115	0.2772540	-1.2711717
H	-5.2471839	0.2661965	-2.1215720
C	-3.2023462	0.2945508	-1.5286713
C	-2.7852112	0.3335218	-2.9823110
H	-3.5965660	0.0070625	-3.6441730
H	-2.5053302	1.3485175	-3.2837221
H	-1.9162949	-0.3017749	-3.1734195
C	-2.7852112	0.3335218	2.9823110
H	-2.5053302	1.3485175	3.2837221
H	-3.5965660	0.0070625	3.6441730
H	-1.9162949	-0.3017749	3.1734195
S	-6.8790974	0.1414972	0.0000000
C	-7.1167807	-1.6194625	0.0000000
N	-7.2651692	-2.7866259	0.0000000
O	-7.4642590	0.5597775	-1.2480485
O	-7.4642590	0.5597775	1.2480485

Complex 72 ($X = SO_2CN$, $Y = NMe_2$)

C	5.8230823	-0.2622019	0.0000000
C	5.0911657	-0.2301977	1.1997948

C	3.6989220	-0.1870220	1.1887468
C	2.9612736	-0.1628782	0.0000000
C	3.6989220	-0.1870220	-1.1887468
C	5.0911657	-0.2301977	-1.1997948
H	5.5988149	-0.2437852	2.1553505
H	3.1855884	-0.1716026	2.1473986
H	3.1855884	-0.1716026	-2.1473986
H	5.5988149	-0.2437852	-2.1553505
Sn	0.8227854	-0.0273526	0.0000000
H	0.3306555	-0.7983969	1.4156847
H	0.4474768	1.6163046	0.0000000
H	0.3306555	-0.7983969	-1.4156847
N	7.2211428	-0.3502768	0.0000000
C	7.8909686	0.0697960	1.2148612
H	7.6152148	-0.5740176	2.0497505
H	8.9667820	-0.0248209	1.0705624
H	7.6615381	1.1102550	1.4905861
C	7.8909686	0.0697960	-1.2148612
H	8.9667820	-0.0248209	-1.0705624
H	7.6152148	-0.5740176	-2.0497505
H	7.6615381	1.1102550	-1.4905861
Sn	-3.0202035	0.1892534	0.0000000
C	-4.4702923	0.2508848	1.5290354
C	-5.8288320	0.2526865	1.2714584
H	-6.5154610	0.2542118	2.1215722
C	-6.4419211	0.2648313	0.0000000
C	-5.8288320	0.2526865	-1.2714584
H	-6.5154610	0.2542118	-2.1215722
C	-4.4702923	0.2508848	-1.5290354
C	-4.0508556	0.2972342	-2.9816103
H	-4.8600705	-0.0270540	-3.6470644

H -3.7731731 1.3147753 -3.2765661
H -3.1796459 -0.3344531 -3.1742925
C -4.0508556 0.2972342 2.9816103
H -3.7731731 1.3147753 3.2765661
H -4.8600705 -0.0270540 3.6470644
H -3.1796459 -0.3344531 3.1742925
S -8.1472791 0.1322385 0.0000000
C -8.3901449 -1.6279770 0.0000000
N -8.5375815 -2.7953574 0.0000000
O -8.7306350 0.5532145 -1.2479922
O -8.7306350 0.5532145 1.2479922

Complex 73 (X= tBu, Y= H)

C 8.7481920 -0.0631359 0.0000000
C 8.0464613 -0.0520044 1.2041691
C 6.6512660 -0.0271314 1.1966675
C 5.9217921 -0.0133433 0.0000000
C 6.6512660 -0.0271314 -1.1966675
C 8.0464613 -0.0520044 -1.2041691
H 8.5853026 -0.0644477 2.1466456
H 6.1242476 -0.0272870 2.1482351
H 6.1242476 -0.0272870 -2.1482351
H 8.5853026 -0.0644477 -2.1466456
Sn 3.7530518 0.0430159 0.0000000
H 3.3798811 -0.7517964 1.4376158
H 3.3860078 1.6870785 0.0000000
H 3.3798811 -0.7517964 -1.4376158
H 9.8329695 -0.0854037 0.0000000
Sn 0.1067964 0.0028787 0.0000000
C -1.3541585 0.0335697 1.5048163
C -2.7204604 0.0547316 1.2391906

H	-3.3626692	0.0357335	2.1248733
C	-3.3908557	0.0816276	0.0000000
C	-2.7204604	0.0547316	-1.2391906
H	-3.3626692	0.0357335	-2.1248733
C	-1.3541585	0.0335697	-1.5048163
C	-0.9635546	0.0442679	-2.9686411
H	-1.6293255	-0.5906690	-3.5690059
H	-1.0223754	1.0562896	-3.3884548
H	0.0607344	-0.3060255	-3.1225907
C	-0.9635546	0.0442679	2.9686411
H	-1.0223754	1.0562896	3.3884548
H	-1.6293255	-0.5906690	3.5690059
H	0.0607344	-0.3060255	3.1225907
C	-4.9237066	0.0061650	0.0000000
C	-5.3405485	-1.4704755	0.0000000
H	-4.9394297	-1.9749291	0.8830046
H	-6.4327939	-1.5778507	0.0000000
H	-4.9394297	-1.9749291	-0.8830046
C	-5.5454392	0.6854973	1.2264730
H	-6.6360463	0.6992049	1.1250885
H	-5.3121501	0.1635141	2.1549720
H	-5.1927365	1.7162038	1.3192389
C	-5.5454392	0.6854973	-1.2264730
H	-5.1927365	1.7162038	-1.3192389
H	-5.3121501	0.1635141	-2.1549720
H	-6.6360463	0.6992049	-1.1250885

Complex 74 ($X = tBu$, $Y = F$)

C	8.7030662	-0.0364043	0.0000000
C	8.0330127	-0.0353329	1.2116805
C	6.6369676	-0.0283863	1.1953557

C	5.9053768	-0.0229478	0.0000000
C	6.6369676	-0.0283863	-1.1953557
C	8.0330127	-0.0353329	-1.2116805
H	8.5974178	-0.0411848	2.1373526
H	6.1145550	-0.0352798	2.1489479
H	6.1145550	-0.0352798	-2.1489479
H	8.5974178	-0.0411848	-2.1373526
Sn	3.7318327	0.0275722	0.0000000
H	3.3704396	-0.7706371	1.4381597
H	3.3782057	1.6738177	0.0000000
H	3.3704396	-0.7706371	-1.4381597
F	10.0582771	-0.0439057	0.0000000
Sn	0.1038555	0.0111676	0.0000000
C	-1.3560956	0.0416203	1.5050945
C	-2.7225527	0.0545430	1.2390834
H	-3.3643469	0.0347585	2.1249066
C	-3.3934295	0.0755460	0.0000000
C	-2.7225527	0.0545430	-1.2390834
H	-3.3643469	0.0347585	-2.1249066
C	-1.3560956	0.0416203	-1.5050945
C	-0.9642153	0.0647963	-2.9682937
H	-1.6483593	-0.5392874	-3.5796004
H	-0.9914589	1.0849905	-3.3708934
H	0.0492758	-0.3132976	-3.1281706
C	-0.9642153	0.0647963	2.9682937
H	-0.9914589	1.0849905	3.3708934
H	-1.6483593	-0.5392874	3.5796004
H	0.0492758	-0.3132976	3.1281706
C	-4.9259641	-0.0096441	0.0000000
C	-5.3378539	-1.4878061	0.0000000
H	-4.9364584	-1.9912275	0.8834733

H	-6.4299708	-1.5972253	0.0000000
H	-4.9364584	-1.9912275	-0.8834733
C	-5.5515389	0.6652946	1.2268532
H	-6.6419832	0.6738544	1.1244106
H	-5.3174734	0.1423768	2.1546560
H	-5.2038840	1.6973136	1.3228611
C	-5.5515389	0.6652946	-1.2268532
H	-5.2038840	1.6973136	-1.3228611
H	-5.3174734	0.1423768	-2.1546560
H	-6.6419832	0.6738544	-1.1244106

Complex 75 ($X = tBu$, $Y = CF_3$)

C	7.9806923	0.0149343	0.0000000
C	7.2863307	0.0110530	1.2086470
C	5.8927604	0.0146756	1.1948409
C	5.1601725	0.0175953	0.0000000
C	5.8927604	0.0146756	-1.1948409
C	7.2863307	0.0110530	-1.2086470
H	7.8306521	0.0119947	2.1464422
H	5.3683532	0.0087800	2.1475600
H	5.3683532	0.0087800	-2.1475600
H	7.8306521	0.0119947	-2.1464422
Sn	2.9736360	0.0563865	0.0000000
H	2.6601503	-0.7443381	1.4483203
H	2.6498635	1.7087843	0.0000000
H	2.6601503	-0.7443381	-1.4483203
C	9.4723071	-0.0451777	0.0000000
F	9.9279780	-1.3169338	0.0000000
F	10.0114918	0.5475668	1.0805162
F	10.0114918	0.5475668	-1.0805162
Sn	-0.5565857	0.0039581	0.0000000

C	-2.0105854	0.0272667	1.5067661
C	-3.3766584	0.0397038	1.2391728
H	-4.0189982	0.0192392	2.1243590
C	-4.0468460	0.0628907	0.0000000
C	-3.3766584	0.0397038	-1.2391728
H	-4.0189982	0.0192392	-2.1243590
C	-2.0105854	0.0272667	-1.5067661
C	-1.6200474	0.0440112	-2.9702109
H	-2.2813676	-0.5939503	-3.5717208
H	-1.6858830	1.0565714	-3.3872166
H	-0.5938530	-0.2994978	-3.1257650
C	-1.6200474	0.0440112	2.9702109
H	-1.6858830	1.0565714	3.3872166
H	-2.2813676	-0.5939503	3.5717208
H	-0.5938530	-0.2994978	3.1257650
C	-5.5796274	-0.0174499	0.0000000
C	-5.9949620	-1.4945626	0.0000000
H	-5.5949005	-1.9990184	0.8835306
H	-7.0871842	-1.6015006	0.0000000
H	-5.5949005	-1.9990184	-0.8835306
C	-6.2025710	0.6601997	1.2266254
H	-7.2929432	0.6721430	1.1249190
H	-5.9695736	0.1377646	2.1549315
H	-5.8520793	1.6913726	1.3210181
C	-6.2025710	0.6601997	-1.2266254
H	-5.8520793	1.6913726	-1.3210181
H	-5.9695736	0.1377646	-2.1549315
H	-7.2929432	0.6721430	-1.1249190

Complex 76 (X= tBu, Y= CN)

C	8.3733221	-0.0177216	0.0000000
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C	7.6751409	-0.0162089	1.2132276
C	6.2826924	-0.0100016	1.1955009
C	5.5498030	-0.0049631	0.0000000
C	6.2826924	-0.0100016	-1.1955009
C	7.6751409	-0.0162089	-1.2132276
H	8.2261847	-0.0206882	2.1479415
H	5.7569733	-0.0167107	2.1476941
H	5.7569733	-0.0167107	-2.1476941
H	8.2261847	-0.0206882	-2.1479415
Sn	3.3552418	0.0436118	0.0000000
H	3.0640666	-0.7562438	1.4544371
H	3.0686342	1.7031157	0.0000000
H	3.0640666	-0.7562438	-1.4544371
C	9.8037197	-0.0252534	0.0000000
N	10.9769877	-0.0320072	0.0000000
Sn	-0.1085987	0.0197743	0.0000000
C	-1.5586951	0.0359611	1.5079246
C	-2.9247129	0.0385648	1.2395203
H	-3.5669302	0.0140180	2.1246705
C	-3.5946373	0.0564914	0.0000000
C	-2.9247129	0.0385648	-1.2395203
H	-3.5669302	0.0140180	-2.1246705
C	-1.5586951	0.0359611	-1.5079246
C	-1.1655755	0.0644753	-2.9701760
H	-1.8426693	-0.5460956	-3.5824534
H	-1.2038265	1.0851666	-3.3701424
H	-0.1481664	-0.3026326	-3.1296670
C	-1.1655755	0.0644753	2.9701760
H	-1.2038265	1.0851666	3.3701424
H	-1.8426693	-0.5460956	3.5824534
H	-0.1481664	-0.3026326	3.1296670

C	-5.1273977	-0.0253939	0.0000000
C	-5.5445109	-1.5018493	0.0000000
H	-5.1458737	-2.0073006	0.8835807
H	-6.6369112	-1.6061231	0.0000000
H	-5.1458737	-2.0073006	-0.8835807
C	-5.7498725	0.6528975	1.2265417
H	-6.8399676	0.6676904	1.1231980
H	-5.5196881	0.1291081	2.1547983
H	-5.3969063	1.6831595	1.3218676
C	-5.7498725	0.6528975	-1.2265417
H	-5.3969063	1.6831595	-1.3218676
H	-5.5196881	0.1291081	-2.1547983
H	-6.8399676	0.6676904	-1.1231980

Complex 77 ($X = tBu$, $Y = P(CN)_2$)

C	7.6497135	-0.3773868	0.0000000
C	6.9536298	-0.3547584	1.2118018
C	5.5601957	-0.2912478	1.1937465
C	4.8262739	-0.2611423	0.0000000
C	5.5601957	-0.2912478	-1.1937465
C	6.9536298	-0.3547584	-1.2118018
H	7.4886443	-0.3708145	2.1574276
H	5.0377012	-0.2705908	2.1480029
H	5.0377012	-0.2705908	-2.1480029
H	7.4886443	-0.3708145	-2.1574276
Sn	2.6255630	-0.1546824	0.0000000
H	2.3470365	-0.9513070	1.4599338
H	2.3976237	1.5145714	0.0000000
H	2.3470365	-0.9513070	-1.4599338
P	9.4425889	-0.6801834	0.0000000
C	9.9555645	0.3939070	1.3287172

N	10.3340717	0.9794493	2.2752605
C	9.9555645	0.3939070	-1.3287172
N	10.3340717	0.9794493	-2.2752605
Sn	-0.7798514	-0.1192724	0.0000000
C	-2.2211843	-0.0190004	1.5098584
C	-3.5841645	0.0660872	1.2398026
H	-4.2272457	0.0800102	2.1242735
C	-4.2510771	0.1245986	0.0000000
C	-3.5841645	0.0660872	-1.2398026
H	-4.2272457	0.0800102	-2.1242735
C	-2.2211843	-0.0190004	-1.5098584
C	-1.8277066	-0.0216907	-2.9722774
H	-2.5298516	-0.6104485	-3.5773861
H	-1.8241591	0.9951501	-3.3835775
H	-0.8267688	-0.4327318	-3.1282395
C	-1.8277066	-0.0216907	2.9722774
H	-1.8241591	0.9951501	3.3835775
H	-2.5298516	-0.6104485	3.5773861
H	-0.8267688	-0.4327318	3.1282395
C	-5.7859843	0.1299653	0.0000000
C	-6.3693494	0.8409755	1.2272413
H	-7.4566124	0.9192196	1.1229773
H	-6.1708862	0.3024070	2.1544245
H	-5.9572195	1.8486352	1.3259449
C	-6.3693494	0.8409755	-1.2272413
H	-5.9572195	1.8486352	-1.3259449
H	-6.1708862	0.3024070	-2.1544245
H	-7.4566124	0.9192196	-1.1229773
C	-6.2833823	-1.3213911	0.0000000
H	-5.9125159	-1.8478498	0.8833340
H	-7.3798271	-1.3658797	0.0000000

H -5.9125159 -1.8478498 -0.8833340

Complex 78 (X= tBu, Y= SO₂CN)

C 7.6046283 0.2926432 0.0000000
C 6.9288767 0.2537002 1.2208623
C 5.5373969 0.1898662 1.1968495
C 4.8062656 0.1585963 0.0000000
C 5.5373969 0.1898662 -1.1968495
C 6.9288767 0.2537002 -1.2208623
H 7.4852932 0.2883558 2.1508841
H 5.0096830 0.1598943 2.1477440
H 5.0096830 0.1598943 -2.1477440
H 7.4852932 0.2883558 -2.1508841
Sn 2.5881680 0.1387405 0.0000000
H 2.3903382 -0.6687013 1.4685429
H 2.3310268 1.8051263 0.0000000
H 2.3903382 -0.6687013 -1.4685429
S 9.3376634 0.3601559 0.0000000
O 9.8259528 0.8592204 1.2532403
O 9.8259528 0.8592204 -1.2532403
C 9.7368033 -1.3567755 0.0000000
N 10.0321493 -2.4945883 0.0000000
Sn -0.7329967 0.0384764 0.0000000
C -2.1704226 0.0389631 1.5125060
C -3.5355255 0.0237273 1.2401933
H -4.1781342 -0.0095961 2.1241634
C -4.2042014 0.0308429 0.0000000
C -3.5355255 0.0237273 -1.2401933
H -4.1781342 -0.0095961 -2.1241634
C -2.1704226 0.0389631 -1.5125060
C -1.7760763 0.0688217 -2.9740227

H	-2.4532801	-0.5411788	-3.5862936
H	-1.8135793	1.0894469	-3.3735815
H	-0.7590680	-0.2988974	-3.1335985
C	-1.7760763	0.0688217	2.9740227
H	-1.8135793	1.0894469	3.3735815
H	-2.4532801	-0.5411788	3.5862936
H	-0.7590680	-0.2988974	3.1335985
C	-5.7347790	-0.0858392	0.0000000
C	-6.1123025	-1.5729128	0.0000000
H	-5.7002338	-2.0675470	0.8834841
H	-7.2013582	-1.7063110	0.0000000
H	-5.7002338	-2.0675470	-0.8834841
C	-6.3739252	0.5757489	1.2269484
H	-7.4639503	0.5614969	1.1240967
H	-6.1301636	0.0575652	2.1548659
H	-6.0487156	1.6150363	1.3230744
C	-6.3739252	0.5757489	-1.2269484
H	-6.0487156	1.6150363	-1.3230744
H	-6.1301636	0.0575652	-2.1548659
H	-7.4639503	0.5614969	-1.1240967

Complex 79 ($X= tBu$, $Y= tBu$)

C	6.4491687	0.0487927	0.0000000
C	5.7181974	0.0373608	1.1946076
C	4.3231142	0.0264279	1.1899434
C	3.5851425	0.0230613	0.0000000
C	4.3231142	0.0264279	-1.1899434
C	5.7181974	0.0373608	-1.1946076
H	6.2332634	0.0382513	2.1489121
H	3.8055058	0.0148618	2.1469072
H	3.8055058	0.0148618	-2.1469072

H	6.2332634	0.0382513	-2.1489121
Sn	1.4178038	0.0492573	0.0000000
H	1.0423213	-0.7516920	1.4332639
H	1.0274726	1.6872817	0.0000000
H	1.0423213	-0.7516920	-1.4332639
C	7.9706222	-0.0108433	0.0000000
C	8.5607308	0.6721964	1.2355094
H	8.2920025	0.1554281	2.1580236
H	9.6524278	0.6736857	1.1692157
H	8.2191927	1.7075151	1.3123025
C	8.5607308	0.6721964	-1.2355094
H	9.6524278	0.6736857	-1.1692157
H	8.2920025	0.1554281	-2.1580236
H	8.2191927	1.7075151	-1.3123025
C	8.3933656	-1.4849502	0.0000000
H	8.0027307	-1.9959769	-0.8835030
H	9.4848084	-1.5754632	0.0000000
H	8.0027307	-1.9959769	0.8835030
Sn	-2.2635167	0.0134777	0.0000000
C	-3.7266532	0.0441611	1.5042603
C	-5.0933084	0.0543955	1.2389790
H	-5.7347340	0.0344224	2.1251639
C	-5.7645945	0.0728478	0.0000000
C	-5.0933084	0.0543955	-1.2389790
H	-5.7347340	0.0344224	-2.1251639
C	-3.7266532	0.0441611	-1.5042603
C	-3.3350299	0.0702139	-2.9675886
H	-4.0192779	-0.5321817	-3.5808044
H	-3.3615222	1.0914344	-3.3678199
H	-2.3215554	-0.3077423	-3.1282140
C	-3.3350299	0.0702139	2.9675886

H	-3.3615222	1.0914344	3.3678199
H	-4.0192779	-0.5321817	3.5808044
H	-2.3215554	-0.3077423	3.1282140
C	-7.2966986	-0.0194423	0.0000000
C	-7.9259421	0.6521606	1.2267273
H	-9.0164810	0.6543323	1.1243012
H	-7.6881129	0.1308247	2.1544364
H	-7.5840611	1.6861639	1.3220187
C	-7.9259421	0.6521606	-1.2267273
H	-7.6881129	0.1308247	-2.1544364
H	-9.0164810	0.6543323	-1.1243012
H	-7.5840611	1.6861639	-1.3220187
C	-7.7013590	-1.4996200	0.0000000
H	-8.7929119	-1.6145371	0.0000000
H	-7.2974601	-2.0011744	-0.8833736
H	-7.2974601	-2.0011744	0.8833736

Complex 80 (X= tBu, Y= NH₂)

C	8.3151867	-0.0125970	0.0000000
C	7.6011580	-0.0291759	1.2002080
C	6.2077040	-0.0468532	1.1919806
C	5.4716602	-0.0556192	0.0000000
C	6.2077040	-0.0468532	-1.1919806
C	7.6011580	-0.0291759	-1.2002080
H	8.1420767	-0.0290982	2.1436095
H	5.6891175	-0.0620787	2.1480316
H	5.6891175	-0.0620787	-2.1480316
H	8.1420767	-0.0290982	-2.1436095
Sn	3.3096955	-0.0419754	0.0000000
N	9.7232470	-0.0597995	0.0000000
H	10.1229090	0.3630580	-0.8276979

H	10.1229090	0.3630580	0.8276979
H	2.9322702	-0.8425255	1.4332912
H	2.8971361	1.5917551	0.0000000
H	2.9322702	-0.8425255	-1.4332912
Sn	-0.3718934	-0.1198783	0.0000000
C	-1.8328584	-0.0418140	1.5039379
C	-3.1978843	0.0249790	1.2391402
H	-3.8407125	0.0292896	2.1247011
C	-3.8671315	0.0741729	0.0000000
C	-3.1978843	0.0249790	-1.2391402
H	-3.8407125	0.0292896	-2.1247011
C	-1.8328584	-0.0418140	-1.5039379
C	-1.4431849	-0.0504131	-2.9683391
H	-2.0865618	-0.7216033	-3.5532752
H	-1.5366215	0.9490756	-3.4117033
H	-0.4079573	-0.3704642	-3.1150118
C	-1.4431849	-0.0504131	2.9683391
H	-1.5366215	0.9490756	3.4117033
H	-2.0865618	-0.7216033	3.5532752
H	-0.4079573	-0.3704642	3.1150118
C	-5.4015145	0.0458597	0.0000000
C	-6.0022661	0.7423933	1.2271558
H	-7.0916859	0.7920922	1.1250107
H	-5.7873492	0.2095066	2.1538092
H	-5.6157153	1.7603579	1.3247090
C	-6.0022661	0.7423933	-1.2271558
H	-5.6157153	1.7603579	-1.3247090
H	-5.7873492	0.2095066	-2.1538092
H	-7.0916859	0.7920922	-1.1250107
C	-5.8639987	-1.4173405	0.0000000
H	-5.4790460	-1.9340050	0.8832451

H -6.9591720 -1.4900201 0.0000000
H -5.4790460 -1.9340050 -0.8832451

Complex 81 (X= tBu, Y= NMe₂)

C 7.1178086 -0.1694573 0.0000000
C 6.3854807 -0.1601807 1.1994607
C 4.9919280 -0.1618621 1.1868638
C 4.2505883 -0.1611301 0.0000000
C 4.9919280 -0.1618621 -1.1868638
C 6.3854807 -0.1601807 -1.1994607
H 6.8934024 -0.1582304 2.1552877
H 4.4781442 -0.1633579 2.1459030
H 4.4781442 -0.1633579 -2.1459030
H 6.8934024 -0.1582304 -2.1552877
Sn 2.0907471 -0.1090043 0.0000000
N 8.5216258 -0.2146888 0.0000000
C 9.1716968 0.2409318 -1.2127706
H 10.2511196 0.1885975 -1.0715175
H 8.9194983 -0.4071184 -2.0518494
H 8.8995777 1.2734101 -1.4810165
C 9.1716968 0.2409318 1.2127706
H 8.8995777 1.2734101 1.4810165
H 8.9194983 -0.4071184 2.0518494
H 10.2511196 0.1885975 1.0715175
H 1.6954469 -0.9027944 1.4322791
H 1.7049193 1.5310985 0.0000000
H 1.6954469 -0.9027944 -1.4322791
Sn -1.6101780 -0.1144719 0.0000000
C -3.0724615 -0.0413664 1.5039255
C -4.4379027 0.0156193 1.2390793
H -5.0802314 0.0152614 2.1249664

C	-5.1076583	0.0594387	0.0000000
C	-4.4379027	0.0156193	-1.2390793
H	-5.0802314	0.0152614	-2.1249664
C	-3.0724615	-0.0413664	-1.5039255
C	-2.6821573	-0.0376644	-2.9679743
H	-3.3577283	-0.6624023	-3.5681686
H	-2.7251048	0.9748783	-3.3885816
H	-1.6635706	-0.4042026	-3.1219482
C	-2.6821573	-0.0376644	2.9679743
H	-2.7251048	0.9748783	3.3885816
H	-3.3577283	-0.6624023	3.5681686
H	-1.6635706	-0.4042026	3.1219482
C	-6.6419140	0.0231968	0.0000000
C	-7.2461730	0.7178717	1.2266242
H	-8.3360476	0.7600006	1.1250854
H	-7.0266972	0.1893274	2.1548044
H	-6.8667304	1.7389044	1.3204655
C	-7.2461730	0.7178717	-1.2266242
H	-7.0266972	0.1893274	-2.1548044
H	-8.3360476	0.7600006	-1.1250854
H	-6.8667304	1.7389044	-1.3204655
C	-7.0973295	-1.4420222	0.0000000
H	-6.7097445	-1.9567478	0.8831420
H	-8.1921001	-1.5207099	0.0000000
H	-6.7097445	-1.9567478	-0.8831420

Complex 82 ($X=NH_2$, $Y=H$)

C	7.0724730	-0.0633598	0.0000000
C	6.3705099	-0.0563947	1.2040803
C	4.9750611	-0.0383382	1.1963573
C	4.2446641	-0.0272277	0.0000000

C	4.9750611	-0.0383382	-1.1963573
C	6.3705099	-0.0563947	-1.2040803
H	6.9095698	-0.0663585	2.1465314
H	4.4484318	-0.0417248	2.1482028
H	4.4484318	-0.0417248	-2.1482028
H	6.9095698	-0.0663585	-2.1465314
Sn	2.0728183	0.0262472	0.0000000
H	1.7059949	-0.7686101	1.4389507
H	1.7106120	1.6714615	0.0000000
H	1.7059949	-0.7686101	-1.4389507
H	8.1574420	-0.0792221	0.0000000
Sn	-1.5673289	-0.0323186	0.0000000
C	-3.0192291	-0.0246165	1.5163483
C	-4.3832120	-0.0380576	1.2459613
H	-5.0654024	-0.0627973	2.1095758
C	-5.0255450	-0.0391453	0.0000000
C	-4.3832120	-0.0380576	-1.2459613
H	-5.0654024	-0.0627973	-2.1095758
C	-3.0192291	-0.0246165	-1.5163483
C	-2.6276339	0.0151258	-2.9787038
H	-3.2684631	-0.6369830	-3.5880779
H	-2.7187621	1.0279864	-3.3917008
H	-1.5917043	-0.2993865	-3.1330320
C	-2.6276339	0.0151258	2.9787038
H	-2.7187621	1.0279864	3.3917008
H	-3.2684631	-0.6369830	3.5880779
H	-1.5917043	-0.2993865	3.1330320
N	-6.4610666	-0.1375502	0.0000000
H	-6.8371951	0.3307123	0.8182707
H	-6.8371951	0.3307123	-0.8182707

Complex 83 ($X= NH_2$, $Y= F$)

C	7.0017448	-0.0560217	0.0000000
C	6.3316720	-0.0535322	1.2116852
C	4.9355309	-0.0442011	1.1949864
C	4.2034367	-0.0379414	0.0000000
C	4.9355309	-0.0442011	-1.1949864
C	6.3316720	-0.0535322	-1.2116852
H	6.8958980	-0.0606235	2.1374972
H	4.4128653	-0.0502035	2.1485971
H	4.4128653	-0.0502035	-2.1485971
H	6.8958980	-0.0606235	-2.1374972
Sn	2.0257526	0.0099258	0.0000000
H	1.6832374	-0.7891141	1.4428423
H	1.6845120	1.6591049	0.0000000
H	1.6832374	-0.7891141	-1.4428423
F	8.3573784	-0.0664102	0.0000000
Sn	-1.5561168	-0.0267381	0.0000000
C	-3.0042559	-0.0195468	1.5172469
C	-4.3680566	-0.0371210	1.2461997
H	-5.0503249	-0.0638483	2.1095432
C	-5.0101551	-0.0402371	0.0000000
C	-4.3680566	-0.0371210	-1.2461997
H	-5.0503249	-0.0638483	-2.1095432
C	-3.0042559	-0.0195468	-1.5172469
C	-2.6119559	0.0241973	-2.9791117
H	-3.2417850	-0.6386988	-3.5880379
H	-2.7190767	1.0350034	-3.3930342
H	-1.5709876	-0.2737015	-3.1322106
C	-2.6119559	0.0241973	2.9791117
H	-2.7190767	1.0350034	3.3930342
H	-3.2417850	-0.6386988	3.5880379

H	-1.5709876	-0.2737015	3.1322106
N	-6.4448547	-0.1432306	0.0000000
H	-6.8236100	0.3221644	0.8186347
H	-6.8236100	0.3221644	-0.8186347

Complex 84 ($X=NH_2$, $Y=CF_3$)

C	6.2543734	0.0013602	0.0000000
C	5.5596870	-0.0083973	1.2085773
C	4.1659548	-0.0183244	1.1942975
C	3.4323576	-0.0236343	0.0000000
C	4.1659548	-0.0183244	-1.1942975
C	5.5596870	-0.0083973	-1.2085773
H	6.1039278	-0.0006643	2.1465655
H	3.6420281	-0.0282222	2.1472365
H	3.6420281	-0.0282222	-2.1472365
H	6.1039278	-0.0006643	-2.1465655
Sn	1.2417172	0.0038015	0.0000000
H	0.9396410	-0.8025487	1.4485815
H	0.9254535	1.6577694	0.0000000
H	0.9396410	-0.8025487	-1.4485815
C	7.7465807	-0.0461825	0.0000000
F	8.2138177	-1.3139810	0.0000000
F	8.2813588	0.5511375	1.0803501
F	8.2813588	0.5511375	-1.0803501
Sn	-2.2653692	-0.0206007	0.0000000
C	-3.7089794	-0.0220633	1.5183901
C	-5.0724685	-0.0463150	1.2461773
H	-5.7542575	-0.0766864	2.1094918
C	-5.7145235	-0.0525853	0.0000000
C	-5.0724685	-0.0463150	-1.2461773
H	-5.7542575	-0.0766864	-2.1094918

C -3.7089794 -0.0220633 -1.5183901
C -3.3178712 0.0210127 -2.9804158
H -3.9426766 -0.6494561 -3.5859213
H -3.4342261 1.0295234 -3.3972515
H -2.2748009 -0.2688574 -3.1336872
C -3.3178712 0.0210127 2.9804158
H -3.4342261 1.0295234 3.3972515
H -3.9426766 -0.6494561 3.5859213
H -2.2748009 -0.2688574 3.1336872
N -7.1479244 -0.1631769 0.0000000
H -7.5305588 0.2984762 0.8188212
H -7.5305588 0.2984762 -0.8188212

Complex 85 ($X = NH_2$, $Y = CN$)

C 6.6645779 -0.0400015 0.0000000
C 5.9662310 -0.0402417 1.2131715
C 4.5737165 -0.0364130 1.1950975
C 3.8401789 -0.0318170 0.0000000
C 4.5737165 -0.0364130 -1.1950975
C 5.9662310 -0.0402417 -1.2131715
H 6.5171635 -0.0444365 2.1479381
H 4.0478823 -0.0448328 2.1474126
H 4.0478823 -0.0448328 -2.1474126
H 6.5171635 -0.0444365 -2.1479381
Sn 1.6398342 0.0184610 0.0000000
H 1.3684585 -0.7824721 1.4587546
H 1.3754473 1.6826413 0.0000000
H 1.3684585 -0.7824721 -1.4587546
C 8.0949529 -0.0428899 0.0000000
N 9.2683005 -0.0444113 0.0000000
Sn -1.7799214 -0.0147781 0.0000000

C	-3.2169000	-0.0203169	1.5205287
C	-4.5799550	-0.0457729	1.2467745
H	-5.2622358	-0.0765316	2.1094531
C	-5.2212714	-0.0517386	0.0000000
C	-4.5799550	-0.0457729	-1.2467745
H	-5.2622358	-0.0765316	-2.1094531
C	-3.2169000	-0.0203169	-1.5205287
C	-2.8237660	0.0217542	-2.9818700
H	-3.4465476	-0.6502639	-3.5874662
H	-2.9407432	1.0296696	-3.3997098
H	-1.7801969	-0.2669777	-3.1332488
C	-2.8237660	0.0217542	2.9818700
H	-2.9407432	1.0296696	3.3997098
H	-3.4465476	-0.6502639	3.5874662
H	-1.7801969	-0.2669777	3.1332488
N	-6.6540078	-0.1609343	0.0000000
H	-7.0371528	0.2995696	0.8191191
H	-7.0371528	0.2995696	-0.8191191

Complex 86 ($X = NH_2$, $Y = P(CN)_2$)

C	5.9065238	-0.3800689	0.0000000
C	5.2108583	-0.3465605	1.2118394
C	3.8185642	-0.2591507	1.1932765
C	3.0844825	-0.2151326	0.0000000
C	3.8185642	-0.2591507	-1.1932765
C	5.2108583	-0.3465605	-1.2118394
H	5.7453428	-0.3717004	2.1577084
H	3.2964171	-0.2304536	2.1476057
H	3.2964171	-0.2304536	-2.1476057
H	5.7453428	-0.3717004	-2.1577084
Sn	0.8808248	-0.0642108	0.0000000

H	0.6032466	-0.8539771	1.4645444
H	0.7027448	1.6116361	0.0000000
H	0.6032466	-0.8539771	-1.4645444
P	7.6950925	-0.7066069	0.0000000
C	8.2219291	0.3613043	1.3286070
N	8.6074194	0.9424469	2.2750066
C	8.2219291	0.3613043	-1.3286070
N	8.6074194	0.9424469	-2.2750066
Sn	-2.4933349	-0.0008617	0.0000000
C	-3.9267293	0.0153010	1.5213102
C	-5.2897768	0.0166493	1.2469556
H	-5.9724795	-0.0056287	2.1093980
C	-5.9306849	0.0268046	0.0000000
C	-5.2897768	0.0166493	-1.2469556
H	-5.9724795	-0.0056287	-2.1093980
C	-3.9267293	0.0153010	-1.5213102
C	-3.5311552	0.0414349	-2.9818788
H	-4.1883533	-0.5945406	-3.5897660
H	-3.5937211	1.0552648	-3.3963124
H	-2.5044638	-0.3018917	-3.1339391
C	-3.5311552	0.0414349	2.9818788
H	-3.5937211	1.0552648	3.3963124
H	-4.1883533	-0.5945406	3.5897660
H	-2.5044638	-0.3018917	3.1339391
N	-7.3651603	-0.0491834	0.0000000
H	-7.7373427	0.4203140	0.8189962
H	-7.7373427	0.4203140	-0.8189962

Complex 87 ($X = NH_2$, $Y = SO_2CN$)

C	5.8728625	0.2601765	0.0000000
C	5.1971599	0.2194340	1.2209559

C	3.8057291	0.1528234	1.1963675
C	3.0739916	0.1206193	0.0000000
C	3.8057291	0.1528234	-1.1963675
C	5.1971599	0.2194340	-1.2209559
H	5.7535641	0.2555554	2.1509853
H	3.2778210	0.1212861	2.1473135
H	3.2778210	0.1212861	-2.1473135
H	5.7535641	0.2555554	-2.1509853
Sn	0.8496749	0.1015607	0.0000000
H	0.6749714	-0.7032851	1.4745253
H	0.6144708	1.7724860	0.0000000
H	0.6749714	-0.7032851	-1.4745253
S	7.6050149	0.3329229	0.0000000
O	8.0924956	0.8334246	1.2531384
O	8.0924956	0.8334246	-1.2531384
C	8.0120032	-1.3824823	0.0000000
N	8.3144908	-2.5184055	0.0000000
Sn	-2.4297372	-0.0194863	0.0000000
C	-3.8544386	-0.0492614	1.5239150
C	-5.2161044	-0.0992449	1.2472974
H	-5.8974990	-0.1415287	2.1095608
C	-5.8564555	-0.1177243	0.0000000
C	-5.2161044	-0.0992449	-1.2472974
H	-5.8974990	-0.1415287	-2.1095608
C	-3.8544386	-0.0492614	-1.5239150
C	-3.4606130	0.0031411	-2.9842206
H	-4.0837381	-0.6642749	-3.5940092
H	-3.5780659	1.0141795	-3.3935877
H	-2.4172360	-0.2843930	-3.1380997
C	-3.4606130	0.0031411	2.9842206
H	-3.5780659	1.0141795	3.3935877

H	-4.0837381	-0.6642749	3.5940092
H	-2.4172360	-0.2843930	3.1380997
N	-7.2850766	-0.2545571	0.0000000
H	-7.6796659	0.1945890	0.8197084
H	-7.6796659	0.1945890	-0.8197084

Complex 88 (X= NH₂, Y= tBu)

C	4.6766741	0.0253011	0.0000000
C	3.9457755	0.0064770	1.1946200
C	2.5507093	-0.0127909	1.1896163
C	1.8121890	-0.0179947	0.0000000
C	2.5507093	-0.0127909	-1.1896163
C	3.9457755	0.0064770	-1.1946200
H	4.4608799	0.0102425	2.1489306
H	2.0329980	-0.0278668	2.1466037
H	2.0329980	-0.0278668	-2.1466037
H	4.4608799	0.0102425	-2.1489306
Sn	-0.3586001	0.0202868	0.0000000
H	-0.7249415	-0.7774491	1.4376633
H	-0.7212324	1.6651071	0.0000000
H	-0.7249415	-0.7774491	-1.4376633
C	6.1988271	-0.0127036	0.0000000
C	6.7780883	0.6799864	1.2353296
H	6.5193307	0.1580353	2.1577722
H	7.8695321	0.7009438	1.1677752
H	6.4180342	1.7089543	1.3129588
C	6.7780883	0.6799864	-1.2353296
H	7.8695321	0.7009438	-1.1677752
H	6.5193307	0.1580353	-2.1577722
H	6.4180342	1.7089543	-1.3129588
C	6.6460468	-1.4794005	0.0000000

H 6.2642047 -1.9969464 -0.8835447
H 7.7389218 -1.5512721 0.0000000
H 6.2642047 -1.9969464 0.8835447
Sn -3.9957366 -0.0069518 0.0000000
C -5.4475469 -0.0140098 1.5162864
C -6.8112843 -0.0446454 1.2460295
H -7.4929465 -0.0772046 2.1098128
C -7.4535766 -0.0553653 0.0000000
C -6.8112843 -0.0446454 -1.2460295
H -7.4929465 -0.0772046 -2.1098128
C -5.4475469 -0.0140098 -1.5162864
C -5.0559929 0.0350932 -2.9783056
H -5.6897360 -0.6212744 -3.5904838
H -5.1572576 1.0486805 -3.3870925
H -4.0168770 -0.2682344 -3.1335387
C -5.0559929 0.0350932 2.9783056
H -5.1572576 1.0486805 3.3870925
H -5.6897360 -0.6212744 3.5904838
H -4.0168770 -0.2682344 3.1335387
N -8.8873833 -0.1754642 0.0000000
H -9.2710349 0.2862374 0.8185150
H -9.2710349 0.2862374 -0.8185150

Complex 89 ($X= NH_2$, $Y= NH_2$)

C 6.5874216 -0.0274622 0.0000000
C 5.8730986 -0.0337660 1.2000179
C 4.4793768 -0.0275235 1.1916427
C 3.7425675 -0.0220779 0.0000000
C 4.4793768 -0.0275235 -1.1916427
C 5.8730986 -0.0337660 -1.2000179
H 6.4141428 -0.0434776 2.1433254

H	3.9608044	-0.0340977	2.1479183
H	3.9608044	-0.0340977	-2.1479183
H	6.4141428	-0.0434776	-2.1433254
Sn	1.5782990	0.0437900	0.0000000
H	1.1913095	-0.7490245	1.4353070
H	1.2172900	1.6894380	0.0000000
H	1.1913095	-0.7490245	-1.4353070
N	7.9954466	-0.0934242	0.0000000
H	8.3989664	0.3267443	-0.8273641
H	8.3989664	0.3267443	0.8273641
Sn	-2.0802650	0.0519238	0.0000000
C	-3.5328647	0.0278854	1.5162604
C	-4.8962288	-0.0164664	1.2462084
H	-5.5779955	-0.0465747	2.1101221
C	-5.5378186	-0.0402834	0.0000000
C	-4.8962288	-0.0164664	-1.2462084
H	-5.5779955	-0.0465747	-2.1101221
C	-3.5328647	0.0278854	-1.5162604
C	-3.1396916	0.0726271	-2.9779428
H	-3.7808220	-0.5750340	-3.5920470
H	-3.2286198	1.0875862	-3.3858265
H	-2.1038003	-0.2423383	-3.1323498
C	-3.1396916	0.0726271	2.9779428
H	-3.2286198	1.0875862	3.3858265
H	-3.7808220	-0.5750340	3.5920470
H	-2.1038003	-0.2423383	3.1323498
N	-6.9767889	-0.0368955	0.0000000
H	-7.3207518	-0.5290445	-0.8184346
H	-7.3207518	-0.5290445	0.8184346

Complex 90 (X= NH₂, Y= NMe₂)

C	5.3610128	-0.1482409	0.0000000
C	4.6282255	-0.1389849	1.1991648
C	3.2344140	-0.1390596	1.1865369
C	2.4920038	-0.1369399	0.0000000
C	3.2344140	-0.1390596	-1.1865369
C	4.6282255	-0.1389849	-1.1991648
H	5.1360064	-0.1382567	2.1551314
H	2.7213001	-0.1397211	2.1459456
H	2.7213001	-0.1397211	-2.1459456
H	5.1360064	-0.1382567	-2.1551314
Sn	0.3296827	-0.0710263	0.0000000
H	-0.0728535	-0.8636045	1.4309407
H	-0.0407591	1.5722530	0.0000000
H	-0.0728535	-0.8636045	-1.4309407
N	6.7653653	-0.1940393	0.0000000
C	7.4161320	0.2624621	1.2121808
H	7.1635963	-0.3838347	2.0524638
H	8.4955165	0.2084189	1.0706823
H	7.1459456	1.2958144	1.4790072
C	7.4161320	0.2624621	-1.2121808
H	7.1635963	-0.3838347	-2.0524638
H	7.1459456	1.2958144	-1.4790072
H	8.4955165	0.2084189	-1.0706823
Sn	-3.3845748	-0.0361769	0.0000000
C	-4.8398452	-0.0204472	1.5150455
C	-6.2042030	-0.0269956	1.2456817
H	-6.8863902	-0.0339221	2.1097790
C	-6.8469138	-0.0341344	0.0000000
C	-6.2042030	-0.0269956	-1.2456817
H	-6.8863902	-0.0339221	-2.1097790
C	-4.8398452	-0.0204472	-1.5150455

C	-4.4482104	0.0155582	-2.9774955
H	-5.0740996	-0.6543220	-3.5833009
H	-4.5610101	1.0235367	-3.3971140
H	-3.4057224	-0.2781227	-3.1286764
C	-4.4482104	0.0155582	2.9774955
H	-4.5610101	1.0235367	3.3971140
H	-5.0740996	-0.6543220	3.5833009
H	-3.4057224	-0.2781227	3.1286764
N	-8.2855218	0.0117217	0.0000000
H	-8.6439495	-0.4702278	-0.8183697
H	-8.6439495	-0.4702278	0.8183697

Complex 91 ($X = NMe_2$, $Y = H$)

C	8.2042535	0.0102864	0.0000000
C	7.5026859	-0.0137602	1.2040954
C	6.1077760	-0.0565942	1.1965185
C	5.3777385	-0.0771940	0.0000000
C	6.1077760	-0.0565942	-1.1965185
C	7.5026859	-0.0137602	-1.2040954
H	8.0416156	0.0003435	2.1465796
H	5.5818833	-0.0821332	2.1483849
H	5.5818833	-0.0821332	-2.1483849
H	8.0416156	0.0003435	-2.1465796
Sn	3.2068214	-0.1031506	0.0000000
H	2.8598011	-0.9113818	1.4362313
H	2.7853463	1.5273482	0.0000000
H	2.8598011	-0.9113818	-1.4362313
H	9.2888725	0.0426548	0.0000000
Sn	-0.4502218	-0.2379486	0.0000000
C	-1.9154082	-0.1818053	1.4970146
C	-3.2830311	-0.1515420	1.2411680

H	-3.9166501	-0.1578760	2.1295444
C	-3.9550583	-0.1399362	0.0000000
C	-3.2830311	-0.1515420	-1.2411680
H	-3.9166501	-0.1578760	-2.1295444
C	-1.9154082	-0.1818053	-1.4970146
C	-1.5270552	-0.1499255	-2.9619636
H	-2.1768063	-0.7957331	-3.5688713
H	-1.6085302	0.8636892	-3.3752011
H	-0.4951802	-0.4762552	-3.1188867
C	-1.5270552	-0.1499255	2.9619636
H	-1.6085302	0.8636892	3.3752011
H	-2.1768063	-0.7957331	3.5688713
H	-0.4951802	-0.4762552	3.1188867
N	-5.3939786	-0.1909021	0.0000000
C	-6.0357978	0.3266129	1.1936525
H	-7.1156619	0.3281328	1.0337233
H	-5.8372258	-0.3089565	2.0560839
H	-5.7143019	1.3516056	1.4462370
C	-6.0357978	0.3266129	-1.1936525
H	-5.8372258	-0.3089565	-2.0560839
H	-7.1156619	0.3281328	-1.0337233
H	-5.7143019	1.3516056	-1.4462370

Complex 92 ($X = NMe_2$, $Y = F$)

C	8.1236371	-0.0112963	0.0000000
C	7.4537909	-0.0270730	1.2115754
C	6.0578807	-0.0551594	1.1950070
C	5.3259311	-0.0679544	0.0000000
C	6.0578807	-0.0551594	-1.1950070
C	7.4537909	-0.0270730	-1.2115754
H	8.0181984	-0.0197562	2.1372568

H	5.5355744	-0.0759354	2.1485118
H	5.5355744	-0.0759354	-2.1485118
H	8.0181984	-0.0197562	-2.1372568
Sn	3.1486431	-0.0868552	0.0000000
H	2.8271774	-0.8952367	1.4421909
H	2.7454334	1.5483870	0.0000000
H	2.8271774	-0.8952367	-1.4421909
F	9.4790069	0.0152123	0.0000000
Sn	-0.4382467	-0.2391687	0.0000000
C	-1.8991702	-0.1833520	1.4981377
C	-3.2665101	-0.1496703	1.2414994
H	-3.9004990	-0.1553792	2.1294220
C	-3.9380699	-0.1360435	0.0000000
C	-3.2665101	-0.1496703	-1.2414994
H	-3.9004990	-0.1553792	-2.1294220
C	-1.8991702	-0.1833520	-1.4981377
C	-1.5085530	-0.1574000	-2.9625013
H	-2.1509627	-0.8130229	-3.5664215
H	-1.5976521	0.8525891	-3.3828719
H	-0.4736483	-0.4761243	-3.1148205
C	-1.5085530	-0.1574000	2.9625013
H	-1.5976521	0.8525891	3.3828719
H	-2.1509627	-0.8130229	3.5664215
H	-0.4736483	-0.4761243	3.1148205
N	-5.3766098	-0.1822676	0.0000000
C	-6.0177782	0.3359454	1.1936347
H	-7.0977571	0.3359445	1.0349326
H	-5.8176993	-0.2980406	2.0568170
H	-5.6972543	1.3616642	1.4441306
C	-6.0177782	0.3359454	-1.1936347
H	-5.8176993	-0.2980406	-2.0568170

H -7.0977571 0.3359445 -1.0349326
H -5.6972543 1.3616642 -1.4441306

Complex 93 (X= NMe₂, Y= CF₃)

C 7.3849233 -0.0051608 0.0000000
C 6.6908327 -0.0258116 1.2086475
C 5.2975305 -0.0560811 1.1945757
C 4.5646796 -0.0711882 0.0000000
C 5.2975305 -0.0560811 -1.1945757
C 6.6908327 -0.0258116 -1.2086475
H 7.2352082 -0.0114578 2.1462965
H 4.7732377 -0.0749232 2.1473257
H 4.7732377 -0.0749232 -2.1473257
H 7.2352082 -0.0114578 -2.1462965
Sn 2.3744454 -0.0836617 0.0000000
H 2.0919162 -0.8917717 1.4510019
H 2.0265634 1.5641314 0.0000000
H 2.0919162 -0.8917717 -1.4510019
C 8.8773158 -0.0299695 0.0000000
F 9.3635347 -1.2905573 0.0000000
F 9.4026954 0.5752859 1.0805335
F 9.4026954 0.5752859 -1.0805335
Sn -1.1199908 -0.2087713 0.0000000
C -2.5759523 -0.1665490 1.4994932
C -3.9431598 -0.1427402 1.2413631
H -4.5772028 -0.1539407 2.1290204
C -4.6147385 -0.1325144 0.0000000
C -3.9431598 -0.1427402 -1.2413631
H -4.5772028 -0.1539407 -2.1290204
C -2.5759523 -0.1665490 -1.4994932
C -2.1880265 -0.1411683 -2.9643167

H	-2.8205677	-0.8115101	-3.5621301
H	-2.2967281	0.8647674	-3.3893844
H	-1.1483213	-0.4424140	-3.1181986
C	-2.1880265	-0.1411683	2.9643167
H	-2.2967281	0.8647674	3.3893844
H	-2.8205677	-0.8115101	3.5621301
H	-1.1483213	-0.4424140	3.1181986
N	-6.0520271	-0.1841476	0.0000000
C	-6.6956576	0.3281617	1.1950903
H	-7.7751091	0.3308487	1.0337982
H	-6.4988936	-0.3112575	2.0551475
H	-6.3741548	1.3514811	1.4529516
C	-6.6956576	0.3281617	-1.1950903
H	-6.3741548	1.3514811	-1.4529516
H	-6.4988936	-0.3112575	-2.0551475
H	-7.7751091	0.3308487	-1.0337982

Complex 94 (X= NMe₂, Y= CN)

C	7.7898119	-0.0240197	0.0000000
C	7.0917935	-0.0407720	1.2132777
C	5.6995873	-0.0698051	1.1952469
C	4.9664956	-0.0825341	0.0000000
C	5.6995873	-0.0698051	-1.1952469
C	7.0917935	-0.0407720	-1.2132777
H	7.6428859	-0.0315969	2.1479419
H	5.1735856	-0.0910212	2.1472364
H	5.1735856	-0.0910212	-2.1472364
H	7.6428859	-0.0315969	-2.1479419
Sn	2.7670069	-0.0847058	0.0000000
H	2.5116791	-0.8913956	1.4580869
H	2.4569719	1.5714418	0.0000000

H 2.5116791 -0.8913956 -1.4580869
C 9.2198922 0.0055479 0.0000000
N 10.3929718 0.0303470 0.0000000
Sn -0.6551638 -0.1924099 0.0000000
C -2.1057517 -0.1561360 1.5015069
C -3.4727108 -0.1431698 1.2419550
H -4.1068255 -0.1574031 2.1293837
C -4.1437030 -0.1397595 0.0000000
C -3.4727108 -0.1431698 -1.2419550
H -4.1068255 -0.1574031 -2.1293837
C -2.1057517 -0.1561360 -1.5015069
C -1.7154435 -0.1194828 -2.9651617
H -2.3617911 -0.7667587 -3.5734193
H -1.8009279 0.8947045 -3.3753319
H -0.6822474 -0.4409899 -3.1218689
C -1.7154435 -0.1194828 2.9651617
H -1.8009279 0.8947045 3.3753319
H -2.3617911 -0.7667587 3.5734193
H -0.6822474 -0.4409899 3.1218689
N -5.5795535 -0.2043219 0.0000000
C -6.2289035 0.2989459 1.1958078
H -7.3080507 0.2924094 1.0331748
H -6.0273913 -0.3417221 2.0539332
H -5.9168529 1.3244004 1.4569517
C -6.2289035 0.2989459 -1.1958078
H -5.9168529 1.3244004 -1.4569517
H -6.0273913 -0.3417221 -2.0539332
H -7.3080507 0.2924094 -1.0331748

Complex 95 ($X = NMe_2$, $Y = P(CN)_2$)

C 7.0637834 -0.3972653 0.0000000

C	6.3675223	-0.3790515	1.2118646
C	4.9736006	-0.3243854	1.1934148
C	4.2389428	-0.2990044	0.0000000
C	4.9736006	-0.3243854	-1.1934148
C	6.3675223	-0.3790515	-1.2118646
H	6.9022772	-0.3916218	2.1577966
H	4.4508118	-0.3072760	2.1476275
H	4.4508118	-0.3072760	-2.1476275
H	6.9022772	-0.3916218	-2.1577966
Sn	2.0341570	-0.2089200	0.0000000
H	1.7715851	-1.0077808	1.4619321
H	1.8040429	1.4599711	0.0000000
H	1.7715851	-1.0077808	-1.4619321
P	8.8586888	-0.6871100	0.0000000
C	9.3646896	0.3918085	1.3276629
N	9.7411557	0.9826679	2.2716718
C	9.3646896	0.3918085	-1.3276629
N	9.7411557	0.9826679	-2.2716718
Sn	-1.3561359	-0.2062164	0.0000000
C	-2.8029524	-0.1387433	1.5024492
C	-4.1691735	-0.0954896	1.2420655
H	-4.8038133	-0.0956368	2.1291226
C	-4.8398187	-0.0771114	0.0000000
C	-4.1691735	-0.0954896	-1.2420655
H	-4.8038133	-0.0956368	-2.1291226
C	-2.8029524	-0.1387433	-1.5024492
C	-2.4110780	-0.1094482	-2.9657263
H	-3.0781818	-0.7326609	-3.5765533
H	-2.4629163	0.9085582	-3.3717989
H	-1.3889884	-0.4641450	-3.1234669
C	-2.4110780	-0.1094482	2.9657263

H	-2.4629163	0.9085582	3.3717989
H	-3.0781818	-0.7326609	3.5765533
H	-1.3889884	-0.4641450	3.1234669
N	-6.2764725	-0.1089516	0.0000000
C	-6.9149920	0.4086070	1.1956955
H	-7.9938203	0.4265848	1.0322422
H	-6.7290239	-0.2364931	2.0539824
H	-6.5802961	1.4268099	1.4567247
C	-6.9149920	0.4086070	-1.1956955
H	-6.7290239	-0.2364931	-2.0539824
H	-7.9938203	0.4265848	-1.0322422
H	-6.5802961	1.4268099	-1.4567247

Complex 96 ($X = NMe_2$, $Y = SO_2CN$)

C	7.0065801	0.2531361	0.0000000
C	6.3312020	0.2082389	1.2209422
C	4.9405445	0.1279155	1.1965011
C	4.2095690	0.0853594	0.0000000
C	4.9405445	0.1279155	-1.1965011
C	6.3312020	0.2082389	-1.2209422
H	6.8872617	0.2491269	2.1509379
H	4.4130304	0.0909229	2.1474091
H	4.4130304	0.0909229	-2.1474091
H	6.8872617	0.2491269	-2.1509379
Sn	1.9878469	0.0114239	0.0000000
H	1.8303887	-0.7988964	1.4733115
H	1.7018419	1.6743608	0.0000000
H	1.8303887	-0.7988964	-1.4733115
S	8.7389141	0.3224474	0.0000000
O	9.2281917	0.8210987	1.2531375
O	9.2281917	0.8210987	-1.2531375

C	9.1378896	-1.3949256	0.0000000
N	9.4333611	-2.5326988	0.0000000
Sn	-1.2920131	-0.1896995	0.0000000
C	-2.7304460	-0.1660604	1.5054102
C	-4.0967517	-0.1656317	1.2425970
H	-4.7311930	-0.1861960	2.1292247
C	-4.7669645	-0.1675644	0.0000000
C	-4.0967517	-0.1656317	-1.2425970
H	-4.7311930	-0.1861960	-2.1292247
C	-2.7304460	-0.1660604	-1.5054102
C	-2.3385288	-0.1293181	-2.9682057
H	-2.9719725	-0.7912231	-3.5736098
H	-2.4425926	0.8810270	-3.3829486
H	-1.2997218	-0.4328460	-3.1222412
C	-2.3385288	-0.1293181	2.9682057
H	-2.4425926	0.8810270	3.3829486
H	-2.9719725	-0.7912231	3.5736098
H	-1.2997218	-0.4328460	3.1222412
N	-6.2010013	-0.2435009	0.0000000
C	-6.8565122	0.2526097	1.1956608
H	-7.9352935	0.2322120	1.0330738
H	-6.6476402	-0.3845595	2.0544200
H	-6.5579787	1.2824105	1.4545506
C	-6.8565122	0.2526097	-1.1956608
H	-6.5579787	1.2824105	-1.4545506
H	-6.6476402	-0.3845595	-2.0544200
H	-7.9352935	0.2322120	-1.0330738

Complex 97 ($X = NMe_2$, $Y = tBu$)

C	5.8276642	0.0250328	0.0000000
C	5.0971148	-0.0012924	1.1946413

C	3.7025211	-0.0409677	1.1897306
C	2.9644069	-0.0596260	0.0000000
C	3.7025211	-0.0409677	-1.1897306
C	5.0971148	-0.0012924	-1.1946413
H	5.6120967	0.0100669	2.1489638
H	3.1851641	-0.0634023	2.1467191
H	3.1851641	-0.0634023	-2.1467191
H	5.6120967	0.0100669	-2.1489638
Sn	0.7947409	-0.0817781	0.0000000
H	0.4471177	-0.8908596	1.4357698
H	0.3749512	1.5491166	0.0000000
H	0.4471177	-0.8908596	-1.4357698
C	7.3498940	-0.0048663	0.0000000
C	7.9270227	0.6895742	1.2351746
H	7.6676630	0.1687235	2.1580369
H	9.0185122	0.7109052	1.1686873
H	7.5665585	1.7185419	1.3109755
C	7.9270227	0.6895742	-1.2351746
H	9.0185122	0.7109052	-1.1686873
H	7.6676630	0.1687235	-2.1580369
H	7.5665585	1.7185419	-1.3109755
C	7.8012307	-1.4704151	0.0000000
H	7.4205066	-1.9888791	-0.8834895
H	8.8942522	-1.5395581	0.0000000
H	7.4205066	-1.9888791	0.8834895
Sn	-2.8581913	-0.2059203	0.0000000
C	-4.3235628	-0.1578740	1.4968792
C	-5.6913842	-0.1393334	1.2411907
H	-6.3247504	-0.1495760	2.1296516
C	-6.3635060	-0.1350149	0.0000000
C	-5.6913842	-0.1393334	-1.2411907

H	-6.3247504	-0.1495760	-2.1296516
C	-4.3235628	-0.1578740	-1.4968792
C	-3.9345474	-0.1176289	-2.9613349
H	-4.5844787	-0.7591297	-3.5726188
H	-4.0149222	0.8985997	-3.3682284
H	-2.9026608	-0.4434075	-3.1195247
C	-3.9345474	-0.1176289	2.9613349
H	-4.0149222	0.8985997	3.3682284
H	-4.5844787	-0.7591297	3.5726188
H	-2.9026608	-0.4434075	3.1195247
N	-7.8016081	-0.2007687	0.0000000
C	-8.4490229	0.3085442	1.1940688
H	-9.5288110	0.2991891	1.0338840
H	-8.2440102	-0.3262793	2.0556528
H	-8.1380440	1.3363841	1.4482413
C	-8.4490229	0.3085442	-1.1940688
H	-8.1380440	1.3363841	-1.4482413
H	-8.2440102	-0.3262793	-2.0556528
H	-9.5288110	0.2991891	-1.0338840

Complex 98 ($X = NMe_2$, $Y = NH_2$)

C	7.7502467	-0.0749588	0.0000000
C	7.0359214	-0.0546204	1.1998828
C	5.6434255	0.0033758	1.1917747
C	4.9073448	0.0359656	0.0000000
C	5.6434255	0.0033758	-1.1917747
C	7.0359214	-0.0546204	-1.1998828
H	7.5760323	-0.0844445	2.1432122
H	5.1254573	0.0160372	2.1481565
H	5.1254573	0.0160372	-2.1481565
H	7.5760323	-0.0844445	-2.1432122

Sn	2.7492217	0.1818763	0.0000000
H	2.3193428	-0.5944655	1.4319500
H	2.4390307	1.8378132	0.0000000
H	2.3193428	-0.5944655	-1.4319500
N	9.1543220	-0.1941663	0.0000000
H	9.5746439	0.2086516	-0.8275642
H	9.5746439	0.2086516	0.8275642
Sn	-0.9609364	0.3157354	0.0000000
C	-2.4282337	0.2401856	1.4960096
C	-3.7931765	0.1453785	1.2409548
H	-4.4244299	0.0999766	2.1298161
C	-4.4645293	0.1054378	0.0000000
C	-3.7931765	0.1453785	-1.2409548
H	-4.4244299	0.0999766	-2.1298161
C	-2.4282337	0.2401856	-1.4960096
C	-2.0427682	0.2995979	-2.9609755
H	-2.6609412	-0.3729058	-3.5720010
H	-2.1723761	1.3106191	-3.3679705
H	-0.9963585	0.0247589	-3.1206907
C	-2.0427682	0.2995979	2.9609755
H	-2.1723761	1.3106191	3.3679705
H	-2.6609412	-0.3729058	3.5720010
H	-0.9963585	0.0247589	3.1206907
N	-5.9038387	0.0643713	0.0000000
C	-6.5138840	-0.4890368	1.1938195
H	-6.3522375	0.1576742	2.0557131
H	-7.5918901	-0.5532671	1.0341348
H	-6.1339581	-1.4935524	1.4472710
C	-6.5138840	-0.4890368	-1.1938195
H	-7.5918901	-0.5532671	-1.0341348
H	-6.3522375	0.1576742	-2.0557131

H -6.1339581 -1.4935524 -1.4472710

Complex 99 (X= NMe₂, Y= NMe₂)

C 6.5136644 -0.1431908 0.0000000
C 5.7819873 -0.1041311 1.1993026
C 4.3892556 -0.0507298 1.1866590
C 3.6477262 -0.0211004 0.0000000
C 4.3892556 -0.0507298 -1.1866590
C 5.7819873 -0.1041311 -1.1993026
H 6.2895699 -0.1225478 2.1552234
H 3.8762687 -0.0319953 2.1459282
H 3.8762687 -0.0319953 -2.1459282
H 6.2895699 -0.1225478 -2.1552234
Sn 1.4894160 0.1105998 0.0000000
H 1.0640006 -0.6691882 1.4312714
H 1.1630165 1.7632912 0.0000000
H 1.0640006 -0.6691882 -1.4312714
N 7.9144766 -0.2470679 0.0000000
C 8.5845249 0.1783939 1.2127681
H 8.3053691 -0.4591801 2.0513767
H 9.6605360 0.0792154 1.0702522
H 8.3584206 1.2214576 1.4827909
C 8.5845249 0.1783939 -1.2127681
H 8.3053691 -0.4591801 -2.0513767
H 8.3584206 1.2214576 -1.4827909
H 9.6605360 0.0792154 -1.0702522
Sn -2.2261060 0.2163587 0.0000000
C -3.6946946 0.1733195 1.4957856
C -5.0615679 0.1105743 1.2409987
H -5.6941395 0.0822792 2.1297163
C -5.7335607 0.0852513 0.0000000

C	-5.0615679	0.1105743	-1.2409987
H	-5.6941395	0.0822792	-2.1297163
C	-3.6946946	0.1733195	-1.4957856
C	-3.3083622	0.2219943	-2.9609864
H	-3.9137937	-0.4687622	-3.5642773
H	-3.4554805	1.2256529	-3.3804045
H	-2.2571227	-0.0370305	-3.1152634
C	-3.3083622	0.2219943	2.9609864
H	-3.4554805	1.2256529	3.3804045
H	-3.9137937	-0.4687622	3.5642773
H	-2.2571227	-0.0370305	3.1152634
N	-7.1734820	0.0752801	0.0000000
C	-7.7945684	-0.4647519	1.1943329
H	-7.6224540	0.1813749	2.0547227
H	-8.8734045	-0.5108136	1.0337097
H	-7.4319203	-1.4748425	1.4509585
C	-7.7945684	-0.4647519	-1.1943329
H	-8.8734045	-0.5108136	-1.0337097
H	-7.6224540	0.1813749	-2.0547227
H	-7.4319203	-1.4748425	-1.4509585