Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Unified Classification of Non-Covalent Bonds Formed by Main Group Elements: A Bridge to Chemical Bonding

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Atoms in Molecules Analysis

Atoms in Molecules theory, an electron density topological analysis has been used to look deeper into the nature of chemical bonding. In 1960, R.F.W Bader proposed the name Atoms in Molecules[1] theory. The AIM theory examines the distribution of electron density at each position surrounding a molecule's nucleus. The AIM theory can predict the nature and characteristics of a bond based on the electron densities at the bond critical points.

Any point in space where all the first-order partial derivatives of a function (electron density in our context) vanish is termed as a critical point (CP). The nature of the critical point is determined by the rank and signature of the second derivative of electron density. The rank is defined as the number of non-zero eigenvalues of the hessian matrix. The signature is defined as the algebraic sum of the signs of the non-zero eigenvalues. A critical point is characterised by (ω, σ) where ω is the rank and σ is the signature of the critical point. Based on this, a scalar function can have four types of critical points summarised in Table S1.

Table S1: Types and characteristics of critical points (cps) based on the rank and signature of the Hessian matrix.

(Rank, Signature)	*Types of critical points*	*Curvature*
(3,-3)	Nuclear critical point (NCP)	All negative, local maxima
(3,-1)	Bond critical point (BCP)	Two negative, one positive
(3,+1)	Ring critical point (RCP)	One negative, two positive
(3,+3)	Cage critical point (CCP)	All positive, local minima

Most of the stable nuclear configurations' critical points are of rank three. In a few exceptions, degenerate cps with rank < 3 are observed. A degenerate critical point is unstable. A small change in electron density is caused by slight displacement in nuclear configuration results to vanish or change into stable cps of rank three.

Nature of Interaction using Atoms in molecules topological analysis: Based on the following criteria, Atoms in Molecules analysis has been widely used to understand the nature of interactions in weakly bound complexes.

- Sign of Laplacian: Closed shell interactions are characterised by positive Laplacian ($\nabla^2\rho > 0$), whereas negative Laplacian ($\nabla^2\rho < 0$) indicates shared shell interaction[2].
- The ratio of $|\lambda_1|/\lambda_3$**:** Sosa and co-workers[3] proposed this ratio to measure a closed and shared shell interaction. The $|\lambda_1|/\lambda_3$ less than 0.25 proposed as closed shell and greater than 1 for shared shell interaction. Values between 0.25 and 1 are regarded as the interaction of intermediate kind.
- The ratio of $|V|/G$**:** Cremer and Karka[4] proposed another criterion based on potential (V) and kinetic (G) energy density ratio. For closed-shell interaction, $|V|/G < 1$ and for shared shell $|V|/G > 2$. $|V|/G$ in between the limits proposed as intermediate kind of interaction.

Bader's AIM analysis is now routinely utilized to supplement gas phase experimental spectroscopy[5,6,7]. It has also been used successfully to get experimental charge densities in a large range of organic molecules[8], weak bonds in solids[9], and proteins[10].

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Table S2*. Comparison of slope from other studies and present work. References are from main text.*

Method		Intercept	Slope	Reference
H				
MP2(full)/aug-cc-pVTZ	0.88	-0.4	777	[11]
B3LYP/6-311++G(d,p)	0.86	-2.9(5.6)	911(141)	[54]
MP2(full)/aug-cc-pVTZ	0.98	-5.1	1101	[63]
MP2/aug-cc-pVDZ	**0.95**	**-2.5(1.0)**	**901(38)**	This work
Li				
MP2(full)/aug-cc-pVTZ	0.97	-17.6	3271	[11]
MP2(full)/aug-cc-pVTZ	0.96	-13.1	3218	[63]
MP2/aug-cc-pVDZ	**0.85**	**1.1(5.4)**	**2997(239)**	This work
Na				
MP2(full)/6-311++G(d,p)	0.90	18.0(9.6)	4699(536)	[8]
MP2/aug-cc-pVDZ	**0.91**	**-10.5(3.6)**	**4074(238)**	This work
Be				
CCSD(T)/aug-cc-pVTZ	0.87	-64.1(16.6)	2600(308)	[94]
G4	0.77	-68.0(46.3)	2813(694)	[95]
MP2/aug-cc-pVDZ	**0.88**	**-64.9(9.1)**	**2983(206)**	This work
Mg				
B3LYP/6-311+G(3df,2p)	0.93	-29.2(13.7)	3599(466)	[96]
MP2/aug-cc-pVDZ	**0.93**	**-22.9(5.0)**	**3606(188)**	This work
Ca				
G4	0.97	-3.0(18.6)	3082(566)	[97]
MP2/aug-cc-pVDZ	**0.94**	**-9.2(3.8)**	**3081(143)**	This work
B				
MP2/aug-cc-pVTZ	0.62	1.9(11.2)	608(131)	[81]
MP2/aug-cc-pVDZ	**0.76**	**0.6(3.6)**	**552(58)**	This work
Al				
MP2/aug-cc-pVTZ	0.97	-72.8(14.6)	3753(341)	[52]
MP2/aug-cc-pVDZ	**0.89**	**-44.9(9.2)**	**3564(240)**	This work
Ga				
CCSD(T)/aug-cc-pVTZ	0.89	-14.6(6.1)	1228(118)	[98]
MP2/aug-cc-pVTZ	0.87	-3.6(5.7)	1064(111)	[98]
MP2/aug-cc-pVDZ	**0.91**	**-36.3(6.1)**	**2048(125)**	This work
In				
CCSD(T)/aug-cc-pVTZ-PP	0.93	-23.6(5.5)	1824(139)	[98]

MP2/aug-cc-pVTZ-PP	0.93	-12.7(4.6)	1611(117)	[98]
MP2/aug-cc-pVDZ-PP	**0.93**	**-27.4(4.7)**	**2207(115)**	This work
C				
MP2/6-311+G(3df,2p)	0.85	-8.0(0.9)	2970(181)	[35],[99],[100]
MP2/6-311++G(d,p)	0.97	13.7(1.6)	2273(138)	[101]
MP2/aug-cc-pVDZ	**0.86**	**-9.2(1.1)**	**2827(215)**	This work
Si				
MP2/aug-cc-pVTZ	0.72	0.4(10.8)	1311(312)	[16]
MP2/aug-cc-pVDZ	0.88	-29.9(10)	1078(163)	[102]
MP2/aug-cc-pVDZ	**0.92**	**3.0(0.7)**	**823(45)**	This work
Ge				
MP2/aug-cc-pVTZ	0.71	-4.8(16.9)	1572(380)	[16]
MP2/aug-cc-pVDZ	0.82	-2.8(10.6)	1345(256)	[103]
MP2/aug-cc-pVDZ	**0.92**	**2.7(0.7)**	**828(47)**	This work
Sn				
MP2/aug-cc-pVDZ-PP	0.85	-5.2(10.7)	1590(272)	[103]
MP2/aug-cc-pVDZ-PP	**0.93**	**1.0(1.0)**	**1085(56)**	This work
N				
CCSD(T)/def2-QZVP M062X/def2-QZVP	0.88	0.8(1.3)	589(154)	[104]
MP2/aug-cc-pVDZ	**0.87**	**-0.4(0.6)**	**664(90)**	This work
P				
CCSD (T)/def2-QZVP M062X/def2-QZVP	0.95	-3.2(1.4)	1335(100)	[104]
MP2/aug-cc-pVDZ	**0.93**	**1.0(0.8)**	**865(46)**	This work
As				
CCSD (T)/def2-QZVP M062X/def2-QZVP	0.78	1.1(1.3)	991(178)	[104]
MP2/aug-cc-pVDZ	**0.93**	**2.2(0.9)**	**872(44)**	This work
O				
M06-2X/aug-cc-pVTZ	0.72	1.1(0.9)	452(125)	[88]
MP2/aug-cc-PVTZ	0.82	-2.0(1.4)	906(209)	[89]
MP2/aug-cc-pVDZ	**0.97**	**-0.7(0.4)**	**640(38)**	This work
S				
MP2/CBS	0.92	-0.6(0.9)	1255(64)	[105]
MP2/aug-cc-pVTZ	0.93	0.3(4.1)	839(11)	[106]
MP2/aug-cc-pVDZ	**0.96**	**1.3(0.6)**	**785(29)**	This work
Se				
MP2/aug-cc-pVTZ	0.90	-24.4(10.1)	1418(215)	[106]
MP2/aug-cc-pVTZ	0.86	-3.6(10.8)	1005(207)	[107]
MP2/aug-cc-pVDZ	**0.96**	**1.2(0.8)**	**866(31)**	This work
Te				
MP2/aug-cc-pVTZ-PP	0.88	-1.1(3.7)	862(222)	[108]
MP2/aug-cc-pVDZ-PP	**0.90**	**-3.4(2.2)**	**1194(74)**	This work
F				
M06-2X/aug-cc-pVDZ	0.90	-5.0(1.7)	702(102)	[109]
MP2/aug-cc-pVDZ	**0.84**	**-1.4(0.4)**	**875(71)**	This work
Cl				
MP2(full)/aug-cc-pVDZ	0.96	-0.3	776	[11]

MP2(full)/aug-cc-pVTZ	0.98	9.0	1162	[63]
MP2/aug-cc-pVDZ	**0.93**	**2.0(0.9)**	**681(36)**	This work
Br				
B3LYP/6-311++G(d,p)	0.97	-20.3(5.4)	1776(147)	[54]
MP2/aug-cc-pVDZ	**0.93**	**-5.0(1.5)**	**992(50)**	This work
I				
B3LYP/6-311++G(d,p)	0.90	-21.0(7.5)	1862(237)	[54]
MP2/aug-cc-pVDZ	**0.91**	**-6.2(2.3)**	**1269(75)**	This work

Table S3*: Electron density, dissociation energy, percentage covalency, and ionicity of some diatomic molecules. Blue molecules are predominantly ionic (high slope), cyan molecules are intermediate (intermediate), and green molecules are ionic (low slope).*

Diatomic Molecules	*Electron Density (au)*	*Dissociation Energy (kJ/mol)*	*Covalency*	*Ionicity*
NaF	0.0445	477.0	3.3	96.7
NaCl	0.0286	407.9	2.7	97.3
NaBr	0.0249	362.8	4.2	95.8
LiF	0.065	573.0	2.3	97.7
LiCl	0.0356	464.0	3.4	96.6
LiBr	0.0306	418.0	4.4	95.6
KBr	0.0275	379.1	0	100
KCl	0.0318	433.0	1.8	98.2
KF	0.0521	489.2	2.5	97.5
		y=4610(498)x+270.4(19.9), R^2 = 0.92		
HF	0.3526	569.7	42	57
HCl	0.2401	431.4	71	29
HBr	0.1963	366.2	80	20
FCl	0.1803	256.3	61	39
FBr	0.1459	280.0	52	48
BrCl	0.1143	219.0	88	12
		y =1510(191)x + 44.4(41.8), R^2 = 0.94		
H_2	0.2496	435.8	100	0
Li_2	0.0139	82.4	100	0
B_2	0.1247	290.0	100	0
C_2	0.316	618.3	100	0
N_2	0.7204	944.8	100	0
O_2	0.5505	498.4	100	0
Cl_2	0.1388	243.0	100	0
Br_2	0.0975	193.9	100	0
		y = 1042(179)x + 125.2 (64.3), R^2 = 0.85		

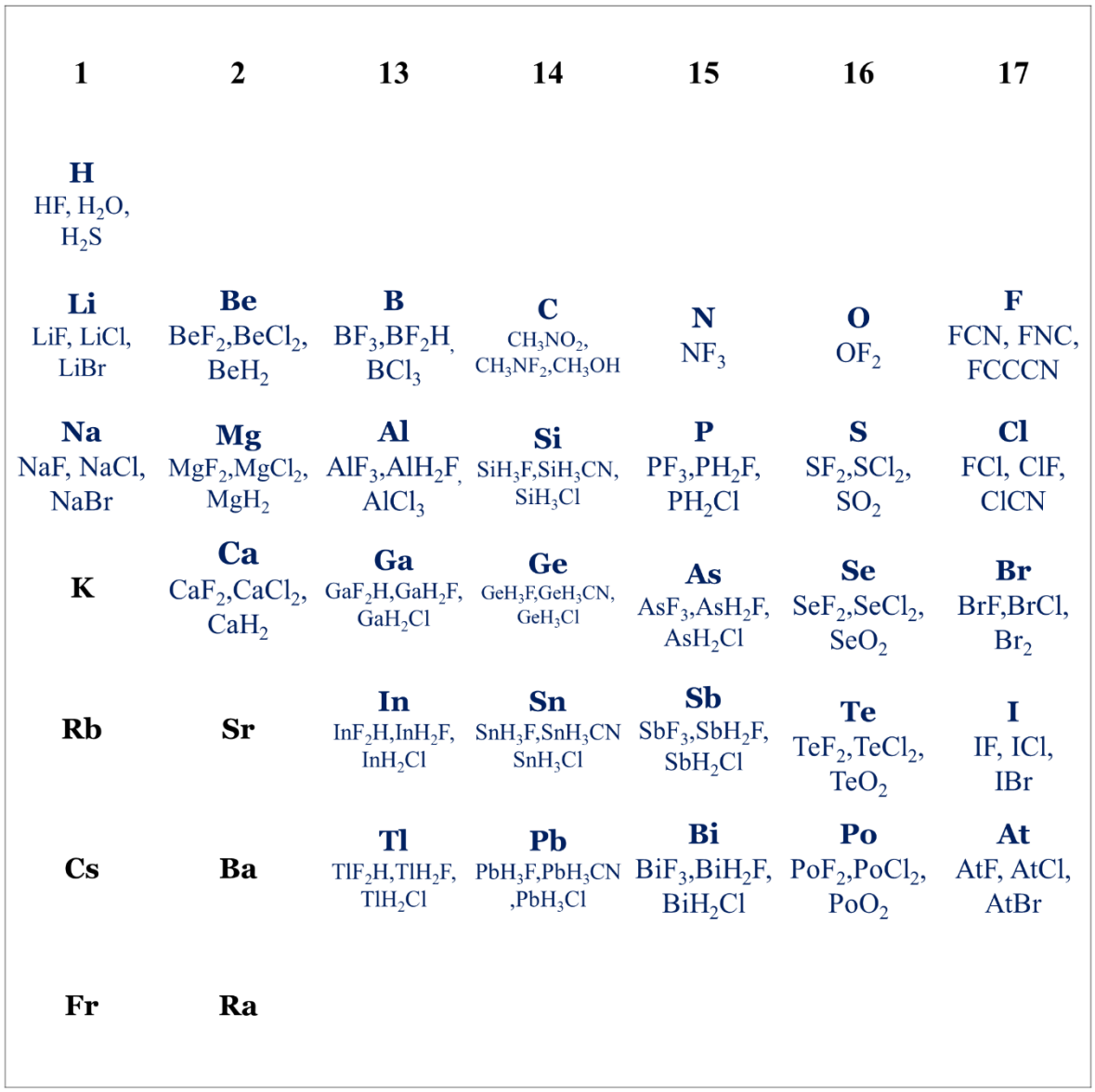

Figure S1*: Non-covalent bond donors used in this study. To obtain a correlation plot of a non-covalent bond, three different donors were combined with ten different acceptors (mostly H_2O, NH_3, H_2S, PH_3, HCHO, C_2H_4, HCN, CO, CH_3OH, CH_3OCH_3).*

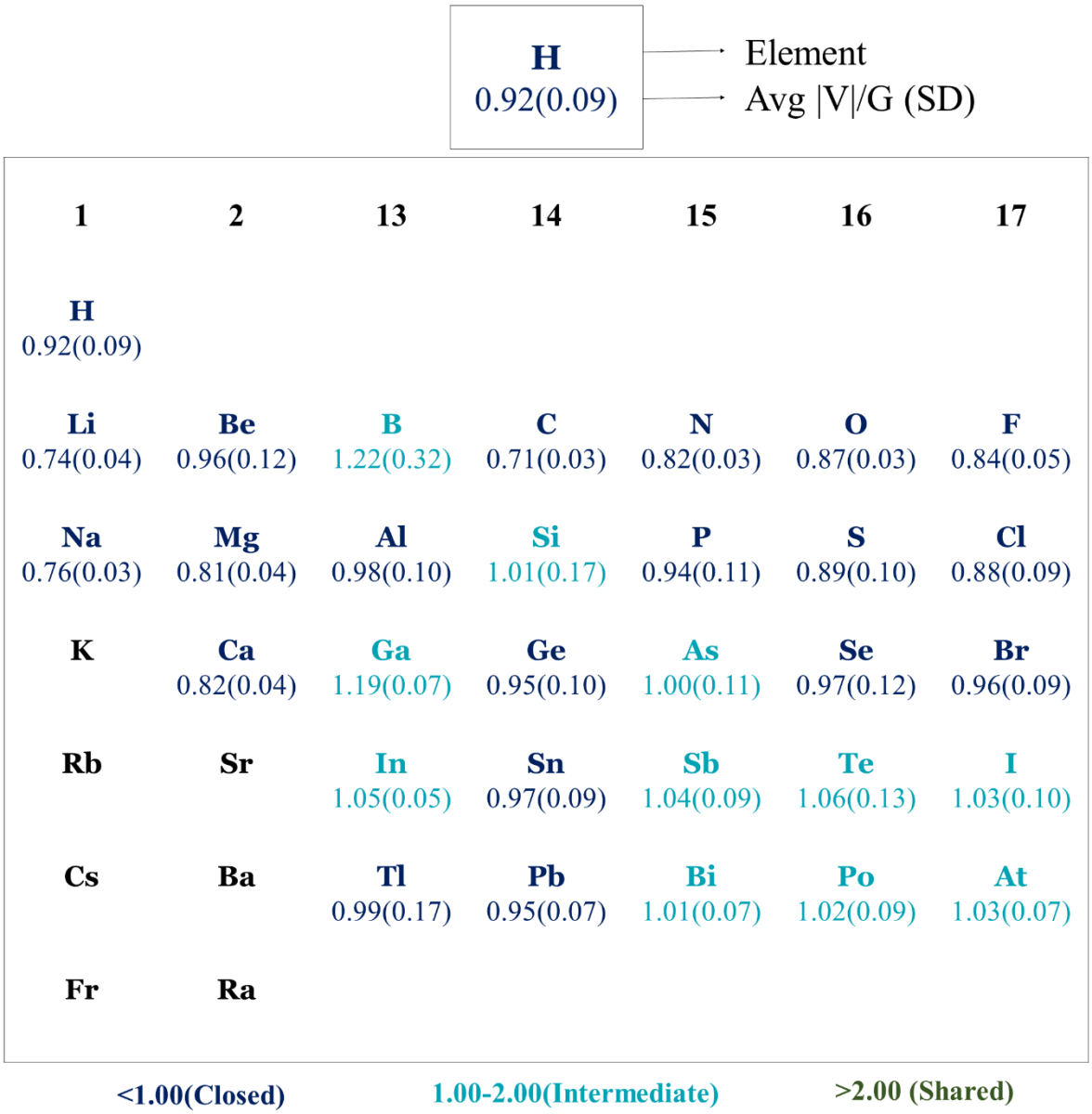

Figure S2. *The ratio of the potential (|V(r)|) and kinetic (G(r)) energy densities of the electrons at BCP for the different non-covalent bonds formed by main group elements of the Periodic Table. The |V(r)|/ G(r) ratio has been used for the characterisation of bonding in three regions, namely closed-shell (<1.00, blue), intermediate (1.00-2.00, cyan), and shared shell (>2.00, green) bond. All the complexes under study fall under the closed or intermediate region.*

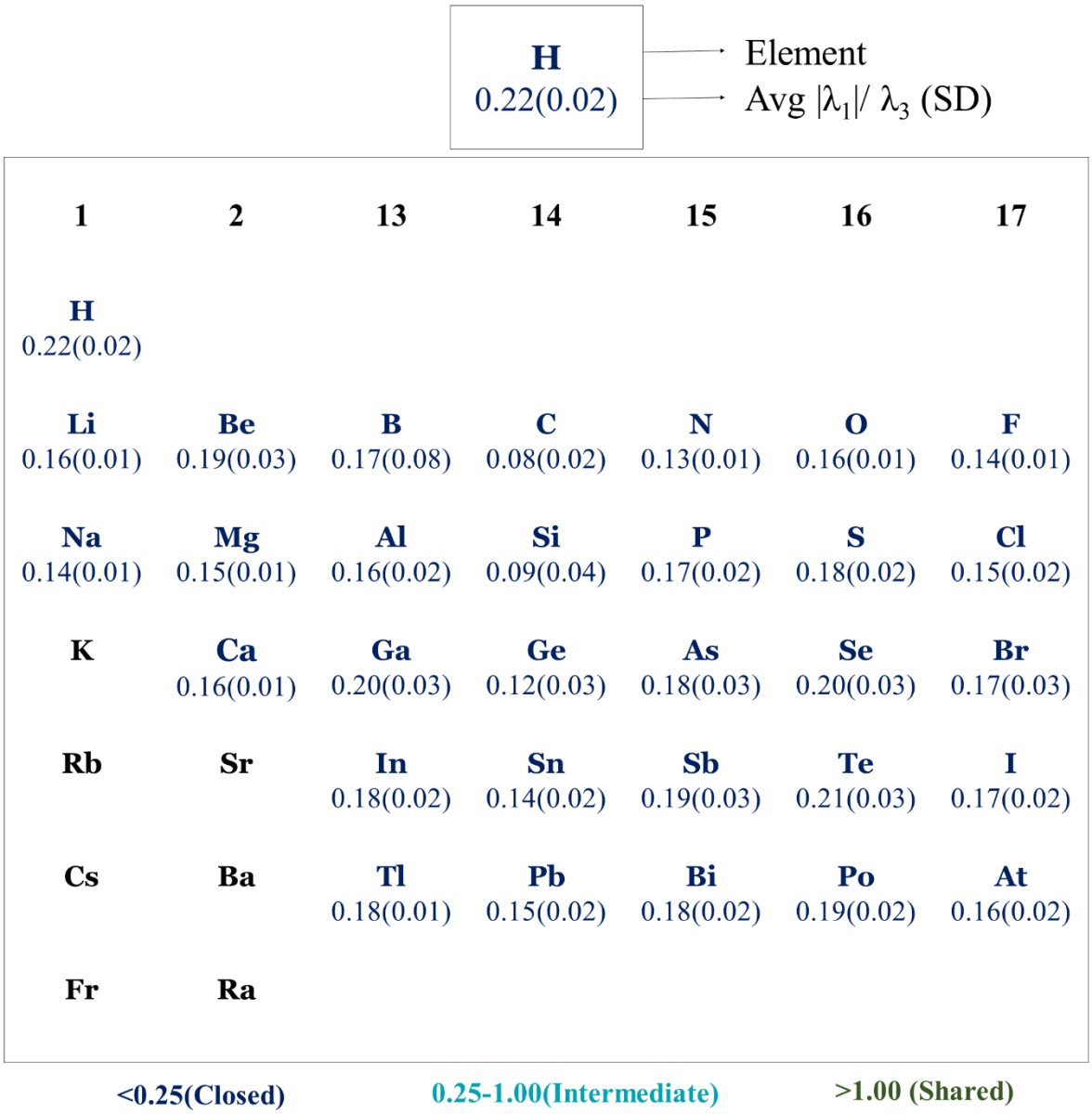

Figure S3. *The ratio of the first ($|\lambda_1|$) and third (λ_3) eigenvalues of the Hessian matrix at BCP for the different non-covalent bonds formed by the main group elements of the Periodic Table. The ($|\lambda_1|$)/λ_3 ratio has been used for the characterisation of bonding in three regions, namely closed-shell (<0.25, blue), intermediate (0.25-1.00, cyan), and shared shell bonding (>1.00, green). All the complexes under study fall under the closed-shell bonding.*

The following section contains all data sets. (Table D1 to Table D31)

All Data Sets

Table D1. *Electron density at BCP (au) and binding energy (kJ/mol) data for H-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
FH•••OH_2	0.0381	32.9
FH•••SH_2	0.0214	19.0
FH•••NH_3	0.0506	48.7
FH•••NCH	0.0288	28.3
FH•••CO	0.0203	13.5
FH•••HCHO	0.0395	31.1
FH•••C_2H_4	0.0183	17.1
FH•••CH_3OH	0.0452	37.4
FH•••PH_3	0.0202	17.6
FH•••$O(CH_3)_2$	0.0510	39.1
HOH•••OH_2	0.0237	18.5
HOH•••SH_2	0.0137	10.7
HOH•••NH_3	0.0275	24.3
HOH•••NCH	0.0174	15.0
HOH•••CO	0.0115	6.4
HOH•••OCH_2	0.0234	19.8
HOH•••C_2H_4	0.0121	9.5
HOH•••$OHCH_3$	0.0277	21.1
HOH•••PH_3	0.0121	8.9
HOH•••$O(CH_3)_2$	0.0306	22.1
HSH•••OH_2	0.0155	10.4
HSH•••SH_2	0.0105	6.5
HSH•••NH_3	0.0197	13.7
HSH•••NCH	0.0124	9.4
HSH•••CO	0.0078	3.6
HSH•••OCH_2	0.0172	11.7
HSH•••C_2H_4	0.0095	6.3
HSH•••$OHCH_3$	0.0189	12.9
HSH•••PH_3	0.0090	5.7
HSH•••$O(CH_3)_2$	0.0239	13.6

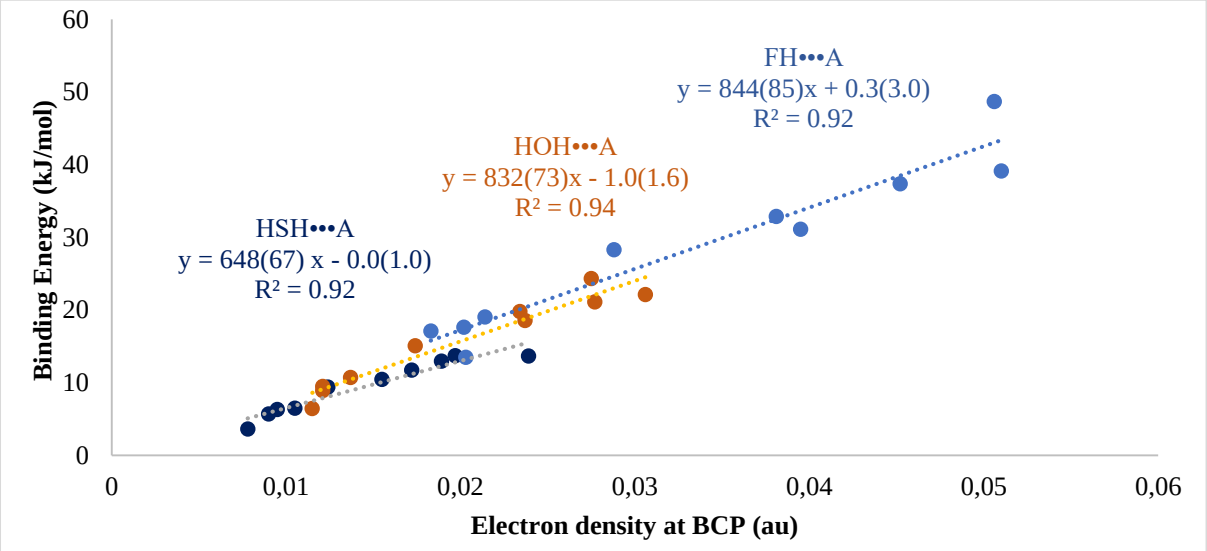

Figure D1*. Binding energy (kJ/mol) versus electron density at BCP (au) plot for H-bonded complexes.*

Table D2. *Electron density at BCP (au) and binding energy (kJ/mol) data for Li-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FLi•••OH_2$	0.0241	65.7
$FLi•••NCCH_3$	0.0222	73.7
$FLi•••NH_3$	0.0234	79.9
FLi•••NCH	0.0203	61.3
$FLi•••OCH_2$	0.0251	75.0
$FLi •••C_2H_4$	0.0112	33.5
$FLi•••OHCH_3$	0.0269	75.9
$FLi•••PH_3$	0.0118	37.0
FLi•••CO	0.0130	28.7
$FLi•••O(CH_3)_2$	0.0275	68.8
$ClLi•••OH_2$	0.0256	74.3
$ClLi •••NCCH_3$	0.0237	84.5
$ClLi•••NH_3$	0.0247	90.3
ClLi•••NCH	0.0218	70.3
$ClLi•••OCH_2$	0.0267	80.9
$ClLi•••C_2H_4$	0.0125	39.7
$ClLi•••OHCH_3$	0.0286	84.8
$ClLi•••PH_3$	0.0132	44.0
ClLi•••CO	0.0142	33.5
$ClLi•••O(CH_3)_2$	0.0297	80.7
$BrLi•••OH_2$	0.0259	76.2
$BrLi•••NCCH_3$	0.0242	86.8
$BrLi•••NH_3$	0.0252	92.4
BrL•••NCH	0.0222	72.2
$BrLi•••OCH_2$	0.0271	81.7
$BrLi •••C_2H_4$	0.0126	41.0
$BrLi•••OHCH_3$	0.0290	86.3
$BrLi•••PH_3$	0.0135	45.4
BrLi•••CO	0.0145	34.4
$BrLi•••O(CH_3)_2$	0.0302	82.7

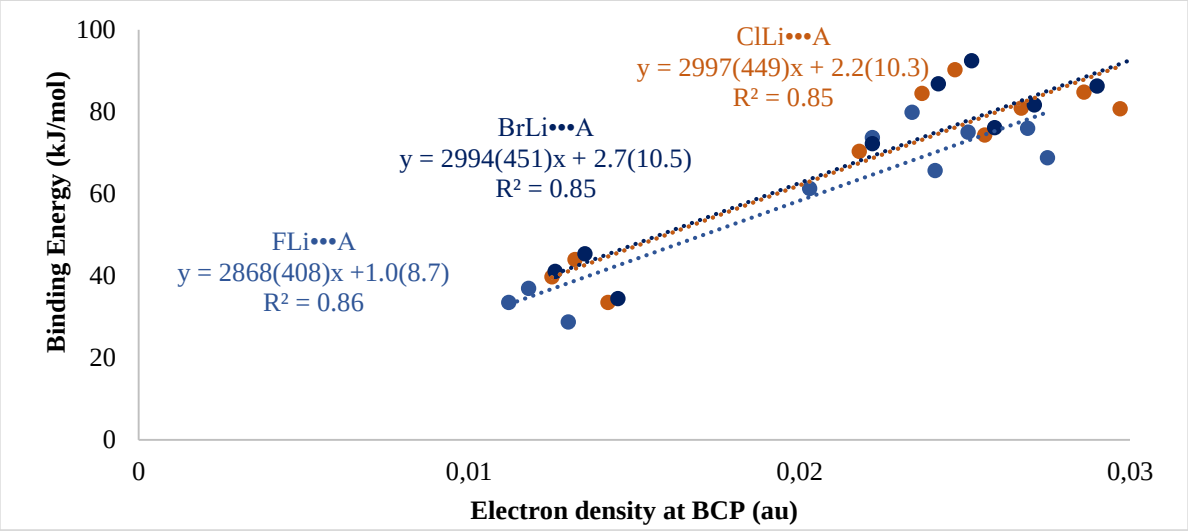

Figure D2*. Binding energy (kJ/mol) versus electron density at BCP (au) plot for Li- bonded complexes.*

Table D3. *Electron density at BCP (au) and binding energy (kJ/mol) data for Na-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FNa\bullet\bullet\bullet OH_2$	0.0128	46.5
$FNa\bullet\bullet\bullet NCCH_3$	0.0162	58.7
$FNa\bullet\bullet\bullet NH_3$	0.0165	58.0
$FNa\bullet\bullet\bullet NCH$	0.0148	48.0
$FNa\bullet\bullet\bullet OCH_2$	0.0165	66.5
$FNa\bullet\bullet\bullet C_2H_4$	0.0082	23.5
$FNa\bullet\bullet\bullet OHCH_3$	0.0176	61.4
$FNa\bullet\bullet\bullet PH_3$	0.0086	26.7
$FNa\bullet\bullet\bullet CO$	0.0093	19.6
$FNa\bullet\bullet\bullet O(CH_3)_2$	0.0175	53.7
$ClNa\bullet\bullet\bullet OH_2$	0.0150	51.9
$ClNa\bullet\bullet\bullet NCCH_3$	0.0171	64.8
$ClNa\bullet\bullet\bullet NH_3$	0.0174	63.6
$ClNa\bullet\bullet\bullet NCH$	0.0156	53.0
$ClNa\bullet\bullet\bullet OCH_2$	0.0173	63.6
$ClNa\bullet\bullet\bullet C_2H_4$	0.0087	26.7
$ClNa\bullet\bullet\bullet OHCH_3$	0.0184	62.4
$ClNa\bullet\bullet\bullet PH_3$	0.0091	30.1
$ClNa\bullet\bullet\bullet CO$	0.0097	21.7
$ClNa\bullet\bullet\bullet O(CH_3)_2$	0.0188	57.4
$BrNa\bullet\bullet\bullet OH_2$	0.0155	52.9
$BrNa\bullet\bullet\bullet NCCH_3$	0.0175	66.1
$BrNa\bullet\bullet\bullet NH_3$	0.0177	64.7
$BrNa\bullet\bullet\bullet NCH$	0.0159	53.9
$BrNa\bullet\bullet\bullet OCH_2$	0.0175	62.8
$BrNa\bullet\bullet\bullet C_2H_4$	0.0089	27.3
$BrNa\bullet\bullet\bullet OHCH_3$	0.0188	62.3
$BrNa\bullet\bullet\bullet PH_3$	0.0094	30.8
$BrNa\bullet\bullet\bullet CO$	0.0099	22.1
$BrNa\bullet\bullet\bullet O(CH_3)_2$	0.0191	57.7

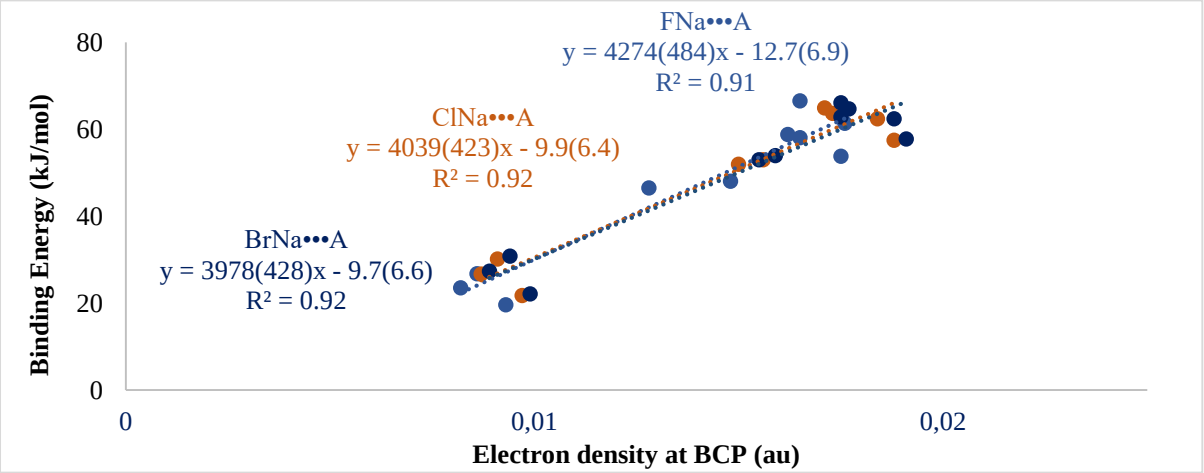

Figure D3. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Na-bonded complexes.*

Table D4. *Electron density at BCP (au) and binding energy (kJ/mol) data for Be-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Be{\bullet\bullet\bullet}OH_2$	0.0470	84.0
$F_2Be{\bullet\bullet\bullet}SH_2$	0.0315	40.0
$F_2Be{\bullet\bullet\bullet}NH_3$	0.0546	113.7
$F_2Be{\bullet\bullet\bullet}NCH$	0.0406	59.8
$F_2Be{\bullet\bullet\bullet}OCH_2$	0.0446	73.4
$F_2Be{\bullet\bullet\bullet}C_2H_4$	0.0250	30.0
$F_2Be{\bullet\bullet\bullet}OHCH_3$	0.0523	100.0
$F_2Be{\bullet\bullet\bullet}PH_3$	0.0335	39.6
$F_2Be{\bullet\bullet\bullet}CO$	0.0321	26.3
$F_2Be{\bullet\bullet\bullet}O(CH_3)_2$	0.0544	107.3
$Cl_2Be{\bullet\bullet\bullet}OH_2$	0.0522	84.7
$Cl_2Be{\bullet\bullet\bullet}SH_2$	0.0369	40.8
$Cl_2Be{\bullet\bullet\bullet}NH_3$	0.0602	119.8
$Cl_2Be{\bullet\bullet\bullet}NCH$	0.0477	61.2
$Cl_2Be{\bullet\bullet\bullet}OCH_2$	0.0481	70.8
$Cl_2Be{\bullet\bullet\bullet}C_2H_4$	0.0278	27.6
$Cl_2Be{\bullet\bullet\bullet}OHCH_3$	0.0575	103.3
$Cl_2Be{\bullet\bullet\bullet}PH_3$	0.0404	43.8
$Cl_2Be{\bullet\bullet\bullet}CO$	0.0401	23.6
$Cl_2Be{\bullet\bullet\bullet}O(CH_3)_2$	0.0578	105.7
$H_2Be{\bullet\bullet\bullet}OH_2$	0.0428	62.7
$H_2Be{\bullet\bullet\bullet}SH_2$	0.0274	24.2
$H_2Be{\bullet\bullet\bullet}NH_3$	0.0496	85.9
$H_2Be{\bullet\bullet\bullet}NCH$	0.0386	40.3
$H_2Be{\bullet\bullet\bullet}OCH_2$	0.0380	50.8
$H_2Be{\bullet\bullet\bullet}NH_2CH_3$	0.0536	99.3
$H_2Be{\bullet\bullet\bullet}OHCH_3$	0.0481	78.2
$H_2Be{\bullet\bullet\bullet}PH_3$	0.0307	24.1
$H_2Be{\bullet\bullet\bullet}CO$	0.0341	13.7
$H_2Be{\bullet\bullet\bullet}O(CH_3)_2$	0.0491	83.3

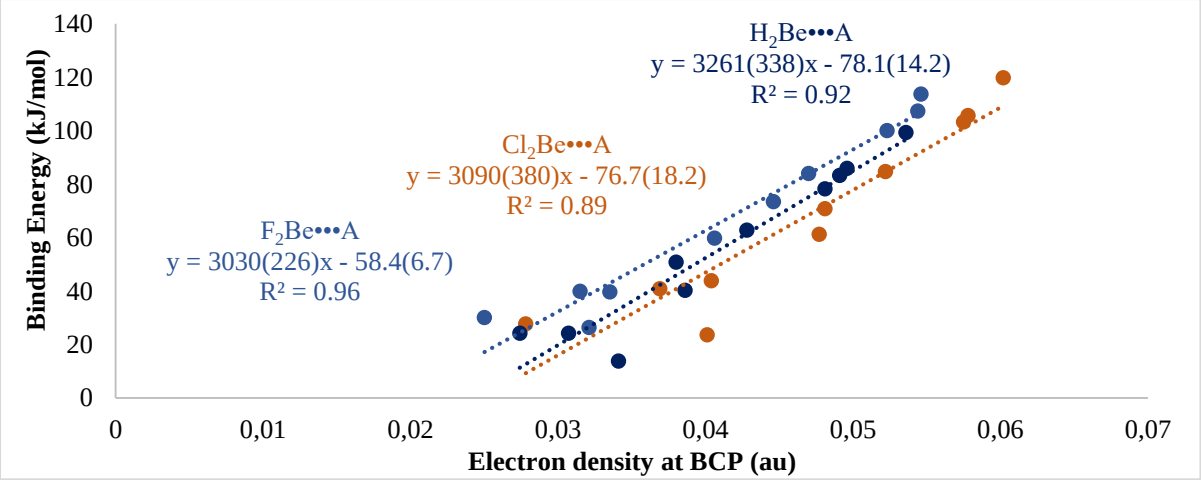

Figure D4*. Binding energy (kJ/mol) versus electron density at BCP (au) plot for Be-bonded complexes.*

Table D5. *Electron density at BCP (au) and binding energy (kJ/mol) data for Mg-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Mg{\bullet\bullet\bullet}OH_2$	0.0324	91.0
$F_2Mg{\bullet\bullet\bullet}SH_2$	0.0200	50.9
$F_2Mg{\bullet\bullet\bullet}NH_3$	0.0320	107.9
$F_2Mg{\bullet\bullet\bullet}NCH$	0.0260	71.9
$F_2Mg{\bullet\bullet\bullet}OCH_2$	0.0307	84.8
$F_2Mg{\bullet\bullet\bullet}C_2H_4$	0.0160	43.1
$F_2Mg{\bullet\bullet\bullet}OHCH_3$	0.0349	103.7
$F_2Mg{\bullet\bullet\bullet}PH_3$	0.0188	48.5
$F_2Mg{\bullet\bullet\bullet}CO$	0.0177	35.5
$F_2Mg{\bullet\bullet\bullet}O(CH_3)_2$	0.0363	109.2
$Cl_2Mg{\bullet\bullet\bullet}OH_2$	0.0341	97.8
$Cl_2Mg{\bullet\bullet\bullet}SH_2$	0.0187	56.7
$Cl_2Mg{\bullet\bullet\bullet}NH_3$	0.0338	117.2
$Cl_2Mg{\bullet\bullet\bullet}NCH$	0.0279	78.9
$Cl_2Mg{\bullet\bullet\bullet}HCHO$	0.0320	88.5
$Cl_2Mg{\bullet\bullet\bullet}C_2H_4$	0.0171	49.6
$Cl_2Mg{\bullet\bullet\bullet}OHCH_3$	0.0368	112.7
$Cl_2Mg{\bullet\bullet\bullet}PH_3$	0.0207	55.7
$Cl_2Mg{\bullet\bullet\bullet}CO$	0.0191	38.5
$Cl_2Mg{\bullet\bullet\bullet}O(CH_3)_2$	0.0368	116.4
$H_2Mg{\bullet\bullet\bullet}OH_2$	0.0274	61.9
$H_2Mg{\bullet\bullet\bullet}SH_2$	0.0140	28.2
$H_2Mg{\bullet\bullet\bullet}NH_3$	0.0272	73.7
$H_2Mg{\bullet\bullet\bullet}NCH$	0.0208	44.5
$H_2Mg{\bullet\bullet\bullet}OCH_2$	0.0252	55.0
$H_2Mg{\bullet\bullet\bullet}C_2H_4$	0.0115	22.4
$H_2Mg{\bullet\bullet\bullet}OHCH_3$	0.0300	72.6
$H_2Mg{\bullet\bullet\bullet}PH_3$	0.0136	25.2
$H_2Mg{\bullet\bullet\bullet}CO$	0.0123	16.5
$H_2Mg{\bullet\bullet\bullet}O(CH_3)_2$	0.0305	75.9

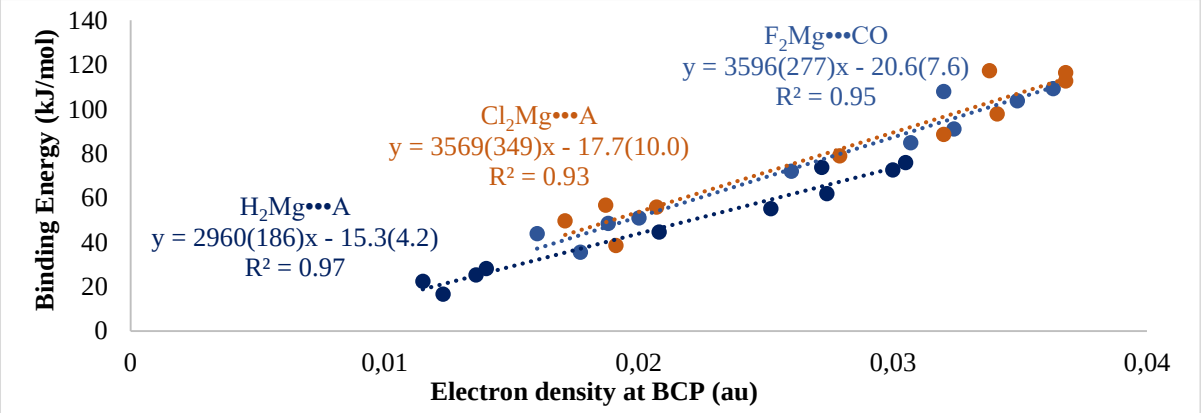

Figure D5. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Mg- bonded complexes.*

Table D6. *Electron density at BCP (au) and binding energy (kJ/mol) data for Ca-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Ca•••OH_2$	0.0312	91.7
$F_2Ca•••SH_2$	0.0173	48.0
$F_2Ca•••NH_3$	0.0287	90.9
$F_2Ca•••NCH$	0.0244	69.1
$F_2Ca•••CO$	0.0161	32.4
$F_2Ca•••OCH_2$	0.0286	80.0
$F_2Ca•••C_2H_4$	0.0146	40.6
$F_2Ca•••OHCH_3$	0.0320	91.3
$F_2Ca•••PH_3$	0.0172	43.4
$F_2Ca•••O(CH_3)_2$	0.0351	92.9
$Cl_2Ca•••OH_2$	0.0336	94.5
$Cl_2Ca•••SH_2$	0.0208	54.8
$Cl_2Ca•••NH_3$	0.0324	102.9
$Cl_2Ca•••NCH$	0.0280	78.3
$Cl_2Ca•••CO$	0.0192	38.2
$Cl_2Ca•••OCH_2$	0.0314	84.4
$Cl_2Ca•••C_2H_4$	0.0166	48.6
$Cl_2Ca•••OHCH_3$	0.0375	103.3
$Cl_2Ca•••PH_3$	0.0190	52.0
$Cl_2Ca•••O(CH_3)_2$	0.0377	106.4
$H_2Ca•••SH_2$	0.0166	40.0
$H_2Ca•••NH_3$	0.0289	85.0
$H_2Ca•••NCH$	0.0238	63.0
$H_2Ca•••CO$	0.0151	27.3
$H_2Ca•••OCH_2$	0.0283	70.1
$H_2Ca•••C_2H_4$	0.0134	34.6
$H_2Ca•••OHCH_3$	0.0328	85.6
$H_2Ca•••PH_3$	0.0148	37.1
$H_2Ca•••O(CH_3)_2$	0.0345	88.3
$H_2Ca•••CH_3CN$	0.0267	77.6

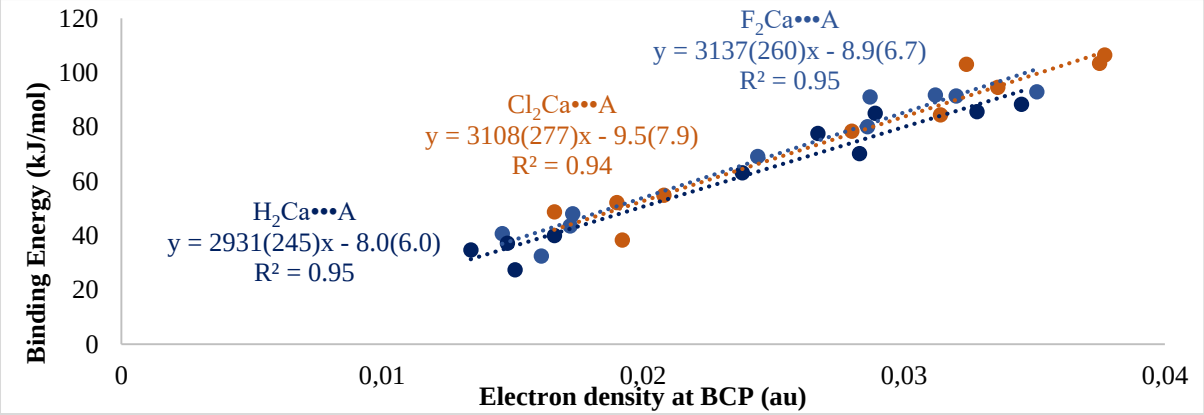

Figure D6. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Ca- bonded complexes.*

Table D7. *Electron density at BCP (au) and binding energy (kJ/mol) data for B-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3B•••OH_2$	0.0696	27.3
$F_3B•••SH_2$	0.0147	11.0
$F_3B•••NH_3$	0.1117	88.1
$F_3B•••NCH$	0.0233	18.6
$F_3B•••CO$	0.0115	8.0
$F_3B•••OCH_2$	0.0663	27.8
$F_3B•••C_2H_4$	0.0107	10.1
$F_3B•••OHCH_3$	0.0845	46.2
$F_3B•••PH_3$	0.0126	9.6
$F_3B•••O(CH_3)_2$	0.0894	55.2
$Cl_3B•••OH_2$	0.0831	16.4
$Cl_3B•••SH_2$	0.0081	8.9
$Cl_3B•••NH_3$	0.1232	101.2
$Cl_3B•••NCH$	0.0109	11.9
$Cl_3B•••CO$	0.0064	5.9
$Cl_3B•••OCH_2$	0.0789	17.6
$Cl_3B•••C_2H_4$	0.007	10.0
$Cl_3B•••OHCH_3$	0.0945	44.1
$Cl_3B•••PH_3$	0.0071	8.2
$Cl_3B•••O(CH_3)_2$	0.0966	50.2
$HF_2B•••OH_2$	0.0613	21.8
$HF_2B•••SH_2$	0.0110	9.1
$HF_2B•••NH_3$	0.1042	71.7
$HF_2B•••NCH$	0.0164	13.5
$HF_2B•••CO$	0.0081	5.5
$HF_2B•••OCH_2$	0.0558	22.0
$HF_2B•••C_2H_4$	0.0087	7.7
$HF_2B•••OHCH_3$	0.0741	33.1
$HF_2B•••PH_3$	0.0086	7.0
$HF_2B•••O(CH_3)_2$	0.0797	42.5

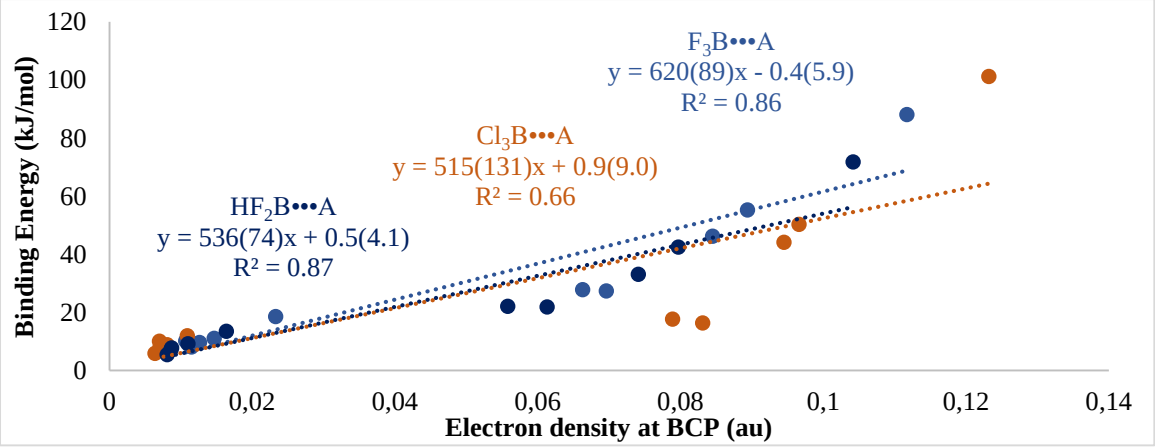

Figure D7*. Binding energy (kJ/mol) versus electron density at BCP (au) plot for B-bonded complexes.*

Table D8. *Electron density at BCP (au) and binding energy (kJ/mol) data for Al-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3Al\cdots OH_3$	0.0436	115.7
$F_3Al\cdots SH_3$	0.0303	72.6
$F_3Al\cdots NH_3$	0.0478	159.4
$F_3Al\cdots NCH$	0.0376	97.7
$F_3Al\cdots CO$	0.0299	54.9
$F_3Al\cdots OCH_2$	0.0429	111.1
$F_3Al\cdots C_2H_4$	0.0245	59.8
$F_3Al\cdots OHCH_3$	0.0478	132.0
$F_3Al\cdots PH_3$	0.0336	78.1
$F_3Al\cdots O(CH_3)_2$	0.0501	140.2
$Cl_3Al\cdots OH_2$	0.0450	102.1
$Cl_3Al\cdots SH_2$	0.0325	66.1
$Cl_3Al\cdots NH_3$	0.0506	150.5
$Cl_3Al\cdots NCH$	0.0399	87.2
$Cl_3Al\cdots CO$	0.0321	44.6
$Cl_3Al\cdots OCH_2$	0.0443	98.7
$Cl_3Al\cdots C_2H_4$	0.0257	49.9
$Cl_3Al\cdots OHCH_3$	0.0500	123.0
$Cl_3Al\cdots PH_3$	0.0375	74.8
$Cl_3Al\cdots O(CH_3)_2$	0.0516	130.9
$H_2FAl\cdots OH_2$	0.0368	81.8
$H_2FAl\cdots SH_2$	0.0241	46.6
$H_2FAl\cdots NH_3$	0.0416	111.9
$H_2FAl\cdots NCH$	0.0309	64.5
$H_2FAl\cdots CO$	0.0234	31.6
$H_2FAl\cdots OCH_2$	0.0365	82.9
$H_2FAl\cdots C_2H_4$	0.0203	39.0
$H_2FAl\cdots OHCH_3$	0.0410	96.1
$H_2FAl\cdots PH_3$	0.0270	47.5
$H_2FAl\cdots O(CH_3)_2$	0.0427	100.2

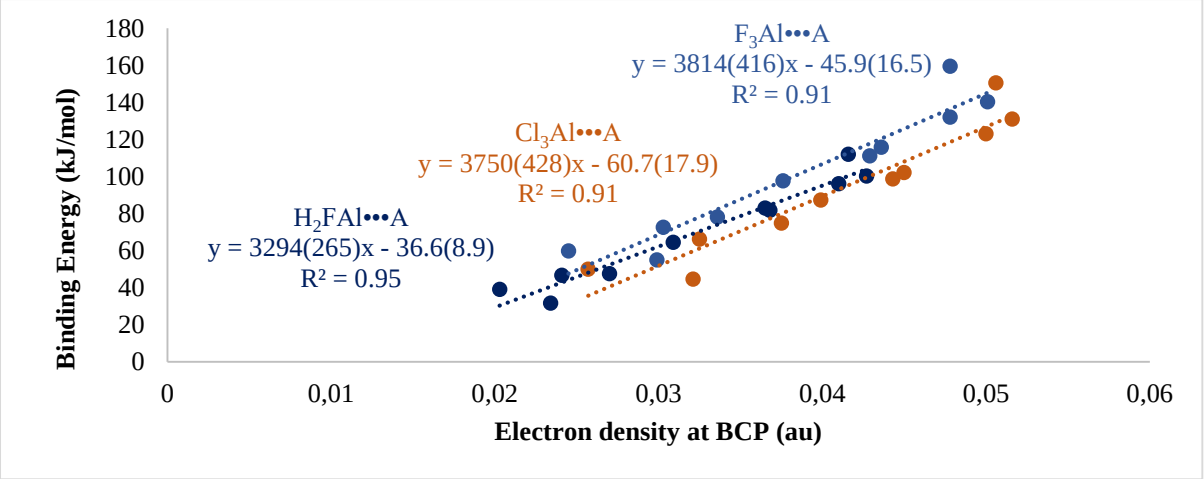

Figure D8. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Al-bonded complexes.*

Table D9. *Electron density at BCP (au) and binding energy (kJ/mol) data for Ga-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$HF_2Ga•••OH_2$	0.0577	82.7
$HF_2Ga•••SH_2$	0.0387	51.2
$HF_2Ga•••NH_3$	0.0661	116.6
$HF_2Ga•••NCH$	0.0485	60.6
$HF_2Ga•••CO$	0.0363	29.2
$HF_2Ga•••OCH_2$	0.0556	77.2
$HF_2Ga•••C_2H_4$	0.031	38.4
$HF_2Ga•••OHCH_3$	0.0621	94.0
$HF_2Ga•••PH_3$	0.0454	51.3
$HF_2Ga•••O(CH_3)_2$	0.064	91.7
$H_2FGa•••OH_2$	0.0500	64.9
$H_2FGa•••SH_2$	0.0337	40.0
$H_2FGa•••NH_3$	0.0597	95.7
$H_2FGa•••NCH$	0.0431	48.5
$H_2FGa•••CO$	0.0326	23.3
$H_2FGa•••OCH_2$	0.0494	67.5
$H_2FGa•••C_2H_4$	0.0290	33.7
$H_2FGa•••OHCH_3$	0.0558	74.6
$H_2FGa•••PH_3$	0.0404	40.7
$H_2FGa•••O(CH_3)_2$	0.0578	76.3
$H_2ClGa•••OH_2$	0.0505	62.8
$H_2ClGa•••SH_2$	0.0354	41.8
$H_2ClGa•••NH_3$	0.0620	98.1
$H_2ClGa•••NCH$	0.0452	49.9
$H_2ClGa•••CO$	0.0356	23.3
$H_2ClGa•••OCH_2$	0.0497	65.0
$H_2ClGa•••C_2H_4$	0.0302	35.2
$H_2ClGa•••OHCH_3$	0.0574	76.2
$H_2ClGa•••PH_3$	0.0442	45.5
$H_2ClGa•••O(CH_3)_2$	0.0587	76.2

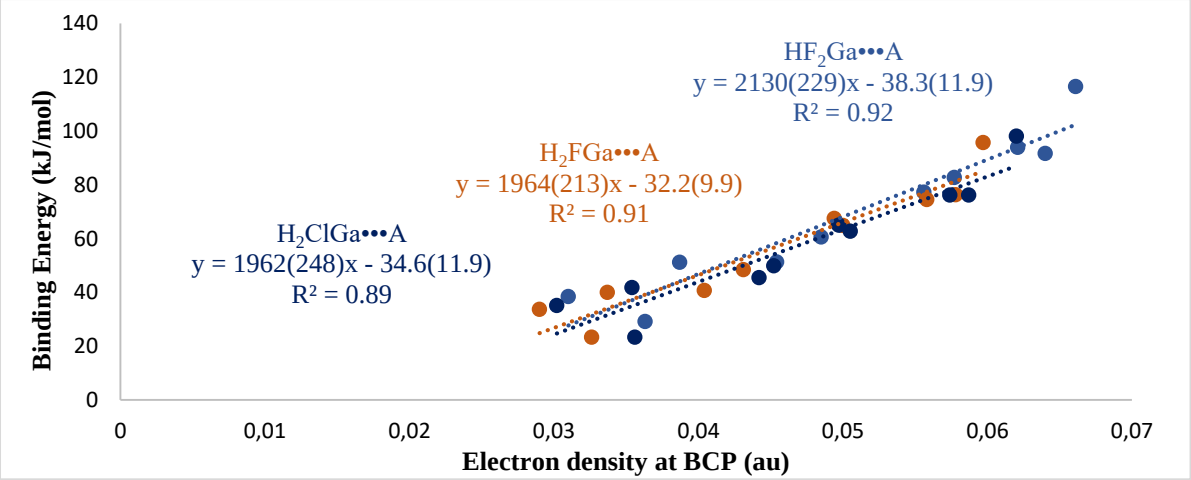

Figure D9. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Ga- bonded complexes.*

Table D10. *Electron density at BCP (au) and binding energy (kJ/mol) data for In-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$HF_2In\cdots OH_2$	0.0495	81.0
$HF_2In\cdots SH_2$	0.0334	55.6
$HF_2In\cdots NH_3$	0.0554	109.0
$HF_2In\cdots NCH$	0.0408	60.2
$HF_2In\cdots CO$	0.0288	29.8
$HF_2In\cdots OCH_2$	0.0469	76.0
$HF_2In\cdots C_2H_4$	0.0278	43.4
$HF_2In\cdots OHCH_3$	0.0527	90.3
$HF_2In\cdots PH_3$	0.0371	52.3
$HF_2In\cdots O(CH_3)_2$	0.0536	90.0
$H_2FIn\cdots OH_2$	0.0422	65.3
$H_2FIn\cdots SH_2$	0.0278	41.1
$H_2FIn\cdots NH_3$	0.0496	88.3
$H_2FIn\cdots NCH$	0.0358	47.0
$H_2FIn\cdots CO$	0.0251	22.7
$H_2FIn\cdots OCH_2$	0.0411	66.0
$H_2FIn\cdots C_2H_4$	0.0249	31.2
$H_2FIn\cdots OHCH_3$	0.0469	73.4
$H_2FIn\cdots PH_3$	0.0323	40.1
$H_2FIn\cdots O(CH_3)_2$	0.0467	69.2
$H_2ClIn\cdots OH_2$	0.0417	60.5
$H_2ClIn\cdots SH_2$	0.0288	42.1
$H_2ClIn\cdots NH_3$	0.0499	88.4
$H_2ClIn\cdots NCH$	0.0369	48.4
$H_2ClIn\cdots CO$	0.0258	22.9
$H_2ClIn\cdots OCH_2$	0.0409	62.6
$H_2ClIn\cdots C_2H_4$	0.0255	36.4
$H_2ClIn\cdots OHCH_3$	0.0472	70.7
$H_2ClIn\cdots PH_3$	0.0337	43.0
$H_2ClIn\cdots O(CH_3)_2$	0.0473	68.0

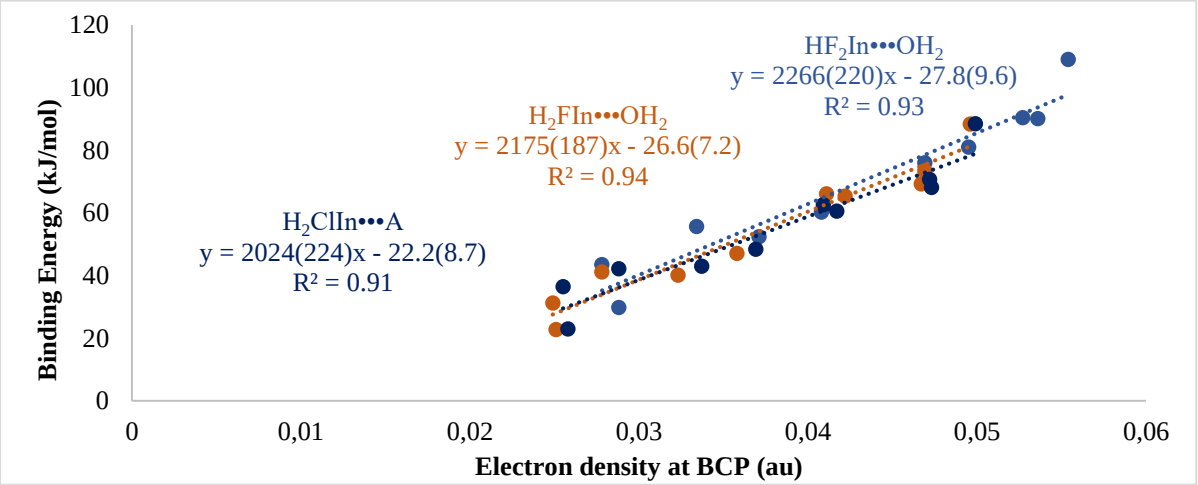

Figure D10. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for In-bonded complexes.*

Table D11. *Electron density at BCP (au) and binding energy (kJ/mol) data for Tl-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$HF_2Tl\cdots OH_2$	0.0420	54.0
$HF_2Tl\cdots SH_2$	0.0335	46.9
$HF_2Tl\cdots NH_3$	0.0569	86.0
$HF_2Tl\cdots NCH$	0.0374	42.8
$HF_2Tl\cdots CO$	0.0262	20.6
$HF_2Tl\cdots OCH_2$	0.0446	61.8
$HF_2Tl\cdots C_2H_4$	0.0283	33.3
$HF_2Tl\cdots OHCH_3$	0.0508	72.2
$HF_2Tl\cdots PH_3$	0.0385	39.9
$HF_2Tl\cdots O(CH_3)_2$	0.0508	68.4
$H_2FTl\cdots OH_2$	0.0382	55.7
$H_2FTl\cdots SH_2$	0.0271	36.5
$H_2FTl\cdots NH_3$	0.0467	66.7
$H_2FTl\cdots NCH$	0.0313	33.0
$H_2FTl\cdots CO$	0.0227	15.6
$H_2FTl\cdots OCH_2$	0.0370	53.5
$H_2FTl\cdots C_2H_4$	0.0244	26.6
$H_2FTl\cdots OHCH_3$	0.0435	61.3
$H_2FTl\cdots PH_3$	0.0303	30.9
$H_2FTl\cdots O(CH_3)_2$	0.0416	49.2
$H_2ClTl\cdots OH_2$	0.0367	48.0
$H_2ClTl\cdots SH_2$	0.0264	34.5
$H_2ClTl\cdots NH_3$	0.0464	66.0
$H_2ClTl\cdots NCH$	0.0323	35.0
$H_2ClTl\cdots CO$	0.0228	16.1
$H_2ClTl\cdots OCH_2$	0.0364	50.1
$H_2ClTl\cdots C_2H_4$	0.0249	28.4
$H_2ClTl\cdots OHCH_3$	0.0428	55.7
$H_2ClTl\cdots PH_3$	0.0311	33.3
$H_2ClTl\cdots O(CH_3)_2$	0.0417	48.0

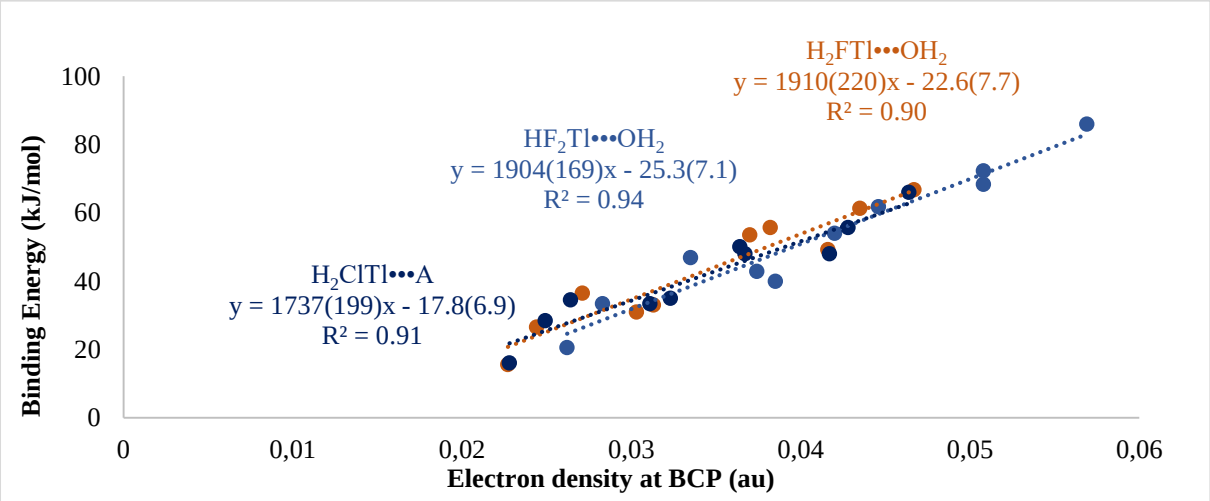

Figure D11. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Tl bonded complexes*

Table D12. *Electron density at BCP (au) and binding energy (kJ/mol) data for C-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$NO_2H_3C\bullet\bullet\bullet OH_2$	0.0069	10.0
$NO_2H_3C\bullet\bullet\bullet SH_2$	0.0051	5.5
$NO_2H_3C\bullet\bullet\bullet NH_3$	0.0069	10.4
$NO_2H_3C\bullet\bullet\bullet NCH$	0.0065	10.9
$NO_2H_3C\bullet\bullet\bullet CO$	0.0045	3.9
$NO_2H_3C\bullet\bullet\bullet OCH_2$	0.0067	10.3
$NO_2H_3C\bullet\bullet\bullet PH_3$	0.0045	5.4
$NO_2H_3C\bullet\bullet\bullet HF$	0.0054	6.8
$NO_2H_3C\bullet\bullet\bullet C_2H_2$	0.0050	5.5
$NO_2H_3C\bullet\bullet\bullet HCl$	0.0049	4.0
$NF_2H_3C\bullet\bullet\bullet OH_2$	0.0064	8.4
$NF_2H_3C\bullet\bullet\bullet SH_2$	0.0048	4.7
$NF_2H_3C\bullet\bullet\bullet NH_3$	0.0064	8.7
$NF_2H_3C\bullet\bullet\bullet NCH$	0.0061	9.2
$NF_2H_3C\bullet\bullet\bullet CO$	0.0043	3.2
$NF_2H_3C\bullet\bullet\bullet C_2H_4$	0.0050	4.7
$NF_2H_3C\bullet\bullet\bullet PH_3$	0.0043	4.6
$NF_2H_3C\bullet\bullet\bullet HF$	0.0052	5.8
$NF_2H_3C\bullet\bullet\bullet C_2H2$	0.0048	4.7
$NF_2H_3C\bullet\bullet\bullet HCl$	0.0047	3.5
$HOH_3C\bullet\bullet\bullet H_2O$	0.0054	4.0
$HOH_3C\bullet\bullet\bullet H_2S$	0.0046	2.8
$HOH_3C\bullet\bullet\bullet NH_3$	0.0055	4.1
$HOH_3C\bullet\bullet\bullet NCH$	0.0054	4.7
$HOH_3C\bullet\bullet\bullet CO$	0.0042	1.9
$HOH_3C\bullet\bullet\bullet OCH_2$	0.0053	4.5
$HOH_3C\bullet\bullet\bullet HCl$	0.0042	2.1
$HOH_3C\bullet\bullet\bullet PH_3$	0.0041	2.7
$HOH_3C\bullet\bullet\bullet HF$	0.0041	2.7
$HOH_3C\bullet\bullet\bullet C_2H_2$	0.0046	3.3

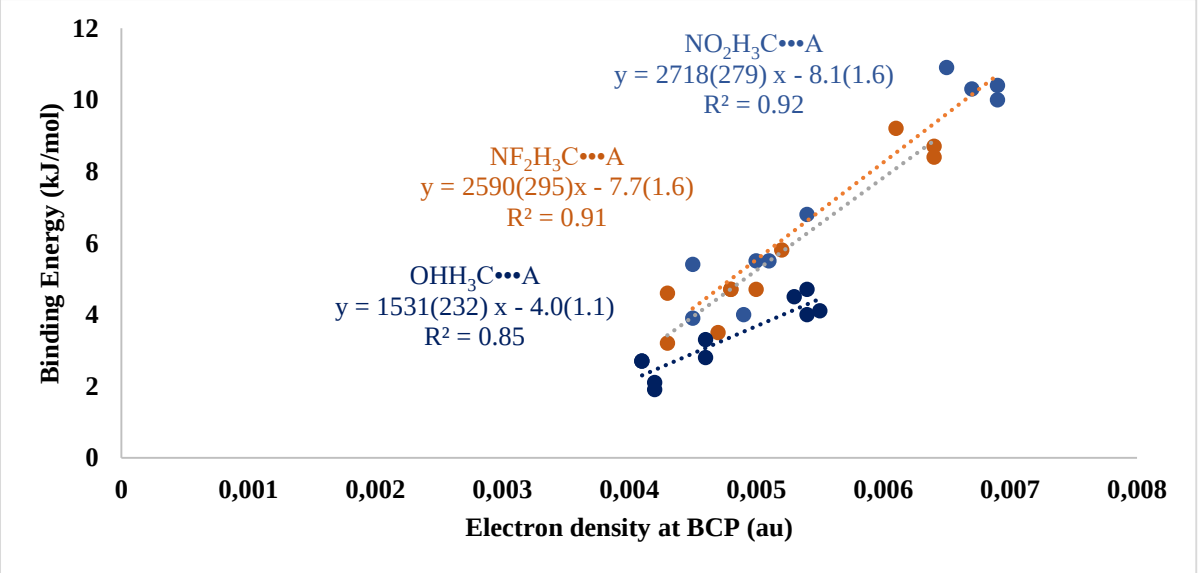

Figure D12. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for C-bonded complexes.*

Table D13. *Electron density at BCP (au) and binding energy (kJ/mol) data for Si-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FH_3Si\bullet\bullet\bullet OH_2$	0.0128	14.4
$FH_3Si\bullet\bullet\bullet SH_2$	0.0081	9.3
$FH_3Si\bullet\bullet\bullet NH_3$	0.0251	23.0
$FH_3Si\bullet\bullet\bullet PH_3$	0.0079	9.2
$FH_3Si\bullet\bullet\bullet CO$	0.0053	3.1
$FH_3Si\bullet\bullet\bullet NCH$	0.0115	14.5
$FH_3Si\bullet\bullet\bullet OHCH_3$	0.0193	19.2
$FH_3Si\bullet\bullet\bullet O(CH_3)_2$	0.0240	22.7
$FH_3Si\bullet\bullet\bullet NCCH_3$	0.0136	17.9
$FH_3Si\bullet\bullet\bullet NH_2CH_3$	0.0374	32.6
$ClH_3Si\bullet\bullet\bullet OH_2$	0.0123	13.6
$ClH_3Si\bullet\bullet\bullet SH_2$	0.0079	8.9
$ClH_3Si\bullet\bullet\bullet NH_3$	0.0259	21.3
$ClH_3Si\bullet\bullet\bullet PH_3$	0.0076	8.8
$ClH_3Si\bullet\bullet\bullet CO$	0.0052	3.0
$ClH_3Si\bullet\bullet\bullet NCH$	0.0112	14.0
$ClH_3Si\bullet\bullet\bullet OHCH_3$	0.0188	18.1
$ClH_3Si\bullet\bullet\bullet OCH_2$	0.0156	15.4
$ClH_3Si\bullet\bullet\bullet C_2H_4$	0.0075	9.4
$ClH_3Si\bullet\bullet\bullet O(CH_3)_2$	0.0242	21.8
$CNH_3Si\bullet\bullet\bullet OH_2$	0.0113	14.6
$CNH_3Si\bullet\bullet\bullet SH_2$	0.0072	8.8
$CNH_3Si\bullet\bullet\bullet NH_3$	0.0193	20.7
$CNH_3Si\bullet\bullet\bullet PH_3$	0.0067	8.5
$CNH_3Si\bullet\bullet\bullet CO$	0.0062	5.9
$CNH_3Si\bullet\bullet\bullet NCH$	0.0103	15.1
$CNH_3Si\bullet\bullet\bullet OHCH_3$	0.0168	18.3
$CNH_3Si\bullet\bullet\bullet OCH_2$	0.0145	15.6
$CNH_3Si\bullet\bullet\bullet C_2H_4$	0.0067	8.9
$CNH_3Si\bullet\bullet\bullet O(CH_3)_2$	0.0219	21.4

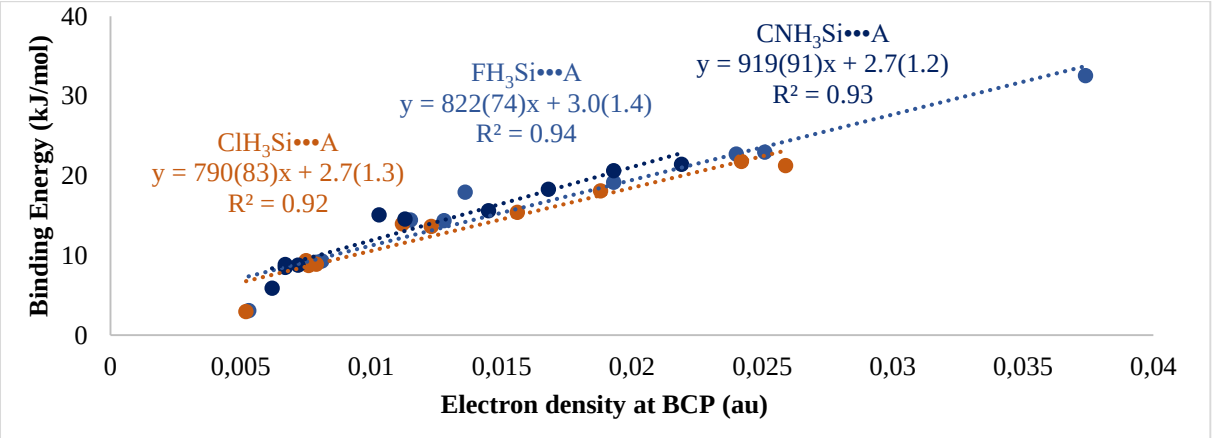

Figure D13. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Si-bonded complexes.*

***Table D14**. Electron density at BCP (au) and binding energy (kJ/mol) data for Ge-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FH_3Ge•••OH_2$	0.0145	16.3
$FH_3Ge•••SH_2$	0.0086	10.5
$FH_3Ge•••NH_3$	0.0252	24.4
$FH_3Ge•••PH_3$	0.0083	10.2
$FH_3Ge•••CO$	0.0058	3.3
$FH_3Ge•••NCH$	0.0139	16.5
$FH_3Ge•••OHCH_3$	0.0216	20.6
$FH_3Ge•••OCH_2$	0.0186	17.7
$FH_3Ge•••C_2H_4$	0.0086	10.6
$FH_3Ge•••O(CH_3)_2$	0.0265	23.8
$ClH_3Ge•••OH_2$	0.0136	15.0
$ClH_3Ge•••SH_2$	0.0083	9.8
$ClH_3Ge•••NH_3$	0.0248	22.1
$ClH_3Ge•••PH_3$	0.008	9.5
$ClH_3Ge•••CO$	0.0055	3.2
$ClH_3Ge•••NCH$	0.0133	15.3
$ClH_3Ge•••OHCH_3$	0.0207	18.8
$ClH_3Ge•••OCH_2$	0.0176	16.30
$ClH_3Ge•••C_2H_4$	0.0084	10.0
$ClH_3Ge•••O(CH_3)_2$	0.0258	21.9
$CNH_3Ge•••OH_2$	0.0112	14.4
$CNH_3Ge•••SH_2$	0.0070	8.8
$CNH_3Ge•••NH_3$	0.0173	19.1
$CNH_3Ge•••PH_3$	0.0067	8.4
$CNH_3Ge•••CO$	0.0064	5.9
$CNH_3Ge•••NCH$	0.0114	14.9
$CNH_3Ge•••OHCH_3$	0.0166	17.2
$CNH_3Ge•••OCH_2$	0.0147	14.9
$CNH_3Ge•••C_2H_4$	0.0072	8.7
$CNH_3Ge•••O(CH_3)_2$	0.0215	19.4

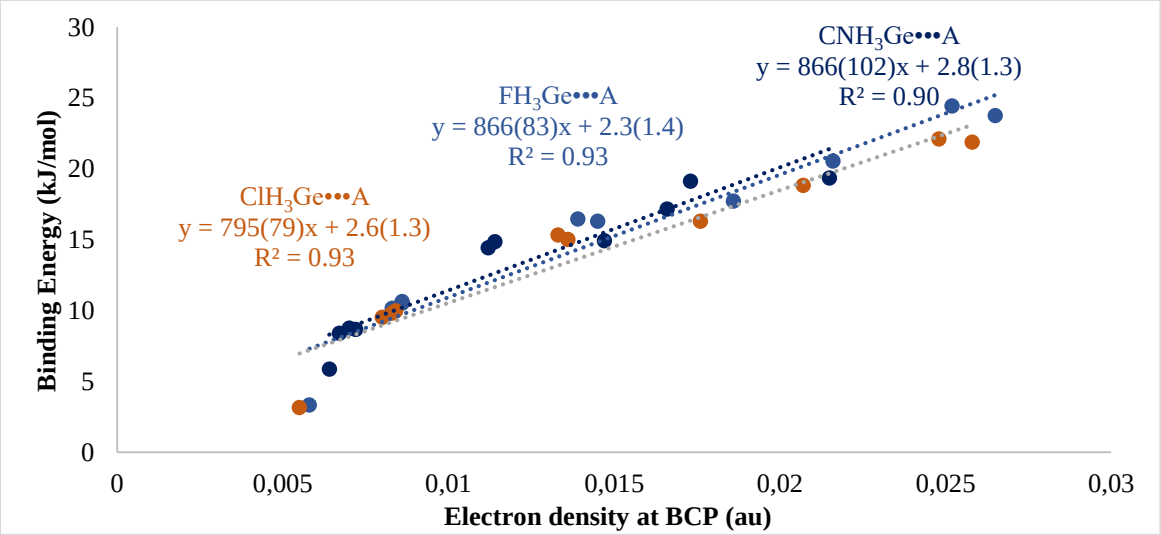

***Figure D14.** Binding energy (kJ/mol) versus electron density at BCP (au) plot for Ge-bonded complexes.*

***Table D15**. Electron density at BCP (au) and binding energy (kJ/mol) data for Sn-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FH_3Sn•••OH_2$	0.0189	22.7
$FH_3Sn•••SH_2$	0.0108	13.9
$FH_3Sn•••NH_3$	0.0286	35.6
$FH_3Sn•••PH_3$	0.0104	13.6
$FH_3Sn•••CO$	0.0062	3.9
$FH_3Sn•••NCH$	0.0164	22.1
$FH_3Sn•••OHCH_3$	0.0254	28.9
$FH_3Sn•••OCH_2$	0.0220	24.6
$FH_3Sn•••C_2H_4$	0.0100	13.3
$FH_3Sn•••O(CH_3)_2$	0.0290	32.9
$ClH_3Sn•••OH_2$	0.0185	21.5
$ClH_3Sn•••SH_2$	0.0104	13.2
$ClH_3Sn•••NH_3$	0.0290	34.0
$ClH_3Sn•••PH_3$	0.0104	13.0
$ClH_3Sn•••CO$	0.0099	3.7
$ClH_3Sn•••NCH$	0.0163	21.1
$ClH_3Sn•••OHCH_3$	0.0254	27.5
$ClH_3Sn•••OCH_2$	0.0218	23.3
$ClH_3Sn•••C_2H_4$	0.0097	12.8
$ClH_3Sn•••O(CH_3)_2$	0.0290	31.5
$CNH_3Sn•••OH_2$	0.0161	19.5
$CNH_3Sn•••SH_2$	0.0088	11.5
$CNH_3Sn•••FH$	0.0082	9.9
$CNH_3Sn•••PH_3$	0.0079	11.0
$CNH_3Sn•••CO$	0.0080	7.3
$CNH_3Sn•••C_2H_2$	0.0070	10.1
$CNH_3Sn•••OHCH_3$	0.0225	24.3
$CNH_3Sn•••OCH_2$	0.0196	20.7
$CNH_3Sn•••C_2H_4$	0.0084	11.0
$CNH_3Sn•••O(CH_3)_2$	0.0290	27.7

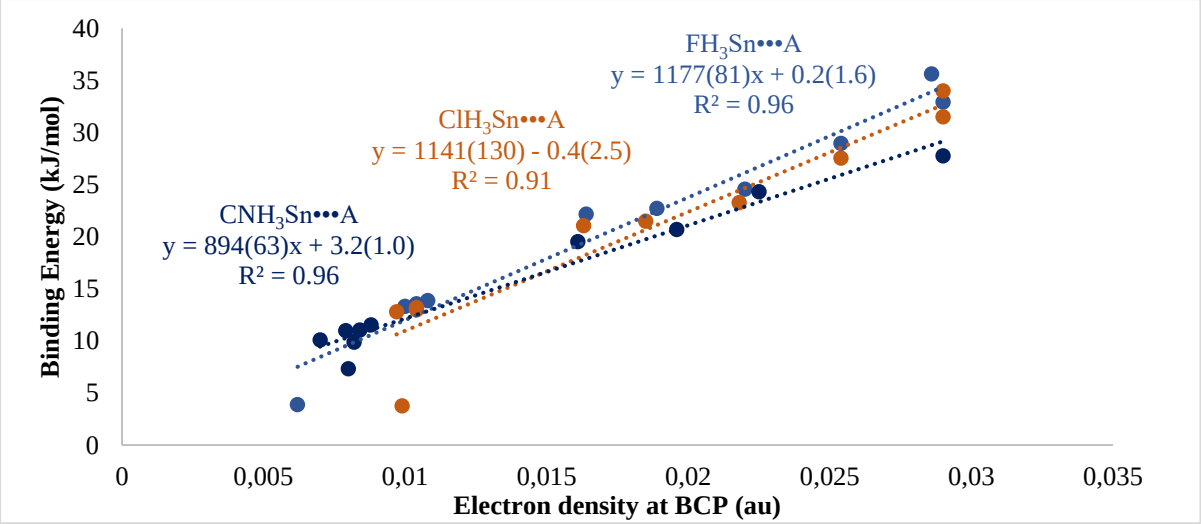

***Figure D15.** Binding energy (kJ/mol) versus electron density at BCP (au) plot for Sn-bonded complexes.*

Table D16. *Electron density at BCP (au) and binding energy (kJ/mol) data for Pb-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$FH_3Pb\bullet\bullet\bullet OH_2$	0.01450	22.1
$FH_3Pb\bullet\bullet\bullet SH_2$	0.0086	14.1
$FH_3Pb\bullet\bullet\bullet NH_3$	0.0252	31.7
$FH_3Pb\bullet\bullet\bullet PH_3$	0.0083	13.9
$FH_3Pb\bullet\bullet\bullet CO$	0.0058	3.8
$FH_3Pb\bullet\bullet\bullet NCH$	0.0139	22.4
$FH_3Pb\bullet\bullet\bullet OHCH_3$	0.0216	26.2
$FH_3Pb\bullet\bullet\bullet OCH_2$	0.0186	22.8
$FH_3Pb\bullet\bullet\bullet C_2H_4$	0.0086	13.4
$FH_3SPb\bullet\bullet\bullet O(CH_3)_2$	0.0264	28.9
$ClH_3Pb\bullet\bullet\bullet OH_2$	0.0172	21.4
$ClH_3Pb\bullet\bullet\bullet SH_2$	0.0110	13.8
$ClH_3Pb\bullet\bullet\bullet NH_3$	0.0249	31.1
$ClH_3Pb\bullet\bullet\bullet PH_3$	0.0103	13.5
$ClH_3Pb\bullet\bullet\bullet CO$	0.0100	8.4
$ClH_3Pb\bullet\bullet\bullet NCH$	0.0167	21.8
$ClH_3Pb\bullet\bullet\bullet OHCH_3$	0.0230	25.6
$ClH_3Pb\bullet\bullet\bullet OCH_2$	0.0209	22.1
$ClH_3Pb\bullet\bullet\bullet C_2H_4$	0.0110	13.2
$ClH_3Pb\bullet\bullet\bullet O(CH_3)_2$	0.0269	28.5
$CNH_3Pb\bullet\bullet\bullet OH_2$	0.0145	18.2
$CNH_3Pb\bullet\bullet\bullet SH_2$	0.0088	11.1
$CNH_3Pb\bullet\bullet\bullet NH_3$	0.0196	24.5
$CNH_3Pb\bullet\bullet\bullet PH_3$	0.0079	10.8
$CNH_3Pb\bullet\bullet\bullet CO$	0.0082	7.0
$CNH_3Pb\bullet\bullet NCH$	0.0139	18.7
$CNH_3Pb\bullet\bullet\bullet OHCH_3$	0.0192	21.1
$CNH_3Pb\bullet\bullet\bullet OCH_2$	0.0178	18.3
$CNH_3Pb\bullet\bullet\bullet C_2H_4$	0.0091	10.6
$CNH_3Pb\bullet\bullet\bullet O(CH_3)_2$	0.0230	23.4

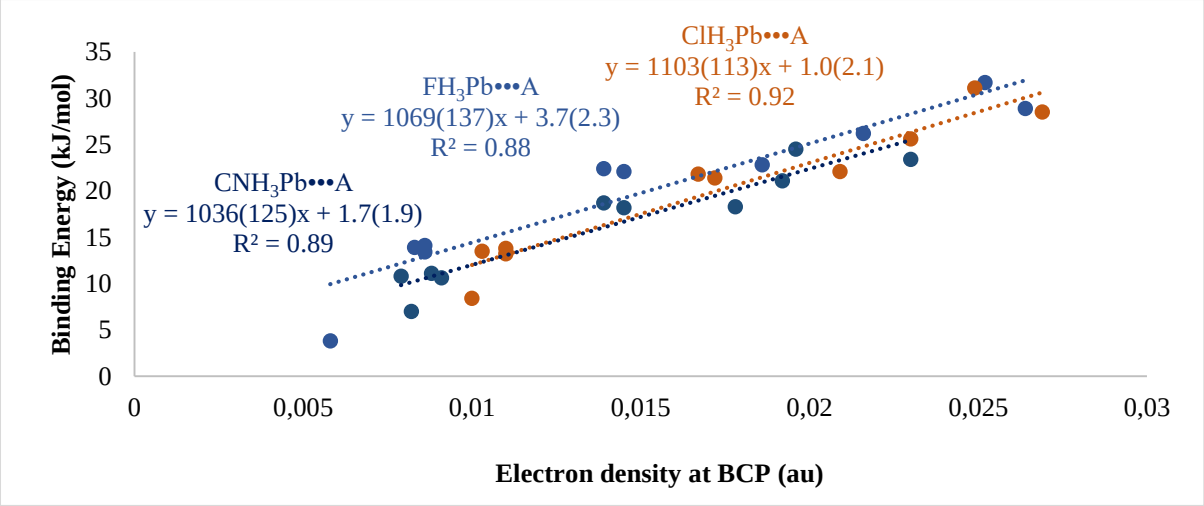

Figure D16. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Pb-bonded complexes.*

Table D17. *Electron density at BCP (au) and binding energy (kJ/mol) data for N-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3N•••OH_2$	0.0065	3.7
$F_3N•••SH_2$	0.0036	2.7
$F_3N•••NH_3$	0.0060	3.9
$F_3N•••NCH$	0.0069	3.8
$F_3N•••CO$	0.0047	1.9
$F_3N•••OCH_2$	0.0073	4.8
$F_3N•••C_2H_4$	0.0053	2.9
$F_3N•••OHCH_3$	0.0078	5.3
$F_3N•••O(CH_3)_2$	0.0105	6.4
$F_3N•••FH$	0.0056	2.9

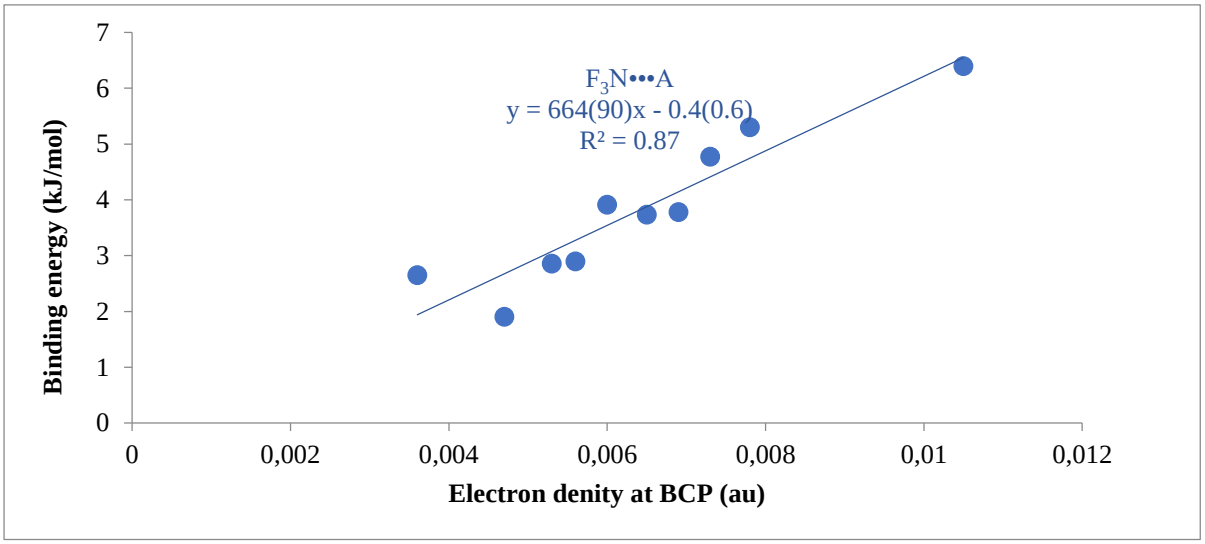

Figure D17. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for N-bonded complexes.*

***Table D18**. Electron density at BCP (au) and binding energy (kJ/mol) data for P-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3P{\bullet\bullet\bullet}OH_2$	0.0158	14.2
$F_3P{\bullet\bullet\bullet}SH_2$	0.0084	8.5
$F_3P{\bullet\bullet\bullet}NH_3$	0.0218	18.7
$F_3P{\bullet\bullet\bullet}NCH$	0.0114	11.5
$F_3P{\bullet\bullet\bullet}CO$	0.0066	4.8
$F_3P\ {\bullet\bullet\bullet}OCH_2$	0.0167	16.4
$F_3P{\bullet\bullet\bullet}C_2H_4$	0.0079	7.4
$F_3P{\bullet\bullet\bullet}OHCH_3$	0.0197	17.6
$F_3P\ {\bullet\bullet\bullet}PH_3$	0.0073	6.7
$F_3P{\bullet\bullet\bullet}O(CH_3)_2$	0.0248	20.5
$FH_2P{\bullet\bullet\bullet}SH_2$	0.0131	12.9
$FH_2P{\bullet\bullet\bullet}NH_3$	0.0269	25.8
$FH_2P{\bullet\bullet\bullet}NCH$	0.0159	17.2
$FH_2P{\bullet\bullet\bullet}CO$	0.0130	8.9
$FH_2P{\bullet\bullet\bullet}OCH_2$	0.0096	11.5
$FH_2P{\bullet\bullet\bullet}C_2H_4$	0.0154	14.5
$FH_2P{\bullet\bullet\bullet}OHCH_3$	0.0226	20.9
$FH_2P{\bullet\bullet\bullet}PH_3$	0.0161	13.5
$FH_2P{\bullet\bullet\bullet}C_2H_2$	0.0120	12.2
$FH_2P{\bullet\bullet\bullet}O(CH_3)_2$	0.0263	24
$ClH_2P{\bullet\bullet\bullet}OH_2$	0.0146	14.8
$ClH_2P{\bullet\bullet\bullet}SH_2$	0.0119	11.4
$ClH_2P{\bullet\bullet\bullet}NH_3$	0.0241	22.3
$ClH_2P{\bullet\bullet\bullet}NCH$	0.0139	15.5
$ClH_2P{\bullet\bullet\bullet}CO$	0.0103	7.2
$ClH_2P{\bullet\bullet\bullet}OCH_2$	0.0098	11.8
$ClH_2P{\bullet\bullet\bullet}C_2H_4$	0.0135	12.7
$ClH_2P{\bullet\bullet\bullet}OHCH_3$	0.0203	18.3
$ClH_2P{\bullet\bullet\bullet}PH_3$	0.0137	11.7
$ClH_2P{\bullet\bullet\bullet}O(CH_3)_2$	0.0253	22

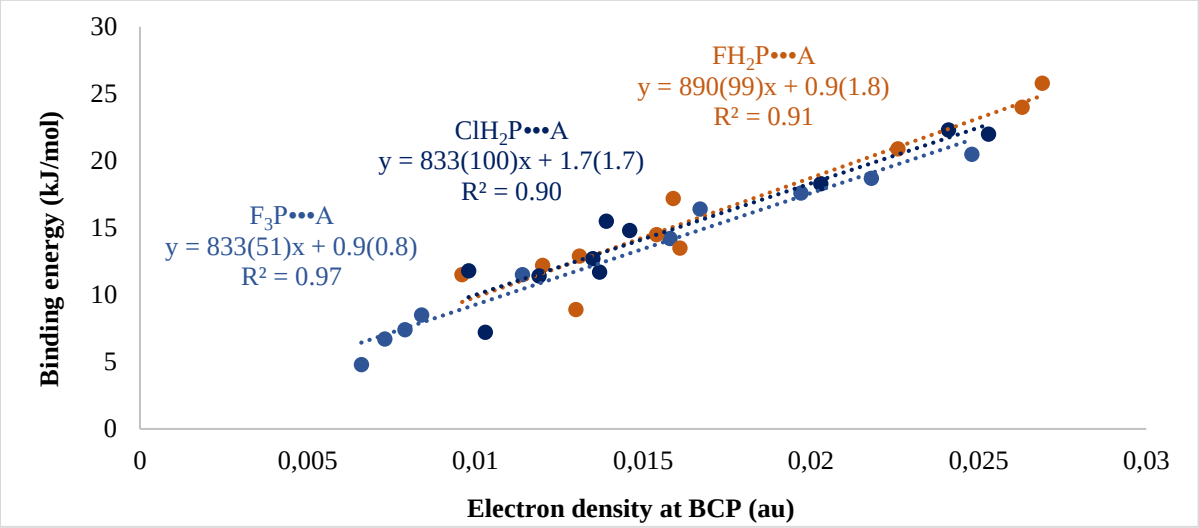

***Figure D18.** Binding energy (kJ/mol) versus electron density at BCP (au) plot for P-bonded complexes.*

Table D19. *Electron density at BCP (au) and binding energy (kJ/mol) data for As-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3As\bullet\bullet\bullet OH_2$	0.0239	23.3
$F_3As\bullet\bullet\bullet SH_2$	0.0113	13.7
$F_3As\bullet\bullet\bullet NH_3$	0.0330	30.6
$F_3As\bullet\bullet\bullet NCH$	0.0157	17.1
$F_3As\bullet\bullet\bullet CO$	0.0085	7.2
$F_3As\bullet\bullet\bullet OCH_2$	0.0239	25.4
$F_3As\bullet\bullet\bullet C_2H_4$	0.0099	10.9
$F_3As\bullet\bullet\bullet OHCH_3$	0.0298	28.3
$F_3As\bullet\bullet\bullet PH_3$	0.0101	10.6
$F_3As\bullet\bullet\bullet O(CH_3)_2$	0.0338	30.1
$FH_2As\bullet\bullet\bullet OH_2$	0.0188	19.8
$FH_2As\bullet\bullet\bullet SH_2$	0.0146	15.2
$FH_2As\bullet\bullet\bullet NH_3$	0.0298	31.4
$FH_2As\bullet\bullet\bullet NCH$	0.0187	20.4
$FH_2As\bullet\bullet\bullet CO$	0.0141	10.4
$FH_2As\bullet\bullet OCH_2$	0.0113	14.3
$FH_2As\bullet\bullet\bullet C_2H_4$	0.0172	16.8
$FH_2As\bullet\bullet\bullet OHCH_3$	0.0253	23.8
$FH_2As\bullet\bullet\bullet PH_3$	0.0131	16.2
$FH_2As\bullet\bullet\bullet O(CH_3)_2$	0.0306	27.8
$ClH_2As\bullet\bullet\bullet OH_2$	0.0170	17.5
$ClH_2As\bullet\bullet\bullet SH_2$	0.0135	13.6
$ClH_2As\bullet\bullet\bullet NH_3$	0.0287	27.9
$ClH_2As\bullet\bullet\bullet NCH$	0.0169	18.3
$ClH_2As\bullet\bullet\bullet CO$	0.0116	8.4
$ClH_2As\bullet\bullet OCH_2$	0.0110	13.6
$ClH_2As\bullet\bullet\bullet C_2H_4$	0.0155	14.9
$ClH_2As\bullet\bullet\bullet OHCH_3$	0.0235	21.2
$ClH_2As\bullet\bullet\bullet PH_3$	0.0153	14.2
$ClH_2As\bullet\bullet\bullet O(CH_3)_2$	0.0290	25.1

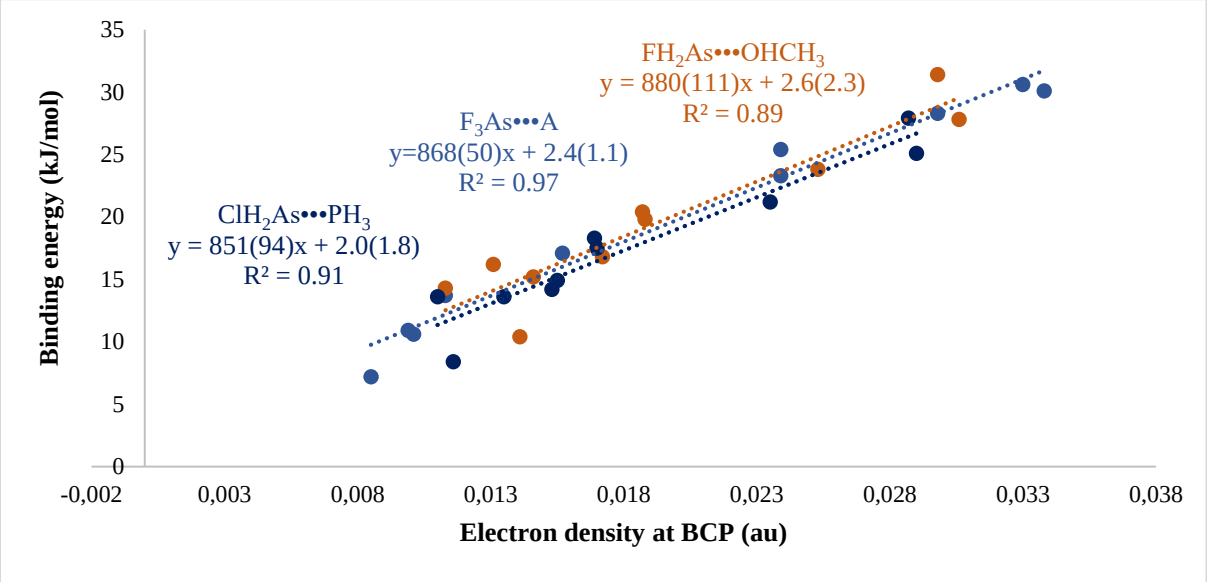

Figure D19. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for As-bonded complexes.*

Table D20. *Electron density at BCP (au) and binding energy (kJ/mol) data for Sb-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3Sb\cdots OH_2$	0.0312	37.1
$F_3Sb\cdots SH_2$	0.0148	21.3
$F_3Sb\cdots NH_3$	0.0375	48.9
$F_3Sb\cdots NCH$	0.0198	24.6
$F_3Sb\cdots CO$	0.0108	10.2
$F_3Sb\cdots OCH_2$	0.0291	37.5
$F_3Sb\cdots C_2H_4$	0.0123	15.6
$F_3Sb\cdots OHCH_3$	0.0349	43.8
$F_3Sb\cdots PH_3$	0.0141	16.3
$F_3Sb\cdots O(CH_3)_2$	0.0367	43.9
$FH_2Sb\cdots OH_2$	0.0207	24.7
$FH_2Sb\cdots SH_2$	0.0150	18.6
$FH_2Sb\cdots NH_3$	0.0303	40.1
$FH_2Sb\cdots NCH$	0.0200	25.1
$FH_2Sb\cdots CO$	0.0145	12.4
$FH_2Sb\cdots OCH_2$	0.0149	19.7
$FH_2Sb\cdots C_2H_4$	0.0168	19.7
$FH_2Sb\cdots OHCH_3$	0.0267	32
$FH_2Sb\cdots PH_3$	0.0172	19.7
$FH_2Sb\cdots O(CH_3)_2$	0.0304	33.5
$ClH_2Sb\cdots OH_2$	0.0202	23
$ClH_2Sb\cdots SH_2$	0.0147	17.5
$ClH_2Sb\cdots NH_3$	0.0309	38.1
$ClH_2Sb\cdots NCH$	0.0196	23.5
$ClH_2Sb\cdots CO$	0.0131	10.6
$ClH_2Sb\cdots OCH_2$	0.0136	18
$ClH_2Sb\cdots C_2H_4$	0.0164	18.3
$ClH_2Sb\cdots OHCH_3$	0.0268	30.1
$ClH_2Sb\cdots PH_3$	0.0166	18.3
$ClH_2Sb\cdots O(CH_3)_2$	0.0306	31.8

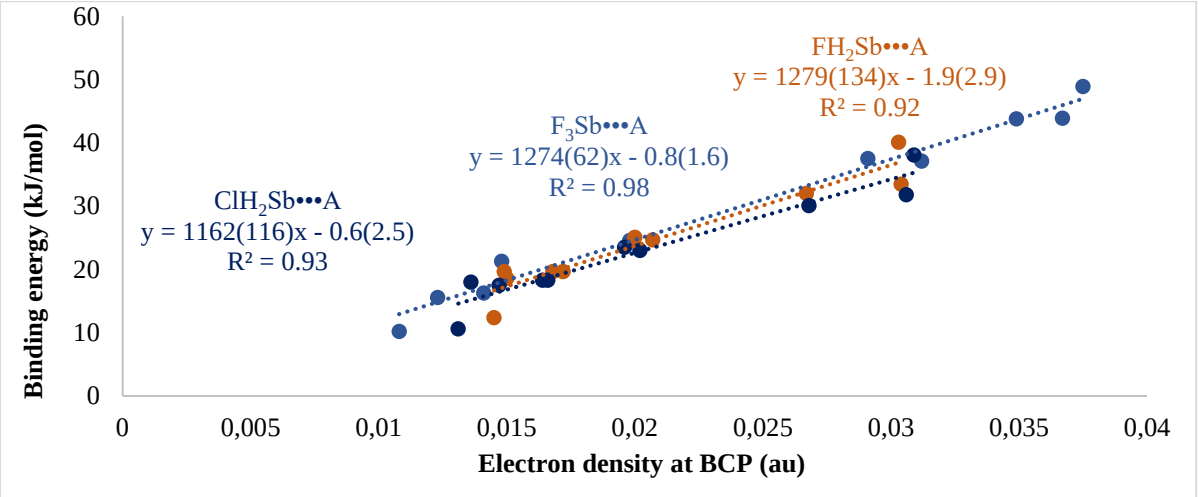

Figure D20. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Sb-bonded complexes.*

Table D21. *Electron density at BCP (au) and binding energy (kJ/mol) data for Bi-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_3Bi\bullet\bullet\bullet OH_2$	0.0322	45.5
$F_3Bi\bullet\bullet\bullet SH_2$	0.0163	27.7
$F_3Bi\bullet\bullet\bullet NH_3$	0.0348	55.3
$F_3Bi\bullet\bullet\bullet NCH$	0.0214	31.3
$F_3Bi\bullet\bullet\bullet CO$	0.0128	13.4
$F_3Bi\bullet\bullet\bullet OCH_2$	0.0298	45
$F_3Bi\bullet\bullet\bullet C_2H_4$	0.0137	19.7
$F_3Bi\bullet\bullet\bullet OHCH_3$	0.0344	51.8
$F_3Bi\bullet\bullet\bullet PH_3$	0.0157	21.2
$F_3Bi\bullet\bullet\bullet O(CH_3)_2$	0.0350	49.3
$FH_2Bi\bullet\bullet\bullet OH_2$	0.0208	27.7
$FH_2Bi\bullet\bullet\bullet SH_2$	0.0153	21.1
$FH_2Bi\bullet\bullet\bullet NH_3$	0.0282	41.9
$FH_2Bi\bullet\bullet\bullet NCH$	0.0207	28
$FH_2Bi\bullet\bullet\bullet CO$	0.0152	13.9
$FH_2Bi\bullet\bullet OCH_2$	0.0157	23.1
$FH_2Bi\bullet\bullet\bullet C_2H_4$	0.0167	21.5
$FH_2Bi\bullet\bullet\bullet OHCH_3$	0.0256	34.2
$FH_2Bi\bullet\bullet\bullet PH_3$	0.0168	21.9
$FH_2Bi\bullet\bullet\bullet O(CH_3)_2$	0.0288	33.3
$ClH_2Bi\bullet\bullet\bullet OH_2$	0.0210	26.6
$ClH_2Bi\bullet\bullet\bullet SH_2$	0.0156	20.5
$ClH_2Bi\bullet\bullet\bullet NH_3$	0.0293	41.3
$ClH_2Bi\bullet\bullet\bullet NCH$	0.0209	27.1
$ClH_2Bi\bullet\bullet\bullet CO$	0.0145	12.4
$ClH_2Bi\bullet\bullet OCH_2$	0.0146	20.9
$ClH_2Bi\bullet\bullet\bullet C_2H_4$	0.0171	20.7
$ClH_2Bi\bullet\bullet\bullet OHCH_3$	0.0263	33.2
$ClH_2Bi\bullet\bullet\bullet PH_3$	0.0171	21.3
$ClH_2Bi\bullet\bullet\bullet O(CH_3)_2$	0.0296	32.6

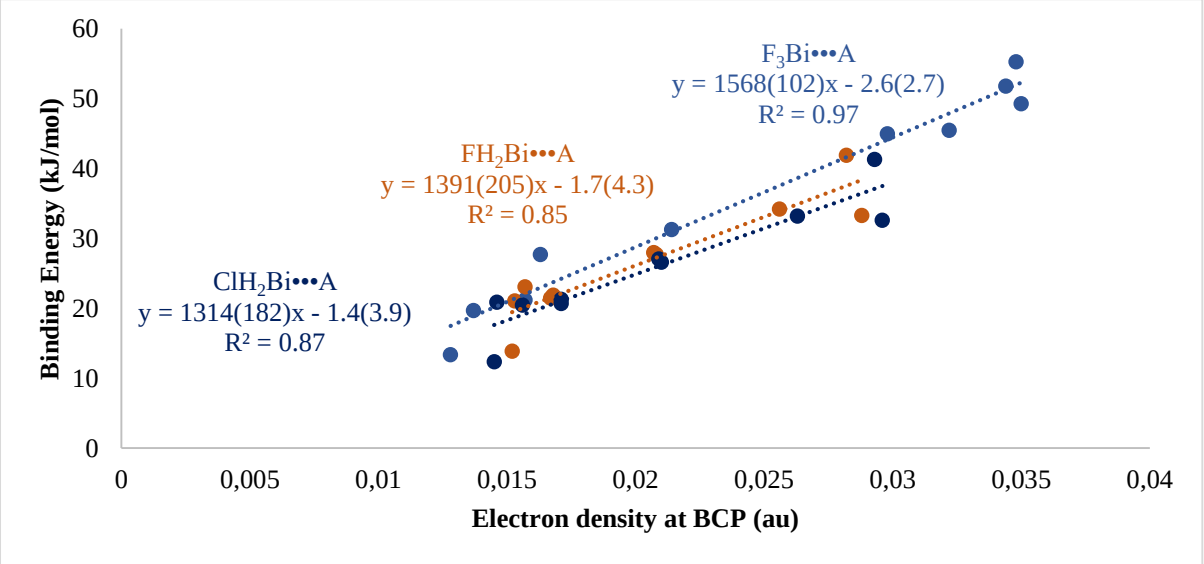

Figure D21. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Bi-bonded complexes.*

***Table D22**. Electron density at BCP (au) and binding energy (kJ/mol) data for O-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2O•••OH_2$	0.0100	5.4
$F_2O•••SH_2$	0.0067	3.8
$F_2O•••NH_3$	0.0111	6.4
$F_2O•••NCH$	0.0091	5.3
$F_2O•••CO$	0.0060	2.5
$F_2O•••OCH_2$	0.0112	6.7
$F_2O•••C_2H_4$	0.0076	4.4
$F_3N•••OHCH_3$	0.0117	6.8
$F_2O•••PH_3$	0.0057	3.3
$F_2O•••O(CH_3)_2$	0.0141	8.3

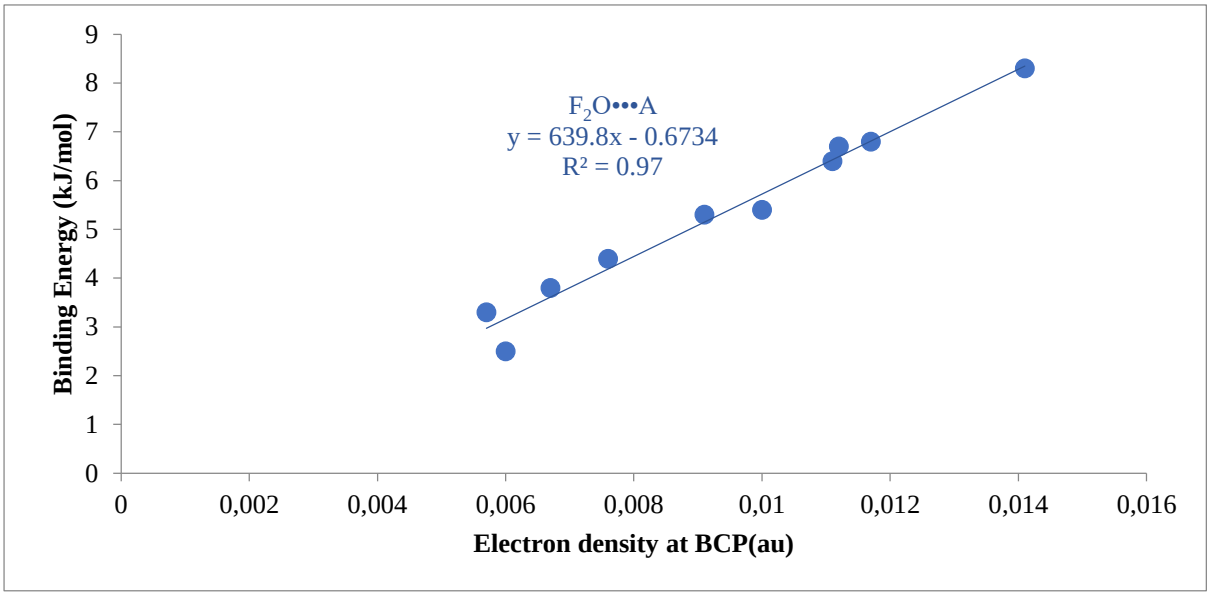

***Figure D22.** Binding energy (kJ/mol) versus electron density at BCP (au) plot for O-bonded complexes.*

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Table D23. *Electron density at BCP (au) and binding energy (kJ/mol) data for S-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2S\bullet\bullet\bullet OH_2$	0.0219	19
$F_2S\bullet\bullet\bullet SH_2$	0.0150	13.1
$F_2S\bullet\bullet\bullet NH_3$	0.0376	29.1
$F_2S\bullet\bullet\bullet NCH$	0.0163	16.2
$F_2S\bullet\bullet\bullet CO$	0.0106	7.5
$F_2S\bullet\bullet\bullet OCH_2$	0.0240	22.1
$F_2S\bullet\bullet\bullet C_2H_4$	0.0164	13.4
$F_2S\bullet\bullet\bullet OHCH_3$	0.0297	24.9
$F_2S\bullet\bullet\bullet PH_3$	0.0144	11.4
$F_2S\bullet\bullet\bullet O(CH_3)_2$	0.0363	29.1
$Cl_2S\bullet\bullet\bullet OH_2$	0.0166	13.1
$Cl_2S\bullet\bullet\bullet SH_2$	0.0130	11.4
$Cl_2S\bullet\bullet\bullet NH_3$	0.0266	20.3
$Cl_2S\bullet\bullet\bullet NCH$	0.0141	12.6
$Cl_2S\bullet\bullet\bullet CO$	0.0094	6.1
$Cl_2S\bullet\bullet OCH_2$	0.0181	16.2
$Cl_2S\bullet\bullet\bullet C_2H_4$	0.0139	12.1
$Cl_2S\bullet\bullet\bullet OHCH_3$	0.0221	18
$Cl_2S\bullet\bullet\bullet PH_3$	0.0129	10.5
$Cl_2S\bullet\bullet\bullet O(CH_3)_2$	0.0271	22.8
$O_2S\bullet\bullet\bullet OH_2$	0.0158	14.4
$O_2S\bullet\bullet\bullet SH_2$	0.0097	9.9
$O_2S\bullet\bullet\bullet NH_3$	0.0203	18.9
$O_2S\bullet\bullet\bullet NCH$	0.0117	12.5
$O_2S\bullet\bullet\bullet CO$	0.0068	5.3
$O_2S\bullet\bullet OCH_2$	0.0200	18.2
$O_2S\bullet\bullet\bullet C_2H_4$	0.0085	8.5
$O_2S\bullet\bullet\bullet OHCH_3$	0.0219	19.1
$O_2S\bullet\bullet\bullet PH_3$	0.0079	7.4
$O_2S\bullet\bullet\bullet O(CH_3)_2$	0.0273	22.9

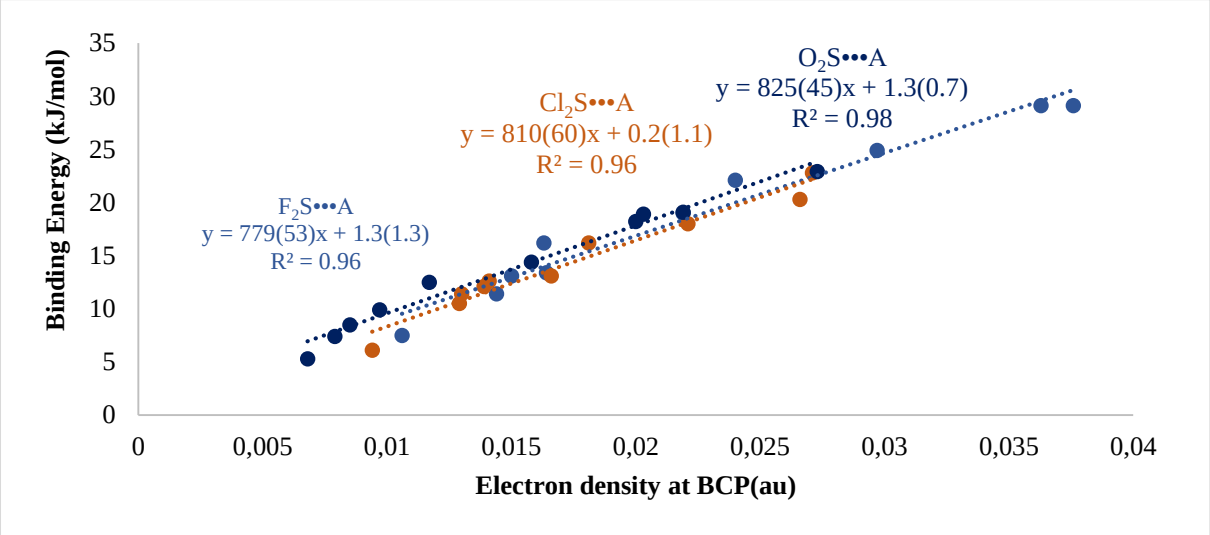

Figure D23. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for S-bonded complexes.*

***Table D24**. Electron density at BCP (au) and binding energy (kJ/mol) data for Se-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Se\cdots OH_2$	0.0297	27.9
$F_2Se\cdots SH_2$	0.0204	20.2
$F_2Se\cdots NH_3$	0.0481	45
$F_2Se\cdots NCH$	0.0231	23.1
$F_2Se\cdots CO$	0.0147	11
$F_2Se\cdots OCH_2$	0.0322	31.8
$F_2Se\cdots C_2H_4$	0.0283	20.5
$F_2Se\cdots OHCH_3$	0.0398	36.3
$F_2Se\cdots PH_3$	0.0239	18.5
$F_2Se\cdots O(CH_3)_2$	0.0459	41.4
$Cl_2Se\cdots OH_2$	0.0218	20.1
$Cl_2Se\cdots SH_2$	0.0170	16.8
$Cl_2Se\cdots NH_3$	0.0381	32.6
$Cl_2Se\cdots NCH$	0.0184	18.2
$Cl_2Se\cdots CO$	0.0068	8.6
$Cl_2Se\cdots OCH_2$	0.0235	23.4
$Cl_2Se\cdots C_2H_4$	0.0198	17.1
$Cl_2Se\cdots OHCH_3$	0.0303	26.8
$Cl_2Se\cdots PH_3$	0.0188	15.9
$Cl_2Se\cdots O(CH_3)_2$	0.0367	32.2
$O_2Se\cdots OH_2$	0.0182	17.2
$O_2Se\cdots SH_2$	0.0112	12
$O_2Se\cdots NH_3$	0.0253	23.4
$O_2Se\cdots NCH$	0.0125	14.7
$O_2Se\cdots CO$	0.0072	6
$O_2Se\cdots OCH_2$	0.0230	22.3
$O_2Se\cdots C_2H_4$	0.0086	9.4
$O_2Se\cdots OHCH_3$	0.0268	23.3
$O_2Se\cdots PH_3$	0.0090	8.2
$O_2Se\cdots O(CH_3)_2$	0.0319	27.7

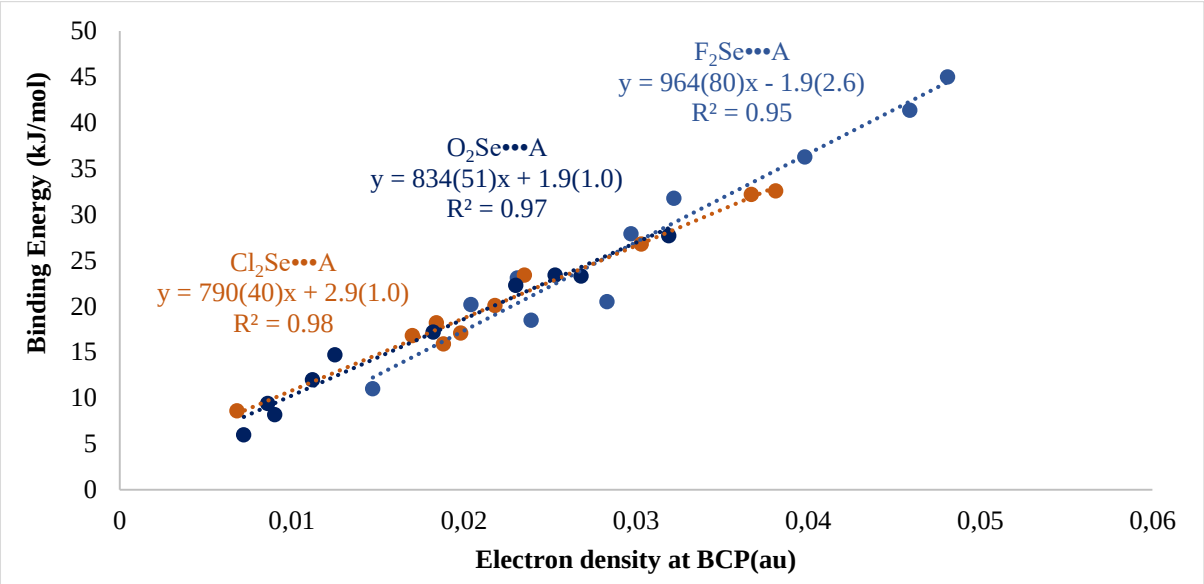

***Figure D24.** Binding energy (kJ/mol) versus electron density at BCP (au) plot for Se-bonded complexes.*

Table D25. *Electron density at BCP (au) and binding energy (kJ/mol) data for Te-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Te{\bullet\bullet\bullet}OH_2$	0.0333	38.2
$F_2Te{\bullet\bullet\bullet}SH_2$	0.0242	29.0
$F_2Te{\bullet\bullet\bullet}C_2H_2$	0.0259	23.8
$F_2Te{\bullet\bullet\bullet}NH_3$	0.0459	60.8
$F_2Te{\bullet\bullet\bullet}O(CH_3)_2$	0.0446	54.3
$F_2Te{\bullet\bullet\bullet}CO$	0.0209	15.7
$F_2Te{\bullet\bullet\bullet}OCH_2$	0.0354	43.4
$F_2Te{\bullet\bullet\bullet}OHCH_3$	0.0410	49.0
$F_2Te{\bullet\bullet\bullet}PH_3$	0.0322	29.0
$F_2Te{\bullet\bullet\bullet}NCH$	0.0284	31.9
$Cl_2Te{\bullet\bullet\bullet}OH_2$	0.0283	29.7
$Cl_2Te{\bullet\bullet\bullet}SH_2$	0.0206	24.5
$Cl_2Te{\bullet\bullet\bullet}NH_3$	0.0419	49.3
$Cl_2Te{\bullet\bullet\bullet}NCH$	0.0245	26.0
$Cl_2Te{\bullet\bullet\bullet}CO$	0.0157	12.2
$Cl_2Te{\bullet\bullet}OCH_2$	0.0296	33.7
$Cl_2Te{\bullet\bullet\bullet}C_2H_4$	0.0273	24.6
$Cl_2Te{\bullet\bullet\bullet}OHCH_3$	0.0365	39.3
$Cl_2Te{\bullet\bullet\bullet}PH_3$	0.0258	24.4
$Cl_2Te{\bullet\bullet\bullet}O(CH_3)_2$	0.0407	45.5
$O_2Te{\bullet\bullet\bullet}OH_2$	0.0230	20.9
$O_2Te{\bullet\bullet\bullet}SH_2$	0.0119	14.5
$O_2Te{\bullet\bullet\bullet}NH_3$	0.0346	30.2
$O_2Te{\bullet\bullet\bullet}NCH$	0.0132	17.0
$O_2Te{\bullet\bullet\bullet}CO$	0.0070	6.7
$O_2Te{\bullet\bullet}OCH_2$	0.0261	27.2
$O_2Te{\bullet\bullet\bullet}C_2H_4$	0.0080	9.9
$O_2Te{\bullet\bullet\bullet}OHCH_3$	0.0335	29.3
$O_2Te{\bullet\bullet\bullet}PH_3$	0.0094	9.6
$O_2Te{\bullet\bullet\bullet}O(CH_3)_2$	0.0363	33.4

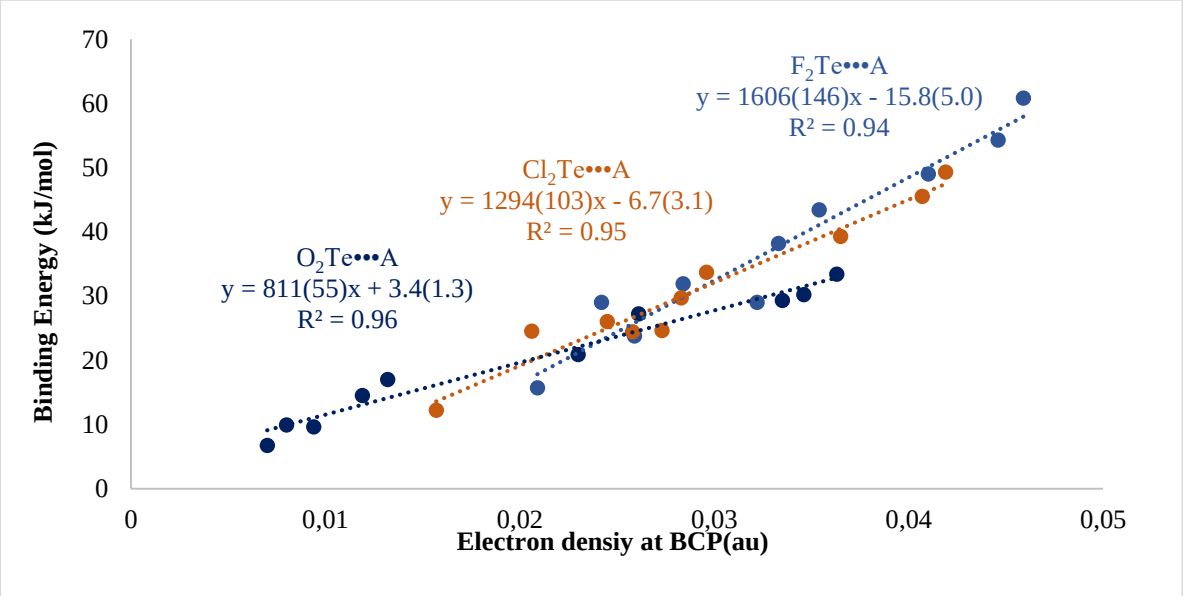

Figure D25. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Te-bonded complexes.*

Table D26. *Electron density at BCP (au) and binding energy (kJ/mol) data for Po-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$F_2Po\cdots OH_2$	0.0329	45.6
$F_2Po\cdots SH_2$	0.0242	35.7
$F_2Po\cdots NH_3$	0.0410	68.4
$F_2Po\cdots NCH$	0.0287	39.9
$F_2Po\cdots OCH_2$	0.0350	51.6
$F_2Po\cdots C_2H_2$	0.0281	31.1
$F_2Po\cdots OHCH_3$	0.0390	56.1
$F_2Po\cdots PH_3$	0.0299	36.0
$F_2Po\cdots O(CH_3)_2$	0.0419	60.4
$F_2Po\cdots CO$	0.0242	21.4
$Cl_2Po\cdots OH_2$	0.0304	38.8
$Cl_2Po\cdots SH_2$	0.0229	32.8
$Cl_2Po\cdots NH_3$	0.0396	59.7
$Cl_2Po\cdots NCH$	0.0281	35.1
$Cl_2Po\cdots OCH_2$	0.0320	43.2
$Cl_2Po\cdots C_2H_4$	0.0316	34.2
$Cl_2Po\cdots OHCH_3$	0.0370	49.1
$Cl_2Po\cdots PH_3$	0.0283	34.0
$Cl_2Po\cdots O(CH_3)_2$	0.0403	54.7
$F_2Po\cdots CO$	0.0211	17.6
$O_2Po\cdots OH_2$	0.0164	32.0
$O_2Po\cdots SH_2$	0.0102	19.4
O_2 o$\cdots NH_3$	0.0195	33.8
$O_2Po\cdots NCH$	0.0141	23.1
$O_2Po\cdots OCH_2$	0.0191	32.2
$O_2Po\cdots C_2H_4$	0.0098	14.4
$O_2Po\cdots OHCH_3$	0.0191	35.2
$O_2Po\cdots PH_3$	0.0112	16.3
$O_2Po\cdots O(CH_3)_2$	0.0230	31.4
$O_2Po\cdots CO$	0.0092	9.8

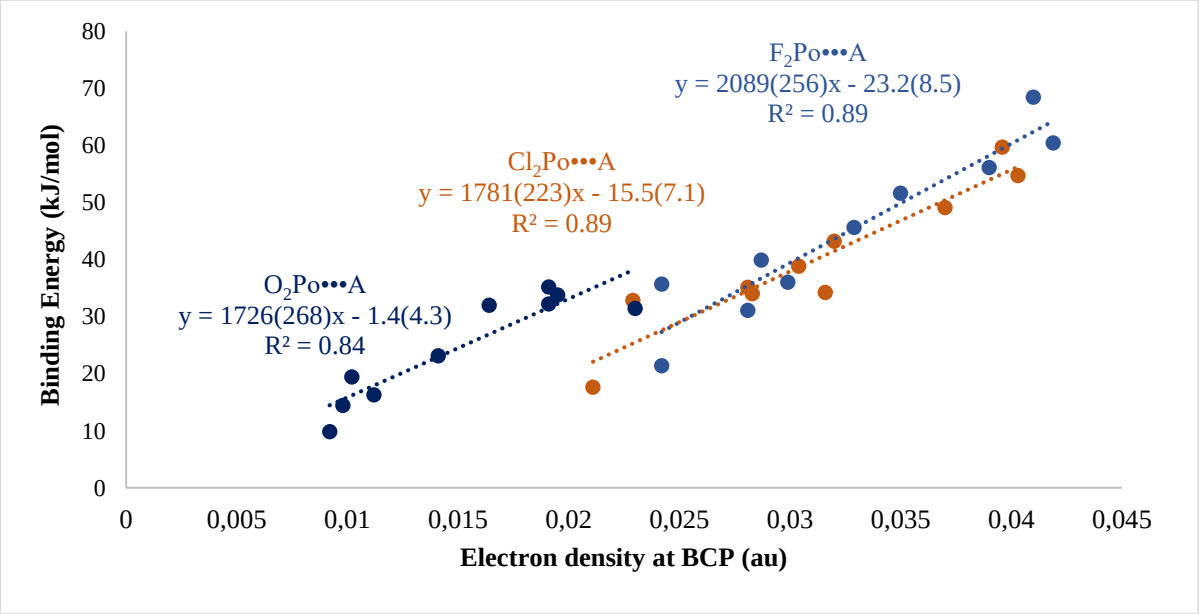

Figure D26. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Po-bonded complexes*

Table D27. *Electron density at BCP (au) and binding energy (kJ/mol) data for F-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy(kJ/mol)
CNF•••OH_2	0.0081	5.6
CNF•••SH_2	0.0056	3.3
CNF•••NH_3	0.0083	6.1
CNF•••NCH	0.0083	6.0
CNF•••OCH_2	0.0065	3.8
CNF•••C_2H_4	0.0085	6.1
CNF•••$OHCH_3$	0.0064	3.5
CNF•••PH_3	0.0092	6.2
CNF•••CO	0.0051	3.2
CNF•••$O(CH_3)_2$	0.0054	2.0
NCF•••OH_2	0.0059	4.4
NCF•••SH_2	0.0041	2.4
NCF•••NH_3	0.0054	4.4
NCF•••NCH	0.0061	4.9
NCF•••FH	0.0054	3.3
NCF•••OCH_2	0.0065	4.8
NCF•••C_2H_4	0.0045	2.5
NCF•••$OHCH_3$	0.0069	4.7
NCF•••PH_3	0.0036	2.4
NCF•••CO	0.0040	1.7
NCCCF•••OH_2	0.0061	4.2
NCCCF•••SH_2	0.0045	2.4
NCCCF•••NH_3	0.0056	4.1
NCCCF•••NCH	0.0065	4.9
NCCCF••OCH_2	0.0071	4.8
NCCCF•••C_2H_4	0.0049	2.4
NCCCF•••$OHCH_3$	0.0069	4.4
NCCCF•••PH_3	0.0040	2.3
NCCCF•••CO	0.0045	1.5
NCCCF•••FH	0.0060	3.2

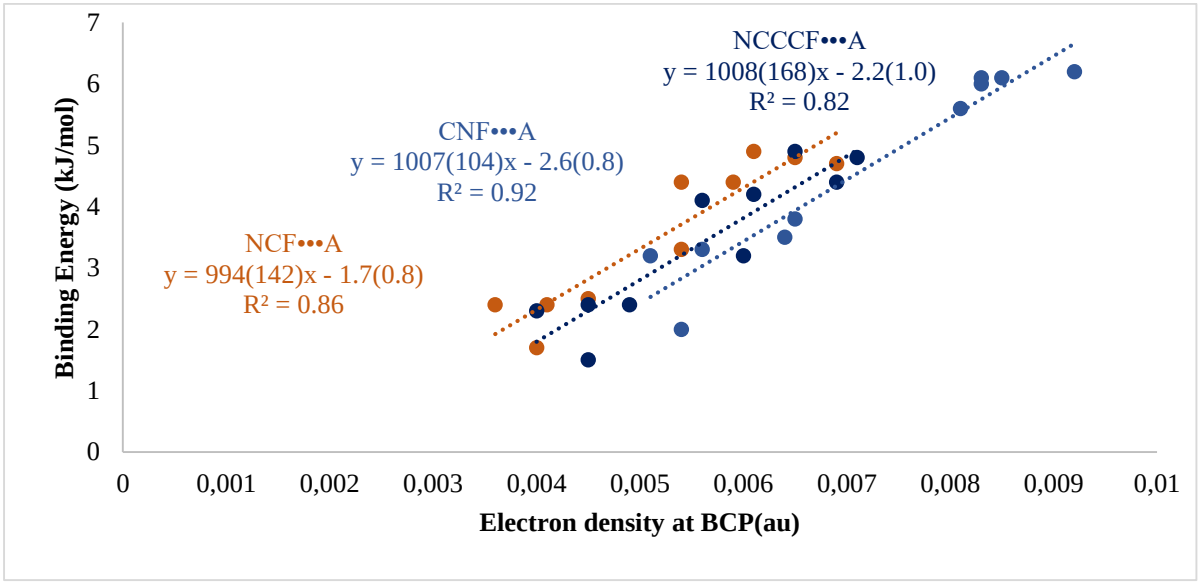

Figure D27. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for F-bonded complexes.*

Table D28. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Cl-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
$ClCl•••OH_2$	0.0167	11.8
$ClCl•••SH_2$	0.0158	11.0
$ClCl•••NH_3$	0.0314	20.9
ClCl•••NCH	0.0154	11.9
ClCl•••CO	0.0073	5.9
$ClCl•••OCH_2$	0.0202	13.5
$ClCl•••C_2H_4$	0.0167	12.2
$ClCl•••OHCH_3$	0.0225	15.4
ClCl•••FH	0.0096	5.7
$ClCl•••O(CH_3)_2$	0.0284	18.7
$FCl•••OH_2$	0.0262	20.9
$FCl•••SH_2$	0.0296	20.4
$FCl•••NH_3$	0.0566	43.4
FCl•••NCH	0.0228	20.3
FCl•••CO	0.0188	11.0
$FCl•••OCH_2$	0.0319	23.3
$FCl•••C_2H_4$	0.0304	22.0
$FCl•••OHCH_3$	0.0362	27.5
FCl•••FH	0.0141	9.5
$FCl•••O(CH_3)_2$	0.0451	32.8
$NCCl•••OH_2$	0.0118	13.2
$NCCl•••SH_2$	0.0085	8.5
$NCCl•••NH_3$	0.0140	16.6
NCCl•••NCH	0.0112	13.8
NCCl•••CO	0.0073	5.8
$NCCl•••OCH_2$	0.0137	12.4
$NCCl•••C_2H_4$	0.0084	8.6
$NCCl•••OHCH_3$	0.0142	14.9
NCCl•••FH	0.0079	7.5
$NCCl•••O(CH_3)_2$	0.0170	15.6

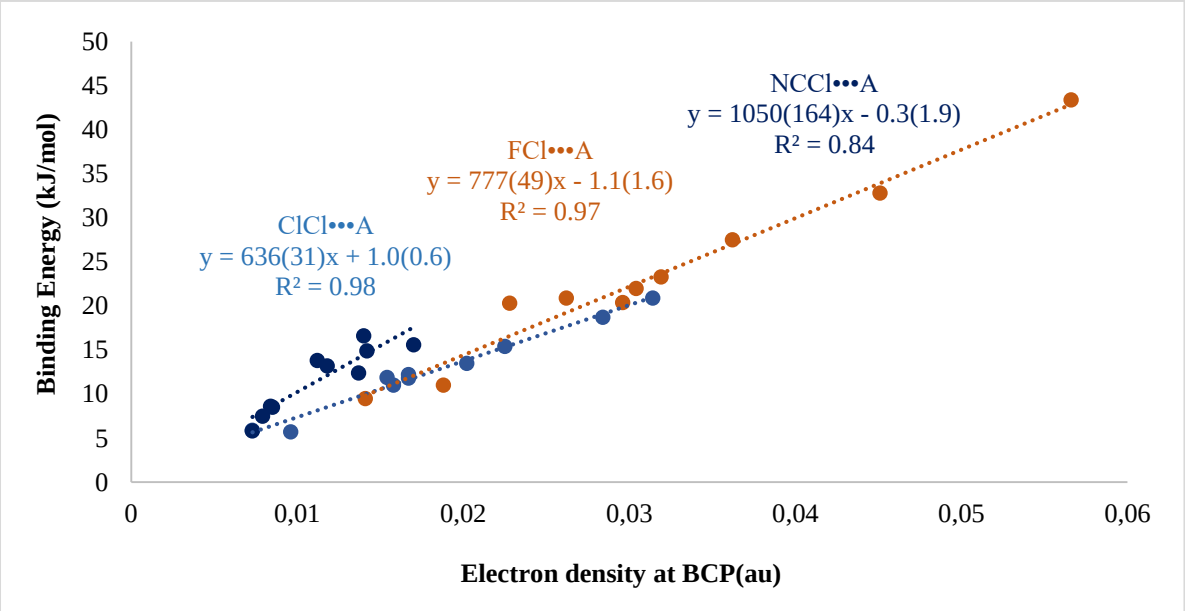

Figure D28*. Binding energy (kJ/mol) versus electron density at BCP (au) plot for Cl-bonded complexes.*

Table D29. Electron density at BCP (au) and binding energy (kJ/mol) data for Br-bonded complexes.

Complexes	Electron Density (au)	Binding Energy(kJ/mol)
$FBr\bullet\bullet\bullet OH_2$	0.0309	29.0
$FBr\bullet\bullet\bullet SH_2$	0.0328	29.6
$FBr\bullet\bullet\bullet NH_3$	0.0569	59.5
FBr•••NCH	0.0310	28.9
$FBr\bullet\bullet\bullet OCH_2$	0.0370	31.9
$FBr\bullet\bullet\bullet C_2H_4$	0.0373	32.6
$FBr\bullet\bullet\bullet OHCH_3$	0.0418	37.8
$FBr\bullet\bullet\bullet O(CH_3)_2$	0.0495	44.3
FBr•••FH	0.0159	12.5
FBr•••CO	0.0306	17.0
$ClBr\bullet\bullet\bullet OH_2$	0.0216	18.4
$ClBr\bullet\bullet\bullet SH_2$	0.0223	18.1
$ClBr\bullet\bullet\bullet NH_3$	0.0442	36.3
ClBr•••NCH	0.0210	18.5
$ClBr\bullet\bullet\bullet OCH_2$	0.0264	20.5
$ClBr\bullet\bullet\bullet\bullet C_2H_4$	0.0246	19.5
$ClBr\bullet\bullet\bullet OHCH_3$	0.0301	24.1
$ClBr\bullet\bullet\bullet O(CH_3)_2$	0.0377	28.7
ClBr•••FH	0.0118	8.4
ClBr•••CO	0.0152	9.2
$BrBr\bullet\bullet\bullet OH_2$	0.0193	15.1
$BrBr\bullet\bullet\bullet SH_2$	0.0195	15.0
$BrBr\bullet\bullet\bullet NH_3$	0.0394	29.1
BrBr•••NCH	0.0191	15.2
$BrBr\bullet\bullet\bullet OCH_2$	0.0236	17.1
$BrBr\bullet\bullet\bullet C_2H_4$	0.0217	16.2
$BrBr\bullet\bullet\bullet OHCH_3$	0.0269	19.9
$BrBr\bullet\bullet\bullet O(CH_3)_2$	0.0342	24.0
BrBr•••FH	0.0106	6.9
BrBr•••CO	0.0131	7.4

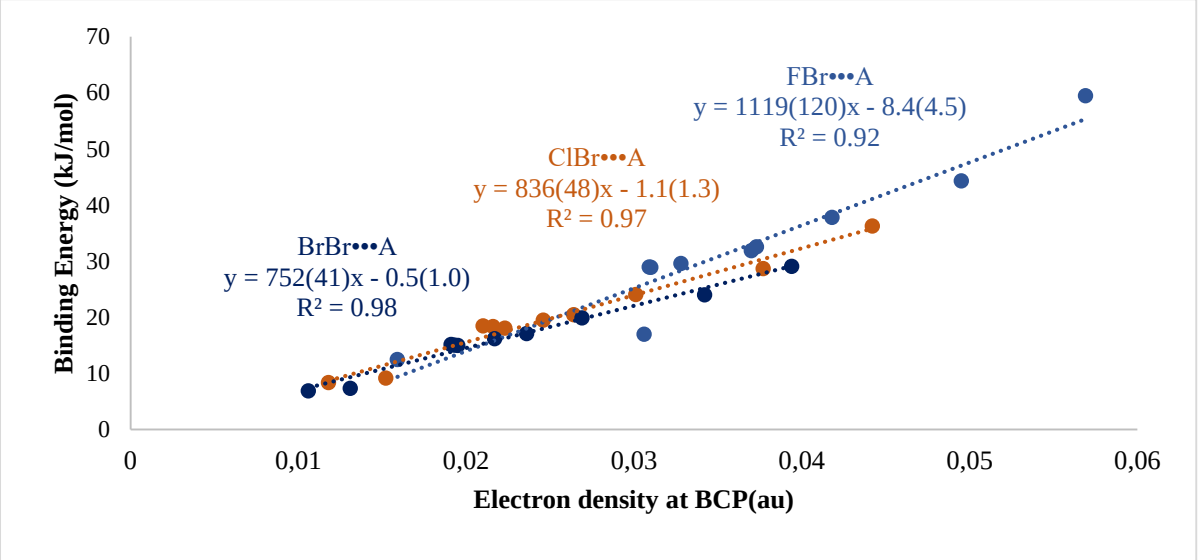

Figure D29. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for Br-bonded complexes.*

Table D30. *Electron density at BCP (au) and binding energy (kJ/mol) data for I-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
FI•••OH_2	0.0315	36.3
FI•••SH_2	0.0296	35.7
FI•••NH_3	0.0489	69.4
FI•••NCH	0.0350	38.1
FI•••OCH_2	0.0363	39.1
FI•••C_2H_4	0.0358	39.9
FI•••$OHCH_3$	0.0400	46.4
FI•••C_2H_2	0.0230	27.3
FI••• $O(CH_3)_2$	0.0452	52.8
FI•••FH	0.0161	15.6
ClI•••OH_2	0.0255	25.7
ClI•••SH_2	0.0239	25.4
ClI•••NH_3	0.0442	51.5
ClI•••NCH	0.0275	26.2
ClI••• OCH_2	0.0304	28.2
ClI••••C_2H_4	0.0280	25.8
ClI•••$OHCH_3$	0.0344	33.8
ClI•••FH	0.0124	11.6
ClI•••$O(CH_3)_2$	0.0403	39.7
ClI•••C_2H_2	0.0177	18.7
BrI•••OH_2	0.0232	22.8
BrI•••SH_2	0.0218	22.3
BrI•••NH_3	0.0417	44.8
BrI•••NCH	0.0247	23.4
BrI•••OCH_2	0.0279	24.9
BrI•••C_2H_4	0.0254	23.8
BrI•••$OHCH_3$	0.0319	29.7
BrI•••FH	0.0112	10.0
BrI•••$O(CH_3)_2$	0.0379	34.8
BrI•••C_2H_2	0.0161	17.4

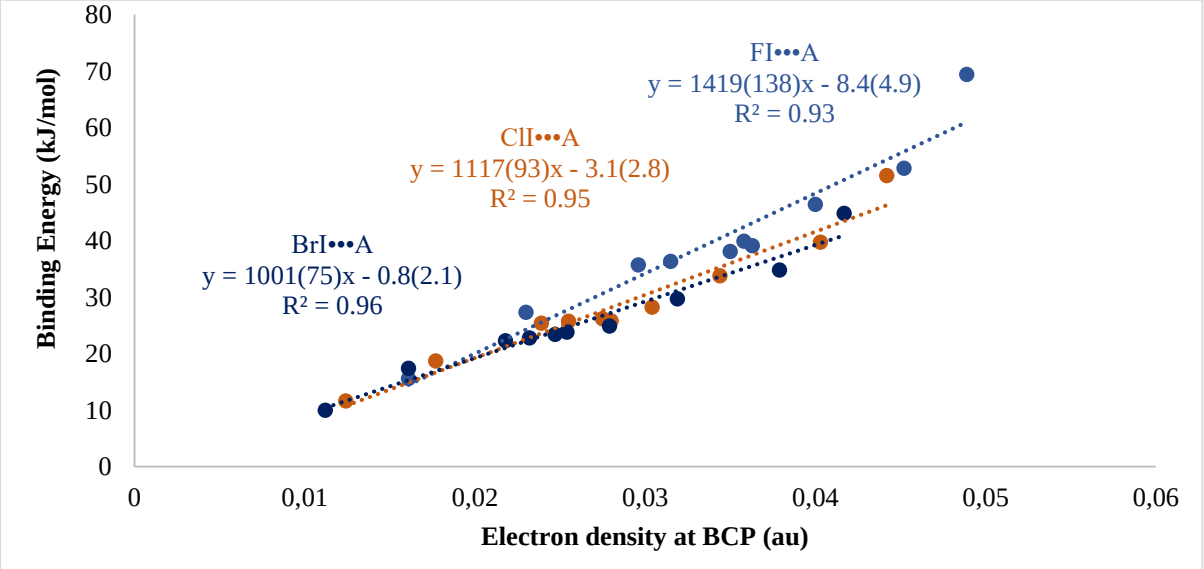

Figure D30. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for I-bonded complexes.*

Table D31. *Electron density at BCP (au) and binding energy (kJ/mol) data for At-bonded complexes.*

Complexes	Electron Density (au)	Binding Energy (kJ/mol)
FAt•••OH_2	0.0320	43.6
FAt•••SH_2	0.0299	43.7
FAt•••NH_3	0.0458	78.5
FAt•••NCH	0.0376	48.1
FAt•••OCH_2	0.0362	46.0
FAt•••C_2H_4	0.0372	50.4
FAt•••$OHCH_3$	0.0390	53.8
FAt•••C_2H_2	0.0258	35.2
FAt••• $O(CH_3)_2$	0.0433	64.1
FAt•••FH	0.0181	19.4
ClAt•••OH_2	0.0286	34.7
ClAt•••SH_2	0.0268	35.1
ClAt•••NH_3	0.0437	65.0
ClAt•••NCH	0.0332	37.5
ClAt••• OCH_2	0.0330	36.9
ClAt••••C_2H_4	0.0329	39.2
ClAt•••$OHCH_3$	0.0362	43.7
ClAt•••C_2H_2	0.0220	27.6
ClAt•••$O(CH_3)_2$	0.0410	49.1
ClAt•••FH	0.0149	15.3
BrAt•••OH_2	0.0268	30.5
BrAt•••SH_2	0.0250	30.8
BrAt•••NH_3	0.0420	57.8
BrAt•••NCH	0.0309	32.5
BrAt•••OCH_2	0.0311	32.4
BrAt•••C_2H_4	0.0305	33.8
BrAt•••$OHCH_3$	0.0344	38.5
BrAt•••C_2H_2	0.0202	24.0
BrAt•••$O(CH_3)_2$	0.0393	43.7
BrAt•••FH	0.0135	13.3

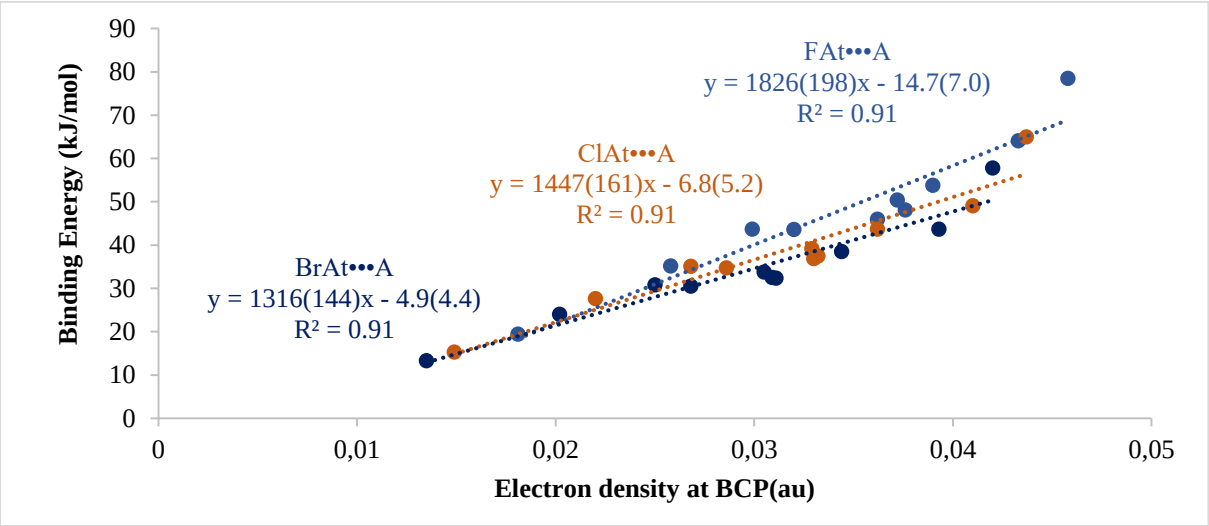

Figure D31. *Binding energy (kJ/mol) versus electron density at BCP (au) plot for At-bonded complexes.*

Optimised Geometries

1. Hydrogen Bonded Complexes:

FH•••OH$_2$			
O	1.24121100	-0.00019300	-0.09632800
H	1.63862400	-0.76392500	0.34342900
H	1.63405100	0.76681700	0.34186100
H	-0.47360300	-0.00130900	-0.04695900
F	-1.41430700	-0.00000500	0.01469900

FH•••SH$_2$			
H	1.23739700	-0.97665300	0.81875300
H	1.23862400	0.97622500	0.81911000
H	-1.17997800	-0.00015900	-0.05574000
F	-2.11419300	0.00005200	0.01172700
S	1.10823100	0.00000800	-0.10547900

FH•••NH$_3$			
H	0.47023900	-0.00045000	0.00088000
F	1.43031000	-0.00000800	0.00008300
N	-1.21945100	-0.00006700	0.00025400
H	-1.60395600	-0.92126200	0.20904100
H	-1.59878900	0.27910300	-0.90432200
H	-1.60412100	0.64315300	0.69187400

FH•••NCH			
H	0.00254500	0.05423300	-1.11594700
N	-0.00161500	-0.03549100	0.73336500
C	-0.00422800	-0.09356300	1.91038400
H	-0.00659400	-0.14630500	2.98700900
F	0.00452400	0.10021000	-2.05188000

FH•••CO			
H	1.23864200	0.00315500	0.00082000
C	-0.82821300	0.00836900	-0.00006300
O	-1.97528200	-0.00462900	0.00001100
F	2.17032100	-0.00181600	-0.00005900

FH•••OCH$_2$			
H	-0.96079200	-0.27682500	0.00005900
C	1.36398800	0.40869700	0.00001200

O	0.72105200	-0.63931100	-0.00000500
H	2.47035800	0.39291000	-0.00003200
H	0.85782400	1.39399800	-0.00001300
F	-1.81330400	0.12802500	-0.00000500

FH•••C_2H_4			
H	-0.99544500	0.00018100	0.00025700
C	1.14662300	-0.67632200	-0.00003200
H	1.15193900	-1.24386200	0.93433200
C	1.14676300	0.67626600	-0.00003200
H	1.15122100	1.24368900	-0.93447600
H	1.15222000	1.24381000	0.93432800
H	1.15097800	-1.24375200	-0.93447100
F	-1.93013700	0.00003000	0.00004600

FH•••CH_3OH			
O	0.53553500	0.67264500	-0.11493400
H	0.76213800	1.31354500	0.57265400
H	-1.05031800	0.18093200	-0.04631300
C	1.40674400	-0.47453900	0.02148200
H	1.28284000	-0.95608500	1.00330400
H	1.10832700	-1.17552800	-0.76669200
H	2.45668200	-0.18297800	-0.12754200
F	-1.92049000	-0.19042300	0.01724100

FH•••PH_3			
H	-1.29504900	-0.00225300	-0.00352800
F	-2.23157600	0.00000600	0.00003700
H	1.79002100	-0.15123400	1.21299600
H	1.79686600	1.12727200	-0.46349900
H	1.81250800	-0.96388500	-0.73236800
P	1.06532200	-0.00066300	-0.00092900

FH•••$O(CH_3)_2$			
O	-0.35714700	-0.00116900	-0.43809000
C	-0.95728900	-1.17956000	0.12112900
H	-0.46030200	-2.04087500	-0.34227200
H	-0.81259100	-1.20803400	1.21514200
H	-2.03557500	-1.20076300	-0.10939200
C	-0.93367800	1.18967000	0.12004600
H	-0.79929700	1.21085500	1.21553200
H	-0.41086700	2.04006500	-0.33480200
H	-2.00870300	1.23801300	-0.12132900
H	1.24493900	-0.01067000	-0.16918700
F	2.16504100	-0.00887800	0.07821900

HOH•••OH_2			
O	-1.39008500	-0.00005900	-0.11242400
H	-1.74768600	0.76286600	0.36129800
H	-1.74768000	-0.76250500	0.36207200
O	1.51701100	0.00006900	0.12285200
H	1.91977200	-0.00045100	-0.75390400
H	0.56019000	0.00001000	-0.05289200

HOH•••SH_2			
H	-1.14389400	0.91010700	-0.89712800
H	-1.18459900	0.73613900	1.04575200
O	2.24538800	0.11265800	0.00600200
H	2.72329200	-0.72538700	-0.03314600
H	1.31061400	-0.14766800	-0.00234400
S	-1.22928200	-0.10465400	-0.01007200

HOH•••NH_3			
O	1.55390500	-0.10683000	0.00051000
H	1.93931700	0.77753900	-0.00258900
H	0.58735400	0.04786000	-0.00767000
N	-1.38082300	0.02216900	-0.00093800
H	-1.73155800	-0.30739600	-0.90028900
H	-1.91168500	0.86295000	0.22561000
H	-1.64890300	-0.68149300	0.68742200

HOH•••NCH			
O	-2.19711500	-0.13708400	0.00007500
H	-2.56290100	0.75586400	0.00101100
H	-1.23722100	0.00434400	-0.00052300
N	0.86593900	0.11539500	-0.00052700
C	2.03540300	-0.04621700	0.00027700
H	3.10305400	-0.19400000	0.00094100

HOH•••CO			
O	2.35272200	-0.10935800	0.00429800
H	2.70047600	0.79119000	0.00609000
H	1.39222500	0.00969400	-0.01421500
C	-0.98056500	0.00954000	-0.01937000
O	-2.12888600	0.00209300	0.01124500

HOH•••OCH_2			
O	1.80164500	0.17766000	0.00008900
H	2.58164700	-0.38989600	-0.00029300
H	1.04836800	-0.43806000	-0.00010300
C	-1.28893200	0.48083100	0.00007900

O	-0.92352300	-0.69161100	-0.00004000
H	-2.36638300	0.74292200	0.00020600
H	-0.55501400	1.31165200	-0.00067800

HOH•••C_2H_4			
O	2.06498700	-0.00014100	0.08760600
H	2.51976000	0.00209400	-0.76420800
H	1.12415700	0.00026400	-0.14578500
C	-1.25995200	0.67555500	0.01302500
H	-1.01071600	1.24326500	0.91343900
C	-1.25940800	-0.67570800	0.01280700
H	-1.51310300	-1.24346200	-0.88636300
H	-1.00969800	-1.24351300	0.91302200
H	-1.51413700	1.24339800	-0.88594900

HOH•••$OHCH_3$			
O	0.73276000	0.74930100	-0.10287600
H	0.95243400	1.23816800	0.70174500
O	-1.93776100	-0.21317800	0.07964100
H	-2.60825300	0.26341200	-0.42430000
H	-1.11228300	0.27950800	-0.08292800
C	1.33097000	-0.56137700	-0.00203600
H	0.91553700	-1.12763000	0.84624500
H	1.08096500	-1.08235200	-0.93394900
H	2.42579100	-0.49182800	0.09128800

HOH•••PH_3			
O	2.40761200	0.10926200	0.00010400
H	2.82283400	-0.76245300	-0.00064300
H	1.45704800	-0.08333000	-0.00060300
H	-2.01196100	-0.41408200	1.09075600
H	-2.04171200	-0.56812900	-0.99807700
H	-1.72119000	1.29301000	-0.08976000
P	-1.18439400	-0.02260800	-0.00016700

HOH•••$O(CH_3)_2$			
O	-0.52797600	0.00002000	-0.54983800
C	-0.93552500	-1.17746400	0.15712600
H	-0.59312000	-2.03929700	-0.42982800
H	-0.47618400	-1.20837400	1.16114100
H	-2.03502900	-1.20870500	0.25497200
C	-0.93605700	1.17726800	0.15720800
H	-0.47754800	1.20781200	1.16161600
H	-0.59309800	2.03929800	-0.42913500
H	-2.03563800	1.20852200	0.25413800
O	2.18714500	0.00005700	0.17079400

H	1.32538200	0.00017200	-0.28827500
H	2.84137600	0.00113000	-0.53827400

HSH•••OH_2			
H	-2.70704500	-0.23318600	0.76137500
H	-2.70318800	-0.23337300	-0.76356600
H	1.52304500	1.24962700	-0.00058800
H	-0.00683900	0.02860800	0.00108100
S	1.34186300	-0.08739400	0.00002900
O	-2.19697300	0.07332900	0.00015400

HSH•••NH_3			
H	-1.53159000	1.25487200	-0.00022400
H	0.00542300	0.02901100	-0.00385000
N	2.19760500	0.01090200	-0.00050600
H	2.55772400	-0.35483300	0.88129800
H	2.64938700	0.91479400	-0.14111700
H	2.55421900	-0.60338200	-0.73299100
S	-1.35115000	-0.08229900	0.00002600

HSH•••NCH			
H	-2.13248100	1.24595800	0.00202700
H	-0.59624100	0.03609900	-0.00179300
N	1.74884000	0.05704000	-0.00297200
C	2.92787800	-0.02403700	0.00157300
H	4.00320600	-0.09816900	0.00565500
S	-1.94272700	-0.08993400	0.00034200

HSH•••CO			
H	-2.28248400	1.24397400	-0.00950200
H	-0.72495900	0.06816600	0.02072800
C	1.92028000	0.04587700	0.01969700
O	3.06731900	-0.02238100	-0.01219900
S	-2.06580000	-0.08802200	-0.00198900

HSH•••OCH_2			
H	-1.95603000	-0.16797200	1.22523800
H	-0.50894500	-0.57928800	-0.02793000
C	1.98815500	0.51034000	0.02364500
O	1.69013600	-0.67873200	-0.01749700
H	3.04814700	0.83892200	0.02430400
H	1.20837700	1.29998400	0.06172400
S	-1.70259800	0.06101100	-0.08032700

HSH•••C_2H_4

H	2.13993500	0.00018400	1.24244800
H	0.54604700	0.00031900	0.11087100
C	-2.05141300	-0.67548700	-0.00185400
H	-1.97604400	-1.24418600	-0.93246300
C	-2.05219900	0.67526000	-0.00185300
H	-2.13137100	1.24363200	0.92868600
H	-1.97749900	1.24403900	-0.93246600
H	-2.12991900	-1.24394400	0.92868900
S	1.88440800	0.00008200	-0.08272000

HSH•••OHCH$_3$

O	-1.47336800	0.72708300	0.03893300
H	-2.08559500	1.31264900	-0.42552500
H	2.13418600	0.34596300	1.16788400
H	0.61416300	0.45176000	-0.06283900
C	-2.02405500	-0.60321300	0.02670600
H	-2.17222800	-0.97212600	-1.00120800
H	-1.28855100	-1.24281900	0.53068800
H	-2.97799600	-0.64925300	0.57610700
S	1.85670600	-0.09022300	-0.07855000

HSH•••PH$_3$

H	2.38031000	1.25616000	0.00092100
H	0.85929300	0.03121000	0.03142100
H	-2.66161100	-1.14967100	-0.51070600
H	-2.79781600	0.92006500	-0.76366800
H	-2.85308300	0.09618800	1.15666400
S	2.20679800	-0.08221200	-0.00078400
P	-2.01572400	0.01076300	0.00652700

HSH•••O(CH$_3$)$_2$

O	-1.19776600	-0.01818700	-0.57738000
C	-1.55648800	-1.15529100	0.21164700
H	-1.33930000	-2.04671300	-0.39105400
H	-0.96497400	-1.18892800	1.14503900
H	-2.63193800	-1.13291900	0.46401000
C	-1.45187400	1.19178100	0.13907200
H	-0.86897300	1.22406800	1.07890600
H	-1.14607100	2.02195800	-0.51081600
H	-2.52565300	1.28653800	0.38120400
H	0.84483500	-0.03317000	-0.40803200
H	2.62317900	-0.69896700	-0.90447200
S	2.10257500	0.03091800	0.10374700

2. Lithium Bonded Complexes

FLi•••OH$_2$			
F	-1.91189700	0.00381200	0.00027100
O	1.68767500	0.00074800	-0.00005900
H	2.25556300	0.78154800	0.00104800
H	2.28960000	-0.75398100	0.00132600
Li	-0.27982900	-0.02262000	-0.00144800

FLi•••NCCH$_3$			
C	1.39718500	0.00140500	-0.00000800
N	0.21790000	0.00249600	-0.00002500
F	-3.47457400	-0.00043400	0.00001300
C	2.86477700	-0.00140200	0.00001500
H	3.22954900	-0.53738600	0.88708300
H	3.22965300	-0.50283200	-0.90699100
H	3.23294100	1.03361100	0.01997100
Li	-1.83935100	-0.00232500	-0.00001400

FLi•••NH$_3$			
F	-1.97385800	-0.00001100	-0.00000400
N	1.75809300	-0.00000200	-0.00000200
H	2.15780900	0.44587500	0.82739000
H	2.15779100	0.49356700	-0.79986900
H	2.15770600	-0.93952800	-0.02754200
Li	-0.33841300	0.00006700	0.00002400

FLi•••NCH			
C	0.00000000	0.00000000	-2.34597500
H	0.00000000	0.00000000	-3.42485900
N	0.00000000	0.00000000	-1.16973300
F	0.00000000	0.00000000	2.54856800
Li	0.00000000	0.00000000	0.91724500

FLi•••OCH$_2$			
F	1.74009300	0.25542900	0.00007000
O	-1.11885000	-0.62251900	0.00001300
C	-1.14158200	0.61532200	-0.00004800
H	-0.19204800	1.18351200	-0.00014000
H	-2.11610200	1.13923000	-0.00000200
Li	0.81586800	-1.11112900	-0.00010000

FLi•••C$_2$H$_4$			
C	-1.56623000	0.67716500	0.00009400

H	-1.58275700	1.24482200	-0.93490600
H	-1.58316600	1.24482000	0.93508900
C	-1.56623000	-0.67716400	0.00009500
H	-1.58316700	-1.24481900	0.93508900
H	-1.58275800	-1.24482200	-0.93490600
F	2.49921600	0.00000000	-0.00030100
Li	0.87788800	0.00000000	0.00040400

$FLi{\bullet\bullet\bullet}OHCH_3$

F	1.93578900	-0.24696700	-0.00007200
O	-0.97047700	0.70570000	-0.00014300
H	-1.82813900	1.14534400	-0.00000800
C	-1.16821800	-0.74150800	0.00007100
H	-0.15760100	-1.17010100	-0.00039100
H	-1.71699700	-1.04541300	0.90283900
H	-1.71781400	-1.04552000	-0.90215900
Li	0.92385800	1.04728000	0.00035900

$FLi{\bullet\bullet\bullet}PH_3$

F	-2.81571900	-0.00000400	-0.00003800
H	2.20228200	1.06057800	-0.61442200
H	2.20225400	-1.06284200	-0.61052900
H	2.20074700	0.00223900	1.22643300
Li	-1.19145800	0.00002200	0.00008200
P	1.48737100	0.00000000	-0.00009200

$FLi{\bullet\bullet\bullet}CO$

F	0.00000000	0.00000000	2.66287700
Li	0.00000000	0.00000000	1.04266600
C	0.00000000	0.00000000	-1.28112800
O	0.00000000	0.00000000	-2.42589000

$FLi{\bullet\bullet\bullet}O(CH_3)_2$

O	0.76766100	-0.00015200	0.57877700
C	0.92845800	-1.18188700	-0.23881000
H	0.83667300	-2.04889000	0.42893300
H	0.14497900	-1.21322100	-1.01342100
H	1.92994700	-1.18022100	-0.69890300
C	0.93090900	1.18081100	-0.23939100
H	0.14741100	1.21353300	-1.01393700
H	0.84127000	2.04838400	0.42793000
H	1.93227800	1.17672600	-0.69973900
F	-2.18527900	0.00057400	-0.25045300
Li	-1.15417600	0.00206500	1.02073600

ClLi•••OH_2			
O	-2.44887300	0.00002000	-0.00031100
H	-3.03315200	0.76885200	0.00165000
H	-3.03377200	-0.76833800	0.00165200
Li	-0.50346500	-0.00040200	-0.00083100
Cl	1.59813500	0.00003200	0.00009900

ClLi•••$NCCH_3$			
C	1.95024300	-0.43780900	1.00190800
N	0.92158200	-0.20686600	0.47442600
C	3.23046200	-0.72522800	1.65864000
H	3.58854500	-1.71501400	1.34340400
H	3.96655400	0.03936700	1.37432400
H	3.09223600	-0.71465500	2.74862000
Li	-0.84804700	0.19040000	-0.43762000
Cl	-2.68461800	0.60267000	-1.37869200

ClLi•••NH_3			
N	2.53733600	-0.00000200	0.00005500
H	2.93807000	0.82289400	-0.45383200
H	2.93805400	-0.80465100	-0.48545800
H	2.93760600	-0.01826700	0.93984800
Li	0.46166500	0.00002300	-0.00059400
Cl	-1.64471000	-0.00000200	0.00004900

ClLi•••NCH			
C	0.00000000	0.00000000	-3.16278800
H	0.00000000	0.00000000	-4.24186400
N	0.00000000	0.00000000	-1.98706500
Li	0.00000000	0.00000000	0.07099500
Cl	0.00000000	0.00000000	2.17147400

ClLi•••OCH_2			
O	-1.74999800	0.57583600	-0.00002300
C	-1.76937000	-0.66036700	0.00033400
H	-0.82588200	-1.23674700	0.00021800
H	-2.73965700	-1.19033400	-0.00009800
Li	0.07691700	1.31063500	0.00005300
Cl	1.64417600	-0.12643000	-0.00012400

ClLi•••C_2H_4			
C	-0.00053400	-2.31935300	-0.67749400
H	0.93465600	-2.33653300	-1.24512800
H	-0.93572000	-2.33675800	-1.24512600
C	-0.00053400	-2.31935300	0.67749400

H	-0.93572000	-2.33675800	1.24512600
H	0.93465600	-2.33653300	1.24512800
Li	-0.00053400	0.08154300	0.00000000
Cl	0.00059600	2.17260000	0.00000000

ClLi•••OHCH$_3$			
O	-1.63959400	0.67092100	0.00018600
H	-2.50841500	1.08916700	0.00029300
C	-1.80566000	-0.77992600	0.00017200
H	-0.79020700	-1.19461800	0.00006100
H	-2.34516500	-1.09593800	0.90373400
H	-2.34534500	-1.09589800	-0.90329500
Li	0.19212300	1.20424100	-0.00000800
Cl	1.84491000	-0.11783800	-0.00019400

ClLi•••PH$_3$			
H	2.98027900	0.61661200	1.06205800
H	2.98024700	0.60972800	-1.06604700
H	2.97730900	-1.22983200	0.00396700
Li	-0.36540700	0.00292500	0.00001700
P	2.27083400	-0.00004300	0.00000000
Cl	-2.46494800	-0.00027300	-0.00000200

ClLi•••CO			
Li	0.00000000	0.00000000	-0.16529300
C	0.00000000	0.00000000	2.12187300
O	0.00000000	0.00000000	3.26621400
Cl	0.00000000	0.00000000	-2.25676900

ClLi•••O(CH$_3$)$_2$			
O	-1.31507900	0.00005600	0.55174600
C	-1.47255200	1.18368300	-0.26541800
H	-1.37378900	2.05107700	0.40044600
H	-0.69109500	1.21227500	-1.04183200
H	-2.47498100	1.18408500	-0.72258300
C	-1.47379000	-1.18321400	-0.26571600
H	-0.69225300	-1.21245700	-1.04203000
H	-1.37597800	-2.05087100	0.39995500
H	-2.47617600	-1.18239100	-0.72294300
Li	0.49972700	-0.00072500	1.23985300
Cl	2.10492800	-0.00016500	-0.13045500

BrLi•••OH$_2$			
O	-3.15553200	0.00003200	-0.00023600

H	-3.73944900	0.76912300	0.00143700
H	-3.74011100	-0.76855300	0.00143900
Li	-1.21576200	-0.00048800	-0.00082300
Br	1.03917400	0.00001800	0.00004200

BrLi•••NCCH$_3$			
C	0.02230500	0.07681100	3.24288000
N	0.01422300	0.04929400	2.06441000
C	0.03236900	0.11131400	4.70955100
H	-0.86333900	-0.39673200	5.09280000
H	0.93164100	-0.39952400	5.08054800
H	0.03631700	1.15597400	5.05007300
Li	0.00028000	-0.00060400	0.04302100
Br	-0.01523000	-0.05233500	-2.21479800

BrLi•••NH$_3$			
N	-0.00077100	-0.03785400	3.26022500
H	-0.46446100	-0.86007200	3.65115500
H	-0.47718600	0.76772200	3.67004300
H	0.93898100	-0.03516000	3.66114600
Li	-0.00008400	-0.01384200	1.19170000
Br	0.00023800	0.01240000	-1.06797200

BrLi•••NCH			
C	0.00000000	0.00000000	-4.01277200
H	0.00000000	0.00000000	-5.09181900
N	0.00000000	0.00000000	-2.83708800
Li	0.00000000	0.00000000	-0.78513600
Br	0.00000000	0.00000000	1.46809900

BrLi•••OCH$_2$			
O	-2.41044600	0.55818900	0.00003400
C	-2.40397900	-0.67807700	0.00002400
H	-1.44881300	-1.23519500	-0.00023500
H	-3.36252400	-1.22857800	-0.00007400
Li	-0.62457200	1.37229700	-0.00010300
Br	1.15407100	-0.05857600	0.00000600

BrLi•••C$_2$H$_4$			
C	0.00003100	-3.13641000	-0.67757600
H	0.93534900	-3.15381800	-1.24505500
H	-0.93527700	-3.15447000	-1.24505200
C	0.00003100	-3.13641000	0.67757600
H	-0.93527700	-3.15447000	1.24505200
H	0.93534900	-3.15381800	1.24505500

Li	-0.00052700	-0.74464300	0.00000000
Br	0.00003100	1.49964100	0.00000000

$BrLi•••OHCH_3$			
O	-2.34297500	0.65885200	0.00025900
H	-3.22206500	1.05536200	0.00039400
C	-2.47380200	-0.79589000	0.00026000
H	-1.44878200	-1.18637700	0.00015300
H	-3.00506400	-1.12459000	0.90407200
H	-3.00524700	-1.12457300	-0.90345100
Li	-0.53874500	1.26363400	0.00005800
Br	1.31097200	-0.05446300	-0.00014200

$BrLi•••PH_3$			
H	-3.86088900	-0.61430600	1.06435800
H	-3.86086200	-0.61381500	-1.06465900
H	-3.85938300	1.22973100	0.00027400
Li	-0.52728500	-0.00075800	0.00002100
P	-3.15318600	-0.00002800	0.00000000
Br	1.72745100	0.00003100	-0.00000100

BrLi•••CO			
Li	0.00000000	0.00000000	0.72017500
C	0.00000000	0.00000000	2.99777300
O	0.00000000	0.00000000	4.14190900
Br	0.00000000	0.00000000	-1.52235500

$BrLi•••O(CH_3)_2$			
O	-1.99048100	0.00004200	0.54408500
C	-2.12715200	1.18352900	-0.27770800
H	-2.04091100	2.05163100	0.38894700
H	-1.32797600	1.20907700	-1.03595400
H	-3.11909400	1.18501200	-0.75706500
C	-2.12698500	-1.18382700	-0.27713500
H	-1.32749700	-1.20978200	-1.03504300
H	-2.04087200	-2.05160500	0.38997000
H	-3.11875500	-1.18555000	-0.75681100
Li	-0.21901800	0.00142400	1.32084200
Br	1.57373800	-0.00004600	-0.06229100

3. Sodium Bonded Complexes

FNa•••OH_2			
F	-2.26970800	0.00007400	0.00037000
O	2.20513200	0.00003200	0.00007000
H	2.79699600	0.76707400	0.00087300
H	2.79730700	-0.76676700	0.00087500
Na	-0.25527100	-0.00011200	-0.00051300

FNa•••$NCCH_3$			
C	-2.01588200	0.00269400	0.00000600
N	-0.83466500	0.00789100	0.00002800
F	3.63047400	0.00570100	-0.00001600
C	-3.48452900	-0.00165900	-0.00001800
H	-3.85020900	-0.53705200	-0.88710600
H	-3.85033100	-0.50372600	0.90630000
H	-3.85459400	1.03274600	-0.01926600
Na	1.61145300	-0.00952000	0.00000800

FNa•••NH_3			
F	2.28801200	-0.00034400	-0.00009300
N	-2.23544000	-0.00018100	-0.00005800
H	-2.63752800	-0.45894400	0.81909600
H	-2.63739000	-0.48065100	-0.80674000
H	-2.63835900	0.93824500	-0.01262200
Na	0.26993100	0.00052000	0.00013700

FNa•••NCH			
C	0.00000000	0.00000000	-2.89596600
H	0.00000000	0.00000000	-3.97501400
N	0.00000000	0.00000000	-1.71785000
F	0.00000000	0.00000000	2.77652800
Na	0.00000000	0.00000000	0.76245600

FNa•••OCH_2			
F	1.34469500	1.05767300	-0.00009100
O	-1.38877400	-0.61738200	0.00033800
C	-1.49574100	0.61935200	0.00015500
H	-0.58116600	1.25166200	0.00048600
H	-2.50935800	1.07015600	-0.00054100
Na	1.00662700	-0.96526600	-0.00025100

FNa•••C_2H_4			
C	-0.00019300	-2.09059400	0.67654500
H	-0.93475300	-2.10862000	1.24479400
H	0.93436000	-2.10909400	1.24479200
C	-0.00019300	-2.09059400	-0.67654500

H	0.93436000	-2.10909400	-1.24479200
H	-0.93475300	-2.10862000	-1.24479400
F	-0.00019300	2.77786200	0.00000000
Na	0.00043900	0.77471000	0.00000000

$FNa\cdots OHCH_3$			
F	-1.58486400	0.98865000	-0.00010900
O	1.27658600	-0.65944700	0.00008600
H	2.14324800	-1.08342100	0.00018600
C	1.47305700	0.79290500	0.00007400
H	0.46013800	1.22636300	0.00000000
H	2.02654000	1.09554300	0.90142700
H	2.02666000	1.09551100	-0.90121600
Na	-1.04034900	-0.97397300	-0.00005000

$FNa\cdots PH_3$			
F	-3.05196700	0.00017800	0.00001300
H	2.77094200	-0.61040500	-1.05672300
H	2.77092100	-0.60922400	1.05742500
H	2.76964600	1.22110300	-0.00067200
P	2.04430500	-0.00001800	0.00000300
Na	-1.04621600	-0.00025500	-0.00001700

FNa•••CO			
F	0.00000000	0.00000000	2.86884500
C	0.00000000	0.00000000	-1.87276500
O	0.00000000	0.00000000	-3.01865300
Na	0.00000000	0.00000000	0.86965500

$FNa\cdots O(CH_3)_2$			
O	1.04039900	0.00031200	-0.58024300
C	1.17844200	1.17498400	0.25092300
H	1.09216700	2.04783000	-0.41214600
H	0.38356900	1.18263000	1.01599000
H	2.17580100	1.18324500	0.72329200
C	1.17815800	-1.17540300	0.24952100
H	0.38315700	-1.18386000	1.01444700
H	1.09188200	-2.04741800	-0.41464000
H	2.17544600	-1.18436300	0.72202500
F	-1.66690000	-0.00067100	1.05476200
Na	-1.34206500	0.00072700	-0.95477700

$ClNa\cdots OH_2$			
O	2.83374600	0.01471100	0.00049100
H	3.40228400	0.79816600	0.00115300

H	3.44788500	-0.73341800	0.00212500
Na	0.43303600	-0.03296300	-0.00137100
Cl	-2.01667900	0.01059800	0.00046300

ClNa•••NCCH$_3$			
C	2.73197200	-0.00022000	0.00035500
N	1.55098800	-0.00152800	0.00024100
C	4.20031500	0.00192600	-0.00024500
H	4.56711100	0.10210800	1.03064000
H	4.56800600	-0.94027500	-0.42960900
H	4.56540100	0.84552400	-0.60221000
Na	-0.87297600	-0.00306100	-0.00005200
Cl	-3.32637800	0.00157500	-0.00003500

ClNa•••NH$_3$			
N	-2.89428800	0.00000900	0.00000500
H	-3.29770200	-0.81297700	-0.46880900
H	-3.29767600	0.81255700	-0.46959000
H	-3.29766200	0.00046600	0.93850400
Na	-0.41145400	-0.00002000	-0.00002600
Cl	2.03994400	0.00000600	0.00000900

ClNa•••NCH			
C	0.00000000	0.00000000	-3.58575200
H	0.00000000	0.00000000	-4.66506000
N	0.00000000	0.00000000	-2.40793500
Na	0.00000000	0.00000000	0.05051500
Cl	0.00000000	0.00000000	2.49879100

ClNa•••OCH$_2$			
O	-1.94943000	0.23455400	0.00006200
C	-1.77754000	-0.99067900	0.00005700
H	-0.75591100	-1.41751100	-0.00003600
H	-2.65562100	-1.66609000	0.00004200
Na	0.12591700	1.43649800	-0.00001600
Cl	1.66394900	-0.50883700	-0.00004000

ClNa•••C$_2$H$_4$			
C	-0.00025100	2.74762500	0.67681300
H	0.93442400	2.76802300	1.24503400
H	-0.93499200	2.76707600	1.24495900
C	-0.00025100	2.74762500	-0.67681300
H	-0.93499200	2.76707600	-1.24495900
H	0.93442400	2.76802300	-1.24503400
Na	0.00076600	-0.09278300	0.00000000

Cl	-0.00025100	-2.53065200	0.00000000

ClNa•••OHCH$_3$			
O	-1.89116600	0.38269500	0.00018400
H	-2.82744700	0.61756100	0.00027800
C	-1.78667900	-1.07523900	0.00015300
H	-0.71236200	-1.30239900	0.00005500
H	-2.26003900	-1.48840500	0.90253400
H	-2.26019700	-1.48837700	-0.90215800
Na	0.21591000	1.37143900	-0.00001400
Cl	1.85496700	-0.47260800	-0.00017300

ClNa•••PH$_3$			
H	-3.44496000	-1.07115700	-0.58853400
H	-3.44493200	1.04574800	-0.63262800
H	-3.44388900	0.02548200	1.22270600
Na	0.34479200	-0.00003500	-0.00060100
P	-2.72234800	0.00000600	0.00009400
Cl	2.78684000	0.00001200	0.00021500

ClNa•••CO			
Na	0.00000000	0.00000000	0.13993700
C	0.00000000	0.00000000	-2.58210100
O	0.00000000	0.00000000	-3.72778500
Cl	0.00000000	0.00000000	2.57503400

ClNa•••O(CH$_3$)$_2$			
O	-1.52975300	-0.38030700	-0.00005600
C	-1.54808700	0.45612900	1.17754100
H	-1.56679500	-0.21341200	2.04879000
H	-0.64796600	1.09246900	1.20404300
H	-2.46013500	1.07657800	1.18047000
C	-1.54799900	0.45637600	-1.17748300
H	-0.64786500	1.09270500	-1.20379400
H	-1.56666300	-0.21298500	-2.04887000
H	-2.46003900	1.07683700	-1.18033900
Na	0.58912800	-1.46512300	-0.00011400
Cl	1.98138800	0.57480000	0.00006200

BrNa•••OH$_2$			
O	3.56434900	0.01484200	0.00057100
H	4.13383400	0.79714700	0.00126800
H	4.17796200	-0.73324200	0.00223500
Na	1.17722300	-0.03199300	-0.00148100
Br	-1.42217300	0.00483700	0.00023500

BrNa•••NCCH$_3$			
C	3.68520900	0.00013000	-0.00003000
N	2.50428000	-0.00188700	-0.00008700
C	5.15347300	0.00222000	0.00002900
H	5.51978600	0.04548500	1.03503900
H	5.52125500	-0.91494100	-0.48045000
H	5.51862600	0.87772100	-0.55445900
Na	0.08842200	-0.00365300	0.00006500
Br	-2.51698200	0.00088700	-0.00000700

BrNa•••NH$_3$			
N	-3.63818000	-0.00001000	0.00005600
H	-4.04167000	0.81231800	0.47003100
H	-4.04164300	-0.81311900	0.46870400
H	-4.04198000	0.00074900	-0.93829600
Na	-1.16343600	0.00002200	-0.00014300
Br	1.43972400	-0.00000300	0.00002100

BrNa•••NCH			
C	0.00000000	0.00000000	-4.41749300
H	0.00000000	0.00000000	-5.49684000
N	0.00000000	0.00000000	-3.23974800
Na	0.00000000	0.00000000	-0.78928200
Br	0.00000000	0.00000000	1.81034700

BrNa••• OCH$_2$			
O	-2.53790700	0.07049300	0.00006300
C	-2.22610800	-1.12640400	-0.00005300
H	-1.16222400	-1.43279800	0.00025300
H	-3.01962000	-1.89891200	0.00020300
Na	-0.66048700	1.55257200	0.00019500
Br	1.28877400	-0.21577500	-0.00008000

BrNa•••C$_2$H$_4$			
C	-0.02181600	3.55253100	0.67681400
H	0.91027600	3.62550500	1.24505600
H	-0.95609800	3.52018000	1.24518900
C	-0.02181600	3.55253100	-0.67681400
H	-0.95609800	3.52018000	-1.24518900
H	0.91027600	3.62550500	-1.24505600
Na	0.10154300	0.72971500	0.00000000

Br	-0.02181600	-1.85567500	0.00000000

$BrNa\bullet\bullet\bullet OHCH_3$			
O	-2.53044400	0.26561300	0.00022700
H	-3.48540600	0.40621400	0.00034700
C	-2.28280900	-1.17429300	0.00020400
H	-1.19160300	-1.29560700	0.00010300
H	-2.71235700	-1.63228900	0.90278400
H	-2.71252200	-1.63228700	-0.90229900
Na	-0.55964900	1.49117600	0.00005700
Br	1.43424100	-0.20937500	-0.00013200

$BrNa\bullet\bullet\bullet PH_3$			
H	-4.30100100	-1.06255400	-0.60477300
H	-4.30097000	1.05535800	-0.61729700
H	-4.30021300	0.00724900	1.22311900
Na	-0.52560700	-0.00002700	-0.00031900
P	-3.57929500	0.00000600	0.00004000
Br	2.06780800	0.00000500	0.00005300

$BrNa\bullet\bullet\bullet CO$			
Na	0.00000000	0.00000000	-0.72196000
C	0.00000000	0.00000000	-3.43782900
O	0.00000000	0.00000000	-4.58332700
Br	0.00000000	0.00000000	1.86386100

$BrNa\bullet\bullet\bullet O(CH_3)_2$			
O	2.12702900	0.27905200	-0.00001300
C	2.05737600	-0.55454600	1.17765700
H	2.14282700	0.10909300	2.04935100
H	1.09604300	-1.09392800	1.20330600
H	2.90014500	-1.26612800	1.18147000
C	2.05733800	-0.55459500	-1.17764700
H	1.09600000	-1.09396900	-1.20324900
H	2.14277200	0.10900800	-2.04937000
H	2.90010300	-1.26618200	-1.18145300
Na	0.18968400	1.64979500	-0.00002300
Br	-1.60196900	-0.26352000	0.00000700

4. Beryllium Bonded Complexes

$F_2Be\bullet\bullet\bullet OH_2$			
Be	-0.00002300	-0.31307900	-0.02679400

F	1.37916500	-0.76996900	0.01068500
F	-1.37927400	-0.76977800	0.01068700
O	0.00009700	1.42225000	-0.07702800
H	-0.78822500	1.86605800	0.26551700
H	0.78851800	1.86597800	0.26553600

$F_2Be•••SH_2$			
Be	-0.84183600	0.00000000	-0.01131500
F	-1.27102800	1.38160300	0.00879800
F	-1.27103500	-1.38160000	0.00879800
S	1.43525200	-0.00000200	-0.10597700
H	1.64094100	-0.98956500	0.79126600
H	1.64094000	0.98955900	0.79126900

$F_2Be•••NH_3$			
Be	-0.29978400	0.00008200	-0.00151700
F	-0.82317100	1.36376800	0.00032000
F	-0.82420800	-1.36319800	0.00032000
N	1.49041200	-0.00051900	-0.00269200
H	1.86613800	0.82814000	-0.46599600
H	1.86562100	-0.83042100	-0.46418500
H	1.86090300	0.00045300	0.94933000

$F_2Be•••NCH$			
C	2.27338300	-0.00000200	0.00001400
H	3.35189800	0.00000000	0.00012200
N	1.10167900	-0.00000400	-0.00012400
Be	-0.73452200	0.00000100	-0.00000900
F	-1.20921100	1.36870400	0.00004500
F	-1.20921800	-1.36870000	0.00003300

$F_2Be•••OCH_2$			
O	0.82100200	-0.81900100	-0.00010100
C	1.87840400	-0.17554800	-0.00026800
H	2.83297800	-0.72462700	0.00049800
H	1.85993800	0.92606100	0.00053200
Be	-0.69952100	0.10681300	0.00004700
F	-1.86195100	-0.74690400	0.00036400
F	-0.33063400	1.52208200	-0.00023200

$F_2Be•••C_2H_4$			
C	1.45254200	-0.00036300	0.67913800
H	1.46268700	0.93806300	1.23967800
H	1.46418300	-0.93860900	1.23993700

C	1.45221500	-0.00053400	-0.67929900
H	1.46361700	-0.93892200	-1.23986900
H	1.46212800	0.93775600	-1.24007700
Be	-0.73173100	0.00011200	0.00039100
F	-1.12995000	1.38497500	-0.00005600
F	-1.13163100	-1.38423700	0.00002600

$F_2Be{\bullet\bullet\bullet}OHCH_3$

O	-0.69242700	-0.68411700	-0.19133500
H	-0.67241100	-1.62598100	0.02848500
C	-1.97936000	-0.06945100	0.10375000
H	-2.22921400	-0.21069100	1.16343300
H	-1.84720500	0.99401800	-0.11676100
H	-2.74538500	-0.51386200	-0.54370600
Be	0.78956600	0.14052600	-0.03152400
F	1.86529600	-0.83580200	0.07601900
F	0.55154000	1.57847500	-0.02015000

$F_2Be{\bullet\bullet\bullet}PH_3$

Be	-0.89333300	0.00787100	-0.00001900
F	-1.41438500	-1.34326300	0.00000200
F	-1.26885900	1.40870900	0.00000200
H	2.08427400	0.61083200	1.07253400
H	2.08440600	0.61235400	-1.07154500
H	2.14359100	-1.25905900	-0.00080800
P	1.42735000	-0.03897500	-0.00001000

$F_2Be{\bullet\bullet\bullet}CO$

Be	0.84085700	0.00000200	-0.00002700
F	1.23322300	-1.38674700	-0.00003900
F	1.23319500	1.38675800	-0.00004100
C	-1.17317200	-0.00000900	0.00004200
O	-2.31527000	-0.00000800	0.00007300

$F_2Be{\bullet\bullet\bullet}O(CH_3)_2$

O	0.64625300	0.00000000	0.00031800
C	1.43357000	-1.21265900	0.00023200
H	2.06240400	-1.23274300	0.90291800
H	0.71879100	-2.04181000	0.00034100
H	2.06221100	-1.23276800	-0.90259200
Be	-1.04210200	0.00000000	0.00103200
F	-1.54951400	1.36861500	-0.00052000
F	-1.54951700	-1.36861400	-0.00054300
C	1.43357100	1.21265800	0.00010600
H	0.71879200	2.04181000	0.00040100

H	2.06260100	1.23270600	0.90265700
H	2.06201500	1.23280200	-0.90285300

$Cl_2Be•••OH_2$			
Be	-0.00000900	0.07478700	-0.03223300
O	0.00003500	1.77831000	-0.06900700
Cl	1.76877100	-0.55873800	0.00558900
Cl	-1.76879300	-0.55870600	0.00558900
H	-0.79413700	2.23551200	0.24550700
H	0.79428100	2.23541600	0.24545900

$Cl_2Be•••SH_2$			
Be	0.00000000	-0.34201800	-0.00609200
S	0.00000100	1.88468400	-0.10542300
H	0.99376700	2.12168800	0.78124300
H	-0.99376400	2.12168900	0.78124300
Cl	-1.76387200	-0.97147700	0.00437200
Cl	1.76387100	-0.97147900	0.00437200

$Cl_2Be•••NH_3$			
Be	-0.00615300	0.11419400	-0.00009900
Cl	-1.76226600	-0.57900700	-0.00002700
Cl	1.73614900	-0.61776300	0.00005100
N	0.03883900	1.87674600	-0.00003100
H	0.54655800	2.22840400	-0.81536600
H	0.54393300	2.22828900	0.81698800
H	-0.89375600	2.29440700	-0.00141700

$Cl_2Be•••NCH$			
C	-0.01537700	2.73340000	0.00005300
H	-0.02156500	3.81227600	0.00002400
N	-0.00866000	1.56182800	0.00008100
Be	0.00126600	-0.22225300	-0.00001100
Cl	1.75706400	-0.88014400	-0.00002400
Cl	-1.74710100	-0.89964800	-0.00002700

$Cl_2Be•••OCH_2$			
O	0.61509500	-1.43945900	0.00013000
C	1.85195500	-1.49920600	0.00038100
H	2.32852700	-2.49134000	0.00063400
H	2.45998800	-0.57989800	0.00063100
Be	-0.25676400	0.08219300	-0.00005600
Cl	0.93819100	1.54655700	0.00009400
Cl	-2.10254100	-0.17871100	-0.00035000

$Cl_2Be\cdots C_2H_4$			
C	-0.00026400	1.89921700	-0.68061600
H	0.93845800	1.91595700	-1.24084100
H	-0.93906300	1.91492900	-1.24074800
C	-0.00020700	1.89963000	0.68041000
H	-0.93895500	1.91564400	1.24061100
H	0.93855800	1.91667100	1.24054700
Be	0.00006400	-0.26209200	0.00048000
Cl	1.76315400	-0.86479700	-0.00001300
Cl	-1.76294400	-0.86508100	-0.00000200

$Cl_2Be\cdots OHCH_3$			
O	0.62098800	-1.23790700	-0.19599700
H	0.11285700	-2.04399300	-0.01585300
C	2.04028100	-1.38999500	0.11168300
H	2.43712200	-2.22682900	-0.47549100
H	2.50732300	-0.44615100	-0.18407900
H	2.16917500	-1.56095400	1.18810100
Be	-0.29295700	0.16039300	-0.05390500
Cl	0.74748100	1.72651600	-0.00288400
Cl	-2.11596600	-0.32183500	0.03822600

$Cl_2Be\cdots PH_3$			
Be	0.29274700	0.22628100	-0.00010900
H	-2.33303300	-1.13900800	-1.07760900
H	-2.33194400	-1.13996700	1.07860700
H	-1.18843300	-2.63931500	-0.00071700
P	-1.42214800	-1.24443300	-0.00000900
Cl	1.96180300	-0.62617300	0.00000900
Cl	-0.43152900	1.96027100	0.00000900

$Cl_2Be\cdots CO$			
Be	-0.00002900	-0.31732800	-0.00000500
C	0.00014300	1.61883600	0.00002700
O	0.00024600	2.76106300	0.00004600
Cl	1.77143200	-0.89816100	-0.00001500
Cl	-1.77159200	-0.89785200	-0.00001500

$Cl_2Be\cdots O(CH_2)_2$			
O	1.15002200	0.00000000	-0.00006300
C	1.96722100	-1.20319100	0.00001700
H	2.59406200	-1.19954900	0.90371500
H	1.28069900	-2.05437700	-0.00003400
H	2.59421100	-1.19955700	-0.90357800
Be	-0.52420200	0.00000000	-0.00002000
C	1.96722100	1.20319200	-0.00003600

H	1.28069800	2.05437700	-0.00010900
H	2.59407200	1.19958200	0.90365500
H	2.59419900	1.19952700	-0.90363800
Cl	-1.28376400	1.72941600	-0.00001700
Cl	-1.28376300	-1.72941700	0.00005800

$H_2Be•••OH_2$			
Be	-0.03976500	1.10177700	0.00000000
H	0.26756500	-1.11564800	0.78834600
H	0.26756500	-1.11564800	-0.78834600
O	-0.03976500	-0.64827500	0.00000000
H	-0.02897300	1.50519300	-1.30422700
H	-0.02897300	1.50519300	1.30422700

$H_2Be•••SH_2$			
Be	1.72955100	0.00000000	0.02903700
S	-0.58289100	0.00000000	-0.10684500
H	-0.88616600	0.99013000	0.76062700
H	-0.88616500	-0.99012900	0.76062800
H	2.09018800	-1.30831400	0.03605800
H	2.09018900	1.30831400	0.03605800

$H_2Be•••NH_3$			
Be	1.14586300	0.00113100	0.00006900
N	-0.66853400	0.01040100	-0.00004000
H	-1.02431500	-0.49421800	0.81464800
H	-1.02423700	-0.49460800	-0.81451900
H	-1.08787500	0.94057600	-0.00027900
H	1.65551600	1.27369300	-0.00013100
H	1.57719700	-1.30277200	0.00028400

$H_2Be•••NCH$			
C	-1.30322800	-0.00000800	-0.00009800
H	-2.38150500	0.00000400	-0.00042500
N	-0.12963000	0.00000100	0.00025900
Be	1.70836100	-0.00000100	-0.00009900
H	2.13747700	-1.29258900	-0.00020200
H	2.13736300	1.29263400	-0.00020200

$H_2Be•••OCH_2$			
O	-0.08641200	-0.53189300	-0.00001600
C	-1.06888900	0.21858600	0.00000600
H	-2.08001300	-0.22038900	-0.00013200
H	-0.93431300	1.31356600	-0.00002500
Be	1.56821200	0.24127200	0.00005500
H	1.30641600	1.58843200	0.00005900

H	2.53969500	-0.70306800	-0.00003200

$H_2Be•••NH_2CH_3$			
Be	-1.63008700	0.40522800	-0.00003500
N	-0.08833200	-0.52069200	-0.00010800
H	-0.11556500	-1.14940500	-0.80755500
H	-0.11602200	-1.14919800	0.80749700
H	-1.40006400	1.75919100	-0.00028800
H	-2.68500400	-0.47698800	0.00046500
C	1.17270200	0.26580900	0.00008600
H	1.17780500	0.91065000	-0.88708700
H	1.17634500	0.91253400	0.88588400
H	2.06496800	-0.37770000	0.00146300

$H_2Be•••OHCH_3$			
O	-0.11297700	-0.42582800	-0.07346800
H	-0.07596600	-1.37511200	0.10518300
C	1.18825800	0.21089600	0.02913500
H	1.86523900	-0.21493700	-0.72299100
H	1.00530100	1.27157100	-0.16961300
H	1.59404300	0.07710300	1.04086300
Be	-1.64314100	0.33619500	0.01797500
H	-1.46020400	1.69051900	-0.05526000
H	-2.58157900	-0.65267400	0.14285600

$H_2Be•••PH_3$			
Be	-1.80819000	0.00231500	-0.00003500
H	1.15449700	-0.67874800	-1.06769200
H	1.15443600	-0.67820800	1.06808500
H	1.34544800	1.17542600	-0.00026500
P	0.53122300	0.01513300	0.00000300
H	-2.10309200	-1.32717400	0.00022000
H	-2.28686900	1.27245000	-0.00024600

$H_2Be•••CO$			
Be	1.79884400	0.00000100	0.00008500
C	-0.17086900	-0.00000100	0.00000500
O	-1.31472500	0.00000000	-0.00004500
H	2.17382200	-1.30281400	-0.00000300
H	2.17381500	1.30281700	-0.00000300

$H_2Be•••O(CH_3)_2$			
O	-0.13792000	0.00000000	-0.00005800
C	0.66369700	-1.20319700	0.00004400
H	1.29431200	-1.21840400	0.90243500
H	-0.03946300	-2.04177200	-0.00000900

H	1.29448500	-1.21843300	-0.90222400
Be	-1.84636400	0.00000000	-0.00004900
C	0.66369700	1.20319700	-0.00001500
H	-0.03946400	2.04177200	-0.00010200
H	1.29431700	1.21844500	0.90237100
H	1.29447900	1.21839200	-0.90228800
H	-2.28711000	1.29615600	0.00012100
H	-2.28710900	-1.29615600	0.00018200

5. Magnesium Bonded Complexes

$F_2Mg•••OH_2$			
Mg	-0.05420400	-0.38102500	-0.00063300
F	1.66454600	-0.90106600	0.00034800
F	-1.83815400	-0.56968500	0.00041400
O	0.20295600	1.66968500	-0.00113900
H	-0.47839400	2.35265700	0.00523200
H	1.06766300	2.09893500	0.00461000

$F_2Mg•••SH_2$			
Mg	0.88009700	0.00013100	-0.02881300
F	1.21420100	-1.75820500	0.02209800
F	1.21313800	1.75867500	0.02209900
H	-1.95064400	-0.99025400	0.80190000
S	-1.78161200	-0.00033700	-0.10346900
H	-1.95076600	0.98983800	0.80159600

$F_2Mg•••NH_3$			
N	0.63298800	1.69511900	-0.00006100
H	0.35010900	2.24421700	-0.81323800
H	1.65416100	1.66345500	-0.00025700
H	0.35042900	2.24415600	0.81326900
Mg	-0.14418700	-0.34970700	0.00001700
F	-1.93699500	-0.22033500	0.00015300
F	1.37528800	-1.31535100	-0.00010300

$F_2Mg•••NCH$			
C	-2.64390500	0.00005400	0.00004300
H	-3.72229400	0.00000700	-0.00013800
N	-1.47008100	0.00010200	0.00023700
F	1.16766200	-1.74035100	-0.00000900
F	1.16785700	1.74026200	-0.00014900
Mg	0.73805200	-0.00002000	-0.00003000

$F_2Mg\bullet\bullet\bullet OCH_2$			
O	1.03803300	-1.03418700	-0.00045800
C	2.13998200	-0.46945600	-0.00031400
H	3.05620700	-1.08392500	0.00055900
H	2.20017800	0.63218200	0.00125200
F	-2.24562900	-0.70737600	0.00052300
F	0.24752500	1.73321800	-0.00020600
Mg	-0.70146700	0.19244900	0.00007400

$F_2Mg\bullet\bullet\bullet C_2H_4$			
C	-1.77980100	-0.00421600	-0.67869400
H	-1.79458800	0.93589300	-1.23827500
H	-1.79305400	-0.94356700	-1.23956300
C	-1.77978800	-0.00509400	0.67872100
H	-1.79300100	-0.94516000	1.23838700
H	-1.79459200	0.93430000	1.23950600
F	1.07739700	1.76067000	0.00021200
F	1.09025700	-1.75472000	-0.00022700
Mg	0.75199000	0.00173700	-0.00000700

$F_2Mg\bullet\bullet\bullet OHCH_3$			
O	-0.90977500	-0.88879300	-0.00239900
H	-0.92729500	-1.85414400	0.00006700
C	-2.25810100	-0.33660000	0.00143200
H	-2.78943600	-0.65832800	0.90705200
H	-2.12494600	0.75074400	-0.00125700
H	-2.79597200	-0.66221400	-0.89891000
F	2.16083800	-0.92477700	0.00103600
F	0.04675500	1.88180000	-0.00008200
Mg	0.79967700	0.24505600	-0.00041200

$F_2Mg\bullet\bullet\bullet PH_3$			
F	-1.50402600	-1.65116800	0.00000000
F	-1.07784500	1.83064000	0.00000000
H	2.48573600	0.50579500	1.06726100
H	2.48570900	0.50539600	-1.06750900
H	2.48684600	-1.35606600	0.00021800
P	1.79591300	-0.12020300	0.00000200
Mg	-0.93001200	0.04438900	0.00000000

$F_2Mg\bullet\bullet\bullet CO$			
F	-1.14281800	-1.76412900	0.00029300
F	-1.14414300	1.76357300	0.00043800
C	1.56145900	0.00084200	0.00089600
O	2.70487100	0.00025800	-0.00027900
Mg	-0.86875600	-0.00017600	-0.00081000

$F_2Mg\bullet\bullet\bullet O(CH_3)_2$			
O	0.94341800	-0.00000100	-0.00006700
C	1.73848300	-1.20618400	0.00001900
H	2.37046600	-1.22870900	0.90168400
H	1.03144700	-2.04444800	-0.00003200
H	2.37062500	-1.22872900	-0.90153400
F	-1.48612200	1.75832400	0.00003300
F	-1.48612800	-1.75832000	0.00002900
C	1.73848500	1.20618100	-0.00003800
H	1.03145000	2.04444500	-0.00007100
H	2.37050800	1.22872100	0.90159800
H	2.37058700	1.22870900	-0.90161900
Mg	-1.10033200	0.00000100	0.00000600

$Cl_2Mg\bullet\bullet\bullet OH_2$			
Mg	0.00006600	-0.11695100	0.00004100
O	-0.00031800	1.93780700	-0.00055600
H	0.78550300	2.49983800	0.00178700
H	-0.78654700	2.49927100	0.00177500
Cl	2.19849500	-0.56159400	0.00001200
Cl	-2.19833100	-0.56182800	0.00001200

$Cl_2Mg\bullet\bullet\bullet SH_2$			
Mg	-0.00004100	-0.51429200	-0.03936600
H	-0.99187000	2.30965300	0.80154800
S	0.00013700	2.13469500	-0.10127200
H	0.99219000	2.30948200	0.80153000
Cl	-2.19317500	-0.95880500	0.01440800
Cl	2.19305600	-0.95900400	0.01439700

$Cl_2Mg\bullet\bullet\bullet NH_3$			
N	-0.03322400	2.10161600	0.00012100
H	0.43438000	2.50795100	0.81309100
H	-0.99425500	2.44979800	0.00027700
H	0.43415600	2.50806500	-0.81292100
Mg	0.00625600	-0.07038300	-0.00003700
Cl	2.18707300	-0.61488400	-0.00024200
Cl	-2.17041400	-0.63997000	0.00019300

$Cl_2Mg\bullet\bullet\bullet NCH$			
C	0.00017700	-3.01068400	-0.00008100
H	0.00027100	-4.08935100	0.00050400
N	0.00007000	-1.83687400	-0.00070700

Mg	-0.00002300	0.35203200	-0.00000900
Cl	-2.17081400	0.90541500	0.00001000
Cl	2.17072200	0.90559700	0.00028700

$Cl_2Mg{\bullet\bullet\bullet}OCH_2$			
O	0.62528000	1.67866600	0.00017900
C	1.85002300	1.85112400	0.00040900
H	2.24595400	2.88062700	0.00050400
H	2.54146700	0.99075100	0.00048600
Mg	-0.31646000	-0.21106100	-0.00006600
Cl	-2.53933200	-0.01379600	-0.00041400
Cl	1.53390400	-1.50824700	0.00017400

$Cl_2Mg{\bullet\bullet\bullet}C_2H_4$			
C	-0.00169500	2.11294900	0.67937100
H	-0.94201300	2.12698800	1.23896300
H	0.93831200	2.12983900	1.23939500
C	-0.00140600	2.11296800	-0.67937800
H	0.93883600	2.12986400	-1.23900500
H	-0.94148900	2.12702800	-1.23936500
Mg	0.00042200	-0.40727300	-0.00003500
Cl	2.19072200	-0.85151700	0.00016300
Cl	-2.18955200	-0.85330300	-0.00013500

$Cl_2Mg{\bullet\bullet\bullet}OHCH_3$			
O	0.33102700	1.54282600	-0.00031800
H	-0.34122300	2.23881500	0.00017100
C	1.67620600	2.10166700	0.00068300
H	1.82541700	2.70576700	0.90508000
H	2.35349200	1.24080700	-0.00009200
H	1.82588100	2.70781000	-0.90226600
Mg	-0.28064100	-0.40050600	0.00010200
Cl	-2.51074000	-0.12328200	-0.00007100
Cl	1.62830800	-1.58493800	-0.00026300

$Cl_2Mg{\bullet\bullet\bullet}PH_3$			
H	-1.34004600	2.54673900	1.07000600
H	-1.34021700	2.54672900	-1.06981600
H	0.43348400	3.13719300	-0.00005100
P	-0.52784600	2.09787900	0.00003300
Mg	0.15448500	-0.52039700	-0.00001400
Cl	2.39195200	-0.55638800	-0.00028000
Cl	-1.90309000	-1.41149900	0.00025300

$Cl_2Mg\cdots CO$			
C	-0.00046200	1.90133700	0.00000500
O	-0.00081000	3.04481400	0.00014200
Mg	0.00015100	-0.51184100	-0.00003000
Cl	-2.19960900	-0.87174000	-0.00009000
Cl	2.20004700	-0.87087400	0.00004200

$Cl_2Mg\cdots O(CH_3)_2$			
O	0.33102700	1.54282600	-0.00031800
H	-0.34122300	2.23881500	0.00017100
C	1.67620600	2.10166700	0.00068300
H	1.82541700	2.70576700	0.90508000
H	2.35349200	1.24080700	-0.00009200
H	1.82588100	2.70781000	-0.90226600
Mg	-0.28064100	-0.40050600	0.00010200
Cl	-2.51074000	-0.12328200	-0.00007100
Cl	1.62830800	-1.58493800	-0.00026300

$H_2Mg\cdots OH_2$			
Mg	-0.90820300	0.00001100	0.00000700
O	1.22492600	-0.00003500	-0.00043300
H	1.79339700	-0.78055700	0.00149400
H	1.79322700	0.78061200	0.00149300
H	-1.24398300	-1.70135500	0.00019900
H	-1.24361900	1.70145500	0.00019900

$H_2Mg\cdots SH_2$			
Mg	1.57936900	0.00000000	0.00490900
H	-1.46134300	-0.98604700	0.78943300
S	-1.23536500	-0.00000100	-0.10620700
H	-1.46131900	0.98605100	0.78943300
H	1.86805700	-1.70139100	0.03076600
H	1.86802000	1.70139900	0.03076300

$H_2Mg\cdots NH_3$			
N	1.30325800	0.00312300	0.00009600
H	1.69219300	-0.47788800	0.81321100
H	1.69045100	0.94799400	0.00025100
H	1.69231100	-0.47766800	-0.81309300
Mg	-0.95472400	-0.00074300	-0.00006800
H	-1.36169200	-1.69204100	-0.00027700
H	-1.37937800	1.68665800	0.00005600

$H_2Mg\cdots NCH$			
C	-2.02195200	0.00000300	-0.00000400

H	-3.10000100	0.00004500	-0.00012100
N	-0.84584300	-0.00002200	0.00012300
Mg	1.45717300	0.00000600	-0.00004000
H	1.83323800	1.68921500	-0.00021300
H	1.83329400	-1.68919100	-0.00002300

$H_2Mg\cdots OCH_2$			
O	0.72979900	-0.59054100	-0.00024700
C	1.63749700	0.24628700	-0.00013500
H	2.68973400	-0.08924100	-0.00050700
H	1.40498600	1.32703300	0.00008100
Mg	-1.36549700	0.11803600	0.00036600
H	-0.91153300	1.80455100	-0.00069900
H	-2.46060100	-1.21216600	-0.00048200

$H_2Mg\cdots C_2H_4$			
C	-1.29042100	-0.67774800	0.00002000
H	-1.29926800	-1.25006800	-0.93141000
H	-1.29889700	-1.25005100	0.93146500
C	-1.29041900	0.67774500	0.00001000
H	-1.29889300	1.25006300	0.93144600
H	-1.29926500	1.25005100	-0.93142900
Mg	1.43797900	0.00000100	-0.00001800
H	1.71282600	-1.70066600	-0.00003500
H	1.71278200	1.70067600	0.00000100

$H_2Mg\cdots OHCH_3$			
O	-0.52200600	-0.51473400	0.00004900
H	-0.73180700	-1.45813700	0.00012400
C	-1.73378500	0.28342500	0.00002700
H	-2.32503600	0.07628800	0.90276800
H	-1.39904900	1.32692000	-0.00005900
H	-2.32509100	0.07615600	-0.90264700
Mg	1.47891500	0.15500100	-0.00005500
H	2.35788700	-1.34257100	0.00006000
H	1.25487100	1.87864600	-0.00013700

$H_2Mg\cdots PH_3$			
H	-1.88185600	-0.65878400	1.05987400
H	-1.88191000	-0.65898300	-1.05962700
H	-2.02772500	1.18164900	-0.00004500
P	-1.21959500	0.01493000	0.00004400
Mg	1.67760500	-0.00346900	-0.00005800
H	1.87379600	-1.71986700	0.00009700
H	2.08036600	1.67365700	-0.00025300

$H_2Mg\cdots CO$			
C	-0.99395200	-0.00044500	-0.00041500
O	-2.13986300	0.00018300	0.00033600
Mg	1.61607600	0.00007700	-0.00000400
H	1.84530000	-1.70476300	-0.00005400
H	1.84440500	1.70504200	-0.00009400

$H_2Mg\cdots O(CH_3)_2$			
O	0.36724000	0.00000000	0.00001700
C	1.17199400	1.19724800	0.00010200
H	1.80527500	1.21801500	-0.90142500
H	0.47574000	2.04425200	-0.00000200
H	1.80504900	1.21804400	0.90178800
C	1.17199400	-1.19724800	0.00012200
H	0.47574000	-2.04425200	0.00003200
H	1.80527500	-1.21803000	-0.90140400
H	1.80504900	-1.21802900	0.90180800
Mg	-1.74504100	0.00000000	-0.00028200
H	-2.11674500	1.69779400	0.00053600
H	-2.11674600	-1.69779400	0.00056400

6. Calcium Bonded Complexes

$F_2Ca\cdots OH_2$			
F	1.26696900	1.34039700	0.00001000
F	-2.38821900	-0.21915200	0.00001600
O	1.66994200	-1.12511800	0.00000200
H	2.38180400	-1.76695100	0.00003200
H	2.03369800	-0.20474600	0.00001400
Ca	-0.38418900	0.04407200	-0.00001500

$F_2Ca\cdots SH_2$			
F	-0.25276100	1.84418600	0.05831000
F	2.60204700	-0.84399300	0.07632800
H	-2.21993900	-0.84222600	1.25023100
H	-1.84987900	0.67497000	0.05725100
Ca	0.81684500	0.08418700	-0.06943300
S	-2.08816600	-0.65738900	-0.07066000

$F_2Ca\cdots NH_3$			
N	1.76372700	-1.23903700	0.00001300
H	2.08059200	-1.76003700	0.81207600
H	2.25272200	-0.34044200	0.00009400
H	2.08065700	-1.75992400	-0.81209700
F	-2.33401700	-0.42513200	-0.00014600
F	1.07377200	1.57862500	0.00014900

Ca	-0.37089300	0.10761100	-0.00001000

$F_2Ca•••NCH$			
C	3.05342300	-0.00002000	0.00002700
H	4.12314800	-0.00002300	0.00003800
N	1.89315700	-0.00001800	0.00001000
F	-1.26354000	1.93861500	-0.00001100
F	-1.26359700	-1.93859200	-0.00001100
Ca	-0.64757800	0.00000300	-0.00000300

$F_2Ca•••CO$			
F	-1.23310900	-1.97240100	0.00068300
F	-1.23175200	1.97290600	0.00082500
C	2.02237400	-0.00040000	-0.00019300
O	3.15376200	-0.00048800	0.00031400
Ca	-0.75903000	0.00008800	-0.00074600

$F_2Ca•••OCH_2$			
O	1.44719600	-1.12480100	-0.00007100
C	2.46503500	-0.44379100	0.00002700
H	3.44464200	-0.93893700	0.00005900
H	2.39471200	0.65146800	0.00008500
F	-2.59932200	-0.59213100	-0.00006000
F	0.55001500	1.73177000	0.00014000
Ca	-0.68816900	0.08459400	-0.00002300

$F_2Ca•••C_2H_4$			
C	-2.18433400	-0.00457100	-0.66878400
H	-2.20269300	0.92509200	-1.22851600
H	-2.20126700	-0.93302800	-1.23054300
C	-2.18433200	-0.00600100	0.66878300
H	-2.20123200	-0.93564500	1.22857400
H	-2.20272000	0.92247600	1.23048400
F	1.17777700	1.97129800	0.00024000
F	1.19299400	-1.96478800	-0.00024100
Ca	0.68414800	0.00129800	0.00000100

$F_2Ca•••OHCH_3$			
O	-1.26420500	-1.08316100	-0.00000900
H	-1.43865200	-2.03018200	-0.00002400
C	-2.51926600	-0.36173700	0.00001000
H	-3.09178100	-0.60804800	0.89389500
H	-2.25465000	0.69383700	0.00000600
H	-3.09180700	-0.60804900	-0.89385800
F	2.54078000	-0.81204500	0.00000900
F	-0.32199700	1.91912800	0.00000000

Ca	0.75685400	0.17122000	-0.00000400

$F_2Ca•••PH_3$			
F	-2.68905500	-0.83078800	0.00000100
F	0.25341000	1.78668900	0.00000100
H	2.66349100	0.13049200	1.05391500
H	2.66347000	0.13049200	-1.05392500
H	2.97654300	-1.67608600	-0.00000700
P	2.08130600	-0.59011400	0.00000100
Ca	-0.88011500	0.08318500	-0.00000100

$F_2Ca•••O(CH_3)_2$			
O	1.25450900	-0.17294300	0.00000300
C	2.10089400	0.98248200	-0.00001400
H	2.73100000	0.98010000	-0.89307000
H	1.44605900	1.85310000	-0.00003300
H	2.73099200	0.98013300	0.89304800
C	1.99266400	-1.39348500	0.00003000
H	1.27129900	-2.20924400	0.00004200
H	2.62065500	-1.45257100	-0.89271500
H	2.62064600	-1.45253700	0.89278400
Ca	-1.07913100	0.09296600	-0.00000700
F	-1.03730400	2.14582400	-0.00004500
F	-1.89997000	-1.78012800	0.00004100

$Cl_2Ca•••OH_2$			
O	0.92039300	1.99007700	0.00010300
H	0.84661200	2.94868800	0.00008100
H	1.86051100	1.74969500	0.00013000
Ca	-0.16461700	-0.09162500	-0.00000400
Cl	-2.64256800	-0.25819100	-0.00011700
Cl	2.24386600	-0.84689700	0.00006100

$Cl_2Ca•••SH_2$			
H	-0.98498500	2.43560600	0.81687700
H	0.98450000	2.43583000	0.81694400
Ca	0.00005900	-0.59897800	-0.16573900
S	-0.00019900	2.32513200	-0.08716500
Cl	2.45735200	-0.88498200	0.09046000
Cl	-2.45720600	-0.88525200	0.09045900

$Cl_2Ca•••NH_3$			
N	-0.48741700	2.25575700	0.00000000
H	-0.18713600	2.79092900	0.81102400
H	-1.50649800	2.25992700	0.00000200
H	-0.18714200	2.79091500	-0.81103600

Ca	0.08248600	-0.16339900	0.00000400
Cl	2.56251500	-0.42409100	-0.00000200
Cl	-2.34822300	-0.77379600	-0.00000200

$Cl_2Ca\bullet\bullet\bullet NCH$			
C	0.00006900	-3.28477200	0.00003300
H	0.00009700	-4.35474000	0.00004800
N	0.00004000	-2.12494600	0.00001900
Ca	-0.00000900	0.36266600	-0.00000800
Cl	2.42368500	0.93193900	-0.00000300
Cl	-2.42372000	0.93186600	-0.00001000

$Cl_2Ca\bullet\bullet\bullet CO$			
C	-0.00116500	2.15377100	-0.00004200
O	-0.00187800	3.28480500	-0.00000600
Ca	0.00034400	-0.55819300	-0.00003500
Cl	2.46762400	-0.82366100	0.00001500
Cl	-2.46673400	-0.82558600	0.00004400

$Cl_2Ca\bullet\bullet\bullet OCH_2$			
O	1.03243200	1.77209800	0.00004800
C	2.25453200	1.80401000	0.00002200
H	2.77153100	2.77128600	0.00004700
H	2.83951200	0.87643500	-0.00002700
Ca	-0.38389600	-0.16911800	-0.00000100
Cl	-2.85043800	0.10099400	0.00014600
Cl	1.69045200	-1.58724200	-0.00017600

$Cl_2Ca\bullet\bullet\bullet C_2H_4$			
C	-0.00379700	2.35069400	0.66942200
H	-0.93450000	2.36691600	1.22815100
H	0.92679900	2.37163800	1.22815700
C	-0.00382300	2.35069400	-0.66942300
H	0.92675200	2.37163800	-1.22819400
H	-0.93454700	2.36691500	-1.22811600
Ca	0.00094200	-0.46350000	0.00000000
Cl	2.45756100	-0.83359800	0.00000300
Cl	-2.45506800	-0.83789800	-0.00000200

$Cl_2Ca\bullet\bullet\bullet OHCH_3$			
O	-0.18165800	1.73094600	-0.00000400
H	0.57147200	2.33508700	-0.00000300
C	-1.42099000	2.46601900	0.00000200
H	-1.49243600	3.08424100	-0.89424400
H	-2.21536200	1.72367500	-0.00000400
H	-1.49243600	3.08422700	0.89425900

Ca	0.23155400	-0.55015900	-0.00000100
Cl	-2.12980900	-1.37742400	0.00000000
Cl	2.71668500	-0.26185400	0.00000100

$Cl_2Ca•••PH_3$			
H	-2.52260900	1.70588600	1.05594700
H	-2.52270200	1.70581700	-1.05580700
H	-1.49146600	3.22994800	-0.00002800
P	-1.60570100	1.82927900	0.00002600
Ca	0.45465200	-0.37754000	0.00000500
Cl	-1.58904300	-1.80886300	0.00024800
Cl	2.85546900	0.24827300	-0.00028400

$Cl_2Ca•••O(CH_3)_2$			
O	0.00000000	1.56485200	-0.00000400
C	-1.18770700	2.36816800	-0.00002400
H	-1.20669100	2.99660600	-0.89352500
H	-2.03861100	1.68935500	-0.00003700
H	-1.20672100	2.99660700	0.89347600
C	1.18770700	2.36816800	0.00001500
H	2.03861100	1.68935500	0.00002900
H	1.20672100	2.99660700	-0.89348500
H	1.20669200	2.99660600	0.89351600
Ca	0.00000000	-0.75941600	0.00000100
Cl	-2.46124800	-1.20922500	-0.00008000
Cl	2.46124800	-1.20922500	0.00008600

$H_2Ca•••SH_2$			
H	1.85361700	0.98061200	0.79247000
H	1.85362700	-0.98060200	0.79248400
Ca	-1.34878400	0.00000100	-0.01622000
S	1.66718300	-0.00000200	-0.10240700
H	-1.70326400	-2.00648600	0.18897900
H	-1.70322200	2.00649600	0.18898000

$H_2Ca•••NH_3$			
N	1.73011800	-0.08211400	0.00000000
H	2.19020800	-0.48525400	0.81207000
H	1.94569100	0.91388500	0.00000600
H	2.19020900	-0.48524300	-0.81207500
Ca	-0.79662300	0.01740900	0.00000000
H	-1.76141200	-1.79678500	0.00000100
H	-0.74306200	2.08002000	0.00000100

$H_2Ca•••NCH$			
C	2.49388800	-0.00000700	0.00002200

H	3.56353200	-0.00003200	0.00004900
N	1.33342900	0.00002000	-0.00000600
Ca	-1.21573800	-0.00000300	-0.00000600
H	-1.77307100	1.97143400	-0.00000400
H	-1.77304400	-1.97144700	-0.00001100

$H_2Ca•••CO$			
C	-1.47825000	-0.00003600	-0.00000800
O	-2.61020200	-0.00000200	0.00000300
Ca	1.32682100	0.00000800	0.00000200
H	1.60751700	-2.02719000	-0.00000300
H	1.60718400	2.02725400	-0.00000600

$H_2Ca•••OCH_2$			
O	1.17784900	-0.60939400	-0.00011600
C	2.06381100	0.23338800	-0.00000800
H	3.11472900	-0.08253100	-0.00007600
H	1.81347900	1.30170300	0.00015400
Ca	-1.17669500	0.07335900	0.00003600
H	-2.75937900	-1.21720200	-0.00005500
H	-0.44059000	2.00568000	0.00023700

$H_2Ca•••C_2H_4$			
C	-1.70659300	-0.00174000	-0.66856100
H	-1.72065900	0.92585000	-1.23163000
H	-1.72233800	-0.93210000	-1.22698200
C	-1.70659300	0.00162700	0.66856100
H	-1.72233900	-0.92590800	1.23166100
H	-1.72065800	0.93204100	1.22695100
Ca	1.20572200	0.00000800	0.00000000
H	1.62675400	-2.00186100	0.00500300
H	1.62390800	2.00249100	-0.00500500

$H_2Ca•••OHCH_3$			
O	-0.98458000	-0.58519000	0.00004100
H	-1.29765300	-1.49677200	0.00009000
C	-2.10732100	0.31963200	0.00002700
H	-2.71216200	0.17167200	0.89437100
H	-1.68662000	1.32259500	-0.00002400
H	-2.71220100	0.17159800	-0.89427900
Ca	1.28140200	0.10385700	-0.00002800
H	0.88518700	2.12987600	-0.00009800
H	2.41598200	-1.61238500	0.00000800

$H_2Ca•••PH_3$			
H	2.28901100	0.66893300	1.05154600

H	2.28894600	0.66906000	-1.05153900
H	2.56684600	-1.14001000	-0.00011700
P	1.68710800	-0.04342700	-0.00002100
Ca	-1.43708200	0.01188800	0.00002000
H	-1.41884500	2.06210000	0.00029900
H	-2.29092400	-1.84644700	-0.00028000

$H_2Ca•••O(CH_3)_2$			
O	-0.77422000	0.00000000	0.00001100
C	-1.56968000	1.18753400	0.00004300
H	-2.19880600	1.21459800	0.89340300
H	-0.88403600	2.03356500	0.00005500
H	-2.19882100	1.21463600	-0.89330500
C	-1.56968000	-1.18753400	-0.00000600
H	-0.88403600	-2.03356500	-0.00002900
H	-2.19880500	-1.21463500	0.89335300
H	-2.19882200	-1.21459900	-0.89335400
Ca	1.58154000	0.00000000	-0.00001900
H	1.98122700	2.02318600	0.00001300
H	1.98122700	-2.02318600	-0.00006300

$H_2Ca•••CH_3CN$			
C	1.72606700	-0.00162700	0.00111200
N	0.56266400	-0.00392900	0.00293900
Ca	-1.94389100	0.00076600	-0.00033600
H	-2.54591600	1.96260700	-0.00244400
H	-2.56034200	-1.95652800	-0.00250800
C	3.17666500	0.00157200	-0.00166500
H	3.54514200	-0.15715300	1.01171900
H	3.54360700	-0.79682500	-0.64649200
H	3.54029500	0.96041200	-0.37082400

7. Boron Bonded Complexes

$F_3B•••OH_2$			
B	0.27369500	0.00000200	-0.04393200
F	0.92392400	-0.00001900	1.15393200
F	0.30420000	1.17215600	-0.76966800
F	0.30420700	-1.17212700	-0.76971000
O	-1.43261200	-0.00000900	0.45022400
H	-1.84928200	0.77689900	0.04343400
H	-1.84927400	-0.77692700	0.04344600

$F_3B{\bullet\bullet\bullet}SH_2$			
B	1.02324500	0.00000000	-0.00799800
F	1.10850800	1.16243200	0.65644600
F	1.03001900	-0.00000600	-1.35178500
F	1.10850400	-1.16242700	0.65645600
S	-1.89302800	0.00000100	0.12441400
H	-2.02553600	0.97533300	-0.80034100
H	-2.02552500	-0.97532900	-0.80034500

$F_3B{\bullet\bullet\bullet}NH_3$			
B	-0.19643800	0.00000600	0.00000600
F	-0.54251700	1.08945600	0.80490700
F	-0.54258500	-1.24178600	0.54102000
F	-0.54251800	0.15236800	-1.34594600
N	1.45714900	-0.00003500	0.00001500
H	1.81025700	0.87818500	-0.38261100
H	1.81022500	-0.77051800	-0.56924100
H	1.81024600	-0.10779200	0.95189200

$F_3B{\bullet\bullet\bullet}NCH$			
B	0.86577800	-0.00000500	-0.00000700
F	0.95456500	0.23622100	1.32070000
F	0.95453000	1.02564600	-0.86493900
F	0.95447300	-1.26189000	-0.45577900
H	-3.73988000	0.00000200	0.00002900
C	-2.66233000	0.00002200	0.00001800
N	-1.48387700	0.00001400	0.00000800

$F_3B{\bullet\bullet\bullet}CO$			
B	1.02418300	0.00000100	-0.00000100
F	1.05711000	1.18779900	-0.61823900
F	1.05712400	-1.12931000	-0.71954000
F	1.05711100	-0.05848500	1.33778300

C	-1.74830900	-0.00000600	-0.00000500
O	-2.89664600	-0.00000100	0.00000000

$F_3B{\bullet\bullet\bullet}OCH_2$

B	-0.61141000	0.06315200	-0.00000100
F	-1.09366300	-0.44603800	1.17060600
F	-1.09365100	-0.44604400	-1.17061100
F	-0.29008500	1.40519900	-0.00000200
C	2.03245700	0.00934300	0.00000100
H	1.94552500	1.10691300	-0.00001300
H	3.02185400	-0.47233600	0.00000900
O	1.02394000	-0.70305700	0.00000700

$F_3B{\bullet\bullet\bullet}C_2H_4$

B	-0.93412100	0.00000100	0.00810500
F	-0.90166200	-0.00001100	1.34800900
F	-1.01372100	-1.16020500	-0.65764200
F	-1.01371300	1.16021900	-0.65762200
C	1.93939000	0.67555700	-0.02106200
H	1.83963200	1.24278600	0.90807200
H	2.04027200	1.24329200	-0.94931100
C	1.93938800	-0.67556100	-0.02106300
H	2.04026700	-1.24329300	-0.94931400
H	1.83962800	-1.24279300	0.90806900

$F_3B{\bullet\bullet\bullet}OHCH_3$

B	-0.62099800	0.08318800	0.01922700
F	-1.52406100	-0.92552600	-0.24761600
F	-0.60810700	1.16167700	-0.83576400
F	-0.47388000	0.39739700	1.36288400
C	2.03361300	0.04871100	0.00479500
H	2.04091900	0.23059900	1.08624800
H	2.90564100	-0.53152400	-0.31840700

H	1.97088100	0.99186200	-0.54635500
O	0.82830000	-0.69339600	-0.36801400
H	0.81390100	-1.55390100	0.08218000

$F_3B{\bullet\bullet\bullet}PH_3$			
B	-1.11193300	0.00000200	0.00000000
F	-1.16289400	-1.14180200	-0.70223000
F	-1.16287300	1.17905300	-0.63771600
F	-1.16288300	-0.03724500	1.33994600
H	2.67326700	-1.06718500	0.57720300
H	2.67323100	1.03347400	0.63561800
H	2.67325500	0.03373300	-1.21281400
P	1.92918400	-0.00000600	-0.00000100

$F_3B{\bullet\bullet\bullet}O(CH_3)_2$			
B	-0.81655000	0.00000100	0.02407700
F	-1.29086300	-1.17143900	-0.53269700
F	-1.29085800	1.17144400	-0.53269500
F	-0.75277900	-0.00000200	1.41322000
C	1.49052700	1.20315200	-0.01358700
H	1.54354000	1.22153200	1.08453800
H	2.49338700	1.18168700	-0.45954300
H	0.90992500	2.04919200	-0.39227100
O	0.78915900	0.00000000	-0.44415200
C	1.49052200	-1.20315600	-0.01358900
H	1.54353300	-1.22154000	1.08453600
H	0.90991800	-2.04919300	-0.39227700
H	2.49338400	-1.18169300	-0.45954300

$Cl_3B{\bullet\bullet\bullet}OH_2$			
B	0.00000100	-0.02590000	0.04155300
O	0.00000400	-0.01631900	1.74320200
H	0.78221100	0.48717600	2.03699500

H	-0.78222100	0.48714900	2.03699200
Cl	-0.00007400	1.75186900	-0.40197000
Cl	1.54449500	-0.89688000	-0.33511600
Cl	-1.54442300	-0.89700600	-0.33511100

$Cl_3B{\bullet\bullet\bullet}SH_2$

B	0.78749900	0.00000000	0.01870100
S	-2.55941300	-0.00000100	-0.17645000
H	-2.65269000	-0.97493300	0.75339700
H	-2.65269000	0.97492700	0.75340100
Cl	0.87803800	-1.52226500	-0.85298500
Cl	0.73325000	-0.00000500	1.77789600
Cl	0.87803500	1.52227000	-0.85297600

$Cl_3B{\bullet\bullet\bullet}NH_3$

B	0.00000000	0.00000000	-0.10490900
N	-0.00000100	0.00000000	-1.72743400
H	-0.43038600	-0.85987600	-2.07948900
H	-0.52948300	0.80266200	-2.07948900
H	0.95986500	0.05721400	-2.07949000
Cl	0.98034500	-1.48614300	0.36970700
Cl	0.79686600	1.59207500	0.36970700
Cl	-1.77721000	-0.10593200	0.36970800

$Cl_3B{\bullet\bullet\bullet}NCH$

B	0.00000000	0.00000000	-0.10490900
N	-0.00000100	0.00000000	-1.72743400
H	-0.43038600	-0.85987600	-2.07948900
H	-0.52948300	0.80266200	-2.07948900
H	0.95986500	0.05721400	-2.07949000
Cl	0.98034500	-1.48614300	0.36970700
Cl	0.79686600	1.59207500	0.36970700
Cl	-1.77721000	-0.10593200	0.36970800

$Cl_3B{\bullet\bullet\bullet}CO$			
B	-0.75817400	-0.00003700	0.00002200
C	2.45047700	0.00020900	-0.00017700
O	3.60026300	0.00012000	-0.00003600
Cl	-0.77867100	-1.11809400	-1.35389400
Cl	-0.77854500	-0.61354200	1.64524600
Cl	-0.77890700	1.73151600	-0.29127900

$Cl_3B{\bullet\bullet\bullet}OCH_2$			
B	-0.20853000	0.00000000	0.07469500
C	2.08538500	0.00000200	-1.21131600
H	2.58307700	0.00000300	-0.22983400
H	2.66102500	0.00000500	-2.14725700
O	0.84938900	-0.00000100	-1.29603600
Cl	0.85785500	0.00002900	1.55672600
Cl	-1.12034500	-1.53854800	-0.20070600
Cl	-1.12038400	1.53851800	-0.20073800

$Cl_3B{\bullet\bullet\bullet}C_2H_4$			
B	-0.69695600	0.00000000	0.03502600
C	2.53945400	0.67529000	-0.13729000
H	2.37314500	1.24337300	0.78203800
H	2.70501700	1.24336400	-1.05636000
C	2.53945500	-0.67528900	-0.13729000
H	2.70501800	-1.24336300	-1.05636000
H	2.37314600	-1.24337200	0.78203800
Cl	-0.55371900	0.00000000	1.78709600
Cl	-0.81564000	-1.52121300	-0.83410700
Cl	-0.81564100	1.52121300	-0.83410700

$Cl_3B{\bullet\bullet\bullet}OHCH_3$

B	0.23696800	0.02979800	-0.05721000
C	-2.22736400	-0.12170000	0.98082900
H	-2.47123900	-1.02564700	0.41076900
H	-2.72552100	-0.09586500	1.95655500
H	-2.44567800	0.78150400	0.40310100
O	-0.77874700	-0.07289300	1.23690800
H	-0.49406000	-0.85216900	1.74966800
Cl	-0.22765400	-1.34218200	-1.18453200
Cl	1.86146300	-0.20673100	0.74540500
Cl	-0.07229100	1.68753300	-0.73818300

$Cl_3B{\bullet\bullet\bullet}PH_3$

B	-0.85243100	-0.00000400	0.00000100
H	3.37875900	0.75422400	-0.94196400
H	3.37872500	-1.19287200	-0.18219300
H	3.37874700	0.43865700	1.12415700
P	2.61938200	0.00001400	-0.00000300
Cl	-0.88560200	1.73643400	0.26520000
Cl	-0.88558100	-0.63855400	-1.63639800
Cl	-0.88557000	-1.09789300	1.37120000

$Cl_3B{\bullet\bullet\bullet}O(CH_3)_2$

B	-0.39088400	-0.00180600	0.04064500
C	1.89353300	1.21529000	-0.43664300
H	2.12414000	1.27523500	0.63627100
H	2.80358000	1.11301600	-1.04041400
H	1.29454900	2.06770900	-0.76488500
O	1.08899200	0.01035000	-0.68469900
C	1.90688300	-1.18405700	-0.42692400
H	2.27087600	-1.15087900	0.60907800
H	1.26137600	-2.04981400	-0.59403400
H	2.73219700	-1.15887100	-1.14909200
Cl	-0.05308500	-0.07691300	1.84887700

Cl	-1.19880100	1.54941100	-0.48679900
Cl	-1.22145200	-1.49353000	-0.61155800

$HF_2B•••OH_2$

B	-0.33643700	0.00000000	0.46920500
F	-0.70136800	-1.16754400	-0.18759800
F	-0.70136700	1.16754500	-0.18759800
O	1.43843200	0.00000000	0.05115500
H	1.56025000	-0.77441600	-0.52304800
H	1.56024900	0.77441500	-0.52304900
H	-0.32115400	0.00000000	1.66759600

$HF_2B•••SH_2$

B	-1.24927900	0.00000800	0.48267300
F	-1.37857000	-1.15263100	-0.20904500
F	-1.37858400	1.15262800	-0.20901700
S	1.80996800	-0.00004300	0.08383500
H	1.62137800	-0.97508600	-0.83122400
H	1.62153800	0.97581700	-0.83038600
H	-1.14161700	-0.00005700	1.66943900

$HF_2B•••NH_3$

B	-0.22621100	0.00000000	0.44348900
F	-0.73587000	-1.17699200	-0.15597300
F	-0.73586900	1.17699300	-0.15597300
N	1.36025200	-0.00000100	-0.06894400
H	1.85791500	0.83087900	0.25324800
H	1.35929600	-0.00000100	-1.09165700
H	1.85791500	-0.83088000	0.25324900
H	-0.22018200	0.00000000	1.65783500

$HF_2B•••NCH$

B	-1.09625600	0.00000100	0.45505400
F	-1.25275000	1.15327200	-0.23102700
F	-1.25276300	-1.15326600	-0.23102900
H	3.62251500	0.00000700	-0.34245600
C	2.57283000	0.00000000	-0.09851200
N	1.42304600	-0.00000900	0.16780400
H	-0.98992000	-0.00000100	1.64213000

$HF_2B{\bullet\bullet\bullet}CO$

B	1.28818100	-0.00000200	0.46349100
F	1.36508300	1.15195200	-0.23035500
F	1.36503300	-1.15197100	-0.23034800
C	-1.66513000	0.00003900	0.17238200
O	-2.77960500	-0.00000600	-0.10734400
H	1.21567600	-0.00000600	1.65333700

$HF_2B{\bullet\bullet\bullet}OCH_2$

B	-0.79447900	0.02531800	0.45752100
F	-1.39425800	-0.85849700	-0.40397700
F	-0.61361800	1.30005100	-0.05836400
C	1.81152400	0.05786100	-0.24081300
H	1.54751400	1.04858900	-0.64520800
H	2.83898100	-0.32584300	-0.34722300
O	0.96696600	-0.63452000	0.33384000
H	-0.94809200	-0.09432800	1.64004900

$HF_2B{\bullet\bullet\bullet}C_2H_4$

B	-1.10887900	-0.13145800	0.49045000
F	-1.17854300	-1.13456200	-0.40776700
F	-1.38343300	1.11418100	0.05361400
C	1.69494300	0.59936500	-0.45437800
H	1.82508900	1.62863300	-0.11053300
H	1.31303900	0.45256900	-1.46809200

C	1.99262800	-0.45076600	0.34117000
H	1.86060700	-1.47935000	-0.00462200
H	2.37676400	-0.30448600	1.35419100
H	-0.89875000	-0.34823900	1.64342100

$HF_2B{\bullet\bullet\bullet}OHCH_3$

B	-0.68924100	0.08915800	0.41042500
F	-1.61998300	-0.84272800	-0.03673100
F	-0.75602100	1.33636000	-0.19189300
C	1.97518300	0.05783800	0.11364100
H	2.08262800	-0.05931900	1.20064600
H	2.81427300	-0.40262800	-0.42185000
H	1.88696800	1.11676500	-0.14940500
O	0.73461400	-0.55662600	-0.34272300
H	0.74277400	-1.50928300	-0.15536500
H	-0.42440300	0.07197600	1.59139600

$HF_2B{\bullet\bullet\bullet}PH_3$

B	-1.38762800	0.00000000	0.48143300
F	-1.47835400	-1.15221600	-0.21355900
F	-1.47835800	1.15221500	-0.21355900
H	2.76753200	-1.04778800	0.24865400
H	2.76751300	1.04781700	0.24860500
H	1.95919500	-0.00003100	-1.37516200
P	1.82467600	0.00000100	0.04290800
H	-1.31582800	0.00000000	1.67119300

$HF_2B{\bullet\bullet\bullet}O(CH_3)_2$

B	0.90490200	0.00000000	0.39974500
F	1.44873400	1.17027200	-0.12182400
F	1.44873400	-1.17027200	-0.12182300
C	-1.39093700	-1.20002100	0.03719800
H	-1.54616500	-1.23218900	1.12719000

H	-2.35265900	-1.17634100	-0.49289500
H	-0.78100500	-2.04617400	-0.29302800
O	-0.65171000	0.00000000	-0.31544600
C	-1.39093900	1.20002100	0.03719900
H	-1.54616600	1.23218800	1.12719100
H	-0.78100800	2.04617400	-0.29302600
H	-2.35266100	1.17633900	-0.49289400
H	0.66287900	0.00000100	1.58873500

8. Aluminium Bonded Complexes

$F_3Al•••OH_2$			
F	1.55618000	0.00001500	0.91321500
F	-0.13322400	1.44963000	-0.91669000
F	-0.13319300	-1.44963300	-0.91668900
O	-1.36486200	-0.00001100	1.03583700
H	-1.91459300	0.77926200	0.85259800
H	-1.91456900	-0.77930400	0.85262000
Al	0.24155300	0.00000200	-0.13157300

$F_3Al•••SH_2$			
F	-0.96451700	1.45114800	-0.79560200
F	-0.81177600	0.00000100	1.68616100
F	-0.96451600	-1.45114900	-0.79560000
S	1.83680700	0.00000000	-0.15340300
H	1.99845900	0.98124700	0.76574100
H	1.99845900	-0.98124700	0.76574000
Al	-0.67065800	0.00000000	0.00525700

$F_3Al•••NH_3$			
Al	-0.26849300	-0.00000800	-0.00001000
F	-0.56655900	0.98607800	-1.34261400
F	-0.56669500	0.66963100	1.52526100
F	-0.56646400	-1.65580200	-0.18272800

N	1.76811400	0.00009100	0.00008200
H	2.13705700	-0.94717200	-0.10440700
H	2.13697400	0.38323700	0.87271200
H	2.13703300	0.56424300	-0.76801600

$F_3Al•••NCH$

Al	0.57688700	-0.00000800	-0.00003200
F	0.84019500	-0.14636300	1.65713600
F	0.83999300	1.50834900	-0.70187200
F	0.83987700	-1.36201500	-0.95535800
H	-3.74249700	0.00005100	0.00016200
C	-2.66381900	0.00003100	0.00011500
N	-1.49353000	0.00001900	0.00005800

$F_3Al•••CO$

F	0.84812600	1.45448700	0.81672000
F	0.84815500	-0.01995100	-1.66797400
F	0.84810900	-1.43454100	0.85127200
C	-1.59379900	0.00000500	-0.00001300
O	-2.73478500	0.00000500	-0.00001400
Al	0.65704300	-0.00000200	0.00000200

$F_3Al•••OCH_2$

Al	-0.56702600	-0.00001400	0.07903800
F	-1.21146300	-1.44962500	-0.47799100
F	-1.21139400	1.44986300	-0.47735600
F	0.04581500	-0.00037600	1.66214100
C	2.26571600	0.00000600	-0.17079500
H	2.24528700	-0.00028200	0.93044300
H	3.22159700	0.00014000	-0.71612300
O	1.21294300	0.00019000	-0.82227400

$F_3Al•••C_2H_4$

Al	-0.57321900	0.00000100	0.01699500
F	-0.65987200	0.00003000	1.69796600
F	-0.89243500	-1.44069000	-0.79178500
F	-0.89242700	1.44066800	-0.79182500
C	1.83840400	0.68013600	-0.07896500
H	1.79289400	1.24265400	0.85854300
H	1.90393600	1.24807900	-1.00989300
C	1.83839600	-0.68014700	-0.07895100
H	1.90392900	-1.24811000	-1.00986500
H	1.79288100	-1.24264000	0.85857200

$F_3Al{\bullet\bullet\bullet}OHCH_3$

Al	-0.62978800	0.07397100	0.05696200
F	-1.39944900	-1.43143600	0.09787300
F	-1.04847800	1.17432700	-1.14654200
F	-0.17040900	0.75126600	1.53820200
C	2.32650000	0.06294600	-0.09206000
H	2.42530600	-0.00685700	0.99758500
H	3.17786100	-0.39168800	-0.61169700
H	2.20914000	1.10765500	-0.39772600
O	1.10240600	-0.61578100	-0.52762200
H	1.16171300	-1.56957600	-0.36113400

$F_3Al{\bullet\bullet\bullet}PH_3$

Al	-0.69658800	-0.00000100	0.00000000
F	-0.96221400	-0.64801400	1.53550300
F	-0.96221700	-1.00577900	-1.32894700
F	-0.96222000	1.65379100	-0.20655500
H	2.48924300	0.75669000	0.99985300
H	2.48924400	0.48755300	-1.15523800
H	2.48924300	-1.24423800	0.15538500
P	1.83785100	0.00000100	-0.00000100

$F_3Al•••O(CH_3)_2$			
F	-1.31286700	-1.45874600	-0.68138800
F	-1.31286700	1.45874700	-0.68138700
F	-0.74653900	0.00000000	1.71902500
C	1.77333200	1.20871500	-0.04015700
H	1.90845900	1.23224100	1.05140900
H	2.74279300	1.20028900	-0.55673600
H	1.16019500	2.05194100	-0.37752500
O	1.05034300	0.00000000	-0.41429700
C	1.77333200	-1.20871500	-0.04015700
H	1.90845900	-1.23224100	1.05140900
H	1.16019500	-2.05194100	-0.37752500
H	2.74279300	-1.20028900	-0.55673600
Al	-0.84270500	0.00000000	0.02736200

$Cl_3Al•••OH_2$			
O	0.00000100	-0.32266900	1.91278100
H	-0.78127900	-0.84203600	2.16978600
H	0.78128600	-0.84202500	2.16978900
Al	0.00000000	0.04747600	-0.04041400
Cl	-1.84009100	-0.97810100	-0.46808700
Cl	-0.00000900	2.17078800	-0.18832300
Cl	1.84010000	-0.97808500	-0.46808700

$Cl_3Al•••SH_2$			
S	0.00000200	0.58326000	2.08314200
H	0.98287600	1.50297100	1.92812000
H	-0.98286800	1.50297600	1.92812000
Al	-0.00000100	-0.12639100	-0.32896900
Cl	1.84344200	-1.21127200	-0.32541900
Cl	0.00000600	1.79341400	-1.28503900
Cl	-1.84344900	-1.21126100	-0.32541900

$Cl_3Al•••NH_3$			
Al	0.00000100	-0.00000100	-0.02854400
N	-0.00000900	0.00000400	1.99759000
H	-0.92428200	0.23325200	2.36834800
H	0.66411900	0.68382400	2.36836000
H	0.26012500	-0.91705900	2.36836300
Cl	2.05105900	-0.51759800	-0.40621300
Cl	-0.57727500	2.03506500	-0.40622100
Cl	-1.47377900	-1.51746900	-0.40622000

$Cl_3Al•••NCH$			
Al	0.00007500	-0.00026100	-0.26683500
H	-0.00112600	0.00394700	4.04574300
C	-0.00081800	0.00287900	2.96675300
N	-0.00048600	0.00172100	1.79537600
Cl	-1.78276800	1.12986700	-0.60831900
Cl	1.87063700	0.97824900	-0.60719100
Cl	-0.08737100	-2.10987300	-0.60478700

$Cl_3Al•••CO$			
C	-1.89163700	-0.00014400	-0.00005600
O	-3.03379300	-0.00023000	-0.00009000
Al	0.35329000	0.00002700	0.00000800
Cl	0.60855300	-1.83438200	-1.05455000
Cl	0.60827200	1.83054600	-1.06135400
Cl	0.60831600	0.00397500	2.11596000

$Cl_3Al•••OCH_2$			
Al	0.24103800	0.00000000	-0.15401000
C	-1.99210200	0.00000100	1.70404600
H	-2.65843000	0.00000000	0.82630900
H	-2.40618400	0.00000200	2.72353400

O	-0.76219900	0.00000200	1.56738700
Cl	1.29754100	1.84162500	0.05024200
Cl	1.29756300	-1.84161000	0.05025700
Cl	-1.41973200	-0.00001600	-1.53056300

$Cl_3Al{\bullet\bullet\bullet}C_2H_4$			
Al	0.00000000	-0.08274100	-0.24999100
C	0.68107300	0.57218900	2.09682800
H	1.24572900	1.43761200	1.73632500
H	1.24594500	-0.27843800	2.48434000
C	-0.68107400	0.57218500	2.09682900
H	-1.24594200	-0.27844300	2.48434000
H	-1.24573500	1.43760700	1.73632600
Cl	-0.00000400	1.90754200	-1.03354500
Cl	-1.82105600	-1.19227300	-0.37597400
Cl	1.82106000	-1.19226600	-0.37597500

$Cl_3Al{\bullet\bullet\bullet}OHCH_3$			
Al	0.26891400	0.06716200	-0.17807200
C	-2.13176600	-0.34624300	1.50830500
H	-2.41050000	-1.30096000	1.04621500
H	-2.48125500	-0.27226300	2.54452800
H	-2.50721900	0.49533800	0.91616100
O	-0.67100900	-0.20160400	1.50545300
H	-0.25322700	-0.88311900	2.05712700
Cl	2.24205700	-0.31687700	0.56739300
Cl	-0.60228100	-1.46746700	-1.40620700
Cl	-0.32713000	2.06541300	-0.65192400

$Cl_3Al{\bullet\bullet\bullet}PH_3$			
Al	-0.35474700	0.00000200	0.00000500
H	2.79455700	1.25676200	-0.09796700
H	2.79453000	-0.71321400	-1.03948300

H	2.79456300	-0.54360300	1.13732400
P	2.15533300	-0.00001400	-0.00003300
Cl	-0.70790400	0.91310000	-1.91051100
Cl	-0.70784500	1.19801700	1.74603500
Cl	-0.70789300	-2.11110300	0.16450800

$Cl_3Al{\bullet\bullet\bullet}O(CH_3)_2$

C	-2.03713000	-1.20406300	-0.70812100
H	-2.48430700	-1.22346700	0.29658700
H	-2.81023000	-1.17373500	-1.48761300
H	-1.36688800	-2.05717800	-0.85709500
O	-1.21918600	-0.00000100	-0.84718600
C	-2.03713200	1.20406000	-0.70812100
H	-2.48430900	1.22346200	0.29658700
H	-1.36689200	2.05717500	-0.85709500
H	-2.81023200	1.17372900	-1.48761300
Al	0.46783500	0.00000000	0.12095000
Cl	1.35961200	-1.83048600	-0.54709600
Cl	-0.28156900	0.00000000	2.14118200
Cl	1.35960800	1.83048800	-0.54709600

$H_2FAl{\bullet\bullet\bullet}OH_2$

F	-1.06458300	-0.91493200	0.03021400
O	1.48177700	-0.24051700	-0.11216900
H	2.04429900	-0.09412600	0.66323000
H	1.24114200	-1.18385000	-0.09461400
Al	-0.36995400	0.66196200	0.00067800
H	-0.22965600	1.38292600	1.41160700
H	-0.51935500	1.44806300	-1.36361300

$H_2FAl{\bullet\bullet\bullet}SH_2$

F	-1.46315900	1.01511700	-0.00000100
H	1.41349400	0.91690200	-0.97790100

H	1.41348400	0.91694000	0.97786900
Al	-0.98296700	-0.62835500	0.00000000
H	-1.04341300	-1.36684300	-1.40085600
H	-1.04342300	-1.36684400	1.40085500
S	1.57542900	-0.00422400	0.00000200

$H_2FAl•••NH_3$			
Al	-0.35338000	0.64502100	-0.00002100
F	-1.20651300	-0.84961300	0.00015100
N	1.51597800	-0.29925200	-0.00008900
H	1.59073400	-0.90463500	-0.81994600
H	1.59086800	-0.90452000	0.81984100
H	2.32833000	0.31930200	-0.00019900
H	-0.33451400	1.42303800	1.39079300
H	-0.33470300	1.42282400	-1.39095800

$H_2FAl•••NCH$			
Al	-0.89005900	-0.58860200	0.00001800
F	-1.37577700	1.05149900	-0.00001000
H	3.37608300	0.50901200	-0.00002400
C	2.34136000	0.20545500	-0.00001800
N	1.21536600	-0.12387000	-0.00001200
H	-0.98950500	-1.34312800	1.39213000
H	-0.98954600	-1.34318500	-1.39206000

$H_2FAl•••CO$			
F	1.36011800	1.07176200	0.00006800
C	-1.32033000	-0.11513200	-0.00007900
O	-2.42501000	0.18068900	-0.00014000
Al	0.99818900	-0.59456100	0.00006300
H	1.05217600	-1.33562500	1.39655800
H	1.05235800	-1.33565800	-1.39640700

$H_2FAl{\bullet\bullet\bullet}OCH_2$			
Al	0.97495600	-0.52056400	-0.00000400
F	0.92743400	1.20376100	0.00000600
C	-1.78965600	0.34695900	-0.00000400
H	-1.32619100	1.34661400	-0.00001900
H	-2.88593400	0.23600800	0.00000500
O	-1.08709500	-0.67147500	0.00000600
H	1.31274900	-1.17955800	1.40078600
H	1.31273600	-1.17954500	-1.40080200

$H_2FAl{\bullet\bullet\bullet}C_2H_4$			
Al	-0.82187300	0.65222600	0.00000000
C	1.55952200	-0.16803700	0.67955400
H	1.13782600	-1.00554400	1.24268200
H	2.00353100	0.65364200	1.24673700
C	1.55952200	-0.16803800	-0.67955400
H	2.00353100	0.65364100	-1.24673800
H	1.13782600	-1.00554500	-1.24268100
F	-1.40918300	-0.95164100	0.00000000
H	-0.81498800	1.40303900	1.39443400
H	-0.81498800	1.40303800	-1.39443500

$H_2FAl{\bullet\bullet\bullet}OHCH_3$			
Al	0.99025000	-0.51626700	0.18126900
F	1.14975100	1.15428000	-0.19772600
C	-1.81629200	0.41700700	0.22319000
H	-1.49195800	1.39284600	-0.15872400
H	-2.85964300	0.20125600	-0.03793300
H	-1.68077400	0.37111700	1.30932600
O	-0.96398500	-0.64196800	-0.32211100
H	-1.07243200	-0.67221300	-1.28521900
H	0.90543800	-0.82343600	1.73693000
H	1.58799300	-1.51292000	-0.90359100

$H_2FAl•••PH_3$			
Al	1.02879100	-0.62547000	0.00000000
F	1.51650100	1.01757400	0.00000000
H	-1.95502800	0.86848600	-1.07644700
H	-1.95502900	0.86848500	1.07644800
H	-2.56630300	-0.89343000	-0.00000100
P	-1.51792200	0.05937400	0.00000000
H	1.11120300	-1.38060900	1.39443000
H	1.11120200	-1.38060900	-1.39443000

$H_2FAl•••O(CH_3)_2$			
F	1.94891400	0.66309100	-0.23224700
C	-1.89017300	-0.79674000	-0.07767700
H	-2.08184000	-0.87494800	1.00410800
H	-2.76540200	-0.37900900	-0.59581500
H	-1.63457500	-1.77839600	-0.49566700
O	-0.75260100	0.06694000	-0.31757100
C	-0.98056700	1.41122800	0.18485600
H	-1.14771900	1.37582700	1.27318100
H	-0.07723500	1.98417600	-0.05025700
H	-1.85888400	1.82911200	-0.32790400
Al	1.02908300	-0.72655500	0.17393000
H	0.81070100	-0.93840700	1.74214500
H	1.08190100	-1.96340300	-0.82315900

9. Gallium Bonded Complexes

$HF_2Ga•••OH_2$			
F	-1.47791200	-0.38555400	-0.67635900
O	0.00087500	1.76423100	0.12730800
H	0.77425600	1.91821300	-0.44355900

H	-0.77230500	1.91895100	-0.44363000
H	-0.00038300	-0.79230500	1.79728200
Ga	-0.00016500	-0.32922500	0.33051400
F	1.47752800	-0.38697100	-0.67636200

$HF_2Ga•••SH_2$

F	-0.77854600	1.47219100	-0.65980100
H	1.81212500	-0.98235000	-0.84475800
H	1.81213500	0.98235700	-0.84475200
H	-1.01460200	-0.00001700	1.83419500
Ga	-0.64045300	0.00000000	0.33877600
F	-0.77854200	-1.47219200	-0.65980300
S	1.95363700	0.00000000	0.07685500

$HF_2Ga•••NH_3$

F	-0.55777500	1.47961100	-0.62407600
N	1.79069700	-0.00000300	-0.10173300
H	1.95222100	0.82635400	-0.68192200
H	1.95221600	-0.82634900	-0.68193700
H	2.47623100	-0.00001200	0.65336300
H	-0.56408600	0.00001300	1.86708000
Ga	-0.26811200	0.00000000	0.34802900
F	-0.55777900	-1.47961000	-0.62407500

$HF_2Ga•••NCH$

F	-0.74322200	1.47501700	-0.65600200
H	3.81595200	-0.00000600	-0.34332500
C	2.76296900	-0.00000300	-0.11082600
N	1.61749300	-0.00000500	0.14160200
H	-0.87446400	0.00000400	1.83336000
Ga	-0.56334300	0.00000000	0.32231500
F	-0.74323500	-1.47501200	-0.65600300

$HF_2Ga\cdots CO$			
F	-0.69499100	1.47364100	-0.66626800
C	1.74084100	-0.00000400	0.14536800
O	2.86261500	-0.00000100	-0.07543700
H	-0.97867700	0.00000000	1.82110700
Ga	-0.64056100	0.00000100	0.31945200
F	-0.69499700	-1.47364100	-0.66626800

$HF_2Ga\cdots OCH_2$			
F	-1.47791200	-0.38555400	-0.67635900
O	0.00087500	1.76423100	0.12730800
H	0.77425600	1.91821300	-0.44355900
H	-0.77230500	1.91895100	-0.44363000
H	-0.00038300	-0.79230500	1.79728200
Ga	-0.00016500	-0.32922500	0.33051400
F	1.47752800	-0.38697100	-0.67636200

$HF_2Ga\cdots C_2H_4$			
C	1.79422600	0.57399300	0.60971100
H	1.52290700	0.19605300	1.59907800
H	1.85425400	1.65649700	0.47760100
C	2.04496800	-0.27967400	-0.41821500
H	2.33507100	0.09180000	-1.40472200
H	1.99845000	-1.36284200	-0.27103200
F	-0.59459500	-1.40548100	0.84678400
H	-0.69343600	-0.34778100	-1.85583400
Ga	-0.51878300	-0.08617700	-0.34489300
F	-0.95764200	1.48013300	0.37517400

$HF_2Ga\cdots OHCH_3$			
F	1.17197300	-1.20620300	-0.77354800
C	-2.36437000	0.00989500	-0.13307100
H	-2.15774200	0.43714100	-1.12148200

H	-3.25279100	-0.63377800	-0.14363500
H	-2.48703900	0.81427700	0.59909300
O	-1.22197200	-0.78169600	0.32561700
H	-1.06074000	-1.50492600	-0.30637900
H	1.21048800	0.25949700	1.74403800
Ga	0.64412800	0.11809100	0.31786500
F	0.13267900	1.55744400	-0.60778000

$HF_2Ga{\bullet\bullet\bullet}PH_3$

F	-0.82524700	1.47830700	-0.65181000
H	2.70268900	1.08269400	0.42741000
H	2.20847200	0.00000500	-1.38451300
H	2.70269400	-1.08269800	0.42740100
P	1.90152600	-0.00000200	-0.00525500
H	-1.05158900	0.00001000	1.83269300
Ga	-0.65260200	0.00000000	0.33898100
F	-0.82525300	-1.47830600	-0.65180900

$HF_2Ga{\bullet\bullet\bullet}O(CH_3)_2$

F	-1.17076400	-1.50217800	-0.55217500
F	-1.17076400	1.50217800	-0.55217600
C	1.95015200	1.20730500	-0.00827700
H	2.24488800	1.24529400	1.05302500
H	2.84206000	1.21070900	-0.65167300
H	1.28853500	2.04357500	-0.26224200
O	1.19505300	0.00000000	-0.27070600
C	1.95015200	-1.20730500	-0.00827700
H	2.24488800	-1.24529400	1.05302500
H	1.28853500	-2.04357500	-0.26224200
H	2.84206000	-1.21070900	-0.65167300
H	-0.78272100	0.00000000	1.87526700
Ga	-0.76957200	0.00000000	0.32421400

$H_2FGa•••OH_2$			
F	0.32798000	1.47439900	0.02551800
O	-1.72187500	-0.14789300	-0.11294700
H	-2.19480300	-0.40947000	0.69095200
H	-1.69166900	0.82839600	-0.09081800
H	0.60204700	-0.96344200	1.42304100
H	0.82237300	-0.91493700	-1.38849100
Ga	0.42855600	-0.34280600	0.00126600

$H_2FGa•••SH_2$			
F	-0.91411900	1.42661800	0.00000000
H	1.76191500	0.86535200	-0.97351400
H	1.76191300	0.86533000	0.97353100
H	-0.94447300	-1.00836500	-1.40985700
H	-0.94444800	-1.00835300	1.40986700
S	1.88794400	-0.06557500	-0.00000200
Ga	-0.76177200	-0.37110700	0.00000000

$H_2FGa•••NH_3$			
F	-0.76455400	1.36239200	0.00002500
N	1.73084100	0.19541800	-0.00005900
H	1.62376000	1.21362400	0.00007400
H	2.27200100	-0.06339200	-0.82516300
H	2.27215100	-0.06359900	0.82488200
H	-0.52330600	-1.07986500	-1.39936900
H	-0.52319900	-1.07985500	1.39941100
Ga	-0.33407400	-0.40504400	0.00001100

$H_2FGa•••NCH$			
F	-0.86747900	1.43397200	0.00002800
H	3.73617300	0.38378300	-0.00004800

C	2.68854800	0.12907500	-0.00003700
N	1.54694200	-0.14729200	-0.00002500
H	-0.87366200	-1.00728600	1.40323500
H	-0.87369900	-1.00728200	-1.40321900
Ga	-0.68198000	-0.35543100	0.00000600

$H_2FGa\cdots CO$			
F	0.78269400	1.44703300	0.00001900
C	-1.66948700	-0.15681500	-0.00009600
O	-2.78905600	0.08092400	-0.00019200
H	0.92579200	-0.98796000	1.40716000
H	0.92590800	-0.98801800	-1.40700600
Ga	0.75591700	-0.34689700	0.00005800

$H_2FGa\cdots OCH_2$			
F	-0.36126000	1.50075300	-0.00001000
C	2.16908800	0.19790200	0.00000800
H	1.81558800	1.24210400	0.00003300
H	3.24836600	-0.03046800	0.00000000
O	1.36031800	-0.73783700	-0.00001300
H	-1.14306300	-0.79865200	-1.41283400
H	-1.14302900	-0.79863600	1.41285600
Ga	-0.75560000	-0.27115600	0.00000300

$H_2FGa\cdots C_2H_4$			
C	-0.86635500	-1.61762100	0.67993600
H	-1.52737000	-0.95016800	1.23945400
H	-0.22806900	-2.29990900	1.24695200
C	-0.86635500	-1.61762100	-0.67993600
H	-0.22806900	-2.29990900	-1.24695200
H	-1.52737000	-0.95016800	-1.23945400
F	-0.86635500	1.42351800	0.00000000
H	1.27673100	0.24572200	1.40211000

H	1.27673100	0.24572200	-1.40211000
Ga	0.61777000	0.40672600	0.00000000

$H_2FGa•••OHCH_3$

F	0.65955400	1.48284800	-0.11605500
C	-2.17124000	0.16653400	0.35991000
H	-1.81670000	1.17458700	0.61272000
H	-3.17680300	0.19367400	-0.07929700
H	-2.16512900	-0.47506800	1.24753000
O	-1.25028300	-0.46062800	-0.58868100
H	-1.25571900	0.07962200	-1.39600700
H	0.56658400	-0.76800400	1.57002200
H	1.52480500	-1.01037500	-1.07774700
Ga	0.75537700	-0.31787900	0.08765400

$H_2FGa•••PH_3$

F	1.67845400	0.19262600	0.00000000
H	-0.24248900	-2.38677500	1.07640000
H	-0.24248900	-2.38677500	-1.07640000
H	-2.09434700	-2.14570900	0.00000000
P	-0.77170600	-1.63594600	0.00000000
H	-0.47558400	1.36555400	-1.40176700
H	-0.47558400	1.36555400	1.40176700
Ga	0.00000000	0.87076500	0.00000000

$H_2FGa•••O(CH_3)_2$

F	1.49695000	1.20901400	-0.24314300
C	-2.08216600	-0.91771700	-0.07782600
H	-2.16042300	-1.06839000	1.01141200
H	-3.05797400	-0.62452300	-0.49317000
H	-1.72614200	-1.83428700	-0.56545600

O	-1.11457200	0.11327700	-0.37084900
C	-1.48936400	1.38297500	0.22263200
H	-1.56643500	1.27333200	1.31690900
H	-0.69285500	2.08828500	-0.03700300
H	-2.45533200	1.69683200	-0.20039900
H	0.68256500	-0.72522500	1.62088300
H	1.13358300	-1.49929300	-1.03547100
Ga	0.86181400	-0.44792300	0.08608200

$H_2ClGa•••OH_2$			
Cl	1.62254400	0.27758800	0.01138500
O	-1.22091700	1.44269800	-0.10029200
H	-1.59382800	1.73260200	0.74672200
H	-0.39681400	1.95348400	-0.20148600
H	-0.96396300	-0.95879800	1.42209300
H	-0.86688000	-1.14374300	-1.38198500
Ga	-0.45143300	-0.57561700	0.00075700

$H_2ClGa•••SH_2$			
Cl	-1.50024500	1.07043200	0.00000100
H	1.59696000	1.29796100	-0.97552900
H	1.59705400	1.29791600	0.97559900
H	-0.18966600	-1.46800000	-1.40587200
H	-0.18970300	-1.46803200	1.40586000
S	2.01636700	0.45921400	-0.00000400
Ga	-0.30878600	-0.81305200	0.00000000

$H_2ClGa•••NH_3$			
Cl	-1.63214100	0.37453200	-0.00000100

N	1.35379800	1.32038700	-0.00000400
H	1.02950900	1.83842200	-0.81892300
H	2.37460800	1.33582500	-0.00003600
H	1.02956200	1.83837400	0.81896700
H	0.79383300	-1.16647700	-1.39575000
H	0.79382800	-1.16642500	1.39577600
Ga	0.39511200	-0.58998300	0.00000000

$H_2ClGa\cdots NCH$

Cl	1.35009900	1.17207400	0.00000000
H	-3.65201600	1.33649400	0.00000100
C	-2.73426800	0.77032100	0.00000000
N	-1.73193000	0.15788300	0.00000000
H	0.22073900	-1.45341100	-1.39990800
H	0.22074000	-1.45339900	1.39991400
Ga	0.28348300	-0.77684000	0.00000000

$H_2ClGa\cdots CO$

Cl	1.27550600	1.23669200	0.00029300
C	-1.84027700	0.13739500	-0.00019700
O	-2.85169000	0.67317800	-0.00023600
H	0.29092800	-1.45021000	1.40150300
H	0.29129200	-1.44987600	-1.40178800
Ga	0.37385000	-0.78495100	-0.00005200

$H_2ClGa\cdots OCH_2$

Cl	-1.15795400	1.26834700	-0.00001500
C	2.11963900	0.94574900	0.00001600
H	1.39687700	1.77939200	0.00003600
H	3.20357600	1.15022500	0.00001000
O	1.73250900	-0.22742500	-0.00000800
H	-0.38570700	-1.47477300	-1.40888000
H	-0.38568900	-1.47473700	1.40890700

Ga	-0.34586200	-0.81926100	0.00000500

$H_2ClGa•••C_2H_4$

C	-0.82250100	-1.83427400	0.68055300
H	-1.46135700	-1.14746200	1.24261700
H	-0.20950400	-2.54036100	1.24618600
C	-0.82250100	-1.83427400	-0.68055300
H	-0.20950400	-2.54036100	-1.24618600
H	-1.46135700	-1.14746200	-1.24261700
Cl	-0.82250100	1.60619600	0.00000000
H	1.42181600	-0.17196900	1.39701300
H	1.42181600	-0.17196900	-1.39701300
Ga	0.78550400	0.07824300	0.00000000

$H_2ClGa•••OHCH_3$

Cl	1.34290500	1.17648700	-0.01166600
C	-2.19717400	0.78183700	0.37074200
H	-1.52025200	1.50685600	0.84339200
H	-3.05528500	1.28386100	-0.09403900
H	-2.54043100	0.04465300	1.10406800
O	-1.47813600	0.02174200	-0.65199700
H	-1.17328900	0.65673600	-1.32292800
H	-0.14753300	-1.19464500	1.51146800
H	0.72534500	-1.74086100	-1.11202700
Ga	0.31903900	-0.82005900	0.07290000

$H_2ClGa•••PH_3$

Cl	1.75773100	-0.49073500	0.00000000
H	-1.35173500	-2.04195100	1.07999400
H	-1.35173500	-2.04195100	-1.07999400
H	-2.99038000	-1.12990800	0.00000000
P	-1.57288300	-1.15555300	0.00000000
H	-0.29716600	1.51867400	-1.39816900

H	-0.29716600	1.51867400	1.39816900
Ga	0.00000000	0.89846000	0.00000000

$H_2ClGa\cdots O(CH_3)_2$			
C	-2.49034900	-0.39856100	-0.31373000
H	-2.72140800	-0.67115800	0.72931500
H	-3.30875000	0.19940900	-0.74119100
H	-2.32311000	-1.29883800	-0.91775700
O	-1.26725900	0.37226800	-0.36813200
C	-1.38732800	1.60502300	0.38761100
H	-1.58472800	1.37426600	1.44726700
H	-0.43110300	2.12857100	0.27886600
H	-2.20981600	2.19881000	-0.03802900
H	0.08066500	-0.96335600	1.67597800
H	0.30056200	-1.87929500	-0.95579000
Ga	0.40575900	-0.78825800	0.15320700
Cl	1.94254700	0.77239300	-0.21919400

10. Indium Bonded Complexes

$HF_2In\cdots OH_2$			
O	0.00388400	-1.90239700	-0.48866400
H	0.77540900	-2.11182000	0.06901700
H	-0.76679000	-2.11495900	0.06900700
H	-0.00285400	1.40465000	-1.56265400
In	-0.00079100	0.38847100	-0.21415800
F	-1.60313900	-0.05847100	0.87931200
F	1.60335400	-0.05195100	0.87932100

$HF_2In\cdots SH_2$			
F	-0.46489300	1.59913300	0.89977400
H	2.00556700	0.98181800	0.75228700
H	2.00553700	-0.98174700	0.75234100

H	-1.28401700	-0.00002000	-1.81856400
F	-0.46485600	-1.59914200	0.89977200
S	2.19091100	0.00000700	-0.16474400
In	-0.60028400	-0.00000200	-0.27032800

$HF_2In•••NH_3$			
F	0.24983200	1.61512000	-0.89355500
N	-1.99139200	-0.00023800	0.11776300
H	-2.19371200	0.82506700	-0.45182000
H	-2.62343000	-0.00032200	0.91751500
H	-2.19352100	-0.82557800	-0.45183900
H	1.02418900	0.00010300	1.81630200
F	0.25024200	-1.61506600	-0.89355300
In	0.31480700	0.00003900	0.27407100

$HF_2In•••NCH$			
F	-0.53254400	1.61086200	-0.87830600
H	4.08125200	-0.00001700	-0.31220300
C	3.03096600	-0.00001600	-0.06701600
N	1.88758700	-0.00001600	0.20049000
H	-0.97501100	0.00002500	1.90016200
F	-0.53259200	-1.61085900	-0.87830300
In	-0.50854900	0.00000300	0.26980000

$HF_2In•••CO$			
F	-0.41586000	1.60516700	0.87781400
C	2.02935800	-0.00000100	-0.22038000
O	3.15386000	-0.00000200	-0.00958200
H	-1.14863900	0.00005700	-1.85125800
F	-0.41586700	-1.60516000	0.87781200
In	-0.58720100	-0.00000200	-0.25613100

$HF_2In\cdots OCH_2$			
F	0.05283600	1.57345800	0.86935800
C	2.43028800	-0.07927300	0.16022300
H	2.06241000	0.26341400	1.14132300
H	3.50960400	-0.25165800	0.01064200
O	1.65394800	-0.26620800	-0.78451800
H	-1.56519500	0.14845500	-1.59542500
F	-0.41190900	-1.51136800	0.99558800
In	-0.58343800	0.03849600	-0.22502500

$HF_2In\cdots C_2H_4$			
C	2.25617200	0.27155100	-0.47180100
H	2.22309500	1.34679500	-0.26995100
H	2.50973800	-0.05490600	-1.48455300
C	2.03989600	-0.62756600	0.52551400
H	2.08884600	-1.70409900	0.34525600
H	1.81062100	-0.29172800	1.54088600
F	-0.32819900	1.47728400	1.11565300
H	-0.86280200	0.40322500	-1.90421900
F	-0.79576400	-1.66380100	0.58972800
In	-0.47816800	0.08398900	-0.28363500

$HF_2In\cdots OHCH_3$			
F	-0.01883800	1.62192800	-0.84291200
C	-2.60383200	0.13160800	-0.01848400
H	-2.36216600	0.56850800	-0.99543200
H	-3.52080000	-0.47047000	-0.05907800
H	-2.71204100	0.92889900	0.72469800
O	-1.50461700	-0.71148300	0.44771700
H	-1.37179400	-1.43557200	-0.19413200
H	1.52347600	0.23177500	1.65879900
F	0.65282600	-1.52273400	-0.95445700
In	0.62035400	0.08543600	0.23613500

$HF_2In•••PH_3$			
F	-0.54205400	1.61297500	0.88488500
H	2.48337200	-0.00004200	1.31054600
H	2.97227200	1.08024400	-0.49860300
H	2.97226900	-1.08023900	-0.49865600
P	2.16593100	-0.00000700	-0.06673700
H	-1.27238300	0.00000900	-1.83581400
F	-0.54208000	-1.61296900	0.88488700
In	-0.60994500	0.00000100	-0.27355900

$HF_2In•••O(CH_3)_2$			
F	1.14968400	1.69726200	0.16603800
C	-2.30527600	-0.90753500	-0.37400100
H	-2.21481400	-1.33664000	0.63525600
H	-3.34602200	-0.62377200	-0.59085500
H	-1.95171500	-1.62420000	-1.12704300
O	-1.46547200	0.26968900	-0.48565900
C	-1.89813200	1.30076300	0.44812600
H	-1.85624300	0.90549900	1.47485800
H	-1.19997300	2.13707200	0.33390400
H	-2.92420600	1.59815500	0.18537200
H	1.31252100	-1.07099100	-1.56481000
In	0.74268700	-0.20464300	-0.22244800
F	0.26509300	-1.08331900	1.49993900

$H_2FIn•••OH_2$			
F	-0.72139100	1.54297100	0.02330600
O	-1.79646200	-0.78826700	-0.11744400
H	-2.21377200	-1.18467200	0.66031300
H	-1.98538400	0.17742100	-0.05986400
H	0.90354200	-0.55800500	1.59727100
H	1.07451600	-0.40292300	-1.56656500

In	0.47112900	-0.11453900	0.00201300

$H_2FIn•••SH_2$

F	-0.38794300	1.73929000	-0.00001300
H	2.07910700	0.73681000	-0.96886800
H	2.07913400	0.73674600	0.96891000
H	-0.98108500	-0.83534900	-1.58109100
H	-0.98106600	-0.83532400	1.58111300
S	2.19052600	-0.20137000	-0.00001100
In	-0.68883700	-0.24968500	0.00000500

$H_2FIn•••NH_3$

F	-0.10639600	1.74296800	-0.00006500
N	-1.95138300	-0.36755200	0.00008200
H	-2.10033400	0.64718300	0.00004000
H	-2.41250100	-0.75348500	0.82382500
H	-2.41256500	-0.75356400	-0.82358700
H	0.84639200	-0.75241300	1.57227100
H	0.84628700	-0.75253600	-1.57227000
In	0.40510100	-0.21936800	-0.00000500

$H_2FIn•••NCH$

F	-0.45904800	1.74211200	-0.00013700
H	4.05287900	0.26485700	-0.00004100
C	3.00298100	0.01897200	-0.00001900
N	1.85786900	-0.24777200	0.00000500
H	-0.85754900	-0.88165200	1.57400300
H	-0.85756700	-0.88191100	-1.57384800
In	-0.59651600	-0.25632100	0.00002500

$H_2FIn•••CO$

F	0.22308200	1.71656900	0.00003400

C	-2.00307200	-0.30093900	-0.00014900
O	-3.12800200	-0.08599000	-0.00021000
H	0.95200400	-0.82496700	1.57817800
H	0.95227900	-0.82491900	-1.57806000
In	0.67613100	-0.23072800	0.00004400

$H_2FIn•••OCH_2$			
F	0.11526200	1.69634800	-0.00000300
C	2.48019800	0.04704300	-0.00000300
H	2.17874400	1.10859700	-0.00000600
H	3.54819300	-0.23485700	-0.00000600
O	1.62409200	-0.84612400	-0.00000300
H	-1.09895800	-0.64106900	-1.58523100
H	-1.09895000	-0.64106500	1.58523800
In	-0.66204700	-0.17085700	0.00000100

$H_2FIn•••C_2H_4$			
C	-1.16910200	-1.77006200	0.67961500
H	-1.77488900	-1.04849200	1.23523700
H	-0.58897800	-2.50228600	1.24786800
C	-1.16910200	-1.77006200	-0.67961500
H	-0.58897800	-2.50228600	-1.24786800
H	-1.77488900	-1.04849200	-1.23523700
F	-1.16910200	1.35675500	0.00000000
H	1.20707300	0.16912400	1.57263100
H	1.20707300	0.16912400	-1.57263100
In	0.54826000	0.32231100	0.00000000

$H_2FIn•••OHCH_3$			
F	0.29243100	1.74034200	0.17128100
C	-2.60322000	-0.30615800	0.27407800
H	-2.34458100	-0.07298000	1.31792900
H	-3.53570900	0.20153300	-0.00868300

H	-2.72499700	-1.38942200	0.15597800
O	-1.53712000	0.09387400	-0.62375500
H	-1.34934400	1.04803700	-0.47561800
H	0.45971800	-1.02927000	1.53055300
H	1.53344000	-0.60556500	-1.42156300
In	0.67848700	-0.25978500	0.01439700

$H_2FIn•••PH_3$

F	1.70534200	-0.31502300	0.00000000
H	-0.18588000	-2.64024000	1.07256200
H	-0.18588000	-2.64024000	-1.07256200
H	-2.05116200	-2.64179500	0.00000000
P	-0.80753900	-1.95775100	0.00000000
H	-0.40603100	1.30418100	-1.57445800
H	-0.40603100	1.30418100	1.57445800
In	0.00000000	0.76562000	0.00000000

$H_2FIn•••O(CH_3)_2$

F	1.07164100	1.66279800	-0.13437000
C	-2.34018700	-1.04221100	-0.01481400
H	-2.39764000	-1.16576400	1.07975200
H	-3.34301200	-0.84251000	-0.42384000
H	-1.92673000	-1.94866500	-0.47667300
O	-1.45814000	0.04490500	-0.35231800
C	-1.94533900	1.30638600	0.16975700
H	-2.05774000	1.23851300	1.26481000
H	-1.19120600	2.05812200	-0.08834400
H	-2.91657200	1.53242500	-0.29705100
H	0.68163500	-0.78330400	1.69007600
H	1.23677300	-1.18718700	-1.38126700
In	0.80914300	-0.32267600	0.03532100

$H_2ClIn•••OH_2$

Cl	1.88645800	-0.16968700	0.01027800
O	-0.31749700	2.02363800	-0.10836000
H	-0.56450300	2.52600500	0.68239900
H	0.65917600	2.03345100	-0.12146600
H	-1.17641700	-0.47831500	1.59161100
H	-1.14835500	-0.70787000	-1.55474100
In	-0.55713700	-0.34036100	0.00192500

$H_2ClIn•••SH_2$

Cl	-1.14547400	1.63975300	0.00000100
H	1.91223400	1.21476200	-0.97210800
H	1.91223700	1.21476100	0.97210300
H	-0.41436200	-1.33795900	-1.57636800
H	-0.41435700	-1.33795900	1.57637000
S	2.27810700	0.34708400	-0.00000300
In	-0.40760000	-0.67719900	0.00000100

$H_2ClIn•••NH_3$

Cl	1.91876000	0.17021300	-0.00004900
N	-0.84330300	1.89899100	0.00007900
H	0.11639900	2.25709000	0.00000200
H	-1.31332100	2.27750300	0.82336800
H	-1.31347900	2.27755500	-0.82309500
H	-0.99093200	-0.88096300	1.56687300
H	-0.99102000	-0.88087000	-1.56687000
In	-0.45354000	-0.43340500	0.00000000

$H_2ClIn•••NCH$

Cl	-1.06679800	1.66625000	0.00000000
H	3.96142300	1.18092300	0.00000400
C	3.01349000	0.66666400	0.00000100
N	1.97748600	0.11045700	-0.00000300
H	-0.36782800	-1.32678000	1.56938200

H	-0.36783200	-1.32678700	-1.56937800
In	-0.34721500	-0.64544500	0.00000000

$H_2ClIn•••CO$

Cl	0.80073900	1.77741400	0.00000000
C	-2.13106900	-0.05237300	-0.00000600
O	-3.20448500	0.34719600	0.00000100
H	0.53653500	-1.28087500	1.57125900
H	0.53657500	-1.28087900	-1.57125400
In	0.48442100	-0.61464500	0.00000000

$H_2ClIn•••OCH_2$

Cl	-0.23288600	1.90907200	-0.00000500
C	2.57854700	0.05764700	-0.00000200
H	2.25314500	1.11282500	-0.00000100
H	3.65550300	-0.18731300	-0.00000300
O	1.75171400	-0.85991700	-0.00000200
H	-0.92073600	-1.07436900	-1.57890600
H	-0.92072600	-1.07436100	1.57891500
In	-0.60394100	-0.50403200	0.00000200

$H_2ClIn•••C_2H_4$

C	-1.13510700	-1.91190200	0.67997900
H	-1.72074000	-1.17628800	1.23909300
H	-0.57641600	-2.66139400	1.24712700
C	-1.13510700	-1.91190200	-0.67997900
H	-0.57641600	-2.66139400	-1.24712700
H	-1.72074000	-1.17628800	-1.23909300
Cl	-1.13510700	1.63165600	0.00000000
H	1.34615200	-0.18809400	1.56708500
H	1.34615200	-0.18809400	-1.56708500
In	0.71061400	0.06645300	0.00000000

$H_2ClIn\cdots OHCH_3$			
Cl	1.01663800	1.70399800	0.05344200
C	-2.61363700	0.40540400	0.35702300
H	-2.17341800	0.91350800	1.22748600
H	-3.46378400	0.97894500	-0.03590100
H	-2.94176100	-0.60179100	0.63790800
O	-1.61640200	0.23552500	-0.69084800
H	-1.26208200	1.12216500	-0.89517100
H	-0.07938000	-1.20096100	1.58091800
H	1.01701300	-1.44897100	-1.36809000
In	0.41293100	-0.67443800	0.02712200

$H_2ClIn\cdots PH_3$			
Cl	1.78362500	-0.84039400	0.00000000
H	-1.28601300	-2.36851200	1.07452000
H	-1.28601300	-2.36851200	-1.07452000
H	-3.01957400	-1.66930800	0.00000000
P	-1.60972400	-1.50594000	0.00000000
H	-0.29208300	1.44102300	-1.56931100
H	-0.29208300	1.44102300	1.56931100
In	0.00000000	0.82449100	0.00000000

$H_2ClIn\cdots O(CH_3)_2$			
C	-2.71364200	-0.35150700	-0.25424600
H	-2.90564600	-0.61894700	0.79861500
H	-3.57285300	0.20140400	-0.66443400
H	-2.53471800	-1.25585000	-0.85054500
O	-1.52697000	0.46194200	-0.35788700
C	-1.67358200	1.70226300	0.37541400
H	-1.83407600	1.48904100	1.44561400
H	-0.74131100	2.26033300	0.23200300
H	-2.53023700	2.25979800	-0.03376800
H	0.10049100	-1.02664500	1.73578700

H	0.42702500	-1.72906600	-1.30079900
In	0.43610200	-0.71219800	0.07774500
Cl	1.80949400	1.26573900	-0.17858200

11. Thallium Bonded Complexes

$HF_2Tl•••OH_2$			
F	1.10548800	0.53893500	1.42485100
O	1.93141600	-0.78715900	-0.65767500
H	2.57379200	-0.39392600	-1.26463900
H	2.17955400	-0.46446700	0.23777700
H	-0.68969800	1.34157300	-1.22579400
F	-0.95918300	-1.58276200	0.55219000
Tl	-0.25718200	0.18776000	-0.12690500

$HF_2Tl•••SH_2$			
F	0.08727100	1.54933600	1.10984400
H	-2.16173200	-0.97718300	0.63845600
H	-2.16173500	0.97718600	0.63845100
F	0.08727300	-1.54933600	1.10984400
H	1.32204800	0.00000100	-1.61666700
S	-2.38208800	-0.00000100	-0.27743600
Tl	0.48819700	0.00000000	-0.18763500

$HF_2Tl•••NH_3$			
F	0.27168300	1.57369700	1.05958500
N	2.04300900	-0.00000300	-0.52725000
H	2.30110800	0.82522000	0.02019200
H	2.56575300	0.00000600	-1.40159500
H	2.30111100	-0.82523100	0.02018200
H	-1.45256000	0.00004000	-1.35414000
F	0.27168100	-1.57368200	1.05959300
Tl	-0.30749100	-0.00000200	-0.15637600

$HF_2Tl•••NCH$			
F	0.16090700	1.55621400	1.11097200

H	-4.25472200	-0.00002300	0.26142600
C	-3.22030300	-0.00002700	-0.04286300
N	-2.09182300	-0.00002400	-0.37456200
H	1.03766200	0.00005300	-1.73003100
F	0.16099500	-1.55624500	1.11094000
Tl	0.42326600	0.00000700	-0.19320400

$HF_2Tl•••CO$

F	-0.03778900	1.54727600	1.07792800
C	2.26320200	-0.00000800	-0.36199700
O	3.38340600	-0.00000300	-0.12266600
H	-1.19147800	0.00000700	-1.67044900
F	-0.03780600	-1.54727600	1.07792800
Tl	-0.47869900	0.00000100	-0.17998700

$HF_2Tl•••OCH_2$

F	0.22497400	1.50218300	1.07263500
C	2.61376600	-0.00001200	0.01083500
H	2.25223000	-0.00006800	1.05182400
H	3.70038600	0.00000600	-0.18749100
O	1.82597300	0.00003000	-0.94186600
H	-1.55873000	0.00003400	-1.38492700
F	0.22495900	-1.50223700	1.07256800
Tl	-0.47819300	0.00000400	-0.13970800

$HF_2Tl•••C_2H_4$

C	2.25073800	0.68846800	0.31061900
H	2.03431900	0.58187800	1.37680500
H	2.33435900	1.70052200	-0.09288700
C	2.40628100	-0.40705500	-0.47940600
H	2.64154500	-0.31151900	-1.54354100
H	2.33617200	-1.41264100	-0.05353000
F	-0.04444900	-1.15196700	1.52466400

H	-0.88916000	-0.62437200	-1.68656000
Tl	-0.38711600	-0.09157800	-0.19840900
F	-0.51588100	1.79590800	0.59572900

$HF_2Tl•••OHCH_3$

F	0.21496800	1.54090800	1.02767000
C	2.80578100	0.27726900	-0.12619300
H	2.54128300	0.77974200	0.81324700
H	3.74778300	-0.28007100	-0.03112600
H	2.89562200	1.01791800	-0.92939600
O	1.74648900	-0.63757500	-0.52963200
H	1.61235400	-1.29081200	0.18996300
H	-1.53088800	0.01136800	-1.45606000
Tl	-0.50936400	0.04083400	-0.15949800
F	-0.08322300	-1.55298700	1.11977000

$HF_2Tl•••PH_3$

F	-0.08816800	-1.49388300	1.15430700
H	-2.61801400	0.36399500	1.15559200
H	-3.06072500	-1.10726500	-0.36252800
H	-3.23377300	0.99491000	-0.82030300
P	-2.33041300	0.09455900	-0.20102600
H	1.39267700	-0.21880600	-1.57100300
Tl	0.49992900	-0.03173900	-0.18556300
F	0.30836400	1.61829200	1.02838200

$HF_2Tl•••O(CH_3)_2$

F	0.75951500	1.86940600	0.12564900
C	-2.45723200	-1.05061800	-0.27850300
H	-2.32119100	-1.32164200	0.77986700
H	-3.52234400	-0.89021000	-0.50780900
H	-2.05665300	-1.83941100	-0.92994200
O	-1.71916900	0.15705700	-0.57735300

C	-2.22157700	1.26687700	0.21702700
H	-2.12485700	1.02519400	1.28665900
H	-1.59915900	2.13378700	-0.02811200
H	-3.27461200	1.44155000	-0.05301100
H	1.26544500	-1.16051900	-1.28052400
Tl	0.60728200	-0.15858000	-0.13778100
F	-0.06288200	-0.65805200	1.74999800

$H_2FTl{\bullet\bullet\bullet}OH_2$			
F	-1.17038700	1.47724400	0.01712800
O	-1.98519900	-0.91422500	-0.10965800
H	-2.41837000	-1.26895200	0.67867700
H	-2.11078700	0.07217000	-0.06061300
H	0.64397600	-0.25978500	1.63527100
H	0.69818500	-0.16335900	-1.62778100
Tl	0.36545800	-0.05384500	0.00120400

$H_2FTl{\bullet\bullet\bullet}SH_2$			
F	0.33583800	1.83086200	0.00942100
H	1.90258200	0.94417700	-0.05846000
H	2.55761900	-0.37277200	1.26097300
H	-0.81818800	-0.37105200	-1.62998600
H	-0.77198500	-0.41326900	1.63228700
S	2.41777300	-0.33587400	-0.08266200
Tl	-0.55033300	-0.13445500	0.00040700

$H_2FTl{\bullet\bullet\bullet}NH_3$			
F	-0.82354600	1.70964900	-0.00005700
N	-2.04620200	-0.73705800	0.00008800
H	-2.25877700	0.27002200	0.00003900
H	-2.47628900	-1.15677200	0.82357000
H	-2.47634500	-1.15686600	-0.82331700
H	0.69134500	-0.31312000	1.62660200

H	0.69126500	-0.31326600	-1.62660800
Tl	0.34029800	-0.09330200	-0.00000500

$H_2FTl•••NCH$

F	0.23190200	1.84935500	-0.00014100
H	4.18840400	0.25804500	0.00001300
C	3.18580100	-0.13856400	0.00003600
N	2.08808700	-0.56598000	0.00006200
H	-0.70387500	-0.46253100	1.62786200
H	-0.70384500	-0.46278700	-1.62780200
Tl	-0.47653400	-0.13807000	0.00000700

$H_2FTl•••CO$

F	-0.40194500	1.76223700	0.00001400
C	-2.26555700	-0.48503800	-0.00016300
O	-3.38061200	-0.21793500	-0.00019700
H	0.75400100	-0.43787400	1.62802800
H	0.75434400	-0.43773800	-1.62794700
Tl	0.52774600	-0.12754100	0.00002900

$H_2FTl•••OCH_2$

F	0.49074500	1.78081400	0.00001900
C	2.73741500	-0.01676500	-0.00000600
H	2.42107900	1.04219000	-0.00001600
H	3.81109000	-0.28444100	-0.00000900
O	1.89165700	-0.91892900	0.00000900
H	-0.76372100	-0.36327600	-1.63160900
H	-0.76381000	-0.36342800	1.63156400
Tl	-0.50221100	-0.10625100	-0.00000200

$H_2FTl•••C_2H_4$

C	0.16507900	-2.34899800	0.67907000

H	-0.75301000	-2.12245500	1.22810800
H	1.06583800	-2.59622300	1.24816600
C	0.16507900	-2.34899800	-0.67907000
H	1.06583800	-2.59622300	-1.24816600
H	-0.75301000	-2.12245500	-1.22810800
F	-1.89065800	-0.02962000	0.00000000
H	0.51896600	0.66245600	1.62480000
H	0.51896600	0.66245600	-1.62480000
Tl	0.16507900	0.45144400	0.00000000

$H_2FTl{\bullet\bullet\bullet}OHCH_3$

F	0.33393200	1.83849300	-0.17045100
C	2.82078500	-0.47866000	-0.28266000
H	2.51817500	-0.25954200	-1.31950200
H	3.78727000	0.00317700	-0.07278300
H	2.92261300	-1.56379900	-0.15200100
O	1.82336700	-0.02630200	0.65573300
H	1.61939200	0.92441800	0.44630700
H	-0.29768300	-0.73591600	-1.55673300
H	-1.25465600	-0.07746500	1.49473900
Tl	-0.54089100	-0.14512300	-0.01056600

$H_2FTl{\bullet\bullet\bullet}PH_3$

F	1.65015600	-0.76158700	0.00000000
H	-0.11327700	-2.84855700	1.06711600
H	-0.11327700	-2.84855700	-1.06711600
H	-1.95597900	-3.09403900	0.00000000
P	-0.81694500	-2.24104400	0.00000000
H	-0.20734800	0.92771500	-1.62655900
H	-0.20734800	0.92771500	1.62655900
Tl	0.00000000	0.58525500	0.00000000

$H_2FTl{\bullet\bullet\bullet}O(CH_3)_2$

F	0.61137900	1.90915500	0.00105200
C	-2.55805600	-1.13594800	0.08930700
H	-2.50261700	-1.18647400	1.19108000
H	-3.61058600	-1.03600700	-0.22303600
H	-2.13090000	-2.04817400	-0.34923500
O	-1.79186900	-0.02774300	-0.40451900
C	-2.31586500	1.22843800	0.08589300
H	-2.33246900	1.22173300	1.18925200
H	-1.63211500	2.00958600	-0.26374000
H	-3.33625600	1.37078100	-0.30530900
H	0.42822700	-0.56971300	1.63901200
H	1.11819000	-0.60665200	-1.54505900
Tl	0.64289600	-0.20580800	0.01040200

$H_2ClTl{\bullet\bullet\bullet}OH_2$

Cl	2.03775600	-0.57105800	0.00814900
O	0.56574400	2.15451000	-0.10158600
H	0.57211400	2.70584400	0.69432200
H	1.45038700	1.73440200	-0.11793400
H	-0.87022500	-0.12842700	1.62988000
H	-0.87172800	-0.23316900	-1.62065100
Tl	-0.48701700	-0.14329300	0.00109300

$H_2ClTl{\bullet\bullet\bullet}SH_2$

Cl	-0.22059200	2.13705300	0.00324500
H	2.19293200	0.98481700	-0.45528900
H	2.52831300	0.10831500	1.24422300
H	-0.64357000	-0.75381700	-1.62622900
H	-0.64680200	-0.77536800	1.62174300
S	2.50964200	-0.27191900	-0.05301100
Tl	-0.49179100	-0.38942200	0.00010600

$H_2ClTl\bullet\bullet\bullet NH_3$			
Cl	2.11487400	-0.29366900	-0.00005300
N	0.06667600	2.21785000	0.00008400
H	1.08627800	2.10985900	0.00001500
H	-0.18657400	2.76577600	0.82286200
H	-0.18667900	2.76588200	-0.82259100
H	-0.84541700	-0.38182300	1.62065800
H	-0.84548000	-0.38169800	-1.62065500
Tl	-0.43755200	-0.21494500	0.00000000

$H_2ClTl\bullet\bullet\bullet NCH$			
Cl	-0.13026100	2.12642800	0.00000000
H	4.30934300	0.17022400	0.00000300
C	3.27957100	-0.14961200	0.00000100
N	2.15229700	-0.49106800	-0.00000100
H	-0.59851200	-0.76995200	1.62119100
H	-0.59851000	-0.76996100	-1.62118800
Tl	-0.44001700	-0.37585700	0.00000000

$H_2ClTl\bullet\bullet\bullet CO$			
Cl	-0.11204400	2.09462200	-0.00002200
C	-2.29965300	-0.58172700	-0.00014300
O	-3.43249500	-0.40449900	-0.00024200
H	0.68262900	-0.72220400	1.62117400
H	0.68275100	-0.72224400	-1.62107700
Tl	0.51601500	-0.33873800	0.00003800

$H_2ClTl\bullet\bullet\bullet OCH_2$			
Cl	-0.72540600	-1.98524300	-0.00000500
C	-2.71807300	0.75575600	0.00001300
H	-2.71665200	-0.34954700	0.00006500
H	-3.67992700	1.30229300	-0.00001000
O	-1.65916400	1.38970900	-0.00002100

H	0.86519500	0.47087800	-1.62525700
H	0.86516400	0.47088900	1.62526400
Tl	0.57506000	0.20003000	0.00000100

$H_2ClTl{\bullet\bullet\bullet}C_2H_4$

C	-1.42280800	-1.93273000	0.67937800
H	-1.95126500	-1.15207400	1.23391100
H	-0.92096700	-2.72155400	1.24698200
C	-1.42280800	-1.93273000	-0.67937800
H	-0.92096700	-2.72155400	-1.24698200
H	-1.95126500	-1.15207400	-1.23391100
Cl	-1.42280800	1.60768400	0.00000000
H	0.96382200	-0.11111100	1.61878700
H	0.96382200	-0.11111100	-1.61878700
Tl	0.55652100	0.04730400	0.00000000

$H_2ClTl{\bullet\bullet\bullet}OHCH_3$

Cl	0.31284700	2.11367300	-0.05181900
C	2.71547700	-0.76056400	-0.37151100
H	2.48789200	-0.13053500	-1.24505200
H	3.75212400	-0.59324700	-0.04630900
H	2.57777600	-1.81850700	-0.62699900
O	1.80040100	-0.47299100	0.71597800
H	1.82334700	0.49693300	0.84754000
H	-0.29035500	-0.81877500	-1.58839500
H	-1.28557900	-0.41061400	1.48105600
Tl	-0.55653900	-0.30012800	-0.01777400

$H_2ClTl{\bullet\bullet\bullet}PH_3$

Cl	1.73919700	-1.19842500	0.00000000
H	-1.15952100	-2.64294500	1.06802100
H	-1.15952100	-2.64294500	-1.06802100
H	-2.96783800	-2.19596200	0.00000000

P	-1.59572000	-1.82154400	0.00000000
H	-0.17183000	1.04309400	-1.62109100
H	-0.17183000	1.04309400	1.62109100
Tl	0.00000000	0.65545700	0.00000000

$H_2ClTl\cdots O(CH_3)_2$			
C	-2.85896700	-0.49676400	-0.07169700
H	-2.87532300	-0.68536000	1.01627000
H	-3.83763500	-0.10551900	-0.39395400
H	-2.64049400	-1.42851600	-0.61111700
O	-1.82163200	0.43881200	-0.40738700
C	-2.03971800	1.71049200	0.24267600
H	-2.04164800	1.57883600	1.33868700
H	-1.20841600	2.36030500	-0.05243900
H	-3.00517500	2.12688100	-0.08748100
H	0.08945700	-0.73108600	1.66707700
H	0.63668300	-1.18314300	-1.49871700
Tl	0.41956700	-0.52742500	0.02886600
Cl	1.46251600	1.76448100	-0.08724900

12. Carbon Bonded Complexes

$NO_2H_3C\cdots OH_2$			
C	0.26483000	-0.00167400	0.08610200
H	0.57842500	0.90425500	0.61264700
H	0.64101800	0.00676700	-0.94380100
H	0.57722600	-0.91627900	0.59808300
H	3.86736500	0.76041400	-0.06831500
H	3.86744600	-0.76024500	-0.06807400
N	-1.22612400	0.00007200	0.01117500
O	-1.79662200	-1.09885700	-0.03422300
O	-1.79343600	1.10062500	-0.03400100
O	3.27285800	0.00006000	-0.02244800

$NO_2H_3C\bullet\bullet\bullet SH_2$			
C	-0.45729800	0.03536500	-0.07055600
H	-0.15578400	1.02997700	-0.41195100
H	-0.13203500	-0.76037400	-0.74863700
H	-0.08492500	-0.16091100	0.94245200
H	3.50827000	0.97189800	0.76756200
H	3.48804800	-0.97935800	0.76877000
S	3.12638400	-0.00040900	-0.08728100
N	-1.94891400	-0.00137600	-0.00541500
O	-2.55011800	1.08112900	0.03588000
O	-2.48232200	-1.11828500	0.03156200

$NO_2H_3C\bullet\bullet\bullet NH_3$			
C	0.22679700	-0.00811600	0.03052100
H	0.56532900	0.12834600	-1.00337300
H	0.55889900	-0.97398400	0.41974400
H	0.56102700	0.83234400	0.64552800
N	3.40247600	-0.00093900	-0.00958700
H	3.79683500	0.86810900	-0.37172700
H	3.79567400	-0.74587900	-0.58608200
H	3.80901900	-0.12467900	0.91846200
N	-1.26670900	-0.00044300	0.01005600
O	-1.82711500	1.10426800	-0.01290200
O	-1.84762600	-1.09500400	-0.01321900

$NO_2H_3C\bullet\bullet\bullet NCH$			
C	0.22530000	-0.02238800	0.02132000
H	-0.09895000	-1.01551000	0.34382400
H	-0.10989700	0.18536000	-1.00210700
H	-0.11775600	0.77146100	0.69197700
H	-5.13968400	0.01147900	-0.00913600
N	-2.88003900	-0.00614000	-0.00244400

C	-4.06199400	0.00304100	-0.00588400
N	1.71824000	0.00063100	0.00849600
O	2.31252500	-1.08682500	-0.01031400
O	2.26485600	1.11205800	-0.00962900

$NO_2H_3C\cdots CO$			
C	-0.30653300	0.00675400	-0.02618200
H	0.02457600	-0.82304100	-0.65894000
H	0.02606400	-0.15226800	1.00732500
H	0.02561300	0.98098900	-0.39679100
C	3.07530200	-0.01290600	0.01452600
O	4.22458700	0.00917500	0.00004200
N	-1.79989500	0.00133400	-0.00956600
O	-2.37729900	1.09717800	0.01174000
O	-2.35848700	-1.10361600	0.01138100

$NO_2H_3C\cdots OCH_2$			
C	-0.33372000	0.00552900	0.05139100
H	-0.00295300	-0.90978900	0.55066700
H	-0.01302400	0.91136500	0.57414000
H	0.01699300	0.02191200	-0.98769300
H	4.42111700	0.10865900	0.95000900
H	4.45795100	-0.16505000	-0.92189000
C	3.85886600	-0.01252400	0.00029900
O	2.63478800	0.02056300	-0.02866000
N	-1.82572700	-0.00203200	0.01130700
O	-2.39132100	-1.10430100	-0.00587100
O	-2.39982600	1.09487400	-0.03478400

$NO_2H_3C\cdots PH_3$			
C	-0.53433600	-0.01524600	0.02429500
H	-0.19910500	0.22028000	-0.99361000
H	-0.20579600	-1.01438900	0.32484200

H	-0.19985300	0.76493600	0.71615100
P	3.18116300	-0.00129400	-0.00342400
H	3.93386100	0.27027500	-1.18302800
H	3.95041100	-1.14884000	0.34741600
H	3.94299600	0.88638800	0.81103900
N	-2.02778100	-0.00063500	0.00817200
O	-2.57764800	1.10863300	-0.01066100
O	-2.61478600	-1.09154700	-0.01114200

$NO_2H_3C\bullet\bullet\bullet HF$

C	0.28243400	-0.00662700	0.01955900
H	0.61188100	0.23570000	-0.99838600
H	0.61767200	-1.00486300	0.31456500
H	0.61369700	0.77247800	0.71381100
H	4.17197500	0.02786600	0.03710700
F	3.24871000	-0.00649100	-0.01264700
N	-1.21045100	-0.00110300	0.00870200
O	-1.76771500	1.10460300	-0.00823900
O	-1.79166700	-1.09526400	-0.00820400

$NO_2H_3C\bullet\bullet\bullet C_2H_2$

C	0.10958200	-0.09842400	0.03108800
H	-0.26184500	0.30603800	-0.91800200
H	-0.24905300	0.51765200	0.86306400
H	-0.15870800	-1.15214400	0.15128800
C	-3.29525900	-0.60562600	0.00289500
H	-3.35059900	-1.67972100	0.02175200
C	-3.24899000	0.62528800	-0.01936700
H	-3.21967100	1.70048200	-0.03907800
N	1.59919800	0.00298200	0.00412900
O	2.07893800	1.14426700	0.00043600
O	2.25274900	-1.04934300	-0.02488900

$NO_2H_3C\bullet\bullet\bullet HCl$			
C	-0.41593500	0.10153800	0.00345100
H	-0.15291500	1.16333200	0.02229000
H	-0.05017900	-0.39567100	-0.90255100
H	-0.05022200	-0.42936800	0.88995400
H	3.50547100	-1.14144300	-0.00901100
Cl	3.06599000	0.06991300	-0.00014400
N	-1.90525200	-0.00937300	0.00062100
O	-2.56677400	1.03817800	-0.00227900
O	-2.37592700	-1.15430200	-0.00063100

$NF_2H_3C\bullet\bullet\bullet OH_2$			
C	-0.28206600	0.00036700	0.19110700
H	-0.70931900	-0.89728400	0.65318500
H	-0.43828100	0.00017400	-0.89609100
H	-0.70885900	0.89844200	0.65278700
H	-4.06127300	0.00170500	0.53700800
H	-3.74219200	-0.00215600	-0.94958400
N	1.14688100	0.00008100	0.51468000
O	-3.31865400	0.00000100	-0.08110200
F	1.65990500	1.10100400	-0.22790000
F	1.65935900	-1.10141100	-0.22742100

$NF_2H_3C\bullet\bullet\bullet SH_2$			
C	0.42612000	-0.00179900	-0.29744100
H	0.03982000	-0.90240800	-0.79055300
H	0.04002000	0.89462600	-0.79834200
H	0.18211900	0.00260600	0.77345800
H	-3.44099800	-1.06793700	0.73215100
H	-3.37760800	0.86301000	0.99892500
S	-3.18816500	0.01450000	-0.03359100
N	1.87709400	-0.00275000	-0.50617700
F	2.32609700	-1.10063900	0.27946400

F	2.32622500	1.10154300	0.27050400

$NF_2H_3C\bullet\bullet\bullet NH_3$			
C	-0.23865100	0.00013100	-0.24489500
H	-0.43963800	0.00011200	0.83434300
H	-0.64817100	-0.89665100	-0.72422300
H	-0.64796600	0.89693300	-0.72433600
N	-3.44223500	0.00003600	0.09907100
H	-3.74547600	0.81450700	0.63422000
H	-3.74482600	-0.81394000	0.63533900
H	-4.00645300	-0.00076500	-0.75140000
N	1.20220700	-0.00006300	-0.51366500
F	1.68594300	1.10143400	0.24821600
F	1.68568400	-1.10152200	0.24818300

$NF_2H_3C\bullet\bullet\bullet NCH$			
C	-0.19895000	0.00100600	-0.24065900
H	0.20830500	-0.89611800	-0.72218800
H	0.00537000	0.00089400	0.83832700
H	0.20673200	0.89911100	-0.72170800
H	5.18933800	-0.00114100	0.20694900
N	2.93801500	0.00059900	0.00977700
C	4.11573700	-0.00036400	0.11223300
N	-1.64032500	-0.00017900	-0.50518200
F	-2.12279900	1.10076500	0.25784900
F	-2.12101300	-1.10182500	0.25737500

$NF_2H_3C\bullet\bullet\bullet CO$			
C	-0.27870800	-0.00094100	-0.27073400
H	0.11431700	-0.90030000	-0.76107400
H	-0.05348800	-0.00090600	0.80451900
H	0.11547600	0.89765200	-0.76124300
C	3.13138700	0.00134000	-0.01820500

O	4.27047700	-0.00076600	0.13727700
N	-1.72617800	-0.00003000	-0.50261700
F	-2.18664500	1.10146400	0.27044900
F	-2.18812700	-1.10063000	0.27083300

$NF_2H_3C\bullet\bullet\bullet C_2H_4$			
C	0.21950300	-0.01863400	-0.25299900
H	0.01564100	0.16923800	0.81004000
H	-0.20473400	-0.97758400	-0.57580200
H	-0.16675000	0.79272200	-0.88240200
C	-3.15485200	0.62526100	0.37062900
H	-3.03405500	0.73080000	1.45208100
H	-3.22290900	1.54345600	-0.21890800
C	-3.22992200	-0.59005200	-0.21176100
H	-3.36076100	-0.69510100	-1.29218600
H	-3.17189200	-1.50800500	0.37932100
N	1.66125400	-0.09272900	-0.50675200
F	2.11639500	-1.05743400	0.43455700
F	2.16230500	1.11233700	0.05876600

$NF_2H_3C\bullet\bullet\bullet PH_3$			
C	-0.50112300	-0.00130800	-0.29210900
H	-0.26321600	-0.00118700	0.78050300
H	-0.11146700	0.89684700	-0.78726100
H	-0.11317300	-0.90050900	-0.78672100
P	3.23307600	-0.00007400	0.03899400
H	3.70223300	0.00213700	1.38525200
H	4.11200600	1.04297700	-0.37552500
H	4.11332800	-1.04318200	-0.37256500
N	-1.95102800	-0.00001100	-0.50762400
F	-2.40502100	-1.10039600	0.27131900
F	-2.40297000	1.10172500	0.27061700

$NF_2H_3C\bullet\bullet\bullet HF$			
C	0.29927600	0.00096300	-0.19486600
H	0.46010800	0.00091200	0.89170900
H	0.72086200	0.89995300	-0.66101500
H	0.72199500	-0.89732700	-0.66120000
H	4.19767700	0.01570600	0.22157800
F	3.28189100	-0.00219100	0.09147800
N	-1.13102300	0.00011500	-0.51351300
F	-1.63911400	-1.10137000	0.23042100
F	-1.64045900	1.10069200	0.23062500

$NF_2H_3C\bullet\bullet\bullet C_2H_2$			
C	0.07726200	-0.00803500	-0.18779700
H	-0.07234800	0.01018200	0.90077900
H	-0.34740800	-0.91696600	-0.63152100
H	-0.35394300	0.88185100	-0.66263100
C	-3.39672300	-0.01670900	-0.52567500
H	-3.53342800	-0.04898400	-1.59206500
C	-3.25272300	0.02038500	0.69727800
H	-3.13821500	0.05281600	1.76630300
N	1.50472400	-0.00868000	-0.51947100
F	2.02315900	-1.09482700	0.23864100
F	2.01521600	1.10682900	0.20053700

$NF_2H_3C\bullet\bullet\bullet HCl$			
C	-0.38043500	-0.05983500	-0.25839300
H	-0.01707600	-0.99428300	-0.70443700
H	-0.16807400	-0.02317200	0.81893200
H	0.05228800	0.80225800	-0.78100600
H	3.40326000	0.49300100	1.14312000
Cl	3.12119100	-0.02695300	-0.00158800
N	-1.82408700	-0.01534300	-0.50814500
F	-2.33578100	-1.06312700	0.30596900

F	-2.25082300	1.13499500	0.21155900

$HOH_3C\bullet\bullet\bullet OH_2$

C	0.72490600	0.00764400	0.00785600
H	0.35440800	0.91927300	-0.48749900
H	0.34162500	-0.01244300	1.03457900
H	0.33817400	-0.87337900	-0.52905700
O	-2.40229800	0.00404800	-0.03982800
H	-3.02239100	0.72776500	0.11883200
H	-2.93771700	-0.78989200	0.08856800
O	2.15996900	-0.00779000	0.10484100
H	2.51509300	0.01275200	-0.79266400

$HOH_3C\bullet\bullet\bullet SH_2$

C	1.49943500	0.00623400	-0.00086300
H	1.12475500	-0.52818200	-0.88952400
H	1.10917700	1.03115300	-0.01967600
H	1.12313000	-0.49581100	0.90578800
H	-2.47750000	0.73899600	-0.99217100
H	-2.47813500	0.78396800	0.95702700
S	-2.13424700	-0.10615100	0.00255900
O	2.93181500	0.11392600	-0.00153000
H	3.29539300	-0.78052400	0.01503800

$HOH_3C\bullet\bullet\bullet NH_3$

C	0.78348200	-0.00899400	0.00022000
H	0.41094100	-0.52890700	0.89702300
H	0.41050500	-0.52951100	-0.89605300
H	0.38575800	1.01268700	-0.00003200
N	-2.50711200	-0.02088800	0.00010000
H	-2.81210300	0.50968800	0.81667800
H	-3.06517400	-0.87517800	-0.00501100
H	-2.80808900	0.51675200	-0.81334200

O	2.21763500	0.10967700	-0.00018400
H	2.58597800	-0.78276700	0.00018900

$HOH_3C{\bullet\bullet\bullet}NCH$

C	-1.31164700	-0.00498200	0.00011000
H	-0.93752200	0.51334500	0.89757100
H	-0.93732900	0.51358800	-0.89707300
H	-0.91930000	-1.02895200	0.00002000
H	4.13961300	-0.11738900	0.00027100
N	1.88692400	0.06708600	-0.00017900
C	3.06555300	-0.02923200	0.00006500
O	-2.74603600	-0.11550100	-0.00007900
H	-3.10907900	0.77910500	0.00005200

$HOH_3C{\bullet\bullet\bullet}CO$

C	-1.40330300	-0.00471700	-0.00920700
H	-1.04020800	0.53069200	-0.90199800
H	-1.01810700	-1.03160000	-0.03715200
H	-1.01185900	0.49293300	0.89359100
C	2.01436500	0.04500800	-0.04574000
O	3.16003400	-0.02005400	0.03085100
O	-2.83509500	-0.10764800	0.01176300
H	-3.19570900	0.78784800	0.03433200

$HOH_3C{\bullet\bullet\bullet}OCH_2$

C	-1.41383400	0.01044800	0.00056400
H	-1.03824100	1.04026500	-0.00236100
H	-1.03186900	-0.50534100	-0.89499500
H	-1.03255400	-0.50002400	0.89950800
H	3.47611300	0.93473100	-0.00228500
H	3.46542000	-0.95713500	0.00180900
C	2.88806100	-0.00785800	-0.00017100
O	1.66384500	-0.00069800	-0.00002400

O	-2.84957000	0.09753500	0.00009600
H	-3.19842800	-0.80273800	-0.00461200

$HOH_3C•••HCl$

C	-1.40627700	0.04829500	0.00658000
H	-0.99617400	-0.45950800	-0.88273700
H	-1.01087500	-0.43473600	0.91603500
H	-1.07994200	1.09617400	-0.00509900
H	3.29150800	0.07015700	0.02404200
O	-2.84114700	0.07114500	-0.00567200
H	-3.15153800	-0.84328200	0.00357100
Cl	2.00669800	-0.01692600	-0.00293600

$HOH_3C•••PH_3$

C	1.55927500	-0.04902600	-0.00215900
H	1.20996200	-0.58430300	0.89642500
H	1.21533700	-0.59099000	-0.89883900
H	1.11617800	0.95506900	-0.00720100
P	-2.13557400	-0.07733900	0.00079400
H	-3.10695200	-0.00570900	1.04274100
H	-3.10901400	-0.01905800	-1.04006400
H	-1.90435400	1.33038200	-0.00846000
O	2.98271600	0.13801000	0.00131900
H	3.39508000	-0.73523800	0.00588800

$HOH_3C•••HF$

C	0.70417100	-0.01367700	-0.00082500
H	0.32337800	0.50006600	-0.89830400
H	0.32120900	0.49577500	0.89834900
H	0.33216100	-1.04533000	-0.00405000
H	-3.30952500	-0.05487700	0.02094500
F	-2.38801800	0.01903700	-0.00247700
O	2.13907800	-0.09837700	0.00099300

H	2.48729100	0.80210800	0.00235200

$HOH_3C\cdots C_2H_2$			
C	-1.12007100	0.00372600	-0.00573100
H	-0.73674000	-0.11115300	-1.02697900
H	-0.73834300	-0.82769200	0.61012400
H	-0.74276000	0.95472500	0.40624000
C	2.31470100	0.61289700	0.00098600
H	2.33795000	1.68794100	-0.00967200
C	2.29368800	-0.61874500	0.01018800
H	2.27986600	-1.69401100	0.01581000
O	-2.55248000	-0.01095700	-0.10216200
H	-2.91004600	0.09057500	0.78911400

13. Silicon Bonded Complexes

$FH_3Si\cdots OH_2$			
H	0.00860200	1.23600300	-0.68957000
H	0.04102300	-0.00030900	1.44339200
H	0.00865000	-1.23577000	-0.69006700
F	2.09163400	0.00002300	-0.01022300
O	-2.38325700	0.00000100	-0.08214400
H	-2.86778000	0.76303900	0.25993000
H	-2.86793600	-0.76291800	0.25997500
Si	0.42277100	-0.00001800	0.01182200

$FH_3Si\cdots SH_2$			
H	0.69211100	1.22940000	-0.71991200
H	0.66463500	-0.00005900	1.40623500
H	0.69214700	-1.22938900	-0.71998700
F	2.77481200	0.00001300	0.01696700
H	-2.52964400	0.97543600	0.81241000
H	-2.52975300	-0.97532000	0.81251700
Si	1.11124500	-0.00001100	-0.00704300

S	-2.34501500	-0.00000200	-0.10283500

$FH_3Si•••NH_3$			
H	-0.02127000	-0.24337000	-1.42455900
H	-0.02124300	-1.11200100	0.92303300
H	-0.02126300	1.35539200	0.50149200
F	-2.03302800	-0.00000600	0.00000900
N	2.20810000	0.00000000	0.00000000
H	2.59661600	0.72675500	-0.60241000
H	2.59653000	-0.88512400	-0.32816400
H	2.59650400	0.15831800	0.93064000
Si	-0.34895200	0.00000600	-0.00000800

$FH_3Si•••PH_3$			
H	0.74889300	0.86177500	-1.12640400
H	0.74889700	0.54460600	1.30951900
H	0.74889200	-1.40639000	-0.18311700
F	2.84298900	0.00000000	-0.00000100
P	-2.33780800	-0.00000100	0.00000100
H	-3.09209500	1.19859200	0.15609200
H	-3.09212100	-0.73446900	0.95995200
H	-3.09210400	-0.46410200	-1.11605700
Si	1.17927500	0.00000100	0.00000100

$FH_3Si•••CO$			
H	0.57707100	1.39051400	0.27014900
H	0.57634700	-0.92829300	1.06928700
H	0.57566100	-0.46096900	-1.33838700
F	2.67498500	-0.00050400	-0.00042200
Si	1.01352000	0.00024000	0.00020100
C	-2.20001400	0.00093700	0.00077400
O	-3.34914200	-0.00071100	-0.00059000

$FH_3Si\bullet\bullet\bullet NCH$			
H	0.49491000	0.94741000	1.06091400
H	0.49527000	-1.39269700	0.29006800
H	0.49505300	0.44493600	-1.35108000
F	2.57494500	0.00018100	0.00003400
H	-4.25907000	0.00078000	0.00008200
N	-2.00001000	-0.00036700	-0.00003400
C	-3.18113900	0.00023900	0.00002900
Si	0.90616000	-0.00006600	-0.00001600

$FH_3Si\bullet\bullet\bullet OHCH_3$			
H	0.37578600	-0.59947300	1.18199500
H	0.43625700	-0.46662300	-1.28772600
H	0.84608100	1.57219900	0.07982000
F	2.56038500	-0.24875700	0.01947300
O	-1.63819600	0.63130600	-0.10829800
C	-2.44645300	-0.55451700	0.02467900
H	-2.11735600	-1.23776100	-0.76827200
H	-2.29451600	-1.03729400	1.00344600
H	-3.51372300	-0.32617700	-0.11804000
H	-1.91779700	1.26445300	0.56735500
Si	0.92329200	0.09615300	-0.00825200

$FH_3Si\bullet\bullet\bullet O(CH_3)_2$			
H	-0.64905800	-0.00205800	1.30039500
H	-0.94021500	1.25079600	-0.82796300
H	-0.94042600	-1.24795800	-0.83191400
F	-2.86012400	-0.00005000	0.15338500
O	1.29364400	0.00003500	-0.42047600
C	1.88142900	1.17750100	0.14564400
H	1.39858000	2.03995400	-0.33075800
H	1.71236700	1.21015700	1.23732800

H	2.96570100	1.19962600	-0.05725700
C	1.88097600	-1.17773500	0.14560400
H	1.39804500	-2.03995000	-0.33120100
H	2.96528100	-1.20003900	-0.05702100
H	1.71156400	-1.21052500	1.23720800
Si	-1.20030800	0.00011200	-0.07878300

$FH_3Si{\bullet\bullet\bullet}NCCH_3$

H	1.27564500	-0.80331100	-1.17857900
H	1.27564800	1.42233500	-0.10638700
H	1.27565800	-0.61903500	1.28497900
F	3.34447800	0.00000100	-0.00000700
N	-1.14730900	0.00000700	0.00001000
C	-2.33080000	0.00000200	0.00000300
Si	1.67191400	-0.00000200	0.00000200
C	-3.80063500	-0.00000300	-0.00000700
H	-4.17141600	-0.58421800	-0.85376400
H	-4.17142700	-0.44727100	0.93281200
H	-4.17142700	1.03147600	-0.07907500

$FH_3Si{\bullet\bullet\bullet}NH_2CH_3$

H	0.38067700	-0.54305000	-1.26437700
H	0.88908900	1.59602400	-0.00000400
H	0.38067000	-0.54307200	1.26436000
F	2.45843900	-0.28081200	0.00000200
N	-1.47315900	0.62257900	0.00000300
H	-1.68779100	1.19889400	-0.81590000
H	-1.68779000	1.19888100	0.81591700
Si	0.80913900	0.11171400	-0.00000100
C	-2.31457400	-0.59155900	-0.00000200
H	-2.06698500	-1.18700000	-0.89004600
H	-2.06696800	-1.18701500	0.89002700
H	-3.39524100	-0.37905200	0.00001000

$ClH_3Si\cdots OH_2$			
H	-0.53653400	1.23466600	-0.68473600
H	-0.50672100	-0.00043600	1.44677600
H	-0.53650700	-1.23431400	-0.68544500
O	-2.96136500	0.00001100	-0.08120100
H	-3.46381400	0.76292400	0.23431400
H	-3.46389800	-0.76284100	0.23432700
Si	-0.12393800	-0.00002200	0.01720900
Cl	1.99609000	0.00001300	-0.00803300

$ClH_3Si\cdots SH_2$			
H	0.12826600	1.22922200	-0.72544600
H	0.10294800	-0.00190300	1.39708300
H	0.12844400	-1.22761700	-0.72858800
H	-3.10508400	0.97568600	0.81963600
H	-3.10555100	-0.97503100	0.82025700
S	-2.94069500	-0.00000500	-0.09923500
Cl	2.65997600	0.00004800	0.01291200
Si	0.54875000	-0.00007900	-0.01533500

$ClH_3Si\cdots NH_3$			
H	-0.51591500	0.16162800	1.43710600
H	-0.51589900	-1.32540000	-0.57859200
H	-0.51590300	1.16376200	-0.85854500
Cl	1.94760400	0.00000200	0.00000500
N	-2.75317900	0.00000100	0.00000200
H	-3.14201300	0.86484500	0.37862800
H	-3.14203300	-0.76029300	0.55969000
H	-3.14209600	-0.10452900	-0.93825200
Si	-0.20451100	-0.00000300	-0.00001000

$ClH_3Si\cdots PH_3$			
H	0.83971800	0.84412800	-0.78887200
H	-0.39457400	-1.26227800	-0.53942000
H	-0.82830000	0.60319400	0.99503200
P	2.09212700	-1.01041700	1.81974500
H	3.22487700	-1.73078700	1.34196500
H	1.80233400	-1.93622300	2.86340800
H	2.85501800	-0.13978400	2.65060400
Si	-0.43345500	0.20934000	-0.37701800
Cl	-1.93015300	0.93219000	-1.67886100

$ClH_3Si\cdots CO$			
Si	0.42718900	-0.00001000	-0.00000800
H	-0.01213500	-0.65538300	1.25360200
H	-0.01211700	-0.75799300	-1.19438200
H	-0.01214100	1.41333200	-0.05925200
Cl	2.53425400	0.00000800	0.00000700
C	-2.84519200	-0.00001500	-0.00001700
O	-3.99442800	0.00001700	0.00001600

$ClH_3Si\cdots NCH$			
H	-0.08312300	-1.12015400	-0.87489100
H	-0.08284100	1.31802100	-0.53277100
H	-0.08306100	-0.19735700	1.40764800
Cl	2.44641700	-0.00012600	0.00001000
H	-4.87112200	-0.00083500	0.00003800
N	-2.61183000	0.00033800	-0.00001400
C	-3.79314500	-0.00028400	0.00001600
Si	0.32662400	0.00012900	-0.00001400

$ClH_3Si\cdots OHCH_3$			
H	-0.12504500	-0.55177500	1.16899900

H	-0.07998600	-0.38344200	-1.29674000
H	0.24382000	1.65124900	0.09512800
O	-2.22407600	0.60461900	-0.10174700
C	-2.97263500	-0.62066700	0.02458100
H	-2.60200500	-1.28698800	-0.76454300
H	-2.80617500	-1.09498200	1.00518200
H	-4.04872800	-0.44721900	-0.12855300
H	-2.54450700	1.22420300	0.56839700
Cl	2.48326400	-0.16380100	0.01113500
Si	0.38396800	0.18290100	-0.01219100

$ClH_3Si\bullet\bullet\bullet OCH_2$

H	0.02163600	-0.92949700	-1.23677800
H	-0.27940900	1.18376600	-0.00001800
H	0.02163600	-0.92947800	1.23678700
H	-4.24867900	0.37827500	0.00000900
H	-2.72306700	1.50378000	-0.00000500
C	-3.14467800	0.47681900	0.00000100
O	-2.41807200	-0.51131300	-0.00000100
Si	0.31546900	-0.17456400	-0.00000100
Cl	2.41199800	0.14509700	0.00000100

$ClH_3Si\bullet\bullet\bullet C_2H_4$

H	-0.06022200	0.00108300	1.41111200
H	-0.06074200	-1.22658800	-0.71147500
H	-0.06080300	1.22537100	-0.71344200
C	-2.95460300	0.67551800	0.00645200
H	-2.84981800	1.24344100	0.93494000
H	-3.06788000	1.24375300	-0.92038200
C	-2.95450600	-0.67551200	0.00645400
H	-3.06770500	-1.24376500	-0.92037800
H	-2.84964700	-1.24341600	0.93494600
Si	0.37452900	-0.00002800	-0.00471400

Cl	2.48400400	0.00002800	-0.00157500

$ClH_3Si\bullet\bullet\bullet O(CH_3)_2$			
H	-0.18457000	-0.00040000	1.26129400
H	-0.41548900	1.24921000	-0.87570600
H	-0.41546800	-1.24918300	-0.87594200
O	1.81831700	0.00001900	-0.41062400
C	2.39200800	1.17803100	0.16929300
H	1.91958400	2.04025500	-0.31815200
H	2.19787100	1.21045900	1.25683300
H	3.48057400	1.20125600	-0.00852000
C	2.39183000	-1.17803100	0.16925900
H	1.91945900	-2.04023600	-0.31827100
H	3.48042800	-1.20138400	-0.00839200
H	2.19759700	-1.21059800	1.25678500
Cl	-2.81033400	0.00003600	0.10275100
Si	-0.68956400	-0.00001100	-0.13307200

$CNH_3Si\bullet\bullet\bullet OH_2$			
Si	0.02562500	-0.00059800	0.01867300
H	0.40857000	1.24669500	-0.67367500
H	0.40793500	-1.23300300	-0.70011600
H	0.37643200	-0.01595600	1.45403100
O	2.77736800	0.00040400	-0.07561400
H	3.30168100	0.76444000	0.19910700
H	3.30322700	-0.76252700	0.19921700
N	-1.78327900	0.00025400	-0.00373600
C	-2.98209800	0.00062000	-0.01815300

$CNH_3Si\bullet\bullet\bullet SH_2$			
Si	0.68672300	0.00001400	-0.01055000
H	0.28907800	1.23281500	-0.72332800

H	0.27197600	-0.00018000	1.40885800
H	0.28911200	-1.23260500	-0.72366400
H	-2.96236300	0.97580900	0.81014300
H	-2.96238000	-0.97580400	0.81016400
S	-2.75408900	-0.00001000	-0.09974400
N	2.48699600	0.00003400	0.00640600
C	3.68615100	-0.00005100	0.01943100

$CNH_3Si\bullet\bullet\bullet NH_3$

Si	-0.11270100	0.00295100	-0.02040000
H	-0.20487300	1.24096200	-0.82324400
H	-0.63134800	0.06393100	1.36271600
H	-0.28538000	-1.27552500	-0.74248400
N	-2.53002900	0.06624500	-0.45793100
H	-2.74560400	0.04085400	-1.45591400
H	-2.97016600	0.91091400	-0.08928500
H	-3.02252000	-0.72296800	-0.03640600
N	1.69783400	-0.04445500	0.30730500
C	2.87717900	-0.07533600	0.52076700

$CNH_3Si\bullet\bullet\bullet PH_3$

Si	0.73869800	0.01789100	-0.14554800
H	0.32614500	1.42678500	0.03164000
H	0.58785700	-0.78245500	1.08866000
H	0.10897400	-0.61952400	-1.32186800
P	-2.71004800	-0.06559300	0.53395400
H	-3.65669800	0.59500800	-0.30028300
H	-3.24902300	0.44443000	1.74963200
H	-3.43587100	-1.28981200	0.58837600
N	2.50537800	0.06063400	-0.49363300
C	3.68165300	0.08909200	-0.72539200

$CNH_3Si\cdots CO$			
Si	0.51571500	-0.00027800	-0.24345600
H	-0.41935100	0.53972200	-1.25417600
H	0.62120000	0.86723400	0.94977400
H	0.22115300	-1.40723500	0.10469200
C	-2.40466200	0.00119000	1.13515800
O	-3.44349100	0.00178100	1.62554400
N	2.14049100	-0.00107800	-1.01044300
C	3.22491000	-0.00161100	-1.52235100

$CNH_3Si\cdots NCH$			
Si	-0.40862900	-0.06419500	0.17052200
H	0.04328300	1.22083800	0.74177200
H	-0.60991400	-0.02404500	-1.29226100
H	0.38035900	-1.22603300	0.62822700
H	4.25808200	0.66897000	-1.77690700
N	2.19496300	0.34487900	-0.91595000
C	3.27343900	0.51429500	-1.36600700
N	-2.06054200	-0.32374800	0.85986000
C	-3.15543000	-0.49578000	1.31675400

$CNH_3Si\cdots OHCH_3$			
Si	0.49096100	0.18077400	-0.01155900
H	0.02961800	-0.55915800	1.18383400
H	0.06694400	-0.40960900	-1.29715600
H	0.38529100	1.65096900	0.08558000
O	-2.01443000	0.58159600	-0.09778700
C	-2.79509700	-0.62628200	0.02510900
H	-2.41787600	-1.31252000	-0.74344600
H	-2.66744000	-1.08655400	1.01765100
H	-3.86063100	-0.42729200	-0.16251700
H	-2.34589400	1.22351400	0.54592500
N	2.28606600	-0.10581900	0.00651900

C	3.47001700	-0.29408900	0.01966200

$CNH_3Si\bullet\bullet\bullet OCH_2$			
Si	-0.42367900	-0.17090300	-0.00023000
H	0.12365900	1.20537100	-0.00080800
H	-0.15883600	-0.92324800	-1.24275100
H	-0.15923100	-0.92215200	1.24303400
H	2.56120200	1.51803000	-0.00038200
H	4.05941800	0.35561100	0.00025900
C	2.95918100	0.48202700	0.00006200
O	2.20914400	-0.48948200	0.00032500
N	-2.21571900	0.08794600	-0.00055300
C	-3.40215100	0.26118300	0.00079400

$CNH_3Si\bullet\bullet\bullet C_2H_4$			
Si	0.50968800	-0.00070100	-0.00457300
H	0.10039400	-1.17974900	-0.79754700
H	0.09961000	1.27535300	-0.62921900
H	0.09952600	-0.09692200	1.41293900
C	-2.79053800	-0.67488700	0.00597200
H	-2.89931600	-1.24276700	-0.92162500
H	-2.69859400	-1.24306200	0.93570100
C	-2.78610800	0.67636700	0.00590800
H	-2.69030900	1.24412900	0.93555100
H	-2.89116800	1.24497000	-0.92171100
N	2.30832000	-0.00062200	-0.00161000
C	3.50764400	0.00055700	-0.00168100

$CNH_3Si\bullet\bullet\bullet O(CH_3)_2$			
Si	-0.79109000	0.00027700	-0.13128200
H	-0.55975500	-1.25525800	-0.87540400
H	-0.34203500	-0.00420300	1.28121500

H	-0.55893400	1.26028500	-0.86752600
O	1.61557400	0.00008600	-0.39099600
C	2.20811500	-1.18058300	0.17126800
H	1.72498800	-2.04240100	-0.30590600
H	3.29014800	-1.19740400	-0.03871300
H	2.04371400	-1.21402300	1.26319500
C	2.20954400	1.17996600	0.17142200
H	1.72828200	2.04243100	-0.30644800
H	2.04423500	1.21397600	1.26320100
H	3.29179500	1.19492000	-0.03758100
N	-2.60504900	0.00027700	0.05865000
C	-3.79706400	-0.00018700	0.18720000

14. Germanium Bonded Complexes

$FH_3Ge\bullet\bullet\bullet OH_2$			
H	0.15030400	1.45294800	0.07997300
H	0.08860000	-0.68695700	-1.32600500
H	0.09212700	-0.83730700	1.23187900
O	2.52896600	0.01186900	0.06539500
H	2.98972900	0.81534000	-0.21048200
H	3.09713200	-0.70784100	-0.23965400
Ge	-0.25851700	-0.01460800	-0.00139800
F	-2.04189700	0.03736900	-0.00157200

$FH_3Ge\bullet\bullet\bullet SH_2$			
H	-0.38655300	-1.27711500	-0.74865700
H	-0.34887800	-0.00009500	1.45954900
H	-0.38655500	1.27721600	-0.74848700
F	-2.54867900	-0.00000300	0.02668400
H	2.85060100	-0.97544500	0.81975600
H	2.85063000	0.97542700	0.81977000
S	2.69015900	0.00000000	-0.10024500
Ge	-0.77136500	0.00000100	-0.00744200

$FH_3Ge\bullet\bullet\bullet NH_3$			
H	-0.08163700	-1.33132400	0.67998500
H	-0.08170600	0.07677900	-1.49291800
H	-0.08166100	1.25452000	0.81298300
F	2.02529500	0.00001400	-0.00002600
N	-2.40196700	0.00000300	-0.00000600
H	-2.79290100	-0.04867500	0.94183800
H	-2.79282200	-0.79131400	-0.51315500
H	-2.79273300	0.84006600	-0.42880200
Ge	0.22529900	-0.00000600	0.00001100

$FH_3Ge\bullet\bullet\bullet PH_3$			
H	0.42184800	1.47277900	-0.02505800
H	0.42183000	-0.71468800	1.28798100
H	0.42184500	-0.75808200	-1.26293800
F	2.59971800	-0.00000600	0.00000800
P	-2.70605200	0.00000100	-0.00000100
H	-3.45860100	1.20910700	-0.02044900
H	-3.45853700	-0.58684700	1.05738300
H	-3.45859600	-0.62230100	-1.03687300
Ge	0.82198500	0.00000200	-0.00000300

$FH_3Ge\bullet\bullet\bullet CO$			
H	-0.27015900	1.39271800	-0.47415400
H	-0.26950700	-1.10664600	-0.96891900
H	-0.26953200	-0.28545200	1.44292800
F	-2.45186700	-0.00039400	0.00011600
Ge	-0.67697600	0.00010600	-0.00003000
O	3.67374400	-0.00045200	0.00015400
C	2.52488100	0.00052500	-0.00019300

$FH_3Ge\bullet\bullet\bullet NCH$			
H	-0.21903900	-1.07393800	-1.01560700
H	-0.21930700	-0.34262200	1.43798200
H	-0.21916200	1.41660200	-0.42214800
F	-2.37823100	-0.00004800	-0.00015000
H	4.52363500	-0.00022900	-0.00045500
N	2.26489200	0.00010800	0.00019300
C	3.44563900	-0.00006900	-0.00015300
Ge	-0.59344200	0.00000900	0.00003600

$FH_3Ge\bullet\bullet\bullet OHCH_3$			
H	0.10677500	-0.67036500	1.21890600
H	0.17353600	-0.49587300	-1.34107500
H	0.61679400	1.59567900	0.10660600
F	2.38393000	-0.31188600	0.02186600
O	-1.92689100	0.61402500	-0.10188200
C	-2.72298400	-0.58159400	0.02367800
H	-2.35810100	-1.27242900	-0.74678600
H	-2.59635800	-1.04605400	1.01471500
H	-3.78757700	-0.37043200	-0.15817400
H	-2.23989600	1.25557400	0.55090300
Ge	0.63695300	0.07463200	-0.00527800

$FH_3Ge\bullet\bullet\bullet OCH_2$			
H	0.36366400	-0.86559600	-1.28557000
H	-0.05650700	1.31447300	-0.00103100
H	0.36331300	-0.86380900	1.28661500
F	2.32878400	0.28254500	0.00000100
H	-3.94914300	0.29510500	0.00012700
H	-2.47156700	1.48472400	-0.00010400
C	-2.85103500	0.44167700	0.00000400
O	-2.08309100	-0.51515100	-0.00001700
Ge	0.58006600	-0.07614500	0.00000200

$FH_3Ge\bullet\bullet\bullet C_2H_4$			
H	-0.21486900	0.00000400	1.46341200
H	-0.22623500	1.27491200	-0.74589700
H	-0.22623300	-1.27492200	-0.74588000
C	2.63906400	-0.67568200	0.01175400
H	2.50450200	-1.24337800	0.93660300
H	2.78396700	-1.24380400	-0.91073300
C	2.63904800	0.67568600	0.01175600
H	2.78394000	1.24381400	-0.91073000
H	2.50448500	1.24337800	0.93660700
Ge	-0.62396100	-0.00000100	-0.00722200
F	-2.40127700	0.00000000	0.00740700

$FH_3Ge\bullet\bullet\bullet O(CH_3)_2$			
H	-0.33850100	0.00002800	1.37013700
H	-0.66129500	1.29546500	-0.83636100
H	-0.66133700	-1.29553900	-0.83627500
F	-2.65312600	0.00002300	0.20630000
O	1.63246400	0.00000500	-0.41448400
C	2.21164400	1.17841200	0.15949500
H	1.73239100	2.04012300	-0.32217400
H	2.02939300	1.20968300	1.24912100
H	3.29799000	1.20300000	-0.03069500
Ge	-0.88060900	-0.00000600	-0.06077500
C	2.21161800	-1.17841400	0.15949800
H	2.02932800	-1.20969900	1.24911700
H	1.73238000	-2.04011500	-0.32220300
H	3.29797100	-1.20300700	-0.03065400

$ClH_3Ge\bullet\bullet\bullet OH_2$			
H	0.52367500	1.44506000	0.05172900
H	0.47647900	-0.71385400	-1.30946100

H	0.48396300	-0.81466100	1.24256500
O	2.93915200	0.02424700	0.05877700
H	3.41208000	0.83090000	-0.18547700
H	3.53146300	-0.69109900	-0.20823800
Cl	-2.09409200	0.02552700	0.00030100
Ge	0.11433400	-0.02138400	-0.00207600

$ClH_3Ge\bullet\bullet\bullet SH_2$			
H	0.01078500	-1.27303300	-0.75238500
H	0.04385500	-0.00002300	1.44756400
H	0.01078900	1.27305000	-0.75234900
H	3.24685200	-0.97531900	0.83078100
H	3.24684100	0.97533700	0.83076300
S	3.11323000	0.00000000	-0.09364300
Ge	-0.38769500	-0.00000100	-0.01495200
Cl	-2.58615000	0.00000200	0.02190400

$ClH_3Ge\bullet\bullet\bullet NH_3$			
H	0.46418600	1.36879500	0.59152700
H	0.46420800	-0.17211600	-1.48115400
H	0.46419800	-1.19665700	0.88965200
N	2.79579200	-0.00000500	-0.00000600
H	3.18732600	0.10904100	0.93669500
H	3.18726900	0.75667000	-0.56284400
H	3.18720400	-0.86578200	-0.37393800
Ge	0.15327400	0.00000600	0.00000800
Cl	-2.08410100	-0.00000700	-0.00000800

$ClH_3Ge\bullet\bullet\bullet PH_3$			
H	0.02088900	1.39871400	-0.44521800
H	0.02088700	-0.31377800	1.43393500
H	0.02087900	-1.08493300	-0.98869700

P	-3.13317600	-0.00000100	-0.00000300
H	-3.88688700	1.15187700	-0.36654300
H	-3.88687800	-0.25851200	1.18082700
H	-3.88687400	-0.89338000	-0.81429100
Cl	2.63182600	-0.00000200	-0.00000500
Ge	0.43295500	0.00000200	0.00000300

$ClH_3Ge\bullet\bullet\bullet CO$

H	-0.13698500	1.44278600	0.25968000
H	-0.13745800	-0.94584400	1.11948200
H	-0.13747800	-0.49614800	-1.37900600
Ge	0.28329100	0.00018500	0.00003900
Cl	2.47726900	-0.00029600	-0.00006200
C	-2.96963200	0.00046800	0.00011600
O	-4.11864600	-0.00056300	-0.00012800

$ClH_3Ge\bullet\bullet\bullet NCH$

H	-0.18187400	-0.79226000	-1.24201800
H	-0.18185900	1.47175700	-0.06505500
H	-0.18182900	-0.67954000	1.30714400
H	-4.94686500	0.00009900	-0.00013300
N	-2.68781000	-0.00003400	0.00004100
C	-3.86881700	0.00003100	-0.00004700
Ge	0.20319700	-0.00000800	0.00001600
Cl	2.41280500	0.00001500	-0.00002700

$ClH_3Ge\bullet\bullet\bullet OHCH_3$

H	-0.23955900	-0.65192100	1.19064900
H	-0.18429700	-0.40637400	-1.35426800
H	0.15866900	1.65788000	0.14326000
O	-2.35341700	0.56316600	-0.09371600
C	-3.07948700	-0.67686500	0.02353100
H	-2.66843900	-1.34424900	-0.74446600

H	-2.93463600	-1.13535800	1.01494400
H	-4.15318300	-0.52876800	-0.16715400
H	-2.70955200	1.18430100	0.55674500
Ge	0.26309000	0.14608500	-0.00809300
Cl	2.44802100	-0.22908100	0.01340000

$ClH_3Ge\bullet\bullet\bullet OCH_2$

H	-0.05933500	-0.91431900	-1.28185100
H	-0.38059800	1.27274900	-0.00001300
H	-0.05934000	-0.91429700	1.28186400
H	-4.33903800	0.43256800	-0.00000300
H	-2.80787500	1.55162400	0.00000700
C	-3.23501500	0.52691700	0.00000000
O	-2.51227500	-0.46433700	-0.00000400
Ge	0.20492900	-0.13734100	0.00000000
Cl	2.38804400	0.20704600	0.00000200

$ClH_3Ge\bullet\bullet\bullet C_2H_4$

H	-0.17106300	-0.00095300	1.46094800
H	-0.16882800	-1.27011400	-0.74050800
H	-0.16888600	1.27097900	-0.73889400
C	-3.05265100	0.67566200	0.01083300
H	-2.91799300	1.24334700	0.93568500
H	-3.19616100	1.24380100	-0.91189000
C	-3.05277500	-0.67559700	0.01082900
H	-3.19639800	-1.24370000	-0.91189800
H	-2.91823800	-1.24331000	0.93568100
Ge	0.24517800	-0.00002300	-0.00593000

Cl	2.44261400	0.00001800	0.00180500

$ClH_3Ge\bullet\bullet\bullet O(CH_3)_2$

H	-0.01131200	-0.00001700	1.33083700
H	-0.26717500	1.29182600	-0.87651900
H	-0.26717200	-1.29179600	-0.87656000
O	2.02275700	-0.00000100	-0.39393200
C	2.58230200	1.17829100	0.19882000
H	2.11811400	2.04008100	-0.29747700
H	2.36536300	1.20923600	1.28219900
H	3.67428500	1.20451300	0.04402100
Ge	-0.51918300	0.00000200	-0.10962900
Cl	-2.72504000	-0.00000300	0.15520600
C	2.58230000	-1.17829400	0.19881900
H	2.11810200	-2.04008300	-0.29747200
H	3.67428100	-1.20452300	0.04401000
H	2.36537000	-1.20923500	1.28220000

$CNH_3Ge\bullet\bullet\bullet OH_2$

H	0.46758800	1.43614700	0.00975500
H	0.42040400	-0.75562500	-1.27843800
H	0.42199000	-0.77453500	1.26545700
O	2.95933800	0.03136400	0.00448900
H	3.48126000	0.84434800	-0.01082600
H	3.61786000	-0.67533900	-0.01060600
Ge	0.03654500	-0.02404900	-0.00069400
C	-1.91719600	0.01974200	0.00049500
N	-3.10715400	0.04645700	0.00114200

$CNH_3Ge\bullet\bullet\bullet SH_2$

H	-0.08368400	-1.26828400	-0.74520300
H	-0.06173400	-0.00002700	1.44848600

H	-0.08368000	1.26830600	-0.74515800
H	3.29045100	-0.97542400	0.82080200
H	3.29044100	0.97544300	0.82078500
S	3.10777700	0.00000000	-0.09485200
Ge	-0.49838700	-0.00000100	-0.01103200
C	-2.44594700	0.00000100	0.01242900
N	-3.63602200	0.00000300	0.02805000

$CNH_3Ge\bullet\bullet\bullet NH_3$

H	0.41524900	1.46528100	0.20082800
H	0.41527200	-0.55870800	-1.36936100
H	0.41526200	-0.90653900	1.16855600
N	2.90104100	-0.00000900	-0.00000600
H	3.29594100	0.35588200	0.87173700
H	3.29588300	0.57697200	-0.74414000
H	3.29580400	-0.93296400	-0.12767100
Ge	0.05539300	0.00000900	0.00000600
C	-1.91370900	-0.00000700	-0.00000400
N	-3.10443100	-0.00001700	-0.00001100

$CNH_3Ge\bullet\bullet\bullet PH_3$

H	-0.12404100	-1.10074500	-0.96380600
H	-0.12403400	-0.28431000	1.43516700
H	-0.12403700	1.38505100	-0.47137100
P	3.13439200	0.00000000	0.00000300
H	3.88990400	1.14352000	-0.38915300
H	3.88989100	-0.90879100	-0.79573400
H	3.88988100	-0.23474400	1.18491100
Ge	-0.54804400	0.00000100	-0.00000400
C	-2.49575100	0.00000200	0.00000100
N	-3.68593300	-0.00000400	0.00001100

$CNH_3Ge\bullet\bullet\bullet CO$			
H	-0.03985000	1.46106200	0.04946500
H	-0.04023200	-0.77296500	1.24043400
H	-0.04028600	-0.68736900	-1.28975900
Ge	0.38977400	0.00017100	0.00003600
O	-4.13757000	-0.00056000	-0.00007100
C	-2.98840900	0.00042700	0.00001400
C	2.33442300	-0.00020500	-0.00002400
N	3.52458100	-0.00043500	-0.00009300

$CNH_3Ge\bullet\bullet\bullet NCH$			
H	-0.10092800	-0.22048700	-1.45126500
H	-0.10078500	1.36720200	0.53470500
H	-0.10086700	-1.14654900	0.91669500
H	-4.94767300	-0.00026600	-0.00039700
N	-2.68837200	0.00006400	0.00014700
C	-3.86966400	-0.00011100	-0.00014200
Ge	0.30075700	0.00004100	0.00003300
C	2.25618000	-0.00004100	-0.00005200
N	3.44650400	-0.00010900	-0.00009200

$CNH_3Ge\bullet\bullet\bullet OHCH_3$			
H	-0.15659100	-0.67467700	1.16370500
H	-0.10421100	-0.34911100	-1.36035600
H	0.22717300	1.65621100	0.19272500
O	-2.37600200	0.54546100	-0.09150300
C	-3.05982900	-0.71737600	0.02103900
H	-2.57548400	-1.39302100	-0.69553800
H	-2.96427500	-1.14002700	1.03433800
H	-4.12419800	-0.62182300	-0.24299800
H	-2.80186000	1.17249900	0.50878000
Ge	0.36737200	0.15349600	-0.00360500
C	2.29962000	-0.17134500	0.00489000

Ge	0.35006900	0.13947200	-0.00671200

$CNH_3Ge\bullet\bullet\bullet OCH_2$			
H	0.01033400	-0.91416200	-1.27606900
H	-0.29004400	1.26671000	-0.00039200
H	0.01023100	-0.91350000	1.27643800
H	-4.33820300	0.48032300	0.00005700
H	-2.78995600	1.57321700	-0.00005200
C	-3.23227000	0.55449000	0.00000300
O	-2.52578900	-0.44774400	0.00000600
Ge	0.30276200	-0.13915600	-0.00000500
C	2.23641600	0.15022100	0.00000400
N	3.41295700	0.33058500	0.00001200

$CNH_3Ge\bullet\bullet\bullet C_2H_4$			
H	0.08373000	0.00132800	1.45551000
H	0.07861700	1.26597400	-0.73949400
H	0.07862100	-1.26738500	-0.73713000
C	3.05860600	-0.67534100	0.01104600
H	2.92974700	-1.24333000	0.93653700
H	3.19645100	-1.24367500	-0.91247200
C	3.05861700	0.67539000	0.01104700
H	3.19647300	1.24372100	-0.91246900
H	2.92975800	1.24337500	0.93653900
Ge	-0.34559700	-0.00002200	-0.00632500
C	-2.29279400	-0.00000500	0.00191100
N	-3.48298100	0.00006400	0.00447800

$CNH_3Ge\bullet\bullet\bullet O(CH_3)_2$			
H	-0.10282500	-0.00005700	1.31491600
H	-0.34995400	1.28469500	-0.88243200
H	-0.34997500	-1.28462700	-0.88254700

O	2.01729000	0.00000000	-0.39322000
C	2.55550200	1.17699800	0.21712500
H	2.10765200	2.03927600	-0.29367800
H	2.30396300	1.20958700	1.29333400
H	3.65251900	1.20733400	0.10027600
Ge	-0.63358100	0.00000200	-0.11594700
C	-2.58321900	0.00000300	0.11506100
N	-3.76511500	-0.00000300	0.25863100
C	2.55548500	-1.17700600	0.21712400
H	2.10761400	-2.03927600	-0.29367600
H	3.65250000	-1.20736300	0.10026400
H	2.30395400	-1.20958700	1.29333500

15. Tin Bonded Complexes

$FH_3Sn•••OH_2$			
H	-0.20916400	1.43771900	0.80227000
H	-0.20893400	-1.43525000	0.80691500
H	-0.12667800	-0.00280200	-1.68152600
O	-2.60404700	0.00008100	-0.04776400
H	-3.06475900	0.76566700	0.32187200
H	-3.06524500	-0.76495600	0.32240300
F	2.13728900	0.00023400	0.06392500
Sn	0.16543100	-0.00006300	-0.01530300

$FH_3Sn•••SH_2$			
H	0.19469500	1.43100600	-0.82921500
H	0.16901100	-0.00029600	1.64301700
H	0.19470100	-1.43071000	-0.82972600
S	-2.87106400	0.00000100	-0.10076500
H	-3.05074700	0.97585600	0.81567800
H	-3.05071900	-0.97588600	0.81565000
F	2.53874200	-0.00000300	0.02232400
Sn	0.57262800	0.00000100	-0.00408200

$FH_3Sn\bullet\bullet\bullet NH_3$			
H	-0.13374300	1.64949200	-0.28295500
H	-0.13378300	-0.57969700	1.56996400
H	-0.13376300	-1.06978200	-1.28702300
F	2.13779500	-0.00001700	0.00001400
N	-2.51701200	-0.00000500	0.00000400
H	-2.90571100	0.32727000	-0.88565400
H	-2.90565300	0.60334300	0.72630800
H	-2.90559300	-0.93069300	0.15941300
Sn	0.14994300	0.00000500	-0.00000400

$FH_3Sn\bullet\bullet\bullet PH_3$			
H	0.22143500	-0.00152800	-1.64994300
H	0.22145500	1.42966300	0.82365200
H	0.22145400	-1.42813500	0.82629900
F	2.57695400	0.00000000	-0.00001000
P	-2.89661000	0.00000000	0.00000100
H	-3.64135000	-1.05107900	-0.60565600
H	-3.64135100	1.05003300	-0.60746500
H	-3.64140500	0.00104500	1.21305500
Sn	0.61032700	0.00000000	0.00000300

$FH_3Sn\bullet\bullet\bullet CO$			
H	-0.09266200	1.58713600	0.43365700
H	-0.09274900	-0.41804600	-1.59136100
H	-0.09275800	-1.16917500	1.15768300
F	-2.46197600	0.00006100	0.00001300
O	3.87866300	0.00005000	0.00000600
C	2.73037200	-0.00004000	0.00000000
Sn	-0.49951200	-0.00001200	-0.00000300

$FH_3Sn\cdots NCH$			
H	-0.07629100	-0.01524100	-1.65580900
H	-0.07652700	-1.42642100	0.84116400
H	-0.07647400	1.44162600	0.81478600
F	-2.40731000	0.00003900	-0.00014100
H	4.70272200	0.00013500	-0.00040500
N	2.44456500	-0.00005800	0.00016000
C	3.62453100	0.00004500	-0.00013800
Sn	-0.43333600	-0.00000600	0.00002500

$FH_3Sn\cdots OHCH_3$			
H	-0.04527600	-0.78131100	1.37390300
H	0.02897500	-0.62466600	-1.48917400
H	0.49183900	1.75026900	0.10762400
F	2.41888200	-0.33856100	0.02971500
O	-2.10758400	0.58817300	-0.09788100
C	-2.94077700	-0.58598200	0.02679100
H	-2.59771600	-1.28425300	-0.74674800
H	-2.82522800	-1.05274000	1.01746700
H	-3.99665500	-0.33707000	-0.15413600
H	-2.40961900	1.24680700	0.54363800
Sn	0.48178200	0.05881000	-0.00595400

$FH_3Sn\cdots OCH_2$			
H	0.25166800	-0.94073600	-1.44141900
H	-0.23916000	1.49437200	0.00000400
H	0.25167300	-0.94074600	1.44141300
F	2.35783700	0.34902800	0.00000000
H	-4.12028200	0.32010600	-0.00000500
H	-2.64235000	1.51259500	0.00000500
C	-3.02381800	0.47113900	0.00000000
O	-2.25577900	-0.48745100	0.00000000
Sn	0.42934100	-0.07028100	0.00000000

$FH_3Sn\cdots C_2H_4$			
H	0.04929300	-0.00002500	1.63617500
H	0.07845800	-1.42708600	-0.83825800
H	0.07842300	1.42710300	-0.83820800
C	-2.82223700	0.67603800	0.01525900
H	-2.69977200	1.24324400	0.94222900
H	-2.95745900	1.24432000	-0.90857900
C	-2.82221500	-0.67604000	0.01526400
H	-2.95741300	-1.24433500	-0.90857000
H	-2.69971200	-1.24323700	0.94223400
Sn	0.46247100	-0.00000100	-0.00805300
F	2.42792400	0.00001000	0.02138900

$FH_3Sn\cdots O(CH_3)_2$			
H	0.15749400	-0.00000700	1.56239600
H	0.50215100	-1.45182100	-0.90162700
H	0.50214300	1.45180500	-0.90164300
F	2.66395200	0.00000800	0.23153600
O	-1.86964300	0.00000100	-0.38704000
C	-2.47354700	-1.18154100	0.16200300
H	-1.97678000	-2.04196700	-0.30382300
H	-2.33455800	-1.21388300	1.25740900
H	-3.55044600	-1.20036900	-0.07378300
Sn	0.70451700	-0.00000200	-0.04900500
C	-2.47353800	1.18154700	0.16200200
H	-1.97678000	2.04196900	-0.30384000
H	-3.55044100	1.20037200	-0.07376500
H	-2.33453100	1.21390100	1.25740500

$ClH_3Sn\cdots OH_2$			
H	-0.53569200	1.61195600	0.21295900
H	-0.49781300	-1.03864900	1.28944500

H	-0.47375000	-0.65035600	-1.54361200
O	-2.91598600	0.03385300	-0.04158500
H	-3.34106400	0.85364200	0.24533700
H	-3.45407200	-0.66958900	0.34644700
Cl	2.26845600	0.03213300	0.02543300
Sn	-0.13866900	-0.01848200	-0.01300500

$ClH_3Sn{\bullet\bullet\bullet}SH_2$

H	-0.13547900	1.42475300	-0.83001700
H	-0.15845000	0.00006600	1.63123900
H	-0.13547900	-1.42481800	-0.82990600
S	-3.20596800	0.00000000	-0.09435700
H	-3.36230600	0.97575700	0.82647800
H	-3.36230300	-0.97574400	0.82649300
Cl	2.65993800	0.00000100	0.01919500
Sn	0.26461100	0.00000000	-0.00881800

$ClH_3Sn{\bullet\bullet\bullet}NH_3$

H	-0.45134900	1.51100200	-0.70862300
H	-0.45136200	-0.14181700	1.66286800
H	-0.45135100	-1.36918200	-0.95425900
Cl	2.27500600	-0.00000200	0.00000800
N	-2.82108000	-0.00000200	0.00000800
H	-3.21018400	0.08046500	-0.94074500
H	-3.21013100	0.77448800	0.54009700
H	-3.21012200	-0.85496900	0.40071800
Sn	-0.15886100	0.00000100	-0.00000500

$ClH_3Sn{\bullet\bullet\bullet}PH_3$

H	-0.10838200	1.64312200	-0.02088400
H	-0.11013900	-0.80219500	1.43262000
H	-0.11011200	-0.83833000	-1.41180200
Cl	2.69756700	-0.00115900	0.00003000

P	-3.24327300	-0.00027100	0.00000700
H	-3.99213300	0.58985800	-1.05729100
H	-3.99203000	0.61620000	1.04224000
H	-3.98543800	-1.21515200	0.01528700
Sn	0.30177400	0.00060500	-0.00001600

$ClH_3Sn•••CO$			
H	-0.24501100	0.96555300	-1.32270900
H	-0.24502200	0.66271300	1.49754600
H	-0.24499800	-1.62828400	-0.17484900
Cl	2.57310900	0.00000800	0.00000600
O	-4.22265400	0.00000300	0.00001000
C	-3.07424500	0.00001000	-0.00000600
Sn	0.18437700	-0.00000400	-0.00000300

$ClH_3Sn•••NCH$			
H	0.25551000	0.91713600	-1.37127700
H	0.25532900	-1.64624700	-0.10862000
H	0.25542000	0.72894500	1.47998800
Cl	-2.52592100	0.00009900	-0.00004900
H	5.02448200	0.00042600	-0.00024500
N	2.76612600	-0.00012200	0.00007900
C	3.94622400	0.00017000	-0.00009300
Sn	-0.11780600	-0.00004200	0.00002000

$ClH_3Sn•••OHCH_3$			
H	0.32369200	-0.80125300	-1.32929500
H	0.25731100	-0.52908900	1.51488600
H	-0.08536100	1.79409800	-0.16852000
Cl	-2.56142600	-0.25266700	-0.02082300
O	2.43787500	0.52197100	0.08444500
C	3.21708900	-0.68995200	-0.02800500
H	2.83812800	-1.36681000	0.74788000

H	3.08547900	-1.15737800	-1.01635600
H	4.28222900	-0.48856400	0.15747700
H	2.76996700	1.15999300	-0.56319400
Sn	-0.17465500	0.11296600	0.01007200

$ClH_3Sn\cdots OCH_2$

H	-0.11936800	-0.98150100	-1.43639500
H	-0.47939000	1.46604400	0.00002800
H	-0.11936400	-0.98152100	1.43638800
Cl	2.49943800	0.25717200	-0.00000300
H	-4.41378200	0.47858800	-0.00000200
H	-2.88374300	1.60298800	0.00000000
C	-3.31154900	0.57953100	-0.00000200
O	-2.58731300	-0.41251600	-0.00000400
Sn	0.12186000	-0.12267200	0.00000100

$ClH_3Sn\cdots C_2H_4$

H	-0.26768100	0.00001200	1.63074900
H	-0.25472200	-1.42050700	-0.83158700
H	-0.25472300	1.42047700	-0.83162800
C	-3.15312900	0.67600200	0.01634000
H	-3.03067300	1.24334100	0.94323400
H	-3.28755100	1.24418300	-0.90771500
C	-3.15314100	-0.67599100	0.01633800
H	-3.28757400	-1.24416700	-0.90771900
H	-3.03069400	-1.24333700	0.94322900
Sn	0.15770600	-0.00000300	-0.00817800
Cl	2.55093700	0.00000400	0.01025000

$ClH_3Sn\cdots O(CH_3)_2$

H	-0.10589100	-0.00001100	1.53295000
H	0.16082000	-1.44762700	-0.93164100
H	0.16081200	1.44759100	-0.93167600

Cl	2.80631200	0.00000900	0.17710200
O	-2.17777300	0.00000300	-0.35558300
C	-2.76881400	-1.18149500	0.20759500
H	-2.28270600	-2.04209000	-0.26911900
H	-2.60494400	-1.21317400	1.29961100
H	-3.85076800	-1.20062100	-0.00355000
Sn	0.40403100	-0.00000600	-0.08761400
C	-2.76879300	1.18151300	0.20759000
H	-2.28270000	2.04209800	-0.26915700
H	-3.85075400	1.20063600	-0.00351900
H	-2.60488900	1.21321500	1.29960100

$CNH_3Sn\bullet\bullet\bullet OH_2$

H	-0.50210500	1.61198900	-0.07045500
H	-0.43996800	-0.78567700	1.46524200
H	-0.44744300	-0.92364200	-1.37842700
O	-2.92091600	0.05066500	-0.05211900
H	-3.38423700	0.87198800	0.16048000
H	-3.53995400	-0.64940000	0.19467100
Sn	-0.07457200	-0.02298000	0.00085900
C	2.08222500	0.03128800	-0.00025500
N	3.27375700	0.06152600	0.00057800

$CNH_3Sn\bullet\bullet\bullet SH_2$

H	0.06738400	-1.41872200	-0.82650400
H	0.08794900	-0.00003400	1.62442000
H	0.06738300	1.41876300	-0.82644000
S	3.22363700	-0.00000200	-0.09278500
H	3.38106500	-0.97565300	0.82777600
H	3.38106800	0.97564200	0.82778100
Sn	-0.35422500	0.00000200	-0.00885200
C	-2.50079000	-0.00000300	0.01511100
N	-3.69243400	-0.00000600	0.02992300

$CNH_3Sn\bullet\bullet\bullet FH$			
H	-0.47116700	-0.83630900	-1.41216300
H	-0.50408000	1.61742600	-0.00029000
H	-0.47116400	-0.83577000	1.41251400
Sn	-0.04512400	-0.00850600	0.00001700
C	2.09765000	0.01014300	-0.00000100
N	3.28916900	0.01854800	-0.00006300
F	-3.11842000	0.08677900	-0.00004100
H	-3.84168300	-0.49174000	-0.00009900

$CNH_3Sn\bullet\bullet\bullet PH_3$			
H	-0.03161900	1.56144500	0.48440200
H	-0.03166400	-1.20017300	1.11005600
H	-0.03168800	-0.36119700	-1.59439600
P	-3.28950600	-0.00000900	-0.00001100
H	-4.04063000	-0.26735200	-1.18004100
H	-4.04092700	1.15541100	0.35846100
H	-4.04072700	-0.88835300	0.82135600
Sn	0.40185800	0.00001700	0.00001600
C	2.54807500	-0.00002600	-0.00001900
N	3.73978700	-0.00005300	-0.00005100

$CNH_3Sn\bullet\bullet\bullet CO$			
H	0.17915500	-1.39669500	0.84342000
H	0.17913300	1.42882300	0.78780700
H	0.17915100	-0.03209900	-1.63129500
O	4.23594500	-0.00003300	0.00003200
C	3.08728700	0.00002000	-0.00003200
Sn	-0.26608000	0.00000800	-0.00000300
C	-2.40792000	-0.00001100	0.00001500
N	-3.59959800	-0.00002900	0.00001100

$CNH_3Sn\bullet\bullet\bullet C_2H_2$			
H	0.26328300	-0.82300900	1.41509300
H	0.27936200	1.62456000	0.00001600
H	0.26329200	-0.82294100	-1.41513000
C	3.30079500	-0.60573900	-0.00000300
H	3.31614000	-1.68168300	-0.00000800
C	3.30198600	0.62679600	0.00000200
H	3.31705600	1.70263000	0.00000500
Sn	-0.17235600	-0.00611500	0.00000100
C	-2.31514600	0.00908000	0.00000500
N	-3.50673300	0.01790700	-0.00000500

$CNH_3Sn\bullet\bullet\bullet OHCH_3$			
H	0.26383000	-0.80785900	-1.31778700
H	0.20675100	-0.50675800	1.51306600
H	-0.12704000	1.79010500	-0.18377000
O	2.43381600	0.50538900	0.08185200
C	3.18921800	-0.72028800	-0.02620200
H	2.77374200	-1.40126300	0.72726800
H	3.07820100	-1.17189800	-1.02463700
H	4.25319900	-0.54807700	0.19348800
H	2.80132000	1.14549900	-0.54378700
Sn	-0.25049900	0.11397300	0.00807900
C	-2.39066900	-0.20641500	-0.01269700
N	-3.56955500	-0.38304100	-0.02703100

$CNH_3Sn\bullet\bullet\bullet OCH_2$			
H	0.07547400	-0.98012500	1.43055300
H	0.41767300	1.46066100	0.00011900
H	0.07548500	-0.97988500	-1.43071900
H	4.39430700	0.52651400	0.00005300
H	2.84740000	1.62555500	0.00021300
C	3.29010600	0.60793600	0.00007900

O	2.58135500	-0.39446700	-0.00003700
Sn	-0.19414700	-0.12221100	-0.00001200
C	-2.32704900	0.20568900	0.00001000
N	-3.50459500	0.39025600	0.00002000

$CNH_3Sn\bullet\bullet\bullet C_2H_4$			
H	0.20703200	-0.00010800	1.62265100
H	0.19076200	1.41507700	-0.82920000
H	0.19076400	-1.41494400	-0.82940200
C	3.16906600	-0.67567700	0.01862400
H	3.04036400	-1.24332900	0.94446900
H	3.30837200	-1.24397600	-0.90470900
C	3.16907300	0.67565000	0.01862600
H	3.30838400	1.24395000	-0.90470600
H	3.04037500	1.24330000	0.94447300
Sn	-0.23943500	0.00000800	-0.00904500
C	-2.38471500	-0.00000200	0.00968100
N	-3.57640800	-0.00002800	0.01815200

$CNH_3Sn\bullet\bullet\bullet O(CH_3)_2$			
H	0.03991300	0.00001100	1.52557200
H	-0.21460900	1.44144500	-0.93139100
H	-0.21461900	-1.44149400	-0.93133400
O	2.15525900	0.00000300	-0.35063000
C	2.73752200	1.18027000	0.22009800
H	2.25626900	2.04140900	-0.26094000
H	2.56130200	1.21213600	1.31047600
H	3.82238900	1.20357500	0.02327900
Sn	-0.48701400	-0.00000600	-0.08783200
C	-2.64115200	0.00000600	0.14247600
N	-3.82650400	0.00001400	0.27029600
C	2.73754500	-1.18025100	0.22010500

H	2.56129400	-1.21212900	1.31047800
H	2.25633400	-2.04140000	-0.26095500
H	3.82241900	-1.20351700	0.02331600

16. Lead Bonded Complexes

$FH_3Pb\bullet\bullet\bullet OH_2$			
H	-0.26197300	1.67147600	0.03124100
H	-0.15036400	-0.89953900	1.45754900
H	-0.14494700	-0.84941700	-1.48770400
O	-2.76152400	0.03584000	-0.02950500
H	-3.24476700	0.86277000	0.09982600
H	-3.41399000	-0.65736400	0.13622100
F	2.19143200	0.08435700	0.00797900
Pb	0.11689500	-0.01431500	-0.00088900

$FH_3Pb\bullet\bullet\bullet SH_2$			
H	0.09602600	1.47238100	-0.85158600
H	0.06233500	-0.00182800	1.69011100
H	0.09621800	-1.47064100	-0.85471800
S	-3.09070100	0.00000500	-0.09822200
H	-3.26271800	0.97599800	0.81959200
H	-3.26283100	-0.97558300	0.82000200
F	2.47775900	0.00010000	0.03071300
Pb	0.40759000	-0.00001600	-0.00400300

$FH_3Pb\bullet\bullet\bullet NH_3$			
H	-0.14957000	1.65053600	-0.44050900
H	-0.14959400	-0.44377400	1.64965400
H	-0.14958200	-1.20675400	-1.20915200
F	2.20211600	-0.00001100	0.00001100
N	-2.72600300	-0.00000400	0.00000400
H	-3.11851500	0.24506700	-0.91017900

H	-3.11848700	0.66569500	0.66735600
H	-3.11845800	-0.91080400	0.24286400
Pb	0.11057500	0.00000200	-0.00000200

$FH_3Pb\bullet\bullet\bullet PH_3$

H	0.10999400	0.00012100	-1.69714600
H	0.11000900	1.46971500	0.84868100
H	0.11000900	-1.46983500	0.84847200
F	2.50568500	0.00000000	-0.00000900
P	-3.12684800	0.00000000	-0.00000100
H	-3.87266800	-1.04985400	-0.60645000
H	-3.87266900	1.05011900	-0.60599000
H	-3.87268900	-0.00026600	1.21241000
Pb	0.43462900	0.00000000	0.00000100

$FH_3Pb\bullet\bullet\bullet CO$

H	-0.00930500	1.65865200	0.34725200
H	-0.00862800	-0.52825100	-1.60993900
H	-0.00822700	-1.12980400	1.26253900
F	-2.41395100	-0.00066700	0.00010500
O	4.08324200	-0.00055300	0.00001600
C	2.93498400	0.00043600	0.00005900
Pb	-0.34785500	0.00008800	-0.00001600

$FH_3Pb\bullet\bullet\bullet NCH$

H	0.00310000	1.14433100	1.25725400
H	0.00330600	-1.66104500	0.36237400
H	0.00321800	0.51663900	-1.61968800
F	2.38485800	0.00012000	0.00006300
H	-4.91557300	0.00031600	0.00018500
N	-2.65698000	-0.00011800	-0.00007100
C	-3.83729400	0.00011200	0.00006400
Pb	0.30566900	-0.00001400	-0.00000700

$FH_3Pb\cdots OHCH_3$			
H	-0.15636300	-0.80740300	1.41107400
H	-0.08709800	-0.64538200	-1.52098000
H	0.44187300	1.77183100	0.10815100
F	2.38068000	-0.41410300	0.02636300
O	-2.37998900	0.58461500	-0.09071600
C	-3.13441900	-0.64106300	0.02268100
H	-2.72184700	-1.32312100	-0.73150200
H	-3.01873000	-1.09123200	1.02142100
H	-4.19991900	-0.47157700	-0.19256700
H	-2.75515900	1.22935800	0.52517300
Pb	0.35265300	0.05163300	-0.00327300

$FH_3Pb\cdots OCH_2$			
H	0.20161800	-0.93901800	-1.47980700
H	-0.36129600	1.54024800	0.00004900
H	0.20163600	-0.93910800	1.47975400
F	2.32871700	0.43226700	0.00000200
H	-4.33062000	0.40662200	0.00000000
H	-2.80950300	1.54173000	-0.00000100
C	-3.22842100	0.51390500	0.00000100
O	-2.49622500	-0.47159400	0.00000100
Pb	0.31073200	-0.05867700	0.00000000

$FH_3Pb\cdots C_2H_4$			
H	-0.03091900	-0.00001500	1.68649100
H	0.00342800	-1.46885100	-0.86108300
H	0.00342700	1.46886600	-0.86105600
C	-2.96899200	0.67609800	0.01855800
H	-2.84125800	1.24300000	0.94511200
H	-3.11002500	1.24441700	-0.90449600
C	-2.96899000	-0.67609900	0.01855800

H	-3.11002100	-1.24441900	-0.90449600
H	-2.84125400	-1.24300000	0.94511300
Pb	0.31776600	0.00000000	-0.00650500
F	2.38863500	0.00000000	0.02946100

$FH_3Pb{\bullet\bullet\bullet}O(CH_3)_2$

H	0.02540400	-0.00000400	1.59928200
H	-0.38264100	1.48436400	-0.91445200
H	-0.38261100	-1.48435800	-0.91445500
F	-2.58446300	-0.00000700	0.30433700
O	2.17499300	-0.00000100	-0.39986500
C	2.73819600	1.18034300	0.18805300
H	2.27017600	2.04059000	-0.30786000
H	2.52838400	1.21297300	1.27269200
H	3.82898200	1.20705100	0.02564300
Pb	-0.53065200	0.00000100	-0.04326900
C	2.73820600	-1.18034100	0.18805100
H	2.27019300	-2.04059200	-0.30786000
H	3.82899300	-1.20704000	0.02563600
H	2.52840200	-1.21297300	1.27269100

$ClH_3Pb{\bullet\bullet\bullet}OH_2$

H	0.48556600	1.66201100	-0.00241300
H	0.40561900	-0.87660200	-1.46707300
H	0.40633600	-0.87447800	1.46779400
O	2.97590700	0.06946000	0.00941100
H	3.46220800	0.90379300	-0.03030000
H	3.65736400	-0.61394000	-0.03988300
Cl	-2.39792500	0.06006100	-0.00063200
Pb	0.10415100	-0.02167700	0.00008900

$ClH_3Pb{\bullet\bullet\bullet}SH_2$

H	-0.16165900	1.46491100	-0.85151800

H	-0.18637700	-0.00007200	1.67996300
H	-0.16165900	-1.46483800	-0.85164300
S	-3.32331000	0.00000000	-0.09073000
H	-3.48021700	0.97572900	0.83013600
H	-3.48020800	-0.97573600	0.83013000
Cl	2.67753800	-0.00000100	0.02420000
Pb	0.18445000	0.00000000	-0.00727800

$ClH_3Pb\bullet\bullet\bullet NH_3$

H	-0.39359600	1.64511700	-0.44100600
H	-0.39360700	-0.44063400	1.64521000
H	-0.39360100	-1.20447600	-1.20421000
Cl	2.41389300	-0.00000500	0.00000500
N	-2.93423500	-0.00000600	0.00000600
H	-3.32684100	0.24407200	-0.91053800
H	-3.32681800	0.66650400	0.66667400
H	-3.32679500	-0.91061700	0.24390400
Pb	-0.11384500	0.00000200	-0.00000200

$ClH_3Pb\bullet\bullet\bullet PH_3$

H	-0.14492000	1.62687000	0.45396700
H	-0.14492500	-1.20654900	1.18195800
H	-0.14499600	-0.42030000	-1.63584600
Cl	2.70647200	-0.00001600	-0.00005400
P	-3.37627100	-0.00000500	-0.00001600
H	-4.12388100	1.16691200	0.32549000
H	-4.12386300	-0.86550800	0.84767400
H	-4.12359600	-0.30152200	-1.17354300
Pb	0.21268600	0.00000500	0.00001800

$ClH_3Pb\bullet\bullet\bullet CO$

H	-0.25159400	0.91556700	-1.41571800
H	-0.25159700	0.76827700	1.50075600

H	-0.25154900	-1.68385000	-0.08503600
Cl	2.60764200	0.00002000	0.00000200
O	-4.31739300	0.00001300	0.00000300
C	-3.16907800	0.00001600	-0.00000100
Pb	0.12168800	-0.00000700	-0.00000100

$ClH_3Pb\bullet\bullet\bullet NCH$			
H	0.25030300	0.64542100	-1.56580100
H	0.25011800	-1.67882700	0.22395100
H	0.25024900	1.03328000	1.34191700
Cl	-2.58449300	0.00010900	-0.00006700
H	5.13228400	0.00040200	-0.00030300
N	2.87358300	-0.00009300	0.00009000
C	4.05392500	0.00017200	-0.00012200
Pb	-0.07786800	-0.00003100	0.00001800

$ClH_3Pb\bullet\bullet\bullet OHCH_3$			
H	-0.36188400	-0.88492900	1.33190700
H	-0.28176700	-0.50874100	-1.56864400
H	0.08938800	1.80361900	0.22915000
Cl	2.60446400	-0.31692900	0.01908800
O	-2.61531600	0.49020200	-0.07711900
C	-3.32108300	-0.76532300	0.02372700
H	-2.86512000	-1.43116300	-0.71997400
H	-3.20728200	-1.20855800	1.02568600
H	-4.38777600	-0.63975100	-0.21414200
H	-3.02377500	1.11806700	0.53522300
Pb	0.12940700	0.09523900	-0.00572100

$ClH_3Pb\bullet\bullet\bullet OCH_2$			
H	-0.10697600	-0.97239100	-1.47440800
H	-0.50690400	1.52719400	0.00005300
H	-0.10696700	-0.97245800	1.47437400

Cl	2.55414300	0.32327700	-0.00000400
H	-4.52731000	0.58197800	-0.00000500
H	-2.96253000	1.65595600	0.00000600
C	-3.42179700	0.64544800	-0.00000200
O	-2.72913300	-0.36827500	-0.00000600
Pb	0.08724500	-0.10051800	0.00000100

$ClH_3Pb{\bullet\bullet\bullet}C_2H_4$

H	-0.27317000	-0.00008700	1.67962300
H	-0.25742200	-1.46172900	-0.85546300
H	-0.25743400	1.46181500	-0.85531600
C	-3.19956400	0.67611300	0.02196200
H	-3.06875300	1.24309400	0.94804800
H	-3.34385800	1.24437200	-0.90064900
C	-3.19956200	-0.67612400	0.02196000
H	-3.34385600	-1.24437900	-0.90065300
H	-3.06875600	-1.24310300	0.94804700
Pb	0.09724700	0.00000200	-0.00735900
Cl	2.59021900	-0.00000600	0.01625200

$ClH_3Pb{\bullet\bullet\bullet}O(CH_3)_2$

H	0.20419600	-0.00001300	1.57825200
H	-0.10158500	1.47982900	-0.93947000
H	-0.10157200	-1.47979300	-0.93951500
Cl	-2.80215900	-0.00001100	0.23650600
O	2.39529000	-0.00000400	-0.34990300
C	2.94925100	1.18039800	0.24710200
H	2.48989500	2.04078700	-0.25662000
H	2.72178300	1.21283300	1.32818600
H	4.04247200	1.20635600	0.10242100
Pb	-0.31007300	0.00000400	-0.07602200
C	2.94925200	-1.18041000	0.24709500
H	2.48989300	-2.04079700	-0.25662800

H	4.04247200	-1.20636700	0.10240900
H	2.72179100	-1.21284800	1.32818100

$CNH_3Pb•••OH_2$

H	0.47359700	1.65109500	-0.00006500
H	0.39858800	-0.86913600	-1.45755300
H	0.39858100	-0.86902000	1.45762600
O	3.01709200	0.07082400	-0.00000600
H	3.50817300	0.90328500	-0.00000100
H	3.70102000	-0.61188100	-0.00002600
Pb	0.04952500	-0.02013100	0.00000200
C	-2.17948600	0.04826200	-0.00000500
N	-3.37154500	0.08432100	-0.00000800

$CNH_3Pb•••SH_2$

H	-0.13393000	1.45467200	-0.84424200
H	-0.15682900	-0.00122100	1.66749100
H	-0.13379900	-1.45355900	-0.84631100
S	-3.38866200	0.00002000	-0.08967300
H	-3.54636400	0.97585600	0.83061000
H	-3.54657000	-0.97520900	0.83121700
Pb	0.25827000	-0.00002500	-0.00699900
C	2.47781400	0.00006600	0.01992200
N	3.67014800	0.00011300	0.03576800

$CNH_3Pb•••NH_3$

H	1.29605900	1.02184000	-0.53525500
H	0.48323200	-1.36002400	0.96293700
H	-1.41356500	0.83522200	0.56094500
N	0.94552000	1.28503200	2.55594800
H	0.21415000	1.82628500	3.01977600
H	1.72335300	1.93034400	2.40917500
H	1.27073500	0.60363800	3.24364700

Pb	0.01690400	0.02297100	0.04569200
C	-0.68905600	-0.93646900	-1.86266100
N	-1.06348000	-1.44533500	-2.87480800

$CNH_3Pb\cdots PH_3$			
H	0.11235100	-1.45117000	-0.83924800
H	0.11234700	-0.00122800	1.67637600
H	0.11235200	1.45239700	-0.83712100
P	3.45759200	0.00000000	-0.00000300
H	4.21048400	1.04742700	-0.60378100
H	4.21048600	-1.04660700	-0.60519900
H	4.21046700	-0.00081800	1.20899500
Pb	-0.29086500	0.00000000	0.00000100
C	-2.51034400	0.00000100	-0.00000200
N	-3.70276400	0.00000000	-0.00000400

$CNH_3Pb\cdots CO$			
H	0.22534400	1.67424600	0.00144300
H	0.22581200	-0.83553100	-1.45054900
H	0.22597000	-0.83812200	1.44894500
O	4.37225600	-0.00071300	0.00014000
C	3.22353800	0.00029800	-0.00000500
Pb	-0.18807300	0.00012400	-0.00003200
C	-2.40213700	-0.00036900	0.00008700
N	-3.59451000	-0.00065800	0.00016800

$CNH_3Pb\cdots NCH$			
H	0.23323500	-0.84044000	-1.45677200
H	0.23323700	-0.84139500	1.45622000
H	0.23321900	1.68182800	0.00055100
H	5.17401200	-0.00001200	0.00001200
N	2.91489300	-0.00000300	-0.00000400
C	4.09576000	-0.00000800	0.00000300

Pb	-0.14193100	0.00000200	0.00000000
C	-2.37425700	-0.00000700	0.00000100
N	-3.56694800	-0.00001100	0.00000200

$CNH_3Pb\bullet\bullet\bullet OHCH_3$			
H	-0.34388700	0.89260600	-1.30785100
H	-0.26898100	0.46542500	1.56611300
H	0.10320100	-1.79603500	-0.25837300
O	-2.65284900	-0.47563400	0.07868300
C	-3.31557200	0.80109800	-0.02098900
H	-2.79569500	1.47064700	0.67625000
H	-3.24199900	1.21416000	-1.03976000
H	-4.37206800	0.72688600	0.27777900
H	-3.11827100	-1.10300600	-0.49143900
Pb	0.19225400	-0.09539800	0.00317100
C	2.39654900	0.27444900	-0.00959000
N	3.57283000	0.47196100	-0.01838800

$CNH_3Pb\bullet\bullet\bullet OCH_2$			
H	0.09583400	-0.97070900	1.46401200
H	0.48395300	1.51317700	0.00008700
H	0.09583500	-0.97055000	-1.46410600
H	4.54077800	0.63316600	-0.00003800
H	2.95398700	1.67215300	0.00000500
C	3.43354500	0.67049100	-0.00002000
O	2.76239900	-0.35660800	-0.00002800
Pb	-0.14796500	-0.09739400	0.00000100
C	-2.34670100	0.27255600	0.00001900
N	-3.52250600	0.47195000	0.00002800

$CNH_3Pb\bullet\bullet\bullet C_2H_4$			
H	-0.25282600	-0.00001500	1.66575000
H	-0.23343900	-1.45136800	-0.84935000

H	-0.23344100	1.45138100	-0.84932400
C	-3.25859400	0.67564600	0.02487500
H	-3.11181100	1.24303300	0.94825300
H	-3.41619700	1.24403500	-0.89551500
C	-3.25859500	-0.67564300	0.02487500
H	-3.41619900	-1.24403300	-0.89551400
H	-3.11181300	-1.24303000	0.94825300
Pb	0.16503600	0.00000000	-0.00793200
C	2.38454900	0.00000100	0.01561100
N	3.57695100	0.00000200	0.02653400

$CNH_3Pb\bullet\bullet\bullet O(CH_3)_2$			
H	0.18099600	-0.00000200	1.56206400
H	-0.11926000	1.46904400	-0.93889800
H	-0.11931100	-1.46908100	-0.93888600
O	2.41563700	0.00001200	-0.35231900
C	2.94998200	1.17853600	0.26100000
H	2.50313600	2.03966700	-0.25292100
H	2.69320200	1.21021800	1.33592900
H	4.04729900	1.20974800	0.14864600
Pb	-0.37899500	-0.00001000	-0.07457300
C	-2.59927700	0.00002200	0.20184900
N	-3.78304200	0.00004700	0.34894800
C	2.94998000	-1.17850400	0.26102400
H	2.50311100	-2.03963800	-0.25287100
H	4.04729400	-1.20972900	0.14865900
H	2.69320300	-1.21015400	1.33595300

17. Nitrogen Bonded Complexes

$F_3N\bullet\bullet\bullet OH_2$			
N	-0.50950400	0.02088900	-0.36131500
F	-0.42131600	1.13737500	0.44475200
F	-1.88728600	-0.16412600	-0.42787600

F	-0.14597600	-0.99179400	0.52468900
O	2.47470600	0.06020400	-0.28398000
H	3.41859600	0.23538700	-0.38904300
H	2.44148600	-0.69634200	0.31600300

$F_3N•••SH_2$

N	-1.10856200	0.00001300	-0.37254400
F	-0.88243300	1.07367300	0.47858300
F	-2.49247700	0.00216400	-0.45657100
F	-0.88558500	-1.07588900	0.47653000
H	2.09688800	0.97568600	0.58176100
H	2.09508200	-0.97141200	0.58653100
S	2.61952600	-0.00024400	-0.19046000

$F_3N•••NH_3$

N	0.56488600	-0.00000100	-0.38539500
F	0.29094400	-1.07398600	0.44954700
F	1.95683600	-0.00006600	-0.37836300
F	0.29104400	1.07405700	0.44948400
N	-2.59724500	0.00001100	-0.28232100
H	-2.54079500	-0.81569200	0.32849600
H	-3.54133500	0.00009200	-0.66929500
H	-2.54077900	0.81548800	0.32879700

$F_3N•••NCH$

N	0.87712100	0.00000100	0.33340800
F	0.74274600	-1.07302000	-0.52997900
F	0.74270900	1.07299900	-0.53000300
F	2.25591500	0.00002700	0.55517400
N	-2.17549900	-0.00002600	0.16238000
C	-3.35801100	0.00001300	0.15431100
H	-4.43561600	0.00004600	0.14688400

$F_3N{\bullet\bullet\bullet}CO$			
N	0.96062800	-0.00001800	-0.34209500
F	0.80653500	-1.07361500	0.52036100
F	2.33608900	-0.00091600	-0.54076500
F	0.80782200	1.07435100	0.51960100
C	-2.36346600	0.00112300	-0.18194000
O	-3.51220100	-0.00062400	-0.12580800

$F_3N{\bullet\bullet\bullet}OCH_2$			
N	0.92292200	-0.00000500	0.39064600
F	0.56893700	-1.07400700	-0.41397800
F	0.56892800	1.07401400	-0.41395200
F	2.30698200	0.00000200	0.24954500
O	-2.06160800	-0.00002200	0.77935900
C	-2.56200900	0.00001200	-0.33770700
H	-1.93574400	0.00003600	-1.25540700
H	-3.66341100	0.00002000	-0.48228000

$F_3N{\bullet\bullet\bullet}C_2H_4$			
N	0.85872800	0.00000000	0.30450600
F	0.76648300	1.07406000	-0.56582200
F	2.21828700	0.00000000	0.59895600
F	0.76648400	-1.07405300	-0.56583100
C	-2.48602800	0.67462600	0.16642500
H	-2.31145700	1.24267800	1.08392400
H	-2.65866700	1.24294800	-0.75114500
C	-2.48600700	-0.67463300	0.16643200
H	-2.65863000	-1.24297000	-0.75113100
H	-2.31141900	-1.24267000	1.08393800

$F_3N{\bullet\bullet\bullet}OHCH_3$			
N	-1.01391100	-0.05678400	0.38368800
F	-0.70319700	-1.02131600	-0.55795100

F	-2.39770400	0.03334900	0.23489300
F	-0.59904400	1.10212800	-0.25824800
C	2.47807700	0.16410000	-0.45794500
H	1.95083300	-0.35980900	-1.26502900
H	3.55449200	-0.06230700	-0.53215000
H	2.32303600	1.24903300	-0.57968800
O	1.91551700	-0.31973300	0.77132500
H	2.37592400	0.11638600	1.49988100

$F_3N•••O(CH_3)_2$

N	-1.21587300	-0.22443200	-0.23631600
F	-1.21882000	1.12837400	-0.51269000
F	-2.58245100	-0.48870300	-0.14667100
F	-0.85294300	-0.23415200	1.10639500
O	1.60772000	0.07913200	-0.57428300
C	1.96669200	-1.25910300	-0.24469200
H	3.06490000	-1.38997300	-0.25100900
H	1.51777400	-1.91092800	-1.00588200
H	1.58076900	-1.53916300	0.75347700
C	2.13106000	0.99317600	0.38467800
H	1.81052300	1.99850500	0.08089600
H	3.23597400	0.95226300	0.41175500
H	1.74081400	0.77315600	1.39602100

$F_3N•••FH$

N	-0.46771100	0.00000000	-0.32389900
F	-1.84499100	0.00000100	-0.52727500
F	-0.31832300	1.07340300	0.53808900
F	-0.31832500	-1.07340400	0.53808800
F	2.46942200	-0.00000100	-0.28090700
H	3.38392800	0.00000400	-0.14466800

18. Phosphorus Bonded Complexes

$F_3P{\bullet\bullet\bullet}OH_2$			
F	-0.09767100	1.23889500	0.59306400
F	-2.00878400	-0.03496500	-0.20087200
F	-0.03720900	-1.21106800	0.59508400
O	2.46002600	-0.01744600	-0.33231300
H	2.81078100	0.79707500	0.05346300
H	2.62919500	-0.68801200	0.34427800
P	-0.38848100	0.00631700	-0.44164900

$F_3P{\bullet\bullet\bullet}SH_2$			
F	-0.60221500	1.22210800	0.60493300
F	-2.52133100	0.00000000	-0.26501300
F	-0.60221500	-1.22210800	0.60493200
H	2.41705800	0.97444300	0.70178600
H	2.41704700	-0.97440900	0.70182500
P	-0.89638400	0.00000000	-0.43898600
S	2.63397000	-0.00000200	-0.20765600

$F_3P{\bullet\bullet\bullet}NH_3$			
F	-0.08888900	1.22867200	0.60310200
F	-2.00212400	-0.00000900	-0.23020200
F	-0.08887400	-1.22866300	0.60310800
H	2.90137100	0.81842800	-0.59649800
H	2.90128600	-0.81858500	-0.59624900
H	2.52549700	0.00014800	0.76889300
P	-0.36897000	0.00000000	-0.44315600
N	2.40362600	0.00000100	-0.24469600

$F_3P{\bullet\bullet\bullet}NCH$			
F	-0.46494300	-1.22306100	0.61146800
F	-0.46494000	1.22306200	0.61146900
F	-2.38129900	0.00000100	-0.25737600

N	2.27811900	0.00000600	-0.28745200
C	3.43807600	-0.00000300	-0.06303600
H	4.49589800	-0.00001200	0.14335700
P	-0.75137000	-0.00000100	-0.42953500

$F_3P\bullet\bullet\bullet CO$			
F	0.50979800	-1.22154100	0.57811900
F	2.47069000	-0.00000300	-0.20291400
F	0.50980500	1.22154300	0.57811900
C	-2.52351300	0.00001000	-0.29183200
O	-3.63973100	-0.00000500	-0.01770200
P	0.85641900	-0.00000100	-0.44582000

$F_3P\bullet\bullet\bullet OCH_2$			
F	-0.30453500	-1.22009500	0.52244900
F	-0.30451200	1.22010800	0.52239600
F	-2.33734400	0.00001400	-0.01436600
O	2.05078800	-0.00004300	-0.74641700
C	2.62596800	0.00002600	0.33703000
H	2.06153400	0.00010400	1.29139800
H	3.73314100	0.00000900	0.39793400
P	-0.76261800	-0.00001100	-0.46763200

$F_3P\bullet\bullet\bullet C_2H_4$			
F	0.45195300	-0.99107100	0.92328100
F	2.38093300	-0.15091600	-0.30700300
F	0.56603100	1.36424900	0.27948100
C	-2.66247900	-0.60218300	-0.47195800
H	-2.94109000	-0.59474200	-1.52911600
H	-2.46781500	-1.57308000	-0.00835000
C	-2.56914100	0.54314800	0.23747000
H	-2.29143300	0.53501000	1.29458400
H	-2.76578400	1.51480000	-0.22311500

P	0.75103900	-0.10187500	-0.41259400

$F_3P\bullet\bullet\bullet OHCH_3$

F	-0.32093800	1.26462200	0.33335400
F	-2.40962300	0.07552500	-0.00137600
F	-0.43800900	-1.15328800	0.70602600
C	2.58859600	0.18957000	0.42226500
H	2.33683200	1.24245800	0.59314300
H	3.67847000	0.09269600	0.29959400
H	2.25399000	-0.40555600	1.28650800
O	1.89466300	-0.19927700	-0.78176800
H	2.14149500	-1.11299300	-0.98114500
P	-0.83883600	-0.06943600	-0.45464000

$F_3P\bullet\bullet\bullet PH_3$

F	-0.66343300	1.22337800	0.59032100
F	-2.59668500	-0.00312000	-0.24547700
F	-0.65847500	-1.22021400	0.59259100
H	3.61005800	1.03474800	-0.38503900
H	3.59071500	-1.05549500	-0.36488000
H	2.82432800	0.01251900	1.26275900
P	-0.97471600	0.00002300	-0.44449600
P	2.65753200	0.00049900	-0.15215500

$F_3P\bullet\bullet\bullet O(CH_3)_2$

F	-0.91389300	1.37911400	-0.25473000
F	-2.63901100	-0.31267400	-0.07489200
F	-0.58052300	-0.57998300	1.18199300
C	2.11181300	1.05168200	0.42675700
H	1.61174500	2.00456300	0.21553500
H	3.20316900	1.16597500	0.30508700
H	1.88847700	0.73578800	1.46109400
O	1.60389000	0.09674000	-0.51248000

P	-1.02236000	-0.24771800	-0.36111000
C	2.20919100	-1.18363200	-0.31328600
H	2.02766700	-1.54783500	0.71379100
H	1.75118800	-1.87230300	-1.03626200
H	3.29684000	-1.13075400	-0.49492200

$FH_2P{\bullet\bullet\bullet}SH_2$			
F	-2.66961300	0.02999800	0.08258200
H	2.33319300	0.50197500	-1.16376000
H	2.57454000	1.02765300	0.70233600
P	-1.00639100	-0.03375500	-0.16374700
S	2.22523800	-0.09690800	0.04139400
H	-0.70598400	-0.88944500	0.93927500
H	-0.68317200	1.14668700	0.57281000

$FH_2P{\bullet\bullet\bullet}NH_3$			
F	2.03583200	-0.00000200	-0.07988400
N	-2.26231600	0.00000200	-0.03429100
H	-2.61901700	0.81617000	0.46364600
H	-2.61899800	-0.81618200	0.46363500
H	-2.70836000	-0.00000700	-0.95243800
H	0.07893300	1.03948900	-0.76815000
H	0.07893400	-1.03956300	-0.76806900
P	0.35348200	0.00000600	0.16802400

$FH_2P{\bullet\bullet\bullet}NCH$			
F	-2.51277900	0.00000000	-0.09294200
N	1.93772500	0.00000100	-0.10226100
C	3.11263900	0.00000000	0.01823200
H	4.18483400	-0.00000200	0.12865700
H	-0.52926400	-1.03406300	-0.74263200
H	-0.52926500	1.03406500	-0.74263000
P	-0.85008100	0.00000000	0.18663500

$FH_2P\cdots CO$			
F	-2.56647500	-0.00015500	0.07255600
H	-0.59402000	1.03385300	0.76543400
H	-0.59363900	-1.03247900	0.76685200
C	2.05692400	0.00046100	0.12791400
O	3.19189900	-0.00032200	-0.05088500
P	-0.90605300	-0.00001100	-0.16971300

$FH_2P\cdots OCH_2$			
F	0.75842300	1.10745000	-0.10166000
O	-1.66040900	-0.75792900	-0.07754700
C	-2.25018200	0.30706200	0.06800400
H	-1.69718000	1.26192700	0.17385900
H	-3.35963600	0.35068900	0.09836400
H	1.02536700	-0.99434500	-1.09244200
H	2.72639500	-0.09173800	-0.33089700
P	1.41757400	-0.41816800	0.15189400

$FH_2P\cdots C_2H_4$			
F	-2.45568800	0.12245000	0.00000400
C	2.13657500	-0.66467900	-0.00000300
H	2.10920700	-1.23299800	0.93329100
H	2.10922900	-1.23299600	-0.93329800
C	2.23649100	0.68515800	0.00000500
H	2.28501900	1.25107100	-0.93405900
H	2.28500100	1.25105800	0.93407700
H	-0.45779600	0.73979700	-1.03533100
H	-0.45781000	0.73964400	1.03543700
P	-0.80067000	-0.18270000	-0.00001100

$FH_2P\cdots OHCH_3$			
F	-2.52805000	0.25505100	-0.05292200

C	2.39721600	0.58267100	0.02494500
H	2.24798100	1.15215000	-0.90088200
H	3.47456300	0.40737200	0.16824300
H	1.99674800	1.16015600	0.87438900
O	1.68359600	-0.65804700	-0.14674700
H	1.84610200	-1.20068600	0.63774300
H	-0.40851900	0.79478400	-0.84014800
H	-0.86715100	-1.22382700	-0.73341200
P	-0.89262300	-0.10780400	0.15297800

$FH_2P{\bullet\bullet\bullet}PH_3$			
F	2.68931300	-0.00007800	0.04667700
H	-2.70584500	-1.04984500	-0.75212400
H	-2.70643400	1.04902900	-0.75286100
H	-3.20130300	0.00006600	0.99970000
H	0.74102600	-1.03520800	0.80847600
H	0.74117500	1.03504000	0.80888200
P	1.01507900	0.00008400	-0.13676800
P	-2.15324100	0.00002400	0.03462400

$FH_2P{\bullet\bullet\bullet}C_2H_2$			
F	-2.49291594	0.04819023	0.00128828
C	2.14363429	-0.59214201	0.31027599
H	2.07413592	-1.54382204	0.79386572
C	2.23467449	0.61430235	-0.30581785
H	2.31484731	1.56021370	-0.79908987
H	-0.40870928	0.66886710	-1.10264654
H	-0.40764395	0.66677616	1.10204649
P	-0.86269483	0.03535750	-0.00058923

$FH_2P{\bullet\bullet\bullet}O(CH_3)_2$			
F	-2.85900100	0.10094400	0.16752900
O	1.32227300	0.01264700	-0.41765800

C	1.90549400	-1.16515300	0.15113700
H	2.99129100	-1.19086000	-0.04587400
H	1.41774200	-2.02467000	-0.32488000
H	1.73227100	-1.19793900	1.24257200
C	1.90547100	1.19251900	0.14387000
H	1.40997800	2.05182600	-0.32618400
H	2.98864400	1.22743500	-0.06774700
H	1.74730100	1.22528800	1.23752300
H	-1.01639600	0.95181700	-0.95879700
H	-0.75505500	0.49950200	1.05283500
P	-1.21524900	-0.18108500	-0.11639900

$ClH_2P\cdots OH_2$			
H	3.33638200	-0.74424100	-0.26027200
H	3.54679500	0.76766000	-0.22926000
P	0.14216600	-0.20498900	-0.05686000
H	0.41315000	0.46172400	1.17050600
H	0.40223100	0.95384300	-0.84239500
Cl	-1.97020800	0.06225500	0.01602100
O	2.95781000	0.07218900	0.09274500

$ClH_2P\cdots SH_2$			
H	2.91462900	-0.71780400	-1.02245100
H	3.13396000	1.15787400	-0.52436300
P	-0.47263900	-0.19918200	-0.09022300
S	2.83181600	0.00675200	0.11378500
H	-0.20569500	0.16204300	1.26201500
H	-0.18532200	1.10912200	-0.57727400
Cl	-2.58100300	0.06873200	0.02322700

$ClH_2P\cdots NH_3$			
N	-2.86133600	-0.00001200	0.06959000
H	-3.22885300	-0.81616600	-0.42072100

H	-3.22888100	0.81632600	-0.42039400
H	-3.28873500	-0.00020400	0.99672300
H	-0.41453900	-1.03809800	0.73485000
H	-0.41450200	1.03803400	0.73499100
P	-0.18041500	0.00002500	-0.20888200
Cl	1.95947500	-0.00001100	0.06003900

$ClH_2P{\bullet\bullet\bullet}NCH$

N	-2.57057400	0.00005000	0.12268600
C	-3.74779300	0.00006700	0.02225100
H	-4.82182600	0.00008000	-0.06948000
H	0.00495200	-1.03361200	0.68583300
H	0.00491000	1.03473400	0.68405200
P	0.29669900	-0.00023800	-0.24929400
Cl	2.40248500	0.00009500	0.08510000

$ClH_2P{\bullet\bullet\bullet}CO$

H	-0.07826500	1.03318800	0.72183900
H	-0.07825900	-1.03316800	0.72184700
C	2.74059000	0.00001300	0.16236800
O	3.87328200	-0.00001200	-0.03182000
P	-0.36098500	0.00000500	-0.21884000
Cl	-2.46226500	-0.00000500	0.06583900

$ClH_2P{\bullet\bullet\bullet}OCH_2$

O	1.97217200	-0.70394300	0.17540500
C	2.50130200	0.36002700	-0.12566000
H	1.89647900	1.26883100	-0.32183100
H	3.60491800	0.45108700	-0.21256600
H	-0.64539800	-1.31625600	1.14095500
H	-2.48828600	-1.05888200	0.22510200
P	-1.11394500	-0.98998800	-0.16322100
Cl	-0.96727800	1.11626000	0.05690400

$ClH_2P\cdots C_2H_4$			
C	2.75774300	-0.62502000	-0.00000800
H	2.74381700	-1.19370700	0.93349300
H	2.74383400	-1.19368900	-0.93352100
C	2.81854500	0.72652000	0.00000500
H	2.84910500	1.29382200	-0.93411200
H	2.84908700	1.29380500	0.93413400
H	0.02476800	0.67875500	-1.03477000
H	0.02476800	0.67864000	1.03484900
P	-0.28057600	-0.25258200	-0.00001200
Cl	-2.38143900	0.09541800	0.00000800

$ClH_2P\cdots OHCH_3$			
C	2.93107300	-0.65209400	-0.02239000
H	2.71366800	-1.24962900	0.87187400
H	4.02204400	-0.54231600	-0.12223100
H	2.52663100	-1.16785000	-0.90899200
O	2.29150200	0.62331300	0.18078800
H	2.51089800	1.18630400	-0.57489900
H	0.05051100	-0.78086400	0.73964000
H	-0.31506800	1.25810900	0.76892500
P	-0.37299100	0.20975300	-0.19106700
Cl	-2.46072200	-0.17200000	0.04586600

$ClH_2P\cdots PH_3$			
H	3.30867700	1.04775700	-0.75626400
H	3.30895100	-1.04843600	-0.75516800
H	3.86601600	0.00063800	0.97552700
H	-0.24858400	1.03452400	0.78587200
H	-0.24863500	-1.03452500	0.78595600
P	-0.48929400	-0.00003200	-0.16440500
P	2.78127800	0.00001400	0.05127200

Cl	-2.60977600	0.00001800	0.03888700

$ClH_2P\cdots O(CH_3)_2$			
C	2.40567300	1.17672300	0.15547400
H	1.97189600	2.03937000	-0.36704000
H	3.50566700	1.20640700	0.06640600
H	2.12289000	1.20779900	1.22341500
O	1.88348300	0.00000100	-0.47100200
H	-0.52915100	1.03705100	-0.88243100
H	-0.52916000	-1.03700100	-0.88250300
P	-0.67804100	-0.00000800	0.08087200
Cl	-2.81811300	0.00000300	0.03580000
C	2.40567300	-1.17672100	0.15547600
H	1.97188900	-2.03936800	-0.36703200
H	3.50566600	-1.20640900	0.06640200
H	2.12289400	-1.20779100	1.22341900

19. Arsenic Bonded Complexes

$F_3As\cdots OH_2$			
F	-0.11341900	-1.30704900	0.74832000
F	1.98029600	-0.00001200	0.02872900
F	-0.11339700	1.30705600	0.74831900
O	-2.41878700	-0.00000100	-0.29115500
H	-2.60763700	-0.76263100	0.27561500
H	-2.60766800	0.76264800	0.27557900
As	0.26619100	0.00000100	-0.36212900

$F_3As\cdots SH_2$			
F	-0.32324300	1.29889700	0.77278000
F	-2.38992900	0.00000000	-0.07240800
F	-0.32324300	-1.29889700	0.77278000
H	2.52254800	0.97443100	0.71664800
H	2.52254300	-0.97442500	0.71665500

S	2.75436300	0.00000000	-0.18992800
As	-0.66021700	0.00000000	-0.35311600

$F_3As{\bullet\bullet\bullet}NH_3$

F	-0.07866400	-1.31348500	0.75794100
F	1.97876700	-0.00044700	-0.00029500
F	-0.07794000	1.31388500	0.75772100
H	-2.83778000	-0.82476400	-0.52573300
H	-2.84122800	0.81863400	-0.53555700
H	-2.43817100	0.00588300	0.83008600
N	-2.34146200	0.00004000	-0.18651400
As	0.24569500	0.00001200	-0.36671200

$F_3As{\bullet\bullet\bullet}NCH$

F	0.19919100	1.30001700	0.77048800
F	0.19919000	-1.30001700	0.77048700
F	2.27547200	-0.00000100	-0.03903700
N	-2.36150700	0.00000300	-0.32639300
C	-3.49851800	-0.00000200	-0.00867300
H	-4.53591000	-0.00000500	0.28427600
As	0.54523900	0.00000000	-0.34742200

$F_3As{\bullet\bullet\bullet}CO$

F	-0.21648500	1.29787700	0.73473800
F	-2.34114900	-0.00026700	0.02609100
F	-0.21606300	-1.29767000	0.73481100
C	2.64949500	0.00019800	-0.30189100
O	3.75134300	-0.00011000	0.02324600
As	-0.63468000	0.00000700	-0.35864800

$F_3As{\bullet\bullet\bullet}OCH_2$

F	-0.04990000	-1.29497800	0.69545000

F	-0.04990000	1.29499600	0.69541700
F	-2.21911000	0.00000300	0.20559200
O	2.10501700	-0.00001900	-0.71362400
C	2.73406400	0.00001200	0.34185900
H	2.21662800	0.00006000	1.32021200
H	3.84153700	-0.00000800	0.33955300
As	-0.55856000	-0.00000500	-0.37485000

$F_3As{\bullet\bullet\bullet}C_2H_4$

F	0.20356100	-0.99942600	1.12165800
F	2.28980600	-0.12888900	-0.13411600
F	0.34790800	1.49123500	0.39683200
C	-2.77982100	-0.60571400	-0.44072100
H	-3.07424300	-0.62042500	-1.49375000
H	-2.57847700	-1.56602900	0.04210800
C	-2.68171200	0.55461400	0.24510700
H	-2.39130000	0.56780500	1.29861000
H	-2.88754300	1.51639000	-0.23197200
As	0.54937200	-0.08658800	-0.33032400

$F_3As{\bullet\bullet\bullet}OHCH_3$

F	-0.00131100	-1.19788900	0.79812300
F	2.27426800	-0.32781400	-0.01221200
F	0.49979700	1.36652500	0.73426200
C	-2.88725100	-0.41166200	-0.02976400
H	-2.85104600	-1.07180200	-0.90532700
H	-3.89847000	0.01260500	0.05923900
H	-2.63316400	-0.98903300	0.87103400
O	-1.91705200	0.63168500	-0.27107700
H	-1.90179200	1.21994000	0.49910600
As	0.57544300	-0.00977600	-0.35934600

$F_3As{\bullet\bullet\bullet}PH_3$			
F	0.30414900	-1.27119900	0.77077700
F	2.43868600	-0.05435600	-0.03282000
F	0.39208500	1.32446900	0.73742100
H	-3.55974900	-1.17852300	-0.19094500
H	-3.83667500	0.87841500	-0.50153500
H	-2.92943800	0.19505600	1.26688400
P	-2.77187100	0.00644000	-0.13487300
As	0.71786800	0.00055200	-0.35847600

$F_3As{\bullet\bullet\bullet}O(CH_3)_2$			
F	-0.64044200	1.54495000	-0.14891400
F	-2.49573900	-0.20217300	0.10013500
F	-0.28625300	-0.56468800	1.35256700
C	2.29439500	1.07678000	0.40039800
H	1.79229600	2.02531600	0.18018700
H	3.37713900	1.16518900	0.21010700
H	2.11990800	0.79525100	1.45240900
O	1.72578400	0.09080300	-0.47963900
C	2.34148200	-1.18872300	-0.27557700
H	2.22760900	-1.51181900	0.77329300
H	1.83468600	-1.90083600	-0.94171600
H	3.41165400	-1.14139200	-0.53738000
As	-0.77524000	-0.19664500	-0.29644900

$FH_2As{\bullet\bullet\bullet}OH_2$			
F	2.01432700	0.17404800	0.00369800
H	-2.98359000	0.83108000	-0.27683100
H	-2.92783700	-0.69673600	-0.28432000
H	-0.05956300	0.96336100	-1.02891900
H	-0.05244300	0.79894500	1.16199100
O	-2.48934800	0.08239400	0.08342000

As	0.23664500	-0.12491600	-0.00826000

$FH_2As•••SH_2$

F	2.46777600	0.19504100	0.01154600
H	-2.69619000	-0.89475300	0.85992000
H	-2.79109400	1.05332400	0.74705000
S	-2.53056000	0.03702800	-0.10336200
H	0.39579300	0.81529600	-1.15260500
H	0.36395100	0.93643200	1.03670500
As	0.69716700	-0.12903400	0.00178200

$FH_2As•••NH_3$

F	2.00963400	0.17496200	-0.00009400
N	-2.38761300	0.08682000	-0.00005000
H	-2.77692600	-0.38412800	0.81738000
H	-2.77699100	-0.38545700	-0.81668100
H	-2.76670900	1.03447500	-0.00080500
H	-0.05007000	0.88416400	1.10304400
H	-0.05005600	0.88290800	-1.10405700
As	0.21355600	-0.12770800	0.00007000

$FH_2As•••NCH$

F	2.33388300	0.20799700	-0.00003700
N	-2.19518100	0.09471700	-0.00001800
C	-3.37449700	0.04096100	-0.00000600
H	-4.45133000	-0.00785100	0.00000600
H	0.24078100	0.86638600	1.09639600
H	0.24081100	0.86581100	-1.09687500
As	0.56297100	-0.13651800	0.00002900

$FH_2As•••CO$

F	-2.37399700	-0.21480000	0.00002900

H	-0.27087800	-0.86338900	1.09482800
H	-0.27085300	-0.86385700	-1.09444000
C	2.35777500	-0.10312300	0.00002500
O	3.50404200	-0.02943500	-0.00000300
As	-0.61428100	0.13680800	-0.00002400

$FH_2As•••OCH_2$			
F	-0.18306900	1.34206800	0.05959800
O	2.00383200	-0.79208300	0.04210000
C	2.68719000	0.22389800	-0.03693300
H	2.21999900	1.22682200	-0.09033100
H	3.79610400	0.16742200	-0.05696400
H	-0.64200200	-0.72658100	1.32352700
H	-2.35563400	0.30074400	0.42666200
As	-1.01589800	-0.24405300	-0.06831800

$FH_2As•••C_2H_4$			
F	-2.30724600	0.21800800	0.00001000
C	2.38529300	-0.63191000	-0.00000200
H	2.36148500	-1.19997300	0.93374300
H	2.36150800	-1.19995600	-0.93375800
C	2.48430800	0.71893400	0.00001200
H	2.53265100	1.28447300	-0.93418500
H	2.53262800	1.28445600	0.93422000
H	-0.20419600	0.86557600	-1.09855100
H	-0.20420100	0.86545000	1.09865000
As	-0.54037200	-0.13285600	-0.00000800

$FH_2As•••OHCH_3$			
F	-2.36468500	-0.30019200	0.13139300
C	2.67502500	-0.59561500	-0.02340300
H	2.46546400	-1.23751100	0.84105900
H	3.75721000	-0.40317800	-0.07539300

H	2.33901300	-1.10249700	-0.94267900
O	1.93978300	0.62686700	0.19720400
H	2.16628600	1.24015300	-0.51646200
H	-0.14995700	-0.80440000	1.04294300
H	-0.63760600	1.32011900	0.74695800
As	-0.61292900	0.06811500	-0.11261100

$FH_2As{\bullet\bullet\bullet}PH_3$

F	-2.49042700	0.00020300	0.16556300
H	3.11120000	1.05064300	-0.66243500
H	3.11152600	-1.05227800	-0.65958300
H	3.38572100	0.00167200	1.14268500
H	-0.41307800	1.09785300	0.89395400
H	-0.41312700	-1.09606500	0.89619100
P	2.47048100	0.00005000	0.05227300
As	-0.70986700	-0.00013400	-0.11772600

$FH_2As{\bullet\bullet\bullet}O(CH_3)_2$

C	2.18967800	1.17896000	0.13586400
H	1.73665200	2.04018800	-0.37189000
H	3.28444500	1.20247800	0.00146500
H	1.94880100	1.21103400	1.21377800
O	1.63998100	-0.00000200	-0.46766600
H	-0.71176900	1.10246800	-0.97016800
H	-0.71174700	-1.10241900	-0.97021000
C	2.18968200	-1.17896200	0.13586400
H	1.73664600	-2.04019400	-0.37187500
H	3.28444700	-1.20248400	0.00144900
H	1.94882200	-1.21102800	1.21378300
As	-0.84831800	0.00000200	0.06733100
F	-2.65753600	-0.00001000	0.01585500

$ClH_2As\cdots OH_2$			
H	-3.41977900	0.89778100	-0.27556200
H	-3.39292000	-0.62927300	-0.22503300
H	-0.38214800	0.93090100	-1.03603200
H	-0.38412900	0.77853700	1.15222400
O	-2.91642000	0.15384400	0.08207200
As	-0.13802900	-0.16176300	-0.01121900
Cl	2.08619300	0.12526300	0.00576800

$ClH_2As\cdots SH_2$			
H	-3.11535900	-0.86010300	0.84710600
H	-3.18230100	1.09032400	0.76642900
S	-2.96406300	0.08351100	-0.10698900
H	0.06129100	0.67908300	-1.21615200
H	0.03207400	0.98176300	0.95270300
As	0.31915900	-0.17584700	0.01188300
Cl	2.53512200	0.15151100	-0.00178800

$ClH_2As\cdots NH_3$			
N	-2.79601600	0.15060000	-0.00001800
H	-3.19986700	-0.30819600	0.81746300
H	-3.19994100	-0.30896000	-0.81703200
H	-3.14507800	1.10998100	-0.00045000
H	-0.37723700	0.86227700	1.10061900
H	-0.37722900	0.86184400	-1.10097700
As	-0.17077600	-0.16022300	0.00002200
Cl	2.08865100	0.11860000	-0.00001300

$ClH_2As\cdots NCH$			
N	2.64145200	0.13946900	-0.00037500
C	3.82214300	0.11233800	0.00016500
H	4.89989500	0.08795800	0.00064300
H	0.10268300	0.82186900	-1.09597700

H	0.10291200	0.82393500	1.09419200
As	-0.17712300	-0.18944400	0.00009000
Cl	-2.39314400	0.16868100	-0.00001100

$ClH_2As\bullet\bullet\bullet CO$			
H	-0.06437300	0.82463700	1.09130300
H	-0.06383100	0.81999700	-1.09536800
C	-2.84860200	0.15991700	-0.00080900
O	-3.99527400	0.08827300	0.00042300
As	0.23540600	-0.18898100	0.00018500
Cl	2.43609400	0.17212100	-0.00003400

$ClH_2As\bullet\bullet\bullet OCH_2$			
O	2.12786300	-0.86931200	0.10961300
C	2.85945800	0.09687300	-0.07835800
H	2.44363800	1.11684000	-0.20403300
H	3.96286000	-0.01880300	-0.12854700
H	-0.52045500	-0.93219200	1.34271900
H	-2.38825700	-0.33165500	0.36805000
As	-0.95269500	-0.60034200	-0.07290900
Cl	-0.36697000	1.55002100	0.03653200

$ClH_2As\bullet\bullet\bullet C_2H_4$			
C	2.83770800	-0.56609900	-0.00000500
H	2.83010400	-1.13453300	0.93388300
H	2.83012400	-1.13451400	-0.93390400
C	2.89191300	0.78675800	0.00000900
H	2.91976100	1.35384300	-0.93424900
H	2.91974000	1.35382500	0.93427900
H	0.12001700	0.82128900	-1.09638300
H	0.12001700	0.82116600	1.09647700
As	-0.16976400	-0.18904900	-0.00001000
Cl	-2.38325000	0.16668200	0.00001200

$ClH_2As\bullet\bullet\bullet OHCH_3$			
C	-3.04501600	0.69594700	-0.02250000
H	-2.78198900	1.36996600	0.80210800
H	-4.13799800	0.57024600	-0.04930100
H	-2.69498400	1.13130400	-0.97284100
O	-2.38288500	-0.55594600	0.25544200
H	-2.65802000	-1.19196400	-0.42023800
H	-0.16001400	0.87234800	0.89870500
H	0.22956600	-1.28774500	0.87203000
As	0.24205500	-0.15850200	-0.13924300
Cl	2.44404700	0.23754600	0.09153000

$ClH_2As\bullet\bullet\bullet PH_3$			
H	3.55371300	-0.63475900	-1.05035000
H	3.55377000	-0.63514500	1.05006800
H	3.85693700	1.16229400	0.00018300
H	-0.08238800	0.86812300	-1.09501700
H	-0.08238700	0.86798600	1.09513200
P	2.92135800	0.08860800	0.00000900
As	-0.33539000	-0.15361600	-0.00000800
Cl	-2.56189100	0.12421800	0.00000600

$ClH_2As\bullet\bullet\bullet O(CH_3)_2$			
C	2.58276000	1.17886900	0.13824700
H	2.13149300	2.04025500	-0.37107400
H	3.67856500	1.20598100	0.01190500
H	2.33521900	1.20941500	1.21483000
O	2.03977300	-0.00000100	-0.47075000
H	-0.36652800	1.09975600	-0.97107600
H	-0.36652200	-1.09970200	-0.97113100
Cl	-2.74531700	-0.00000200	0.00904600
C	2.58276100	-1.17887000	0.13824800

H	2.13148300	-2.04025800	-0.37106100
H	3.67856400	-1.20598800	0.01189200
H	2.33523400	-1.20940800	1.21483400
As	-0.49086200	0.00000000	0.06618600

20. Antimony Bonded Complexes

$F_3Sb•••OH_2$			
F	-0.28996600	-1.43724200	0.84828400
F	2.02691000	-0.00000200	0.34350200
F	-0.28996300	1.43724300	0.84828400
O	-2.39484700	0.00000000	-0.20432900
H	-2.52946200	-0.76476300	0.37867800
H	-2.52947600	0.76476500	0.37867100
Sb	0.21950800	0.00000000	-0.34281100

$F_3Sb•••SH_2$			
F	-0.06905100	1.41701000	0.88675500
F	-2.38506800	0.00000000	0.22016800
F	-0.06905100	-1.41701000	0.88675500
H	2.55875300	0.97470400	0.74326900
H	2.55875100	-0.97470200	0.74327100
S	2.81679900	0.00000000	-0.15727200
Sb	-0.53878000	0.00000000	-0.33163300

$F_3Sb•••NH_3$			
F	-0.22253700	-1.44530500	0.87026500
F	2.04347000	-0.00000200	0.28680600
F	-0.22253400	1.44530700	0.87026500
H	-2.55462200	-0.82214900	0.48100800
H	-3.05512800	0.00003700	-0.86059700
H	-2.55460300	0.82211000	0.48107000
N	-2.37620300	0.00000000	-0.09885600
Sb	0.20416000	0.00000000	-0.34618700

$F_3Sb\bullet\bullet\bullet NCH$			
F	-0.03589000	1.41867700	0.88109800
F	-0.03589600	-1.41867500	0.88109800
F	2.28811000	-0.00000400	0.25804800
N	-2.41845100	0.00000200	-0.33437600
C	-3.53210900	-0.00000100	0.05398300
H	-4.54904300	-0.00000300	0.41215900
Sb	0.44556800	0.00000000	-0.32505100

$F_3Sb\bullet\bullet\bullet CO$			
F	0.06044700	1.41344800	0.82818200
F	-2.32170200	0.00017800	0.35650000
F	0.06016100	-1.41357700	0.82817700
C	2.71401100	-0.00011900	-0.29624100
O	3.79869900	0.00006400	0.07999700
Sb	-0.52674100	-0.00000500	-0.33290700

$F_3Sb\bullet\bullet\bullet OCH_2$			
F	0.16856000	-1.40625100	0.81534200
F	0.16854100	1.40621900	0.81541200
F	-2.20815600	-0.00002500	0.49079600
O	2.17116700	0.00003600	-0.67538900
C	2.81394800	-0.00002300	0.37492000
H	2.30810400	-0.00009300	1.35672800
H	3.91967900	-0.00000700	0.34938100
Sb	-0.46355500	0.00000900	-0.34600900

$F_3Sb\bullet\bullet\bullet C_2H_4$

F	-0.03076400	-1.08707600	1.25492000
F	2.32536600	-0.07809600	0.12535000
F	0.14305700	1.63828200	0.50008100
C	-2.85298000	-0.58823300	-0.42541300
H	-3.15897500	-0.57545200	-1.47542500
H	-2.64911000	-1.56000600	0.03324000
C	-2.75206000	0.55435900	0.29168500
H	-2.45316800	0.53836700	1.34263600
H	-2.96323300	1.52872100	-0.15654900
Sb	0.44932900	-0.07816400	-0.31107200

$F_3Sb{\bullet\bullet\bullet}OHCH_3$

F	-0.22277000	-1.35160200	0.84677400
F	2.28597600	-0.30639000	0.31112600
F	0.25346400	1.47692300	0.88783700
C	-3.00137300	-0.38924200	0.03758300
H	-3.00553000	-1.07632200	-0.81722900
H	-3.98895100	0.08545400	0.12697200
H	-2.74851400	-0.94318700	0.95164000
O	-1.99443100	0.61322400	-0.25262800
H	-1.93795400	1.22520000	0.49974600
Sb	0.48616900	-0.00454600	-0.34073000

$F_3Sb{\bullet\bullet\bullet}PH_3$

F	0.01859800	-1.39363900	0.86437000
F	2.40596500	-0.05243700	0.28978800
F	0.10489500	1.44035700	0.84713000
H	-3.63530800	-1.14991400	-0.20762400
H	-3.83880100	0.94206400	-0.40539200
H	-2.90749600	0.12700100	1.30993200
P	-2.81166200	0.00516300	-0.10221900
Sb	0.58414500	0.00107600	-0.33676900

$F_3Sb\cdots O(CH_3)_2$			
F	-0.43877400	1.72422000	-0.08274000
F	-2.49317000	-0.07576000	0.33963500
F	-0.03736800	-0.63046000	1.49306000
C	2.43836000	1.09989800	0.43198400
H	1.92390300	2.04317000	0.22204200
H	3.51614400	1.19019100	0.22083100
H	2.27776400	0.80646100	1.48172300
O	1.86432700	0.10815300	-0.44917600
C	2.50749000	-1.16583400	-0.26363000
H	2.40714500	-1.49853500	0.78238600
H	2.01039300	-1.88101900	-0.93433300
H	3.57184200	-1.08906800	-0.53803900
Sb	-0.65829600	-0.18044700	-0.28237100

$FH_2Sb\cdots OH_2$			
F	2.09105600	0.30206800	-0.03467700
H	-2.95265300	1.00148100	-0.19591000
H	-3.14993900	-0.50278800	-0.40047800
H	-0.16543200	0.85699300	-1.34276200
H	-0.17984200	1.15499800	1.08262400
O	-2.59693400	0.14032600	0.06369800
Sb	0.16478100	-0.12454700	0.01292200

$FH_2Sb\cdots SH_2$			
F	2.44971700	0.36240200	0.02859400
H	-3.00704700	-0.55679800	1.08470000
H	-2.84162400	1.28703800	0.46055100
S	-2.76504500	0.05763900	-0.09377700
H	0.15539600	1.03622300	-1.18454100
H	0.14072600	0.94450800	1.25143200
Sb	0.54403600	-0.13519300	-0.00723600

$FH_2Sb•••NH_3$			
F	2.09427600	0.30771400	-0.00006300
N	-2.51632900	0.16059500	-0.00007300
H	-2.96163100	-0.25554300	0.81871400
H	-2.96209700	-0.25676500	-0.81798300
H	-2.76801700	1.14977300	-0.00073000
H	-0.15273800	1.01131500	1.23063600
H	-0.15258800	1.01007200	-1.23173000
Sb	0.15221300	-0.12847900	0.00004300

$FH_2Sb•••NCH$			
F	-2.33919900	0.35596700	-0.00001000
N	2.39283300	0.08542500	0.00001500
C	3.57220800	0.12102800	-0.00001200
H	4.64974700	0.15605700	-0.00002700
H	-0.04708800	0.99398900	-1.22234800
H	-0.04701400	0.99435300	1.22199600
Sb	-0.42521400	-0.13082800	0.00000900

$FH_2Sb•••CO$			
F	2.35611800	0.41396200	0.00000000
H	0.02635400	0.96677100	1.21684500
H	0.02635200	0.96678400	-1.21683000
C	-2.58273900	0.07409900	0.00000300
O	-3.72887900	0.14283000	-0.00000200
Sb	0.47195500	-0.14208700	0.00000000

$FH_2Sb•••OCH_2$			
F	0.23062900	1.50210600	0.00500500
O	2.14511100	-0.82231800	-0.02533400
C	2.92305200	0.12764400	0.01680200
H	2.55063400	1.16939600	0.03494600
H	4.02012100	-0.03883400	0.03784300

H	-0.37609400	-0.64240100	1.54038300
H	-2.20527800	0.61367700	0.55210500
Sb	-0.79929900	-0.17270800	-0.04134200

$FH_2Sb•••C_2H_4$			
F	2.33436200	0.32614200	0.07815000
C	-2.62882900	-0.58352400	0.05069000
H	-2.70606500	-1.18385300	-0.85966200
H	-2.56048300	-1.11881100	1.00210900
C	-2.66832800	0.77053300	0.00822900
H	-2.61666800	1.36853400	0.92174400
H	-2.76376900	1.30569300	-0.94004500
H	0.04193000	0.68959400	1.41816000
H	0.03178800	1.25351600	-0.95994000
Sb	0.41856800	-0.12494100	-0.03214200

$FH_2Sb•••OHCH_3$			
F	-2.29013400	-0.67303000	-0.00065100
C	2.92336200	-0.68610600	-0.02039500
H	2.54108500	-1.37991500	0.73772200
H	3.98510600	-0.47605100	0.17753500
H	2.80325400	-1.13600800	-1.01812400
O	2.13104800	0.51702200	0.10691400
H	2.47357700	1.17528400	-0.51436500
H	0.09679300	-0.92849100	-1.14742600
H	0.03565000	-0.76976900	1.29498500
Sb	-0.50809400	0.18730700	-0.00504700

$FH_2Sb•••PH_3$			
F	-2.47153700	0.35158500	0.00000100
H	3.46287700	-0.50905400	-1.05427100
H	3.46289200	-0.50912800	1.05422100
H	3.41843600	1.31973600	0.00003900

H	-0.16857200	0.99617200	-1.21966600
H	-0.16857600	0.99614700	1.21968900
P	2.71443800	0.08398100	0.00000100
Sb	-0.55842700	-0.13172300	-0.00000100

$FH_2Sb\cdots O(CH_3)_2$

C	2.48313200	1.18232400	0.09247900
H	1.97737700	2.04064100	-0.36812700
H	3.55638600	1.20318600	-0.16026800
H	2.36155700	1.21796800	1.19008700
O	1.87223200	0.00000000	-0.44574100
H	-0.50539300	1.23255700	-1.07495700
H	-0.50538700	-1.23256300	-1.07494500
C	2.48311500	-1.18233200	0.09247900
H	1.97734000	-2.04064200	-0.36811900
H	3.55636700	-1.20321600	-0.16027800
H	2.36154800	-1.21797000	1.19008800
Sb	-0.69721900	0.00000200	0.08525500
F	-2.66633000	-0.00000400	-0.11836800

$ClH_2Sb\cdots OH_2$

Cl	2.25690300	0.20403400	-0.01294800
H	-3.24663500	1.12631000	-0.18191200
H	-3.50349500	-0.36960100	-0.38268600
H	-0.39818300	0.90574600	-1.29360100
H	-0.41120900	1.08189300	1.13759400
O	-2.91051300	0.25232800	0.06076200
Sb	-0.14752400	-0.16140300	0.00891400

$ClH_2Sb\cdots SH_2$

Cl	2.61118200	0.27893400	0.01030700
H	-3.34400700	-0.46336100	1.08559500
H	-3.11776400	1.37496900	0.46398000

S	-3.09416600	0.14509600	-0.09438500
H	-0.08839600	0.93786300	-1.23454200
H	-0.10163500	0.96808800	1.19702800
Sb	0.23075200	-0.19374500	-0.00347300

$ClH_2Sb\bullet\bullet\bullet NH_3$			
Cl	2.26954000	0.19935400	0.00003000
N	-2.81495400	0.26928300	-0.00016600
H	-3.27922600	-0.12598200	0.81869800
H	-3.27976200	-0.12694600	-0.81825800
H	-3.02040800	1.26937700	-0.00067700
H	-0.38463500	0.99652200	1.22642200
H	-0.38445000	0.99519200	-1.22761600
Sb	-0.16723600	-0.16239500	0.00004100

$ClH_2Sb\bullet\bullet\bullet NCH$			
Cl	-2.49665800	0.27154300	0.00000200
N	2.72289800	0.16261800	0.00000200
C	3.90079000	0.23603300	0.00000100
H	4.97679400	0.30505500	-0.00000100
H	0.20173200	0.96105800	-1.21872200
H	0.20170400	0.96088000	1.21889100
Sb	-0.10592300	-0.18427000	-0.00000400

$ClH_2Sb\bullet\bullet\bullet CO$			
Cl	2.51529400	0.32829700	0.00000000
H	-0.21565900	0.92487200	1.21380700
H	-0.21566800	0.92489400	-1.21378500
C	-2.95148500	0.16770700	0.00000500
O	-4.09492400	0.27390200	-0.00000300
Sb	0.15960000	-0.20839700	-0.00000100

$ClH_2Sb\cdots OCH_2$			
Cl	0.18960900	1.78920100	0.00811900
O	2.16007700	-1.07187000	-0.00030600
C	3.05569900	-0.23231600	-0.00232700
H	2.82512100	0.85102500	-0.01522900
H	4.12308900	-0.53661900	0.00918500
H	-0.37816200	-0.79366800	1.54310700
H	-2.33244900	0.23042600	0.53130200
Sb	-0.84462300	-0.39605400	-0.04294100

$ClH_2Sb\cdots C_2H_4$			
Cl	2.49802300	0.24818300	0.02579000
C	-2.98007400	-0.48113600	0.04334100
H	-3.05004700	-1.07655800	-0.87103800
H	-2.96544900	-1.02031600	0.99478200
C	-2.96304900	0.87327400	0.00270100
H	-2.91750700	1.46782300	0.91890900
H	-3.00309200	1.41296300	-0.94707200
H	-0.20239400	0.83497900	1.30958800
H	-0.20773200	1.08151600	-1.11616700
Sb	0.10859900	-0.18181100	-0.01968000

$ClH_2Sb\cdots OHCH_3$			
Cl	-2.48997400	0.51370500	-0.00018700
C	3.14174200	0.90581600	0.02056200
H	2.68685200	1.55842200	-0.73415100
H	4.21860000	0.80747900	-0.18223000
H	2.98036400	1.33841100	1.02016200
O	2.47743800	-0.37286000	-0.10736100
H	2.88937000	-0.99437200	0.50990300
H	0.28799500	0.87483600	1.14028300
H	0.24379200	0.70303200	-1.29472900

Sb	-0.18916400	-0.30338800	0.00548000

$ClH_2Sb•••PH_3$			
Cl	-2.63472100	0.26836700	-0.00000600
H	3.81033400	-0.42093000	-1.05316300
H	3.80999400	-0.41974800	1.05402500
H	3.74298600	1.40734200	-0.00060300
H	0.07548400	0.96095200	-1.21683700
H	0.07554400	0.96136500	1.21645400
P	3.05298200	0.16330300	-0.00001900
Sb	-0.24546700	-0.18629000	0.00001000

$ClH_2Sb•••O(CH_3)_2$			
C	2.78929600	1.18249900	0.07337000
H	2.28040500	2.04115200	-0.38326900
H	3.86087500	1.20407800	-0.18602800
H	2.67441600	1.21685900	1.17173100
O	2.17547200	0.00000300	-0.46219800
H	-0.23345600	1.22858800	-1.06355100
H	-0.23346100	-1.22855100	-1.06359700
Cl	-2.82630100	0.00000500	-0.08396200
C	2.78928900	-1.18249800	0.07336900
H	2.28038000	-2.04114600	-0.38325900
H	3.86086400	-1.20409100	-0.18604300
H	2.67442200	-1.21685000	1.17173100
Sb	-0.39201200	-0.00000300	0.10131000

21. Bismuth Bonded Complexes

$F_3Bi•••OH_2$			
F	-0.43736900	-1.52014300	0.94871400
F	2.04194900	0.00002600	0.54437500
F	-0.43746000	1.52009700	0.94874200
O	-2.47477200	-0.00002400	-0.17013600

H	-2.57195500	-0.76473800	0.42188200
H	-2.57196900	0.76471900	0.42184300
Bi	0.17395200	0.00000500	-0.25854400

$F_3Bi•••SH_2$			
F	-0.13620700	-1.49703600	1.00783000
F	2.33418500	0.00000000	0.37123400
F	-0.13620700	1.49703600	1.00783000
H	-2.62300400	-0.97459000	0.74206300
H	-2.62300300	0.97459000	0.74206400
S	-2.92388800	0.00000000	-0.14702500
Bi	0.40328000	0.00000000	-0.24835900

$F_3Bi•••NH_3$			
F	-0.36213900	-1.52013000	0.98481200
F	2.07830500	-0.00002400	0.46674200
F	-0.36213600	1.52013000	0.98482500
H	-2.63150700	-0.82056500	0.51277600
H	-3.23861900	-0.00001400	-0.78409900
H	-2.63151300	0.82053600	0.51277900
N	-2.49819500	-0.00001300	-0.08231100
Bi	0.16629800	0.00000400	-0.26015300

$F_3Bi•••NCH$			
F	-0.19815400	1.49780000	1.01453900
F	-0.19814100	-1.49782800	1.01450700
F	2.27080500	-0.00000400	0.36312500
N	-2.52980500	0.00002600	-0.37341900
C	-3.61981700	-0.00001600	0.07591200
H	-4.61525500	-0.00005100	0.49066900
Bi	0.32737600	0.00000300	-0.23929800

$F_3Bi\cdots CO$			
F	0.26409400	1.49430900	0.94645200
F	-2.26467200	0.00032200	0.50495200
F	0.26356200	-1.49454100	0.94645000
C	2.79123200	-0.00017600	-0.29200600
O	3.87380000	0.00008800	0.08854100
Bi	-0.38680300	-0.00000600	-0.24743300

$F_3Bi\cdots OCH_2$			
F	0.34865200	-1.47758400	0.94308900
F	0.34858400	1.47753200	0.94321800
F	-2.18323100	-0.00006400	0.63537200
O	2.30363600	0.00006900	-0.67063300
C	2.95189000	-0.00003800	0.37716800
H	2.45086000	-0.00016300	1.36093200
H	4.05736500	-0.00001800	0.34443800
Bi	-0.35270700	0.00001100	-0.25660700

$F_3Bi\cdots C_2H_4$			
F	-0.21760200	-1.11489500	1.40561700
F	2.30119900	-0.09075100	0.23388400
F	0.01438600	1.76120000	0.59816400
C	-2.92912900	-0.59466700	-0.41214100
H	-3.27244100	-0.60246600	-1.45084900
H	-2.69172300	-1.55490000	0.05540100
C	-2.83104400	0.55930700	0.28853800
H	-2.49953600	0.56111400	1.32995200
H	-3.07857000	1.52359200	-0.16296400
Bi	0.32796900	-0.05680900	-0.23095100

$F_3Bi\cdots OHCH_3$			
F	-0.39107200	-1.47261500	0.90352900

F	2.25252300	-0.25022400	0.52213500
F	-0.01613900	1.53430800	1.02719000
C	-3.16742500	-0.38176400	0.08658900
H	-3.24359200	-1.07905900	-0.75646700
H	-4.13629300	0.11648200	0.23433500
H	-2.86585200	-0.92994100	0.98932700
O	-2.15922200	0.59428000	-0.28148400
H	-2.05816200	1.22543100	0.45212000
Bi	0.38523400	-0.00120200	-0.25617700

$F_3Bi•••PH_3$			
F	-0.26965800	-1.43588100	0.98786600
F	2.33483700	-0.13965600	0.45242700
F	-0.04414600	1.55228100	0.95622300
H	-3.63025000	-1.22390900	-0.08118800
H	-4.03309000	0.82009600	-0.46375600
H	-3.00112200	0.25037100	1.30171000
P	-2.92411800	0.00944600	-0.09490100
Bi	0.43779400	0.00266300	-0.25183000

$F_3Bi•••O(CH_3)_2$			
F	-0.24104100	1.86356600	0.08266500
F	-2.43969900	-0.04023500	0.47328700
F	0.19126600	-0.71523900	1.59079600
C	2.65646200	1.10723100	0.41276100
H	2.15589700	2.05366300	0.18374400
H	3.73750900	1.17786200	0.21021200
H	2.48115800	0.83439100	1.46578700
O	2.07502600	0.10717800	-0.45521600
C	2.69214000	-1.17330300	-0.22996700
H	2.56380600	-1.48163000	0.82003600
H	2.19643100	-1.89515700	-0.89551500
H	3.76275300	-1.12311800	-0.48671500

Bi	-0.52029100	-0.12048000	-0.21775100

$FH_2Bi•••OH_2$			
F	-2.13060400	0.36921200	0.07290700
H	2.94230300	1.09127300	-0.03340000
H	3.29249100	-0.25093500	0.61056600
H	0.19111700	0.63122700	1.58245100
H	0.27585800	1.47160600	-0.79026700
O	2.69952700	0.15482900	-0.03653000
Bi	-0.10991000	-0.09041800	-0.02088300

$FH_2Bi•••SH_2$			
F	2.38720200	0.42840100	0.03202300
H	-3.17389600	-0.26071400	1.21127400
H	-2.90399900	1.38230300	0.19104700
S	-2.95425900	0.06039700	-0.08260800
H	-0.01202900	1.16710000	-1.19856600
H	-0.01742700	1.03678400	1.31140000
Bi	0.38422500	-0.09816200	-0.00580300

$FH_2Bi•••NH_3$			
F	2.14677100	0.36456300	-0.00000200
N	-2.65210400	0.19120100	-0.00000200
H	-3.13077600	-0.18732800	0.81820400
H	-3.13080300	-0.18740400	-0.81815700
H	-2.82787500	1.19665600	-0.00004400
H	-0.21003800	1.12435000	1.26399600
H	-0.21003700	1.12434000	-1.26399700
Bi	0.10546200	-0.09265200	0.00000000

$FH_2Bi•••NCH$			
F	-2.31078200	0.41071700	0.00000000

N	2.55995000	0.06111800	0.00000000
C	3.73487500	0.16695900	0.00000000
H	4.80839100	0.26730500	0.00000000
H	0.07759900	1.11079900	-1.25945600
H	0.07759700	1.11078500	1.25947200
Bi	-0.29512600	-0.09174600	0.00000000

$FH_2Bi\cdots CO$			
F	2.29950700	0.50782800	0.00000200
H	-0.13838700	1.07292700	1.25455100
H	-0.13842100	1.07305600	-1.25442500
C	-2.74663400	0.05129300	-0.00000400
O	-3.88352000	0.20994400	0.00000200
Bi	0.32685800	-0.10486400	-0.00000200

$FH_2Bi\cdots OCH_2$			
F	0.55819400	1.61481000	-0.02575300
O	2.36539200	-0.85901000	-0.06062000
C	3.15102000	0.08058000	0.04701200
H	2.78491300	1.12241100	0.10920300
H	4.24545300	-0.10046400	0.08337800
H	-0.15975400	-0.51632900	1.65973100
H	-2.01083200	0.79048000	0.57118900
Bi	-0.57485300	-0.11374400	-0.02396200

$FH_2Bi\cdots C_2H_4$			
F	2.31232900	0.34051200	0.14617200
C	-2.78861400	-0.56709800	0.10324200
H	-2.93034100	-1.19859000	-0.77799900
H	-2.67612500	-1.06587900	1.07047100
C	-2.80055000	0.78511100	0.01046300
H	-2.68340200	1.41488400	0.89609800
H	-2.93995400	1.28682600	-0.95064000

H	-0.07075300	0.55680100	1.58748100
H	-0.08560500	1.51260900	-0.74135400
Bi	0.29048400	-0.08288400	-0.03713100

$FH_2Bi\bullet\bullet\bullet OHCH_3$

F	2.24152100	0.76065600	0.02057800
C	-3.10738100	0.72974100	0.01515900
H	-2.70079900	1.40153800	-0.74987200
H	-2.98298900	1.19157300	1.00679200
H	-4.17233600	0.54289600	-0.18854300
O	-2.34423300	-0.49587000	-0.08552800
H	-2.72438500	-1.13786600	0.53056600
H	-0.22586900	1.00375500	-1.23858200
H	-0.22977600	0.95432500	1.28106900
Bi	0.36458600	-0.13510400	-0.00281200

$FH_2Bi\bullet\bullet\bullet PH_3$

F	-2.39770700	0.45749300	-0.00000100
H	3.74320500	-0.37877200	-1.05486500
H	3.74305700	-0.37830400	1.05518500
H	3.43241300	1.42486000	-0.00025900
H	0.02601800	1.09250500	-1.25512900
H	0.02605300	1.09263500	1.25499800
P	2.91802100	0.09994700	-0.00000400
Bi	-0.39953900	-0.10204300	0.00000200

$FH_2Bi\bullet\bullet\bullet O(CH_3)_2$

C	2.74877700	1.18316900	0.08294300
H	2.23236200	2.03940400	-0.37011800
H	3.81730300	1.20721300	-0.18975800
H	2.65107700	1.22264400	1.18328000
O	2.12899500	0.00000100	-0.43985300
H	-0.34027000	1.26827900	-1.17681200

H	-0.34026000	-1.26828900	-1.17679600
C	2.74874400	-1.18318500	0.08294300
H	2.23228500	-2.03940500	-0.37009700
H	3.81726300	-1.20727300	-0.18978300
H	2.65106800	-1.22264400	1.18328200
Bi	-0.52278100	0.00000300	0.05932700
F	-2.59412100	-0.00000700	-0.14376000

$ClH_2Bi\bullet\bullet\bullet OH_2$

Cl	-2.38464900	0.24376000	0.03114100
H	3.13202900	1.23153400	-0.03551000
H	3.53832400	-0.10454500	0.58955400
H	0.33499500	0.72412600	1.53543900
H	0.39405300	1.41694700	-0.87614200
O	2.90949300	0.29000400	-0.03020900
Bi	0.11884000	-0.11725300	-0.01808500

$ClH_2Bi\bullet\bullet\bullet SH_2$

Cl	2.63706300	0.32408900	0.01402200
H	-3.40083600	-0.15286000	1.21242200
H	-3.08451200	1.48331100	0.19388900
S	-3.17646300	0.16391700	-0.08181900
H	-0.15958100	1.10595100	-1.23575400
H	-0.16208700	1.06312500	1.26979500
Bi	0.15422100	-0.14014100	-0.00445300

$ClH_2Bi\bullet\bullet\bullet NH_3$

Cl	2.40787100	0.23020600	0.00000000
N	-2.85261000	0.31246800	0.00000200
H	-3.34441800	-0.04973700	0.81806000
H	-3.34413500	-0.04873800	-0.81866800
H	-2.99263900	1.32375700	0.00059300
H	-0.34447500	1.12233300	1.25932700

H	-0.34450900	1.12254700	-1.25911200
Bi	-0.12765500	-0.11531300	-0.00000300

$ClH_2Bi•••NCH$

Cl	-2.55910600	0.30410200	0.00000000
N	2.78391200	0.15572700	-0.00000300
C	3.95583800	0.29185100	0.00000200
H	5.02661900	0.41915200	0.00000600
H	0.22614700	1.09678000	-1.25519100
H	0.22614400	1.09679900	1.25516700
Bi	-0.06260900	-0.12799600	0.00000000

$ClH_2Bi•••CO$

Cl	2.55296800	0.39422000	-0.00000100
H	-0.27596200	1.05454900	1.25068600
H	-0.27595400	1.05445900	-1.25077200
C	-2.99929200	0.17140600	-0.00001200
O	-4.13017900	0.36866000	0.00000600
Bi	0.09865800	-0.15407800	0.00000200

$ClH_2Bi•••OCH_2$

Cl	0.65117800	1.91575400	-0.00759900
O	2.27314000	-1.22093700	-0.05757600
C	3.23401600	-0.46204300	0.03996100
H	3.09185800	0.63403500	0.10601500
H	4.27073900	-0.85771800	0.06416100
H	-0.22207200	-0.62624000	1.65652200
H	-2.12423200	0.59405800	0.56388700
Bi	-0.64669300	-0.23821900	-0.02458500

$ClH_2Bi•••C_2H_4$

Cl	2.55956600	0.25819600	0.08367100

C	-3.03012000	-0.45678300	0.14359700
H	-3.19192900	-1.10919700	-0.71881000
H	-2.93864000	-0.92996300	1.12579800
C	-2.99476100	0.89179000	0.01011200
H	-2.85746100	1.54361400	0.87682900
H	-3.11354800	1.36876500	-0.96627700
H	-0.22106600	0.67439700	1.52647600
H	-0.23982700	1.42669700	-0.86744800
Bi	0.06264000	-0.12016500	-0.04001500

$ClH_2Bi{\bullet\bullet\bullet}OHCH_3$

Cl	2.53501300	0.59209800	0.01106000
C	-3.23141300	0.98264800	0.01361200
H	-2.76050200	1.60568500	-0.75585700
H	-3.06185400	1.43610600	1.00239100
H	-4.30951300	0.90089100	-0.18948100
O	-2.59353000	-0.31385800	-0.07886300
H	-3.03512600	-0.91164100	0.54112500
H	-0.32545700	0.95896600	-1.25130500
H	-0.32966400	0.94800200	1.25985600
Bi	0.13088700	-0.22155100	-0.00295800

$ClH_2Bi{\bullet\bullet\bullet}PH_3$

Cl	-2.65041600	0.35114800	-0.00000200
H	3.97995900	-0.24833300	-1.05478400
H	3.97931100	-0.24658100	1.05602100
H	3.61680400	1.54677100	-0.00097600
H	0.17176300	1.07175900	-1.25168100
H	0.17183900	1.07219100	1.25126300
P	3.14160100	0.20712500	-0.00001600
Bi	-0.16851400	-0.14785800	0.00000500

$ClH_2Bi{\bullet\bullet\bullet}O(CH_3)_2$

C	2.95949300	1.18343300	0.06836000
H	2.44615300	2.04012200	-0.38734700
H	4.02958000	1.20716000	-0.19748500
H	2.85404600	1.22137200	1.16796200
O	2.34281400	-0.00000200	-0.45969100
H	-0.15213900	1.26336100	-1.17452300
H	-0.15213100	-1.26337800	-1.17449900
Cl	-2.82897300	-0.00000600	-0.08924500
C	2.95947700	-1.18344600	0.06836100
H	2.44611300	-2.04012800	-0.38733200
H	4.02955900	-1.20719500	-0.19749900
H	2.85404500	-1.22137200	1.16796500
Bi	-0.29541000	0.00000300	0.06695300

22. Oxygen Bonded Complexes

$F_2O\bullet\bullet\bullet OH_2$			
O	0.42408600	-0.25305100	0.00003100
F	0.53528400	1.16690900	0.00003800
F	1.79445800	-0.66090400	-0.00003700
O	-2.33429500	-0.31482300	-0.00003900
H	-2.84284100	-0.00509600	-0.76085600
H	-2.84316100	-0.00595800	0.76091400

$F_2O\bullet\bullet\bullet SH_2$			
O	1.06163300	-0.28279000	-0.02263000
F	1.13157400	1.14099600	0.01285000
F	2.43912900	-0.65418600	0.00636500
H	-1.98036600	1.06877100	-0.39271100
H	-2.23169200	0.07713800	1.26544900
S	-2.27608300	-0.20405500	-0.05404000

$F_2O•••NH_3$			
O	-0.47971400	-0.32473500	0.00000300
F	-0.39346300	1.09968700	0.00000000
F	-1.89753900	-0.53453300	-0.00000100
N	2.33984400	-0.30002300	0.00000000
H	2.48818100	0.29532800	-0.81544700
H	3.10144800	-0.97900800	-0.00000500
H	2.48819000	0.29532400	0.81544800

$F_2O•••NCH$			
O	0.90040300	-0.27350900	-0.00001700
F	0.98412800	1.14686700	0.00000300
F	2.27827200	-0.65636300	0.00002000
N	-1.94547800	-0.20932600	-0.00003100
C	-3.12453700	-0.12041600	-0.00001400
H	-4.19925500	-0.03867600	0.00023600

$F_2O•••CO$			
O	1.00311100	-0.30235800	-0.00001600
F	1.00123600	1.12092300	0.00000100
F	2.39576500	-0.60555700	0.00001100
C	-2.10887100	-0.26673800	-0.00001000
O	-3.24308300	-0.07737500	0.00001000

$F_2O•••OCH_2$			
O	-1.77691600	-0.77989800	-0.00003600
C	-2.45033800	0.24271400	-0.00000500
H	-1.97849800	1.24817700	0.00003100
H	-3.56053700	0.20707500	-0.00001100
O	0.92540300	-0.34823200	-0.00000900
F	0.65180200	1.05250000	0.00004900
F	2.35410600	-0.37322200	-0.00000700

$F_2O\cdots C_2H_4$			
C	-2.19299900	-0.12757200	-0.67499300
H	-2.55746500	-0.98756100	-1.24288500
H	-1.83015300	0.73307100	-1.24289800
C	-2.19300600	-0.12762100	0.67504000
H	-1.83016600	0.73298100	1.24301200
H	-2.55747900	-0.98765200	1.24286600
O	0.84876800	-0.28739200	-0.00004100
F	0.91500100	1.13682900	0.00006500
F	2.22957200	-0.65466700	-0.00007000

$F_2O\cdots OHCH_3$			
C	-2.10042300	0.16465900	-0.63124600
H	-3.13695500	-0.04683500	-0.94136000
H	-1.41809000	-0.17958900	-1.41852600
H	-1.97076300	1.25169500	-0.50102700
O	-1.74245500	-0.56031000	0.55638000
H	-2.33005400	-0.27407800	1.26768700
O	0.92714100	-0.31623200	0.17625800
F	0.85853900	1.10402400	0.27332600
F	2.25045200	-0.51811400	-0.32670300

$F_2O\cdots PH_3$			
O	-1.16364400	-0.36937600	0.00012300
F	-0.95669300	1.04141700	-0.00001400
F	-2.58509300	-0.46902700	-0.00006400
H	2.28539200	0.75525700	-1.04180700
H	3.60145200	-0.48393500	0.00000100
H	2.28560100	0.75611000	1.04105700
P	2.20085200	-0.21492900	0.00003100

$F_2O\cdots O(CH_3)_2$			
C	-1.65122000	1.20088400	0.33469200

H	-2.74047900	1.37277000	0.41769900
H	-1.16440300	2.11337900	-0.03400000
H	-1.25157900	0.94920300	1.33465300
O	-1.36746400	0.16566200	-0.60333800
O	1.26831700	0.05862700	-0.33299300
F	1.07352700	-0.51879000	0.95722900
F	2.69291100	0.19946600	-0.38401200
C	-1.95500500	-1.06471900	-0.18789800
H	-3.05546400	-0.97624600	-0.12274100
H	-1.69312500	-1.81854500	-0.94202500
H	-1.56236700	-1.37794700	0.79734400

23. Sulfur Bonded Complexes

$F_2S\bullet\bullet\bullet OH_2$			
S	-0.32197700	-0.36265500	-0.00004100
O	2.32975200	-0.38092100	-0.00000400
H	2.65444800	0.11766800	0.76285000
H	2.65447100	0.11778200	-0.76277500
F	-0.10425300	1.28250000	0.00013100
F	-1.98411500	-0.32534500	-0.00006300

$F_2S\bullet\bullet\bullet SH_2$			
S	0.83631800	-0.36119400	-0.00002900
H	-2.28757400	0.69654000	-0.97525900
H	-2.28759900	0.69635600	0.97544500
S	-2.33013200	-0.23678200	0.00000500
F	0.66657100	1.28803400	0.00007300
F	2.49745100	-0.37973300	-0.00005200

$F_2S\bullet\bullet\bullet NH_3$			
S	-0.29241400	-0.39554200	0.00001600
H	2.46906400	0.26160300	0.82054900
H	2.46909100	0.26151100	-0.82049400

N	2.18473200	-0.27389800	0.00005300
H	2.72162900	-1.14134100	0.00011000
F	-0.05788900	1.25568100	-0.00007100
F	-1.97258800	-0.27077100	-0.00001700

$F_2S•••NCH$			
S	-0.73444300	-0.35990700	0.00002400
N	2.06874500	-0.28573000	0.00069800
C	3.23497100	-0.10003500	-0.00040900
H	4.29909500	0.07101900	-0.00144300
F	-2.39598100	-0.36157600	-0.00021400
F	-0.54169100	1.28244300	0.00006000

$F_2S•••CO$			
S	0.81802100	-0.36915600	-0.00015000
C	-2.25674600	-0.27124400	-0.00002300
O	-3.39049300	-0.08508600	0.00041000
F	0.59185000	1.26793200	-0.00000900
F	2.47215800	-0.35519200	-0.00007200

$F_2S•••OCH_2$			
S	0.74852200	-0.40549400	-0.00000700
O	-1.83818200	-0.74649500	-0.00000400
C	-2.57957200	0.23221500	0.00000600
H	-2.17265100	1.26226300	0.00001200
H	-3.68088500	0.10964900	0.00000800
F	0.28704200	1.19171400	0.00001700
F	2.38629900	-0.11452900	-0.00000800

$F_2S•••C_2H_4$			
S	0.65284200	-0.35581200	-0.00002300
C	-2.24457900	-0.14926100	-0.67696000

H	-2.42139800	-1.06670000	-1.24454100
H	-2.08040900	0.77072700	-1.24377800
C	-2.24456300	-0.14931700	0.67699400
H	-2.08037900	0.77062400	1.24388500
H	-2.42136800	-1.06680300	1.24450400
F	0.51688100	1.29510900	0.00005200
F	2.31566700	-0.39770800	-0.00004200

$F_2S{\bullet\bullet\bullet}OHCH_3$

S	-0.77412600	-0.39398100	-0.02849800
C	2.43636600	0.17694900	0.51531300
H	3.52118600	0.08840000	0.35147400
H	2.18357500	-0.23438300	1.50007600
H	2.13237900	1.23391200	0.47447800
O	1.70462800	-0.61502300	-0.44603100
H	1.89315200	-0.26496000	-1.32869200
F	-2.40005000	-0.17846700	0.27559900
F	-0.44433800	1.21615600	-0.28282100

$F_2S{\bullet\bullet\bullet}PH_3$

S	0.90124200	-0.37375200	0.00000900
H	-2.85174500	0.63620400	-1.04953400
H	-2.85266400	0.63352900	1.05109200
H	-3.37335900	-1.10964200	-0.00166300
P	-2.31209400	-0.15980800	0.00000300
F	0.69739000	1.27074700	0.00000000
F	2.56253300	-0.35773900	-0.00001000

$F_2S{\bullet\bullet\bullet}O(CH_3)_2$

S	-1.03324100	-0.00006600	-0.39676100
C	1.94632400	-1.18235900	0.03724300
H	3.03744000	-1.21779800	-0.12313800
H	1.46840700	-2.03927900	-0.45393500

H	1.72924000	-1.20264500	1.11895400
O	1.39755300	-0.00006100	-0.56370600
F	-2.69436400	-0.00003900	-0.19645500
F	-0.69160200	0.00016300	1.23304100
C	1.94622800	1.18239400	0.03702500
H	1.46821500	2.03918500	-0.45428700
H	1.72916700	1.20284700	1.11873700
H	3.03733600	1.21790800	-0.12339200

$Cl_2S{\bullet\bullet\bullet}OH_2$

S	-0.03322600	-0.53478000	-0.00001000
O	2.73699000	-1.04357300	-0.00002100
H	3.15421300	-0.61795300	0.76176100
H	3.15421600	-0.61758200	-0.76159400
Cl	-2.10345300	-0.40676200	0.00000300
Cl	0.47564500	1.47385600	0.00000600

$Cl_2S{\bullet\bullet\bullet}SH_2$

S	-0.40862900	-0.47139400	0.00001300
H	2.85738000	0.34826500	0.97415200
H	2.85735100	0.34799100	-0.97438800
Cl	-2.47738500	-0.63223800	-0.00000600
Cl	-0.17555400	1.58749500	-0.00000200
S	2.87020600	-0.58708200	0.00001000

$Cl_2S{\bullet\bullet\bullet}NH_3$

S	-0.02954800	-0.57324300	0.00003400
H	2.99068400	-0.45228700	0.81832200
H	2.99071200	-0.45237800	-0.81821100
Cl	-2.11535500	-0.33849700	0.00000800
Cl	0.53678900	1.42609300	-0.00008600
N	2.61654100	-0.93395200	0.00007600
H	3.01120800	-1.87491400	0.00013500

$Cl_2S\cdots NCH$			
S	-0.30519100	-0.49292100	-0.00005600
Cl	-2.37647800	-0.61263300	0.00004500
Cl	-0.02856000	1.55448400	0.00000200
N	2.60142400	-0.59478800	-0.00010800
C	3.78303200	-0.56951900	0.00009500
H	4.86052700	-0.54409300	0.00027500

$Cl_2S\cdots CO$			
S	0.38569800	-0.51773600	-0.00046300
Cl	0.02311300	1.51626000	-0.00004800
Cl	2.45117600	-0.56912800	0.00030500
C	-2.79471400	-0.64894800	-0.00043600
O	-3.93322600	-0.49047200	0.00070500

$Cl_2S\cdots OCH_2$			
S	0.38864800	-0.55163100	0.00001200
O	-2.32896400	-1.05617300	-0.00001900
Cl	2.45686700	-0.37791200	-0.00000300
Cl	-0.16425400	1.44590400	-0.00000400
C	-3.21590600	-0.20916700	0.00000800
H	-2.97903700	0.87446500	0.00002500
H	-4.28660200	-0.49984200	0.00001600

$Cl_2S\cdots C_2H_4$			
S	0.26982700	-0.47564100	-0.00003400
Cl	2.34548000	-0.59041600	0.00000800
Cl	-0.00562500	1.57713300	0.00001300
C	-2.75508800	-0.57285000	-0.67656900
H	-2.89117500	-1.49743300	-1.24385100
H	-2.62585200	0.35287800	-1.24330600
C	-2.75505200	-0.57291400	0.67659200

H	-2.62578700	0.35275900	1.24341100
H	-2.89111100	-1.49755200	1.24379300

$Cl_2S{\bullet\bullet\bullet}OHCH_3$

S	-0.37188400	-0.47368500	-0.25423500
Cl	-0.00075100	1.54992700	0.02201300
Cl	-2.40666800	-0.53974900	0.16873400
C	2.84220500	-0.54621500	0.67998800
H	3.94243800	-0.49867700	0.65747300
H	2.53348800	-1.47261700	1.18006500
H	2.44236000	0.31525600	1.23880900
O	2.29405900	-0.60777700	-0.65193000
H	2.55227600	0.20146400	-1.11578200

$Cl_2S{\bullet\bullet\bullet}PH_3$

S	0.48258500	-0.52419300	-0.00000600
H	-3.24323800	0.35108100	-1.04711600
H	-3.24321500	0.35105600	1.04714700
Cl	2.55736400	-0.52777400	0.00000400
Cl	0.08986400	1.51077600	0.00000000
H	-4.00378800	-1.30280500	0.00000400
P	-2.81559900	-0.51488400	0.00000000

$Cl_2S{\bullet\bullet\bullet}O(CH_3)_2$

S	-0.65861900	-0.51072200	-0.00000400
Cl	-0.27098800	1.52774600	0.00000900
Cl	-2.74581700	-0.48508300	-0.00000300
C	2.53121000	-0.23295600	1.17924400
H	3.59687000	-0.51932100	1.22728500
H	1.99368700	-0.65734100	2.03734500
H	2.44657800	0.86824000	1.19666200
O	1.92184300	-0.76770800	-0.00000700
C	2.53121700	-0.23292900	-1.17924300

H	3.59687600	-0.51929500	-1.22728500
H	1.99369700	-0.65729300	-2.03735600
H	2.44658600	0.86826700	-1.19663400

$O_2S•••OH_2$			
S	0.64108500	0.00003400	0.39147600
O	0.77012200	1.28533800	-0.37899000
O	0.77063400	-1.28519800	-0.37902300
O	-2.21129300	-0.00016100	0.08928700
H	-2.44671400	-0.76305000	-0.45678100
H	-2.44633900	0.76267100	-0.45702600

$O_2S•••SH_2$			
S	-1.20072500	0.00000600	-0.39763600
O	-1.27877600	1.28705100	0.37917400
O	-1.27886400	-1.28703400	0.37917300
H	1.89795600	-0.97548600	0.78878600
H	1.89786400	0.97543100	0.78878500
S	2.24230600	-0.00001200	-0.08013500

$O_2S•••NH_3$			
S	0.62045300	-0.00000200	-0.39788300
O	0.80762600	-1.28265700	0.36549500
O	0.80765600	1.28264900	0.36549500
N	-2.18181700	0.00001100	0.00040900
H	-2.31525200	-0.81898300	0.59535900
H	-2.94631400	0.00006800	-0.67546600
H	-2.31521800	0.81893800	0.59545800

$O_2S•••NCH$			
S	-1.06427700	0.00002800	-0.37086100
O	-1.19699200	1.28658700	0.39800000

O	-1.19768300	-1.28632300	0.39822600
N	1.96193300	-0.00043000	-0.27224600
C	3.06390000	0.00000800	0.15426200
H	4.06891100	0.00040500	0.54412900

$O_2S•••CO$			
S	-1.19053600	0.00000000	-0.38052500
O	-1.26494800	1.28901300	0.39279400
O	-1.26494700	-1.28901300	0.39279400
C	2.17745000	-0.00000300	-0.20367900
O	3.27787900	0.00000100	0.12822200

$O_2S•••OCH_2$			
S	-0.99801600	0.02192200	-0.38041800
O	-0.61087500	1.37002500	0.17090300
O	-1.40419600	-1.03133500	0.61284100
C	2.25032200	0.16278100	0.31795200
H	1.68908600	1.00282100	0.77833900
H	3.32960900	0.07081300	0.55324500
O	1.69602400	-0.63882400	-0.42782000

$O_2S•••C_2H_4$			
S	-1.04388300	0.00004200	-0.39926500
O	-1.21416500	1.28760500	0.36030800
O	-1.21428800	-1.28761400	0.36012100
C	2.25792500	-0.67537900	0.03924200
H	1.95194800	-1.24428500	0.92131100
H	2.56483800	-1.24366300	-0.84306200
C	2.25803600	0.67530300	0.03897500
H	2.56504500	1.24318600	-0.84355500
H	1.95215300	1.24460900	0.92081800

$O_2S•••OHCH_3$			
S	1.09165000	0.00663800	-0.36577100
O	0.77969300	1.38745600	0.14314600
O	1.30290600	-1.07074700	0.66387100
C	-2.16308500	0.30291800	0.39825600
H	-3.22994800	0.07252300	0.54335800
H	-2.06228700	1.31918900	-0.00134600
H	-1.63348400	0.24469200	1.36280500
O	-1.57395200	-0.57666800	-0.58223900
H	-1.63134900	-1.48045500	-0.24025300

$O_2S•••PH_3$			
S	1.29829700	0.00007100	-0.39446500
O	1.37459600	-1.28788500	0.38052200
O	1.37357900	1.28808300	0.38053200
H	-3.23750900	1.04647300	-0.11952700
H	-2.19594900	-0.00012000	1.36313100
H	-3.23869000	-1.04582700	-0.11933300
P	-2.27240000	-0.00021700	-0.06008400

$O_2S•••O(CH_3)_2$			
S	1.28700800	-0.22673700	-0.35896000
O	1.60098200	1.20437300	-0.01622000
O	1.10009700	-1.17826100	0.79379400
C	-1.50462300	1.22029000	0.46353900
H	-2.57937000	1.44285200	0.58019900
H	-0.97116600	2.11712400	0.12443100
H	-1.09162100	0.88856600	1.43345900
O	-1.31442600	0.21301600	-0.53868300
C	-1.94888400	-1.01159500	-0.15002200
H	-3.03573900	-0.85920900	-0.03084300
H	-1.76414300	-1.73779600	-0.95252100
H	-1.52226300	-1.38894500	0.79640900

24. Selenium Bonded Complexes

$F_2Se\bullet\bullet\bullet OH_2$			
O	-2.34870200	-0.32968900	0.00001300
H	-2.65156600	0.18285800	-0.76388700
H	-2.65154000	0.18290500	0.76389300
Se	0.21153200	-0.29350000	-0.00001700
F	-0.10643900	1.45739000	0.00007600
F	1.98428900	-0.09619500	-0.00002600

$F_2Se\bullet\bullet\bullet SH_2$			
H	2.44303200	0.72283000	0.97589100
H	2.44291500	0.72308100	-0.97576200
Se	-0.59350200	-0.29060800	0.00001500
S	2.47548700	-0.21088600	-0.00005700
F	-0.33003200	1.46740400	-0.00001900
F	-2.37159900	-0.15530200	0.00004800

$F_2Se\bullet\bullet\bullet NH_3$			
H	-2.48975100	0.34111300	-0.82202700
H	-2.48975000	0.34110900	0.82203000
N	-2.21107500	-0.19539000	0.00000000
H	-2.74106600	-1.06753300	-0.00000200
Se	0.19135800	-0.32122800	-0.00000100
F	-0.12348200	1.43985600	0.00000600
F	1.97813900	-0.03154600	-0.00000300

$F_2Se\bullet\bullet\bullet NCH$			
N	2.18330300	-0.26528100	0.00001000
C	3.34637500	-0.06729800	0.00000300
H	4.40861300	0.11616600	-0.00000500
Se	-0.50813600	-0.28795200	-0.00001200
F	-0.21571400	1.46006900	0.00005300

F	-2.28354800	-0.13396400	-0.00001500

$F_2Se\bullet\bullet\bullet CO$			
C	-2.39635000	-0.24852000	0.00007600
O	-3.52857000	-0.05766500	0.00010900
Se	0.57229500	-0.29292400	-0.00000800
F	2.33678800	-0.12181700	-0.00006000
F	0.23528300	1.44535700	-0.00005500

$F_2Se\bullet\bullet\bullet OCH_2$			
O	-1.95700800	-0.69418100	0.00000800
C	-2.74654200	0.24919000	0.00003200
H	-2.38780300	1.29482900	0.00004600
H	-3.83735800	0.06320500	0.00004100
Se	0.53396500	-0.31832900	-0.00001000
F	-0.01810600	1.37613200	0.00002100
F	2.26318100	0.12647500	-0.00002000

$F_2Se\bullet\bullet\bullet C_2H_4$			
C	2.24917700	-0.11305500	0.68068700
H	2.41093700	-1.03427400	1.24665200
H	2.12597300	0.81390500	1.24584600
C	2.24918200	-0.11303600	-0.68067300
H	2.12598200	0.81393900	-1.24580700
H	2.41094500	-1.03424000	-1.24666200
Se	-0.41737300	-0.29244900	-0.00000600
F	-0.22308200	1.47509100	0.00002000
F	-2.20728700	-0.17059500	-0.00001100

$F_2Se\bullet\bullet\bullet OHCH_3$			
C	2.61918700	0.17085300	0.53105200
H	3.69015900	0.06196500	0.30612500

H	2.39471500	-0.30304200	1.49377200
H	2.33761900	1.23293200	0.56773000
O	1.82508400	-0.53883300	-0.45323100
H	1.98540600	-0.13304800	-1.31886600
Se	-0.55740500	-0.31491400	-0.02410300
F	-0.13706300	1.40199100	-0.26524300
F	-2.28204000	0.05732200	0.28860700

$F_2Se{\bullet\bullet\bullet}PH_3$

H	3.43593900	-1.09845800	-0.00003100
H	2.91195300	0.66396100	1.05941300
H	2.91193500	0.66401100	-1.05938400
P	2.39502600	-0.12908200	0.00000000
Se	-0.61841100	-0.30869900	0.00000000
F	-2.39256400	-0.08539300	0.00000000
F	-0.29179700	1.44122400	0.00000000

$F_2Se{\bullet\bullet\bullet}O(CH_3)_2$

C	2.16562900	-1.18758100	0.05514100
H	3.24449900	-1.21109200	-0.16927300
H	1.66305300	-2.04235100	-0.41348600
H	2.00389500	-1.20608400	1.14512900
O	1.58028700	0.00000800	-0.51485400
Se	-0.77902900	0.00000500	-0.31806100
F	-0.34613300	-0.00002700	1.41433000
F	-2.53892900	-0.00000400	0.04634800
C	2.16560900	1.18758400	0.05517700
H	3.24448300	1.21112000	-0.16922400
H	1.66303100	2.04236400	-0.41343100
H	2.00386000	1.20606400	1.14516300

$Cl_2Se{\bullet\bullet\bullet}OH_2$

O	2.68138800	-0.96039100	-0.00000100
H	3.07254700	-0.50977100	0.76228500
H	3.07253000	-0.50986500	-0.76235100
Cl	-2.19442500	-0.18675600	-0.00000600
Cl	0.59403700	1.64216200	-0.00000100
Se	-0.01145800	-0.47173900	0.00000600

$Cl_2Se\cdots SH_2$			
H	2.90196700	0.38103300	0.97469300
H	2.90166000	0.38124200	-0.97456300
Cl	-2.49868400	-0.44183100	-0.00002800
Cl	0.01808300	1.75695600	0.00000000
Se	-0.29423800	-0.41904500	0.00002600
S	2.89816600	-0.55449300	-0.00003500

$Cl_2Se\cdots NH_3$			
H	2.89942900	-0.34295200	0.82057300
H	2.89942400	-0.34295900	-0.82058000
Cl	-2.20189400	-0.11441200	0.00000000
Cl	0.63843600	1.60903200	0.00000000
N	2.52572800	-0.82133100	0.00000000
H	2.89663600	-1.77219700	0.00000300
Se	0.00597700	-0.50591500	0.00000000

$Cl_2Se\cdots NCH$			
Cl	2.41720600	-0.40803400	0.00002100
Cl	-0.15041000	1.72512100	-0.00005900
N	-2.61070700	-0.58398200	0.00000900
C	-3.78943700	-0.50912300	0.00000700
H	-4.86504800	-0.43741400	0.00000400
Se	0.21591400	-0.43560200	0.00001500

$Cl_2Se\bullet\bullet\bullet CO$			
Cl	-0.15273700	1.69998300	-0.00005400
Cl	2.46759100	-0.38080900	-0.00006300
C	-2.83507000	-0.59443800	0.00010500
O	-3.97567400	-0.45622100	0.00012200
Se	0.27833200	-0.44734000	0.00001100

$Cl_2Se\bullet\bullet\bullet OCH_2$			
O	2.35691700	-0.99495000	-0.00002100
Cl	-2.46574200	-0.17638900	0.00005100
Cl	0.33621100	1.63265700	-0.00003800
C	3.26324800	-0.16617900	-0.00003300
H	3.04841400	0.92056300	-0.00004500
H	4.32424100	-0.48658900	-0.00002500
Se	-0.28251300	-0.47746600	0.00000600

$Cl_2Se\bullet\bullet\bullet C_2H_4$			
Cl	2.38425900	-0.40245400	-0.00000100
Cl	-0.16616300	1.75096700	-0.00000400
C	-2.71618100	-0.53814700	-0.67845200
H	-2.80465900	-1.46915600	-1.24493000
H	-2.64522700	0.39424600	-1.24440200
C	-2.71619600	-0.53812500	0.67844600
H	-2.64525300	0.39428500	1.24436800
H	-2.80468600	-1.46911700	1.24495200
Se	0.17019000	-0.42109800	0.00000400

$Cl_2Se\bullet\bullet\bullet OHCH_3$			
Cl	0.19097300	1.70612900	-0.02610000
Cl	-2.44757100	-0.30764800	0.24256200
C	2.95307400	-0.41973800	0.70864000
H	4.04509000	-0.42216500	0.57147900
H	2.66628100	-1.25746300	1.35579600

H	2.63037900	0.52608200	1.17068300
O	2.27732700	-0.63899300	-0.55104700
H	2.50656800	0.09370500	-1.14248200
Se	-0.27715400	-0.44364600	-0.16114100

$Cl_2Se•••PH_3$

H	3.33593800	0.34263700	1.05379800
H	3.33595100	0.34264800	-1.05378200
Cl	-2.54363700	-0.34128100	0.00000300
Cl	0.10234800	1.70204200	0.00000000
H	3.90134200	-1.40025000	0.00000300
P	2.82641500	-0.46577200	0.00000100
Se	-0.33728100	-0.45386500	-0.00000200

$Cl_2Se•••O(CH_3)_2$

Cl	-0.05198900	1.70709200	-0.00002000
Cl	-2.71214600	-0.29339500	0.00000100
C	2.61534000	-0.20508300	1.18476900
H	3.66475000	-0.54313900	1.22682500
H	2.05686100	-0.60641800	2.04004100
H	2.57665800	0.89748700	1.19760800
O	1.98273200	-0.71478300	0.00001400
Se	-0.49565100	-0.45143600	0.00000700
C	2.61533300	-0.20514800	-1.18477300
H	3.66474400	-0.54320200	-1.22681400
H	2.05685200	-0.60653400	-2.04001900
H	2.57664500	0.89742200	-1.19767600

$O_2Se•••OH_2$

Se	0.46656400	0.00000400	-0.28764000
O	0.53567900	-1.39050000	0.60023800
O	0.53562100	1.39051100	0.60023500
H	-2.57565200	0.76325000	0.47540700

H	-2.57568100	-0.76329700	0.47538900
O	-2.41028100	-0.00002000	-0.09685300

$O_2Se•••SH_2$			
O	-0.93129400	1.39239600	0.60033000
O	-0.93128500	-1.39239600	0.60033100
H	2.19177800	-0.97537800	0.77964900
H	2.19178600	0.97536800	0.77966900
S	2.55939300	0.00000200	-0.08079600
Se	-0.89509500	-0.00000100	-0.29034900

$O_2Se•••NH_3$			
O	0.58749900	-1.38605100	0.58696400
O	0.58748800	1.38605300	0.58696600
N	-2.32863700	-0.00000400	0.01106700
H	-2.44207000	-0.82106500	0.60811200
H	-3.10245200	0.00000100	-0.65420400
H	-2.44206300	0.82105400	0.60811700
Se	0.43785700	0.00000100	-0.29502700

$O_2Se•••NCH$			
O	0.93519000	-1.39210500	0.59997900
O	0.93510600	1.39212900	0.59996500
N	-2.31079300	-0.00003400	-0.27502500
C	-3.40131300	-0.00001000	0.17933300
H	-4.39615400	0.00001200	0.59480200
Se	0.76521200	0.00000300	-0.27485800

$O_2Se•••CO$			
O	0.95354200	-1.39582000	0.60345600
O	0.95047500	1.39638900	0.60324300
C	-2.57186300	-0.00098800	-0.21655600

O	-3.66257900	-0.00037200	0.14578700
Se	0.86763700	0.00012800	-0.28001600

$O_2Se•••OCH_2$			
O	-0.23131900	1.46083500	0.37427700
O	-1.18284800	-1.10384100	0.83626400
C	2.53010200	0.10791900	0.31723500
H	1.98621000	0.94188300	0.80811800
H	3.61467600	-0.00072300	0.51424100
O	1.94759700	-0.67628600	-0.42771500
Se	-0.73673300	0.02840200	-0.27907000

$O_2Se•••C_2H_4$			
O	0.93822200	-1.39509500	0.57134600
O	0.91971600	1.39170600	0.58984500
C	-2.60427100	0.67024000	0.03619300
H	-2.22199300	1.25862900	0.87491200
H	-2.99783400	1.21880800	-0.82407300
C	-2.59325200	-0.68038600	0.06160500
H	-2.97731800	-1.26739600	-0.77730500
H	-2.20186100	-1.23060200	0.92177000
Se	0.78590100	0.00319300	-0.29622400

$O_2Se•••OHCH_3$			
O	0.38740000	1.47670000	0.43452900
O	1.08027400	-1.18628700	0.79533100
C	-2.54942400	0.29050300	0.24134100
H	-3.52144500	-0.10971100	0.56717300
H	-2.71220300	1.08530900	-0.49645600
H	-2.00083600	0.70534400	1.10154500
O	-1.77683500	-0.73045100	-0.43084400
H	-1.65743600	-1.46749500	0.18842000
Se	0.81358100	0.04599600	-0.27061300

$O_2Se\cdots PH_3$			
O	-0.46523400	1.35383400	0.61678700
O	-1.45176400	-1.25480500	0.59024200
H	3.92758700	-0.66113500	-0.04280100
H	2.37910800	-0.29768600	1.32917800
H	2.91989700	1.18210200	-0.04461100
P	2.57931900	-0.20078700	-0.07832400
Se	-0.95824700	0.05871500	-0.28597500

$O_2Se\cdots O(CH_3)_2$			
O	-1.25731800	-1.41793700	0.17237500
O	-0.74890100	1.17296100	1.01786400
C	1.85456300	-1.22638900	0.44443800
H	2.93681100	-1.43544500	0.48225200
H	1.30550300	-2.12347800	0.13280700
H	1.50237400	-0.90389300	1.44011700
O	1.59168300	-0.20869900	-0.53706300
Se	-0.99781100	0.15375900	-0.25815000
C	2.21224800	1.03029100	-0.15785200
H	1.98731700	1.75683600	-0.94976400
H	1.80497600	1.38928300	0.80342200
H	3.30402700	0.89487000	-0.07665200

25. Tellurium Bonded Complexes

$F_2Te\cdots OH_2$			
O	2.41636000	-0.26932700	-0.00001500
H	2.70232800	0.25409200	0.76423200
H	2.70227900	0.25441600	-0.76405800
Te	-0.16873500	-0.27401700	-0.00000500
F	0.29557200	1.61244300	0.00000600
F	-2.06904600	0.15366400	0.00001500

$F_2Te\cdots SH_2$			
S	2.60272300	-0.17916000	0.00000100
H	2.57977400	0.75544900	0.97609900
H	2.57977500	0.75545500	-0.97608700
Te	-0.47720000	-0.27388200	-0.00000100
F	-0.05710300	1.62130200	-0.00000100
F	-2.38609000	0.11175400	0.00000400

$F_2Te\cdots C_2H_2$			
C	-2.50251400	-0.11215400	-0.61937400
H	-2.57679900	-0.09212300	-1.69371500
C	-2.50250900	-0.11213900	0.61938900
H	-2.57675300	-0.09214400	1.69373400
Te	0.28367200	-0.25173100	-0.00000400
F	0.04803300	1.66694100	-0.00000300
F	2.22227000	-0.04249500	0.00001200

$F_2Te\cdots NH_3$			
H	-2.59313500	0.42544600	-0.82068200
H	-2.59297900	0.42585800	0.82047100
N	-2.33046100	-0.12179700	0.00000700
H	-2.88917400	-0.97626500	0.00027400
Te	0.16152800	-0.29575400	-0.00000400
F	-0.28480100	1.60228500	-0.00000400
F	2.06136200	0.21512900	0.00001300

$F_2Te\cdots O(CH_3)_2$			
C	2.38062800	0.07863900	1.18954100
H	3.45712500	-0.15507200	1.19716500
H	1.88363700	-0.39289700	2.04569600
H	2.22269900	1.16831800	1.21188700
O	1.78015400	-0.48320600	-0.00010200
Te	-0.66298600	-0.29173700	-0.00006200

F	-0.07890300	1.56573800	0.00032800
F	-2.52781300	0.30611000	0.00006600
C	2.38063100	0.07915000	-1.18950300
H	1.88364300	-0.39201900	-2.04586200
H	2.22270100	1.16883800	-1.21138100
H	3.45712900	-0.15455600	-1.19722400

$F_2Te•••CO$			
C	2.44776700	-0.23124500	0.00000600
O	3.57518100	-0.01828100	-0.00000500
Te	-0.44253000	-0.27424000	0.00000100
F	0.07701900	1.58835500	0.00000200
F	-2.32996500	0.16655500	-0.00000400

$F_2Te•••OCH_2$			
O	2.09015000	-0.64937500	-0.00000200
C	2.89837700	0.28141900	0.00000000
H	2.55596200	1.33075200	-0.00002400
H	3.98252500	0.06624300	0.00002500
Te	-0.43450000	-0.29015600	0.00000000
F	0.25825100	1.52775500	0.00000200
F	-2.26446800	0.38309100	0.00000000

$F_2Te•••OHCH_3$			
C	2.79609900	0.19458700	0.54384300
H	3.85984200	0.09382200	0.28616300
H	2.59392100	-0.31218500	1.49441200
H	2.50723300	1.25218800	0.61430100
O	1.98116400	-0.48950600	-0.44892200
H	2.13136900	-0.05970600	-1.30562200
Te	-0.46204000	-0.28947200	-0.01609200
F	0.10801500	1.55337900	-0.27543900
F	-2.29603500	0.31628400	0.28386800

$F_2Te•••PH_3$			
H	-2.95788500	0.70524400	-1.06949800
H	-2.95798400	0.70529400	1.06941200
H	-3.48103000	-1.07835600	-0.00002500
P	-2.46597600	-0.08448400	-0.00000200
Te	0.48566000	-0.29743700	0.00000500
F	-0.01939300	1.58393100	0.00000700
F	2.36742100	0.23849200	-0.00002100

$F_2Te•••NCH$			
N	-2.27785600	-0.24023100	0.00000300
C	-3.43714000	-0.02745200	0.00000600
H	-4.49695700	0.17060900	0.00000800
Te	0.39792800	-0.26862100	-0.00000100
F	2.30628500	0.12282200	-0.00000100
F	-0.04267200	1.61540300	0.00000000

$Cl_2Te•••OH_2$			
O	-2.65965000	-0.85045000	0.00000000
H	-3.02873000	-0.38018600	-0.76299900
H	-3.02872900	-0.38017700	0.76299400
Cl	2.33805400	0.06164500	0.00000000
Cl	-0.74188700	1.80426200	0.00000000
Te	0.00384300	-0.46454700	0.00000000

$Cl_2Te•••SH_2$			
S	2.95597700	-0.50686500	0.00000100
H	2.96707100	0.42948600	0.97470500
H	2.96707000	0.42950900	-0.97468000
Cl	-2.62276900	-0.20215600	-0.00000500
Cl	0.22014400	1.91951500	0.00001000
Te	-0.23817600	-0.42200500	-0.00000200

$Cl_2Te\bullet\bullet\bullet NH_3$			
H	-2.91510300	-0.17017600	-0.82019800
H	-2.91510600	-0.17019000	0.82020400
Cl	2.34344200	0.10281900	-0.00000100
Cl	-0.72987900	1.79330800	0.00000000
N	-2.56951800	-0.67090900	-0.00000100
H	-2.99082600	-1.60120600	-0.00000900
Te	-0.01197900	-0.49223500	0.00000000

$Cl_2Te\bullet\bullet\bullet NCH$			
Cl	-2.54106700	-0.16771300	0.00000100
Cl	0.34174600	1.89268800	0.00000000
N	2.61081100	-0.54549400	0.00000200
C	3.78672800	-0.44896100	0.00000000
H	4.86090600	-0.35553800	-0.00000100
Te	-0.16285600	-0.43186200	-0.00000100

$Cl_2Te\bullet\bullet\bullet CO$			
Cl	-0.37316900	1.85995300	0.00000000
Cl	2.57791500	-0.12569400	-0.00000100
C	-2.84586300	-0.55093800	-0.00000600
O	-3.98494000	-0.40649600	0.00000200
Te	0.22065400	-0.44086200	0.00000100

$Cl_2Te\bullet\bullet\bullet OCH_2$			
O	-2.39317000	-0.92483700	-0.00000200
Cl	2.56089200	0.05330700	0.00006400
Cl	-0.50708700	1.80869400	-0.00013100
C	-3.30953200	-0.10325900	-0.00007900
H	-3.10270900	0.98303800	-0.00014200
H	-4.36255700	-0.44366100	-0.00008400
Te	0.22217600	-0.46490700	0.00003500

$Cl_2Te{\bullet\bullet\bullet}C_2H_4$			
Cl	-2.51220200	-0.17343200	-0.00008100
Cl	0.31568600	1.91853000	0.00027900
C	2.69133800	-0.46189800	0.68204800
H	2.79131900	-1.39262100	1.24736100
H	2.63754600	0.47262000	1.24626200
C	2.69134000	-0.46171900	-0.68207500
H	2.63754000	0.47294800	-1.24604100
H	2.79131600	-1.39229300	-1.24763300
Te	-0.11178900	-0.42857000	-0.00006100

$Cl_2Te{\bullet\bullet\bullet}OHCH_3$			
Cl	0.37833200	1.86331500	-0.07417300
Cl	-2.56697400	-0.04532800	0.27181100
C	3.06731800	-0.30719800	0.72449800
H	4.14558100	-0.34647000	0.51250800
H	2.80538000	-1.08601100	1.45029300
H	2.78631200	0.68000600	1.11982300
O	2.30993200	-0.61130500	-0.47655400
H	2.50838900	0.07555200	-1.13298000
Te	-0.22927100	-0.45183100	-0.11238600

$Cl_2Te{\bullet\bullet\bullet}PH_3$			
H	3.36057800	0.38332000	1.06373600
H	3.36078700	0.38294100	-1.06366400
Cl	-2.63865700	-0.08301400	-0.00000600
Cl	0.31000900	1.86586900	-0.00031500
H	3.84025600	-1.40524800	0.00040000
P	2.83646700	-0.39724000	0.00012300
Te	-0.26003100	-0.45598000	0.00006000

$Cl_2Te\cdots O(CH_3)_2$			
Cl	0.14535500	1.87486800	0.00001900
Cl	-2.79611200	-0.06252400	0.00000600
C	2.73028200	-0.15773600	1.18854700
H	3.77649900	-0.50370700	1.21214100
H	2.17755400	-0.56459600	2.04440800
H	2.69186400	0.94361000	1.20427800
O	2.08476900	-0.65973800	-0.00001100
Te	-0.41674000	-0.44981600	-0.00000800
C	2.73028000	-0.15766600	-1.18854000
H	3.77649800	-0.50362800	-1.21214700
H	2.17755800	-0.56448800	-2.04442500
H	2.69184200	0.94367900	-1.20421800

$O_2Te\cdots OH_2$			
O	0.24765100	-1.52804500	0.78521000
O	0.24757000	1.52804800	0.78521200
H	-2.57543200	0.76434100	0.39889700
H	-2.57544900	-0.76441700	0.39888100
O	-2.46595000	-0.00003300	-0.18819600
Te	0.40224500	0.00000600	-0.22799200

$O_2Te\cdots SH_2$			
O	0.60615800	-1.52949900	0.78387100
O	0.60612300	1.52949800	0.78387400
H	-2.38600500	0.97515600	0.73220400
H	-2.38601000	-0.97516200	0.73221600
S	-2.78488300	-0.00000700	-0.11571100
Te	0.76215200	0.00000200	-0.23375000

$O_2Te\cdots NH_3$			
O	0.38030200	-1.52425100	0.77769200
O	0.38030100	1.52425200	0.77769200

N	-2.33747800	0.00000000	-0.01929600
H	-2.46568900	-0.82523400	0.57081700
H	-3.07135100	0.00000200	-0.72897400
H	-2.46568700	0.82523100	0.57082100
Te	0.35154300	0.00000000	-0.24462800

$O_2Te•••NCH$			
O	0.80607600	-1.53001500	0.77308600
O	0.80486000	1.53036100	0.77287700
N	-2.56479100	-0.00049300	-0.25671100
C	-3.65671200	-0.00016100	0.19333400
H	-4.65302300	0.00013700	0.60564200
Te	0.60883400	0.00002900	-0.23723800

$O_2Te•••CO$			
O	0.70565500	-1.53524200	0.79099900
O	0.69748100	1.53602700	0.79072000
C	-2.86960800	-0.00265100	-0.27108500
O	-3.93900500	-0.00116500	0.14998200
Te	0.72124200	0.00036400	-0.23513600

$O_2Te•••OCH_2$			
O	0.10395600	1.54246300	0.57924600
O	-1.07800200	-1.23167400	1.00043700
C	2.72549400	0.02246300	0.29453700
H	2.22199400	0.86377100	0.81462200
H	3.80997500	-0.13480000	0.44876800
O	2.09161400	-0.72827500	-0.44677700
Te	-0.60241300	0.04761800	-0.23257400

$O_2Te•••C_2H_4$			
O	-0.83043800	1.56970800	0.62976500

O	-0.41218300	-1.45036500	0.92395100
C	2.94611700	-0.54348300	-0.17355900
H	2.53506100	-1.35823000	0.42934700
H	3.49770000	-0.81271400	-1.07883100
C	2.78230300	0.74740700	0.18945700
H	3.19253800	1.56425200	-0.41084600
H	2.23818600	1.01857600	1.09881100
Te	-0.69025100	-0.04981100	-0.24160800

$O_2Te•••OHCH_3$			
O	0.12630500	1.57052900	0.66771600
O	0.75659600	-1.40303500	0.90393100
C	-2.76004700	0.26410000	0.14623200
H	-3.64795900	-0.22219500	0.57511700
H	-3.06194800	0.91060300	-0.68629400
H	-2.23913000	0.86362700	0.90899300
O	-1.86990900	-0.73291700	-0.42017600
H	-1.68256400	-1.39593300	0.26798200
Te	0.67476800	0.05351300	-0.21451800

$O_2Te•••PH_3$			
O	-0.03448900	1.37563400	0.82726300
O	-1.43547000	-1.34939100	0.74700600
H	4.21364100	-0.69273800	-0.11653200
H	2.69724300	-0.41081100	1.31697400
H	3.14652900	1.12119000	-0.03516000
P	2.85232800	-0.27083400	-0.09178100
Te	-0.79005100	0.07374800	-0.23812900

$O_2Te•••O(CH_3)_2$			
O	1.01596600	1.63026700	0.29709900
O	0.46028100	-1.21852500	1.22191400
C	-2.10212400	1.22780000	0.43651600

H	-3.17675200	1.45635100	0.35366200
H	-1.49826600	2.11299100	0.20216200
H	-1.86512500	0.87694800	1.45508400
O	-1.75951500	0.21361300	-0.53374100
Te	0.83751400	-0.12637000	-0.20812100
C	-2.40672800	-1.03390300	-0.21007500
H	-3.49867500	-0.88646400	-0.18984900
H	-2.14305300	-1.74588900	-1.00345700
H	-2.04960500	-1.40894500	0.76385000

26. Polonium Bonded Complexes

$F_2Po\cdots OH_2$			
O	2.50172500	-0.26165000	-0.00028100
H	2.79670600	0.25589000	0.76451000
H	2.79543400	0.26165000	-0.76165400
Po	-0.12450800	-0.19865400	-0.00004300
F	0.43107600	1.76023400	0.00011400
F	-2.11411000	0.26894800	0.00022200

$F_2Po\cdots SH_2$			
S	2.75355400	-0.17530900	0.00000300
H	2.72678200	0.76018500	0.97554700
H	2.72680000	0.76013200	-0.97559400
Po	-0.35335300	-0.19858300	0.00000000
F	0.15036500	1.77352000	0.00000000
F	-2.35356600	0.22265700	0.00000000

$F_2Po\cdots NH_3$			
H	2.95619800	-0.46737500	0.82387700
H	2.54186000	0.89917500	-0.00004300
N	2.46378300	-0.12123000	0.00000200
H	2.95622100	-0.46745100	-0.82382700
F	0.41986600	1.75772400	-0.00000100
F	-2.11324200	0.33149200	0.00000300
Po	-0.12452800	-0.21331800	0.00000000

$F_2Po\cdots NCH$			
N	2.40201700	-0.24068100	-0.00000300
C	3.56024900	-0.02479800	-0.00000700
H	4.61944800	0.17724800	-0.00001300
F	-2.29423400	0.19387400	0.00000300

F	0.19825300	1.77899600	-0.00002700
Po	-0.28489600	-0.19166100	0.00000300

$F_2Po\bullet\bullet\bullet OCH_2$			
O	-2.23388200	-0.63842900	0.00000700
C	-3.05513900	0.28167000	-0.00001100
H	-2.72465100	1.33479700	-0.00002200
H	-4.13578000	0.04990900	-0.00001900
F	-0.46326200	1.67257200	0.00000900
F	2.23847900	0.50851800	-0.00000900
Po	0.32244500	-0.20948900	0.00000100

$F_2Po\bullet\bullet\bullet C_2H_2$			
C	-2.57686700	-0.11347000	-0.62056100
H	-2.68652900	-0.08918900	-1.69217000
C	-2.57688000	-0.11345400	0.62056800
H	-2.68649000	-0.08915500	1.69218100
Po	0.19460600	-0.17490900	-0.00000100
F	-0.02436300	1.83953700	-0.00000700
F	2.24087200	-0.03595100	0.00000600

$F_2Po\bullet\bullet\bullet OHCH_3$			
C	2.96622100	0.19624300	0.55817600
H	4.03031400	0.10008200	0.30028600
H	2.76597500	-0.31857800	1.50494500
H	2.67306100	1.25216700	0.63550900
O	2.15215900	-0.48200800	-0.44064300
H	2.31568300	-0.05200300	-1.29454800
F	0.32099000	1.69962900	-0.27349900
F	-2.26887300	0.43921300	0.29573500
Po	-0.34843700	-0.20896000	-0.01393100

$F_2Po\bullet\bullet\bullet PH_3$			
H	3.13141100	0.71560000	1.06898200
H	3.13145000	0.71562000	-1.06889300
H	3.68117800	-1.05910800	0.00003400
P	2.65100500	-0.08100000	0.00002800
F	0.26088000	1.72452700	0.00003000
F	-2.33087000	0.38767900	0.00000700
Po	-0.36999100	-0.21627300	-0.00001000

$F_2Po\bullet\bullet\bullet O(CH_3)_2$			
C	2.59811600	0.08165600	1.18840600
H	3.67614200	-0.14551900	1.19129700
H	2.10902100	-0.39478300	2.04656500
H	2.43251600	1.17015000	1.21372400

O	1.99462200	-0.48070000	-0.00008100
Po	-0.51136100	-0.21043100	-0.00004800
F	0.17237400	1.71153900	0.00034700
F	-2.46300000	0.43037900	0.00006500
C	2.59814000	0.08216900	-1.18831300
H	2.10906200	-0.39390000	-2.04668800
H	2.43254000	1.17067300	-1.21316600
H	3.67616600	-0.14500600	-1.19128000

$F_2Po\cdots CO$			
C	2.53310200	-0.21988100	0.00000000
O	3.66175400	-0.01592100	-0.00000300
Po	-0.31326600	-0.19915000	0.00000100
F	0.27332800	1.74239700	0.00000100
F	-2.29314300	0.27707800	-0.00000500

$Cl_2Po\cdots OH_2$			
O	2.64065200	-0.81070900	0.00015900
H	3.02176900	-0.34919800	0.76295600
H	3.02179500	-0.34941800	-0.76275900
Po	-0.00308800	-0.35911000	0.00004900
Cl	0.84173100	1.97563300	-0.00025500
Cl	-2.42463700	0.22139900	-0.00007500

$Cl_2Po\cdots SH_2$			
S	2.97824800	-0.49662100	-0.00000700
H	3.01200500	0.43973300	0.97483400
H	3.01198700	0.43975000	-0.97483000
Po	-0.17584200	-0.32614100	0.00000300
Cl	0.36825100	2.09540900	0.00000100
Cl	-2.65679500	-0.06821200	-0.00000700

$Cl_2Po\cdots NH_3$			
H	2.95009100	-0.12924800	0.81805700
H	2.95006700	-0.12897000	-0.81794000
N	2.61023400	-0.63756900	-0.00002300
H	3.05432500	-1.55717000	-0.00018500
Cl	0.83942300	1.96590400	0.00012500
Cl	-2.43920500	0.26280900	-0.00001000
Po	-0.00035500	-0.37630700	-0.00002100

$Cl_2Po\cdots NCH$			
N	-2.61336200	-0.53067200	0.00000400
C	-3.78872000	-0.43806400	0.00000500
H	-4.86332600	-0.34745800	0.00000700
Cl	2.58968100	-0.05985700	-0.00000400

Cl	-0.44162900	2.08206800	0.00000000
Po	0.11157500	-0.32960800	0.00000000

$Cl_2Po\cdots OCH_2$			
O	-2.42267000	-0.89185600	-0.00002300
C	-3.35762100	-0.08977000	0.00005600
H	-3.17276900	0.99990600	0.00013200
H	-4.40083900	-0.45716400	0.00005100
Cl	-0.64944700	1.98612300	-0.00001600
Cl	2.59574400	0.20434900	0.00002900
Po	0.16682900	-0.35842000	-0.00000700

$Cl_2Po\cdots C_2H_4$			
C	-2.66385700	-0.45317100	-0.68502400
H	-2.74897900	-1.38576400	-1.25009800
H	-2.65250600	0.48440400	-1.24698500
C	-2.66385800	-0.45315800	0.68502800
H	-2.65250800	0.48442800	1.24697000
H	-2.74898200	-1.38573900	1.25012000
Po	0.07273500	-0.32778900	0.00000300
Cl	-0.42196000	2.10162800	-0.00002100
Cl	2.57840400	-0.05604500	0.00000300

$Cl_2Po\cdots OHCH_3$			
C	3.15342500	-0.26774500	0.74424200
H	4.22702600	-0.34457900	0.52042800
H	2.88127500	-1.00611000	1.50754300
H	2.90007200	0.74343500	1.09427600
O	2.37320700	-0.60747200	-0.43473500
H	2.58871800	0.03935200	-1.12575700
Cl	0.53750900	2.02983100	-0.08358000
Cl	-2.60897500	0.11758600	0.29451500
Po	-0.18200500	-0.35085600	-0.07821400

$Cl_2Po\cdots PH_3$			
H	3.41573600	0.38476800	1.06796600
H	3.41580600	0.38490500	-1.06777200
H	3.83568000	-1.42518300	-0.00000600
P	2.87611600	-0.37634400	0.00003100
Cl	0.47612900	2.04119300	0.00017000
Cl	-2.66913300	0.07223600	-0.00004400
Po	-0.19676100	-0.35271000	-0.00003300

$Cl_2Po\cdots O(CH_3)_2$			
C	2.85397700	-0.14842200	1.18865700
H	3.89830600	-0.49995600	1.20373000

H	2.30478400	-0.55659900	2.04603400
H	2.81930600	0.95281500	1.20832200
O	2.19845600	-0.64230000	-0.00000800
Po	-0.33149100	-0.34540600	0.00000300
Cl	0.32911300	2.04999100	0.00000600
Cl	-2.80174900	0.07594300	-0.00001000
C	2.85397100	-0.14840700	-1.18867100
H	2.30477100	-0.55657100	-2.04605000
H	2.81930200	0.95283000	-1.20832000
H	3.89829900	-0.49994300	-1.20375500

$Cl_2Po•••CO$			
C	2.78192700	-0.51633400	0.00000100
O	3.92369900	-0.40191400	0.00000000
Po	-0.14958000	-0.34178400	0.00000000
Cl	0.51311300	2.04072200	-0.00000200
Cl	-2.60231400	0.01946500	0.00000000

$O_2Po•••OH_2$			
O	2.74334000	-0.36069500	-0.00003600
H	3.70279000	-0.46551200	0.00016000
H	2.57173800	0.59939200	0.00000100
Po	-0.19864900	-0.13633200	0.00000300
O	0.69622300	1.59614700	0.00000200
O	-2.13806500	0.17929900	-0.00001400

$O_2Po•••SH_2$			
S	3.15462000	-0.20620100	-0.06901700
H	3.35102200	-0.21599100	1.26715500
H	2.46959100	0.96507400	-0.02398300
Po	-0.46457400	-0.12910500	-0.00636300
O	0.26241600	1.68344900	0.00027500
O	-2.42120200	-0.00908000	0.04916800

$O_2Po•••NH_3$			
H	3.38288600	-0.57614800	0.81627700
H	2.69482700	0.67214200	0.00002800
N	2.81462000	-0.34506500	0.00000600
H	3.38290900	-0.57612000	-0.81625800
O	0.52611100	1.68700500	0.00000000
O	-2.16569100	0.01519900	0.00001700
Po	-0.19102800	-0.12764300	-0.00000300

$O_2Po•••NCH$			
N	-2.76551900	-0.47826600	-0.00003400
C	-3.87682400	-0.07941300	0.00005100

H	-4.89051900	0.28888900	0.00012900
O	2.30112100	-0.35253900	0.00011200
O	-0.02412400	1.81689200	0.00002100
Po	0.34874000	-0.09737300	-0.00001500

$O_2Po\bullet\bullet\bullet OCH_2$			
O	-2.52726900	-0.79849800	0.00000400
C	-3.22170300	0.21770500	-0.00001400
H	-2.75323400	1.22137500	-0.00005300
H	-4.32746200	0.14121900	0.00001200
O	-0.41103600	1.66459800	0.00001000
O	2.33758700	0.06856700	-0.00001600
Po	0.37162700	-0.12078800	0.00000200

$O_2Po\bullet\bullet\bullet C_2H_4$			
C	3.07461600	-0.17693800	0.67626800
H	3.44550300	-1.03411300	1.24543700
H	2.71982200	0.69382600	1.23485400
C	3.07461600	-0.17692200	-0.67626600
H	2.71982300	0.69385700	-1.23483000
H	3.44550300	-1.03408200	-1.24545600
Po	-0.37502200	-0.11193700	-0.00000200
O	0.12092400	1.77389400	0.00001300
O	-2.33645200	-0.24809800	0.00000500

$O_2Po\bullet\bullet\bullet OHCH_3$			
C	3.84233100	-0.23756400	0.00000900
H	4.29041400	0.21356600	-0.89964600
H	4.05015400	-1.31513000	0.00000200
H	4.29038400	0.21354900	0.89968700
O	2.41316700	-0.09046500	-0.00001400
H	2.17733400	0.85615300	-0.00000800
O	0.22682100	1.68895000	0.00000100
O	-2.43684300	-0.02936200	0.00000400
Po	-0.47008900	-0.13209200	0.00000000

$O_2Po\bullet\bullet\bullet PH_3$			
H	3.30130900	0.73021000	1.04869000
H	3.30130800	0.73005400	-1.04878300
H	4.41345100	-0.72350000	0.00006100
P	3.08497000	-0.20515700	0.00002300
O	0.40098100	1.59760800	-0.00011500
O	-2.43044000	0.15203700	-0.00009500
Po	-0.48874900	-0.13876900	0.00001600

$O_2Po•••O(CH_3)_2$			
C	2.78476500	-1.17665000	0.02953500
H	3.88430900	-1.20789300	-0.06078600
H	2.35398100	-2.04600800	-0.48609000
H	2.49343900	-1.18874200	1.09383100
O	2.26579300	-0.00378800	-0.61690400
Po	-0.58479100	-0.00070800	-0.11500200
O	0.07906700	0.01057500	1.71757500
O	-2.56463700	-0.00034700	-0.05654100
C	2.78476500	1.17692000	0.01509100
H	2.35398100	2.03988300	-0.51116400
H	2.49343800	1.20207400	1.07915900
H	3.88430900	1.20705200	-0.07560500

$O_2Po•••CO$			
C	2.97886700	-0.48297000	0.00000100
O	4.01423500	0.01479500	0.00000300
Po	-0.41325200	-0.13231600	0.00000000
O	0.44502100	1.61979800	-0.00000200
O	-2.35426200	0.11695600	0.00000200

27. Fluorine Bonded Complexes

$CNF•••OH_2$			
F	-0.17001200	0.00073500	0.03330100
O	2.75205100	-0.00200800	-0.01301500
H	3.36030500	-0.75258300	-0.01621100
H	3.33616300	0.76750700	-0.01661500
C	-1.45177100	-0.00010300	0.00251500
N	-2.63887700	-0.00069400	-0.02540700

$CNF•••SH_2$			
F	0.97728600	-0.01255300	-0.03063700
H	-2.90673300	0.99539600	0.74106300
H	-2.92694100	-0.95354500	0.77907900
S	-2.54097400	0.00036500	-0.09410800
C	2.26040500	-0.00036200	0.00323200
N	3.44732300	0.00963600	0.03456100

CNF•••NH_3			
F	-0.23803800	-0.00234100	0.00020900
N	2.90350800	0.00037300	0.00007400
H	3.30285600	-0.93623800	0.06676300
H	3.29570600	0.53031500	0.77886000
H	3.29377400	0.41371200	-0.84727900
C	-1.52015200	-0.00026600	0.00003600
N	-2.70766200	0.00175100	-0.00013700

CNF•••NCH			
C	3.44648500	0.00144600	0.00016200
H	4.52439200	0.00355300	0.00062500
N	2.26397400	-0.00086100	-0.00042700
F	-0.73054500	-0.00233300	0.00021500
C	-2.01261900	-0.00004900	0.00003800
N	-3.20007200	0.00215500	-0.00011100

CNF•••OCH_2			
F	0.83411600	0.22252800	-0.00505600
O	-2.00512300	-0.10332300	0.02390800
C	-3.22633500	-0.02047700	-0.01186800
H	-3.74331700	0.96274600	-0.01372000
H	-3.87157500	-0.92439500	-0.04512100
C	2.10013200	0.01806700	-0.00243300
N	3.27229200	-0.17143800	-0.00016000

CNF•••C_2H_4			
C	-2.57614900	-0.67052100	-0.00552600
H	-2.59556000	-1.23871800	0.92820900
H	-2.58309800	-1.23864700	-0.93948200
C	-2.55119700	0.67876400	-0.00532100
H	-2.53702200	1.24661100	-0.93936700
H	-2.54948200	1.24755800	0.92821300

F	0.72857300	-0.00672300	0.02115200
C	2.01241600	-0.00237300	0.00150800
N	3.19965500	0.00121100	-0.01598600

CNF•••OHCH$_3$

F	-0.80623400	-0.24040900	-0.02878200
O	2.02344500	-0.66711900	0.00926500
H	2.77096400	-1.27775900	0.04545100
C	2.55003200	0.66864800	0.00069300
H	1.68401300	1.34180400	-0.04163400
H	3.12414100	0.88927100	0.91593400
H	3.18447900	0.85397200	-0.88193200
C	-2.06480800	0.00539800	-0.00238300
N	-3.22948400	0.23558100	0.02246300

CNF•••PH$_3$

F	1.05740700	-0.01629500	-0.13278200
H	-3.23199900	-0.93854800	1.09556000
H	-3.45569400	-0.04551900	-0.77381900
H	-3.22185500	1.13821600	0.92506600
P	-2.54369900	0.03975600	0.31916500
C	2.33096900	-0.03642400	-0.29263300
N	3.50893600	-0.05504200	-0.44049200

CNF•••CO

F	0.00000000	-0.82761000	0.00000000
C	-0.00974300	2.42934200	0.00000000
O	-0.03318200	3.57899400	0.00000000
C	0.01660700	-2.11141500	0.00000000
N	0.03203900	-3.29871800	0.00000000

$CNF\bullet\bullet\bullet O(CH_3)_2$			
F	1.12735000	-0.00094700	-0.15514300
O	-1.74530600	0.00011100	-0.56770200
C	-1.96367900	-1.17092500	0.21283500
H	-1.77872900	-2.03466200	-0.43928400
H	-1.27326000	-1.20740900	1.07707400
H	-3.00300800	-1.21142100	0.58888500
C	-1.96281500	1.17145600	0.21261000
H	-1.27235700	1.20760700	1.07683100
H	-1.77724900	2.03493300	-0.43967900
H	-3.00210700	1.21278200	0.58867000
C	2.40226100	-0.00022200	-0.00469200
N	3.58120100	0.00056500	0.13727000

$NCF\bullet\bullet\bullet OH_2$			
F	0.14465600	-0.00888800	0.00031000
O	-2.62901900	-0.00138800	-0.00987800
H	-3.25990000	-0.73205300	0.03540200
H	-3.18603500	0.78681700	0.03283600
N	1.45791700	-0.00072000	0.00111700
C	2.66179400	0.00689600	0.00002900

$NCF\bullet\bullet\bullet SH_2$			
F	0.91427800	-0.00353300	0.00449200
H	-2.76654100	0.97175600	0.77290600
H	-2.75977600	-0.97772800	0.76617000
S	-2.43173100	0.00118200	-0.10311500
N	2.22917700	-0.00005200	0.00446900
C	3.43354500	0.00320200	0.00650800

NCF•••NH_3			
F	-0.19081300	0.00173200	-0.00044800
N	2.73273400	-0.00032200	-0.00007000
H	3.13111400	0.86017100	-0.37702000
H	3.12506300	-0.76027800	-0.55666000
H	3.12384200	-0.10560900	0.93651700
N	-1.50528900	0.00012200	-0.00004000
C	-2.70913700	-0.00141200	0.00032600

NCF•••NCH			
C	0.00000000	0.00000000	-3.32884900
H	0.00000000	0.00000000	-4.40679300
N	0.00000000	0.00000000	-2.14645200
F	0.00000000	0.00000000	0.68634800
N	0.00000000	0.00000000	2.00031200
C	0.00000000	0.00000000	3.20428900

NCF•••FH			
F	0.00000000	0.00000000	-0.12310400
F	0.00000000	0.00000000	2.60790700
H	0.00000000	0.00000000	3.53273200
N	0.00000000	0.00000000	-1.43628000
C	0.00000000	0.00000000	-2.64033200

NCF•••OCH_2			
F	0.79026300	-0.00036400	0.00006400
O	-1.91988700	-0.00264800	0.00007500
C	-3.14426000	0.00177100	-0.00006900
H	-3.72302900	0.95002100	-0.00012500
H	-3.72987300	-0.94226300	-0.00012900
N	2.10323100	0.00027400	-0.00001600
C	3.30709500	0.00069200	-0.00006600

NCF•••C_2H_4			
C	2.43262600	-0.67412100	0.00000400
H	2.44004000	-1.24221500	-0.93394300
H	2.43815200	-1.24225000	0.93394300
C	2.42361200	0.67562600	0.00000700
H	2.42148200	1.24375400	0.93396300
H	2.42337400	1.24376200	-0.93394500
F	-0.66037400	0.00079300	0.00019000
N	-1.97620200	-0.00092700	-0.00014600
C	-3.18061600	-0.00212100	-0.00012800

NCF•••$OHCH_3$			
F	-0.78686100	-0.27355100	-0.00026000
O	1.90766000	-0.64277000	0.00070200
H	2.61174000	-1.30402600	-0.00258500
C	2.52190000	0.65557100	-0.00011700
H	1.70148300	1.38481200	0.00488000
H	3.14265100	0.81562400	0.89696900
H	3.13424500	0.81842900	-0.90246900
N	-2.06633300	0.02552600	-0.00007100
C	-3.23945300	0.29619500	0.00018800

NCF•••PH_3			
F	0.99828000	-0.00020000	-0.00018100
H	-3.20689200	1.07028300	0.55238700
H	-3.20974400	-1.01226600	0.64969900
H	-3.20798000	-0.05526800	-1.20246700
P	-2.44379300	-0.00012200	0.00006800
N	2.31313900	-0.00001000	-0.00000100
C	3.51750200	0.00015900	0.00016500

NCF•••CO			
F	0.00000000	0.78551800	0.00000000

C	0.00198500	-2.31440800	0.00000000
O	0.00406900	-3.46410200	0.00000000
N	-0.00332900	2.10030300	0.00000000
C	-0.00352600	3.30458000	0.00000000

NCCCF•••OH$_2$			
F	-1.16891200	-0.00041400	0.01803100
O	-4.08050600	-0.00225400	-0.01331400
H	-4.65903900	0.77154600	-0.01293100
H	-4.69467700	-0.74807400	-0.01316700
C	0.11352400	-0.00033200	0.01049800
C	1.34207700	-0.00024200	0.00309200
C	2.72571500	-0.00002400	-0.00512600
N	3.91858200	0.00026800	-0.01149200

NCCCF•••SH$_2$			
F	0.35657900	0.00169900	-0.01565300
H	4.27755200	-0.97353000	0.72610200
H	4.27352400	0.97621500	0.72340100
S	3.81909200	-0.00073100	-0.08922800
C	-0.92767600	0.00069600	-0.00814700
C	-2.15590800	-0.00049700	-0.00065200
C	-3.53960800	-0.00087400	0.00901000
N	-4.73237200	-0.00031900	0.01682300

NCCCF•••NH$_3$			
F	1.12009200	-0.00186800	-0.00076000
N	4.24764700	0.00119000	-0.00034400
H	4.63989200	-0.73434200	0.58811700
H	4.63773700	0.87783500	0.34675000
H	4.64777100	-0.13726800	-0.92872100
C	-0.16227200	-0.00123100	-0.00001100
C	-1.39099600	-0.00059800	0.00054500

C	-2.77459300	0.00053900	0.00022300
N	-3.96751400	0.00142800	-0.00020500

NCCCF•••NCH

F	0.64369300	-0.00479600	0.00009800
C	-0.63855700	-0.00268900	0.00001700
C	-1.86715700	-0.00043700	-0.00033500
C	-3.25071100	0.00161500	-0.00006700
N	-4.44360900	0.00335100	0.00018900
N	3.60676600	-0.00028200	0.00001200
C	4.78934600	0.00385700	0.00001200
H	5.86714900	0.00760200	-0.00005500

NCCCF••OCH_2

F	-0.51753800	0.00070100	-0.02348600
O	-3.32584900	-0.00010600	0.07257100
C	-4.54596500	-0.00044600	-0.02891200
H	-5.12673900	0.94540000	-0.07742500
H	-5.12620100	-0.94661600	-0.07755500
C	0.76465900	0.00040700	-0.01462100
C	1.99310300	0.00016600	-0.00708200
C	3.37669800	-0.00021200	0.00261100
N	4.56951500	-0.00053200	0.01054400

NCCCF•••C_2H_4

C	-3.84044400	0.67511100	0.00000600
H	-3.84184400	1.24335300	-0.93386000
H	-3.84252200	1.24335700	0.93386700
C	-3.84281600	-0.67435000	0.00000900
H	-3.84689400	-1.24258500	0.93387100
H	-3.84621500	-1.24258900	-0.93385200
F	-0.59737300	-0.00041200	0.00052200
C	0.68708300	-0.00029800	0.00024800

C	1.91529300	-0.00029000	-0.00001800
C	3.29919200	-0.00003000	-0.00033100
N	4.49199800	0.00018800	-0.00060200

NCCCF•••$OHCH_3$

F	0.49658900	-0.08452800	0.00156500
O	3.29316300	-0.68499000	-0.00067400
H	4.05387100	-1.28026200	-0.00164400
C	3.78916000	0.66226000	-0.00051500
H	2.90722700	1.31563600	0.00093600
H	4.39000700	0.87849500	0.89840400
H	4.38780300	0.87949500	-0.90065900
C	-0.78550300	-0.04452800	0.00090000
C	-2.01316600	-0.00444300	0.00031300
C	-3.39621800	0.03853000	-0.00044300
N	-4.58845000	0.07662900	-0.00103700

NCCCF•••PH_3

F	0.29064600	-0.00022400	-0.00495800
H	4.60069200	-0.83753300	0.88831500
H	4.62160400	1.16656200	0.31925000
H	4.67507200	-0.32862600	-1.13062700
C	-0.99358500	-0.00013400	-0.00294800
C	-2.22182600	-0.00012100	-0.00078000
C	-3.60572200	0.00003200	0.00135100
N	-4.79854400	0.00023600	0.00317300
P	3.86689500	0.00008600	-0.00268500

NCCCF•••CO

F	-0.57866900	0.00460100	-0.00125700
C	-3.77967300	0.00354400	0.00242500
O	-4.92955000	-0.00581700	-0.00064000
C	0.70584100	0.00244500	-0.00060100

C	1.93400000	0.00054000	-0.00022100
C	3.31796500	-0.00166300	0.00034000
N	4.51080300	-0.00343800	0.00068200

NCCCF•••FH			
F	-1.20412900	0.11800500	0.00002400
C	0.07813600	0.06972900	-0.00001200
C	1.30552600	0.02413400	0.00030600
C	2.68832200	-0.03044800	-0.00022300
N	3.88021600	-0.07765000	-0.00031000
F	-3.98317500	-0.09068900	0.00208700
H	-4.90767300	-0.08277600	-0.01725800

28. Chlorine Bonded Complexes

ClCl•••OH_2			
O	-2.90348000	-0.00111700	-0.07445300
H	-3.28542500	0.76131300	0.38096000
H	-3.28772100	-0.76341900	0.37922600
Cl	-0.14822900	0.00159600	-0.03105200
Cl	1.90122800	-0.00094700	0.02137200

ClCl•••SH_2			
H	2.82025900	-0.97043900	0.83895800
H	2.81882300	0.98058200	0.82902300
Cl	-0.40983400	-0.00213500	-0.03216300
S	2.70574500	0.00027100	-0.09294600
Cl	-2.46846000	0.00128300	0.02152400

ClCl•••NH_3			
N	2.75131300	0.00000700	-0.00002400
H	3.12587600	-0.82673100	0.46509100
H	3.12575200	0.81613900	0.48355800
H	3.12625000	0.01069700	-0.94841400
Cl	0.20085400	-0.00001900	0.00000000
Cl	-1.88538800	0.00000900	-0.00000400

ClCl•••NCH			
C	0.01152100	-3.70281800	0.00000000
H	0.01125500	-4.78058300	0.00000000
N	0.01076400	-2.52116400	0.00000000
Cl	0.00000000	0.28844200	0.00000000

Cl	-0.00916100	2.33777200	0.00000000

ClCl•••CO			
C	0.00000000	0.00000000	-2.69738800
O	0.00000000	0.00000000	-3.84685600
Cl	0.00000000	0.00000000	0.35884500
Cl	0.00000000	0.00000000	2.40345900

ClCl•••OCH_2			
O	2.41652800	-0.54408200	0.00002500
C	2.88245700	0.59042100	0.00013000
H	2.22530900	1.48529800	0.00024200
H	3.97839500	0.76273800	0.00020200
Cl	-0.25944800	-0.27293200	0.00002600
Cl	-2.26000400	0.18834900	-0.00011000

ClCl•••C_2H_4			
C	2.65285500	-0.67704400	0.00001400
H	2.65745200	-1.24380200	-0.93464700
H	2.65700800	-1.24379300	0.93468100
C	2.65286000	0.67703900	0.00001400
H	2.65701800	1.24378700	0.93468100
H	2.65746200	1.24379600	-0.93464700
Cl	-0.21577800	0.00000500	-0.00049100
Cl	-2.28205900	-0.00000200	0.00047700

ClCl•••$OHCH_3$			
O	2.26198500	-0.63690000	-0.08245700
H	2.52866400	-1.12390000	0.70951900
C	2.78845400	0.70049000	0.01818500
H	2.47294500	1.22112600	-0.89437600
H	2.37927300	1.23150700	0.89292000
H	3.88897200	0.69502900	0.06741200
Cl	-0.35200500	-0.25419100	-0.03844000
Cl	-2.35955200	0.18763200	0.02520900

ClCl•••FH			
F	-0.91837800	2.87637800	0.00000000
H	-1.81003400	3.12485900	0.00000000
Cl	0.00000000	0.12389100	0.00000000
Cl	0.59267300	-1.83049400	0.00000000

ClCl•••$O(CH_3)_2$			
O	1.87333000	-0.00000100	-0.47189200
C	2.30147000	1.17773300	0.21890500

H	1.93081600	2.03739600	-0.35391500
H	1.88298600	1.20528900	1.24147100
H	3.40406700	1.21466500	0.27498300
Cl	-0.66096200	-0.00000100	-0.21190700
Cl	-2.69433600	0.00000000	0.14268300
C	2.30147400	-1.17772900	0.21890500
H	1.88299600	-1.20528700	1.24147400
H	1.93082000	-2.03739600	-0.35390900
H	3.40407200	-1.21466200	0.27498000

$FCl•••OH_2$			
F	-1.99234700	-0.00001500	0.02885500
O	2.23464100	0.00000300	-0.09108900
H	2.57056800	-0.76402700	0.39824300
H	2.57081200	0.76386000	0.39834500
Cl	-0.29925800	0.00001600	-0.01926900

$FCl•••SH_2$			
F	2.51048100	-0.00001200	0.03140900
H	-2.11924600	0.97683800	0.82816400
H	-2.11913100	-0.97693400	0.82807600
Cl	0.79569500	0.00001300	-0.02243400
S	-1.99267300	-0.00000100	-0.09734700

$FCl•••NH_3$			
F	-1.97307900	0.00005400	0.00002900
N	2.04897000	0.00000900	0.00001200
H	2.40450500	-0.64396600	-0.70575500
H	2.40417700	-0.28904400	0.91076800
H	2.40380200	0.93348900	-0.20485500
Cl	-0.22338600	-0.00006000	-0.00002900

FCl•••NCH			
C	0.00000000	0.00000000	3.02062600
H	0.00000000	0.00000000	4.09847500
N	0.00000000	0.00000000	1.84033000
F	0.00000000	0.00000000	-2.45647500
Cl	0.00000000	0.00000000	-0.76448600

FCl•••CO

F	0.00000000	0.00000000	2.50078400
C	0.00000000	0.00000000	-1.94009700
O	0.00000000	0.00000000	-3.08836000
Cl	0.00000000	0.00000000	0.81414100

$FCl•••OCH_2$			
F	-2.35115500	0.24931200	-0.00025200
O	1.72177500	-0.56941300	-0.00022300
C	2.34169900	0.49130600	-0.00006100
H	1.81453000	1.46669400	0.00011300
H	3.44922000	0.50083400	0.00034200
Cl	-0.70163200	-0.15316900	0.00023300

$FCl•••C_2H_4$			
C	1.94715400	0.68017500	-0.00000900
H	1.96002800	1.24514500	0.93518400
H	1.96023400	1.24515600	-0.93519200
C	1.94715300	-0.68017500	-0.00000900
H	1.96023300	-1.24515600	-0.93519200
H	1.96002700	-1.24514500	0.93518300
F	-2.32871800	0.00000000	0.00012700
Cl	-0.60281800	0.00000000	-0.00006000

$FCl•••OHCH_3$			
F	-2.43716300	0.27307300	0.03764300
O	1.56794600	-0.65196200	-0.10011300
H	1.75006300	-1.18087300	0.69032500
C	2.27728200	0.60133600	0.02259900
H	2.04492500	1.16922300	-0.88602800
H	1.93656100	1.16857800	0.90271300
H	3.36307400	0.43035500	0.07930500
Cl	-0.78631900	-0.14336800	-0.02704700

FCl•••FH			
F	-2.02551000	0.04065200	0.00002000
Cl	-0.34555200	-0.02770500	-0.00001700
F	2.36598700	-0.07079600	0.00001300
H	2.81009300	0.74226800	-0.00000900

$FCl•••O(CH_3)_2$			
F	-2.73522300	-0.00000100	0.18306000
O	1.24903900	-0.00000200	-0.45654100
C	1.76166900	1.18421300	0.17515000
H	1.31948800	2.03964600	-0.34999400
H	1.47438200	1.20893700	1.24080600
H	2.86071200	1.21239200	0.08446600

Cl	-1.04852500	-0.00001000	-0.12044800
C	1.76171300	-1.18419400	0.17515500
H	1.47440300	-1.20893700	1.24080400
H	1.31958700	-2.03964600	-0.35000300
H	2.86076000	-1.21231800	0.08449600

NCCl•••OH_2			
O	-2.87688600	-0.00011500	-0.00013100
H	-3.47157500	0.76128600	0.00252000
H	-3.46972000	-0.76296200	0.00250900
Cl	0.00516400	0.00030700	-0.00059800
C	1.65645400	-0.00006000	0.00043700
N	2.84712500	-0.00032400	0.00050900

NCCl•••SH_2			
H	2.96758200	-0.97659300	0.81785000
H	2.96820700	0.97397500	0.82034200
Cl	-0.68100800	0.00041700	-0.02785100
S	2.76908000	-0.00003000	-0.09292300
C	-2.33319400	-0.00010400	0.00942000
N	-3.52353800	-0.00048100	0.03793200

NCCl•••NH_3			
N	2.93064600	-0.00013600	-0.00007800
H	3.32636100	0.63261100	0.69614300
H	3.32420000	0.28543800	-0.89743500
H	3.32250400	-0.92105700	0.20001800
Cl	-0.02129600	0.00044700	0.00021300
C	-1.67612500	-0.00005800	-0.00005400
N	-2.86697400	-0.00047000	-0.00021000

NCCl•••NCH			
C	-0.00388900	-3.67527600	0.00000000
H	-0.00361800	-4.75296700	0.00000000
N	-0.00413000	-2.49358500	0.00000000
Cl	0.00000000	0.48192600	0.00000000
C	0.00300000	2.13320200	0.00000000
N	0.00540800	3.32396600	0.00000000

NCCl•••CO			
C	0.05395700	2.68821700	0.00000000
O	0.07443300	3.83724600	0.00000000
Cl	0.00000000	-0.56806600	0.00000000
C	-0.05037300	-2.21844400	0.00000000
N	-0.08813900	-3.40849800	0.00000000

NCCl•••OCH_2			
O	-2.39078300	-0.51298300	-0.00028100
C	-2.95917900	0.57272100	-0.00004200
H	-2.38956600	1.52660800	0.00113500
H	-4.06618700	0.64721500	-0.00081800
Cl	0.47230200	-0.25654100	0.00028800
C	2.08927800	0.08461200	0.00002800
N	3.25318400	0.33532000	-0.00041200

NCCl•••C_2H_4			
C	2.76897300	-0.67527600	0.00046100
H	2.77407100	-1.24328900	-0.93361000
H	2.77281900	-1.24325500	0.93455700
C	2.76885200	0.67539000	0.00043800
H	2.77259300	1.24340000	0.93451600
H	2.77384400	1.24337600	-0.93364900
Cl	-0.48318900	-0.00012400	-0.00104300
C	-2.13625400	0.00020600	0.00051100
N	-3.32693500	-0.00000600	0.00106600

NCCl•••$OHCH_3$			
O	2.22461200	-0.59056500	-0.07434000
H	2.80096600	-1.22909000	0.36560100
C	2.84330100	0.70544900	0.01423900
H	2.17533500	1.40141400	-0.50927500
H	2.95199200	1.03377100	1.06083400
H	3.82767700	0.71899100	-0.48030000
Cl	-0.58342600	-0.26284200	0.00203400
C	-2.19689200	0.09374100	0.00259500
N	-3.35901100	0.35323100	0.00318300

NCCl•••FH			
Cl	-0.01210600	0.00292500	0.00000000
F	2.92178000	-0.00340100	0.00000000
H	3.84696100	0.00579500	-0.00000100
C	-1.66180100	-0.00046300	0.00000000
N	-2.85233900	-0.00316200	0.00000000

NCCl•••$O(CH_3)_2$			
O	1.87553400	0.00000000	-0.46715500
C	2.27981100	1.17475100	0.23701800
H	1.94053500	2.03705700	-0.35187300
H	1.82076800	1.21013600	1.24284100
H	3.37901000	1.21133000	0.34365900
Cl	-0.91083600	-0.00000500	-0.23740500
C	-2.53629300	-0.00000100	0.06856300

N	-3.70582100	0.00000500	0.29260400
C	2.27982000	-1.17474500	0.23702200
H	1.94054800	-2.03705500	-0.35186500
H	3.37901900	-1.21131700	0.34366000
H	1.82078000	-1.21012900	1.24284600

29. Bromine Bonded Complexes

$FBr\bullet\bullet\bullet OH_2$			
F	1.99052100	-0.00000700	0.03938200
O	-2.34726100	-0.00000300	-0.08350000
H	-2.67948600	0.76540900	0.40760800
H	-2.67946900	-0.76543200	0.40759300
Br	0.17778100	0.00000300	-0.01433300

$FBr\bullet\bullet\bullet SH_2$			
F	2.38721500	-0.00001400	0.03968000
H	-2.39821200	0.97718300	0.82864000
H	-2.39816400	-0.97724300	0.82858300
Br	0.55411700	0.00000600	-0.01445100
S	-2.25516700	-0.00000200	-0.09428500

$FBr\bullet\bullet\bullet NH_3$			
F	-1.94466300	0.10488000	0.45696700
Br	-0.13653600	0.00735600	0.03208800
N	2.12371400	-0.11451800	-0.49905200
H	2.25372500	-0.12124900	-1.51048700
H	2.53596200	-0.96505900	-0.11619300
H	2.62502700	0.68654600	-0.11573600

$FBr\bullet\bullet\bullet NCH$			
F	-2.03316100	-0.41175500	1.00672000
Br	-0.43302000	-0.08766400	0.21442500
N	1.80189900	0.36491700	-0.89221300
C	2.84147100	0.57532500	-1.40703300

H	3.79204400	0.76767600	-1.87768400

$FBr\cdots OCH_2$

F	-2.24787500	0.31418900	-0.00000300
O	1.93916200	-0.52772400	-0.00000100
C	2.60523500	0.50671300	0.00000000
H	2.11949300	1.50210700	0.00000900
H	3.71051000	0.46136200	-0.00001000
Br	-0.47839500	-0.10313300	0.00000100

$FBr\cdots C_2H_4$

C	2.11984800	0.68319200	0.00000400
H	2.14587900	1.24663100	0.93562400
H	2.14592300	1.24663500	-0.93561300
C	2.11984800	-0.68319200	0.00000300
H	2.14592300	-1.24663500	-0.93561300
H	2.14587900	-1.24663100	0.93562300
F	-2.24500200	0.00000000	0.00003500
Br	-0.39476500	0.00000000	-0.00001100

$FBr\cdots OHCH_3$

F	-2.31642900	0.33882900	0.04888000
O	1.80221800	-0.61503500	-0.08989100
H	1.98451600	-1.15804500	0.69190000
C	2.55940900	0.61539900	0.02371900
H	2.32472700	1.19450400	-0.87674500
H	2.25609500	1.18477200	0.91523100
H	3.63719900	0.39826500	0.05418900
Br	-0.54653900	-0.09831600	-0.01850500

$FBr\cdots O(CH_3)_2$

F	2.58512200	0.00000100	0.23043800

O	-1.53315300	0.00000000	-0.42088500
C	-2.08235400	-1.18801000	0.18130700
H	-1.61293700	-2.04155200	-0.32209800
H	-1.85120900	-1.21267600	1.25985300
H	-3.17368300	-1.20812500	0.02775300
Br	0.77893900	-0.00000200	-0.08038700
C	-2.08233800	1.18801800	0.18130500
H	-1.61292600	2.04155300	-0.32211600
H	-3.17366900	1.20813700	0.02776900
H	-1.85117500	1.21269300	1.25984700

FBr•••FH

Br	0.00000000	0.21507900	0.00000000
H	0.48225900	-3.00864000	0.00000000
F	0.23902700	1.99741100	0.00000000
F	-0.29261100	-2.49953600	0.00000000

FBr•••CO

F	0.00000000	0.00000000	2.31575000
Br	0.00000000	0.00000000	0.50397500
C	0.00000000	0.00000000	-2.09309400
O	0.00000000	0.00000000	-3.24028800

ClBr•••OH_2

O	-2.86180900	-0.00002400	-0.06565000
H	-3.22691200	0.76351300	0.40290200
H	-3.22662500	-0.76382000	0.40270500
Br	-0.15364200	0.00003100	-0.02171500
Cl	2.04267600	-0.00003400	0.02821300

ClBr•••SH_2

H	-2.86928100	0.97620200	0.84869700

H	-2.86927400	-0.97617700	0.84872100
Br	0.24120400	0.00000000	-0.02905400
S	-2.77830600	-0.00000200	-0.08104100
Cl	2.45584100	0.00000000	0.03624300

ClBr•••NH_3			
Br	0.20459400	0.00000300	0.00000200
N	2.66131400	-0.00000300	0.00000000
H	3.02506700	-0.82137500	0.48297500
H	3.02509100	0.82895500	0.46981600
H	3.02505400	-0.00760600	-0.95282400
Cl	-2.05089300	-0.00000300	-0.00000200

ClBr•••NCH			
Br	0.00000000	0.00000000	-0.15631200
N	0.00000000	0.00000000	2.58175300
C	0.00000000	0.00000000	3.76248600
H	0.00000000	0.00000000	4.84045700
Cl	0.00000000	0.00000000	-2.35392400

ClBr••• OCH_2			
O	-2.46879400	-0.47128000	-0.00006000
C	-3.01652200	0.62817200	0.00003900
H	-2.42506500	1.56649600	0.00013900
H	-4.12119600	0.71402500	0.00003400
Br	0.14821500	-0.18613600	-0.00001400
Cl	2.30636600	0.24914400	0.00003200

ClBr••••C_2H_4			
C	0.00000000	-2.65552300	0.67957800
H	-0.93538500	-2.66685900	1.24486600
H	0.93538500	-2.66686600	1.24486600

C	0.00000000	-2.65552300	-0.67957800
H	0.93538500	-2.66686600	-1.24486600
H	-0.93538500	-2.66685900	-1.24486600
Br	0.00000000	0.08911700	0.00000000
Cl	0.00000000	2.31850700	0.00000000

ClBr•••OHCH$_3$

O	2.32771400	-0.56983900	-0.06780900
H	2.57087300	-1.07142600	0.72390200
C	2.94064800	0.73580100	0.02038200
H	2.64488900	1.26974600	-0.89060600
H	2.57601300	1.29036400	0.89923000
H	4.03769800	0.65224600	0.05445300
Br	-0.21749000	-0.18073600	-0.02656300
Cl	-2.38134900	0.25463100	0.03311300

ClBr•••O(CH$_3$)$_2$

O	-2.00018800	-0.00000200	-0.41264200
C	-2.49054300	-1.18317600	0.23706000
H	-2.06636300	-2.03968400	-0.30145300
H	-2.16663700	-1.20768800	1.29246600
H	-3.59233000	-1.21373800	0.18564500
Br	0.46613800	-0.00001200	-0.14605400
C	-2.49046100	1.18321500	0.23704500
H	-2.06619800	2.03968700	-0.30146100
H	-3.59224400	1.21386500	0.18560500
H	-2.16657500	1.20770400	1.29245800
Cl	2.66017800	0.00000300	0.18912600

ClBr•••FH			
Br	0.00000000	0.12834700	0.00000000
H	1.43486100	3.30259000	0.00000000
F	0.57804900	2.95068300	0.00000000
Cl	-0.39043000	-2.02063900	0.00000000

ClBr•••CO			
Br	0.00000000	0.00000000	0.20187000
C	0.00000000	0.00000000	-2.75249100
O	0.00000000	0.00000000	-3.90106200
Cl	0.00000000	0.00000000	2.39164700

BrBr•••OH_2			
O	3.43584500	0.00001300	-0.05450900
H	3.80278500	-0.76311900	0.41288200
H	3.80276700	0.76318100	0.41283800
Br	0.66743400	-0.00001100	-0.02802100
Br	-1.67007100	0.00000600	0.01688800

BrBr•••SH_2			
H	-3.46351500	0.97582200	0.86135100
H	-3.46351300	-0.97583300	0.86134000
Br	-0.30164300	0.00000100	-0.04079700
S	-3.39569600	-0.00000100	-0.07045300
Br	2.05187600	-0.00000100	0.02378400

BrBr•••NH_3			
Br	0.71728700	0.00000400	0.00000200
N	3.23339000	-0.00000600	-0.00000100
H	3.60029700	-0.81825600	0.48597800
H	3.60032800	0.82999100	0.46560900
H	3.60027700	-0.01177300	-0.95162300

Br	-1.67256200	-0.00000200	-0.00000100

BrBr•••NCH			
Br	0.00000000	0.00000000	-0.39770700
N	0.00000000	0.00000000	-3.18994000
C	0.00000000	0.00000000	-4.37110900
H	0.00000000	0.00000000	-5.44899300
Br	0.00000000	0.00000000	1.94071300

BrBr•••OCH_2			
O	-3.07939100	-0.42054800	-0.00000100
C	-3.54276700	0.71635700	-0.00000700
H	-2.88210600	1.60781400	-0.00001400
H	-4.63798000	0.88775500	-0.00000600
Br	-0.39055800	-0.25004100	0.00000100
Br	1.91661000	0.15206000	0.00000100

BrBr•••C_2H_4			
C	0.00000000	-3.25392500	0.67877800
H	-0.93526100	-3.26257100	1.24445800
H	0.93526100	-3.26257200	1.24445800
C	0.00000000	-3.25392500	-0.67877800
H	0.93526100	-3.26257200	-1.24445800
H	-0.93526100	-3.26257100	-1.24445800
Br	0.00000000	-0.43893600	0.00000000
Br	0.00000000	1.92743300	0.00000000

BrBr•••$OHCH_3$			
O	2.94299300	-0.52962800	-0.05287100
H	3.20821000	-0.99815400	0.75155700
C	3.46525300	0.81436900	0.01800200
H	3.14629700	1.31157300	-0.90604900

H	3.05288400	1.36025700	0.88136700
H	4.56523500	0.80881300	0.06670300
Br	0.32398800	-0.24033100	-0.03256800
Br	-1.98993300	0.15085400	0.01889300

BrBr•••O(CH$_3$)$_2$			
O	-2.60281700	-0.00001000	-0.39907100
C	-3.05300900	-1.18133000	0.27869800
H	-2.66061400	-2.03884500	-0.28219800
H	-2.66789600	-1.20559100	1.31367600
H	-4.15622400	-1.21533000	0.29399800
Br	-0.07639900	-0.00000800	-0.19792600
C	-3.05285500	1.18138300	0.27867900
H	-2.66030000	2.03883600	-0.28219900
H	-4.15606600	1.21555800	0.29393100
H	-2.66778400	1.20558500	1.31367400
Br	2.26001600	-0.00000500	0.11785200

BrBr•••FH			
Br	0.00000000	0.64477900	0.00000000
H	0.91805800	4.08506000	0.00000000
Br	-0.06297800	-1.68167700	0.00000000
F	0.14290700	3.57848800	0.00000000

BrBr•••CO			
Br	0.00000000	0.00000000	-0.35580800
C	0.00000000	0.00000000	-3.39401600
O	0.00000000	0.00000000	-4.54293400
Br	0.00000000	0.00000000	1.97602400

30. Iodine Bonded Complexes

FI•••OH$_2$

F	-2.09645600	-0.00000400	0.04437200
O	2.48034700	0.00000000	-0.07434400
H	2.84236200	-0.76672700	0.39367900
H	2.84240700	0.76669200	0.39370000
I	-0.12565000	0.00000100	-0.01116900

FI•••SH_2			
F	-2.43008300	-0.00000100	0.04319000
S	2.51365100	-0.00000100	-0.09277600
H	2.67611400	-0.97741200	0.82699800
H	2.67610700	0.97742600	0.82698500
I	-0.44716800	0.00000000	-0.01053400

FI•••NH_3			
F	-0.15699200	-0.87336200	1.91815600
N	0.17575000	0.97790400	-2.14770600
H	-0.68240500	0.84323300	-2.68284000
H	0.94299000	0.56338300	-2.67727900
H	0.34826300	1.98121800	-2.08036800
I	-0.00804100	-0.04477200	0.09832100

FI•••NCH			
F	0.00000000	0.00000000	-2.33884400
N	0.00000000	0.00000000	2.20778100
C	0.00000000	0.00000000	3.38585700
H	0.00000000	0.00000000	4.46400500
I	0.00000000	0.00000000	-0.36196300

FI•••OCH_2			
F	2.30325000	0.34709100	0.00000200
O	-2.14056500	-0.49343700	-0.00000500
C	-2.85175400	0.51184100	0.00000800

H	-2.40946100	1.52664300	0.00001900
H	-3.95276400	0.41449700	0.00000700
I	0.37486800	-0.07902800	-0.00000100

FI•••C_2H_4

C	0.00000000	-2.31783200	0.68484200
H	-0.93582900	-2.35491400	1.24750100
H	0.93582900	-2.35491500	1.24750100
C	0.00000000	-2.31783200	-0.68484200
H	0.93582900	-2.35491500	-1.24750100
H	-0.93582900	-2.35491400	-1.24750100
F	0.00000000	2.31047200	0.00000000
I	0.00000000	0.31017700	0.00000000

FI•••$OHCH_3$

F	-2.36391800	0.36683800	0.05504300
O	2.01953300	-0.58514200	-0.08164500
H	2.23061200	-1.15956400	0.67008700
C	2.81872200	0.62182500	0.02485600
H	2.55948700	1.22832400	-0.85034500
H	2.57269000	1.17570300	0.94299400
H	3.88839700	0.36922500	-0.00055400
I	-0.43480200	-0.07481200	-0.01421800

FI•••C_2H_2

C	-2.55204100	-0.61844700	0.00000700
C	-2.55206300	0.61844200	-0.00000400
F	2.26580500	0.00000200	-0.00000100
H	-2.60695300	-1.69419600	-0.00000300
H	-2.60698200	1.69419100	0.00000700

I	0.29144000	0.00000000	0.00000000

FI•••O(CH$_3$)$_2$

F	2.61050700	-0.00000600	0.24640800
O	-1.78661800	0.00000200	-0.38845300
C	-2.37341600	-1.18942600	0.17924200
H	-1.88383200	-2.04328200	-0.30384300
H	-2.19771600	-1.21990200	1.26783900
H	-3.45489000	-1.20016500	-0.03153200
C	-2.37346200	1.18940300	0.17924800
H	-1.88386400	2.04328200	-0.30378300
H	-3.45492500	1.20013300	-0.03158200
H	-2.19781900	1.21985000	1.26785500
I	0.64816400	0.00000500	-0.05898000

FI•••FH

F	2.10860800	0.06324700	0.00000400
I	0.15433700	-0.01586100	-0.00000100
F	-2.66976800	-0.05345100	0.00000300
H	-3.12943900	0.75248400	-0.00000400

ClI•••OH$_2$

Cl	-2.23440500	-0.00000900	0.03054500
O	2.88473000	-0.00000800	-0.05672700
H	3.26329200	-0.76546800	0.39926300
H	3.26335100	0.76539500	0.39930800
I	0.15812100	0.00000500	-0.01630200

ClI•••SH$_2$

Cl	-2.57792100	-0.00000300	0.03998500
S	2.92193400	-0.00002100	-0.07712200

H	3.03724900	-0.97672000	0.85011600
H	3.03714600	0.97703700	0.84976000
I	-0.16982400	0.00000100	-0.02161700

ClI•••NH_3

Cl	-2.25570200	-0.00001100	0.00001500
N	2.72863600	-0.00001300	0.00002400
H	3.09505600	-0.45480800	-0.83669400
H	3.09506000	-0.49726900	0.81222500
H	3.09513600	0.95197200	0.02453700
I	0.18794800	0.00000700	-0.00000900

ClI•••NCH

Cl	0.00000000	0.00000000	-2.47524900
N	0.00000000	0.00000000	2.63263600
C	0.00000000	0.00000000	3.81213600
H	0.00000000	0.00000000	4.89030600
I	0.00000000	0.00000000	-0.07759100

ClI••• OCH_2

Cl	2.45029700	0.27720000	0.00000500
O	-2.55447200	-0.41681300	0.00000300
C	-3.17286900	0.64664300	0.00000200
H	-2.64269300	1.61965400	-0.00004000
H	-4.27937100	0.65443400	0.00004300
I	0.08943400	-0.14211000	-0.00000200

ClI••••C_2H_4

C	0.00000000	-2.74041400	0.68182100
H	-0.93576600	-2.76145200	1.24619600
H	0.93576600	-2.76145600	1.24619700

C	0.00000000	-2.74041400	-0.68182100
H	0.93576600	-2.76145600	-1.24619700
H	-0.93576600	-2.76145200	-1.24619600
Cl	0.00000000	2.46547900	0.00000000
I	0.00000000	0.03806900	0.00000000

ClI•••OHCH$_3$			
Cl	-2.51585100	0.28327000	0.03644300
O	2.42303800	-0.51842500	-0.05888500
H	2.67477100	-1.05502400	0.70779700
C	3.12116200	0.74890700	0.02329800
H	2.81800300	1.31552800	-0.86484700
H	2.82940600	1.30351800	0.92810500
H	4.20922700	0.58913600	0.00559700
I	-0.14855100	-0.13801500	-0.02009200

ClI•••FH			
Cl	2.24747400	0.04202900	-0.00058900
I	-0.12739000	-0.02183600	0.00034300
F	-3.09320300	-0.03222600	-0.00098600
H	-3.61657800	0.73283800	0.00072500

ClI•••O(CH$_3$)$_2$			
Cl	2.76347600	0.00000200	0.20233700
O	-2.14875700	-0.00000100	-0.36398800
C	-2.69909400	-1.18723600	0.23788900
H	-2.23485200	-2.04237500	-0.26819900
H	-2.46460000	-1.21583400	1.31592200
H	-3.79139900	-1.20597500	0.08980300
C	-2.69908000	1.18724500	0.23788000
H	-2.23482600	2.04237400	-0.26821600
H	-3.79138400	1.20599700	0.08979300
H	-2.46458600	1.21584900	1.31591200

I	0.36946500	-0.00000200	-0.10674400

ClI•••C_2H_2			
C	-2.98701700	-0.61769200	0.00000500
C	-2.98701700	0.61769200	-0.00000100
Cl	2.41188800	0.00000000	-0.00000200
H	-3.02006600	-1.69405000	-0.00000200
H	-3.02006500	1.69405000	0.00000600
I	0.01664600	0.00000000	0.00000000

BrI•••OH_2			
Br	-1.92250200	0.00000500	0.01822300
O	3.39641800	0.00000900	-0.04397200
H	3.77762100	-0.76479000	0.41047600
H	3.77755100	0.76487700	0.41042000
I	0.61435900	-0.00000600	-0.02088500

BrI•••SH_2			
Br	-2.24598900	0.00001200	0.02649500
S	3.45596800	0.00000700	-0.06443900
H	3.54948800	-0.97642600	0.86528900
H	3.54931000	0.97668900	0.86504900
I	0.30595000	-0.00001500	-0.03069100

BrI•••NH_3			
Br	-1.58358100	-0.59529300	0.94560400
N	2.63603500	0.99092700	-1.57405300
H	3.21100200	0.19882600	-1.86242700
H	3.20998500	1.59504100	-0.98515800
H	2.38719600	1.51726700	-2.41203700
I	0.53141400	0.19976700	-0.31732300

BrI•••NCH			
Br	0.00000000	0.00000000	-2.14108500
N	0.00000000	0.00000000	3.17097300
C	0.00000000	0.00000000	4.35103100
H	0.00000000	0.00000000	5.42916300
I	0.00000000	0.00000000	0.40011000

BrI•••OCH_2			
Br	2.13240800	0.17093200	0.00000700
O	-3.08769600	-0.35275400	0.00001400
C	-3.63707600	0.74723800	0.00000500
H	-3.04617700	1.68512900	-0.00012700
H	-4.74119700	0.82806500	0.00013200
I	-0.38345100	-0.19164600	-0.00000800

BrI•••C_2H_4			
C	0.00000100	3.26708400	0.68080800
H	0.93568100	3.28348200	1.24565300
H	-0.93567900	3.28349000	1.24565300
C	0.00000100	3.26708400	-0.68080800
H	-0.93567900	3.28349000	-1.24565300
H	0.93568100	3.28348200	-1.24565300
Br	0.00000100	-2.14231500	0.00000000
I	-0.00000100	0.42720900	0.00000000

BrI•••$OHCH_3$			
Br	-2.19635600	0.17170700	0.02060400
O	2.95748900	-0.46481700	-0.04331700
H	3.23094200	-0.97034900	0.73666000
C	3.57861200	0.84147600	0.02177300
H	3.25115800	1.37433600	-0.87873400
H	3.24649500	1.39517300	0.91340300

H	4.67485300	0.74897000	0.01617500
I	0.32712200	-0.18656900	-0.02439200

BrI•••FH

Br	-1.93470500	0.02375400	0.00012400
I	0.58642500	-0.02627600	-0.00015100
F	3.60842100	-0.01845500	0.00044500
H	4.15835600	0.72734500	-0.00032900

BrI•••O(CH$_3$)$_2$

Br	2.43519600	-0.00000200	0.12919300
O	-2.66976800	0.00000000	-0.34148300
C	-3.18911400	-1.18596900	0.28656800
H	-2.74737600	-2.04159700	-0.23876900
H	-2.90489400	-1.21339800	1.35284200
H	-4.28749500	-1.20898100	0.19084900
C	-3.18914400	1.18595000	0.28657700
H	-2.74743600	2.04159400	-0.23876000
H	-4.28752700	1.20893000	0.19086700
H	-2.90491600	1.21338200	1.35284900
I	-0.10801000	0.00000500	-0.14789900

BrI•••C$_2$H$_2$

C	-3.51240200	-0.61745500	0.00000400
C	-3.51240200	0.61745500	0.00000000
Br	2.08888200	0.00000000	-0.00000100
H	-3.53918900	-1.69383800	-0.00000200
H	-3.53918800	1.69383800	0.00000600
I	-0.45063500	0.00000000	0.00000000

31. Astatine Bonded Complexes

FAt•••OH_2			
F	-2.13943100	-0.00002700	0.04624700
O	2.54225200	-0.00000700	-0.06804700
H	2.92799400	-0.76718500	0.37953600
H	2.92818400	0.76702000	0.37963100
At	-0.08163900	0.00000500	-0.00742400

FAt•••SH_2			
F	-2.38604300	0.00000500	0.04431000
S	2.66623600	0.00000000	-0.09202600
H	2.85079800	-0.97757800	0.82363100
H	2.85077900	0.97760800	0.82360300
At	-0.31631700	-0.00000100	-0.00674800

FAt•••NH_3			
F	-2.16319100	-0.00002200	-0.00000100
N	2.46365600	-0.00001400	-0.00000100
H	2.83485000	0.47058200	0.82567900
H	2.83486000	0.47973200	-0.82039500
H	2.83479500	-0.95039200	-0.00528200
At	-0.07389900	0.00000400	0.00000000

FAt•••NCH			
F	0.00000000	0.00000000	2.31325300
N	0.00000000	0.00000000	-2.31848600
C	0.00000000	0.00000000	-3.49593500
H	0.00000000	0.00000000	-4.57413600
At	0.00000000	0.00000000	0.24658700

FAt•••OCH_2			
F	2.28244500	0.37264500	-0.00000300
O	-2.27712900	-0.46557900	0.00000500

C	-3.02438400	0.51360300	-0.00000300
H	-2.61932900	1.54356900	-0.00001500
H	-4.12060200	0.37483200	0.00000400
At	0.26542700	-0.05446100	0.00000000

FAt•••C_2H_4			
C	0.00000000	-2.41723500	0.68704800
H	-0.93616300	-2.46783200	1.24810300
H	0.93616300	-2.46783600	1.24810300
C	0.00000000	-2.41723500	-0.68704800
H	0.93616300	-2.46783600	-1.24810300
H	-0.93616300	-2.46783200	-1.24810300
F	-0.00000100	2.30356300	0.00000000
At	0.00000000	0.21348300	0.00000000

FAt•••$OHCH_3$			
F	-2.32713600	0.39914500	0.05755100
O	2.18134200	-0.56263000	-0.07612700
H	2.41713900	-1.15818500	0.65107100
C	2.99994100	0.63261200	0.02508900
H	2.72178100	1.25657900	-0.83183000
H	2.78904500	1.17331100	0.95958600
H	4.06451500	0.36601900	-0.03772600
At	-0.31174900	-0.05323100	-0.00941800

FAt•••C_2H_2			
C	-2.61574700	-0.61935500	0.00001000
C	-2.61574700	0.61935500	-0.00000700
F	2.25826800	0.00000000	-0.00000100
H	-2.70014600	-1.69358700	-0.00000400
H	-2.70014400	1.69358700	0.00000800
At	0.19370400	0.00000000	0.00000000

FAt•••O(CH$_3$)$_2$			
F	2.53112500	0.00000600	0.26662500
O	-2.00070200	0.00000000	-0.36800800
C	-2.60546900	-1.18958700	0.18134900
H	-2.10746700	-2.04376500	-0.29253800
H	-2.45621600	-1.22384200	1.27380500
H	-3.68149700	-1.19593300	-0.05562700
C	-2.60545800	1.18959500	0.18134600
H	-2.10744000	2.04376700	-0.29253500
H	-3.68148300	1.19595600	-0.05564000
H	-2.45621400	1.22384700	1.27380300
At	0.48213400	-0.00000200	-0.04097600

FAt•••FH			
F	-2.13713200	0.06487300	0.00000400
F	2.69685100	-0.04964500	0.00000400
H	3.17632500	0.74535300	-0.00000200
At	-0.09663300	-0.01038100	-0.00000100

ClAt•••OH$_2$			
Cl	-2.35858100	-0.00002300	0.03189700
O	2.82246800	-0.00002400	-0.04976600
H	3.21572600	-0.76649200	0.39234500
H	3.21587500	0.76630200	0.39245800
At	0.13040600	0.00000900	-0.01092800

ClAt•••SH$_2$			
Cl	-2.61190400	-0.00000400	0.04119600
S	2.95175700	-0.00000500	-0.07512400
H	3.09634100	-0.97731600	0.84785000
H	3.09639300	0.97732100	0.84784500
At	-0.10610000	0.00000200	-0.01404700

ClAt•••NH_3			
Cl	-2.38885400	0.00000300	0.00000100
N	2.71764500	0.00000300	0.00000200
H	3.08785200	0.46988300	0.82675900
H	3.08785400	0.48106800	-0.82029600
H	3.08787900	-0.95091800	-0.00645600
At	0.14498100	-0.00000100	0.00000000

ClAt•••NCH			
Cl	0.00000000	0.00000000	-2.53066000
N	0.00000000	0.00000000	2.60718800
C	0.00000000	0.00000000	3.78558700
H	0.00000000	0.00000000	4.86388200
At	0.00000000	0.00000000	-0.03301800

ClAt••• OCH_2			
Cl	2.51285400	0.30325100	-0.00000600
O	-2.57207800	-0.37072100	0.00000700
C	-3.23999900	0.66349500	0.00000000
H	-2.75578900	1.65944100	-0.00000600
H	-4.34469600	0.61550600	0.00000000
At	0.05174800	-0.09935800	0.00000100

ClAt••••C_2H_4			
C	0.00000000	-2.70748700	0.68484300
H	-0.93629100	-2.74431000	1.24732800
H	0.93629000	-2.74431200	1.24732800
C	0.00000000	-2.70748700	-0.68484300
H	0.93629000	-2.74431200	-1.24732800
H	-0.93629100	-2.74431000	-1.24732800
Cl	0.00000000	2.53504700	0.00000000
At	0.00000000	0.00436800	0.00000000

ClAt•••OHCH$_3$			
Cl	-2.56167400	0.31947200	0.03823800
O	2.47130800	-0.47450200	-0.05222600
H	2.74203100	-1.03195300	0.69292000
C	3.20115400	0.77747300	0.02432700
H	2.88402500	1.36094300	-0.84771800
H	2.94786000	1.32454400	0.94480300
H	4.28331200	0.59019300	-0.02823200
At	-0.09748400	-0.10051200	-0.01341100

ClAt•••C_2H_2			
C	-2.92478100	-0.61863600	0.00000800
C	-2.92478100	0.61863600	-0.00000400
Cl	2.48262400	0.00000000	-0.00000100
H	-2.98512000	-1.69434200	-0.00000300
H	-2.98512000	1.69434200	0.00000700
At	-0.01337700	0.00000000	0.00000000

ClAt•••O(CH$_3$)$_2$			
Cl	2.76008900	0.00001200	0.22663300
O	-2.26179900	-0.00000100	-0.33103300
C	-2.83647600	-1.18857400	0.24912000
H	-2.36032500	-2.04340500	-0.24609500
H	-2.63525400	-1.22110000	1.33354100
H	-3.92318600	-1.20002600	0.06575300
C	-2.83638800	1.18862600	0.24910000
H	-2.36014300	2.04341300	-0.24609900
H	-3.92309100	1.20017600	0.06569700
H	-2.63519800	1.22113500	1.33352700
At	0.27114400	-0.00000800	-0.07647200

ClAt•••FH			
Cl	-2.35799900	0.04378600	0.00000200
F	3.01252300	-0.02658300	0.00000400
H	3.53602300	0.73928100	-0.00000300
At	0.11102700	-0.01464000	-0.00000100

BrAt•••OH_2			
Br	-2.13962600	-0.00000300	0.01895200
O	3.22374200	-0.00000900	-0.03633400
H	3.61704600	-0.76593200	0.40641500
H	3.61706000	0.76589300	0.40644000
At	0.49250400	0.00000300	-0.01394700

BrAt•••SH_2			
Br	2.38332300	-0.00000600	0.02776100
S	-3.36699400	-0.00000300	-0.06063600
H	-3.49069100	0.97696800	0.86552800
H	-3.49067000	-0.97708400	0.86541600
At	-0.26544800	0.00000400	-0.02038100

BrAt•••NH_3			
Br	-0.97035800	-0.64761000	-1.82404600
N	1.39362700	0.93009800	2.61969400
H	0.82393700	1.61321000	3.11987800
H	2.29626900	1.36447000	2.42493900
H	1.55863800	0.14495400	3.25032200
At	0.22974500	0.15333000	0.43186600

BrAt•••NCH			
Br	0.00000000	0.00000000	-2.30014600
N	0.00000000	0.00000000	3.02260900
C	0.00000000	0.00000000	4.20151800

H	0.00000000	0.00000000	5.27981000
At	0.00000000	0.00000000	0.33950500

BrAt•••OCH_2

Br	2.29670100	0.19081600	0.00000000
O	-2.98968500	-0.28996500	0.00000100
C	-3.59282900	0.78275600	0.00000000
H	-3.04845700	1.74754600	0.00000000
H	-4.69880000	0.80492600	0.00000000
At	-0.31956300	-0.13656300	0.00000000

BrAt•••C_2H_4

C	0.00000000	3.12115800	0.68364000
H	0.93624800	3.15177100	1.24675100
H	-0.93624800	3.15177400	1.24675200
C	0.00000000	3.12115800	-0.68364000
H	-0.93624800	3.15177400	-1.24675200
H	0.93624800	3.15177100	-1.24675100
Br	0.00000000	-2.30960000	0.00000000
At	0.00000000	0.36205900	0.00000000

BrAt•••$OHCH_3$

Br	-2.34564900	0.19899200	0.02161300
O	2.88989000	-0.40103400	-0.03600900
H	3.18336800	-0.92694900	0.72319400
C	3.54537600	0.89118800	0.02332400
H	3.20202500	1.44076400	-0.86086400
H	3.25398900	1.43974400	0.93177300
H	4.63740100	0.76828100	-0.01843200
At	0.27564200	-0.13912200	-0.01628200

BrAt•••C_2H_2

C	-3.34163400	-0.61830400	0.00000700
C	-3.34163400	0.61830400	-0.00000300
Br	2.25937800	0.00000000	-0.00000100
H	-3.39234500	-1.69435700	-0.00000300
H	-3.39234500	1.69435700	0.00000700
At	-0.37875200	0.00000000	0.00000000

$BrAt{\bullet\bullet\bullet}O(CH_3)_2$

Br	2.53525900	0.00000100	0.14938700
O	-2.66828900	0.00000000	-0.29569000
C	-3.21586700	-1.18770100	0.30926300
H	-2.75892200	-2.04278400	-0.20353800
H	-2.97003500	-1.21880900	1.38467500
H	-4.30957400	-1.20317800	0.17210000
C	-3.21585200	1.18770800	0.30926000
H	-2.75889500	2.04278400	-0.20354200
H	-4.30955900	1.20320000	0.17209500
H	-2.97002200	1.21881500	1.38467200
At	-0.10259300	-0.00000100	-0.10918400

BrAt•••FH

Br	-2.14133100	0.02562000	0.00000100
F	3.42737700	-0.00952200	0.00000500
H	3.97021600	0.74231500	-0.00000300
At	0.47211700	-0.01827400	-0.00000100