

Supplementary Information

Heavy Pnictogen Atoms as Electron Donors in Sigma-Hole Bonds

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Table S1. E_{def} (kcal/mol) of individual subunits, base listed first followed by acid.

perfluoro											
	FH	FBr	F ₂ Se	F ₃ As	F ₄ Ge		FH	FBr	F ₂ Se	F ₃ As	F ₄ Ge
NH ₃	0.01+0.79	0.09+1.09	0.06+1.29	0.03+0.79	0.07+16.14	NMe ₃	0.20+1.95	0.49+2.22	0.45+2.51	0.28+1.68	1.44+21.74
PH ₃	0.19+0.08	1.30+1.67	0.26+0.41	0.09+0.71	0.17+1.69	PMe ₃	0.29+0.30	4.15+10.47	3.00+6.10	0.37+0.57	4.93+22.16
AsH ₃	0.14+0.05	1.06+1.71	0.19+0.22	0.04+0.06	0.09+0.90	AsMe ₃	0.26+0.05	3.42+7.06	1.29+2.51	0.25+0.30	3.93+18.43
SbH ₃	0.11+0.04	0.78+1.84	0.13+0.18	0.05+0.05	0.04+0.55	SbMe ₃	0.18+0.10	2.27+5.77	0.75+1.67	0.16+0.15	0.28+2.95
monofluoro											
	FH	FBr	FHSe	FH ₂ As	FH ₃ Ge		FH	FBr	FHSe	FH ₂ As	FH ₃ Ge
NH ₃	0.01+0.79	0.09+1.09	0.02+0.55	0.01+0.28	0.01+0.01	NMe ₃	0.20+1.95	0.49+2.22	0.30+1.33	0.15+0.74	0.16+2.59
PH ₃	0.19+0.08	1.30+1.67	0.32+0.41	0.08+0.05	0.06+0.06	PMe ₃	0.29+0.30	4.15+10.47	1.93+3.44	0.41+0.43	0.12+0.34
AsH ₃	0.14+0.05	1.06+1.71	0.23+0.16	0.06+0.04	0.05+0.03	AsMe ₃	0.26+0.05	3.42+7.06	1.19+1.73	0.25+0.19	0.11+0.18
SbH ₃	0.11+0.04	0.78+1.84	0.11+0.14	0.06+0.03	0.03+0.03	SbMe ₃	0.18+0.10	2.27+5.77	0.63+0.99	0.11+0.09	0.05+0.05

Table S2. Intermolecular distances R(Å)

Perfluoro											
	FH	FBr	F ₂ Se	F ₃ As	F ₄ Ge		FH	FBr	F ₂ Se	F ₃ As	F ₄ Ge
NH ₃	1.680	2.361	2.449	2.656	2.121	NMe ₃	1.572	2.248	2.303	2.456	2.116
PH ₃	2.357	2.499	3.059	3.437	3.243	PMe ₃	2.239	2.307	2.520	3.179	2.467
AsH ₃	2.472	2.668	3.240	3.569	3.429	AsMe ₃	2.379	2.484	2.824	3.360	2.627
SbH ₃	2.668	2.814	3.426	3.738	3.651	SbMe ₃	2.604	2.674	3.054	3.611	3.393
Monofluoro											
	FH	FBr	FHSe	FH ₂ As	FH ₃ Ge		FH	FBr	FHSe	FH ₂ As	FH ₃ Ge
NH ₃	1.680	2.361	2.527	2.725	2.731	NMe ₃	1.572	2.248	2.348	2.501	2.469
PH ₃	2.357	2.499	2.871	3.291	3.451	PMe ₃	2.239	2.307	2.515	2.922	3.269
AsH ₃	2.472	2.668	3.116	3.391	3.564	AsMe ₃	2.379	2.484	2.718	3.132	3.413
SbH ₃	2.668	2.814	3.250	3.556	3.752	SbMe ₃	2.604	2.674	2.957	3.411	3.655

Cartesian Coordinates of Complexes

NH₃···HF

1	1.580863000	0.014455000	0.944407000
1	1.582703000	-0.824218000	-0.461339000
1	1.576427000	0.813011000	-0.484489000
9	-1.419981000	-0.000099000	0.000004000
1	-0.464673000	-0.000948000	0.000412000
7	1.214929000	-0.000202000	0.000139000

NH₃···BrF

1	2.552206000	-0.014890000	0.951059000
1	2.552972000	-0.816215000	-0.489924000
1	2.549177000	0.833047000	-0.463024000
9	-1.965532000	0.000171000	-0.000380000
7	2.206684000	0.000041000	-0.000128000
35	-0.154610000	-0.000108000	0.000177000

NH₃···SeF₂

9	-0.119080000	1.393867000	-0.000031000
9	1.941503000	-0.005036000	0.000122000
1	-2.761957000	-1.043427000	0.000977000
1	-2.494644000	0.361588000	0.820055000
1	-2.495243000	0.360161000	-0.820658000
34	0.206413000	-0.321906000	-0.000050000
7	-2.238286000	-0.176143000	0.000071000

NH₃···AsF₃

1	-2.624551000	0.901987000	0.225796000
1	-3.017022000	-0.192348000	-0.935209000
1	-2.538859000	-0.700732000	0.551341000
33	0.263339000	-0.000270000	-0.368101000
9	-0.065299000	-1.286144000	0.729713000
9	1.948239000	0.011496000	0.032410000
9	-0.084642000	1.275802000	0.735142000
7	-2.384919000	-0.001482000	-0.167139000

NH₃···GeF₄

32	-0.163208000	-0.000322000	0.000038000
9	0.056148000	0.967234000	1.408993000
9	-1.881964000	-0.000661000	0.000205000
9	0.056266000	0.739505000	-1.540711000
9	0.056673000	-1.704573000	0.131098000
1	2.311569000	-0.413146000	0.858213000
1	2.311715000	0.949028000	-0.070993000

1	2.311918000	-0.536663000	-0.786313000
7	1.957619000	-0.000353000	0.000232000

NH₃···SeFH

9	-1.971175000	0.131749000	0.000007000
1	2.672813000	-0.881917000	0.005840000
1	2.691722000	0.529781000	-0.825379000
1	2.692540000	0.540044000	0.819265000
34	-0.195156000	-0.094594000	0.000003000
7	2.326460000	0.070085000	0.000020000
1	0.033574000	1.351954000	-0.000020000

NH₃···AsFH₂

1	-2.831149000	-0.152537000	-0.903229000
1	-2.862372000	-0.571499000	0.675129000
1	-2.827688000	1.007803000	0.249524000
33	0.243661000	-0.132772000	-0.020285000
9	1.988997000	0.194918000	0.026825000
7	-2.472239000	0.088938000	0.013111000
1	-0.053419000	0.667597000	1.242096000
1	-0.061495000	1.053278000	-0.927323000

NH₃···GeFH₃

32	-0.250968000	-0.000486000	-0.000505000
9	-2.015585000	0.001267000	0.001382000
1	2.852150000	-0.792535000	-0.509070000
1	2.848546000	-0.044783000	0.943534000
1	2.851385000	0.839501000	-0.430373000
7	2.479667000	0.000557000	0.000534000
1	0.089458000	1.247585000	0.828587000
1	0.086329000	-1.343852000	0.664114000
1	0.085717000	0.094327000	-1.496815000

PH₃···HF

1	1.793781000	-0.951226000	-0.735381000
1	1.797346000	1.112330000	-0.452641000
1	1.791035000	-0.164373000	1.192561000
9	-2.225120000	0.000014000	0.000069000
1	-1.294244000	0.000689000	-0.001533000
15	1.062544000	0.000164000	-0.000242000

PH₃···BrF

1	2.692577000	1.223985000	-0.062838000
1	2.669137000	-0.562250000	1.103841000
1	2.683847000	-0.679869000	-1.026140000
9	-2.338613000	-0.003094000	0.001768000

15	2.009352000	-0.000344000	-0.000025000
35	-0.489667000	0.001461000	-0.000869000

PH₃···SeF₂

9	0.345270000	1.410597000	-0.000189000
9	2.362256000	-0.097731000	0.001035000
1	-3.276634000	-0.525184000	-1.043576000
1	-3.273854000	-0.528448000	1.044769000
1	-2.830836000	1.231633000	0.002855000
15	-2.424797000	-0.115137000	0.000109000
34	0.628986000	-0.301963000	-0.000391000

PH₃···AsF₃

1	3.641187000	-1.037422000	-0.278679000
1	3.640303000	1.038315000	-0.277889000
1	2.753046000	-0.000595000	1.288840000
33	-0.727883000	0.000001000	-0.372721000
9	-0.283911000	1.268271000	0.692704000
9	-2.378234000	-0.000012000	0.098513000
9	-0.283875000	-1.268275000	0.692684000
15	2.699985000	-0.000013000	-0.119172000

PH₃···GeF₄

32	-0.668206000	-0.000064000	-0.000426000
9	-0.217547000	-0.359095000	-1.594706000
9	-2.366983000	-0.001536000	0.006068000
9	-0.213619000	-1.203119000	1.103386000
9	-0.219610000	1.561983000	0.483279000
1	3.328954000	-1.060269000	-0.538309000
1	3.287710000	0.067581000	1.211749000
1	3.301451000	1.021482000	-0.639025000
15	2.574955000	-0.000724000	-0.000202000

PH₃···SeFH

9	2.385078000	0.141153000	0.001801000
1	-2.976324000	-0.554501000	-1.052570000
1	-2.964537000	-0.585224000	1.043079000
1	-2.977468000	1.242607000	0.021851000
15	-2.253456000	0.035507000	-0.000058000
34	0.614556000	-0.095727000	-0.000707000
1	0.359564000	1.348835000	-0.003655000

PH₃···AsFH₂

1	-3.377561000	0.324312000	-1.115429000
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1	-3.211809000	-1.129683000	0.355792000
1	-3.234797000	0.877371000	0.878511000
33	0.750229000	-0.129516000	0.040949000
9	2.476792000	0.210017000	-0.055573000
15	-2.535579000	0.047366000	-0.019846000
1	0.384582000	1.205997000	0.682045000
1	0.424574000	0.395376000	-1.354379000

PH₃···GeFH₃

32	0.803572000	-0.003769000	0.001163000
9	2.553630000	0.010438000	-0.003093000
1	-3.362076000	1.213837000	0.015052000
1	-3.422984000	-0.599127000	1.013712000
1	-3.394194000	-0.557599000	-1.056653000
15	-2.646971000	-0.000732000	0.000854000
1	0.386609000	0.780488000	-1.254112000
1	0.392713000	0.688694000	1.311027000
1	0.407512000	-1.488661000	-0.051217000

AsH₃···HF

1	-1.510329000	-1.188533000	0.423062000
1	-1.465335000	1.004440000	0.806847000
1	-1.434242000	0.239572000	-1.283097000
9	2.734008000	0.000631000	-0.000281000
1	1.805154000	-0.014533000	0.010130000
33	-0.666707000	-0.001413000	0.001381000

AsH₃···BrF

1	-2.399369000	0.176722000	1.297677000
1	-2.393243000	1.035490000	-0.807354000
1	-2.389488000	-1.217384000	-0.498332000
9	2.849903000	-0.000900000	-0.001108000
35	1.023073000	0.000409000	0.000521000
33	-1.644684000	-0.000032000	-0.000008000

AsH₃···SeF₂

9	0.941595000	1.423160000	-0.000025000
9	2.931229000	-0.142394000	0.000184000
1	-2.961453000	-0.513384000	-1.111372000
1	-2.959361000	-0.508904000	1.114914000
1	-2.527532000	1.373097000	-0.002428000
34	1.197378000	-0.291432000	-0.000071000
33	-2.033877000	-0.059667000	-0.000004000

AsH₃···AsF₃

1	2.833058000	-0.994862000	0.950484000
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1	3.553426000	-0.002486000	-0.899205000
1	2.690191000	1.211643000	0.748680000
33	-1.272674000	0.000266000	-0.361171000
9	-0.843150000	1.239323000	0.741634000
9	-2.946363000	0.050412000	0.014500000
9	-0.927981000	-1.291741000	0.709824000
33	2.284212000	-0.006212000	-0.062876000

AsH₃···GeF₄

32	1.188199000	0.000123000	0.000235000
9	0.719933000	-0.724726000	1.456848000
9	2.884782000	0.002208000	-0.012270000
9	0.698456000	-0.897474000	-1.350009000
9	0.703602000	1.620160000	-0.096158000
33	-2.240499000	-0.000782000	0.002170000
1	-3.068441000	0.903173000	0.896826000
1	-3.068294000	-1.238259000	0.293514000
1	-3.010122000	0.355455000	-1.255164000

AsH₃···SeFH

9	2.993530000	0.144870000	0.002959000
1	-2.633259000	-0.705153000	-1.095991000
1	-2.619354000	-0.651363000	1.138902000
1	-2.768759000	1.248403000	-0.024007000
34	1.236970000	-0.095028000	-0.001103000
33	-1.876678000	0.020909000	-0.000054000
1	0.952974000	1.345222000	-0.006256000

AsH₃···AsFH₂

1	1.003080000	0.801138000	1.135263000
1	0.996149000	0.898393000	-1.054487000
33	-2.015950000	0.028645000	0.001847000
33	1.370699000	-0.145630000	-0.004848000
9	3.087249000	0.244840000	0.006597000
1	-2.805246000	-0.840378000	0.964615000
1	-2.900832000	1.245049000	0.212172000
1	-2.785088000	-0.447275000	-1.217899000

AsH₃···GeFH₃

32	-1.453210000	0.003978000	-0.000183000
9	-3.201886000	-0.011069000	0.000719000
33	2.110484000	0.000593000	0.000714000
1	2.954371000	0.366224000	1.209755000
1	2.945663000	0.837660000	-0.952887000

1	2.892155000	-1.271217000	-0.279423000
1	-1.034428000	-0.689810000	-1.307397000
1	-1.051714000	1.487680000	0.050223000
1	-1.032320000	-0.777776000	1.255557000

SbH₃···HF

1	-1.442437000	-0.711374000	-1.227811000
1	-1.389542000	-0.721417000	1.259113000
1	-1.409536000	1.438957000	0.024252000
9	3.090490000	-0.000027000	0.000606000
51	-0.504623000	-0.000098000	-0.000940000
1	2.162880000	-0.000945000	-0.013084000

SbH₃···BrF

1	2.275345000	-0.360244000	1.409267000
1	2.252204000	-1.045439000	-1.030405000
1	2.252296000	1.411435000	-0.403523000
9	-3.238373000	-0.000061000	-0.003303000
35	-1.408595000	-0.000008000	0.001520000
51	1.405223000	-0.000097000	0.000023000

SbH₃···SeF₂

9	1.348952000	1.411227000	-0.002517000
9	3.371788000	-0.116409000	0.015641000
1	-2.845801000	-0.321802000	-1.291746000
1	-2.837315000	-0.673736000	1.168497000
1	-2.272448000	1.566504000	0.229563000
34	1.643497000	-0.297358000	-0.005863000
51	-1.772745000	-0.041454000	-0.000492000

SbH₃···AsF₃

1	2.254990000	-0.232843000	1.624505000
1	3.318005000	-0.992662000	-0.489746000
1	2.931996000	1.423696000	-0.096877000
51	2.002759000	-0.003898000	-0.042744000
33	-1.721110000	0.000290000	-0.366506000
9	-1.239308000	1.227944000	0.728541000
9	-3.381562000	0.072254000	0.053829000
9	-1.362362000	-1.301195000	0.688378000

SbH₃···GeF₄

32	-1.624175000	-0.000130000	-0.000169000
9	-1.126436000	1.128290000	-1.160188000
9	-3.318991000	0.001045000	0.003535000
9	-1.126519000	-1.569087000	-0.398020000

9	-1.120993000	0.440130000	1.555219000
1	2.921493000	0.379352000	1.397671000
1	2.952145000	1.018654000	-1.003061000
1	2.961454000	-1.378679000	-0.356530000
51	2.026960000	-0.000364000	-0.000737000

SbH₃···SeFH

9	3.419379000	0.103210000	-0.039120000
1	-2.499213000	0.609493000	-1.309841000
1	-2.218195000	-1.560915000	-0.110940000
1	-2.712168000	0.519741000	1.176808000
34	1.657992000	-0.078037000	0.014753000
51	-1.590887000	0.015411000	0.000584000
1	1.418635000	1.370083000	0.064636000

SbH₃···AsFH₂

1	2.772987000	1.355352000	0.063750000
1	2.571180000	-0.848474000	1.191600000
1	2.553752000	-0.717201000	-1.286434000
51	1.717388000	0.019786000	0.001073000
33	-1.834956000	-0.139204000	-0.005302000
9	-3.554134000	0.230617000	0.007619000
1	-1.469764000	0.910115000	-1.053454000
1	-1.474232000	0.809304000	1.136185000

SbH₃···GeFH₃

32	1.948326000	0.003490000	0.004833000
9	3.695363000	-0.009788000	-0.013542000
1	-2.672040000	-1.421177000	-0.358491000
1	-2.711150000	0.948723000	-1.086735000
1	-2.800629000	0.392703000	1.326476000
51	-1.804089000	0.000758000	0.001203000
1	1.534719000	-0.851091000	1.214701000
1	1.542003000	1.480771000	0.145306000
1	1.510959000	-0.612170000	-1.335409000

N(CH₃)₃···HF

9	2.283762000	-0.004286000	0.002955000
1	1.307447000	-0.004317000	0.002634000
7	-0.264491000	-0.000489000	0.000354000
6	-0.712587000	-1.338164000	0.366498000
1	-0.325311000	-2.060004000	-0.351975000
1	-0.327701000	-1.592002000	1.353663000
1	-1.808908000	-1.405334000	0.383265000
6	-0.700179000	0.353087000	-1.344874000

1	-0.304685000	1.333450000	-1.608679000
1	-0.314420000	-0.377594000	-2.055174000
1	-1.795808000	0.378672000	-1.419715000
6	-0.704366000	0.989737000	0.975236000
1	-0.320675000	0.724925000	1.959999000
1	-0.309368000	1.967744000	0.702178000
1	-1.800201000	1.048501000	1.023575000

N(CH₃)₃···BrF

9	2.769963000	0.000020000	-0.000092000
7	-1.316050000	-0.000167000	-0.000060000
35	0.931878000	-0.000031000	0.000079000
6	-1.755794000	-0.465955000	1.312776000
1	-1.361985000	-1.465672000	1.488083000
1	-1.365825000	0.202552000	2.078581000
1	-2.850067000	-0.489199000	1.371734000
6	-1.755668000	-0.904123000	-1.059996000
1	-1.362096000	-0.555051000	-2.013083000
1	-1.364546000	-1.901199000	-0.864880000
1	-2.849890000	-0.944499000	-1.109165000
6	-1.755473000	1.370190000	-0.253065000
1	-1.364836000	2.021121000	0.527361000
1	-1.362468000	1.701159000	-1.212861000
1	-2.849739000	1.432189000	-0.265572000

N(CH₃)₃···SeF₂

9	0.772758000	1.440706000	-0.000030000
9	2.653785000	-0.151816000	0.000657000
34	0.878985000	-0.308894000	-0.000443000
6	-1.827995000	0.667081000	-1.205214000
1	-1.380767000	1.659184000	-1.203345000
1	-1.478740000	0.124727000	-2.082873000
1	-2.919955000	0.758232000	-1.245331000
6	-1.892007000	-1.421234000	-0.000084000
1	-1.519896000	-1.933026000	-0.888577000
1	-1.518083000	-1.933682000	0.887296000
1	-2.986844000	-1.459992000	0.001064000
6	-1.826748000	0.666149000	1.206248000
1	-1.476609000	0.123084000	2.083155000
1	-1.379511000	1.658250000	1.204743000
1	-2.918667000	0.757208000	1.247500000
7	-1.409260000	-0.046225000	0.000013000

N(CH₃)₃···AsF₃

33	-0.888139000	-0.000022000	0.353496000
9	-0.703766000	-1.297071000	-0.773703000
9	-2.615456000	0.000035000	0.125404000
9	-0.703743000	1.297069000	-0.773654000
7	1.549474000	-0.000014000	0.050704000
6	2.021695000	1.201950000	0.724475000
1	1.623050000	2.079672000	0.216736000
1	1.670069000	1.202782000	1.757900000
1	3.117482000	1.257130000	0.728692000
6	2.021737000	-1.202355000	0.723747000
1	1.669972000	-1.203876000	1.757126000
1	1.623297000	-2.079829000	0.215418000
1	3.117536000	-1.257383000	0.728107000
6	1.924812000	0.000457000	-1.359628000
1	1.511631000	-0.884092000	-1.840977000
1	1.510316000	0.884576000	-1.840608000
1	3.016137000	0.001244000	-1.476670000

N(CH₃)₃···GeF₄

32	-0.738474000	0.000949000	-0.000128000
9	-0.576459000	1.722563000	0.048497000
9	-2.462744000	0.001969000	0.000856000
9	-0.578388000	-0.820545000	-1.513873000
9	-0.575959000	-0.905431000	1.464385000
7	1.377022000	0.000275000	-0.000220000
6	1.878655000	0.726810000	-1.186212000
1	1.513974000	0.237475000	-2.086152000
1	1.518051000	1.752086000	-1.155685000
1	2.971541000	0.720886000	-1.181306000
6	1.872227000	-1.392270000	-0.036510000
1	1.504988000	-1.923735000	0.838142000
1	1.507557000	-1.876493000	-0.939255000
1	2.965096000	-1.390288000	-0.035007000
6	1.875847000	0.663405000	1.223409000
1	1.513057000	1.688192000	1.247025000
1	1.510607000	0.125725000	2.095188000
1	2.968720000	0.659188000	1.219768000

N(CH₃)₃···SeFH

9	-2.776022000	-0.163106000	0.000442000
34	-0.984276000	0.105912000	-0.000139000
7	1.360146000	-0.025687000	0.000049000
1	-0.776109000	-1.345670000	0.000548000
6	1.810521000	-0.710523000	1.207179000

1	1.422010000	-0.191505000	2.082169000
1	1.426138000	-1.730384000	1.210363000
1	2.906243000	-0.744315000	1.259713000
6	1.810068000	-0.722644000	-1.200271000
1	1.426086000	-1.742653000	-1.192636000
1	1.420804000	-0.212857000	-2.080316000
1	2.905760000	-0.756684000	-1.253137000
6	1.796160000	1.366417000	-0.006934000
1	1.404105000	1.860590000	-0.895642000
1	1.402825000	1.869914000	0.875998000
1	2.890212000	1.440839000	-0.006482000

N(CH₃)₃···AsFH₂

33	-1.058333000	-0.137954000	0.002235000
1	-0.784937000	0.850793000	-1.127760000
9	-2.812680000	0.212820000	-0.003584000
1	-0.785182000	0.887253000	1.099798000
7	1.437038000	0.030538000	-0.000571000
6	1.873450000	-0.646225000	1.212137000
1	1.491894000	-0.113049000	2.083430000
1	1.474776000	-1.660708000	1.224637000
1	2.968678000	-0.692685000	1.278676000
6	1.873838000	-0.689071000	-1.188209000
1	1.475882000	-1.703621000	-1.164112000
1	1.491743000	-0.187877000	-2.078077000
1	2.969094000	-0.737100000	-1.253159000
6	1.895422000	1.412129000	-0.025038000
1	1.515703000	1.906503000	-0.918994000
1	1.513349000	1.938320000	0.849509000
1	2.992576000	1.474524000	-0.024801000

N(CH₃)₃···GeFH₃

32	-0.738474000	0.000949000	-0.000128000
9	-0.576459000	1.722563000	0.048497000
9	-2.462744000	0.001969000	0.000856000
9	-0.578388000	-0.820545000	-1.513873000
9	-0.575959000	-0.905431000	1.464385000
7	1.377022000	0.000275000	-0.000220000
6	1.878655000	0.726810000	-1.186212000
1	1.513974000	0.237475000	-2.086152000
1	1.518051000	1.752086000	-1.155685000
1	2.971541000	0.720886000	-1.181306000
6	1.872227000	-1.392270000	-0.036510000
1	1.504988000	-1.923735000	0.838142000
1	1.507557000	-1.876493000	-0.939255000

1	2.965096000	-1.390288000	-0.035007000
6	1.875847000	0.663405000	1.223409000
1	1.513057000	1.688192000	1.247025000
1	1.510607000	0.125725000	2.095188000
1	2.968720000	0.659188000	1.219768000

P(CH₃)₃···HF

9	3.053129000	-0.010842000	0.004129000
1	2.111840000	-0.015656000	0.006698000
15	-0.126934000	-0.005880000	0.001934000
6	-0.953974000	0.780523000	-1.434338000
1	-0.637508000	1.820906000	-1.513797000
1	-0.662459000	0.269086000	-2.351867000
1	-2.040376000	0.744329000	-1.333354000
6	-0.966879000	0.861824000	1.383088000
1	-0.682747000	0.402312000	2.330067000
1	-0.649617000	1.904276000	1.403683000
1	-2.052862000	0.819282000	1.276659000
6	-0.992655000	-1.622500000	0.044206000
1	-0.702526000	-2.214604000	-0.824118000
1	-0.700166000	-2.170836000	0.939780000
1	-2.076673000	-1.492400000	0.042349000

P(CH₃)₃···BrF

9	-3.117460000	-0.000171000	-0.000089000
15	1.147482000	0.000431000	0.000167000
35	-1.159821000	0.000653000	0.000526000
6	1.858104000	-1.129242000	-1.225205000
1	1.505793000	-2.139234000	-1.017919000
1	1.510286000	-0.839131000	-2.216230000
1	2.948355000	-1.107039000	-1.197657000
6	1.862941000	-0.497294000	1.588418000
1	1.515612000	0.187627000	2.361412000
1	1.512386000	-1.499356000	1.834085000
1	2.953044000	-0.487771000	1.551864000
6	1.863652000	1.623768000	-0.365384000
1	1.517663000	1.949017000	-1.346104000
1	1.513596000	2.339213000	0.378167000
1	2.953736000	1.585492000	-0.354715000

P(CH₃)₃···SeF₂

9	0.976502000	1.365447000	0.000214000
9	2.956925000	-0.009520000	0.000131000
15	-1.309727000	-0.068986000	-0.000053000
34	1.188473000	-0.399820000	-0.000132000

6	-1.872223000	0.896484000	-1.433168000
1	-1.300373000	1.823592000	-1.461426000
1	-1.665760000	0.337144000	-2.345068000
1	-2.938019000	1.121392000	-1.373102000
6	-2.363465000	-1.554554000	0.001489000
1	-2.147328000	-2.153389000	-0.883065000
1	-2.146538000	-2.152104000	0.886728000
1	-3.420651000	-1.284389000	0.001869000
6	-1.871496000	0.898618000	1.431897000
1	-1.664951000	0.340399000	2.344472000
1	-1.299081000	1.825455000	1.458530000
1	-2.937211000	1.123944000	1.371938000

P(CH₃)₃···AsF₃

33	-1.437060000	0.011286000	0.440398000
9	-1.116041000	-1.370394000	-0.531554000
9	-3.091671000	0.088960000	-0.048651000
9	-0.940538000	1.164632000	-0.742825000
6	2.398085000	1.659325000	-0.030126000
1	1.670070000	2.245098000	-0.591675000
1	2.552657000	2.140221000	0.935860000
1	3.343661000	1.642873000	-0.575486000
6	3.187887000	-0.870622000	0.958752000
1	3.361526000	-0.484462000	1.963111000
1	2.992163000	-1.940059000	1.035937000
1	4.085778000	-0.715899000	0.357345000
6	1.804667000	-0.672426000	-1.500455000
1	1.550853000	-1.732273000	-1.502366000
1	1.060259000	-0.150985000	-2.102551000
1	2.793524000	-0.532128000	-1.940844000
15	1.733526000	-0.032751000	0.215051000

P(CH₃)₃···GeF₄

32	-1.024473000	0.000076000	0.000230000
9	-0.852841000	0.863938000	-1.502056000
9	-2.746719000	-0.000536000	-0.000688000
9	-0.852644000	-1.732771000	0.003345000
9	-0.854474000	0.869375000	1.499508000
6	2.137735000	-0.838621000	-1.446699000
1	1.781500000	-1.868412000	-1.459116000
1	1.782575000	-0.336544000	-2.346300000
1	3.227680000	-0.826262000	-1.423866000
6	2.140485000	-0.833516000	1.448825000
1	1.788240000	-0.327741000	2.347491000

1	1.783526000	-1.862985000	1.466232000
1	3.230373000	-0.822014000	1.423011000
6	2.140072000	1.671703000	-0.003425000
1	1.784722000	2.197201000	-0.889497000
1	1.785666000	2.201005000	0.880713000
1	3.229983000	1.644164000	-0.003916000
15	1.442614000	0.000113000	0.000314000

P(CH₃)₃···SeFH

9	-3.136985000	-0.150503000	0.000051000
34	-1.290000000	0.059232000	0.000018000
1	-1.164655000	-1.399588000	-0.000043000
6	2.095822000	-0.770345000	1.429745000
1	1.706013000	-0.323028000	2.343719000
1	1.903427000	-1.842530000	1.466267000
1	3.172072000	-0.600172000	1.369136000
6	2.095644000	-0.771302000	-1.429262000
1	1.904948000	-1.843860000	-1.463745000
1	1.704266000	-0.326199000	-2.343641000
1	3.171672000	-0.599313000	-1.369981000
6	1.768688000	1.687593000	-0.000591000
1	1.370047000	2.183746000	-0.885590000
1	1.366617000	2.185442000	0.881895000
1	2.856386000	1.767699000	0.001428000
15	1.222742000	-0.049148000	0.000010000

P(CH₃)₃···AsFH₂

33	-1.505377000	0.025455000	-0.010190000
1	-1.344920000	0.930189000	1.204594000
9	-3.284519000	-0.037795000	0.106747000
1	-1.294620000	-1.247631000	0.801320000
6	1.869902000	-1.329716000	-1.046247000
1	1.710724000	-2.301682000	-0.578619000
1	1.224737000	-1.266311000	-1.923110000
1	2.912013000	-1.250764000	-1.360892000
6	1.977219000	1.479899000	-0.788860000
1	1.333343000	1.626206000	-1.656590000
1	1.892060000	2.360454000	-0.151819000
1	3.011738000	1.378571000	-1.121721000
6	2.746516000	-0.167533000	1.380476000
1	2.683105000	0.655453000	2.092106000
1	2.616515000	-1.100005000	1.929450000
1	3.733628000	-0.161767000	0.914187000
15	1.413197000	-0.001231000	0.130296000

P(CH₃)₃···GeFH₃

32	-1.690360000	0.005914000	0.128879000
9	-3.429001000	-0.012362000	-0.126290000
1	-1.492886000	-0.675825000	1.489879000
1	-1.131133000	-0.791207000	-1.064893000
1	-1.314797000	1.496840000	0.099264000
6	1.888765000	1.069375000	-1.313646000
1	1.210869000	0.783644000	-2.119299000
1	1.685518000	2.109559000	-1.057131000
1	2.917858000	0.982712000	-1.668287000
6	2.980588000	0.513033000	1.223597000
1	2.823327000	1.535730000	1.566710000
1	3.024428000	-0.133070000	2.100474000
1	3.932397000	0.457835000	0.691450000
6	2.225791000	-1.596423000	-0.485077000
1	2.265792000	-2.324133000	0.325721000
1	1.550985000	-1.981089000	-1.250574000
1	3.223869000	-1.484083000	-0.913372000
15	1.579030000	0.001945000	0.150886000

As(CH₃)₃···HF

9	-3.244763000	0.004465000	0.002480000
1	-2.308936000	0.005629000	0.004791000
33	0.069788000	0.001942000	0.001393000
6	1.020857000	-1.263934000	1.157519000
1	0.747373000	-1.084167000	2.196011000
1	0.735004000	-2.281136000	0.894576000
1	2.098441000	-1.148328000	1.040850000
6	1.015877000	-0.378606000	-1.673277000
1	0.730141000	-1.364653000	-2.035824000
1	0.738572000	0.360038000	-2.423633000
1	2.093767000	-0.348450000	-1.515226000
6	1.035433000	1.631441000	0.508326000
1	0.755147000	2.443284000	-0.160820000
1	0.765819000	1.911721000	1.525307000
1	2.111518000	1.468384000	0.450273000

As(CH₃)₃···BrF

9	3.410219000	0.000614000	0.000315000
35	1.494727000	-0.000670000	-0.000510000
33	-0.988921000	-0.000371000	-0.000186000
6	-1.814396000	0.808307000	1.559985000
1	-1.489050000	0.272450000	2.449563000
1	-1.489137000	1.844164000	1.633782000
1	-2.900046000	0.766019000	1.478376000

6	-1.817605000	0.948404000	-1.477701000
1	-1.491195000	1.986356000	-1.457384000
1	-1.494880000	0.495836000	-2.413331000
1	-2.903089000	0.899870000	-1.397446000
6	-1.819598000	-1.753710000	-0.080154000
1	-1.494745000	-2.256980000	-0.988767000
1	-1.496277000	-2.336434000	0.780232000
1	-2.905007000	-1.659135000	-0.076655000

As(CH₃)₃···SeF₂

9	1.393241000	1.372209000	-0.000302000
9	3.363125000	-0.103289000	0.000018000
34	1.603127000	-0.368787000	0.000093000
6	-1.642627000	1.812988000	-0.005679000
1	-1.207243000	2.275690000	0.877771000
1	-1.198849000	2.272850000	-0.886386000
1	-2.722603000	1.956207000	-0.010871000
6	-2.296823000	-0.712508000	-1.496382000
1	-1.886961000	-0.319161000	-2.424894000
1	-2.273293000	-1.800084000	-1.536143000
1	-3.326360000	-0.374785000	-1.379057000
6	-2.294451000	-0.702661000	1.502137000
1	-2.270280000	-1.789940000	1.549314000
1	-1.883288000	-0.302833000	2.427286000
1	-3.324369000	-0.366303000	1.384154000
33	-1.206574000	-0.085456000	-0.000067000

As(CH₃)₃···AsF₃

33	1.807242000	0.013463000	-0.440604000
9	1.448970000	-1.369432000	0.511551000
9	3.442106000	0.100092000	0.090716000
9	1.253214000	1.154962000	0.724026000
6	-2.228709000	1.758128000	0.218246000
1	-1.449466000	2.312175000	0.739677000
1	-2.485852000	2.290010000	-0.696439000
1	-3.110610000	1.684675000	0.854523000
6	-3.229170000	-0.841194000	-0.824866000
1	-3.519000000	-0.411939000	-1.782623000
1	-3.090124000	-1.913570000	-0.952388000
1	-4.019106000	-0.663891000	-0.095139000
6	-1.509647000	-0.758841000	1.600690000
1	-1.281345000	-1.822539000	1.560063000
1	-0.721086000	-0.260296000	2.162477000
1	-2.468736000	-0.604846000	2.094930000
33	-1.545065000	-0.029491000	-0.219582000

As(CH₃)₃···GeF₄

32	-1.334834000	-0.000171000	0.000128000
9	-1.133565000	-0.062863000	-1.718304000
9	-3.054758000	-0.000698000	0.003598000
9	-1.129639000	-1.459628000	0.910023000
9	-1.132491000	1.521145000	0.803037000
6	2.108049000	-1.555501000	-0.821706000
1	1.777592000	-2.446691000	-0.291192000
1	1.777728000	-1.617039000	-1.857088000
1	3.193752000	-1.480802000	-0.782063000
6	2.106133000	0.067741000	1.760235000
1	1.765299000	0.967741000	2.268823000
1	1.783788000	-0.803386000	2.327900000
1	3.192047000	0.076072000	1.678442000
6	2.104656000	1.489965000	-0.938589000
1	1.770419000	1.474154000	-1.974430000
1	1.775074000	2.417589000	-0.474178000
1	3.190689000	1.419471000	-0.897937000
33	1.291799000	0.000107000	0.000388000

As(CH₃)₃···SeFH

6	2.132800000	0.788409000	-1.467212000
1	1.723935000	0.428586000	-2.409619000
1	2.082003000	1.875613000	-1.455664000
1	3.170888000	0.471019000	-1.371861000
6	1.549433000	-1.817521000	-0.096239000
1	1.132519000	-2.337477000	0.764797000
1	1.124025000	-2.245662000	-1.002481000
1	2.632045000	-1.937076000	-0.107611000
6	2.142669000	0.630347000	1.536394000
1	2.094096000	1.712954000	1.637988000
1	1.738535000	0.175256000	2.438793000
1	3.179511000	0.322959000	1.402412000
9	-3.472692000	0.120372000	0.005593000
33	1.064395000	0.069086000	0.004330000
1	-1.523736000	1.430850000	0.080521000
34	-1.652178000	-0.025518000	-0.000240000

As(CH₃)₃···AsFH₂

33	1.895662000	0.025755000	0.006007000
1	1.725425000	0.914977000	-1.219738000
9	3.663977000	-0.039746000	-0.098599000
1	1.670588000	-1.248705000	-0.800275000
6	-1.691586000	-1.383717000	1.175019000

1	-1.585377000	-2.368045000	0.721476000
1	-1.004958000	-1.313466000	2.017727000
1	-2.714632000	-1.255904000	1.528184000
6	-1.829682000	1.562601000	0.883698000
1	-1.143875000	1.725274000	1.714089000
1	-1.817151000	2.444174000	0.244663000
1	-2.837462000	1.408612000	1.268890000
6	-2.794173000	-0.191588000	-1.317033000
1	-2.807975000	0.625366000	-2.036508000
1	-2.726011000	-1.132473000	-1.860545000
1	-3.713936000	-0.175870000	-0.732515000
33	-1.232867000	-0.001209000	-0.139588000

As(CH₃)₃···GeFH₃

32	-2.065816000	0.007640000	-0.132041000
9	-3.798599000	-0.013879000	0.135772000
1	-1.878631000	-0.439968000	-1.588332000
1	-1.640294000	1.460429000	0.139850000
1	-1.498858000	-0.986128000	0.899959000
6	1.538575000	0.906948000	1.577307000
1	1.300577000	1.963902000	1.465406000
1	0.839340000	0.469211000	2.289228000
1	2.554288000	0.802295000	1.958624000
6	2.144996000	-1.716642000	0.356913000
1	1.465320000	-2.239941000	1.028331000
1	2.296221000	-2.330118000	-0.529904000
1	3.100622000	-1.562460000	0.857892000
6	2.923215000	0.780343000	-1.040560000
1	3.100896000	0.267691000	-1.984564000
1	2.741254000	1.833819000	-1.247096000
1	3.802831000	0.682805000	-0.404437000
33	1.347552000	0.004090000	-0.158895000

Sb(CH₃)₃···HF

9	-3.501092000	0.001238000	-0.001667000
51	0.034434000	0.000626000	-0.000756000
1	-2.569157000	0.002151000	-0.002263000
6	1.136210000	-1.022744000	-1.538491000
1	0.882668000	-2.081555000	-1.535575000
1	0.886239000	-0.608107000	-2.513667000
1	2.205074000	-0.908254000	-1.362121000
6	1.138211000	1.843194000	-0.112185000
1	0.889303000	2.370789000	-1.031460000
1	0.884937000	2.480161000	0.733684000
1	2.206868000	1.632305000	-0.096452000
6	1.128855000	-0.825080000	1.656423000

1	0.876167000	-0.292074000	2.571528000
1	0.873334000	-1.875682000	1.784231000
1	2.198574000	-0.734996000	1.471185000

Sb(CH₃)₃···BrF

9	-3.697469000	-0.000509000	-0.000242000
35	-1.799769000	0.000681000	0.000269000
51	0.874151000	0.000326000	0.000207000
6	1.857511000	-0.403658000	-1.851912000
1	1.560061000	-1.385454000	-2.214763000
1	1.570489000	0.345635000	-2.586949000
1	2.936736000	-0.378986000	-1.706888000
6	1.857965000	-1.403664000	1.273490000
1	1.566748000	-1.224104000	2.306454000
1	1.565064000	-2.414025000	0.995167000
1	2.937137000	-1.295222000	1.173661000
6	1.862336000	1.803623000	0.576625000
1	1.569565000	2.608844000	-0.094170000
1	1.573587000	2.067981000	1.591917000
1	2.941163000	1.661636000	0.528552000

Sb(CH₃)₃···SeF₂

9	-1.532716000	-1.294359000	0.000190000
9	-3.652218000	-0.007799000	0.000093000
34	-1.939989000	0.413320000	-0.000099000
6	1.606214000	-1.169978000	-1.611963000
1	0.854377000	-1.955182000	-1.669936000
1	1.617618000	-0.622664000	-2.552756000
1	2.585884000	-1.613313000	-1.438179000
6	2.900895000	1.326753000	0.000736000
1	2.933222000	1.959522000	-0.884263000
1	2.932991000	1.958493000	0.886480000
1	3.763943000	0.661858000	0.000468000
6	1.605386000	-1.170596000	1.611603000
1	1.616347000	-0.623585000	2.552575000
1	0.853494000	-1.955798000	1.668909000
1	2.585109000	-1.613938000	1.438144000
51	1.102080000	0.148119000	-0.000056000

Sb(CH₃)₃···AsF₃

33	2.170993000	0.019950000	-0.445454000
9	1.771259000	-1.388080000	0.447093000
9	3.759926000	0.135962000	0.192090000
9	1.498730000	1.118996000	0.695781000
6	-2.051495000	1.908394000	0.461476000

1	-1.203681000	2.404648000	0.931670000
1	-2.399981000	2.518710000	-0.370190000
1	-2.855095000	1.799869000	1.189139000
6	-3.415458000	-0.764907000	-0.663341000
1	-3.816563000	-0.265962000	-1.544283000
1	-3.385117000	-1.836559000	-0.853872000
1	-4.067874000	-0.570435000	0.187314000
6	-1.266342000	-0.915649000	1.717265000
1	-1.104988000	-1.988821000	1.629997000
1	-0.412057000	-0.478949000	2.232474000
1	-2.174120000	-0.727599000	2.289544000
51	-1.433191000	-0.032984000	-0.237233000

Sb(CH₃)₃···GeF₄

32	-1.997489000	-0.001831000	-0.000208000
9	-3.698628000	0.009923000	0.000971000
6	2.514528000	-1.839700000	-0.056884000
1	2.266651000	-2.450995000	0.809212000
1	2.266977000	-2.396561000	-0.959043000
1	3.581336000	-1.619210000	-0.050077000
6	2.472259000	0.990569000	-1.572324000
1	2.227951000	0.539523000	-2.532584000
1	2.196543000	2.043374000	-1.601174000
1	3.543570000	0.903331000	-1.394985000
6	2.466478000	0.888269000	1.635081000
1	2.190585000	1.937211000	1.729316000
1	2.217753000	0.377471000	2.563784000
1	3.538523000	0.811917000	1.457154000
51	1.395469000	-0.005309000	-0.000825000
9	-1.586260000	-0.874314000	1.397382000
9	-1.587785000	-0.782803000	-1.451567000
9	-1.571632000	1.641470000	0.052314000

Sb(CH₃)₃···SeFH

9	3.801072000	-0.086107000	0.045422000
6	-2.229679000	0.251722000	1.741980000
1	-2.272720000	-0.650579000	2.349350000
1	-1.832560000	1.063803000	2.348282000
1	-3.233445000	0.507632000	1.404786000
6	-1.465369000	1.712645000	-1.037208000
1	-1.047475000	2.579880000	-0.528421000
1	-1.049454000	1.664122000	-2.042261000
1	-2.547801000	1.816755000	-1.098208000
6	-2.247442000	-1.423500000	-1.019147000
1	-1.861231000	-1.587211000	-2.023543000

1	-2.290311000	-2.379385000	-0.500142000
1	-3.249318000	-1.000289000	-1.080643000
1	1.867487000	-1.257650000	0.721315000
51	-0.959260000	-0.069679000	0.040060000
34	1.996600000	0.009597000	-0.003415000

Sb(CH₃)₃···AsFH₂

33	-2.297424000	0.010480000	-0.041868000
1	-2.060954000	1.029327000	1.068558000
9	-4.054573000	-0.017215000	0.133593000
1	-2.043859000	-1.162244000	0.900677000
6	1.806832000	-1.516350000	-1.250356000
1	1.713629000	-2.500321000	-0.793353000
1	1.208479000	-1.497376000	-2.160044000
1	2.851100000	-1.334995000	-1.502460000
6	1.894742000	1.668563000	-0.999601000
1	1.308285000	1.817091000	-1.905072000
1	1.842898000	2.575267000	-0.398930000
1	2.932269000	1.475974000	-1.270475000
6	2.762238000	-0.154492000	1.485517000
1	2.743975000	0.680000000	2.184624000
1	2.691800000	-1.082943000	2.049851000
1	3.700909000	-0.139960000	0.932648000
51	1.110485000	-0.000727000	0.110979000

Sb(CH₃)₃···GeFH₃

32	2.444206000	0.000016000	-0.128010000
9	4.173012000	-0.000031000	0.142155000
1	2.261216000	0.000894000	-1.652732000
1	1.924538000	-1.280292000	0.551014000
1	1.924396000	1.279465000	0.552526000
6	-1.236939000	0.000682000	1.992293000
1	-0.723818000	-0.883163000	2.369452000
1	-0.724450000	0.885135000	2.368884000
1	-2.264624000	0.000429000	2.354138000
6	-2.640292000	1.596634000	-0.393162000
1	-2.189636000	2.543662000	-0.100222000
1	-2.956379000	1.669253000	-1.432606000
1	-3.509961000	1.403807000	0.234094000
6	-2.639602000	-1.597369000	-0.392137000
1	-2.956231000	-1.670216000	-1.431401000
1	-2.188332000	-2.544149000	-0.099355000
1	-3.509027000	-1.404893000	0.235565000
51	-1.210949000	0.000003000	-0.164204000

Optimized coordinates of the monomers

NH₃

1	2.558688	-0.014591	0.941223
1	2.559356	-0.807151	-0.484853
1	2.555678	0.823913	-0.458145
7	2.187317	-0.000188	-0.000242

PH₃

1	1.801963	-0.939007	-0.726161
1	1.805583	1.097843	-0.446652
1	1.799266	-0.162011	1.177375
15	1.037894	0.000070	-0.000265

AsH₃

1	-2.968647	-0.501406	-1.095521
1	-2.966587	-0.497005	1.099036
1	-2.542072	1.357325	-0.002392
33	-2.004918	-0.067771	-0.000013

SbH₃

1	2.297066	-0.349431	1.370789
1	2.274742	-1.016156	-1.003698
1	2.275069	1.371936	-0.392851
51	1.338192	-0.000694	0.001122

N(CH₃)₃

7	1.428240	0.030616	-0.000731
6	1.868541	-0.641102	1.204206
1	1.494496	-0.111549	2.081179
1	1.477896	-1.659141	1.225134
1	2.969187	-0.692208	1.275500
6	1.869609	-0.683513	-1.180617
1	1.480654	-1.702259	-1.163931
1	1.494370	-0.186894	-2.076169
1	2.970309	-0.735400	-1.250086
6	1.891416	1.402448	-0.024902
1	1.517798	1.904138	-0.918312
1	1.517538	1.935413	0.850053
1	2.993390	1.471129	-0.025896

P(CH₃)₃

6	1.868323	-1.317709	-1.034914
1	1.723814	-2.297224	-0.578036
1	1.243219	-1.269129	-1.927013

1	2.915382	-1.213570	-1.328363
6	1.974264	1.466384	-0.779474
1	1.353075	1.627845	-1.661027
1	1.900935	2.354632	-0.151240
1	3.012438	1.338939	-1.094755
6	2.738095	-0.166026	1.361598
1	2.698672	0.657430	2.075386
1	2.626929	-1.097063	1.918220
1	3.712512	-0.161629	0.867543
15	1.357037	-0.001306	0.150732

As(CH₃)₃

6	-1.691010	-1.374405	1.163664
1	-1.594198	-2.362572	0.715634
1	-1.021164	-1.317874	2.020808
1	-2.718391	-1.230036	1.499058
6	-1.829169	1.551282	0.874966
1	-1.162817	1.727621	1.718469
1	-1.823658	2.437046	0.240985
1	-2.840433	1.378874	1.244372
6	-2.785669	-0.189274	-1.296891
1	-2.815594	0.625065	-2.019705
1	-2.734610	-1.131160	-1.841679
1	-3.694389	-0.170091	-0.694619
33	-1.188584	-0.000721	-0.157505

Sb(CH₃)₃

6	1.809742	-1.501892	-1.253461
1	1.737296	-2.495803	-0.813542
1	1.211075	-1.482311	-2.163167
1	2.850048	-1.296716	-1.505350
6	1.858760	1.663533	-0.967628
1	1.263586	1.825001	-1.865452
1	1.814891	2.564716	-0.357348
1	2.893464	1.475159	-1.253403
6	2.791597	-0.166118	1.458652
1	2.780947	0.653056	2.176299
1	2.759962	-1.106380	2.007517
1	3.712384	-0.121690	0.877565
51	1.083889	-0.020824	0.142644

HF

9	2.729702	0.000561	-0.000233
1	1.809460	-0.014463	0.010082

BrF

9	2.812059	-0.000873	-0.001074
35	1.060917	0.000382	0.000487

SeF₂

9	0.921751	1.425538	-0.000028
9	2.935003	-0.161339	0.000184
34	1.213448	-0.274865	-0.000068

AsF₃

33	-1.726184	-0.000142	-0.359150
9	-1.236907	1.226146	0.727077
9	-3.384453	0.074445	0.048831
9	-1.356798	-1.301156	0.687485

GeF₄

32	-0.736336	-0.000478	-0.000652
9	-0.178335	-0.348391	-1.557523
9	-2.426511	-0.003796	0.002743
9	-0.170301	-1.169993	1.079708
9	-0.174482	1.520826	0.473325

SeFH

9	2.375021	0.129655	0.001805
34	0.637775	-0.088432	-0.000681
1	0.346402	1.353038	-0.003684

AsFH₂

33	0.758105	-0.130548	0.042359
9	2.471816	0.207555	-0.056305
1	0.381903	1.206738	0.678940
1	0.424354	0.398128	-1.351952

GeFH₃

32	1.958809	0.002824	0.003675
9	3.700544	-0.009972	-0.012557
1	1.530315	-0.847258	1.212659
1	1.536547	1.474861	0.145076
1	1.505154	-0.609243	-1.332964