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

Supporting Information

Tetrel Bonding Interaction: An Analysis with the Block-Localized Wavefunction (BLW) Approach

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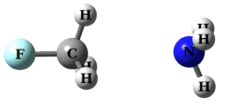
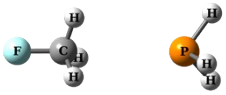
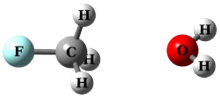


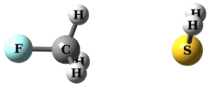
$FH_3C\cdots NH_3$ (1)



$FH_3C\cdots PH_3$ (2)



$FH_3C\cdots OH_2$ (3)



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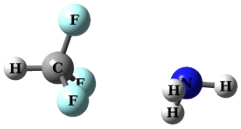
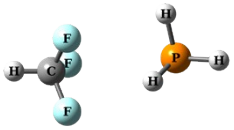


$F_3HC\cdots NH_3$ (5)



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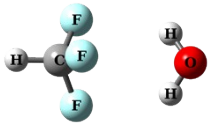
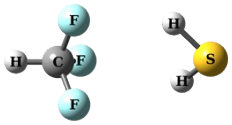
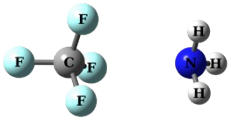


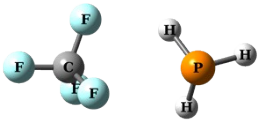
$F_3HC\cdots OH_2$ (7)



$F_3HC\cdots SH_2$ (8)



$F_4C\cdots NH_3$ (9)



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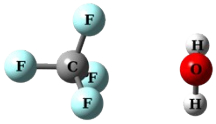
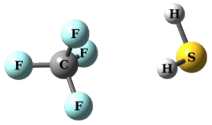
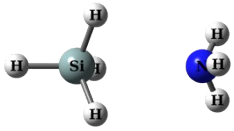


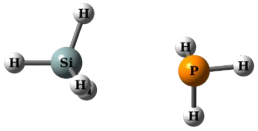
$F_4C\cdots OH_2$ (11)



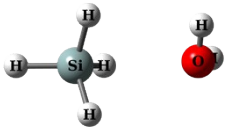
$F_4C\cdots SH_2$ (12)



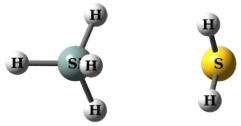
$H_4Si\cdots NH_3$ (13)



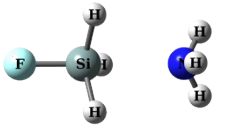
$H_4Si\cdots PH_3$ (14)



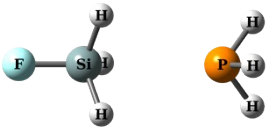
$H_4Si\cdots OH_2$ (15)



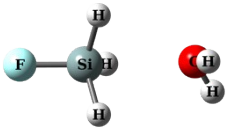
$H_4Si\cdots SH_2$ (16)



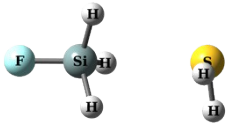
$FH_3Si\cdots NH_3$ (17)



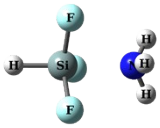
$FH_3Si\cdots PH_3$ (18)



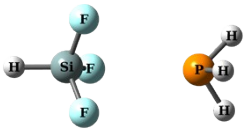
$FH_3Si\cdots OH_2$ (19)



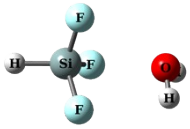
$FH_3Si\cdots SH_2$ (20)



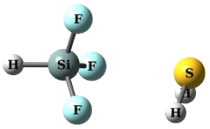
$F_3HSi\cdots NH_3$ (21)



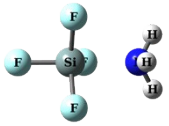
$F_3HSi\cdots PH_3$ (22)



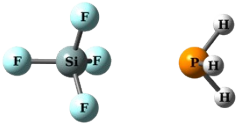
$F_3HSi\cdots OH_2$ (23)



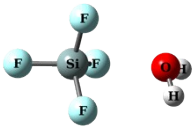
$F_3HSi\cdots SH_2$ (24)



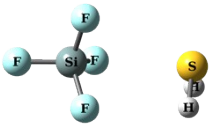
$F_4Si\cdots NH_3$ (25)



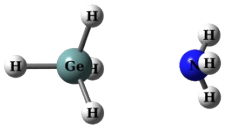
$F_4Si\cdots PH_3$ (26)



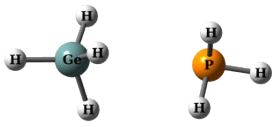
$F_4Si\cdots OH_2$ (27)



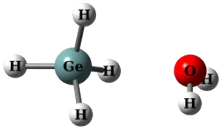
$F_4Si\cdots SH_2$ (28)



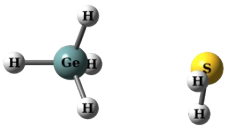
$H_4Ge\cdots NH_3$ (29)



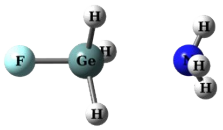
$H_4Ge\cdots PH_3$ (30)



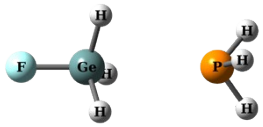
$H_4Ge\cdots OH_2$ (31)



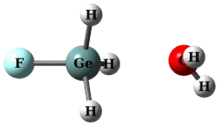
$H_4Ge\cdots SH_2$ (32)



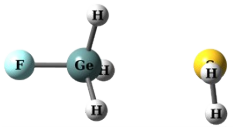
$FH_3Ge\cdots NH_3$ (33)



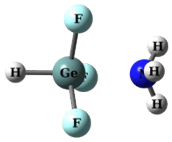
$FH_3Ge\cdots PH_3$ (34)



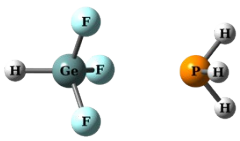
$FH_3Ge\cdots OH_2$ (35)



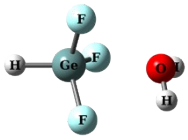
$FH_3Ge\cdots SH_2$ (36)



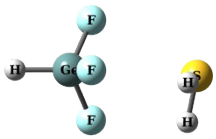
$F_3HGe\cdots NH_3$ (37)



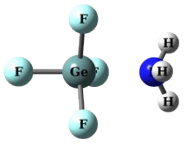
$F_3HGe\cdots PH_3$ (38)



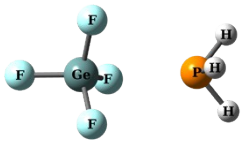
$F_3HGe\cdots OH_2$ (39)



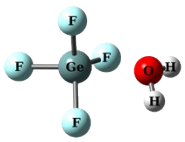
$F_3HGe\cdots SH_2$ (40)



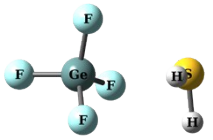
$F_4Ge\cdots NH_3$ (41)



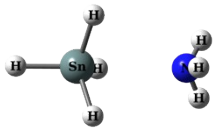
$F_4Ge\cdots PH_3$ (42)



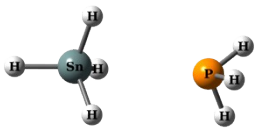
$F_4Ge\cdots OH_2$ (43)



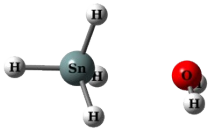
$F_4Ge\cdots SH_2$ (44)



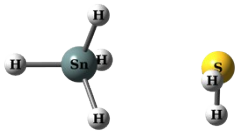
$H_4Sn\cdots NH_3$ (45)



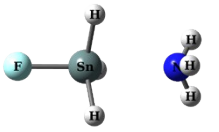
$H_4Sn\cdots PH_3$ (46)



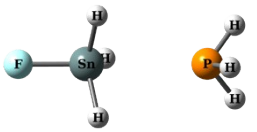
$H_4Sn\cdots OH_2$ (47)



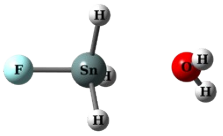
$H_4Sn\cdots SH_2$ (48)



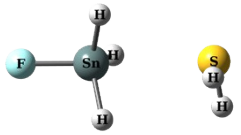
$FH_3Sn\cdots NH_3$ (49)



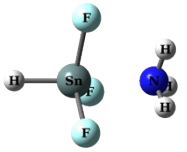
$FH_3Sn\cdots PH_3$ (50)



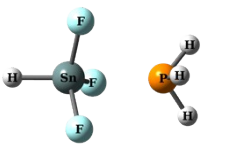
$FH_3Sn\cdots OH_2$ (51)



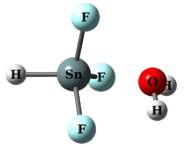
$FH_3Sn\cdots SH_2$ (52)



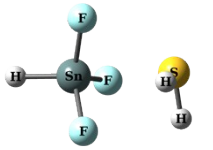
$F_3HSn\cdots NH_3$ (53)



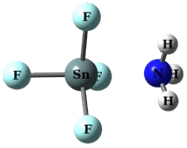
$F_3HSn\cdots PH_3$ (54)



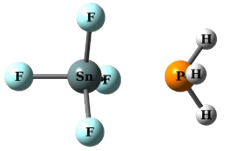
$F_3HSn\cdots OH_2$ (55)



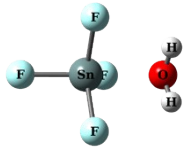
$F_3HSn\cdots SH_2$ (56)



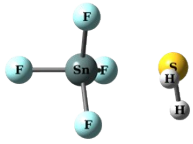
$F_4Sn\cdots NH_3$ (57)



$F_4Sn\cdots PH_3$ (58)



$F_4Sn\cdots OH_2$ (59)



$F_4Sn\cdots SH_2$ (60)

Figure S1. Optimal structures of all complexes studied.

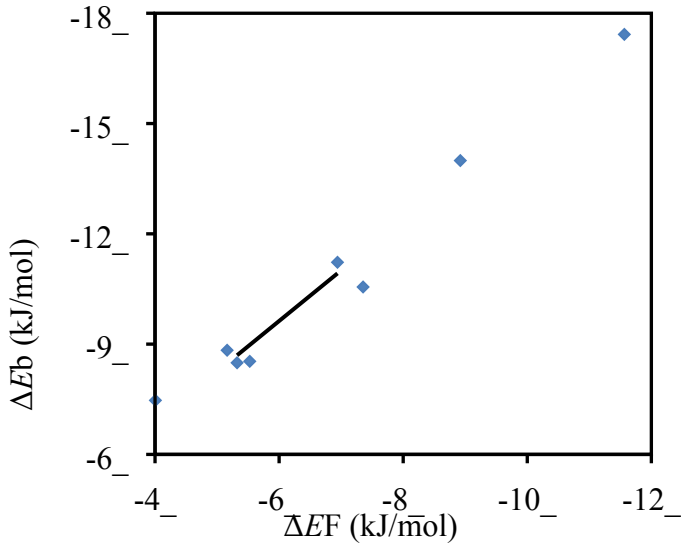
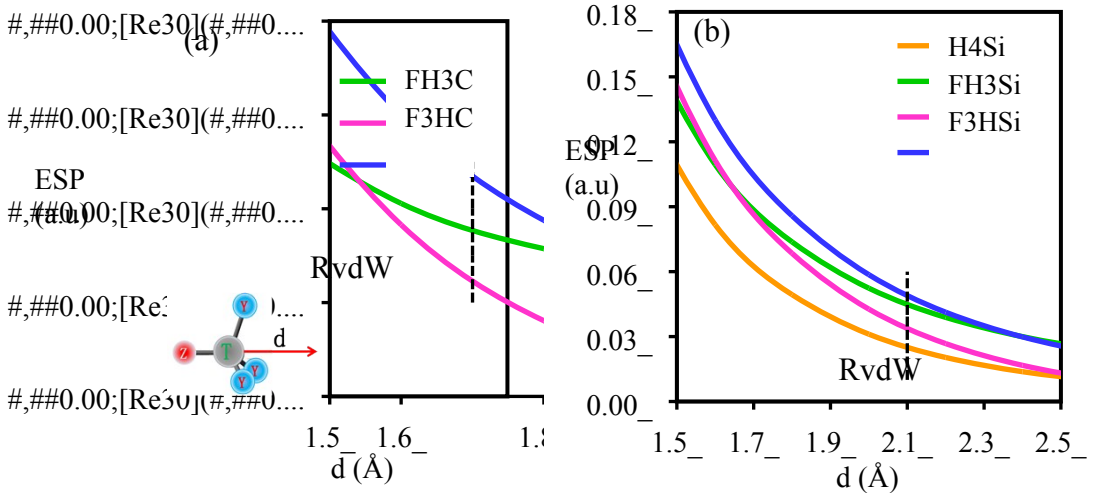


Figure S2. Correlation between the overall binding energy and the frozen energy of complexes formed with H4T.



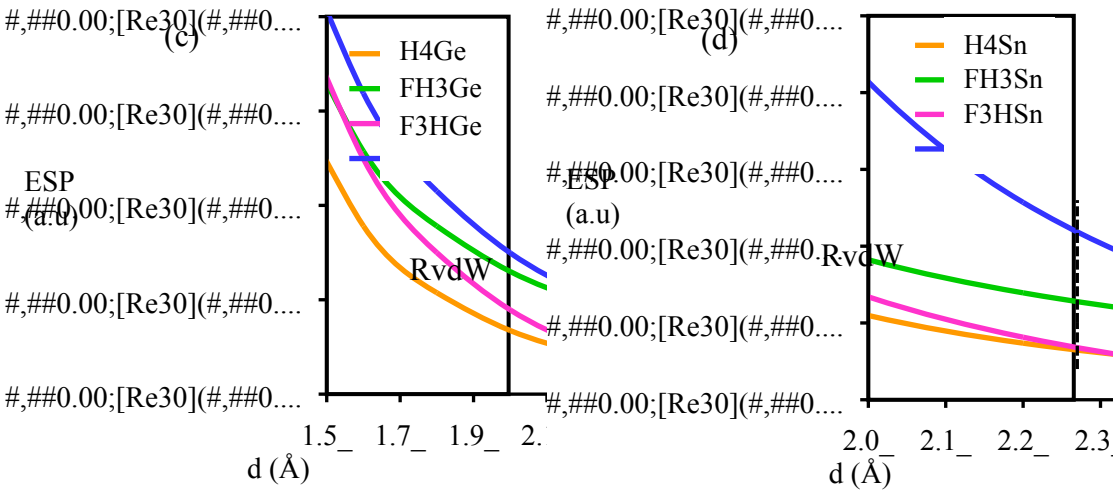


Figure S3. Distribution of ESP along the binding direction of the Lewis acids.

2) Additional Tables

Table S1. Intermolecular distance (R_1 in Å), variation of the X-T bond length upon formation of complex (ΔR_2 in Å) and the difference between the tetrel bond length and the summary of corresponding atomic van der Waals radii (R_1-R_{vdW} in Å) of the optimal geometries of both the adiabatic and diabatic states.

No	Complex	R_1	R_1'[1)]	ΔR_2	ΔR_2'[2)]	R_1-R_{vdW}	R_1'-R_{vdW}
1	$FH_3C\cdots NH_3$	3.080	3.135	0.005	0.004	-0.170	-0.115
2	$FH_3C\cdots PH_3$	3.606	3.838	0.002	0.001	0.106	0.338
3	$FH_3C\cdots OH_2$	2.912	2.980	0.005	0.004	-0.308	-0.240
4	$FH_3C\cdots SH_2$	3.528	3.685	0.002	0.001	0.028	0.185
9	$F_4C\cdots NH_3$	3.238	3.247	0.008	0.007	-0.012	-0.003
13	$H_4Si\cdots NH_3$	3.095	3.192	0.008	0.005	-0.555	-0.458
15	$H_4Si\cdots OH_2$	3.063	3.092	0.005	0.004	-0.557	-0.528
16	$H_4Si\cdots SH_2$	3.681	3.802	0.003	0.002	-0.219	-0.098
17	$FH_3Si\cdots NH_3$	2.574	2.926	0.021	0.011	-1.076	-0.724
18	$FH_3Si\cdots PH_3$	3.431	3.677	0.005	0.003	-0.469	-0.223
19	$FH_3Si\cdots OH_2$	2.736	2.852	0.011	0.009	-0.884	-0.768
20	$FH_3Si\cdots SH_2$	3.387	3.573	0.005	0.003	-0.513	-0.327

21	$F_3HSi\cdots NH_3$	2.136	2.987	0.016	0.004	-1.514	-0.663
22	$F_3HSi\cdots PH_3$	3.659	3.854	0.001	0.001	-0.241	-0.046
23	$F_3HSi\cdots OH_2$	2.855	2.936	0.003	0.003	-0.765	-0.684
24	$F_3HSi\cdots SH_2$	3.613	3.730	0.001	0.001	-0.287	-0.170
25	$F_4Si\cdots NH_3$	2.088	2.876	0.036	0.010	-1.562	-0.774
26	$F_4Si\cdots PH_3$	3.544	3.744	0.004	0.003	-0.356	-0.156
27	$F_4Si\cdots OH_2$	2.663	2.820	0.011	0.008	-0.957	-0.800
28	$F_4Si\cdots SH_2$	3.478	3.626	0.004	0.003	-0.422	-0.274
29	$H_4Ge\cdots NH_3$	3.179	3.236	0.011	0.008	-0.561	-0.504
31	$H_4Ge\cdots OH_2$	3.114	3.125	0.007	0.006	-0.596	-0.585
32	$H_4Ge\cdots SH_2$	3.745	3.844	0.004	0.002	-0.245	-0.146
33	$FH_3Ge\cdots NH_3$	2.727	2.920	0.023	0.014	-1.013	-0.820
34	$FH_3Ge\cdots PH_3$	3.460	3.676	0.008	0.004	-0.530	-0.314
35	$FH_3Ge\cdots OH_2$	2.749	2.842	0.014	0.011	-0.961	-0.868
36	$FH_3Ge\cdots SH_2$	3.406	3.571	0.008	0.004	-0.584	-0.419
37	$F_3HGe\cdots NH_3$	2.164	2.862	0.016	0.006	-1.576	-0.878
38	$F_3HGe\cdots PH_3$	3.556	3.814	0.002	0.002	-0.434	-0.176
39	$F_3HGe\cdots OH_2$	2.594	2.867	0.007	0.004	-1.116	-0.843
40	$F_3HGe\cdots SH_2$	3.551	3.721	0.002	0.001	-0.439	-0.269
41	$F_4Ge\cdots NH_3$	2.127	2.604	0.029	0.015	-1.613	-1.136
42	$F_4Ge\cdots PH_3$	3.203	3.613	0.009	0.004	-0.787	-0.377
43	$F_4Ge\cdots OH_2$	2.215	2.638	0.021	0.010	-1.495	-1.072
44	$F_4Ge\cdots SH_2$	3.150	3.499	0.009	0.004	-0.840	-0.491
45	$H_4Sn\cdots NH_3$	3.081	3.176	0.019	0.014	-0.739	-0.644
46	$H_4Sn\cdots PH_3$	3.833	3.989	0.006	0.004	-0.237	-0.081
47	$H_4Sn\cdots OH_2$	3.038	3.087	0.013	0.011	-0.752	-0.703
48	$H_4Sn\cdots SH_2$	3.754	3.855	0.006	0.004	-0.316	-0.215
49	$FH_3Sn\cdots NH_3$	2.684	2.882	0.027	0.018	-1.136	-0.938
50	$FH_3Sn\cdots PH_3$	3.437	3.700	0.012	0.006	-0.633	-0.370
51	$FH_3Sn\cdots OH_2$	2.706	2.817	0.018	0.014	-1.084	-0.973
52	$FH_3Sn\cdots SH_2$	3.386	3.592	0.011	0.006	-0.684	-0.478
53	$F_3HSn\cdots NH_3$	2.281	2.562	0.013	0.014	-1.539	-1.258
54	$F_3HSn\cdots PH_3$	2.871	3.662	0.011	0.003	-1.199	-0.408
55	$F_3HSn\cdots OH_2$	2.306	2.580	0.012	0.010	-1.484	-1.210

56	$F_3HSn\cdots SH_2$	2.925	3.549	0.010	0.003	-1.145	-0.521
57	$F_4Sn\cdots NH_3$	2.268	2.473	0.016	0.015	-1.552	-1.347
58	$F_4Sn\cdots PH_3$	2.769	3.406	0.013	0.005	-1.301	-0.664
59	$F_4Sn\cdots OH_2$	2.266	2.446	0.013	0.012	-1.524	-1.344
60	$F_4Sn\cdots SH_2$	2.783	3.316	0.012	0.005	-1.287	-0.754

1) R_1' and R_2' are the bond lengths in the optimal geometry of an electron-localized state with the BLW method.

2) ΔR_2=R_2(complex) - R_2(monomer).

Table S2. Classifications of the sixty complexes studied according to their optimal geometries and BLW-ED results.

Atypical cases		Dominated by ΔE_F		Dominated by ΔE_{pol}		Dominated by ΔE_{CT}	
Complex	No	Complex	No	Complex	No	Complex	No
$F_3HC\cdots NH_3$	(5)	$FH_3C\cdots NH_3$	(1)	$FH_3Si\cdots NH_3$	(17)	$FH_3Si\cdots PH_3$	(18)
$F_3HC\cdots PH_3$	(6)	$FH_3C\cdots PH_3$	(2)	$F_3HSi\cdots NH_3$	(21)	$FH_3Ge\cdots PH_3$	(34)
$F_3HC\cdots OH_2$	(7)	$FH_3C\cdots OH_2$	(3)	$F_4Si\cdots NH_3$	(25)	$F_3HGe\cdots PH_3$	(38)
$F_3HC\cdots SH_2$	(8)	$FH_3C\cdots SH_2$	(4)	$F_3HGe\cdots NH_3$	(37)	$F_4Ge\cdots PH_3$	(42)
$F_4C\cdots PH_3$	(10)	$F_4C\cdots NH_3$	(9)	$F_4Ge\cdots NH_3$	(41)	$F_4Ge\cdots SH_2$	(44)
$F_4C\cdots OH_2$	(11)	$H_4Si\cdots NH_3$	(13)	$F_4Ge\cdots OH_2$	(43)	$FH_3Sn\cdots PH_3$	(50)
$F_4C\cdots SH_2$	(12)	$H_4Si\cdots OH_2$	(15)	$F_3HSn\cdots NH_3$	(53)	$F_3HSn\cdots PH_3$	(54)
$H_4Si\cdots PH_3$	(14)	$H_4Si\cdots SH_2$	(16)	$F_3HSn\cdots OH_2$	(55)	$F_3HSn\cdots SH_2$	(56)
$H_4Ge\cdots PH_3$	(30)	$FH_3Si\cdots OH_2$	(19)	$F_4Sn\cdots NH_3$	(57)	$F_4Sn\cdots PH_3$	(58)
		$FH_3Si\cdots SH_2$	(20)	$F_4Sn\cdots OH_2$	(59)	$F_4Sn\cdots SH_2$	(60)
		$F_3HSi\cdots PH_3$	(22)				
		$F_3HSi\cdots OH_2$	(23)				
		$F_3HSi\cdots SH_2$	(24)				
		$F_4Si\cdots PH_3$	(26)				
		$F_4Si\cdots OH_2$	(27)				
		$F_4Si\cdots SH_2$	(28)				
		$H_4Ge\cdots NH_3$	(29)				
		$H_4Ge\cdots OH_2$	(31)				
		$H_4Ge\cdots SH_2$	(32)				

$FH_3Ge\cdots NH_3$	(33)
$FH_3Ge\cdots OH_2$	(35)
$FH_3Ge\cdots SH_2$	(36)
$F_3HGe\cdots OH_2$	(39)
$F_3HGe\cdots SH_2$	(40)
$H_4Sn\cdots NH_3$	(45)
$H_4Sn\cdots PH_3$	(46)
$H_4Sn\cdots OH_2$	(47)
$H_4Sn\cdots SH_2$	(48)
$FH_3Sn\cdots NH_3$	(49)
$FH_3Sn\cdots OH_2$	(51)
$FH_3Sn\cdots SH_2$	(52)

Table S3. Energy of the lone pair orbital (in a.u) of Lewis bases studied.

	NH_3	PH_3	OH_2	SH_2
E(LP)	-0.32880	-0.28380	-0.39260	-0.32020

Table S4. Energy decomposation results (in kJ/mol) of the point charge model.

No	Complex	ΔE_{pol}	ΔE_{es}	ΔE_{int}(PC)	No	Complex	ΔE_{pol}	ΔE_{es}	ΔE_{int}(PC)
1	$FH_3C\cdots NH_3$	-0.5	-14.7	-15.2	31	$H_4Ge\cdots OH_2$	-0.1	-5.3	-5.4
2	$FH_3C\cdots PH_3$	-0.7	-5.9	-6.6	32	$H_4Ge\cdots SH_2$	-0.1	-2.4	-2.4
3	$FH_3C\cdots OH_2$	-0.4	-13.3	-13.7	33	$FH_3Ge\cdots NH_3$	-6.1	-51.4	-57.4
4	$FH_3C\cdots SH_2$	-0.6	-6.0	-6.6	34	$FH_3Ge\cdots PH_3$	-3.7	-15.9	-19.6
5	$F_3HC\cdots NH_3$	-0.1	0.4	0.3	35	$FH_3Ge\cdots OH_2$	-3.1	-33.6	-36.7
6	$F_3HC\cdots PH_3$	-0.2	-0.1	-0.3	36	$FH_3Ge\cdots SH_2$	-3.1	-15.7	-18.8
7	$F_3HC\cdots OH_2$	-0.1	-6.3	-6.4	37	$F_3HGe\cdots NH_3$	-76.6	-175.0	-251.6
8	$F_3HC\cdots SH_2$	-0.1	-3.0	-3.1	38	$F_3HGe\cdots PH_3$	-1.2	-11.3	-12.6
9	$F_4C\cdots NH_3$	-0.2	-10.4	-10.6	39	$F_3HGe\cdots OH_2$	-8.6	-52.9	-61.5
10	$F_4C\cdots PH_3$	-0.2	-0.9	-1.1	40	$F_3HGe\cdots SH_2$	-1.3	-12.6	-13.9
11	$F_4C\cdots OH_2$	-0.2	-6.1	-6.3	41	$F_4Ge\cdots NH_3$	-129.7	-224.1	-353.8
12	$F_4C\cdots SH_2$	-0.1	-2.5	-2.7	42	$F_4Ge\cdots PH_3$	-16.2	-37.5	-53.7
13	$H_4Si\cdots NH_3$	-0.2	-8.7	-8.9	43	$F_4Ge\cdots OH_2$	-53.2	-130.7	-183.9

14	$H_4Si\cdots PH_3$	-0.1	-1.2	-1.3	44	$F_4Ge\cdots SH_2$	-14.3	-37.0	-51.3
15	$H_4Si\cdots OH_2$	-0.1	-5.7	-5.8	45	$H_4Sn\cdots NH_3$	-0.6	-17.0	-17.6
16	$H_4Si\cdots SH_2$	-0.1	-2.6	-2.7	46	$H_4Sn\cdots PH_3$	-0.2	-4.3	-4.6
17	$FH_3Si\cdots NH_3$	-7.9	-58.9	-66.8	47	$H_4Sn\cdots OH_2$	-0.4	-11.7	-12.1
18	$FH_3Si\cdots PH_3$	-3.1	-14.8	-17.9	48	$H_4Sn\cdots SH_2$	-0.2	-4.7	-5.0
19	$FH_3Si\cdots OH_2$	-2.7	-30.7	-33.4	49	$FH_3Sn\cdots NH_3$	-11.1	-69.1	-80.2
20	$FH_3Si\cdots SH_2$	-2.6	-14.6	-17.2	50	$FH_3Sn\cdots PH_3$	-6.4	-21.4	-27.8
21	$F_3HSi\cdots NH_3$	-73.2	-171.3	-244.5	51	$FH_3Sn\cdots OH_2$	-5.6	-45.8	-51.4
22	$F_3HSi\cdots PH_3$	-0.6	-8.1	-8.7	52	$FH_3Sn\cdots SH_2$	-5.4	-20.8	-26.2
23	$F_3HSi\cdots OH_2$	-2.4	-27.7	-30.1	53	$F_3HSn\cdots NH_3$	-84.0	-183.4	-267.4
24	$F_3HSi\cdots SH_2$	-0.8	-9.6	-10.5	54	$F_3HSn\cdots PH_3$	-44.4	-67.3	-111.7
25	$F_4Si\cdots NH_3$	-123.6	-219.2	-342.8	55	$F_3HSn\cdots OH_2$	-41.1	-116.9	-158.0
26	$F_4Si\cdots PH_3$	-3.7	-17.6	-21.3	56	$F_3HSn\cdots SH_2$	-27.3	-52.9	-80.2
27	$F_4Si\cdots OH_2$	-8.7	-54.1	-62.9	57	$F_4Sn\cdots NH_3$	-125.7	-220.9	-346.6
28	$F_4Si\cdots SH_2$	-3.7	-18.6	-22.3	58	$F_4Sn\cdots PH_3$	-101.8	-99.7	-201.5
29	$H_4Ge\cdots NH_3$	-0.1	-7.7	-7.8	59	$F_4Sn\cdots OH_2$	-65.7	-148.1	-213.9
30	$H_4Ge\cdots PH_3$	-0.1	-1.1	-1.2	60	$F_4Sn\cdots SH_2$	-74.6	-79.6	-154.1

3) The xyz coordinates of all complexes optimized at M062x-D3/cc-pVTZ level of theory (in Å) and charges (obtained from NPA results of distorted yet unpolarized monomers) used in the point charge model

Complex	X (Å)	Y (Å)	Z (Å)	Net Charge
FH3C···NH3 (1)				
C	-0.741193864	0.000518058	0.000320952	-0.1186
F	-2.123583951	0.001626248	0.001241752	-0.36063
H	-0.381368298	0.692493211	-0.757783189	0.15974
H	-0.380311146	0.310704393	0.978437606	0.15974
H	-0.382223773	-1.002266659	-0.220279142	0.15974
N	2.335967802	-0.001846323	-0.001336364	
H	2.718803061	-0.597254291	0.723175832	
H	2.719785034	-0.330636217	-0.879157006	
H	2.717822136	0.92359458	0.152876559	

$FH_3C\cdots PH_3$ (2)

C	0.025521131	-0.00158263	0.512074667	-0.11822
F	0.020126508	0.001937391	1.890738381	-0.36015
H	0.045271557	-1.030472764	0.155917493	0.15948
H	-0.872491644	0.495584389	0.148596864	0.15945
H	0.907836899	0.527397474	0.155164894	0.15944
P	0.002205715	-0.026643265	-3.093467724	
H	-1.216580341	-0.110756808	-3.804463762	
H	0.62341103	-1.043474984	-3.853555441	
H	0.509120456	1.016604168	-3.901125143	

$FH_3C\cdots OH_2$ (3)

C	0.024444616	0.01224265	0.193276893	-0.11839
F	-0.009385554	-0.084261155	1.571242068	-0.36068
H	-0.02145129	-0.984666575	-0.238737283	0.15983
H	-0.828049897	0.597215626	-0.14574917	0.15954
H	0.946067787	0.504005928	-0.109937831	0.1597
O	0.160607219	0.142143175	-2.713000208	
H	-0.515520193	0.389118807	-3.347142732	
H	0.898177002	-0.167388486	-3.242519137	

$FH_3C\cdots SH_2$ (4)

C	0.004469553	0.052052453	0.241517324	-0.11825
F	0.018219951	0.06191054	1.620381181	-0.36023
H	0.043982135	-0.977714088	-0.109987996	0.15954
H	-0.909910859	0.526235111	-0.111593272	0.15948
H	0.868639245	0.600650633	-0.129802636	0.15947
S	-0.024195401	-0.029614372	-3.285895153	
H	-0.942588197	-0.987624487	-3.463857137	
H	0.989248533	-0.882440929	-3.480522103	

$F_3HC\cdots NH_3$ (5)

C	0.010852997	0.037693499	0.272522577	0.87773
H	-0.080587359	-0.127484262	1.344304433	0.1078
F	0.125241978	-1.132564485	-0.361572512	-0.33124
F	-1.070852533	0.658877424	-0.192059345	-0.32871
F	1.080077603	0.772680767	0.002658803	-0.32558
N	0.106989801	0.130322257	-3.08046454	
H	-0.838135027	-0.066764826	-2.774352917	
H	0.641103099	-0.714522545	-2.91876246	
H	0.069730762	0.27035518	-4.082393819	

$F_3HC\cdots PH_3$ (6)

C	0.00908438	-0.095166518	0.491219057	0.87722
H	0.383779596	-0.209289388	1.506207194	0.10917
F	-0.422126994	-1.262075007	0.018099535	-0.32866
F	-0.995657887	0.773017261	0.45598945	-0.32734
F	0.976928644	0.348520084	-0.312961466	-0.33039
P	-0.44943199	0.231548098	-3.207234886	
H	-0.434986712	-0.019890065	-4.59971736	
H	0.251493368	-0.955709865	-2.894048062	
H	0.725338914	1.01763842	-3.247673242	

$F_3HC\cdots OH_2$ (7)

C	0.033546553	-0.003582336	0.095135901	0.87726
H	-0.12027542	0.001827296	1.171711682	0.10925
F	0.133681894	-1.258614246	-0.351142508	-0.33096
F	-1.002442858	0.570270354	-0.522659413	-0.33099
F	1.136681476	0.651252055	-0.230886469	-0.32456
O	0.192722196	-0.218698907	-3.231750986	
H	-0.562903105	0.240203955	-2.859394008	
H	0.237759375	-1.041686402	-2.74093517	

$F_3HC\cdots SH_2$ (8)

C	-0.023429877	0.007977731	0.216333247	0.87708
H	-0.026170497	-0.049334594	1.302396557	0.10967
F	0.532488404	-1.085884223	-0.306859318	-0.3302
F	-1.269223878	0.101356453	-0.248724529	-0.32973
F	0.661869738	1.065997918	-0.199926453	-0.32682
S	0.073263282	-0.121327329	-3.712422609	
H	-0.891674985	-0.288505464	-2.799454515	
H	0.991647924	-0.689308733	-2.92126335	

$F_4C\cdots NH_3$ (9)

C	-0.011677117	-0.014622942	0.247979699	1.22917
F	0.015904748	0.016467905	1.571592438	-0.31284
F	-1.079235725	-0.674714036	-0.139032678	-0.30478
F	-0.053181796	1.220228507	-0.203045932	-0.30578
F	1.075323612	-0.616372025	-0.183545464	-0.30577
N	-0.01438825	-0.048094985	-2.990143457	
H	-0.790266987	-0.436651567	-3.51180237	

H	0.818964292	-0.533724172	-3.298261754	
H	0.082978553	0.916076305	-3.283860251	

$F_4C\cdots PH_3$ (10)

C	-0.025241297	-0.060216039	0.475113246	1.22907
F	0.383134506	-0.205521377	1.718703039	-0.30754
F	-0.495180447	-1.207308347	0.031536131	-0.30704
F	-0.967830435	0.854116211	0.425515615	-0.30575
F	0.993177162	0.314771471	-0.276020675	-0.30875
P	-0.394080089	0.192059699	-3.20255181	
H	-0.560413803	-0.057052866	-4.584461594	
H	0.351453377	-0.990232133	-2.986046727	
H	0.759402366	0.987976381	-3.391907004	

$F_4C\cdots OH_2$ (11)

C	0.007509684	0.021173792	0.08586529	1.22916
F	0.015805653	-0.024791758	1.40505018	-0.31006
F	0.005646676	-1.214568923	-0.382321727	-0.30936
F	-1.072853753	0.648732212	-0.318287634	-0.3048
F	1.082325827	0.650051564	-0.331723566	-0.30495
O	-0.002478619	0.0102951	-3.050102917	
H	-0.753749252	-0.586623436	-3.04442057	
H	0.766563883	-0.563296791	-3.033980026	

$F_4C\cdots SH_2$ (12)

C	0.006497169	0.045275786	0.208108483	1.22909
F	-0.031830724	-0.085610178	1.518620059	-0.3081
F	0.093559554	-1.151010178	-0.343680219	-0.30899
F	-1.093215688	0.637980886	-0.204052394	-0.30642
F	1.054367427	0.762464375	-0.12998697	-0.30559
S	0.048891691	0.117569191	-3.537373541	
H	-0.974769082	-0.595616115	-3.051091228	
H	0.945269751	-0.790082006	-3.130465161	

$H_4Si\cdots NH_3$ (13)

Si	0.007578572	0.003693818	0.175513998	0.6141
H	0.010167999	0.028267703	1.660281271	-0.15621
H	0.006062172	-1.408805507	-0.251408773	-0.15276
H	-1.20974727	0.699601372	-0.284325479	-0.15257
H	1.224254748	0.698250239	-0.288472287	-0.15256

N	0.001808082	-0.044578489	-2.918668956	
H	-0.811667251	-0.521796416	-3.287414368	
H	0.817288132	-0.516890818	-3.289084749	
H	-0.001323875	0.890851087	-3.306540437	

$H_4Si\cdots PH_3$ (14)

Si	0.002364637	0.06369399	0.487526738	0.61533
H	0.042884853	-0.362573469	-1.903218967	0.15407
H	0.531345353	-1.029519064	-0.357494892	-0.15388
H	-1.394067898	0.350041632	0.100947222	-0.15368
H	0.83213302	1.271875656	0.31194246	-0.1537
P	-0.010429053	0.300806069	-3.169589801	
H	-0.881747598	-0.812382645	-3.134771075	
H	1.139923823	-0.492799352	-3.383762102	
H	-0.217985828	0.539450183	-4.548137298	

$H_4Si\cdots OH_2$ (15)

Si	0.054977948	-0.013597014	0.099437262	0.61496
H	-0.073286643	0.00407851	1.575588733	-0.15556
H	0.172702679	-1.421899594	-0.332119757	-0.15335
H	-1.165435999	0.591601764	-0.47288674	-0.15327
H	1.251870678	0.754640423	-0.285741644	-0.15278
O	0.232960729	-0.108138896	-2.956871782	
H	-0.648788038	0.190398348	-3.190555076	
H	0.223768747	-1.056111771	-3.106771968	

$H_4Si\cdots SH_2$ (16)

Si	0.0043589859	0.0517472144	0.2601421495	0.61533
H	0.033906949	-0.065839285	1.735032745	-0.15446
H	-0.002581032	-1.306029449	-0.324707023	-0.15391
H	-1.21601722	0.776698141	-0.145086834	-0.15346
H	1.205027259	0.782835204	-0.191992852	-0.1535
S	-0.034919041	0.177572928	-3.418703085	
H	-0.934617233	-0.80782563	-3.306213861	
H	0.993611442	-0.668187363	-3.278392211	

$FH_3Si\cdots NH_3$ (17)

Si	0.00814523	-0.000696428	-0.107973772	1.2833
F	0.011989475	0.024681523	1.517233352	-0.65565

H	0.008140635	-1.436882427	-0.430653538	-0.20937
H	-1.232373473	0.708936608	-0.461422341	-0.20914
H	1.246394181	0.709850478	-0.467575633	-0.20915
N	0.001364523	-0.040433938	-2.681762397	
H	-0.815577558	-0.517963008	-3.043161397	
H	0.81735368	-0.515651179	-3.048590532	
H	-0.001015383	0.89675136	-3.066213523	

$FH_3Si\cdots PH_3$

(18)

Si	0.007122203	0.019980614	0.432527619	1.29384
F	0.001420467	0.056058109	2.041893088	-0.64656
H	0.011139378	-1.395106521	0.025467485	-0.2159
H	-1.209804249	0.710534548	-0.026734052	-0.21571
H	1.224418355	0.71536749	-0.018629633	-0.21567
P	0.006677784	-0.059364131	-2.997954368	
H	-1.033695811	-0.672937741	-3.730459415	
H	1.038486286	-0.668865229	-3.745575803	
H	-0.001343102	1.122925841	-3.770654689	

$FH_3Si\cdots OH_2$

(19)

Atom	X (Å)	Y (Å)	Z (Å)	Q
Si	0.008094017	-0.007019737	-0.012248486	1.29156
F	0.008314735	0.057809865	1.601501053	-0.64963
H	0.008687697	-1.439463502	-0.355565109	-0.21455
H	-1.219735115	0.674587436	-0.449009813	-0.2137
H	1.235052225	0.67602573	-0.449476574	-0.21368
O	0.004517258	-0.04851314	-2.747786176	
H	-0.762772231	-0.485038039	-3.124895913	
H	0.766611504	-0.487416854	-3.132439953	

$FH_3Si\cdots SH_2$

(20)

F	0.035763871	-0.03694473	1.793817326	-0.64672
H	0.057389307	-1.34596957	-0.314410395	-0.21597
H	-1.224706016	0.720525472	-0.208534608	-0.21557
H	1.211057243	0.795983683	-0.230306099	-0.21555
S	-0.01729449	0.197930843	-3.196720249	
H	-0.984181283	-0.717406488	-3.341132764	
H	0.951671739	-0.712179589	-3.358575195	

$F_3HSi\cdots NH_3$

(21)

Si	0.00834929	-0.024548628	-0.320328908	2.23526
H	0.012298788	-0.032425099	1.14816161	-0.33777
F	0.002578366	-1.613287147	-0.583052778	-0.63244
F	-1.367689501	0.776224256	-0.565394386	-0.63252
F	1.38807844	0.767272273	-0.573075712	-0.63252
N	0.001391059	-0.012551499	-2.45621737	
H	-0.819682178	-0.489115488	-2.812288991	
H	0.823931962	-0.481147075	-2.819376121	
H	-0.004834907	0.938171407	-2.808547113	

$F_3HSi\cdots PH_3$

(22)

Si	0.014619001	0.01507273	0.584673373	2.21454
H	-0.006524168	-0.001240703	2.038635326	-0.28826
F	0.021471709	-1.462807043	0.03434322	-0.64211
F	-1.262450531	0.76321609	0.040539687	-0.64212
F	1.307094372	0.761667903	0.076804315	-0.64206
P	0.014323451	-0.018348188	-3.074383186	
H	-1.044715946	-0.671127123	-3.745122161	
H	1.019377486	-0.670632438	-3.82421585	
H	-0.018774053	1.112791772	-3.921394505	

$F_3HSi\cdots OH_2$

(23)

Si	0.051471042	0.000384685	0.035898887	2.21903
H	-0.110733919	0.055872485	1.481448662	-0.29583
F	0.042966103	-1.519690984	-0.400640409	-0.64154
F	-1.170749441	0.75675717	-0.624191978	-0.64159
F	1.413322706	0.68820943	-0.346324306	-0.64007
O	0.256376062	-0.163854199	-2.807050511	
H	-0.579967288	0.23127351	-3.065318604	
H	0.146084845	-1.107980336	-2.943742712	

$F_3HSi\cdots SH_2$

(24)

Si	0.052702322	0.034390185	0.23852833	2.21445
H	-0.032805553	-0.10034766	1.68365527	-0.28794
F	0.729938135	-1.251645497	-0.378682292	-0.64262

F	-1.395810089	0.178763135	-0.371376105	-0.64241
F	0.907983002	1.301585024	-0.135723204	-0.64148
S	0.149986537	0.153175306	-3.371100069	
H	-1.080254557	-0.330212601	-3.155885695	
H	0.717030313	-1.044736122	-3.179337206	

$F_4Si\cdots NH_3$ (25)

Si	0.007775973	-0.009264025	-0.370245591	2.52454
F	0.012572297	0.007788598	1.229996463	-0.66858
F	0.006205247	-1.59556705	-0.561788372	-0.61859
F	-1.364334636	0.781333344	-0.584420245	-0.61868
F	1.379654969	0.779483387	-0.592651096	-0.61869
N	0.001491645	-0.031667051	-2.458379456	
H	-0.821795142	-0.508476667	-2.810825826	
H	0.822211776	-0.509117135	-2.815859978	
H	0.000639202	0.914079589	-2.825945679	

$F_4Si\cdots PH_3$ (26)

Si	0.013653219	0.005957312	0.502511699	2.53656
F	0.030433103	0.028473936	2.070508684	-0.63819
F	0.042456569	-1.489150204	0.040391853	-0.63276
F	-1.296723611	0.714914005	0.022384562	-0.63279
F	1.280562367	0.772018031	-0.006149798	-0.63283
P	-0.010748777	-0.044609652	-3.040924723	
H	-1.05978528	-0.616540596	-3.794262261	
H	1.01036778	-0.684238228	-3.77816906	
H	0.034205971	1.141768395	-3.806410736	

$F_4Si\cdots OH_2$ (27)

Si	0.054079217	-0.020281907	-0.043430669	2.53573
F	-0.086976247	0.036074395	1.523827409	-0.64472
F	0.010816796	-1.546113983	-0.412904473	-0.63068
F	-1.179521516	0.774247087	-0.60352446	-0.63066
F	1.42328711	0.653549467	-0.382426424	-0.62967
O	0.214946087	-0.155637523	-2.698194725	
H	-0.552544215	0.274696436	-3.083348944	
H	0.164682867	-1.075562222	-2.969918682	

$F_4Si\cdots SH_2$ (28)

Si	0.044301541	0.012306371	0.21239625	2.5366

F	-0.155725011	-0.042287499	1.766761024	-0.63834
F	0.151002492	-1.460480107	-0.311007572	-0.63311
F	-1.202769514	0.728244841	-0.408430409	-0.6329
F	1.357606167	0.807811198	-0.08159308	-0.63226
S	0.376540965	0.077731737	-3.249006366	
H	-0.960134991	0.077727811	-3.332408626	
H	0.437948451	-1.260082601	-3.266632181	

$H_4Ge\cdots NH_3$ (29)

Ge	0.006734507	0.00266288	0.21358668	0.56019
H	0.009723982	0.027542271	1.764298737	-0.14302
H	0.006211828	-1.468744312	-0.236552879	-0.13906
H	-1.26242486	0.726326482	-0.269222613	-0.13907
H	1.273426288	0.727298122	-0.274528369	-0.13904
N	0.003924623	-0.043385082	-2.964938443	
H	-0.811313482	-0.518911456	-3.331826341	
H	0.817393247	-0.516419023	-3.338818733	
H	0.000745189	0.89222311	-3.352117829	

$H_4Ge\cdots PH_3$ (30)

Ge	0.003170395	0.06389318	0.500260378	0.56104
H	0.04583377	-0.393275191	1.972940378	-0.14047
H	0.56255344	-1.065253162	-0.390718187	-0.14058
H	-1.453861553	0.356049102	0.095723608	-0.14013
H	0.860970427	1.329939597	0.327605533	-0.13986
P	-0.006571906	0.311543518	-3.195622164	
H	-0.890170068	-0.790759459	-3.131405274	
H	1.134867397	-0.500180766	-3.38910919	
H	-0.212370591	0.516636182	-4.579794861	

$H_4Ge\cdots OH_2$ (31)

Ge	0.05657108	-0.010803516	0.116389672	0.56077
H	-0.07962364	0.004459096	1.657191392	-0.14226
H	0.175344633	-1.478901555	-0.33798607	-0.13984
H	-1.214149512	0.623344333	-0.48235567	-0.13979
H	1.306137602	0.786950386	-0.28503457	-0.13888
O	0.231319067	-0.107366393	-2.991259253	
H	-0.65661777	0.180122976	-3.215207896	

H	0.22978864	-1.056833557	-3.131658575	

$H_4Ge\cdots SH_2$ (32)

Ge	0.056811695	0.006424743	0.290735392	0.56107
H	0.083082362	-0.170139136	1.824406285	-0.14096
H	0.045400901	-1.387396345	-0.368810037	-0.14037
H	-1.213678299	0.778851379	-0.109098898	-0.1399
H	1.31093989	0.78063024	-0.153112487	-0.13984
S	-0.030403258	0.250980017	-3.445356839	
H	-1.048144657	-0.606186691	-3.294986347	
H	0.879597163	-0.728412238	-3.369333246	

$FH_3Ge\cdots NH_3$ (33)

Ge	0.008057691	-0.000928108	-0.055334966	1.22897
F	0.0139963	0.027904662	1.706024338	-0.66934
H	0.005984414	-1.502752454	-0.371923573	-0.18656
H	-1.288538358	0.742916605	-0.40441249	-0.18653
H	1.303456278	0.740938435	-0.412750178	-0.18654
N	0.000480471	-0.041874252	-2.782313726	
H	-0.813370556	-0.519380706	-3.150838993	
H	0.817464238	-0.513508675	-3.151546002	
H	-0.003109167	0.895277484	-3.167024191	

$FH_3Ge\cdots PH_3$ (34)

Ge	0.00899567	0.005107741	0.420083918	1.23778
F	0.01615631	0.034511424	2.166775836	-0.66267
H	-0.002513237	-1.481544236	0.033370114	-0.1917
H	-1.269435913	0.746893064	0.001138865	-0.1917
H	1.29398126	0.729492155	-0.008545655	-0.19171
P	8.95694E-05	-0.045322617	-3.039179632	
H	-1.032279115	-0.661506781	-3.779851958	
H	1.041347591	-0.642744508	-3.783175954	
H	-0.011920827	1.143706737	-3.800735294	

$FH_3Ge\cdots OH_2$ (35)

Ge	0.006382656	-0.015606568	-0.021968043	1.2342
F	0.005164941	0.082581651	1.728541257	-0.66589
H	0.003855136	-1.52491481	-0.308676317	-0.18994

H	-1.283198822	0.700883473	-0.443149	-0.1892
H	1.299303151	0.696376531	-0.441067869	-0.18918
O	0.006125804	-0.079553771	-2.769833979	
H	-0.759941587	-0.460826824	-3.204744269	
H	0.771078811	-0.457967924	-3.20902275	

$FH_3Ge\cdots SH_2$

(36)

Ge	0.01573037	0.039087569	0.17217163	1.23776
F	0.024538815	-0.037478017	1.91732801	-0.66288
H	0.024312391	-1.424161472	-0.297674806	-0.19186
H	-1.274597069	0.783870373	-0.200490348	-0.19151
H	1.29146478	0.802704502	-0.212407137	-0.19151
S	-0.003754288	0.197760779	-3.23050085	
H	-0.982566058	-0.69940662	-3.406926035	
H	0.953641149	-0.721405364	-3.411421433	

$F_3HGe\cdots NH_3$

(37)

Ge	0.009615512	-0.003739394	-0.301098154	2.20339
H	0.016784491	0.020178154	1.232398278	-0.28087
F	0.004687828	-1.725841001	-0.576334034	-0.64086
F	-1.477690393	0.852764972	-0.610560168	-0.64084
F	1.497624814	0.84653817	-0.62459317	-0.64083
N	-0.000440392	-0.036994515	-2.464939599	
H	-0.824366208	-0.520258819	-2.804929336	
H	0.823938358	-0.513985362	-2.812573598	
H	-0.005732691	0.909930803	-2.82748999	

$F_3HGe\cdots PH_3$

(38)

Ge	0.013831861	0.009099088	0.552041539	2.20197
H	0.043811127	0.044753266	2.071580183	-0.24325
F	0.005694375	-1.602070894	-0.007985164	-0.65291
F	-1.381457299	0.793147245	-0.038035252	-0.65286
F	1.384363352	0.79589108	-0.0913629	-0.65296
P	-0.021316944	-0.055780028	-3.002969587	
H	-1.033410043	-0.650734106	-3.789332928	
H	1.034699393	-0.647769254	-3.731790001	
H	-0.001794503	1.142056615	-3.752265671	

$F_3HGe\cdots OH_2$
(39)

Ge	0.062043751	-0.009623268	-0.055954976	2.20835
H	-0.092597726	0.028631884	1.46047196	-0.25862
F	0.116917854	-1.667688126	-0.497883778	-0.65044
F	-1.324567528	0.766179581	-0.706439826	-0.65042
F	1.503695992	0.810741667	-0.447250925	-0.64887
O	0.218622575	-0.138384308	-2.64201728	
H	-0.615142575	0.230479827	-2.94648763	
H	0.179797776	-1.079365496	-2.834358505	

$F_3HGe\cdots SH_2$
(40)

Ge	0.043298714	0.01210938	0.244818214	2.20143
H	-0.033151939	-0.149181394	1.754170908	-0.24242
F	1.00143432	-1.223053715	-0.443264504	-0.65343
F	-1.512971922	-0.099054203	-0.449405451	-0.65334
F	0.71970328	1.516973413	-0.173318687	-0.65223
S	0.14970845	0.201125212	-3.299094096	
H	-1.070560161	-0.331938824	-3.155452034	
H	0.751309378	-0.986008098	-3.148375301	

$F_4Ge\cdots NH_3$ (41)

Ge	0.011819125	-0.00527125	-0.363051176	2.53001
F	0.024397101	0.018627445	1.353578182	-0.67004
F	0.007303373	-1.7143129	-0.562182506	-0.61999
F	-1.465738292	0.84741224	-0.5875105	-0.61998
F	1.489408885	0.841485444	-0.609104632	-0.62
N	-0.003726072	-0.03620297	-2.490213443	
H	-0.826151972	-0.523423677	-2.830805093	
H	0.82130242	-0.509730918	-2.843712234	
H	-0.014193238	0.910009587	-2.857118378	

$F_4Ge\cdots PH_3$ (42)

Ge	0.011448199	0.0021915	0.31660288	2.55435
F	0.037351463	0.038736582	2.012513876	-0.65044
F	0.006048287	-1.640319193	-0.093109542	-0.63462
F	-1.409585486	0.809776844	-0.124696159	-0.63462
F	1.419112859	0.809782824	-0.166614245	-0.63467
P	-0.012039704	-0.048596568	-2.886146392	

H	-1.046498139	-0.651749161	-3.629957707	
H	1.042574384	-0.649515947	-3.603651789	
H	-0.003990524	1.15828612	-3.615060703	

$F_4Ge\cdots OH_2$ (43)

Ge	0.049031015	-0.006165811	-0.270671209	2.54264
F	-0.006675245	-0.065045185	1.435744204	-0.66326
F	1.050173833	-1.359223983	-0.576039028	-0.62633
F	-1.618441664	-0.156867998	-0.621234047	-0.62626
F	0.743479394	1.52024723	-0.527776551	-0.62679
O	0.06648235	-0.046448246	-2.485579993	
H	-0.829364437	-0.15761289	-2.822360656	
H	0.594084854	-0.787911358	-2.802003692	

$F_4Ge\cdots SH_2$ (44)

Ge	0.010733926	0.041323334	0.084981911	2.55464
F	0.023028968	-0.037366355	1.779097595	-0.65016
F	0.001796609	-1.570147102	-0.438111237	-0.63553
F	-1.409257168	0.869379743	-0.315876414	-0.63447
F	1.43007873	0.860504457	-0.336217008	-0.63448
S	-0.005841923	0.203652658	-3.060925777	
H	-0.969226053	-0.718984162	-3.187799166	
H	0.967457013	-0.707390812	-3.195070864	

$H_4Sn\cdots NH_3$ (45)

Sn	0.010677884	0.004179051	0.154730015	0.82619
H	0.001715882	0.0196364	1.890093653	-0.21484
H	0.013480421	-1.644148091	-0.321739448	-0.20384
H	-1.411817629	0.819391877	-0.35119931	-0.20381
H	1.43592884	0.822779839	-0.337344228	-0.2037
N	0.005608238	-0.039410481	-2.925468679	
H	-0.818176362	-0.521495867	-3.264634076	
H	0.811268631	-0.521717277	-3.30519045	
H	-0.004264585	0.889377548	-3.329367267	

$H_4Sn\cdots PH_3$ (46)

Sn	0.0204982	0.017460169	0.634066564	0.82876
H	-0.071078497	-0.050747525	2.352657177	-0.20897
H	0.053992843	-1.585029049	0.019497996	-0.2068
H	-1.36114803	0.842902762	0.038425401	-0.20667

H	1.44972328	0.853061657	0.186106436	-0.20632
P	0.068069436	0.021872222	-3.198681431	
H	-1.058069269	-0.663738379	-3.708229682	
H	0.987364517	-0.696762684	-3.996179984	
H	-0.044931171	1.089573837	-4.117782256	

$H_4Sn\cdots OH_2$ (47)

Sn	0.065918857	0.005123926	0.097095075	0.82743
H	-0.088443033	0.051253035	1.818303625	-0.2126
H	0.130906646	-1.650048871	-0.360871978	-0.2055
H	-1.33029803	0.763332337	-0.557357919	-0.20545
H	1.498327812	0.836472912	-0.331911794	-0.20388
O	0.20694877	-0.157735597	-2.933705205	
H	-0.629398372	0.186682697	-3.255901039	
H	0.19480745	-1.094108659	-3.145575173	

$H_4Sn\cdots SH_2$ (48)

Sn	0.001489204	0.051216517	0.30926191	0.82866
H	0.028613626	-0.069740873	2.027248206	-0.20926
H	-0.001981136	-1.536740675	-0.3467555	-0.20713
H	-1.418450037	0.886736187	-0.165932619	-0.20607
H	1.401948022	0.895418731	-0.208500785	-0.2062
S	-0.021173333	0.18792828	-3.442191991	
H	-0.936080652	-0.789961887	-3.440537138	
H	0.994404415	-0.683884498	-3.402513053	

$FH_3Sn\cdots NH_3$ (49)

Sn	0.009064126	-0.000619927	-0.113553498	1.42189
F	0.015238195	0.026929847	1.846903167	-0.72105
H	0.007604598	-1.690192297	-0.381516291	-0.23362
H	-1.451800285	0.837956635	-0.413247048	-0.23364
H	1.467609419	0.837949504	-0.422479962	-0.23358
N	0.000369192	-0.041216	-2.797166449	
H	-0.816293973	-0.520795673	-3.158161343	
H	0.816511537	-0.516337441	-3.165269949	
H	-0.003881499	0.894918341	-3.185628407	

$FH_3Sn\cdots PH_3$ (50)

Sn	0.015393887	0.010820804	0.37611441	1.43706
F	0.018946636	0.042652912	2.320630623	-0.71345
H	0.010745343	-1.659979024	0.019012474	-0.2412
H	-1.424953773	0.840020821	-0.020949447	-0.24121
H	1.458080329	0.833398025	-0.026694836	-0.2412
P	-0.00196358	-0.049335888	-3.060092133	
H	-1.047139683	-0.670402088	-3.776097331	
H	1.034121164	-0.656952587	-3.800450595	
H	-0.018809013	1.138370005	-3.821592926	

$FH_3Sn\cdots OH_2$

(51)

Sn	0.006892492	-0.030846192	-0.065368341	1.43074
F	0.008865813	0.108787377	1.880778869	-0.71695
H	0.003387068	-1.727043801	-0.283552975	-0.23916
H	-1.448073885	0.768825972	-0.464971601	-0.23732
H	1.464249837	0.763226119	-0.467455963	-0.23731
O	0.004790186	-0.101232485	-2.770558348	
H	-0.764345372	-0.420329053	-3.248696896	
H	0.773003951	-0.420416187	-3.250095715	

$FH_3Sn\cdots SH_2$

(52)

Sn	0.010062892	0.047353869	0.130652041	1.43724
F	0.01696887	-0.020738564	2.073400458	-0.7135
H	-0.021938908	-1.605020261	-0.308306802	-0.24169
H	-1.419283796	0.913310032	-0.221528701	-0.241
H	1.467835419	0.860041002	-0.233856775	-0.24104
S	-0.005742145	0.187497727	-3.252316441	
H	-0.968435453	-0.727859497	-3.426061428	
H	0.96930321	-0.713612771	-3.431903322	

$F_3HSn\cdots NH_3$

(53)

Sn	-0.012161882	-0.007818426	-0.245580645	2.36268
H	-0.038299806	0.008676286	1.452648071	-0.30089
F	0.013739818	-1.912854067	-0.608173795	-0.68735
F	-1.664036312	0.918167661	-0.662378355	-0.68723
F	1.63195423	0.953484899	-0.611417833	-0.68722
N	0.024077343	-0.030015745	-2.526398525	
H	0.034392494	-0.990624165	-2.852985691	

H	0.856344851	0.448827579	-2.854384055	
H	-0.801589405	0.440748988	-2.881448944	

$F_3HSn\cdots PH_3$ (54)

Sn	0.014043721	0.008679637	0.163187541	2.36753
H	0.026183566	0.025035591	1.859257716	-0.29421
F	0.012566488	-1.860371548	-0.295588315	-0.69108
F	-1.60465469	0.93471053	-0.310694327	-0.69113
F	1.623027103	0.939704189	-0.333672609	-0.69111
P	-0.003893913	-0.039118556	-2.707662511	
H	-1.071612387	-0.67395679	-3.364127845	
H	1.056208164	-0.674570054	-3.375533562	
H	-0.007446721	1.168480011	-3.425285869	

$F_3HSn\cdots OH_2$ (55)

Sn	0.107097759	-0.029410591	-0.191653341	2.36823
H	-0.077026138	-0.044113748	1.49523304	-0.29625
F	0.14216231	-1.909734718	-0.638048878	-0.69074
F	-1.448715357	0.950909821	-0.78653695	-0.69077
F	1.758208653	0.871898307	-0.516593036	-0.69048
O	0.140202664	-0.132075602	-2.495603586	
H	-0.665221905	0.300087731	-2.804967802	
H	0.092062134	-1.06658944	-2.731750408	

$F_3HSn\cdots SH_2$ (56)

Sn	0.013028814	0.034099042	0.027512705	2.36962
H	0.021257162	-0.028967542	1.721470951	-0.29183
F	-0.003084579	-1.786919549	-0.574618977	-0.69346
F	-1.60705925	0.947670959	-0.434663473	-0.69215
F	1.641026287	0.925010205	-0.450539913	-0.69217
S	0.001021414	0.226922861	-2.891431037	
H	-0.978118306	-0.678623937	-3.030262078	
H	0.960698589	-0.698220281	-3.037389147	

$F_4Sn\cdots NH_3$ (57)

Sn	0.012582628	-0.004284574	-0.305476394	2.68977
F	0.027237326	0.021017614	1.591557506	-0.70229
F	0.407297896	-1.857198661	-0.562630598	-0.66249

F	-1.789835414	0.571508033	-0.578404466	-0.66254
F	1.411443715	1.262149911	-0.612190812	-0.66245
N	-0.004130022	-0.037106346	-2.572852356	
H	-0.914574268	0.255347826	-2.914544206	
H	0.189295493	-0.977548657	-2.903605513	
H	0.705103975	0.594707855	-2.931972942	

$F_4Sn\cdots PH_3$ (58)

Sn	0.012553091	0.002103782	0.035038262	2.69563
F	0.018888102	0.037431727	1.928985564	-0.69968
F	0.016950399	-1.883001962	-0.25086723	-0.66535
F	-1.618738393	0.931079022	-0.300568198	-0.66528
F	1.636926692	0.938628615	-0.312279942	-0.66532
P	-0.001801536	-0.043870257	-2.73353818	
H	-1.083671178	-0.668721499	-3.370573394	
H	1.066532784	-0.675026958	-3.386703629	
H	-0.003218622	1.18997053	-3.399613033	

$F_4Sn\cdots OH_2$ (59)

Sn	-0.084977969	-0.020619629	-0.261814894	2.69987
F	0.124347378	-0.015784926	1.620760377	-0.69869
F	-0.165172963	-1.900210409	-0.572366968	-0.6663
F	-1.708903917	0.923737334	-0.466499259	-0.66848
F	1.494574832	0.919807944	-0.766917897	-0.6664
O	-0.127255834	-0.155411385	-2.523123296	
H	-0.137224489	-1.07996845	-2.800294434	
H	0.653383071	0.26942128	-2.899664599	

$F_4Sn\cdots SH_2$ (60)

Sn	0.011605885	0.043220401	-0.107499646	2.70061
F	0.017759108	-0.021758771	1.784033717	-0.69813
F	0.008441215	-1.81024533	-0.53672845	-0.66945
F	-1.631112664	0.94721752	-0.416370636	-0.66651
F	1.654123251	0.943181799	-0.427688826	-0.66653
S	0.000961337	0.221002956	-2.884593407	
H	-0.97919956	-0.683637938	-3.035920723	
H	0.966191547	-0.698008877	-3.045152999	

4) The xyz coordinates of all complexes optimized at BLW(M062x-D3)/cc-pVTZ level of theory (in Å)

$FH_3C\cdots NH_3$ (1)

C	6.0	0.0051247809	0.0040219388	0.1783189374
F	9.0	0.0054964676	0.0251788158	1.5595883935
H	1.0	0.0063109490	-1.0279781587	-0.1653317749
H	1.0	-0.8846227164	0.5107009969	-0.1889403162
H	1.0	0.8936797490	0.5126661544	-0.1891849906
N	7.0	0.0046770874	-0.0452593820	-2.9562595102
H	1.0	-0.8064528477	-0.5182698098	-3.3362423825
H	1.0	0.8156646318	-0.5182015207	-3.3366356264
H	1.0	0.0045431985	0.8857339552	-3.3554325101

$FH_3C\cdots PH_3$ (2)

C	6.0	0.0264820443	-0.0005367868	0.6155029101
F	9.0	0.0432850598	0.0146253957	1.9936286621
H	1.0	0.0091348155	-1.0326925415	0.2694904348
H	1.0	-0.8617959877	0.5209342101	0.2628083586
H	1.0	0.9190842872	0.4981857148	0.2414573759
P	15.0	-0.0174833788	-0.0395572303	-3.2220067461
H	1.0	-1.2117744999	-0.1361202294	-3.9720109706
H	1.0	0.6484952938	-1.0263498660	-3.9840481120
H	1.0	0.4889936759	1.0301043036	-3.9949416827

$FH_3C\cdots OH_2$ (3)

C	6.0	0.0247594658	0.0069945150	0.2191217658
F	9.0	-0.0253090835	-0.0600612563	1.5977256659
H	1.0	-0.0170781580	-0.9994676455	-0.1911213326
H	1.0	-0.8227825431	0.5856920114	-0.1421825303
H	1.0	0.9512941382	0.4905917702	-0.0827248141
O	8.0	0.1601502991	0.1192508935	-2.7554506681
H	1.0	-0.5152864944	0.4105851466	-3.3710595826
H	1.0	0.8991420658	-0.1451754648	-3.3068759044

$FH_3C\cdots SH_2$ (4)

C	6.0	0.0044784593	0.0667709650	0.3213273979
F	9.0	0.0179186660	0.0922884665	1.6994187445
H	1.0	0.0453773526	-0.9668553658	-0.0182137453
H	1.0	-0.9109017543	0.5356234012	-0.0362273009
H	1.0	0.8682260812	0.6123890058	-0.0551869599

S	16.0	-0.0220635396	-0.0702923578	-3.3606137830
H	1.0	-0.9434412135	-1.0040141973	-3.6283089788
H	1.0	0.9882709085	-0.9024550574	-3.6419551646

$F_3HC\cdots NH_3$ (5)

C	6.0	0.0140182305	0.0423295318	0.3037817492
H	1.0	-0.0760432907	-0.1130864525	1.3772461674
F	9.0	0.1447400191	-1.1305983527	-0.3197185374
F	9.0	-1.0743301216	0.6464888475	-0.1678166098
F	9.0	1.0739690888	0.7897695272	0.0287230209
N	7.0	0.1065296474	0.1087967138	-3.0984962991
H	1.0	-0.8544533011	-0.0740658692	-2.8365545293
H	1.0	0.6058255949	-0.7652235988	-2.9896729815
H	1.0	0.1041654527	0.3241826628	-4.0876117603

$F_3HC\cdots PH_3$ (6)

C	6.0	0.0126341866	-0.0962008597	0.5690364400
H	1.0	0.4086560357	-0.2169844178	1.5750174106
F	9.0	-0.4204439833	-1.2617031955	0.0942258141
F	9.0	-1.0004461577	0.7639641650	0.5640511789
F	9.0	0.9579411597	0.3630917908	-0.2509465002
P	15.0	-0.4616093424	0.2393181602	-3.3265393043
H	1.0	-0.3879357152	-0.0199536455	-4.7154529520
H	1.0	0.2124887450	-0.9542439964	-2.9792682151
H	1.0	0.7231363915	1.0113050188	-3.3202436520

$F_3HC\cdots OH_2$ (7)

C	6.0	0.0410981503	0.0068014527	0.1601882910
H	1.0	-0.1600990092	-0.0176945320	1.2284397867
F	9.0	0.1736847198	-1.2318202580	-0.3183118649
F	9.0	-0.9660326473	0.5923395486	-0.4908004113
F	9.0	1.1546085073	0.6782625219	-0.0980754907
O	8.0	0.1356465880	-0.2699640310	-3.3730784853
H	1.0	-0.5598736509	0.2366159782	-2.9497772433
H	1.0	0.2297374520	-1.0535689104	-2.8285055522

$F_3HC\cdots SH_2$ (8)

C	6.0	-0.0309259564	0.0212252916	0.2729370093
H	1.0	-0.0128035345	-0.0646033138	1.3570022334
F	9.0	0.3623010773	-1.1214092879	-0.2919874528
F	9.0	-1.2609538843	0.2937529356	-0.1553380127

F	9.0	0.7828592831	0.9893191906	-0.1361177502
S	16.0	0.0242376443	-0.1209446788	-3.7920633922
H	1.0	-0.8676207009	-0.6358582966	-2.9364714805
H	1.0	1.0516761812	-0.4205100806	-2.9878821243

$F_4C\cdots NH_3$ (9)

C	6.0	-0.0124249873	-0.0151810285	0.2551099758
F	9.0	-0.0254320538	-0.0087891281	1.5790569737
F	9.0	-1.0716191969	-0.6630501862	-0.1765821318
F	9.0	-0.0358789795	1.2266935023	-0.1753599993
F	9.0	1.0826730516	-0.6152399326	-0.1557977324
N	7.0	0.0221728162	-0.0253287001	-2.9919721507
H	1.0	-0.8042138300	-0.4544055833	-3.3903832344
H	1.0	0.8177558518	-0.5291995623	-3.3645380420
H	1.0	0.0713886579	0.9130936087	-3.3696534289

$F_4C\cdots PH_3$ (10)

C	6.0	-0.0288771520	-0.0601054666	0.5534188774
F	9.0	0.3861688178	-0.2194501359	1.7932923735
F	9.0	-0.5036508876	-1.2014302340	0.1005808588
F	9.0	-0.9714414943	0.8556610658	0.5197614954
F	9.0	0.9841281835	0.3219124659	-0.1994280089
P	15.0	-0.3837508469	0.1925052433	-3.2937043166
H	1.0	-0.5706373562	-0.0593649672	-4.6724987572
H	1.0	0.3660219044	-0.9893091998	-3.0885182309
H	1.0	0.7664601714	0.9881742288	-3.5030240714

$F_4C\cdots OH_2$ (11)

C	6.0	0.0076559460	0.0096305658	0.1872127712
F	9.0	0.0136623405	0.1275888050	1.5050315068
F	9.0	0.0050700105	-1.2684529367	-0.1257563299
F	9.0	-1.0713456842	0.5898445946	-0.2885840229
F	9.0	1.0836464946	0.5877505534	-0.2981656950
O	8.0	-0.0011065973	-0.1632371509	-2.8864047460
H	1.0	-0.7555961543	-0.4855693207	-3.3829438646
H	1.0	0.7667837442	-0.4565833504	-3.3803105898

$F_4C\cdots SH_2$ (12)

C	6.0	0.0090170611	0.0618757044	0.3007133799
F	9.0	-0.0307519842	-0.0458983287	1.6141634719
F	9.0	0.1070316164	-1.1413617935	-0.2293998735

F	9.0	-1.0943094254	0.6401389685	-0.1224454055
F	9.0	1.0516530696	0.7831458083	-0.0465618137
S	16.0	0.0647048852	0.1488195906	-3.5244142911
H	1.0	-0.9891975459	-0.6462947745	-3.3007119349
H	1.0	0.9306224232	-0.8594534152	-3.3612645030

$H_4Si\cdots NH_3$ (13)

SI	14.0	0.0076802470	0.0046537643	0.2253385950
H	1.0	0.0101154870	0.0282650409	1.7078640025
H	1.0	0.0063521497	-1.4041936473	-0.2139350987
H	1.0	-1.2069148854	0.6987174057	-0.2449921089
H	1.0	1.2211356492	0.6975741191	-0.2495495672
N	7.0	0.0018988415	-0.0451819812	-2.9663955786
H	1.0	-0.8094808959	-0.5212617949	-3.3417055652
H	1.0	0.8146992516	-0.5169284881	-3.3441449853
H	1.0	-0.0010645347	0.8869485715	-3.3625994736

$H_4Si\cdots PH_3$ (14)

SI	14.0	0.0041429169	0.0609849731	0.5897072680
H	1.0	-0.0003404885	-0.2912178954	2.0253876984
H	1.0	0.5666733448	-1.0677001100	-0.1828150095
H	1.0	-1.3799182753	0.3185605025	0.1424598493
H	1.0	0.8312137660	1.2657609528	0.3789200321
P	15.0	0.0195323109	0.2744436855	-3.2662828420
H	1.0	-0.8757090928	-0.8204689398	-3.2637579439
H	1.0	1.1353164445	-0.5264904274	-3.6029863894
H	1.0	-0.2564896165	0.6147202585	-4.6107524431

$H_4Si\cdots OH_2$ (15)

SI	14.0	0.0466972191	-0.0142842679	0.1766201617
H	1.0	-0.0200343072	0.0495225544	1.6553172663
H	1.0	0.1517405569	-1.4321866454	-0.2224695043
H	1.0	-1.1896204058	0.5797220471	-0.3706655149
H	1.0	1.2291405766	0.7402007562	-0.2789466929
O	8.0	0.1373290631	-0.1740077686	-2.9098404824
H	1.0	-0.5859964558	0.2214710423	-3.4000989215
H	1.0	0.2795138531	-1.0294659480	-3.3198372820

$H_4Si\cdots SH_2$ (16)

SI	14.0	0.0046844934	0.0582387915	0.3287751047
H	1.0	0.0283991791	-0.0371677921	1.8043903881

H	1.0	0.0024420342	-1.3061570252	-0.2402112715
H	1.0	-1.2146032483	0.7755587248	-0.0945510484
H	1.0	1.2043103582	0.7859946858	-0.1318450540
S	16.0	-0.0335226225	0.1705843307	-3.4711060273
H	1.0	-0.9360367528	-0.8180016489	-3.4377042680
H	1.0	0.9930966687	-0.6880783065	-3.4276687935

$FH_3Si\cdots NH_3$ (17)

SI	14.0	0.0086238528	0.0022261798	0.0761364349
F	9.0	0.0125887739	0.0269442097	1.6908059992
H	1.0	0.0082572041	-1.4164476416	-0.3125249569
H	1.0	-1.2159467457	0.7019346376	-0.3420260204
H	1.0	1.2304872642	0.7025483013	-0.3487257599
N	7.0	0.0007852468	-0.0428030228	-2.8498554881
H	1.0	-0.8112322048	-0.5183833403	-3.2251447595
H	1.0	0.8124787580	-0.5156692902	-3.2293322077
H	1.0	-0.0016208394	0.8882429566	-3.2494530217

$FH_3Si\cdots PH_3$ (18)

SI	14.0	0.0065123214	0.0222563702	0.5468131437
F	9.0	0.0064786605	0.0597531933	2.1538392869
H	1.0	0.0057924846	-1.3906932553	0.1312560434
H	1.0	-1.2078729643	0.7135707404	0.0810619763
H	1.0	1.2216946226	0.7123866585	0.0813633988
P	15.0	0.0043590205	-0.0617589911	-3.1289795612
H	1.0	-1.0278722178	-0.6777220135	-3.8715997547
H	1.0	1.0392805364	-0.6667217085	-3.8768683425
H	1.0	-0.0039511538	1.1175219859	-3.9070059607

$FH_3Si\cdots OH_2$ (19)

SI	14.0	0.0079155368	-0.0181054837	0.0789769844
F	9.0	0.0103046003	0.1417708769	1.6840130798
H	1.0	0.0076905932	-1.4626525862	-0.2011624967
H	1.0	-1.2143264015	0.6393375309	-0.4098845334
H	1.0	1.2284725854	0.6394880148	-0.4138626996
O	8.0	0.0033795612	-0.2229468651	-2.7657593360
H	1.0	-0.7614978364	-0.3882146776	-3.3200322982
H	1.0	0.7668314511	-0.3877050500	-3.3222096703

$FH_3Si\cdots SH_2$ (20)

SI	14.0	0.0195651838	0.0455985408	0.2676786983

F	9.0	0.0361188173	-0.0154897059	1.8740556861
H	1.0	0.0554913766	-1.3407783582	-0.2299685722
H	1.0	-1.2205867589	0.7251912407	-0.1429011857
H	1.0	1.2101933884	0.7961291991	-0.1651663128
S	16.0	-0.0199647614	0.1815920756	-3.3021518827
H	1.0	-0.9835025342	-0.7322248472	-3.4739873688
H	1.0	0.9514553783	-0.7190463948	-3.4974800322

$F_3HSi\cdots NH_3$ (21)

SI	14.0	0.0094458283	-0.0274414953	0.1462704672
H	1.0	0.0141327239	-0.0346419932	1.6028201309
F	9.0	0.0045469425	-1.5239261952	-0.3514649146
F	9.0	-1.2875121469	0.7282485366	-0.3383821858
F	9.0	1.3078655921	0.7207783695	-0.3459565039
N	7.0	0.0000695184	-0.0112194820	-2.8408695437
H	1.0	-0.8129022963	-0.4798835430	-3.2217849980
H	1.0	0.8133444002	-0.4741772270	-3.2280776039
H	1.0	-0.0045692422	0.9308560294	-3.2126746178

$F_3HSi\cdots PH_3$ (22)

SI	14.0	0.0132675372	0.0165266660	0.6749822294
H	1.0	0.0008112249	-0.0219530905	2.1282463305
F	9.0	0.0080444961	-1.4481939593	0.0928157193
F	9.0	-1.2580353075	0.7778460653	0.1381809961
F	9.0	1.3030678406	0.7615106954	0.1605574629
P	15.0	0.0157117039	-0.0017386724	-3.1790703000
H	1.0	-1.0358210949	-0.6855573597	-3.8307320478
H	1.0	1.0254117884	-0.6686233913	-3.9100822611
H	1.0	-0.0280368686	1.0987760464	-4.0650179094

$F_3HSi\cdots OH_2$ (23)

SI	14.0	0.0477420711	0.0037551805	0.0973779384
H	1.0	-0.0934132989	0.0713011527	1.5442787375
F	9.0	0.0419057068	-1.5117017557	-0.3454913568
F	9.0	-1.1731287745	0.7502995616	-0.5702090834
F	9.0	1.3992008467	0.6881417431	-0.3252650215
O	8.0	0.2310194024	-0.1847158627	-2.8267777800
H	1.0	-0.5538895171	0.2360193067	-3.1843142618
H	1.0	0.1493336734	-1.1121275662	-3.0595201422

$F_3HSi\cdots SH_2$ (24)

SI	14.0	0.0552348679	0.0425211059	0.3032091374
H	1.0	-0.0336110290	-0.0885058325	1.7481832184
F	9.0	0.7325584432	-1.2399816026	-0.3179742191
F	9.0	-1.3862853117	0.1909433268	-0.3192775387
F	9.0	0.9118809793	1.3063086724	-0.0796851404
S	16.0	0.1445537007	0.1462121043	-3.4242676155
H	1.0	-1.0879127788	-0.3558075796	-3.2742515686
H	1.0	0.7123512385	-1.0607184245	-3.3058572435

$F_4Si\cdots NH_3$ (25)

SI	14.0	0.0091115970	-0.0049360528	0.0668790544
F	9.0	0.0138558019	0.0127742766	1.6407108020
F	9.0	0.0067887215	-1.5128799316	-0.3546454659
F	9.0	-1.2933526533	0.7426990960	-0.3769036701
F	9.0	1.3099274693	0.7408746602	-0.3847634965
N	7.0	0.0003806566	-0.0353148258	-2.8088241404
H	1.0	-0.8135912294	-0.5070219246	-3.1846414739
H	1.0	0.8118360420	-0.5074643548	-3.1894924455
H	1.0	-0.0005350757	0.8998620468	-3.1984389443

$F_4Si\cdots PH_3$ (26)

SI	14.0	0.0144132389	0.0077801424	0.5982171659
F	9.0	0.0270310611	0.0255552874	2.1648285446
F	9.0	0.0180070043	-1.4803494212	0.1168740538
F	9.0	-1.2766169837	0.7375248779	0.1005183957
F	9.0	1.2899503159	0.7499824119	0.0793854226
P	15.0	-0.0077391255	-0.0450055457	-3.1449371226
H	1.0	-1.0438220749	-0.6461233185	-3.8945870739
H	1.0	1.0230820124	-0.6582146935	-3.8919711113
H	1.0	0.0001158914	1.1374432593	-3.9184480545

$F_4Si\cdots OH_2$ (27)

SI	14.0	0.0479718850	-0.0154081299	0.0536175240
F	9.0	-0.0633239173	0.0563660449	1.6195283112
F	9.0	0.0006504147	-1.5313100289	-0.3385357509
F	9.0	-1.1766648902	0.7699139338	-0.5275315289
F	9.0	1.4046156139	0.6453861894	-0.3505117816
O	8.0	0.1659952734	-0.1855520936	-2.7586980967
H	1.0	-0.5261076805	0.2723192520	-3.2401948103
H	1.0	0.1956334011	-1.0707434177	-3.1275948368

$F_4Si\cdots SH_2$ (28)

SI	14.0	0.0485096024	0.0130212679	0.2824296784
F	9.0	-0.1570835037	-0.0276495500	1.8351421644
F	9.0	0.2094048101	-1.4552692350	-0.2356836795
F	9.0	-1.2104318921	0.6778269525	-0.3678374553
F	9.0	1.3326219159	0.8467777887	-0.0312671123
S	16.0	0.4018733594	0.0361967097	-3.3258900693
H	1.0	-0.9256479441	0.1514836326	-3.4600902672
H	1.0	0.3495237518	-1.3014158163	-3.3667242191

$H_4Ge\cdots NH_3$ (29)

GE	32.0	0.0070965950	0.0032675521	0.2446319049
H	1.0	0.0092646372	0.0268093933	1.7927603790
H	1.0	0.0076026501	-1.4650670479	-0.2155641410
H	1.0	-1.2592741534	0.7263323883	-0.2468059178
H	1.0	1.2716877510	0.7274520680	-0.2498436702
N	7.0	0.0024532433	-0.0441875993	-2.9913258222
H	1.0	-0.8096719999	-0.5182727335	-3.3676135424
H	1.0	0.8144522242	-0.5163609152	-3.3703253976
H	1.0	0.0008103728	0.8886198842	-3.3860335825

$H_4Ge\cdots PH_3$ (30)

GE	32.0	0.0033108888	0.0616486187	0.6155226072
H	1.0	0.0006244272	-0.2924441844	2.1162991863
H	1.0	0.5860528732	-1.1238223048	-0.1807206959
H	1.0	-1.4404728158	0.3286688757	0.1499804001
H	1.0	0.8677950113	1.3138100226	0.3821847263
P	15.0	0.0218594619	0.2624682761	-3.2884184549
H	1.0	-0.8704213095	-0.8346276557	-3.3110561444
H	1.0	1.1383483961	-0.5253097226	-3.6524658917
H	1.0	-0.2626756231	0.6382010744	-4.6214455132

$H_4Ge\cdots OH_2$ (31)

GE	32.0	0.0454909085	-0.0143063006	0.1949195026
H	1.0	-0.0178753952	0.0605596614	1.7385948743
H	1.0	0.1520894949	-1.4948110070	-0.2147200534
H	1.0	-1.2454308269	0.6034596680	-0.3736039114
H	1.0	1.2767167895	0.7692552665	-0.2888691573
O	8.0	0.1209203639	-0.1881264000	-2.9246240650
H	1.0	-0.5751259049	0.2278726934	-3.4368469376
H	1.0	0.2919846702	-1.0229318116	-3.3647712222

$H_4Ge\cdots SH_2$ (32)

GE	32.0	0.0581573163	0.0099546129	0.3574079009
H	1.0	0.0893854841	-0.1397304503	1.8925300111
H	1.0	0.0409746344	-1.3929025538	-0.2816519433
H	1.0	-1.2102698645	0.7802729468	-0.0528685431
H	1.0	1.3115343067	0.7745755579	-0.1056611643
S	16.0	-0.0344548537	0.2476461576	-3.4785175817
H	1.0	-1.0505183344	-0.6239478704	-3.4440748515
H	1.0	0.8787971082	-0.7311164313	-3.5127200055

$FH_3Ge\cdots NH_3$ (33)

GE	32.0	0.0084549325	0.0008970583	0.0480998036
F	9.0	0.0136653615	0.0279104637	1.8009611338
H	1.0	0.0068905160	-1.4917078970	-0.3080313527
H	1.0	-1.2800730653	0.7388538124	-0.3393204550
H	1.0	1.2949915913	0.7383949149	-0.3467501564
N	7.0	0.0007164545	-0.0425671151	-2.8717728440
H	1.0	-0.8104448403	-0.5179801594	-3.2496910196
H	1.0	0.8125501702	-0.5141659190	-3.2529949227
H	1.0	-0.0023298104	0.8889578312	-3.2706199670

$FH_3Ge\cdots PH_3$ (34)

GE	32.0	0.0095327157	0.0061218873	0.5217915742
F	9.0	0.0154701368	0.0405300512	2.2648756510
H	1.0	0.0052452746	-1.4790697295	0.1282181029
H	1.0	-1.2698437402	0.7390510553	0.0892369206
H	1.0	1.2890264800	0.7339040370	0.0809636027
P	15.0	-0.0003690198	-0.0504560632	-3.1533950869
H	1.0	-1.0349686991	-0.6530184930	-3.9030015677
H	1.0	1.0340959339	-0.6491564811	-3.9062630580
H	1.0	-0.0037677720	1.1406867160	-3.9125458989

$FH_3Ge\cdots OH_2$ (35)

GE	32.0	0.0058628831	-0.0316990471	0.0507682815
F	9.0	0.0075753151	0.1625995314	1.7901357937
H	1.0	-0.0000475549	-1.5493126693	-0.1755999483
H	1.0	-1.2770761536	0.6665916407	-0.4209775623
H	1.0	1.2940688422	0.6565179945	-0.4222593805
O	8.0	0.0052396836	-0.2722375458	-2.7810528764
H	1.0	-0.7577765474	-0.3565023192	-3.3558242065

H	1.0	0.7709236221	-0.3349858252	-3.3551110713

$FH_3Ge\cdots SH_2$ (36)

GE	32.0	0.0149717142	0.0462422789	0.2438592266
F	9.0	0.0284847481	-0.0266748048	1.9857992302
H	1.0	0.0168810916	-1.4145029065	-0.2341118353
H	1.0	-1.2718858664	0.7930474275	-0.1386054021
H	1.0	1.2892535953	0.8052576332	-0.1563349252
S	16.0	-0.0063354499	0.1821828312	-3.3245879393
H	1.0	-0.9788795927	-0.7179894365	-3.5185071282
H	1.0	0.9562798497	-0.7265912728	-3.5274321967

$F_3HGe\cdots NH_3$ (37)

GE	32.0	0.0114284605	0.0019559079	0.0954626763
H	1.0	0.0187281381	0.0258797660	1.6191090345
F	9.0	0.0057456334	-1.6283910170	-0.4109684424
F	9.0	-1.3942531106	0.8086544754	-0.4408458613
F	9.0	1.4153391932	0.8027881382	-0.4541566560
N	7.0	-0.0018389240	-0.0416313776	-2.7665959020
H	1.0	-0.8157700290	-0.5195937523	-3.1335741307
H	1.0	0.8121494845	-0.5136650076	-3.1410090467
H	1.0	-0.0071075265	0.8925958769	-3.1575414418

$F_3HGe\cdots PH_3$ (38)

GE	32.0	0.0151877113	0.0107514053	0.6770454796
H	1.0	0.0444399750	0.0550140735	2.1954579716
F	9.0	-0.0262213521	-1.5921228446	0.1007464511
F	9.0	-1.3543847116	0.8129544538	0.0568486742
F	9.0	1.3909686575	0.7592913708	0.0052510603
P	15.0	-0.0214242303	-0.0644923769	-3.1360179806
H	1.0	-1.0096531538	-0.6848833728	-3.9340603782
H	1.0	1.0517977450	-0.6072039165	-3.8787676315
H	1.0	-0.0462893208	1.1392842175	-3.8766234264

$F_3HGe\cdots OH_2$ (39)

GE	32.0	0.0587986164	0.0000117677	0.0774709897
H	1.0	-0.0858077539	0.0445456586	1.5912633686
F	9.0	0.1152811411	-1.6278666833	-0.4388869472
F	9.0	-1.2940038287	0.7551707004	-0.6431048371
F	9.0	1.4823249395	0.8013308262	-0.3945999026
O	8.0	0.2135390450	-0.1524286881	-2.7816586638

H	1.0	-0.6182499441	0.2098716494	-3.0950137887
H	1.0	0.1768879048	-1.0896634709	-2.9853911790

$F_3HGe\cdots SH_2$ (40)

GE	32.0	0.0454143303	0.0183005663	0.3152674865
H	1.0	-0.0371959906	-0.1516259856	1.8223783731
F	9.0	1.0068406801	-1.1983659445	-0.3957445035
F	9.0	-1.4953144977	-0.0868666199	-0.4089073285
F	9.0	0.7184011613	1.5215339852	-0.1111611730
S	16.0	0.1462652981	0.1841733323	-3.4002749963
H	1.0	-1.0763802367	-0.3409235597	-3.2495021638
H	1.0	0.7407393754	-1.0052540040	-3.2419766445

$F_4Ge\cdots NH_3$ (41)

GE	32.0	0.0138478008	-0.0015875131	-0.0853508261
F	9.0	0.0264799174	0.0219873013	1.6165009346
F	9.0	0.0071217440	-1.6539792658	-0.4530525841
F	9.0	-1.4130175295	0.8210960686	-0.4770954879
F	9.0	1.4394823602	0.8131027839	-0.4978925263
N	7.0	-0.0053945326	-0.0390487404	-2.6891230103
H	1.0	-0.8169038415	-0.5226299304	-3.0556667656
H	1.0	0.8108037382	-0.5055598842	-3.0671704768
H	1.0	-0.0179983269	0.8952121800	-3.0812690376

$F_4Ge\cdots PH_3$ (42)

GE	32.0	0.0137304064	0.0057121322	0.5313658354
F	9.0	0.0348283326	0.0410180488	2.2220806551
F	9.0	0.0219802218	-1.6105140707	0.0447933507
F	9.0	-1.3901886363	0.7856965886	0.0119717381
F	9.0	1.3898777183	0.8106438290	-0.0234014730
P	15.0	-0.0111740680	-0.0508810459	-3.0809721280
H	1.0	-1.0494000154	-0.6334810080	-3.8404722774
H	1.0	1.0218559215	-0.6642930096	-3.8233002796
H	1.0	0.0129114591	1.1446915357	-3.8321852012

$F_4Ge\cdots OH_2$ (43)

GE	32.0	0.0463839334	-0.0041830910	-0.0366619406
F	9.0	0.0147131238	-0.0106711578	1.6603094560
F	9.0	1.0092861948	-1.3286987029	-0.4634985534
F	9.0	-1.5711137578	-0.1692534392	-0.5059231754
F	9.0	0.7205518628	1.4772524080	-0.4780388384

O	8.0	0.0490845493	-0.0954302505	-2.6733784027
H	1.0	-0.8097219549	-0.1485002934	-3.0983290312
H	1.0	0.5895861485	-0.7795437133	-3.0744004843

$F_4Ge\cdots SH_2$ (44)

GE	32.0	0.0081863499	0.0508945208	0.2365581337
F	9.0	0.0329830125	-0.0238261306	1.9259835892
F	9.0	-0.0253213804	-1.5334416361	-0.3497844929
F	9.0	-1.3823750214	0.8878286276	-0.2256929761
F	9.0	1.4093330608	0.8453033056	-0.2672544271
S	16.0	-0.0232036405	0.1845108375	-3.2596824167
H	1.0	-0.9519933516	-0.7749617043	-3.3638222534
H	1.0	0.9811610708	-0.6953360607	-3.3662261167

$H_4Sn\cdots NH_3$ (45)

SN	50.0	0.0088146407	0.0035736982	0.2078708727
H	1.0	0.0112003905	0.0274263460	1.9379703914
H	1.0	0.0096497011	-1.6398234638	-0.2819899664
H	1.0	-1.4099011272	0.8129571517	-0.3147553789
H	1.0	1.4246074893	0.8156175882	-0.3184406678
N	7.0	0.0016656244	-0.0429609845	-2.9678803294
H	1.0	-0.8127571489	-0.5182612483	-3.3380409466
H	1.0	0.8117297911	-0.5180986795	-3.3478085792
H	1.0	-0.0005880412	0.8881625920	-3.3670451859

$H_4Sn\cdots PH_3$ (46)

SN	50.0	0.0142166166	0.0125755258	0.7108367258
H	1.0	0.0233976180	0.0441487969	2.4308615561
H	1.0	0.0128291966	-1.6197852852	0.1825774161
H	1.0	-1.3947064898	0.8117703311	0.1448240053
H	1.0	1.4153985551	0.8147143509	0.1304755900
P	15.0	-0.0034903403	-0.0516603633	-3.2775703932
H	1.0	-1.0399448667	-0.6566702569	-4.0243914002
H	1.0	1.0249574680	-0.6567989532	-4.0354137255
H	1.0	-0.0082364476	1.1302988640	-4.0523195544

$H_4Sn\cdots OH_2$ (47)

SN	50.0	0.0517519374	0.0001712874	0.1716588198
H	1.0	-0.0362474749	0.0999216098	1.8936565325
H	1.0	0.1094886015	-1.6620268417	-0.2513329633
H	1.0	-1.3576429481	0.7443794009	-0.4654693971

H	1.0	1.4666791964	0.8181918272	-0.3395774287
O	8.0	0.1138827110	-0.2225252477	-2.9065277856
H	1.0	-0.5502901830	0.2293055609	-3.4307894311
H	1.0	0.2511482597	-1.0664458167	-3.3415427538

$H_4Sn\cdots SH_2$ (48)

SN	50.0	0.0014361374	0.0544295663	0.3658526382
H	1.0	0.0213434291	-0.0473024990	2.0830475987
H	1.0	-0.0026273397	-1.5372615120	-0.2799403709
H	1.0	-1.4131315262	0.8879087816	-0.1295916799
H	1.0	1.4026001171	0.8912627723	-0.1617138673
S	16.0	-0.0240293730	0.1797094040	-3.4867877549
H	1.0	-0.9335321943	-0.8019272754	-3.5333399528
H	1.0	0.9967108598	-0.6858474577	-3.5274475811

$FH_3Sn\cdots NH_3$ (49)

SN	50.0	0.0093575366	0.0010177230	-0.0020426850
F	9.0	0.0153709706	0.0280835610	1.9490845111
H	1.0	0.0088113776	-1.6758017785	-0.3238791341
H	1.0	-1.4397937932	0.8318400132	-0.3560389246
H	1.0	1.4557780760	0.8327790341	-0.3650123153
N	7.0	-0.0002201001	-0.0426214283	-2.8834070446
H	1.0	-0.8126081559	-0.5186232066	-3.2587955217
H	1.0	0.8108374153	-0.5160915330	-3.2648432837
H	1.0	-0.0031120170	0.8880106051	-3.2851853821

$FH_3Sn\cdots PH_3$ (50)

SN	50.0	0.0153180037	0.0140297876	0.5056800963
F	9.0	0.0231544504	0.0411154641	2.4444317775
H	1.0	0.0148333839	-1.6499057319	0.1179760521
H	1.0	-1.4227514938	0.8366176354	0.0877493599
H	1.0	1.4488530366	0.8381007917	0.0754122263
P	15.0	-0.0045119298	-0.0506409127	-3.1937593423
H	1.0	-1.0460022520	-0.6660583989	-3.9218116116
H	1.0	1.0269975658	-0.6642662580	-3.9373341643
H	1.0	-0.0114694548	1.1296006027	-3.9684641540

$FH_3Sn\cdots OH_2$ (51)

SN	50.0	0.0068776566	-0.0505166316	0.0078959179
F	9.0	0.0092432983	0.1757201258	1.9420085710
H	1.0	0.0028392104	-1.7484885435	-0.1652604963

H	1.0	-1.4379939582	0.7356742898	-0.4509669423
H	1.0	1.4545034312	0.7291757928	-0.4534813926
O	8.0	0.0046752996	-0.2785217363	-2.7996909098
H	1.0	-0.7622535835	-0.3130683627	-3.3746283236
H	1.0	0.7708787357	-0.3090031843	-3.3757973944

$FH_3Sn\cdots SH_2$ (52)

SN	50.0	0.0117189718	0.0538150001	0.2242609810
F	9.0	0.0147421561	-0.0018359905	2.1624765026
H	1.0	-0.0096435561	-1.5941553777	-0.2297408384
H	1.0	-1.4169757612	0.9075728408	-0.1605742466
H	1.0	1.4598951565	0.8713961222	-0.1663144317
S	16.0	0.0036230791	0.1701746120	-3.3655043821
H	1.0	-0.9756247550	-0.7219098244	-3.5644340721
H	1.0	0.9610347988	-0.7440858459	-3.5700904828

$F_3HSn\cdots NH_3$ (53)

SN	50.0	-0.0147940145	-0.0069516965	-0.0773535951
H	1.0	-0.0423080476	0.0075540675	1.6212099019
F	9.0	0.0111993843	-1.8605170764	-0.5457299679
F	9.0	-1.6149895566	0.9012135359	-0.5975104897
F	9.0	1.5856228035	0.9274698905	-0.5473208231
N	7.0	0.0254437231	-0.0323300190	-2.6391911393
H	1.0	0.0424993231	-0.9815987749	-2.9917108732
H	1.0	0.8447362145	0.4465714375	-2.9929336113
H	1.0	-0.7929884998	0.4271816453	-3.0195791723

$F_3HSn\cdots PH_3$ (54)

SN	50.0	0.0171882043	0.0153294118	0.6129696106
H	1.0	0.0289840865	0.0320946118	2.3013400596
F	9.0	0.0214911517	-1.7579669898	-0.0658224500
F	9.0	-1.5225222828	0.8816896587	-0.0823812750
F	9.0	1.5369490830	0.8991906703	-0.1040508118
P	15.0	-0.0065073405	-0.0411609366	-3.0488413343
H	1.0	-1.0510798353	-0.6543758258	-3.7758627076
H	1.0	1.0192624344	-0.6739045439	-3.7857711996
H	1.0	0.0006558285	1.1276969536	-3.8416996719

$F_3HSn\cdots OH_2$ (55)

SN	50.0	0.0966380822	-0.0277184072	-0.0403504720
H	1.0	-0.0355885641	-0.0130796743	1.6497665834

F	9.0	0.1026229915	-1.8626884155	-0.5723584318
F	9.0	-1.4321287645	0.8959911557	-0.7185629374
F	9.0	1.7137880350	0.8489314245	-0.5088487165
O	8.0	0.1445893079	-0.1371876481	-2.6175587128
H	1.0	-0.6412219094	0.2920938540	-2.9656226761
H	1.0	0.1000709413	-1.0553705290	-2.8963855966

$F_3HSn\cdots SH_2$ (56)

SN	50.0	0.0114265570	0.0465387456	0.2986216323
H	1.0	0.0284419266	-0.0406874524	1.9849189077
F	9.0	-0.0232737901	-1.6849707063	-0.4863359997
F	9.0	-1.5251805520	0.9665113570	-0.3297265795
F	9.0	1.5634259492	0.9153067447	-0.3643901009
S	16.0	-0.0153192185	0.1974147383	-3.2473805149
H	1.0	-0.9616042613	-0.7503679402	-3.2611835325
H	1.0	0.9708535193	-0.7087737267	-3.2644447822

$F_4Sn\cdots NH_3$ (57)

SN	50.0	0.0135151022	-0.0026430135	-0.1825458093
F	9.0	0.0260519572	0.0259550611	1.7128331845
F	9.0	0.3951617233	-1.8267218927	-0.5100417053
F	9.0	-1.7571668669	0.5662131449	-0.5309100188
F	9.0	1.3976000090	1.2303108984	-0.5623840892
N	7.0	-0.0054387604	-0.0371211694	-2.6557010034
H	1.0	-0.9118183490	0.2369332038	-3.0170749808
H	1.0	0.2012742415	-0.9643673474	-3.0088540759
H	1.0	0.6852422731	0.6000341148	-3.0354412819

$F_4Sn\cdots PH_3$ (58)

SN	50.0	0.0140581700	0.0118785524	0.4128256118
F	9.0	0.0219334708	0.0224014910	2.2985055650
F	9.0	0.0087721961	-1.8001975735	-0.0974764760
F	9.0	-1.5513552035	0.9185802630	-0.1084053775
F	9.0	1.5781958620	0.9129315655	-0.1219128590
P	15.0	-0.0031512024	-0.0413562462	-2.9927362234
H	1.0	-1.0458858483	-0.6737186668	-3.7007090375
H	1.0	1.0382558464	-0.6597388874	-3.7147932598
H	1.0	-0.0164019511	1.1378125019	-3.7654177235

$F_4Sn\cdots OH_2$ (59)

SN	50.0	-0.0669371254	-0.0233408108	-0.1457492093

F	9.0	0.0885983670	0.0149655698	1.7398811714
F	9.0	-0.1357385915	-1.8801006347	-0.4974450054
F	9.0	-1.6734999993	0.9005841158	-0.4758362577
F	9.0	1.4968248093	0.8914470631	-0.6878801573
O	8.0	-0.0959067373	-0.1775891364	-2.5865296203
H	1.0	-0.1736076001	-1.0594340444	-2.9593224000
H	1.0	0.6090369871	0.2744396376	-3.0570394913

$F_4Sn\cdots SH_2$ (60)

SN	50.0	0.0139808336	0.0523006920	0.1518035794
F	9.0	0.0173077183	-0.0152367191	2.0360311533
F	9.0	0.0160481055	-1.7384126343	-0.4352105097
F	9.0	-1.5665509526	0.9518165254	-0.3333656824
F	9.0	1.5890401719	0.9580468151	-0.3391413263
S	16.0	0.0046274987	0.1886196240	-3.1615171146
H	1.0	-0.9809096192	-0.7102380054	-3.2900468334
H	1.0	0.9552263637	-0.7459245376	-3.2984742364