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Unveiling the role of pyrylium frameworks on π-stacking interactions: A combined *ab initio* and experimental study

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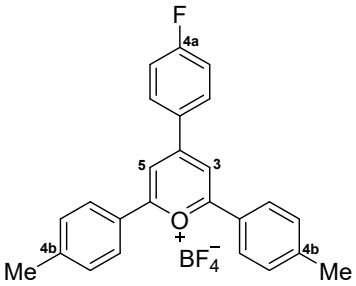
Material and Methods

General methods

All reagents were supplied from commercial sources and were used as received. Solvent evaporation was performed under reduced pressure and at temperatures lower than 50ºC in most of the cases, never being higher than 60ºC. For qualitative purposes, analytical thin-layer chromatography (TLC) was carried out using silica layers on aluminium (MN ALUGRAM Xtra SIL G/UV 254) of 0.2mm thickness. Hexane:AcOEt (4:1) was employed as eluent in all the cases and an ethanolic solution of 10% H_2SO_4 as visualization reagent. Pyrylium salts purification was carried out by crystallization in acetone or 1,2-dichloroethane. For most of the reactions, solvents were directly employed for the commercial source.

Infrared spectroscopy (IR) was recorded on a JASCO spectrophotometer FT/IR-4100. UV-visible spectra were acquired on a V-630 Jasco spectrophotometer in the 250-800 nm range. ^{1}H (and ^{13}C)-NMR spectra were obtained in 300 (75.5 for ^{13}C) and 500 (125.7 and 470 for ^{13}C and ^{19}F, respectively) MHz in Avance and Avance III spectrometers. Chemical shifts (δ) are reported in ppm calibrated with the solvent signals (DMSO-d_6 and acetone-d_6) or using TMS as internal standard. Data are presented according to the following format: chemical shift in ppm (multiplicity, protons number, coupling constant *J* in Hz, assignment). Bidimensional (2D) COSY, ^{1}H ^{13}C-HSQC and NOESY experiments were acquired using standard pulse sequence and employed to facilitate the assignation of NMR signals.

Characterization data for 2,4-di-(4-methylphenyl)-4-(4-fluorophenyl) tetrafluoroborate (1):



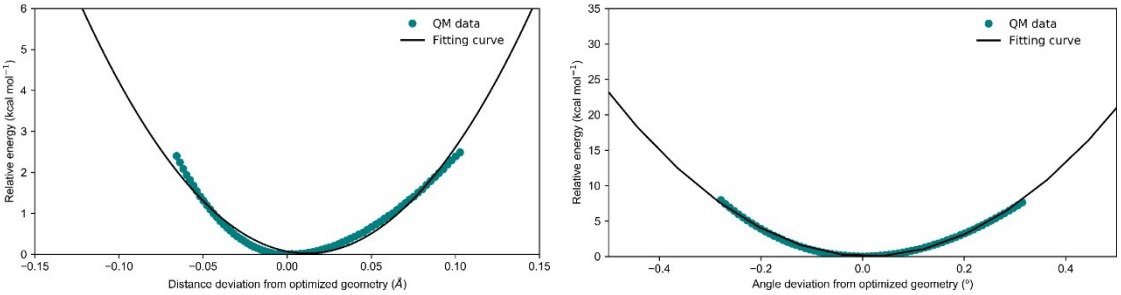
IR: 3043, 1629, 1591, 1494, 1320, 1235, 1161, 1053, 1003, 818 and 724 cm^{-1}; UV-visible (CH_2Cl_2): 445 and 376 nm; ^{1}H NMR (500 MHz, DMSO-d_6): 9.03 (s, 2H, H-3 and H-5), 8.69 (dd, 2H, *J* = 5.2, *J* = 8.9 Hz, H-2a and H-6a), 8.47 (d, 4H, *J* = 8.3 Hz, H-2b and H-6b), 7.65 (t, 2H, *J* = 8.7 Hz, H-3a and H-5a), 7.60 (d, 4H, *J* = 8.1 Hz, H-3b and H-5b) and 2.51 (s, 6H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): 169.7 (C-2 and C-6), 166.3 (d, *J* = 256.4 Hz, C-4a), 163.1 (C-4), 146.2, 133.0 (d, *J* = 9.7 Hz, C-2a and C-6a), 130.5 (C-3b and C-5b), 129.1 (d, *J* = 2.5 Hz, C-1a), 128.7 (C-2b and C-6b), 126.4, 117.0 (*J* = 22.0 Hz, C-3a and C-5a), 114.1 (C-3 and C-5) and 21.4 (CH_3); ^{19}F NMR (470 MHz, DMSO-d_6): −102.87 (m, C-F), −148.33 (br s, $^{10}BF_4^-$) and −148.39 ($J_{F,B11}$ = 1.2 Hz, $^{11}BF_4^-$). ESI-HRMS: *m/z* 355.1478, calculated for $C_{25}H_{20}OF^+$: 355.1493.

Parametrization of BF_4^-

Since Amber force field parameters are not available for boron-containing molecules, in this study we have derived them. Bond length and angle parameters were generated by optimization of tetrafluoroborate anion employing the M06-2X hybrid functional and 6-31+G(d,p) basis set with ultrafine integration grid. Then, scans for angles and bond lengths were carried out at the same level and fitting the obtained energy data to the amber energy function:

$$E_{total} = \sum_{bonds} K_r(r - r_{eq})^2 + \sum_{angles} K_\theta(\theta - \theta_{eq})^2 + \sum_{dihedrals} \frac{V_n}{2} x[1 + \cos(n\varphi - \gamma)] + \sum_{i<j} \left[\frac{A_{ij}}{R_j^{12}} - \frac{B_{ij}}{R_j^6} + \frac{q_i q_j}{\varepsilon R_{ij}} \right]$$

where K_r and K_θ symbols are bond and angle force constants, respectively; n is multiplicity, γ is phase angle, r_{eq} is bond equilibrium distance, θ_{eq} is angle equilibrium, and A, B, and q are non-bond parameters. The obtained bond and angle fitting curves were:



The bond and angle parameters obtained are reported in the following table:

Bond	**K_r** (kcal mol^{-1} Å^{-2})	**r_{eq}**(Å)
B – F	334.1656	1.88219
Angle	**K_θ** (kcal mol^{-1} radian^{-2})	**θ_{eq}**(°)
F – B – F	87.7303	109.48931

Regarding non-bond parameters, previous studies have demonstrated the good performance of the use of non-bonded parameters taken from the MM2 force field. Therefore, in the present study these parameters were used:

Non-bonded	**ε** (kcal mol^{-1})	**r** (Å)
B	0.034	1.98

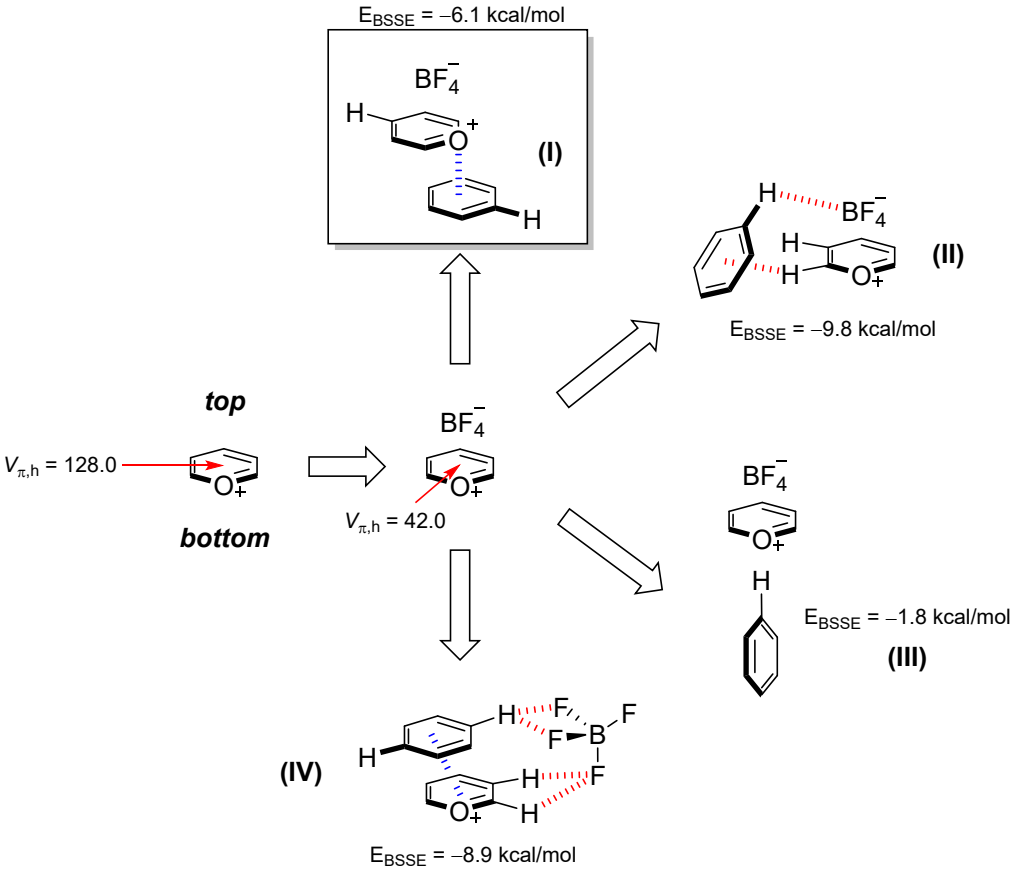
Calculation of β_x and β_y coefficients:

It is possible to obtain a mathematical relation between binding energies (E_{BSSE}) with both $\sigma_p(X)$ and $\sigma_p(Y)$ through coefficients β_x and β_y:

$$E_{BSSE} = \beta_x \times \sigma_p(X) + \beta_y \times \sigma_p(Y) + C$$

These coefficients and intercept C were obtained by a multiple linear regression (MLR) analysis with a good correlation coefficient (r^2 = 0.956). β_x = –1.45 ± 0.08; β_y = 2.41 ± 0.08; C = –5.91 ± 0.05

Figure S1. Feasible geometries (**I**-**IV**) for the interaction of pyrylium tetrafluoroborate model and aromatic moieties. BSSE-corrected energies and the π-hole intensity ($V_{\pi,h}$, in kcal/mol) at MP2(fc)/def2-TZVP are also given. Additional contacts are displayed in red whereas π-π interactions are shown in blue colour.



Note. The pyrylium···BF_4 system in the same geometry of IV, displaying $(C–H)^+$···anion interaction was not found. This geometry seems to be only feasible when the pyrylium complex is substituted at C-2/C-4 position, then making the C–H moiety more acidic. In addition, introducing different substituents on IV-type geometry afforded a disposition similar for geometry (II) which is not found within the CSD.

Table S1. MEP values plotted on the 0.001 a.u. molecular surface for bare pyrylium cations at MP2(fc)/def2-TZVP level.

Substituent	**$V_{\pi,h}$** (kcal/mol)	**Substituent**	**$V_{\pi,h}$** (kcal/mol)
H	128.0	GeF_3	134.0
Br	126.1	Me	120.5
CF_3	133.7	NH_2	109.2
NO_2	138.7	NMe_2	102.2

Figure S2. Geometrical (*d* and θ) and energetic (E_{BSSE}) descriptors that characterize the optimized structures Pyry$^{+}\cdots\pi$, complex **2.10** and benzene dimer at MP2(fc)/def2-TZVP level.

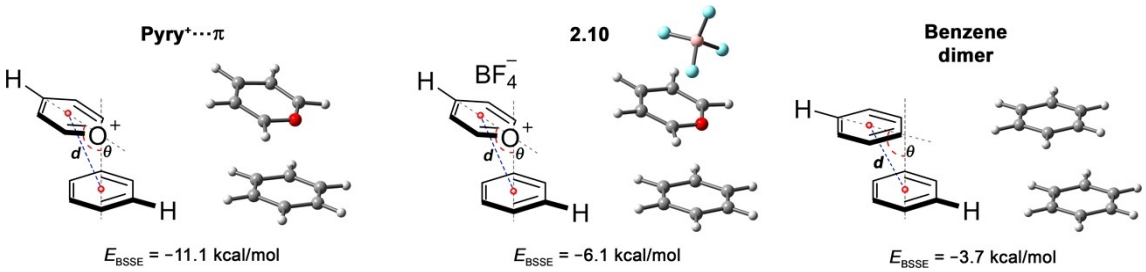


Figure S3. Energy decomposition analysis (EDA) for Pyry$^{+}\cdots\pi$, complex **2.10** and benzene dimer. The plot specifies each contribution on the total interaction energy ($E_{int} = E_{elec} + E_{ex} + E_{rep} + E_{pol} + E_{disp}$)

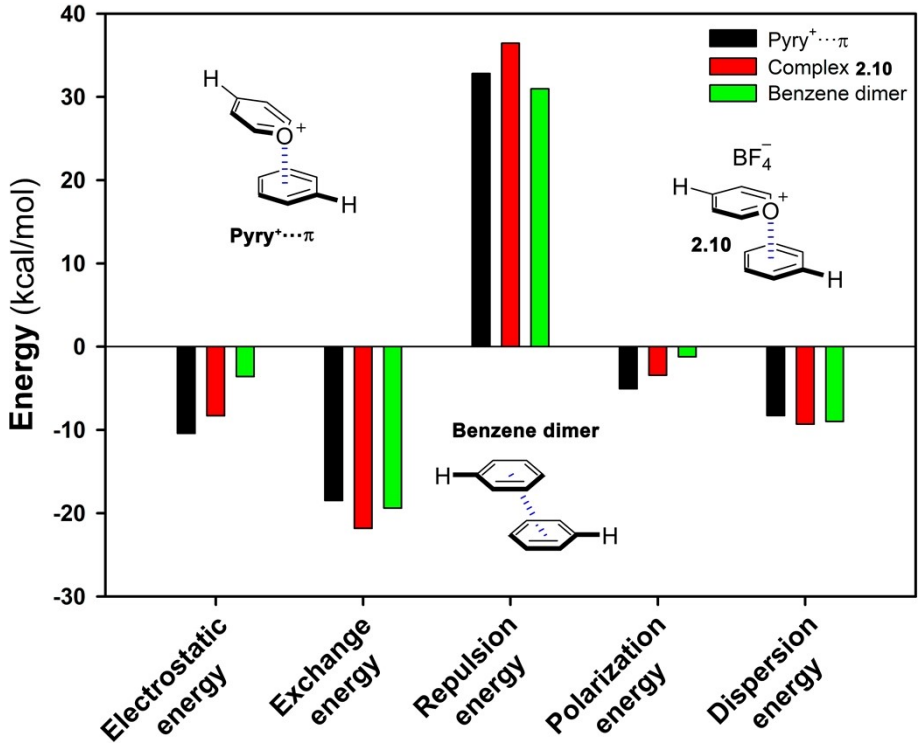
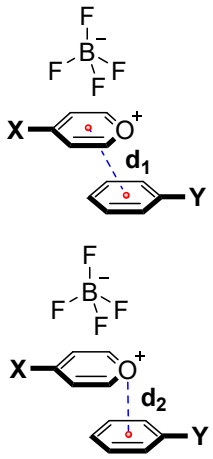


Table S2. Binding energies with BSSE correction (E_{BSSE} in kcal mol^{-1}), equilibrium distances (d, in Å) at the MP2/def2TZVP level of theory for complexes **2.10**–**9.17**.



2.10, X = H, Y = H
2.11, X = H, Y = Br
2.12, X = H, Y = CF_3
2.13, X = H, Y = NO_2
2.14, X = H, Y = GeF_3
2.15, X = H, Y = Me
2.16, X = H, Y = NH_2
2.17, X = H, Y = NMe_2
3.10, X = Br, Y = H
3.11, X = Br, Y = Br
3.12, X = Br, Y = CF_3
3.13, X = Br, Y = NO_2
3.14, X = Br, Y = GeF_3
3.15, X = Br, Y = Me
3.16, X = Br, Y = NH_2
3.17, X = Br, Y = NMe_2
4.10, X = CF_3, Y = H
4.11, X = CF_3, Y = Br
4.12, X = CF_3, Y = CF_3
4.13, X = CF_3, Y = NO_2
4.14, X = CF_3, Y = GeF_3
4.15, X = CF_3, Y = Me
4.16, X = CF_3, Y = NH_2
4.17, X = CF_3, Y = NMe_2
5.10, X = NO_2, Y = H
5.11, X = NO_2, Y = Br
5.12, X = NO_2, Y = CF_3
5.13, X = NO_2, Y = NO_2
5.14, X = NO_2, Y = GeF_3
5.15, X = NO_2, Y = Me
5.16, X = NO_2, Y = NH_2
5.17, X = NO_2, Y = NMe_2
6.10, X = GeF_3, Y = H
6.11, X = GeF_3, Y = Br
6.12, X = GeF_3, Y = CF_3
6.13, X = GeF_3, Y = NO_2
6.14, X = GeF_3, Y = GeF_3
6.15, X = GeF_3, Y = Me
6.16, X = GeF_3, Y = NH_2
6.17, X = GeF_3, Y = NMe_2
7.10, X = Me, Y = H
7.11, X = Me, Y = Br
7.12, X = Me, Y = CF_3
7.13, X = Me, Y = NO_2
7.14, X = Me, Y = GeF_3
7.15, X = Me, Y = Me
7.16, X = Me, Y = NH_2
7.17, X = Me, Y = NMe_2
8.10, X = NH_2, Y = H
8.11, X = NH_2, Y = Br
8.12, X = NH_2, Y = CF_3
8.13, X = NH_2, Y = NO_2
8.14, X = NH_2, Y = GeF_3
8.15, X = NH_2, Y = Me
8.16, X = NH_2, Y = NH_2
8.17, X = NH_2, Y = NMe_2
9.10, X = NMe_2, Y = H
9.11, X = NMe_2, Y = Br
9.12, X = NMe_2, Y = CF_3
9.13, X = NMe_2, Y = NO_2
9.14, X = NMe_2, Y = GeF_3
9.15, X = NMe_2, Y = Me
9.16, X = NMe_2, Y = NH_2
9.17, X = NMe_2, Y = NMe_2

Complex	E_{BSSE}	d_1	d_2	Complex	E_{BSSE}	d_1	d_2
2.10	−6.1	3.588	3.059	**6.10**	−7.4	3.523	3.079
2.11	−5.2	3.572	3.064	**6.11**	−6.4	3.502	3.098
2.12	−4.5	3.580	3.091	**6.12**[a,b]	-	-	-
2.13	−3.7	3.585	3.106	**6.13**	−4.7	3.516	3.173
2.14	−3.5	3.582	3.118	**6.14**	−4.6	3.514	3.168
2.15	−6.7	3.577	3.021	**6.15**	−8.0	3.512	3.042
2.16	−7.1	3.572	3.023	**6.16**	−8.7	3.507	3.032
2.17	−7.8	3.559	2.976	**6.17**	−9.4	3.493	2.981
3.10	−6.6	3.539	3.075	**7.10**	−5.9	3.597	3.078
3.11	−5.7	3.512	3.103	**7.11**	−5.1	3.574	3.083
3.12	−4.9	3.518	3.139	**7.12**	−4.4	3.578	3.110
3.13[a]	-	-	-	**7.13**	−3.7	3.583	3.125
3.14	−4.0	3.518	3.183	**7.14**	−3.5	3.581	3.135
3.15	−7.2	3.523	3.037	**7.15**	−6.4	3.583	3.039
3.16	−7.6	3.521	3.044	**7.16**	−6.8	3.577	3.041
3.17	−8.4	3.507	2.989	**7.17**	−7.5	3.567	2.997
4.10	−7.1	3.520	3.064	**8.10**	−5.1	3.636	3.097
4.11	−6.1	3.501	3.089	**8.11**	−4.5	3.603	3.104
4.12	−5.2	3.495	3.152	**8.12**	−3.9	3.612	3.118
4.13	−4.3	3.502	3.183	**8.13**	−3.3	3.605	3.147
4.14	−4.0	3.523	3.191	**8.14**	−3.2	3.604	3.158
4.15	−7.7	3.507	3.019	**8.15**	−5.6	3.623	3.059
4.16	−8.2	3.503	3.026	**8.16**	−5.9	3.613	3.066
4.17	−9.1	3.489	2.970	**8.17**	−6.5	3.603	3.020
5.10	−7.4	3.523	3.068	**9.10**	−4.8	3.645	3.114
5.11	−6.4	3.499	3.083	**9.11**	−4.4	3.603	3.121
5.12	−5.5	3.507	3.117	**9.12**[b]	−9.9	3.596	4.311
5.13	−4.6	3.505	3.162	**9.13**[a]	-	-	-
5.14	−4.4	3.507	3.164	**9.14**[b]	−10.0	3.534	4.158
5.15	−8.0	3.507	3.026	**9.15**	−5.3	3.631	3.080
5.16	−8.7	3.499	3.020	**9.16**	−5.5	3.622	3.086
5.17	−9.5	3.483	2.978	**9.17**	−6.1	3.611	3.038

[a] Minimum not found; [b] Different geometry showing through-space interaction with the proximal vertex of the arene

Figure S4. (a) Initial (t = 0 ns) MD simulation box containing 35 pyrylium tetrafluoroborates (**1**) solvated in DMSO; (b) MD simulation box (t = 250 ns) for compound **1**. Colour is based on the number of contacts between any atom of the pyrylium core and any atom of a BF_4^- anion along the simulation. Teal colour indicates the presence of contacts whereas atoms in dark grey represent their absence; (c) First (3.4 Å, dark blue colour) and second (5.0 Å, cyan colour) DMSO shell for the pyrylium cation and the BF_4^- anion (red and salmon for the first and second DMSO shell respectively); (d) Distances distribution of the centroid of all pyrylium cations present in the MD box and the closest BF_4^- anion along the whole trajectory.

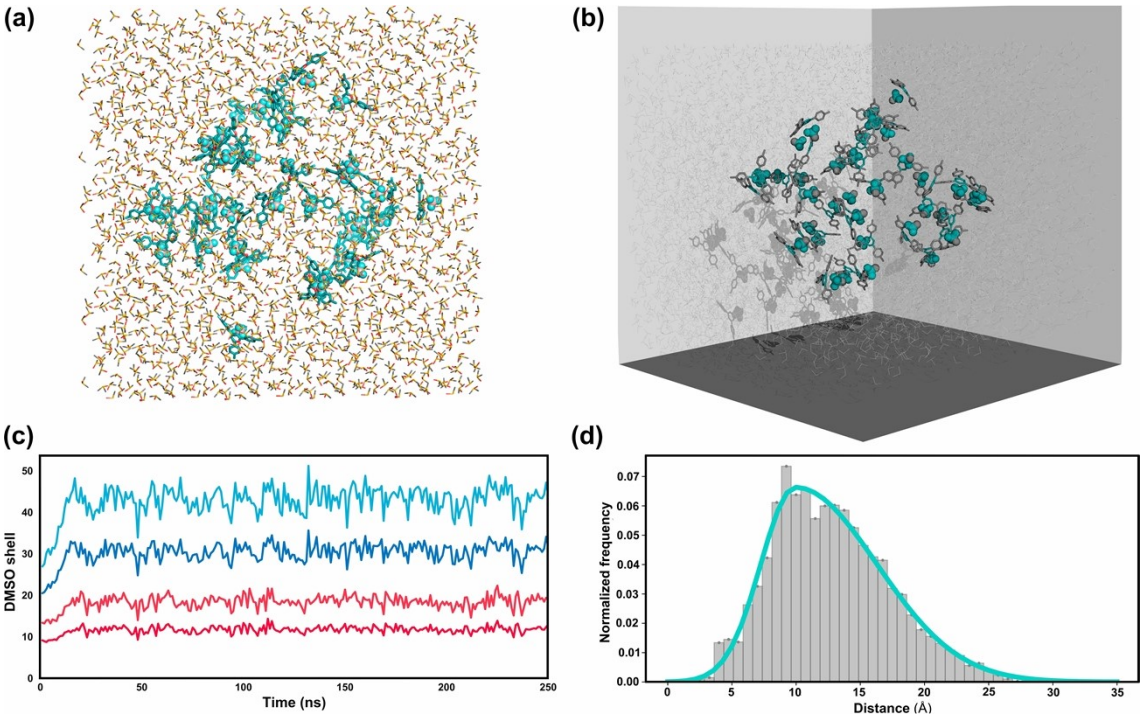
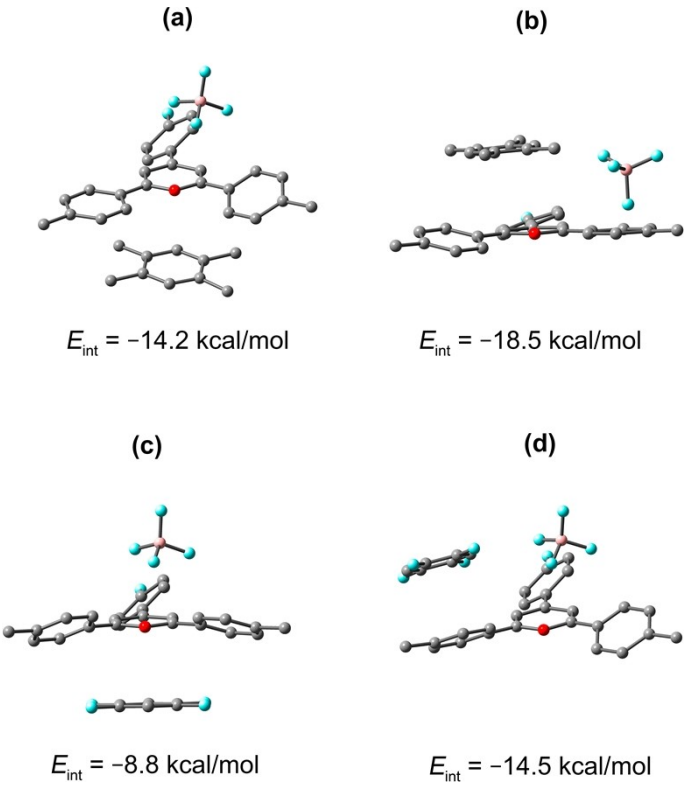


Figure S5. Optimized geometries (N_{imag} = 0) for the interaction of compound **1** at PBE0-D3/def2-TZVP level: (a) and (b) with TMB, (c) and (d) with TFB. Hydrogens are omitted for clarity.



Computational procedure for the calculation of ΔΔG: In order to compare the experimental and theoretical free energy for the association of compound **1** (containing BF_4^- anion) and TMB, solvation free energies (ΔG^{solv}) for each counterpart were computed following the next equations:

$$\Delta G_{1\cdots TMB}^{\ solv} = G^{SMD} - G^{gas\ phase}$$

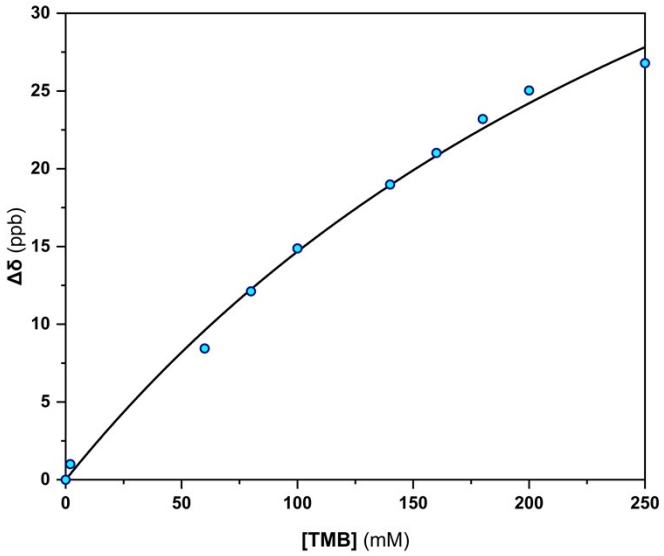
$$\Delta G_{TMB}^{solv} = G^{SMD} - G^{gas\ phase}$$

$$\Delta G_{1}^{solv} = G^{SMD} - G^{gas\ phase}$$

$$\Delta\Delta G = \Delta G_{1\cdots TMB}^{\ solv} - \Delta G_{1}^{solv} - \Delta G_{TMB}^{solv}$$

Environment	$G_{1\cdots TMB}$ (hartrees)	G_{TMB} (hartrees)	G_1 (hartrees)
Gas phase	0.342033	0.175835	0.542523
DMSO	0.343447	0.17517	0.542159
ΔG^{solv} (kcal/mol)	-0.23	-0.42	0.89

Figure S6. Non-linear fit for a 1:1 binding model to determine the association constant (K_a). The concentration of compound **1** was fixed at 20 mM.



NMR spectra

Figure S6. Compound **1**: ^{1}H NMR (DMSO-d_6, 500 MHz)

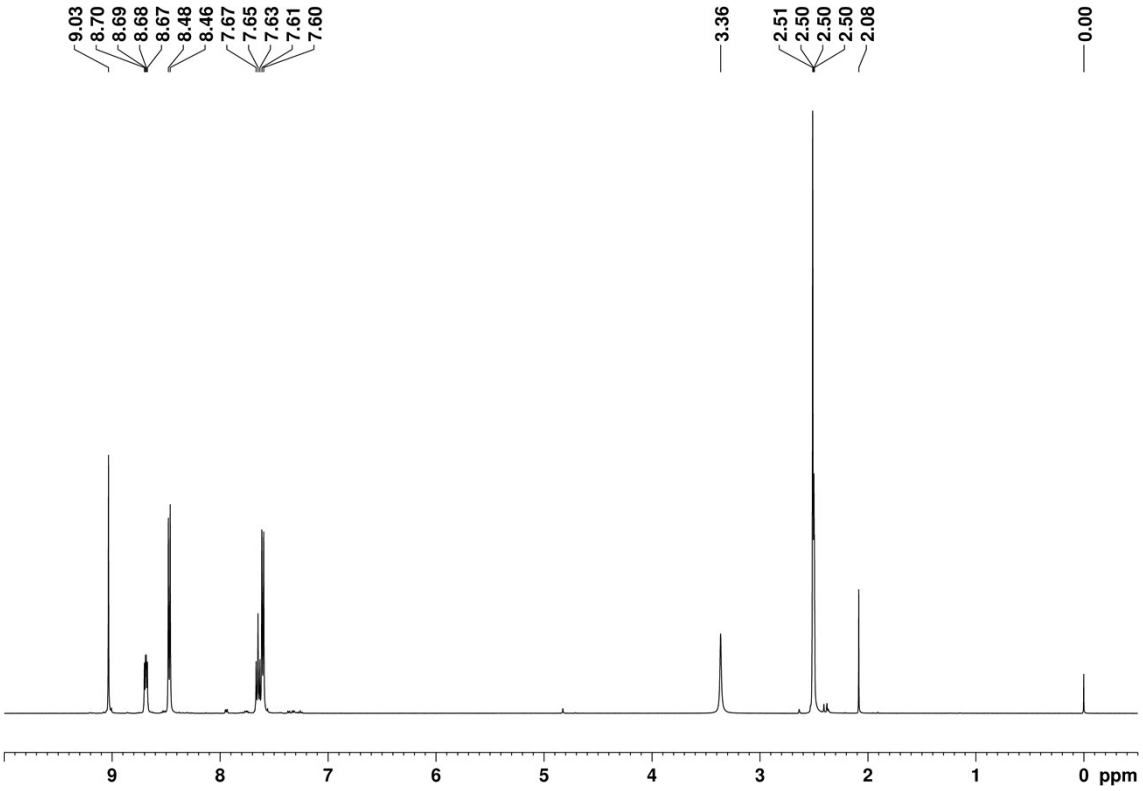


Figure S7. Compound **1**: ^{13}C NMR (DMSO-d_6, 125 MHz)

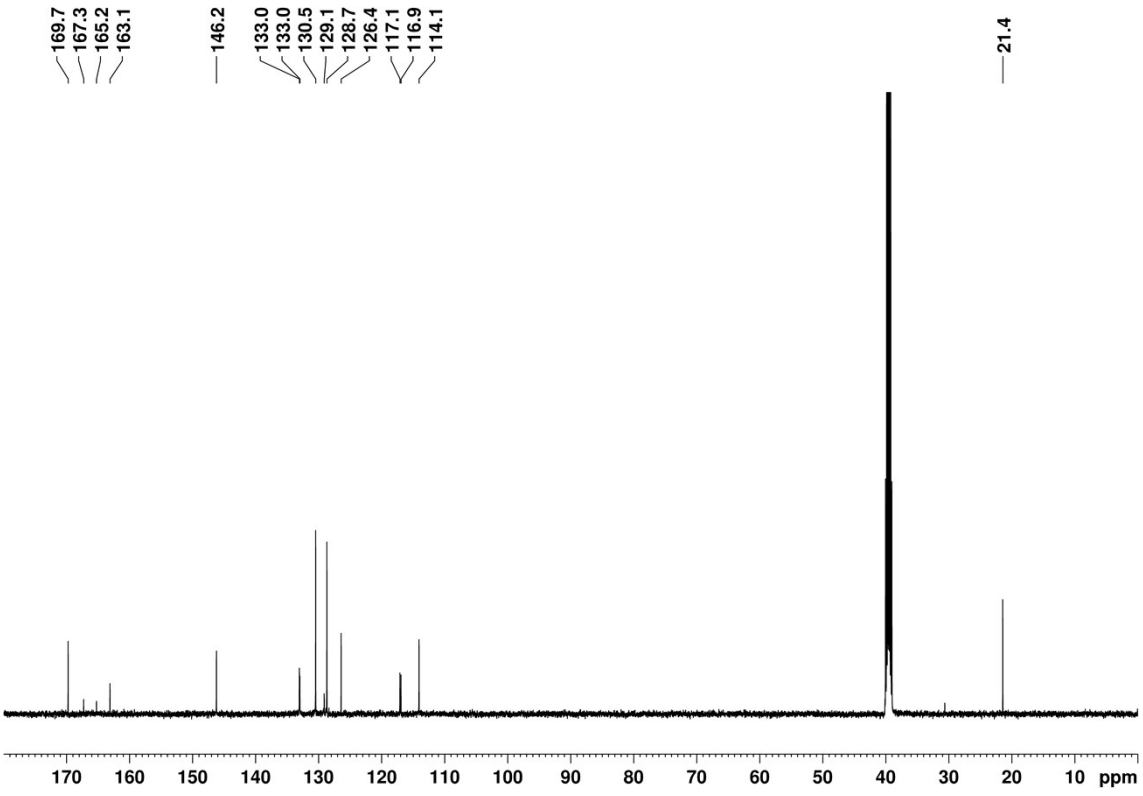
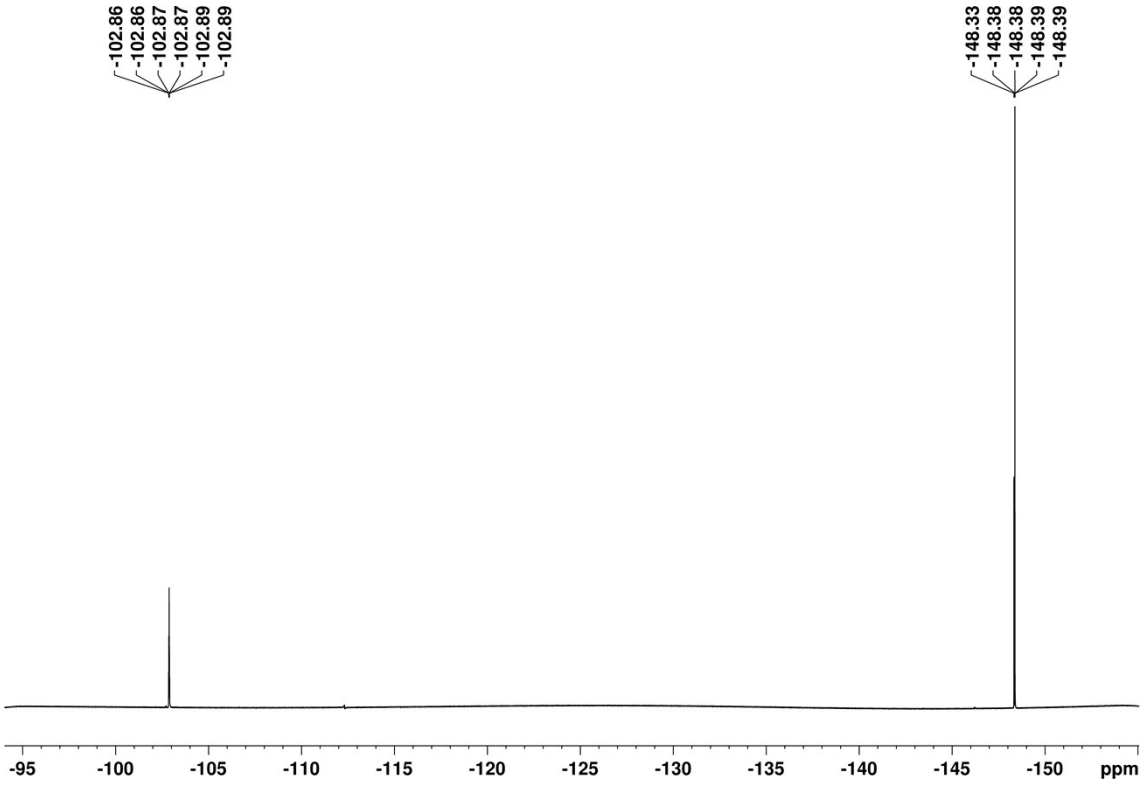


Figure S10. Compound **1**: ^{19}F NMR (DMSO-d_6, 470 MHz)



Cartesian coordinates

Complex ***2.10*** (X = Y = H)

C	-0.03170400	-0.00064200	1.14968700
C	-1.33988000	0.41360600	1.19638800
C	-2.00734900	0.63585500	0.00000000
C	-1.33988000	0.41360600	-1.19638800
C	-0.03170400	-0.00064200	-1.14968700
H	-1.79537800	0.60383700	2.15747300
O	0.58097900	-0.21615900	0.00000000
F	0.88771800	2.42188300	-1.14699000
F	0.88771800	2.42188300	1.14699000
F	1.02111200	4.41493000	0.00000000
F	-0.93856900	3.20340500	0.00000000
B	0.47518600	3.15420900	0.00000000
C	0.93472600	-3.33640200	1.20741100
C	1.62785900	-3.40849000	0.00000000
C	0.93472600	-3.33640200	-1.20741100
C	-0.45106200	-3.18052700	-1.20783300
C	-1.14421400	-3.09641100	0.00000000
C	-0.45106200	-3.18052700	1.20783300
H	1.47305600	-3.40991500	2.14596800
H	2.70487700	-3.53155900	0.00000000
H	1.47305600	-3.40991500	-2.14596800
H	-0.99267500	-3.13897100	-2.14694000
H	-2.22330800	-2.98542600	0.00000000
H	-0.99267500	-3.13897100	2.14694000
H	0.61204800	-0.16976200	-1.99904600
H	0.61204800	-0.16976200	1.99904600
H	-1.79537800	0.60383700	-2.15747300
H	-3.02400100	1.00776700	0.00000000

Complex ***2.11*** (X = H, Y = Br)

C	-0.41499800	0.95575400	1.15009200
C	-1.48881200	1.80985800	1.19650000
C	-2.03302000	2.25586000	0.00000000
C	-1.48881200	1.80985800	-1.19650000
C	-0.41499800	0.95575400	-1.15009200
H	-1.84432900	2.15283500	2.15743800
H	-1.84432900	2.15283500	-2.15743800
O	0.07878100	0.53261600	0.00000000
F	1.25189700	2.94005200	-1.14680200
F	1.25189700	2.94005200	1.14680200
F	2.06644500	4.76419500	0.00000000
F	-0.19132000	4.30550500	0.00000000
B	1.11899800	3.77022900	0.00000000
C	-0.75531200	-2.47311100	1.21337200
C	-0.13675900	-2.76704400	0.00000000
C	-0.75531200	-2.47311100	-1.21337200
C	-2.00541100	-1.85687900	-1.20588100
C	-2.62979500	-1.53864000	0.00000000
C	-2.00541100	-1.85687900	1.20588100
H	-0.26677500	-2.72926500	2.14622700
H	-0.26677500	-2.72926500	-2.14622700
H	-2.49636400	-1.63639100	-2.14786600
H	-3.60598900	-1.06695000	0.00000000
H	-2.49636400	-1.63639100	2.14786600
H	0.12823000	0.56993800	1.99922300
H	0.12823000	0.56993800	-1.99922300
H	-2.84834500	2.96786600	0.00000000
Br	1.55854600	-3.57725700	0.00000000

Complex ***2.12*** (X = H, Y = CF_3)

C	-0.38121000	0.92440500	1.15046200
C	-1.47725400	1.74973800	1.19665500
C	-2.03338100	2.18072000	0.00000000
C	-1.47725400	1.74973800	-1.19665500
C	-0.38121000	0.92440500	-1.15046200
H	-1.84107900	2.08413500	2.15754000
H	-1.84107900	2.08413500	-2.15754000
O	0.12221200	0.51260200	0.00000000
F	1.21858600	2.95855900	-1.14669900
F	1.21858600	2.95855900	1.14669900
F	1.97892400	4.80620000	0.00000000
F	-0.26430500	4.28086600	0.00000000
B	1.06175000	3.78493200	0.00000000
C	-0.69706900	-2.52322100	1.21134400
C	-0.06993900	-2.80928200	0.00000000
C	-0.69706900	-2.52322100	-1.21134400
C	-1.95307800	-1.92184700	-1.20744400
C	-2.57953600	-1.61399000	0.00000000
C	-1.95307800	-1.92184700	1.20744400
H	-0.20573700	-2.76707700	2.14592500
H	-0.20573700	-2.76707700	-2.14592500
H	-2.44841700	-1.70372900	-2.14715600
H	-3.56034100	-1.15140000	0.00000000
H	-2.44841700	-1.70372900	2.14715600
C	1.26732500	-3.49067200	0.00000000
F	1.99010000	-3.16758800	1.08098600
F	1.13272000	-4.82773600	0.00000000
F	1.99010000	-3.16758800	-1.08098600
H	0.17278500	0.55358800	1.99948100
H	0.17278500	0.55358800	-1.99948100
H	-2.86710000	2.87108500	0.00000000

Complex ***2.13*** (X = H, Y = NO_2)

C	0.64896400	0.29834900	1.15115000
C	1.39263400	1.45128600	1.19828300
C	1.78266900	2.03787300	0.00196500
C	1.39305000	1.45330900	-1.19547300
C	0.64937200	0.30028500	-1.15054900
H	1.70093500	1.83696000	2.15941900
H	1.70169400	1.84060300	-2.15584900
O	0.27453000	-0.23248900	-0.00021600
F	2.79215900	-1.14313500	-1.14748700
F	2.79193500	-1.14498800	1.14569300
F	4.69180400	-1.76328700	-0.00121300
F	3.99903400	0.43407200	0.00049700
B	3.60480300	-0.92608500	-0.00063800
C	-2.82243400	0.39095900	1.21820500
C	-3.06354000	-0.23064700	-0.00010700
C	-2.82307600	0.39046000	-1.21880900
C	-2.30344000	1.68242400	-1.20857900
C	-2.03592600	2.32744400	-0.00090500
C	-2.30278400	1.68291900	1.20717300
H	-3.04703700	-0.12945000	2.14010100
H	-3.04813000	-0.13033900	-2.14037400
H	-2.11881100	2.19138300	-2.14812700
H	-1.63923500	3.33659800	-0.00122000
H	-2.11768200	2.19227600	2.14641300
H	0.31927200	-0.28198900	1.99969400
H	0.31999900	-0.27862800	-2.00018700
H	2.41182500	2.91871800	0.00281600
N	-3.60702800	-1.59979400	0.00034000
O	-3.81280900	-2.12247700	1.09116700
O	-3.81484100	-2.12241900	-1.09012700

Complex ***2.14*** (X = H, Y = GeF_3)

C	-0.44475400	1.56950100	1.15086100

C	-1.41877900	2.53582800	1.19683500
C	-1.91069900	3.03875900	0.00000000
C	-1.41877900	2.53582800	-1.19683500
C	-0.44475400	1.56950100	-1.15086100
H	-1.73253800	2.91806700	2.15758700
H	-1.73253800	2.91806700	-2.15758700
O	-0.00213900	1.09279600	0.00000000
F	1.40543600	3.37223500	-1.14654600
F	1.40543600	3.37223500	1.14654600
F	2.40502800	5.10248000	0.00000000
F	0.11182300	4.88031100	0.00000000
B	1.36069400	4.21263700	0.00000000
C	-1.30134200	-1.79895500	1.21282000
C	-0.72405800	-2.19211200	0.00000000
C	-1.30134200	-1.79895500	-1.21282000
C	-2.44741900	-1.00663700	-1.20875400
C	-3.01650000	-0.60628200	0.00000000
C	-2.44741900	-1.00663700	1.20875400
H	-0.86152900	-2.10679500	2.15604000
H	-0.86152900	-2.10679500	-2.15604000
H	-2.90183400	-0.70959400	-2.14773700
H	-3.91274400	0.00454600	0.00000000
H	-2.90183400	-0.70959400	2.14773700
H	0.05465000	1.12774200	1.99999100
H	0.05465000	1.12774200	-1.99999100
H	-2.64208900	3.83673500	0.00000000
Ge	0.83781600	-3.28320600	0.00000000
F	0.52637800	-4.96394500	0.00000000
F	1.80050100	-2.99732900	1.38440800
F	1.80050100	-2.99732900	-1.38440800

*Complex **2.15*** (X = H, Y = Me)

C	-0.24166400	0.23258600	1.14961100
C	-1.48829000	0.80616700	1.19637100
C	-2.12327200	1.10882300	0.00000000
C	-1.48829000	0.80616700	-1.19637100
C	-0.24166400	0.23258600	-1.14961100
H	-1.91713700	1.05036300	2.15750600
H	-1.91713700	1.05036300	-2.15750600
O	0.33950300	-0.05686200	0.00000000
F	1.00252700	2.50430200	-1.14720300
F	1.00252700	2.50430200	1.14720300
F	1.39537500	4.46260500	0.00000000
F	-0.70586700	3.51734500	0.00000000
B	0.68891700	3.28400800	0.00000000
C	0.37860900	-3.14754400	1.20023300
C	1.08306200	-3.28086600	0.00000000
C	0.37860900	-3.14754400	-1.20023300
C	-0.98832200	-2.87481100	-1.20446700
C	-1.67667300	-2.73089100	0.00000000
C	-0.98832200	-2.87481100	1.20446700
H	0.90765700	-3.26200400	2.14193400
H	0.90765700	-3.26200400	-2.14193400
H	-1.51870900	-2.78558500	-2.14693600
H	-2.74156600	-2.52517800	0.00000000
H	-1.51870900	-2.78558500	2.14693600
C	2.55048200	-3.60252000	0.00000000
H	3.04411700	-3.19614500	0.88360700
H	2.70797200	-4.68420100	0.00000000
H	3.04411700	-3.19614500	-0.88360700
H	0.37562700	-0.01622900	1.99885000
H	0.37562700	-0.01622900	-1.99885000
H	-3.08678500	1.60240000	0.00000000

*Complex **2.16*** (X = H, Y = NH_2)

C	-0.20222100	0.21541200	1.14921200
C	-1.44616000	0.79461100	1.19602900
C	-2.07912400	1.10222900	0.00000000
C	-1.44616000	0.79461100	-1.19602900
C	-0.20222100	0.21541200	-1.14921200
H	-1.87336300	1.04136300	2.15721100
H	-1.87336300	1.04136300	-2.15721100
O	0.37942000	-0.07427700	0.00000000
F	0.98246300	2.53453400	-1.14705700
F	0.98246300	2.53453400	1.14705700
F	1.35822700	4.49616700	0.00000000
F	-0.73485400	3.53360000	0.00000000
B	0.66223200	3.31065700	0.00000000
C	0.38814000	-3.17374300	1.20384300
C	1.08906300	-3.32155900	0.00000000
C	0.38814000	-3.17374300	-1.20384300
C	-0.97107700	-2.87637100	-1.20163300
C	-1.66068600	-2.71404600	0.00000000
C	-0.97107700	-2.87637100	1.20163300
H	0.91428800	-3.30096600	2.14550400
H	0.91428800	-3.30096600	-2.14550400
H	-1.49634300	-2.78281700	-2.14655400
H	-2.72166900	-2.49274300	0.00000000
H	-1.49634300	-2.78281700	2.14655400
H	2.82635300	-3.97068400	-0.83713800
H	2.82635300	-3.97068400	0.83713800
N	2.46119900	-3.54019500	0.00000000
H	0.41470800	-0.03483100	1.99833600
H	-3.03891900	1.60272100	0.00000000
H	0.41470800	-0.03483100	-1.99833600

*Complex **2.17*** (X = H, Y = NMe_2)

C	-0.47284700	0.73549600	1.14915300
C	-1.56721900	1.56348800	1.19613300
C	-2.12229100	1.99569300	0.00000000
C	-1.56721900	1.56348800	-1.19613300
C	-0.47284700	0.73549600	-1.14915300
H	-1.93512900	1.89190200	2.15739600
H	-1.93512900	1.89190200	-2.15739600
O	0.03452700	0.33077200	0.00000000
F	1.24808400	2.68139900	-1.14737700
F	1.24808400	2.68139900	1.14737700
F	2.05822900	4.50668500	0.00000000
F	-0.19851300	4.04229900	0.00000000
B	1.11123900	3.50977300	0.00000000
C	-0.50172500	-2.66778200	1.20467700
C	0.19140000	-2.90989000	0.00000000
C	-0.50172500	-2.66778200	-1.20467700
C	-1.79358900	-2.15123600	-1.19764400
C	-2.44988100	-1.87158500	0.00000000
C	-1.79358900	-2.15123600	1.19764400
H	-0.03595200	-2.88468000	2.15677000
H	-0.03595200	-2.88468000	-2.15677000
H	-2.29753400	-1.98567900	-2.14472300
H	-3.46100600	-1.48127800	0.00000000
H	-2.29753400	-1.98567900	2.14472300
N	1.49696300	-3.35697000	0.00000000
H	0.07581700	0.35881800	1.99820300
H	-2.95824900	2.68356100	0.00000000
H	0.07581700	0.35881800	-1.99820300
C	2.03604600	-3.89399800	1.23310600
H	3.06838600	-4.19245100	1.06196200
H	2.04139700	-3.13388800	2.01574600
H	1.47390800	-4.76476800	1.59743500
C	2.03604600	-3.89399800	-1.23310600
H	1.47390800	-4.76476800	-1.59743500
H	2.04139700	-3.13388800	-2.01574600
H	3.06838600	-4.19245100	-1.06196200

*Complex **3.10*** (X = Br, Y = H)

C	-0.72121000	0.41041700	1.14804200
C	0.46038000	-0.28184800	1.20116600
C	1.06514400	-0.63492200	0.00000000
C	0.46038000	-0.28184800	-1.20116600
C	-0.72121000	0.41041700	-1.14804200
H	0.86919800	-0.56866400	2.15958300
O	-1.27062700	0.76658600	0.00000000
F	-2.24492100	-1.66365900	-1.14725400
F	-2.24492100	-1.66365900	1.14725400
F	-2.81050100	-3.57971900	0.00000000
F	-0.63379700	-2.82259700	0.00000000
B	-2.00430300	-2.46870300	0.00000000
C	-0.72629000	3.87331300	1.20746600
C	-1.37199000	4.13545900	0.00000000
C	-0.72629000	3.87331300	-1.20746600
C	0.56116400	3.33717400	-1.20781900
C	1.20357300	3.06297500	0.00000000
C	0.56116400	3.33717400	1.20781900
H	-1.22237500	4.09492200	2.14602100
H	-2.37190900	4.55414500	0.00000000
H	-1.22237500	4.09492200	-2.14602100
H	1.07005400	3.14672800	-2.14690200
H	2.20898100	2.65485100	0.00000000
H	1.07005400	3.14672800	2.14690200
H	-1.30558400	0.71744400	-2.00185300
H	-1.30558400	0.71744400	2.00185300
H	0.86919800	-0.56866400	-2.15958300
Br	2.64757900	-1.59034400	0.00000000

*Complex **3.11*** (X = Br, Y = Br)

C	-0.37886600	-0.29823800	1.14852400
C	0.45518600	-1.38427200	1.20129300
C	0.88439400	-1.93787400	0.00000000
C	0.45518600	-1.38427200	-1.20129300
C	-0.37886600	-0.29823800	-1.14852400
H	0.72392700	-1.80559900	2.15959600
O	-0.75016400	0.24174400	0.00000000
F	-2.54343500	-1.68105300	-1.14710700
F	-2.54343500	-1.68105300	1.14710700
F	-3.78166100	-3.24914900	0.00000000
F	-1.47957400	-3.35659600	0.00000000
B	-2.62053900	-2.51806900	0.00000000
C	1.04127300	2.82683000	1.21339500
C	0.54420800	3.29813400	0.00000000
C	1.04127300	2.82683000	-1.21339500
C	2.03837900	1.85294400	-1.20586200
C	2.53311300	1.35624800	0.00000000
C	2.03837900	1.85294400	1.20586200
H	0.65692800	3.22244200	2.14630200
H	0.65692800	3.22244200	-2.14630200
H	2.43656300	1.49077400	-2.14786900
H	3.31380300	0.60352000	0.00000000
H	2.43656300	1.49077400	2.14786900
H	-0.80649200	0.20559700	-2.00208300
H	-0.80649200	0.20559700	2.00208300
H	0.72392700	-1.80559900	-2.15959600
Br	1.99605400	-3.41393700	0.00000000
Br	-0.81721600	4.59310600	0.00000000

*Complex **3.12*** (X = Br, Y = CF_3)

C	-0.42496000	-0.27446500	1.14891000
C	0.45304300	-1.32522200	1.20144400
C	0.90546800	-1.86012400	0.00000000
C	0.45304300	-1.32522200	-1.20144400
C	-0.42496000	-0.27446500	-1.14891000
H	0.73814500	-1.73587600	2.15969500
O	-0.81624800	0.25133800	0.00000000
F	-2.51539400	-1.75774200	-1.14699200
F	-2.51539400	-1.75774200	1.14699200
F	-3.68761000	-3.37604700	0.00000000
F	-1.38291100	-3.38763900	0.00000000
B	-2.55834800	-2.59768600	0.00000000
C	0.95783600	2.88836200	1.21142300
C	0.44611200	3.35035500	0.00000000
C	0.95783600	2.88836200	-1.21142300
C	1.97359100	1.93566800	-1.20743700
C	2.47768100	1.45250100	0.00000000
C	1.97359100	1.93566800	1.20743700
H	0.56418500	3.27031500	2.14603200
H	0.56418500	3.27031500	-2.14603200
H	2.37979300	1.57782600	-2.14714700
H	3.27193400	0.71372300	0.00000000
H	2.37979300	1.57782600	2.14714700
H	-0.87362400	0.21149800	-2.00215900
H	-0.87362400	0.21149800	2.00215900
H	0.73814500	-1.73587600	-2.15969500
Br	2.07918500	-3.28693500	0.00000000
C	-0.62245300	4.40412600	0.00000000
F	-0.09051500	5.63798400	0.00000000
F	-1.40929100	4.31425500	1.08100400
F	-1.40929100	4.31425500	-1.08100400

*Complex **3.14*** (X = Br, Y = GeF_3)

C	-0.37933700	-0.84766600	1.14929500
C	0.41894700	-1.96008400	1.20156600
C	0.83176800	-2.52628800	0.00000000
C	0.41894700	-1.96008400	-1.20156600
C	-0.37933700	-0.84766600	-1.14929500
H	0.67155400	-2.39172800	2.15976800
O	-0.72859000	-0.29264900	0.00000000
F	-2.56325900	-2.18116300	-1.14686400
F	-2.56325900	-2.18116300	1.14686400
F	-3.84626700	-3.71336600	0.00000000
F	-1.54821200	-3.88677100	0.00000000
B	-2.66576000	-3.01633600	0.00000000
C	1.35035100	2.15553800	1.21286600
C	0.88592900	2.67747200	0.00000000
C	1.35035100	2.15553800	-1.21286600
C	2.26862800	1.10765400	-1.20872000
C	2.72237500	0.57986700	0.00000000
C	2.26862800	1.10765400	1.20872000
H	0.99893600	2.56133200	2.15612700
H	0.99893600	2.56133200	-2.15612700
H	2.63646800	0.70827300	-2.14770400
H	3.44118900	-0.23276400	0.00000000
H	2.63646800	0.70827300	2.14770400
H	-0.79160500	-0.33051000	-2.00282700
H	-0.79160500	-0.33051000	2.00282700
H	0.67155400	-2.39172800	-2.15976800
Br	1.90053800	-4.03278500	0.00000000
F	0.32638400	5.66903800	0.00000000
F	-1.37478500	4.05640800	1.38416700
F	-1.37478500	4.05640800	-1.38416700
Ge	-0.37122000	4.10882100	0.00000000

*Complex **3.15*** (X = Br, Y = Me)

C	-0.30228100	0.50097400	-1.14790700
C	0.62843700	-0.50360600	-1.20114800
C	1.10358300	-1.01784600	-0.00000900

C	0.62844200	-0.50362000	1.20113900
C	-0.30227600	0.50096000	1.14791400
H	0.99595900	-0.84153100	-2.15960300
O	-0.76801600	0.96107100	0.00000700
F	1.37646500	2.45222100	1.14738200
F	1.37646000	2.45223500	-1.14735800
F	3.12208800	3.42353000	0.00001400
F	2.85973400	1.13380400	0.00000100
B	2.21443800	2.39351300	0.00001000
C	-3.66069200	-0.16334100	-1.20027800
C	-4.04455800	0.44226700	0.00000000
C	-3.66070000	-0.16333200	1.20028700
C	-2.90272400	-1.33313900	1.20449500
C	-2.51415600	-1.91955100	0.00001500
C	-2.90271500	-1.33314900	-1.20447100
H	-3.96340800	0.28542300	-2.14196700
H	-3.96342400	0.28544100	2.14196900
H	-2.62423200	-1.79346500	2.14692200
H	-1.92926300	-2.83322900	0.00002100
H	-2.62421600	-1.79348200	-2.14689300
H	-0.72810400	1.00510500	2.00178600
H	-0.72811400	1.00512800	-2.00177100
H	0.99597000	-0.84155600	2.15958900
Br	2.37873000	-2.35637200	-0.00002000
C	-4.88622200	1.68660200	-0.00000700
H	-5.94938000	1.43255400	0.00002200
H	-4.69146100	2.29556500	0.88363700
H	-4.69150000	2.29552900	-0.88368400

*Complex **3.16*** (X = Br, Y = NH_2)

C	-0.52645600	0.30961200	1.14755200
C	0.49479200	-0.60284100	1.20088200
C	1.01709100	-1.06916200	0.00000000
C	0.49479200	-0.60284100	-1.20088200
C	-0.52645600	0.30961200	-1.14755200
H	0.83959900	-0.96385200	2.15931900
O	-0.99692900	0.76501900	0.00000000
F	-2.42075000	-1.44914000	-1.14736700
F	-2.42075000	-1.44914000	1.14736700
F	-3.34639100	-3.21922000	0.00000000
F	-1.06446400	-2.89825500	0.00000000
B	-2.33987200	-2.28446200	0.00000000
C	0.10051400	3.68225700	1.20387300
C	-0.50509600	4.06489300	0.00000000
C	0.10051400	3.68225700	-1.20387300
C	1.27056400	2.92925700	-1.20162200
C	1.86043100	2.53640400	0.00000000
C	1.27056400	2.92925700	1.20162200
H	-0.34830400	3.98476800	2.14557200
H	-0.34830400	3.98476800	-2.14557200
H	1.73061000	2.65876700	-2.14652700
H	2.77750200	1.95825700	0.00000000
H	1.73061000	2.65876700	2.14652700
H	-1.03835900	0.72639600	-2.00121700
H	-1.03835900	0.72639600	2.00121700
H	0.83959900	-0.96385200	-2.15931900
N	-1.71546500	4.74753300	0.00000000
H	-1.90670200	5.27917300	0.83692400
H	-1.90670200	5.27917300	-0.83692400
Br	2.38044400	-2.31799300	0.00000000

*Complex **3.17*** (X = Br, Y = NMe_2)

C	-0.29415400	-0.09395700	1.14749200
C	0.49765100	-1.21145000	1.20097300
C	0.90186500	-1.78280600	0.00000000
C	0.49765100	-1.21145000	-1.20097300
C	-0.29415400	-0.09395700	-1.14749200
H	0.75513200	-1.63897900	2.15946300
O	-0.65292200	0.45315300	0.00000000
F	-2.56313400	-1.33113300	-1.14758500
F	-2.56313400	-1.33113300	1.14758500
F	-3.87235300	-2.83948900	0.00000000
F	-1.57766000	-3.05366600	0.00000000
B	-2.67685300	-2.16253800	0.00000000
C	0.93507000	3.06468800	1.20473200
C	0.37456900	3.53899000	0.00000000
C	0.93507000	3.06468800	-1.20473200
C	1.95668000	2.12014700	-1.19765600
C	2.46955300	1.62389600	0.00000000
C	1.95668000	2.12014700	1.19765600
H	0.57796700	3.43406900	2.15685000
H	0.57796700	3.43406900	-2.15685000
H	2.36823700	1.78526100	-2.14471100
H	3.27395300	0.89713100	0.00000000
H	2.36823700	1.78526100	2.14471100
H	-0.69870600	0.42733400	-2.00117300
H	-0.69870600	0.42733400	2.00117300
H	0.75513200	-1.63897900	-2.15946300
N	-0.68418100	4.42397300	0.00000000
Br	1.94827000	-3.30754800	0.00000000
C	-0.99498500	5.11843800	1.23326200
H	-1.85109100	5.76789800	1.06192100
H	-1.27334100	4.41072900	2.01559400
H	-0.15771600	5.72899700	1.59808200
C	-0.99498500	5.11843800	-1.23326200
H	-0.15771600	5.72899700	-1.59808200
H	-1.27334100	4.41072900	-2.01559400
H	-1.85109100	5.76789800	-1.06192100

*Complex **4.10*** (X = CF_3, Y = H)

C	-0.69421700	0.29852900	1.14996900
C	0.53812100	-0.30832600	1.19899000
C	1.17144800	-0.59900000	0.00000000
C	0.53812100	-0.30832600	-1.19899000
C	-0.69421700	0.29852900	-1.14996900
H	0.97511800	-0.55009000	2.15749000
O	-1.25469700	0.61858200	0.00000000
F	-2.21467600	-1.73961300	-1.14852900
F	-2.21467600	-1.73961300	1.14852900
F	-2.70849100	-3.67525200	0.00000000
F	-0.56245500	-2.83091200	0.00000000
B	-1.94495400	-2.53682700	0.00000000
C	-0.91850900	3.73738700	1.20758700
C	-1.58197900	3.95093100	0.00000000
C	-0.91850900	3.73738700	-1.20758700
C	0.40481300	3.29749900	-1.20811700
C	1.06553200	3.07033400	0.00000000
C	0.40481300	3.29749900	1.20811700
H	-1.42895300	3.92425100	2.14601700
H	-2.60960100	4.29603000	0.00000000
H	-1.42895300	3.92425100	-2.14601700
H	0.92722500	3.14727700	-2.14714700
H	2.09934800	2.74071600	0.00000000
H	0.92722500	3.14727700	2.14714700
H	-1.30019100	0.57134200	-1.99965900
H	-1.30019100	0.57134200	1.99965900
H	0.97511800	-0.55009000	-2.15749000
C	2.53393900	-1.25134100	0.00000000
F	3.23041000	-0.87737700	-1.08180400
F	3.23041000	-0.87737700	1.08180400
F	2.44281800	-2.57246200	0.00000000

*Complex **4.11*** (X = CF_3, Y = Br)

C	-0.35857200	-0.37228700	1.15043800
C	0.48294700	-1.45802800	1.19902700
C	0.92655200	-1.99545800	0.00000000
C	0.48294700	-1.45802800	-1.19902700
C	-0.35857200	-0.37228700	-1.15043800
H	0.76809900	-1.86826100	2.15749100
O	-0.71784700	0.16489700	0.00000000
F	-2.57493300	-1.59047600	-1.14836400
F	-2.57493300	-1.59047600	1.14836400
F	-3.87049500	-3.11127000	0.00000000
F	-1.57185000	-3.29789100	0.00000000
B	-2.68396900	-2.42614700	0.00000000
C	1.05326500	2.74792100	1.21347200
C	0.55450400	3.21793500	0.00000000
C	1.05326500	2.74792100	-1.21347200
C	2.05401600	1.77760500	-1.20607300
C	2.55069400	1.28262500	0.00000000
C	2.05401600	1.77760500	1.20607300
H	0.66922300	3.14393500	2.14637900
H	0.66922300	3.14393500	-2.14637900
H	2.45526200	1.41839900	-2.14800800
H	3.33725300	0.53598400	0.00000000
H	2.45526200	1.41839900	2.14800800
H	-0.78455500	0.13865000	-2.00005100
H	-0.78455500	0.13865000	2.00005100
H	0.76809900	-1.86826100	-2.15749100
C	1.87433300	-3.17218500	0.00000000
F	2.66445700	-3.13271700	-1.08189800
F	2.66445700	-3.13271700	1.08189800
F	1.22575300	-4.32574800	0.00000000
Br	-0.80769000	4.51147800	0.00000000

*Complex **4.12*** (X = CF_3, Y = CF_3)

C	-0.42538100	-0.33307800	1.15085900
C	0.48084700	-1.36518800	1.19926600
C	0.95780800	-1.87292100	0.00000000
C	0.48084700	-1.36518800	-1.19926600
C	-0.42538100	-0.33307800	-1.15085900
H	0.79028500	-1.75779800	2.15759300
O	-0.81355000	0.18348600	0.00000000
F	-2.55381500	-1.69063400	-1.14824300
F	-2.55381500	-1.69063400	1.14824300
F	-3.74914300	-3.29155200	0.00000000
F	-1.44345200	-3.33045700	0.00000000
B	-2.60961600	-2.53185500	0.00000000
C	0.97225500	2.79583700	1.21137100
C	0.44589300	3.24142100	0.00000000
C	0.97225500	2.79583700	-1.21137100
C	2.01727800	1.87536500	-1.20761500
C	2.53561600	1.40741400	0.00000000
C	2.01727800	1.87536500	1.20761500
H	0.56709300	3.16550400	2.14608200
H	0.56709300	3.16550400	-2.14608200
H	2.43517500	1.53090800	-2.14724900
H	3.35435700	0.69587000	0.00000000
H	2.43517500	1.53090800	2.14724900
H	-0.88117700	0.15213000	-2.00022500
H	-0.88117700	0.15213000	2.00022500
H	0.79028500	-1.75779800	-2.15759300
C	1.98095600	-2.98490800	0.00000000
F	2.76672500	-2.89226800	-1.08187900
F	2.76672500	-2.89226800	1.08187900
F	1.41038800	-4.17854700	0.00000000
C	-0.65949800	4.25674000	0.00000000
F	-0.17267400	5.50849900	0.00000000
F	-1.44243000	4.13739300	1.08108500
F	-1.44243000	4.13739300	-1.08108500

*Complex **4.13*** (X = CF_3, Y = NO_2)

C	-0.50498500	-0.10820600	1.15128300
C	0.47374300	-1.07179900	1.19939700
C	0.98697200	-1.54268000	0.00000000
C	0.47374300	-1.07179900	-1.19939700
C	-0.50498500	-0.10820600	-1.15128300
H	0.80992800	-1.44200700	2.15769800
H	0.80992800	-1.44200700	-2.15769800
O	-0.92774700	0.38103100	0.00000000
F	-2.51974200	-1.61769100	-1.14814300
F	-2.51974200	-1.61769100	1.14814300
F	-3.59575400	-3.30133200	0.00000000
F	-1.29335700	-3.17276400	0.00000000
B	-2.51478500	-2.46143700	0.00000000
C	0.73464100	3.11258500	1.21863000
C	0.20813200	3.52131700	0.00000000
C	0.73464100	3.11258500	-1.21863000
C	1.82276500	2.24336200	-1.20800900
C	2.36300600	1.80106500	0.00000000
C	1.82276500	2.24336200	1.20800900
H	0.30131800	3.47830400	2.14048500
H	0.30131800	3.47830400	-2.14048500
H	2.25810400	1.92046400	-2.14733300
H	3.21691100	1.13224700	0.00000000
H	2.25810400	1.92046400	2.14733300
H	-0.99496000	0.34248500	2.00079300
H	-0.99496000	0.34248500	-2.00079300
N	-0.95013400	4.43141900	0.00000000
O	-1.39277000	4.77746600	1.09089400
O	-1.39277000	4.77746600	-1.09089400
C	2.09062200	-2.57519200	0.00000000
F	2.86718900	-2.42288500	1.08192500
F	2.86718900	-2.42288500	-1.08192500
F	1.61189200	-3.80803400	0.00000000

*Complex **4.14*** (X = CF_3, Y = GeF_3)

C	-0.38555200	-0.94451300	1.15077000
C	0.43806600	-2.04378600	1.19926000
C	0.87460600	-2.58719700	0.00000000
C	0.43806600	-2.04378600	-1.19926000
C	-0.38555200	-0.94451300	-1.15077000
H	0.71496000	-2.45974500	2.15777000
O	-0.73227000	-0.39834000	0.00000000
F	-2.58490500	-2.17186800	-1.14819200
F	-2.58490500	-2.17186800	1.14819200
F	-3.89735800	-3.67862700	0.00000000
F	-1.60103400	-3.89060000	0.00000000
B	-2.70451100	-3.00716500	0.00000000
C	1.33139000	2.10601700	1.21283200
C	0.87465800	2.63509300	0.00000000
C	1.33139000	2.10601700	-1.21283200
C	2.22881900	1.04032200	-1.20911000
C	2.67132700	0.50267100	0.00000000
C	2.22881900	1.04032200	1.20911000
H	1.00608600	2.53368200	2.15585200
H	1.00608600	2.53368200	-2.15585200
H	2.59673200	0.64033100	-2.14791900
H	3.38060500	-0.31842500	0.00000000
H	2.59673200	0.64033100	2.14791900
H	-0.80208800	-0.42609500	-2.00058900
H	-0.80208800	-0.42609500	2.00058900
H	0.71496000	-2.45974500	-2.15777000
C	1.81431900	-3.77114100	0.00000000

F	2.60508600	-3.73346000	-1.08158700
F	2.60508600	-3.73346000	1.08158700
F	1.16150200	-4.92084600	0.00000000
Ge	-0.36653100	4.08136200	0.00000000
F	-0.18864700	5.07156100	1.38277900
F	-2.00000400	3.57849400	0.00000000
F	-0.18864700	5.07156100	-1.38277900

*Complex **4.15*** (X = CF_3, Y = Me)

C	-0.45974200	0.21894700	1.14990000
C	0.56731700	-0.69328800	1.19896300
C	1.10025100	-1.14208300	0.00000000
C	0.56731700	-0.69328800	-1.19896300
C	-0.45974200	0.21894700	-1.14990000
H	0.92529100	-1.04152900	2.15744800
O	-0.91681100	0.67419700	0.00000000
F	-2.49758800	-1.31454000	-1.14864100
F	-2.49758800	-1.31454000	1.14864100
F	-3.48524700	-3.05073700	0.00000000
F	-1.19234000	-2.80320800	0.00000000
B	-2.44816700	-2.15390500	0.00000000
C	0.13264700	3.57328900	1.20032100
C	-0.48335200	3.94053800	0.00000000
C	0.13264700	3.57328900	-1.20032100
C	1.32214800	2.84639300	-1.20466000
C	1.91872000	2.47326400	0.00000000
C	1.32214800	2.84639300	1.20466000
H	-0.32380300	3.86434100	2.14200400
H	-0.32380300	3.86434100	-2.14200400
H	1.79104500	2.58221100	-2.14706600
H	2.84938000	1.91576700	0.00000000
H	1.79104500	2.58221100	2.14706600
H	-0.97072800	0.64375500	-1.99954600
H	-0.97072800	0.64375500	1.99954600
H	0.92529100	-1.04152900	-2.15744800
C	2.23710100	-2.13648200	0.00000000
F	3.00849000	-1.96508400	-1.08191500
F	3.00849000	-1.96508400	1.08191500
F	1.79201700	-3.38427800	0.00000000
C	-1.74970700	4.74850900	0.00000000
H	-1.52378300	5.81797600	0.00000000
H	-2.35325300	4.53766400	-0.88362400
H	-2.35325300	4.53766400	0.88362400

*Complex **4.16*** (X = CF_3, Y = NH_2)

C	-0.48698500	0.22413800	1.14945000
C	0.56037700	-0.66471600	1.19863900
C	1.10284600	-1.10232000	0.00000000
C	0.56037700	-0.66471600	-1.19863900
C	-0.48698500	0.22413800	-1.14945000
H	0.92603100	-1.00448900	2.15720700
O	-0.95529700	0.66848200	0.00000000
F	-2.45859600	-1.39655700	-1.14865500
F	-2.45859600	-1.39655700	1.14865500
F	-3.40474700	-3.15549800	0.00000000
F	-1.11856900	-2.85447100	0.00000000
B	-2.38849800	-2.23415700	0.00000000
C	0.05837200	3.59325800	1.20400100
C	-0.55892800	3.95734600	0.00000000
C	0.05837200	3.59325800	-1.20400100
C	1.25007900	2.87495200	-1.20179500
C	1.85114900	2.49902100	0.00000000
C	1.25007900	2.87495200	1.20179500
H	-0.39849600	3.88344600	2.14570800
H	-0.39849600	3.88344600	-2.14570800
H	1.71942700	2.62043100	-2.14664700
H	2.78684300	1.95151900	0.00000000
H	1.71942700	2.62043100	2.14664700
H	-1.00774000	0.63708600	-1.99899400
H	-1.00774000	0.63708600	1.99899400
H	0.92603100	-1.00448900	-2.15720700
C	2.26459900	-2.06737900	0.00000000
F	3.03175500	-1.87534200	-1.08184100
F	3.03175500	-1.87534200	1.08184100
F	1.85436700	-3.32686100	0.00000000
N	-1.78823400	4.60299200	0.00000000
H	-1.99960900	5.12578900	0.83751800
H	-1.99960900	5.12578900	-0.83751800

*Complex **4.17*** (X = CF_3, Y = NMe_2)

C	-0.26406600	-0.16971600	1.14944500
C	0.52389400	-1.29502200	1.19873100
C	0.93711600	-1.85609800	0.00000000
C	0.52389400	-1.29502200	-1.19873100
C	-0.26406600	-0.16971600	-1.14944500
H	0.79325200	-1.71521500	2.15731100
O	-0.60720800	0.37627800	0.00000000
F	-2.61826800	-1.17671400	-1.14885600
F	-2.61826800	-1.17671400	1.14885600
F	-3.98265400	-2.63517300	0.00000000
F	-1.69503100	-2.92797600	0.00000000
B	-2.76456100	-2.00374600	0.00000000
C	0.98075900	2.96265800	1.20493800
C	0.41990100	3.43713300	0.00000000
C	0.98075900	2.96265800	-1.20493800
C	2.00136000	2.01702100	-1.19787100
C	2.51292900	1.51900900	0.00000000
C	2.00136000	2.01702100	1.19787100
H	0.62559400	3.33437300	2.15691800
H	0.62559400	3.33437300	-2.15691800
H	2.41440600	1.68346800	-2.14483000
H	3.31898900	0.79407000	0.00000000
H	2.41440600	1.68346800	2.14483000
H	-0.66237400	0.36224000	-1.99881500
H	-0.66237400	0.36224000	1.99881500
H	0.79325200	-1.71521500	-2.15731100
C	1.80945600	-3.08855000	0.00000000
F	2.59952800	-3.10424800	-1.08187900
F	2.59952800	-3.10424800	1.08187900
F	1.08370600	-4.19772400	0.00000000
N	-0.63714500	4.32197100	0.00000000
C	-0.95611000	5.01071500	1.23444700
H	-1.81325300	5.65818400	1.06141300
H	-1.23608000	4.29910200	2.01271800
H	-0.12246300	5.62233700	1.60520400
C	-0.95611000	5.01071500	-1.23444700
H	-0.12246300	5.62233700	-1.60520400
H	-1.23608000	4.29910200	-2.01271800
H	-1.81325300	5.65818400	-1.06141300

*Complex **5.10*** (X = NO_2, Y = H)

C	-0.60741900	0.30969000	1.15217300
C	0.60948200	-0.32368400	1.20699800
C	1.20084300	-0.64743600	0.00000000
C	0.60948200	-0.32368400	-1.20699800
C	-0.60741900	0.30969000	-1.15217300
H	1.04956600	-0.60503400	2.15265600
H	1.04956600	-0.60503400	-2.15265600
O	-1.17373400	0.62299600	0.00000000
F	-1.72559400	-2.01829300	-1.14577700
F	-1.72559400	-2.01829300	1.14577700
F	-2.06605900	-3.98798600	0.00000000

F	0.01041400	-2.98670700	0.00000000
B	-1.39652000	-2.79392300	0.00000000
C	-0.79556300	3.75163000	1.20768000
C	-1.45256300	3.98370700	0.00000000
C	-0.79556300	3.75163000	-1.20768000
C	0.51539400	3.27552000	-1.20831300
C	1.16969000	3.03089700	0.00000000
C	0.51539400	3.27552000	1.20831300
H	-1.29974600	3.95396400	2.14630100
H	-1.29974600	3.95396400	-2.14630100
H	1.03401100	3.11264200	-2.14734800
H	2.19521000	2.67613600	0.00000000
H	1.03401100	3.11264200	2.14734800
H	-1.21223200	0.58678000	2.00198200
H	-1.21223200	0.58678000	-2.00198200
N	2.48477700	-1.35976000	0.00000000
O	2.96882700	-1.61792700	-1.09663600
O	2.96882700	-1.61792700	1.09663600
H	-2.46966100	4.35857100	0.00000000

Complex ***5.11*** (X = NO_2, Y = Br)

C	-0.24030800	-0.46482900	1.15280100
C	0.66180000	-1.49820400	1.20720500
C	1.09573100	-2.01416800	0.00000000
C	0.66180000	-1.49820400	-1.20720500
C	-0.24030800	-0.46482900	-1.15280100
H	0.96818000	-1.92198200	2.15261000
H	0.96818000	-1.92198200	-2.15261000
O	-0.65066700	0.03590300	0.00000000
F	-2.09576500	-2.26459800	-1.14557200
F	-2.09576500	-2.26459800	1.14557200
F	-3.11457400	-3.98477000	0.00000000
F	-0.81770800	-3.78720500	0.00000000
B	-2.06521300	-3.10675500	0.00000000
C	0.91939500	2.73606100	1.21355900
C	0.38466200	3.16446000	0.00000000
C	0.91939500	2.73606100	-1.21355900
C	1.99301500	1.84709000	-1.20639000
C	2.52622800	1.39205900	0.00000000
C	1.99301500	1.84709000	1.20639000
H	0.50540100	3.10076300	2.14646800
H	0.50540100	3.10076300	-2.14646800
H	2.42208800	1.52115400	-2.14816100
H	3.36981600	0.71047100	0.00000000
H	2.42208800	1.52115400	2.14816100
H	-0.70375000	0.01385400	2.00214500
H	-0.70375000	0.01385400	-2.00214500
N	2.03697400	-3.14104800	0.00000000
O	2.39596500	-3.55528300	-1.09678100
O	2.39596500	-3.55528300	1.09678100
Br	-1.07853600	4.34272500	0.00000000

Complex ***5.12*** (X = NO_2, Y = CF_3)

C	-0.27581400	-0.43940600	1.15317600
C	0.66138500	-1.44101400	1.20740300
C	1.11357000	-1.94092900	0.00000000
C	0.66138500	-1.44101400	-1.20740300
C	-0.27581400	-0.43940600	-1.15317600
H	0.98136500	-1.85497100	2.15270000
H	0.98136500	-1.85497100	-2.15270000
O	-0.70061300	0.04892800	0.00000000
F	-2.06936000	-2.29221500	-1.14552700
F	-2.06936000	-2.29221500	1.14552700
F	-3.02924700	-4.04616400	0.00000000
F	-0.74042900	-3.77062000	0.00000000
B	-2.01076400	-3.13320900	0.00000000
C	0.85313900	2.78964600	1.21158900
C	0.30412900	3.20639200	0.00000000
C	0.85313900	2.78964600	-1.21158900
C	1.94494500	1.92482800	-1.20786500
C	2.48707500	1.48478800	0.00000000
C	1.94494500	1.92482800	1.20786500
H	0.43038500	3.13903600	2.14628500
H	0.43038500	3.13903600	-2.14628500
H	2.38176200	1.60464400	-2.14756100
H	3.34361400	0.81921000	0.00000000
H	2.38176200	1.60464400	2.14756100
H	-0.75603500	0.02306800	2.00231700
H	-0.75603500	0.02306800	-2.00231700
N	2.09415100	-3.03394000	0.00000000
O	2.46753900	-3.43500300	-1.09679800
O	2.46753900	-3.43500300	1.09679800
C	-0.85350800	4.16223900	0.00000000
F	-1.62931500	4.00107000	1.08090000
F	-0.43419300	5.43750600	0.00000000
F	-1.62931500	4.00107000	-1.08090000

Complex ***5.13*** (X = NO_2, Y = NO_2)

C	-0.38768600	-0.18276100	1.15374900
C	0.62550600	-1.10726200	1.20754600
C	1.11607400	-1.56949300	0.00000000
C	0.62550600	-1.10726200	-1.20754600
C	-0.38768600	-0.18276100	-1.15374900
H	0.97669800	-1.49546500	2.15277900
H	0.97669800	-1.49546500	-2.15277900
O	-0.84877000	0.27196100	0.00000000
F	-2.00770500	-2.18983500	-1.14537600
F	-2.00770500	-2.18983500	1.14537600
F	-2.81514500	-4.01918400	0.00000000
F	-0.55794700	-3.55001800	0.00000000
B	-1.87865400	-3.02315900	0.00000000
C	0.60786700	3.09801700	1.21874300
C	0.05502200	3.47013200	0.00000000
C	0.60786700	3.09801700	-1.21874300
C	1.75193900	2.30378100	-1.20834200
C	2.32012700	1.89835500	0.00000000
C	1.75193900	2.30378100	1.20834200
H	0.15143200	3.43442600	2.14065600
H	0.15143200	3.43442600	-2.14065600
H	2.20853400	2.01148000	-2.14761800
H	3.21814700	1.29003300	0.00000000
H	2.20853400	2.01148000	2.14761800
H	-0.90351800	0.23981200	2.00305500
H	-0.90351800	0.23981200	-2.00305500
N	-1.16370700	4.29785100	0.00000000
O	-1.62966500	4.61163700	1.09091600
O	-1.62966500	4.61163700	-1.09091600
N	2.18323700	-2.57840900	0.00000000
O	2.58841200	-2.94675800	-1.09693700
O	2.58841200	-2.94675800	1.09693700

Complex ***5.14*** (X = NO_2, Y = GeF_3)

C	-0.21985900	-1.00984700	1.15369000
C	0.62075700	-2.09367100	1.20752600
C	1.02561100	-2.63260800	0.00000000
C	0.62075700	-2.09367100	-1.20752600
C	-0.21985900	-1.00984700	-1.15369000
H	0.90039300	-2.53628800	2.15272000
H	0.90039300	-2.53628800	-2.15272000
O	-0.59611400	-0.48297100	0.00000000
F	-2.15700800	-2.71295800	-1.14534500
F	-2.15700800	-2.71295800	1.14534500

F	-3.26362600	-4.37854000	0.00000000
F	-0.95957900	-4.29980500	0.00000000
B	-2.17159500	-3.55605400	0.00000000
C	1.32762400	2.04998100	1.21300900
C	0.82667800	2.53706800	0.00000000
C	1.32762400	2.04998100	-1.21300900
C	2.31830500	1.06997400	-1.20917500
C	2.80765700	0.57519900	0.00000000
C	2.31830500	1.06997400	1.20917500
H	0.95009600	2.43158500	2.15635100
H	0.95009600	2.43158500	-2.15635100
H	2.71582000	0.69954200	-2.14803600
H	3.58636500	-0.18029500	0.00000000
H	2.71582000	0.69954200	2.14803600
H	-0.65660400	-0.50568500	2.00287500
H	-0.65660400	-0.50568500	-2.00287500
N	1.90598200	-3.80798800	0.00000000
O	2.24289800	-4.23963000	-1.09694800
O	2.24289800	-4.23963000	1.09694800
Ge	-0.53966200	3.86549900	0.00000000
F	-1.53480500	3.72219800	1.38401400
F	-1.53480500	3.72219800	-1.38401400
F	0.02243800	5.47818200	0.00000000

*Complex **5.15*** (X = NO_2, Y = Me)

C	-0.39853600	0.15469300	1.15200500
C	0.68935500	-0.68113200	1.20693900
C	1.21513900	-1.10307000	0.00000000
C	0.68935500	-0.68113200	-1.20693900
C	-0.39853600	0.15469300	-1.15200500
H	1.07438500	-1.03369800	2.15270700
H	1.07438500	-1.03369800	-2.15270700
O	-0.90251800	0.56072600	0.00000000
F	-1.92161400	-1.92851700	-1.14588800
F	-1.92161400	-1.92851700	1.14588800
F	-2.61032900	-3.80485000	0.00000000
F	-0.38773000	-3.19279600	0.00000000
B	-1.73672300	-2.75060800	0.00000000
C	-0.06895400	3.54660200	1.20052900
C	-0.70548300	3.87663400	0.00000000
C	-0.06895400	3.54660200	-1.20052900
C	1.16260200	2.89347900	-1.20501500
C	1.78088900	2.55798600	0.00000000
C	1.16260200	2.89347900	1.20501500
H	-0.54148900	3.81074800	2.14221400
H	-0.54148900	3.81074800	-2.14221400
H	1.64757300	2.65941600	-2.14725600
H	2.74539800	2.06119400	0.00000000
H	1.64757300	2.65941600	2.14725600
H	-0.94485900	0.53372800	2.00193500
H	-0.94485900	0.53372800	-2.00193500
N	2.35447400	-2.02907900	0.00000000
O	2.78587200	-2.36837400	-1.09659900
O	2.78587200	-2.36837400	1.09659900
C	-2.01533700	4.61209500	0.00000000
H	-1.84922600	5.69244400	0.00000000
H	-2.60609100	4.36865200	-0.88393300
H	-2.60609100	4.36865200	0.88393300

*Complex **5.16*** (X = NO_2, Y = NH_2)

C	-0.41001200	0.16726900	1.15159000
C	0.68325100	-0.66159700	1.20678100
C	1.21122700	-1.08138900	0.00000000
C	0.68325100	-0.66159700	-1.20678100
C	-0.41001200	0.16726900	-1.15159000
H	1.07040400	-1.01134200	2.15267100
H	1.07040400	-1.01134200	-2.15267100
O	-0.91823300	0.56785000	0.00000000
F	-1.90303000	-1.95076800	-1.14592700
F	-1.90303000	-1.95076800	1.14592700
F	-2.56758300	-3.83568400	0.00000000
F	-0.35314700	-3.19538500	0.00000000
B	-1.70767600	-2.76931100	0.00000000
C	-0.10543900	3.55361500	1.20411900
C	-0.74325700	3.88058100	0.00000000
C	-0.10543900	3.55361500	-1.20411900
C	1.12726500	2.90889000	-1.20237500
C	1.74968400	2.56943500	0.00000000
C	1.12726500	2.90889000	1.20237500
H	-0.57800400	3.81737300	2.14586400
H	-0.57800400	3.81737300	-2.14586400
H	1.61187800	2.68450400	-2.14714300
H	2.71768500	2.08114500	0.00000000
H	1.61187800	2.68450400	2.14714300
H	-0.96026300	0.54162900	2.00101000
H	-0.96026300	0.54162900	-2.00101000
N	2.35621000	-1.99934400	0.00000000
O	2.78964200	-2.33656100	-1.09632900
O	2.78964200	-2.33656100	1.09632900
N	-2.00840200	4.45327100	0.00000000
H	-2.24799400	4.96466500	0.83741300
H	-2.24799400	4.96466500	-0.83741300

*Complex **5.17*** (X = NO_2, Y = NMe_2)

C	-0.18008200	-0.27125500	1.15159400
C	0.71403400	-1.31192700	1.20660400
C	1.14173600	-1.83288600	0.00000000
C	0.71403400	-1.31192700	-1.20660400
C	-0.18008200	-0.27125500	-1.15159400
H	1.02060000	-1.73402500	2.15248000
H	1.02060000	-1.73402500	-2.15248000
O	-0.59348700	0.22686300	0.00000000
F	-2.12527900	-1.97062500	-1.14612400
F	-2.12527900	-1.97062500	1.14612400
F	-3.19554200	-3.65833300	0.00000000
F	-0.89387200	-3.53104500	0.00000000
B	-2.11745200	-2.81290500	0.00000000
C	0.74596300	2.97033300	1.20504200
C	0.14928800	3.39880800	0.00000000
C	0.74596300	2.97033300	-1.20504200
C	1.84042700	2.11101600	-1.19795200
C	2.39175400	1.65765400	0.00000000
C	1.84042700	2.11101600	1.19795200
H	0.36248700	3.31243100	2.15717200
H	0.36248700	3.31243100	-2.15717200
H	2.28008100	1.81318000	-2.14484700
H	3.25667000	1.00395300	0.00000000
H	2.28008100	1.81318000	2.14484700
H	-0.63706100	0.21155700	2.00137200
H	-0.63706100	0.21155700	-2.00137200
N	2.06602800	-2.97328000	0.00000000
O	2.41793600	-3.39540000	-1.09677700
O	2.41793600	-3.39540000	1.09677700
N	-0.97418800	4.19846400	0.00000000
C	-1.33919900	4.86619500	1.23377900
H	-2.24251900	5.44787400	1.06181300
H	-1.56268300	4.13865500	2.01553400
H	-0.55191000	5.53914600	1.59942600
C	-1.33919900	4.86619500	-1.23377900
H	-1.56268300	4.13865500	-2.01553400
H	-2.24251900	5.44787400	-1.06181300
H	-0.55191000	5.53914600	-1.59942600

Complex ***6.10*** (X = GeF_3, Y = H)

C	-0.97169100	1.10162000	1.15056900
C	-0.06496500	0.06920100	1.19780000
C	0.38588400	-0.47795200	0.00000000
C	-0.06496500	0.06920100	-1.19780000
C	-0.97169100	1.10162000	-1.15056900
H	0.23839600	-0.31083000	2.16442500
O	-1.39346800	1.59220000	0.00000000
F	-2.80057900	-0.76345700	-1.14585100
F	-2.80057900	-0.76345700	1.14585100
F	-3.83145300	-2.47533000	0.00000000
F	-1.53374600	-2.29547600	0.00000000
B	-2.77692000	-1.60252200	0.00000000
C	0.11793200	4.36879600	1.20775300
C	-0.40887300	4.82486000	0.00000000
C	0.11793200	4.36879600	-1.20775300
C	1.16293700	3.44513300	-1.20833400
C	1.68118800	2.97683600	0.00000000
C	1.16293700	3.44513300	1.20833400
H	-0.27701400	4.74235200	2.14617100
H	-1.21796100	5.54639100	0.00000000
H	-0.27701400	4.74235200	-2.14617100
H	1.58634100	3.10331700	-2.14704700
H	2.50340300	2.26876700	0.00000000
H	1.58634100	3.10331700	2.14704700
H	-1.43251900	1.58103200	-2.00113800
H	-1.43251900	1.58103200	2.00113800
H	0.23839600	-0.31083000	-2.16442500
F	2.61488200	-1.75204700	-1.38716300
F	2.61488200	-1.75204700	1.38716300
F	1.12150200	-3.55780400	0.00000000
Ge	1.63039300	-1.94671200	0.00000000

Complex ***6.11*** (X = GeF_3, Y = Br)

C	-0.66876800	0.33062300	1.15116400
C	0.01203600	-0.86276900	1.19798100
C	0.34543100	-1.48849300	0.00000000
C	0.01203600	-0.86276900	-1.19798100
C	-0.66876800	0.33062300	-1.15116400
H	0.23187800	-1.29691000	2.16445300
O	-0.98004700	0.89793700	0.00000000
F	-2.80998200	-1.17668900	-1.14568000
F	-2.80998200	-1.17668900	1.14568000
F	-4.14626300	-2.66284200	0.00000000
F	-1.85605400	-2.92091900	0.00000000
B	-2.94686400	-2.00443300	0.00000000
C	1.12319600	3.23069000	1.21356300
C	0.68963000	3.76105600	0.00000000
C	1.12319600	3.23069000	-1.21356300
C	1.98792000	2.13737600	-1.20628800
C	2.41381300	1.58046800	0.00000000
C	1.98792000	2.13737600	1.20628800
H	0.79520600	3.67431000	2.14646600
H	0.79520600	3.67431000	-2.14646600
H	2.33967900	1.72894700	-2.14795700
H	3.09508800	0.73668600	0.00000000
H	2.33967900	1.72894700	2.14795700
H	-1.02429100	0.89360500	-2.00138300
H	-1.02429100	0.89360500	2.00138300
H	0.23187800	-1.29691000	-2.16445300
F	2.28679000	-3.16087300	-1.38708900
F	2.28679000	-3.16087300	1.38708900
F	0.48571900	-4.65975500	0.00000000
Ge	1.28267900	-3.17063600	0.00000000
Br	-0.49514500	5.21945600	0.00000000

Complex ***6.13*** (X = GeF_3, Y = NO_2)

C	-0.81710200	0.60407500	1.15208200
C	-0.05404400	-0.53824600	1.19823500
C	0.32447800	-1.13783400	0.00000000
C	-0.05404400	-0.53824600	-1.19823500
C	-0.81710200	0.60407500	-1.15208200
H	0.19484500	-0.95656700	2.16470800
H	0.19484500	-0.95656700	-2.16470800
O	-1.16473200	1.15012300	0.00000000
F	-2.81370900	-1.09692700	-1.14555900
F	-2.81370900	-1.09692700	1.14555900
F	-4.02139300	-2.68986200	0.00000000
F	-1.71784900	-2.75560500	0.00000000
B	-2.88276600	-1.93322800	0.00000000
C	0.94209200	3.57027100	1.21880200
C	0.50643100	4.07456400	0.00000000
C	0.94209200	3.57027100	-1.21880200
C	1.83778500	2.50372000	-1.20820500
C	2.27942100	1.96291400	0.00000000
C	1.83778500	2.50372000	1.20820500
H	0.59082300	4.01537800	2.14068500
H	0.59082300	4.01537800	-2.14068500
H	2.20272000	2.10217000	-2.14723900
H	2.98516800	1.13925600	0.00000000
H	2.20272000	2.10217000	2.14723900
H	-1.21223000	1.14046800	2.00252600
H	-1.21223000	1.14046800	-2.00252600
N	-0.45086700	5.19422900	0.00000000
O	-0.81814000	5.61970200	1.09080500
O	-0.81814000	5.61970200	-1.09080500
F	2.39110600	-2.63853100	1.38721300
F	2.39110600	-2.63853100	-1.38721300
F	0.73318100	-4.29565800	0.00000000
Ge	1.39172300	-2.74122400	0.00000000

Complex ***6.14*** (X = GeF_3, Y = GeF_3)

C	-0.67031400	-0.22124800	1.15198800
C	-0.00556100	-1.42364300	1.19850700
C	0.32126200	-2.05194400	0.00000000
C	-0.00556100	-1.42364300	-1.19850700
C	-0.67031400	-0.22124800	-1.15198800
H	0.20699700	-1.86173300	2.16483100
O	-0.96820600	0.35280000	0.00000000
F	-2.81721000	-1.71105400	-1.14563700
F	-2.81721000	-1.71105400	1.14563700
F	-4.16652700	-3.18578800	0.00000000
F	-1.87854800	-3.46376600	0.00000000
B	-2.96291900	-2.53789100	0.00000000
C	1.34215400	2.56718000	1.21317100
C	0.93017900	3.13074300	0.00000000
C	1.34215400	2.56718000	-1.21317100
C	2.15442100	1.43475200	-1.20915800
C	2.55347300	0.86441200	0.00000000
C	2.15442100	1.43475200	1.20915800
H	1.03411800	3.00662300	2.15651200
H	1.03411800	3.00662300	-2.15651200
H	2.48462000	1.00251200	-2.14772700
H	3.19291400	-0.01204700	0.00000000
H	2.48462000	1.00251200	2.14772700
H	-1.01926400	0.34657400	-2.00209300
H	-1.01926400	0.34657400	2.00209300
H	0.20699700	-1.86173300	-2.16483100
F	2.25187400	-3.72878200	-1.38623000
F	2.25187400	-3.72878200	1.38623000
F	0.44630100	-5.22813300	0.00000000
F	0.63384300	6.16494400	0.00000000

F	-1.19893000	4.69781400	1.38343900
F	-1.19893000	4.69781400	-1.38343900
Ge	1.24647900	-3.74170500	0.00000000
Ge	-0.19280200	4.67040800	0.00000000

Complex ***6.15*** (X = GeF_3, Y = Me)

C	-0.76511500	0.95063700	1.15045000
C	0.00832800	-0.18510600	1.19776200
C	0.38826600	-0.78355600	0.00000000
C	0.00832800	-0.18510600	-1.19776200
C	-0.76511500	0.95063700	-1.15045000
H	0.26349900	-0.59896900	2.16440100
O	-1.12476300	1.48848800	0.00000000
F	-2.81685200	-0.66233300	-1.14589100
F	-2.81685200	-0.66233300	1.14589100
F	-4.05826800	-2.22809300	0.00000000
F	-1.75644700	-2.34383900	0.00000000
B	-2.90008300	-1.49786000	0.00000000
C	0.63076900	4.06592400	1.20060600
C	0.13489000	4.58354300	0.00000000
C	0.63076900	4.06592400	-1.20060600
C	1.58502000	3.04957900	-1.20496000
C	2.06094100	2.53163200	0.00000000
C	1.58502000	3.04957900	1.20496000
H	0.27018000	4.46996600	2.14216300
H	0.27018000	4.46996600	-2.14216300
H	1.96882000	2.67128300	-2.14698000
H	2.81130500	1.74810400	0.00000000
H	1.96882000	2.67128300	2.14698000
H	-1.16225600	1.48387800	-2.00094800
H	-1.16225600	1.48387800	2.00094800
H	0.26349900	-0.59896900	-2.16440100
F	2.44124900	-2.32860700	-1.38732400
F	2.44124900	-2.32860700	1.38732400
F	0.72987400	-3.92879000	0.00000000
Ge	1.44026100	-2.39554400	0.00000000
C	-0.86677700	5.70332600	0.00000000
H	-1.50450700	5.66391800	0.88397800
H	-0.36012700	6.67188500	0.00000000
H	-1.50450700	5.66391800	-0.88397800

Complex ***6.16*** (X = GeF_3, Y = NH_2)

C	-0.77279800	0.96013600	1.15002600
C	0.00502700	-0.17271300	1.19746900
C	0.38703000	-0.77020000	0.00000000
C	0.00502700	-0.17271300	-1.19746900
C	-0.77279800	0.96013600	-1.15002600
H	0.26227600	-0.58506900	2.16416100
O	-1.13693700	1.49515200	0.00000000
F	-2.80710300	-0.69741500	-1.14600100
F	-2.80710300	-0.69741500	1.14600100
F	-4.02923500	-2.27805800	0.00000000
F	-1.72635200	-2.36589900	0.00000000
B	-2.88006700	-1.53269900	0.00000000
C	0.59260500	4.08396200	1.20411700
C	0.09622600	4.60048600	0.00000000
C	0.59260500	4.08396200	-1.20411700
C	1.54807800	3.07237300	-1.20211000
C	2.02533200	2.54826700	0.00000000
C	1.54807800	3.07237300	1.20211000
H	0.23265000	4.48826900	2.14579500
H	0.23265000	4.48826900	-2.14579500
H	1.93347100	2.70207000	-2.14665500
H	2.78060200	1.77054200	0.00000000
H	1.93347100	2.70207000	2.14665500
H	-1.17267500	1.49133000	-2.00051500
H	-1.17267500	1.49133000	2.00051500
H	0.26227600	-0.58506900	-2.16416100
F	2.45075000	-2.29901100	-1.38733400
F	2.45075000	-2.29901100	1.38733400
F	0.76005400	-3.91740900	0.00000000
N	-0.91381900	5.55466300	0.00000000
H	-0.97036700	6.11721600	0.83677400
H	-0.97036700	6.11721600	-0.83677400
Ge	1.44965400	-2.37459400	0.00000000

Complex ***6.17*** (X = GeF_3, Y = NMe_2)

C	-0.56470500	0.52962900	1.14988500
C	0.07686200	-0.68569900	1.19746400
C	0.38681700	-1.32304700	0.00000000
C	0.07686200	-0.68569900	-1.19746400
C	-0.56470500	0.52962900	-1.14988500
H	0.28533700	-1.12470700	2.16416600
O	-0.86473300	1.10282300	0.00000000
F	-2.80293600	-0.81019000	-1.14607300
F	-2.80293600	-0.81019000	1.14607300
F	-4.22491700	-2.21344800	0.00000000
F	-1.95424900	-2.60780200	0.00000000
B	-2.98534800	-1.62968300	0.00000000
C	1.04261300	3.49751200	1.20508800
C	0.55748700	4.04866100	0.00000000
C	1.04261300	3.49751200	-1.20508800
C	1.91804000	2.41564300	-1.19776200
C	2.35403700	1.85064900	0.00000000
C	1.91804000	2.41564300	1.19776200
H	0.74431700	3.91593500	2.15714000
H	0.74431700	3.91593500	-2.15714000
H	2.27982100	2.02661500	-2.14454900
H	3.05004300	1.01946000	0.00000000
H	2.27982100	2.02661500	2.14454900
H	-0.89945700	1.10408700	-2.00027500
H	-0.89945700	1.10408700	2.00027500
H	0.28533700	-1.12470700	-2.16416600
F	2.24755100	-3.10295300	-1.38747600
F	2.24755100	-3.10295300	1.38747600
F	0.35235400	-4.47953900	0.00000000
N	-0.35839200	5.08104300	0.00000000
Ge	1.24599000	-3.04446500	0.00000000
C	-0.55568400	5.81843400	1.23262000
H	-1.30402300	6.58959400	1.06180900
H	-0.93476600	5.16349300	2.01838800
H	0.36592400	6.29590200	1.59191200
C	-0.55568400	5.81843400	-1.23262000
H	0.36592400	6.29590200	-1.59191200
H	-0.93476600	5.16349300	-2.01838800
H	-1.30402300	6.58959400	-1.06180900

Complex ***7.10*** (X = Me, Y = H)

C	-0.21049400	0.11083300	1.14627000
C	1.06469100	-0.38683800	1.18970800
C	1.73380200	-0.67047600	0.00000000
C	1.06469100	-0.38683800	-1.18970800
C	-0.21049400	0.11083300	-1.14627000
H	1.50501900	-0.60188300	2.15411000
O	-0.81910600	0.36228700	0.00000000
F	-1.21122500	-2.32929600	-1.14641600
F	-1.21122500	-2.32929600	1.14641600
F	-1.41992400	-4.31604200	0.00000000
F	0.58431400	-3.18111400	0.00000000
B	-0.83187900	-3.07337800	0.00000000
C	-0.93467600	3.52389800	1.20743600
C	-1.61943100	3.65318400	0.00000000

C	-0.93467600	3.52389800	-1.20743600
C	0.43340800	3.25383900	-1.20777000
C	1.11714200	3.11282500	0.00000000
C	0.43340800	3.25383900	1.20777000
H	-1.46496600	3.64223400	2.14597400
H	-2.68250400	3.86535500	0.00000000
H	-1.46496600	3.64223400	-2.14597400
H	0.96944900	3.16608800	-2.14687000
H	2.18306300	2.91106800	0.00000000
H	0.96944900	3.16608800	2.14687000
H	-0.83623800	0.32066300	-2.00034400
H	-0.83623800	0.32066300	2.00034400
H	1.50501900	-0.60188300	-2.15411000
C	3.06617000	-1.33127700	0.00000000
H	2.88473400	-2.41086200	0.00000000
H	3.64086300	-1.07787700	-0.89058700
H	3.64086300	-1.07787700	0.89058700

*Complex **7.11*** (X = Me, Y = Br)

C	0.17526000	-0.79899700	1.14670100
C	1.18195100	-1.72647700	1.18987500
C	1.70363300	-2.23255500	0.00000000
C	1.18195100	-1.72647700	-1.18987500
C	0.17526000	-0.79899700	-1.14670100
H	1.51205600	-2.08901500	2.15418300
O	-0.29695900	-0.33943000	0.00000000
F	-1.62849900	-2.71468500	-1.14633200
F	-1.62849900	-2.71468500	1.14633200
F	-2.54429200	-4.49030200	0.00000000
F	-0.26483700	-4.16027600	0.00000000
B	-1.54599800	-3.54613200	0.00000000
C	0.80904700	2.59537100	1.21337500
C	0.21869500	2.94217600	0.00000000
C	0.80904700	2.59537100	-1.21337500
C	2.00107300	1.87326600	-1.20580600
C	2.59562000	1.50251600	0.00000000
C	2.00107300	1.87326600	1.20580600
H	0.34430300	2.89240500	2.14623900
H	0.34430300	2.89240500	-2.14623900
H	2.47002900	1.60945600	-2.14782900
H	3.52658200	0.94676500	0.00000000
H	2.47002900	1.60945600	2.14782900
H	-0.33313300	-0.37702400	-2.00047400
H	-0.33313300	-0.37702400	2.00047400
H	1.51205600	-2.08901500	-2.15418300
C	2.70708700	-3.33010300	0.00000000
H	2.14691600	-4.27066700	0.00000000
H	3.33434000	-3.30179700	-0.89070700
H	3.33434000	-3.30179700	0.89070700
Br	-1.39960200	3.89746700	0.00000000

*Complex **7.12*** (X = Me, Y = CF_3)

C	0.14319300	-0.76700200	1.14703700
C	1.17915100	-1.66165600	1.19002500
C	1.71740200	-2.15010500	0.00000000
C	1.17915100	-1.66165600	-1.19002500
C	0.14319300	-0.76700200	-1.14703700
H	1.52002000	-2.01427200	2.15429600
O	-0.34207700	-0.32120000	0.00000000
F	-1.59317200	-2.73735500	-1.14628500
F	-1.59317200	-2.73735500	1.14628500
F	-2.45119300	-4.54180100	0.00000000
F	-0.18364400	-4.13806300	0.00000000
B	-1.48439900	-3.56611200	0.00000000
C	0.74365700	2.64623100	1.21131500
C	0.14208400	2.98271600	0.00000000
C	0.74365700	2.64623100	-1.21131500
C	1.94654200	1.94477600	-1.20735600
C	2.54586100	1.58717600	0.00000000
C	1.94654200	1.94477600	1.20735600
H	0.27352900	2.92860800	2.14593500
H	0.27352900	2.92860800	-2.14593500
H	2.42134700	1.68523400	-2.14710700
H	3.48496000	1.04480400	0.00000000
H	2.42134700	1.68523400	2.14710700
H	-0.37913000	-0.36191800	-2.00073400
H	-0.37913000	-0.36191800	2.00073400
H	1.52002000	-2.01427200	-2.15429600
C	2.75662200	-3.21379600	0.00000000
H	2.22798500	-4.17245800	0.00000000
H	3.38251900	-3.16484900	-0.89076500
H	3.38251900	-3.16484900	0.89076500
C	-1.13515300	3.77043500	0.00000000
F	-0.89262300	5.09244500	0.00000000
F	-1.88211600	3.50748000	-1.08098100
F	-1.88211600	3.50748000	1.08098100

*Complex **7.13*** (X = Me, Y = NO_2)

C	0.06518400	-0.50389900	1.14738500
C	1.16224200	-1.32244700	1.19017800
C	1.73410900	-1.77117100	0.00000000
C	1.16224200	-1.32244700	-1.19017800
C	0.06518400	-0.50389900	-1.14738500
H	1.52665000	-1.65084800	2.15444400
H	1.52665000	-1.65084800	-2.15444400
O	-0.44983600	-0.09235300	0.00000000
F	-1.52562100	-2.58483200	-1.14620500
F	-1.52562100	-2.58483200	1.14620500
F	-2.25444600	-4.44538800	0.00000000
F	-0.02096500	-3.88278100	0.00000000
B	-1.35921900	-3.40443800	0.00000000
C	0.45340900	2.95509600	1.21852200
C	-0.14389000	3.25026400	0.00000000
C	0.45340900	2.95509600	-1.21852200
C	1.69413700	2.32301500	-1.20778700
C	2.31272400	2.00000100	0.00000000
C	1.69413700	2.32301500	1.20778700
H	-0.04596500	3.22334600	2.14034000
H	-0.04596500	3.22334600	-2.14034000
H	2.18394400	2.09205200	-2.14723700
H	3.28213100	1.51410300	0.00000000
H	2.18394400	2.09205200	2.14723700
H	-0.48524600	-0.13803900	2.00126800
H	-0.48524600	-0.13803900	-2.00126800
N	-1.45973600	3.91204100	0.00000000
O	-1.96251000	4.16429300	1.09062900
O	-1.96251000	4.16429300	-1.09062900
C	2.84592400	-2.75844100	0.00000000
H	3.46669600	-2.66589900	0.89088500
H	2.38581800	-3.75188800	0.00000000
H	3.46669600	-2.66589900	-0.89088500

*Complex **7.14*** (X = Me, Y = GeF_3)

C	-0.21060700	1.39996900	1.14735700
C	-1.12734800	2.41645600	1.19013600
C	-1.60120900	2.96777700	0.00000000
C	-1.12734800	2.41645600	-1.19013600
C	-0.21060700	1.39996900	-1.14735700
H	-1.42047800	2.80975600	2.15441700
O	0.21400300	0.89568100	0.00000000
F	1.75047700	3.13677600	-1.14615800
F	1.75047700	3.13677600	1.14615800

F	2.82598000	4.82091600	0.00000000
F	0.52580600	4.70163600	0.00000000
B	1.74617200	3.97305900	0.00000000
C	-1.30265100	-1.90706300	1.21283000
C	-0.75529700	-2.34078500	0.00000000
C	-1.30265100	-1.90706300	-1.21283000
C	-2.38861600	-1.03430500	-1.20868400
C	-2.92722200	-0.59400700	0.00000000
C	-2.38861600	-1.03430500	1.20868400
H	-0.88524100	-2.24459800	2.15605000
H	-0.88524100	-2.24459800	-2.15605000
H	-2.81926800	-0.70391100	-2.14768700
H	-3.77627500	0.08097600	0.00000000
H	-2.81926800	-0.70391100	2.14768700
H	0.25852800	0.93436500	-2.00124500
H	0.25852800	0.93436500	2.00124500
H	-1.42047800	2.80975600	-2.15441700
C	-2.50070700	4.15179900	0.00000000
H	-1.85694700	5.03731600	0.00000000
H	-3.12767600	4.18110200	-0.89088300
H	-3.12767600	4.18110200	0.89088300
Ge	0.72474700	-3.53988800	0.00000000
F	0.29516300	-5.19468300	0.00000000
F	1.70627000	-3.32490000	1.38419200
F	1.70627000	-3.32490000	-1.38419200

*Complex **7.15*** (X = Me, Y = Me)

C	-0.00974800	-0.09890000	1.14615000
C	1.17948500	-0.77666500	1.18968100
C	1.79963600	-1.15531800	0.00000000
C	1.17948500	-0.77666500	-1.18968100
C	-0.00974800	-0.09890000	-1.14615000
H	1.58407400	-1.05293300	2.15412000
O	-0.57589600	0.23743900	0.00000000
F	-1.36649100	-2.36034500	-1.14645400
F	-1.36649100	-2.36034500	1.14645400
F	-1.86843100	-4.29376600	0.00000000
F	0.28246800	-3.47016000	0.00000000
B	-1.10161300	-3.15250500	0.00000000
C	-0.30628300	3.33685900	1.20021200
C	-0.99326100	3.54174400	0.00000000
C	-0.30628300	3.33685900	-1.20021200
C	1.02552500	2.92580900	-1.20438400
C	1.69540900	2.71222600	0.00000000
C	1.02552500	2.92580900	1.20438400
H	-0.82106600	3.50391300	2.14195200
H	-0.82106600	3.50391300	-2.14195200
H	1.54348000	2.78110400	-2.14685400
H	2.73329900	2.39726200	0.00000000
H	1.54348000	2.78110400	2.14685400
H	-0.59797600	0.19967600	-2.00037700
H	-0.59797600	0.19967600	2.00037700
H	1.58407400	-1.05293300	-2.15412000
C	3.01992200	-2.00552600	0.00000000
H	2.68025400	-3.04620500	0.00000000
H	3.62571400	-1.83998600	-0.89061500
H	3.62571400	-1.83998600	0.89061500
C	-2.42027900	4.01132000	0.00000000
H	-2.95272700	3.65731200	0.88363900
H	-2.46710900	5.10342800	0.00000000
H	-2.95272700	3.65731200	-0.88363900

*Complex **7.16*** (X = Me, Y = NH_2)

C	-0.03232600	-0.08852600	1.14581900
C	1.16174800	-0.75789300	1.18937600
C	1.78537100	-1.13106200	0.00000000
C	1.16174800	-0.75789300	-1.18937600
C	-0.03232600	-0.08852600	-1.14581900
H	1.56843500	-1.03080900	2.15387600
H	1.56843500	-1.03080900	-2.15387600
O	-0.60132400	0.24315600	0.00000000
F	-1.34853400	-2.38542400	-1.14651400
F	-1.34853400	-2.38542400	1.14651400
F	-1.82736800	-4.32462300	0.00000000
F	0.31344100	-3.47539000	0.00000000
B	-1.07433000	-3.17352300	0.00000000
C	-0.33319200	3.35033800	1.20380700
C	-1.01777400	3.56060300	0.00000000
C	-0.33319200	3.35033800	-1.20380700
C	0.99366500	2.93169700	-1.20156500
C	1.66565200	2.70790300	0.00000000
C	0.99366500	2.93169700	1.20156500
H	-0.84591200	3.52405200	2.14544100
H	-0.84591200	3.52405200	-2.14544100
H	1.50796400	2.78993900	-2.14648800
H	2.70210400	2.39080400	0.00000000
H	1.50796400	2.78993900	2.14648800
H	-2.68854300	4.36516000	-0.83690600
H	-2.68854300	4.36516000	0.83690600
N	-2.36515300	3.90199700	0.00000000
H	-0.62306100	0.20609400	1.99963500
H	-0.62306100	0.20609400	-1.99963500
C	3.01531200	-1.96751900	0.00000000
H	3.61919200	-1.79407800	0.89046800
H	2.68889400	-3.01233600	0.00000000
H	3.61919200	-1.79407800	-0.89046800

*Complex **7.17*** (X = Me, Y = NMe_2)

C	0.20827800	-0.57343200	1.14576100
C	1.21994700	-1.49551400	1.18947800
C	1.74142700	-2.00131500	0.00000000
C	1.21994700	-1.49551400	-1.18947800
C	0.20827800	-0.57343200	-1.14576100
H	1.55547700	-1.85225300	2.15396900
H	1.55547700	-1.85225300	-2.15396900
O	-0.27240400	-0.12358400	0.00000000
F	-1.61758300	-2.48904500	-1.14659600
F	-1.61758300	-2.48904500	1.14659600
F	-2.52849500	-4.26646900	0.00000000
F	-0.24984500	-3.93142300	0.00000000
B	-1.53089300	-3.31909700	0.00000000
C	0.58247400	2.82229200	1.20453500
C	-0.08077000	3.13656500	0.00000000
C	0.58247400	2.82229200	-1.20453500
C	1.81252400	2.17214700	-1.19754400
C	2.43558700	1.82512400	0.00000000
C	1.81252400	2.17214700	1.19754400
H	0.14181400	3.08613000	2.15670800
H	0.14181400	3.08613000	-2.15670800
H	2.29519900	1.95253600	-2.14467400
H	3.39916800	1.32882300	0.00000000
H	2.29519900	1.95253600	2.14467400
N	-1.33278600	3.71940900	0.00000000
H	-0.29916400	-0.15170400	1.99967100
H	-0.29916400	-0.15170400	-1.99967100
C	2.74616100	-3.09809800	0.00000000
H	3.37373100	-3.06844300	0.89046000
H	2.18802500	-4.03980000	0.00000000
H	3.37373100	-3.06844300	-0.89046000
C	-1.80660100	4.31700900	-1.23212100
H	-1.89108800	3.56547400	-2.01839300
H	-2.80144300	4.72415100	-1.06256700
H	-1.15269600	5.12382200	-1.59083100

C	-1.80660100	4.31700900	1.23212100
H	-1.89108800	3.56547400	2.01839300
H	-1.15269600	5.12382200	1.59083100
H	-2.80144300	4.72415100	1.06256700

Complex ***8.10*** (X = NH_2, Y = H)

C	-0.23532900	0.14839300	1.14526400
C	1.00800800	-0.39270300	1.19997400
C	1.66160200	-0.72898500	0.00000000
C	1.00800800	-0.39270300	-1.19997400
C	-0.23532900	0.14839300	-1.14526400
H	1.43101300	-0.63324800	2.16579100
O	-0.85341600	0.42349600	0.00000000
F	-1.18877200	-2.42775900	-1.14616900
F	-1.18877200	-2.42775900	1.14616900
F	-1.29369500	-4.42263500	0.00000000
F	0.64928100	-3.18781000	0.00000000
B	-0.77719500	-3.14595500	0.00000000
C	-0.89306900	3.60220700	1.20720200
C	-1.57521100	3.74523200	0.00000000
C	-0.89306900	3.60220700	-1.20720200
C	0.46966300	3.30688100	-1.20733000
C	1.15066100	3.15371600	0.00000000
C	0.46966300	3.30688100	1.20733000
H	-1.42125300	3.72890900	2.14585900
H	-2.63452300	3.97553200	0.00000000
H	-1.42125300	3.72890900	-2.14585900
H	1.00333200	3.20619900	-2.14637700
H	2.21199200	2.92911000	0.00000000
H	1.00333200	3.20619900	2.14637700
H	-0.84698600	0.37638800	-2.00501400
H	-0.84698600	0.37638800	2.00501400
H	1.43101300	-0.63324800	-2.16579100
N	2.86829400	-1.30994400	0.00000000
H	3.15480200	-1.77657900	-0.84841600
H	3.15480200	-1.77657900	0.84841600

Complex ***8.11*** (X = NH_2, Y = Br)

C	-0.15767100	0.76268900	1.14573300
C	-1.14693600	1.68985200	1.20023700
C	-1.65190200	2.22429800	0.00000000
C	-1.14693600	1.68985200	-1.20023700
C	-0.15767100	0.76268900	-1.14573300
H	-1.46304000	2.06013700	2.16597600
O	0.32977400	0.29287200	0.00000000
F	1.58872700	2.88130500	-1.14610700
F	1.58872700	2.88130500	1.14610700
F	2.34987400	4.72847500	0.00000000
F	0.10732100	4.20815900	0.00000000
B	1.43984300	3.69559600	0.00000000
C	-0.79117800	-2.64972300	1.21326600
C	-0.19849200	-2.99179800	0.00000000
C	-0.79117800	-2.64972300	-1.21326600
C	-1.98952100	-1.93836000	-1.20543900
C	-2.58756500	-1.57360300	0.00000000
C	-1.98952100	-1.93836000	1.20543900
H	-0.32291000	-2.94111000	2.14611800
H	-0.32291000	-2.94111000	-2.14611800
H	-2.45923300	-1.67606300	-2.14738900
H	-3.52184800	-1.02348000	0.00000000
H	-2.45923300	-1.67606300	2.14738900
H	0.34430200	0.34448100	-2.00529300
H	0.34430200	0.34448100	2.00529300
H	-1.46304000	2.06013700	-2.16597600
N	-2.59644000	3.17297500	0.00000000
H	-2.71184100	3.70841500	-0.84841300
H	-2.71184100	3.70841500	0.84841300
Br	1.42927300	-3.93200300	0.00000000

Complex ***8.12*** (X = NH_2, Y = CF_3)

C	0.13741900	-0.72988500	1.14606000
C	1.14447900	-1.63762400	1.20042800
C	1.66165700	-2.16048900	0.00000000
C	1.14447900	-1.63762400	-1.20042800
C	0.13741900	-0.72988500	-1.14606000
H	1.46553800	-2.00383600	2.16610800
O	-0.35646400	-0.26644200	0.00000000
F	-1.55423300	-2.88946900	-1.14609500
F	-1.55423300	-2.88946900	1.14609500
F	-2.27646500	-4.75237400	0.00000000
F	-0.04533000	-4.18461700	0.00000000
B	-1.38885700	-3.70075100	0.00000000
C	0.72986000	2.70098100	1.21112300
C	0.12532400	3.03226800	0.00000000
C	0.72986000	2.70098100	-1.21112300
C	1.93936500	2.01123800	-1.20696000
C	2.54247400	1.66012400	0.00000000
C	1.93936500	2.01123800	1.20696000
H	0.25627400	2.97725400	2.14579900
H	0.25627400	2.97725400	-2.14579900
H	2.41533600	1.75400800	-2.14663800
H	3.48525400	1.12420900	0.00000000
H	2.41533600	1.75400800	2.14663800
H	-0.37392300	-0.32266100	-2.00550100
H	-0.37392300	-0.32266100	2.00550100
H	1.46553800	-2.00383600	-2.16610800
N	2.62697200	-3.08754800	0.00000000
H	2.75466800	-3.62024800	-0.84845700
H	2.75466800	-3.62024800	0.84845700
C	-1.15980100	3.80617400	0.00000000
F	-1.90466800	3.53616100	1.08092200
F	-1.90466800	3.53616100	-1.08092200
F	-0.93209600	5.13137400	0.00000000

Complex ***8.13*** (X = NH_2, Y = NO_2)

C	0.03533800	-0.46279700	1.14650900
C	1.11415100	-1.28374800	1.20070100
C	1.67118700	-1.76401400	0.00000000
C	1.11415100	-1.28374800	-1.20070100
C	0.03533800	-0.46279700	-1.14650900
H	1.46389200	-1.62271300	2.16642300
H	1.46389200	-1.62271300	-2.16642300
O	-0.49552700	-0.04171000	0.00000000
F	-1.48535800	-2.73491900	-1.14589700
F	-1.48535800	-2.73491900	1.14589700
F	-2.05220000	-4.65111000	0.00000000
F	0.12474900	-3.90240100	0.00000000
B	-1.25458200	-3.53048500	0.00000000
C	0.44251000	3.00202400	1.21834400
C	-0.15782500	3.29127300	0.00000000
C	0.44251000	3.00202400	-1.21834400
C	1.68998100	2.38374000	-1.20741500
C	2.31231600	2.06819000	0.00000000
C	1.68998100	2.38374000	1.20741500
H	-0.06018900	3.26353900	2.14022700
H	-0.06018900	3.26353900	-2.14022700
H	2.18085600	2.15536000	-2.14680300
H	3.28548400	1.58990700	0.00000000
H	2.18085600	2.15536000	2.14680300
H	-0.50829200	-0.10008200	2.00621000
H	-0.50829200	-0.10008200	-2.00621000
N	-1.48090400	3.93732600	0.00000000

O	-1.98724000	4.18414900	1.09043200
O	-1.98724000	4.18414900	-1.09043200
H	2.87912100	-3.13045300	0.84875200
H	2.87912100	-3.13045300	-0.84875200
N	2.70696000	-2.61085000	0.00000000

*Complex **8.14*** (X = NH_2, Y = GeF_3)

C	-0.20020600	1.35306100	1.14651400
C	-1.10371600	2.36378100	1.20066800
C	-1.56073200	2.94008400	0.00000000
C	-1.10371600	2.36378100	-1.20066800
C	-0.20020600	1.35306100	-1.14651400
H	-1.38232100	2.76334500	2.16635900
O	0.24032200	0.83829100	0.00000000
F	1.71562200	3.30533500	-1.14595200
F	1.71562200	3.30533500	1.14595200
F	2.63400000	5.08006700	0.00000000
F	0.35479700	4.75530900	0.00000000
B	1.63923500	4.13008900	0.00000000
C	-1.29773800	-1.96055000	1.21276100
C	-0.74378800	-2.38559200	0.00000000
C	-1.29773800	-1.96055000	-1.21276100
C	-2.39801900	-1.10618800	-1.20834000
C	-2.94412200	-0.67540300	0.00000000
C	-2.39801900	-1.10618800	1.20834000
H	-0.87415200	-2.29028400	2.15596900
H	-0.87415200	-2.29028400	-2.15596900
H	-2.83209300	-0.78043600	-2.14724700
H	-3.80213800	-0.01187100	0.00000000
H	-2.83209300	-0.78043600	2.14724700
H	0.26476500	0.89352600	-2.00608500
H	0.26476500	0.89352600	2.00608500
H	-1.38232100	2.76334500	-2.16635900
N	-2.41956900	3.96601800	0.00000000
H	-2.49036500	4.50905100	-0.84862700
H	-2.49036500	4.50905100	0.84862700
F	1.73913900	-3.31925300	1.38369800
F	1.73913900	-3.31925300	-1.38369800
F	0.36883500	-5.21742100	0.00000000
Ge	0.76038500	-3.55263300	0.00000000

*Complex **8.15*** (X = NH_2, Y = Me)

C	-0.02923600	-0.06690500	1.14515200
C	1.13008900	-0.77014300	1.19994700
C	1.73154400	-1.19245300	0.00000000
C	1.13008900	-0.77014300	-1.19994700
C	-0.02923600	-0.06690500	-1.14515200
H	1.51774700	-1.06404400	2.16581500
O	-0.60558400	0.28725700	0.00000000
F	-1.33833100	-2.47931300	-1.14622200
F	-1.33833100	-2.47931300	1.14622200
F	-1.71602700	-4.44079700	0.00000000
F	0.37810200	-3.48463500	0.00000000
B	-1.02878400	-3.24710600	0.00000000
C	-0.29608100	3.39774100	1.20002300
C	-0.98180200	3.60659900	0.00000000
C	-0.29608100	3.39774100	-1.20002300
C	1.03379400	2.98082000	-1.20398900
C	1.70285200	2.76522700	0.00000000
C	1.03379400	2.98082000	1.20398900
H	-0.81054500	3.56568000	2.14181100
H	-0.81054500	3.56568000	-2.14181100
H	1.55013300	2.83072800	-2.14639800
H	2.73840700	2.44275100	0.00000000
H	1.55013300	2.83072800	2.14639800
H	-0.60387400	0.24219300	-2.00501300
H	-0.60387400	0.24219300	2.00501300
H	1.51774700	-1.06404400	-2.16581500
N	2.84733000	-1.93315400	0.00000000
H	3.06894300	-2.43331400	-0.84865500
H	3.06894300	-2.43331400	0.84865500
C	-2.40690700	4.08205400	0.00000000
H	-2.94075800	3.72988800	0.88358700
H	-2.45005200	5.17436300	0.00000000
H	-2.94075800	3.72988800	-0.88358700

*Complex **8.16*** (X = NH_2, Y = NH_2)

C	-0.06787200	-0.05101600	1.14491900
C	1.09706400	-0.74526000	1.19958500
C	1.70387800	-1.15972000	0.00000000
C	1.09706400	-0.74526000	-1.19958500
C	-0.06787200	-0.05101600	-1.14491900
H	1.48728900	-1.03598400	2.16536800
O	-0.64709600	0.29810100	0.00000000
F	-1.31169100	-2.52026000	-1.14629600
F	-1.31169100	-2.52026000	1.14629600
F	-1.65640700	-4.48776200	0.00000000
F	0.42122900	-3.49636900	0.00000000
B	-0.98954300	-3.28192000	0.00000000
C	-0.31733700	3.41615400	1.20355400
C	-0.99953800	3.63299800	0.00000000
C	-0.31733700	3.41615400	-1.20355400
C	1.00615500	2.98694800	-1.20118700
C	1.67655400	2.75927300	0.00000000
C	1.00615500	2.98694800	1.20118700
H	-0.82931700	3.59217500	2.14519700
H	-0.82931700	3.59217500	-2.14519700
H	1.51826600	2.83776300	-2.14604800
H	2.70941000	2.43068800	0.00000000
H	1.51826600	2.83776300	2.14604800
H	-0.64574400	0.25314500	-2.00437000
H	-0.64574400	0.25314500	2.00437000
H	1.48728900	-1.03598400	-2.16536800
N	2.83065200	-1.88519200	0.00000000
H	3.05152100	-2.38768200	-0.84762900
H	3.05152100	-2.38768200	0.84762900
N	-2.34535200	3.98607100	0.00000000
H	-2.66024600	4.45687000	0.83608700
H	-2.66024600	4.45687000	-0.83608700

*Complex **8.17*** (X = NH_2, Y = NMe_2)

C	0.19183100	-0.53715300	1.14482000
C	1.18457700	-1.46093800	1.19966100
C	1.68794300	-1.99603900	0.00000000
C	1.18457700	-1.46093800	-1.19966100
C	0.19183100	-0.53715300	-1.14482000
H	1.50640400	-1.82567900	2.16552100
O	-0.30256300	-0.07591500	0.00000000
F	-1.57394700	-2.65443900	-1.14634700
F	-1.57394700	-2.65443900	1.14634700
F	-2.33709300	-4.50017700	0.00000000
F	-0.09378900	-3.98343300	0.00000000
B	-1.42389700	-3.46797200	0.00000000
C	0.55892700	2.88072600	1.20417800
C	-0.10753300	3.18736900	0.00000000
C	0.55892700	2.88072600	-1.20417800
C	1.79789000	2.24767500	-1.19714100
C	2.42605500	1.91075000	0.00000000
C	1.79789000	2.24767500	1.19714100
H	0.11412400	3.13709500	2.15643900
H	0.11412400	3.13709500	-2.15643900
H	2.28186000	2.03146900	-2.14427800

H	3.39503500	1.42513300	0.00000000
H	2.28186000	2.03146900	2.14427800
H	-0.30703500	-0.11637600	-2.00442600
H	-0.30703500	-0.11637600	2.00442600
H	1.50640400	-1.82567900	-2.16552100
N	2.63176700	-2.94722200	0.00000000
H	2.74374200	-3.48339300	-0.84820900
H	2.74374200	-3.48339300	0.84820900
N	-1.36888100	3.75413100	0.00000000
C	-1.84181100	4.35628100	1.23043500
H	-2.84086900	4.75398600	1.06272400
H	-1.91644000	3.60930900	2.02183500
H	-1.19279000	5.17083500	1.58094000
C	-1.84181100	4.35628100	-1.23043500
H	-1.19279000	5.17083500	-1.58094000
H	-1.91644000	3.60930900	-2.02183500
H	-2.84086900	4.75398600	-1.06272400

Complex ***9.10*** (X = NMe_2, Y = H)

C	-0.63159700	0.54566700	1.14315600
C	0.49493300	-0.20427500	1.20082700
C	1.10739900	-0.64995600	0.00000000
C	0.49493300	-0.20427500	-1.20082700
C	-0.63159700	0.54566700	-1.14315600
H	0.83670900	-0.51048600	2.17671600
O	-1.20351300	0.92781800	0.00000000
F	-1.69956600	-2.16566300	-1.14683100
F	-1.69956600	-2.16566300	1.14683100
F	-2.10878500	-4.12036600	0.00000000
F	-0.00064900	-3.19651700	0.00000000
B	-1.40736600	-2.93305600	0.00000000
C	-0.65066200	4.08085300	1.20716600
C	-1.29298900	4.35139000	0.00000000
C	-0.65066200	4.08085300	-1.20716600
C	0.63085500	3.53161900	-1.20725600
C	1.26993200	3.25155200	0.00000000
C	0.63085500	3.53161900	1.20725600
H	-1.14549400	4.30442800	2.14592300
H	-2.28885400	4.77976300	0.00000000
H	-1.14549400	4.30442800	-2.14592300
H	1.13435900	3.32852700	-2.14634000
H	2.26856100	2.82772600	0.00000000
H	1.13435900	3.32852700	2.14634000
H	-1.19152300	0.87272800	-2.00678400
H	-1.19152300	0.87272800	2.00678400
H	0.83670900	-0.51048600	-2.17671600
N	2.16632300	-1.45155700	0.00000000
C	2.58394700	-2.08633400	-1.24621200
H	3.50132900	-2.63817100	-1.06008700
H	1.80537000	-2.77255100	-1.58765700
H	2.79040000	-1.33360100	-2.00645100
C	2.58394700	-2.08633400	1.24621200
H	1.80537000	-2.77255100	1.58765700
H	3.50132900	-2.63817100	1.06008700
H	2.79040000	-1.33360100	2.00645100

Complex ***9.11*** (X = NMe_2, Y = Br)

C	-0.23401800	-0.29262000	1.14393300
C	0.62697400	-1.33644300	1.20133100
C	1.09119800	-1.93552200	0.00000000
C	0.62697400	-1.33644300	-1.20133100
C	-0.23401800	-0.29262000	-1.14393300
H	0.86144800	-1.73209200	2.17678500
O	-0.66724100	0.24257000	0.00000000
F	-1.97107300	-2.66352200	-1.14695300
F	-1.97107300	-2.66352200	1.14695300
F	-2.93126500	-4.41481500	0.00000000
F	-0.64551400	-4.14252100	0.00000000
B	-1.91535100	-3.48303200	0.00000000
C	0.86789700	3.00455300	1.21331000
C	0.32700000	3.42316900	0.00000000
C	0.86789700	3.00455300	-1.21331000
C	1.95958700	2.13850100	-1.20539200
C	2.50300900	1.69697700	0.00000000
C	1.95958700	2.13850100	1.20539200
H	0.44243100	3.35534900	2.14619100
H	0.44243100	3.35534900	-2.14619100
H	2.38781300	1.81319000	-2.14739200
H	3.35388900	1.02502800	0.00000000
H	2.38781300	1.81319000	2.14739200
H	-0.67878500	0.18026100	-2.00729700
H	-0.67878500	0.18026100	2.00729700
H	0.86144800	-1.73209200	-2.17678500
N	1.88396100	-2.99996000	0.00000000
Br	-1.16114500	4.57248900	0.00000000
C	2.11567400	-3.72320900	-1.24671300
H	2.52038400	-3.05385900	-2.00525800
H	2.84786100	-4.50397700	-1.05969000
H	1.18026200	-4.17162900	-1.58910500
C	2.11567400	-3.72320900	1.24671300
H	2.52038400	-3.05385900	2.00525800
H	1.18026200	-4.17162900	1.58910500
H	2.84786100	-4.50397700	1.05969000

Complex ***9.12*** (X = NMe_2, Y = CF_3)

C	0.18919200	-1.51212300	1.14435000
C	0.62539200	-0.23159200	1.20349500
O	-0.05412300	-2.15670800	-0.00149900
H	0.01001100	-2.13794400	2.00664100
C	0.87544500	0.48476500	0.00054000
H	0.84677100	0.17785300	2.17639100
C	0.18954000	-1.51048100	-1.14634900
C	0.62571900	-0.22985400	-1.20351600
N	1.31522700	1.73227400	0.00135500
H	0.01053400	-2.13503800	-2.00959500
H	0.84713400	0.18114600	-2.17575800
C	1.67474900	2.38359800	1.25586900
C	1.67520100	2.38475700	-1.25245900
H	1.88730900	3.42965400	1.05152900
H	0.83894200	2.33387500	1.95549200
H	2.55647000	1.90126000	1.68162100
H	2.55488300	1.90043200	-1.68011600
H	0.83824700	2.33899700	-1.95102900
H	1.89149400	3.42971100	-1.04646300
F	3.50276800	-0.03729700	-1.14613900
B	3.78121100	-0.83254300	-0.00027000
F	2.89619500	-1.93037300	-0.00066900
F	5.09457500	-1.24414900	-0.00018200
F	3.50243000	-0.03788500	1.14593700
C	-2.01144100	2.18707900	1.20548900
C	-1.74950400	2.83293100	-0.00176400
C	-2.52975500	0.89459100	1.21046800
H	-1.82728800	2.69504500	2.14566400
C	-2.01227100	2.18589900	-1.20819600
H	-1.35468300	3.84323700	-0.00239200
C	-2.78421200	0.25262400	-0.00014100
H	-2.74093900	0.39067000	2.14624400
C	-2.53067800	0.89343500	-1.21153600
H	-1.82870300	2.69287000	-2.14902800
C	-3.40054200	-1.11382400	0.00075300
H	-2.74254500	0.38861700	-2.14667300
F	-3.04240700	-1.82466900	1.08240800
F	-3.04376000	-1.82548900	-1.08078800

F	-4.74183400	-1.05022100	0.00157900

Complex ***9.14*** (X = NMe_2, Y = GeF_3)

C	-1.47518700	-0.05753000	1.15108700
C	-0.43923500	-0.92530300	1.20648400
C	0.16597000	-1.38712900	0.00000000
C	-0.43923500	-0.92530300	-1.20648400
C	-1.47518700	-0.05753000	-1.15108700
H	-0.13008500	-1.28230800	2.17663300
O	-1.98555200	0.41387500	0.00000000
F	-1.15331900	-3.67516400	-1.14764500
F	-1.15331900	-3.67516400	1.14764500
F	-1.82475000	-5.55638700	0.00000000
F	0.39062500	-4.91940200	0.00000000
B	-0.95767900	-4.48972700	0.00000000
C	1.50599600	1.80024000	1.21306100
C	0.95190900	2.22511200	0.00000000
C	1.50599600	1.80024000	-1.21306100
C	2.61328800	0.95480600	-1.20834200
C	3.16348000	0.52946200	0.00000000
C	2.61328800	0.95480600	1.20834200
H	1.08198900	2.12761500	2.15689700
H	1.08198900	2.12761500	-2.15689700
H	3.05333000	0.63900500	-2.14793700
H	4.03054200	-0.12251700	0.00000000
H	3.05333000	0.63900500	2.14793700
H	-1.99411400	0.34032300	-2.01147500
H	-1.99411400	0.34032300	2.01147500
H	-0.13008500	-1.28230800	-2.17663300
N	1.21349500	-2.18339400	0.00000000
F	-1.53442900	3.15238800	1.38492100
F	-1.53442900	3.15238800	-1.38492100
F	-0.18408900	5.05869300	0.00000000
C	1.76239000	-2.67377200	1.26283800
H	2.60124300	-3.32550700	1.04156500
H	2.10647100	-1.83148000	1.86758200
H	1.00297900	-3.25177900	1.78774600
C	1.76239000	-2.67377200	-1.26283800
H	1.00297900	-3.25177900	-1.78774600
H	2.10647100	-1.83148000	-1.86758200
H	2.60124300	-3.32550700	-1.04156500
Ge	-0.55148800	3.39031300	0.00000000

Complex ***9.15*** (X = NMe_2, Y = Me)

C	-0.41370000	0.35366900	1.14304900
C	0.60607300	-0.53603700	1.20077500
C	1.15341500	-1.05925500	0.00000000
C	0.60607300	-0.53603700	-1.20077500
C	-0.41370000	0.35366900	-1.14304900
H	0.90691000	-0.88231600	2.17674100
O	-0.93255200	0.80500000	0.00000000
F	-1.84887500	-2.17524600	-1.14683000
F	-1.84887500	-2.17524600	1.14683000
F	-2.50793600	-4.06034500	0.00000000
F	-0.29778700	-3.41799700	0.00000000
B	-1.65831900	-2.97389300	0.00000000
C	-0.05026000	3.82840600	1.20001000
C	-0.68440900	4.16228600	0.00000000
C	-0.05026000	3.82840600	-1.20001000
C	1.17799600	3.17001200	-1.20393200
C	1.79459400	2.83311300	0.00000000
C	1.17799600	3.17001200	1.20393200
H	-0.52475200	4.08848500	2.14184700
H	-0.52475200	4.08848500	-2.14184700
H	1.65569300	2.92341000	-2.14634600
H	2.75078500	2.32117200	0.00000000
H	1.65569300	2.92341000	2.14634600
H	-0.92551100	0.75127100	-2.00686000
H	-0.92551100	0.75127100	2.00686000
H	0.90691000	-0.88231600	-2.17674100
N	2.09577300	-1.99525500	0.00000000
C	-1.99537300	4.89617000	0.00000000
H	-2.58568400	4.65017000	0.88366800
H	-1.83374800	5.97734400	0.00000000
H	-2.58568400	4.65017000	-0.88366800
C	2.42430900	-2.67982700	1.24635800
H	3.25735700	-3.35216900	1.05998300
H	2.73277900	-1.96164000	2.00552400
H	1.55992700	-3.25286900	1.59022300
C	2.42430900	-2.67982700	-1.24635800
H	1.55992700	-3.25286900	-1.59022300
H	2.73277900	-1.96164000	-2.00552400
H	3.25735700	-3.35216900	-1.05998300

Complex ***9.16*** (X = NMe_2, Y = NH_2)

C	-0.47431700	0.38754300	1.14310400
C	0.55047400	-0.49628600	1.20082300
C	1.10806000	-1.00905600	0.00000000
C	0.55047400	-0.49628600	-1.20082300
C	-0.47431700	0.38754300	-1.14310400
H	0.85185500	-0.84304400	2.17642100
O	-0.99526400	0.83681100	0.00000000
F	-1.76469000	-2.28186900	-1.14715600
F	-1.76469000	-2.28186900	1.14715600
F	-2.42085200	-4.16790600	0.00000000
F	-0.21197800	-3.51990900	0.00000000
B	-1.57253400	-3.07985500	0.00000000
C	-0.08694900	3.86306300	1.20349500
C	-0.71483400	4.20605400	0.00000000
C	-0.08694900	3.86306300	-1.20349500
C	1.13068700	3.18994400	-1.20111700
C	1.74543600	2.83951600	0.00000000
C	1.13068700	3.18994400	1.20111700
H	-0.55686900	4.13195700	2.14512900
H	-0.55686900	4.13195700	-2.14512900
H	1.60367300	2.94363600	-2.14598400
H	2.69637300	2.31938200	0.00000000
H	1.60367300	2.94363600	2.14598400
H	-0.98870100	0.78293700	-2.00638800
H	-0.98870100	0.78293700	2.00638800
H	0.85185500	-0.84304400	-2.17642100
N	2.06975400	-1.92485500	0.00000000
N	-1.96954900	4.80988600	0.00000000
H	-2.18458900	5.33511100	0.83546500
H	-2.18458900	5.33511100	-0.83546500
C	2.42089100	-2.59789800	1.24647100
H	3.27517300	-3.24282100	1.05938800
H	2.70624600	-1.86934700	2.00470600
H	1.57593600	-3.19907900	1.58949300
C	2.42089100	-2.59789800	-1.24647100
H	1.57593600	-3.19907900	-1.58949300
H	2.70624600	-1.86934700	-2.00470600
H	3.27517300	-3.24282100	-1.05938800

Complex ***9.17*** (X = NMe_2, Y = NMe_2)

C	-0.17699600	-0.08922300	1.14270500
C	0.68063500	-1.13623700	1.20054800
C	1.13425900	-1.74222300	0.00000000
C	0.68063500	-1.13623700	-1.20054800
C	-0.17699600	-0.08922300	-1.14270500
H	0.92123600	-1.52662700	2.17652600
O	-0.61505200	0.44058300	0.00000000

F	-2.00331300	-2.37216400	-1.14699100
F	-2.00331300	-2.37216400	1.14699100
F	-2.96374900	-4.12274000	0.00000000
F	-0.67796800	-3.85321000	0.00000000
B	-1.94619200	-3.19073900	0.00000000
C	0.67770900	3.26109700	1.20403700
C	0.06614500	3.66554900	0.00000000
C	0.67770900	3.26109700	-1.20403700
C	1.80602900	2.44709400	-1.19704400
C	2.37607100	2.01971300	0.00000000
C	1.80602900	2.44709400	1.19704400
H	0.27562800	3.57972200	2.15646700
H	0.27562800	3.57972200	-2.15646700
H	2.24998600	2.15791900	-2.14425600
H	3.25923400	1.39136700	0.00000000
H	2.24998600	2.15791900	2.14425600
H	-0.61402700	0.38953900	-2.00628100
H	-0.61402700	0.38953900	2.00628100
H	0.92123600	-1.52662700	-2.17652600
N	1.91111000	-2.82012200	0.00000000
N	-1.09502800	4.41874900	0.00000000
C	2.12331400	-3.54904700	1.24615800
H	2.83581100	-4.34812700	1.05989200
H	2.54457100	-2.89070200	2.00538300
H	1.17715200	-3.97383600	1.58982900
C	2.12331400	-3.54904700	-1.24615800
H	1.17715200	-3.97383600	-1.58982900
H	2.54457100	-2.89070200	-2.00538300
H	2.83581100	-4.34812700	-1.05989200
C	-1.46471000	5.09076000	1.22945000
H	-2.39098100	5.63768100	1.06344500
H	-1.65094300	4.36707200	2.02405700
H	-0.69641700	5.79647000	1.57528500
C	-1.46471000	5.09076000	-1.22945000
H	-0.69641700	5.79647000	-1.57528500
H	-1.65094300	4.36707200	-2.02405700
H	-2.39098100	5.63768100	-1.06344500