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Electronic Supplementary Information

Strategies toward Realization of Unsupported Transition Metal-Boron Donor-Acceptor Complexes: An Insight from Theory

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Computational Details: Density functional theory calculations were performed to optimize all the molecules in solvent phase using the M062X meta hybrid exchange correlation functional.[1] We used 6-311+G* basis set for lighter main group elements and the SDD basis set with the Stuttgart–Dresden relativistic effective core potential for indium and platinum atoms.[2] Solvent (dichloromethane) and dispersion effects were evaluated for these molecules using polarizable continuum model (PCM)[3] and D3 version of Grimme's dispersion correction coupled with D3 damping function using the keyword "Empirical Dispersion = GD3" as implemented in Gaussian 09 suite of programs.[4] Frequency calculations were carried out at the same level of theory to characterize the nature of the stationary points on the potential energy surface and all of them are found to be minima with real vibrational frequencies.

In order to understand the bonding interactions between the neutral donor (**1**-**2**) and acceptor (**B1**-**B6**) fragments, we performed energy decomposition analysis (EDA) in conjunction with the natural orbital for chemical valence (NOCV) at the Gaussian optimized geometries using the Amsterdam Density Functional (ADF) program.[5] All these calculations were carried out at the BP86(D3)/TZ2P level of theory where dispersion corrections have been incorporated by using the Grimme's DFT-D3-BJDAMP term.[6] Scalar relativistic effects were considered by applying the zero-order regular approximation (ZORA).[7] Core electrons (i.e., 1s for second-, [He]2s2p for third-row elements and [Kr]4d for platinum) were treated by the frozen-core approximation. EDA focuses on the instantaneous interaction energy (ΔE_{int}) associated with the interaction between the donor and acceptor fragments which can be divided into four components: $\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$. The ΔE_{elstat} corresponds to the electrostatic interaction energy between the fragments calculated by means of the frozen electron density distribution of the fragments in the geometry of the molecules. ΔE_{Pauli} refers to the repulsive

interactions between the fragments which are caused by the destabilizing interactions between occupied orbitals of both the fragments while ΔE_{orb} refers to the stabilizing orbital interactions.

Calculation of Preparation Energy: The preparation energy (E_{prep}) is calculated using the following equation:

$$E_{prep} = E_{frag}(SP) - E_{frag}(eq)$$

Here, $E_{frag}(SP)$ is the single point energy of a fragment in a particular donor-acceptor complex while $E_{frag}(eq)$ is the total energy of that fragment in its equilibrium geometry. $E_{frag}(SP)$ is calculated by considering the geometry of the fragment from a particular donor-acceptor complex.

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Table S1: Calculated values of bond angle around boron (θ_B = 360º-Σ(∠EBE), where E=C/O/S) in all the acceptor fragments (**B1**-**B6**).

Fragment	θ_B(°)
B1	21.0
B2	13.9
B3	13.8
B4	14.3
B5	5.7
B6	8.0

Table S2: Calculated values of percentage contribution of platinum (% Pt) and boron (% B) in the Pt→B dative bond.

Molecule	% Pt	%s(Pt)	%p(Pt)	%d(Pt)	% B	%s(B)	%p(B)
1-B1	64.75	47.45	0.97	51.57	35.25	21.14	78.70
1-B2	64.70	47.20	0.99	51.82	35.30	19.55	80.29
1-B3	64.96	47.45	1.00	51.55	35.04	19.38	80.46
1-B4	63.36	47.07	1.00	51.93	36.64	20.25	79.61
1-B5	66.94	46.80	0.96	52.23	33.06	20.92	78.80
1-B6	58.24	48.13	1.04	50.83	41.76	24.31	75.52
2-B1	64.93	50.57	0.61	48.82	35.07	20.86	78.99
2-B2	64.82	50.73	0.67	48.59	35.18	19.23	80.63
2-B3	65.28	50.72	0.65	48.63	34.72	18.99	80.86
2-B4	63.52	50.39	0.65	48.96	36.48	19.92	79.96
2-B5	65.97	48.01	0.40	51.59	34.03	29.49	70.28
2-B6	57.83	50.13	0.44	49.44	42.17	24.36	75.48

Table S3: Calculated (BP86(D3)/TZ2P) values of NOCV stabilization energies (in kcal mol^{-1}) corresponding to σ-donation (E_σ) and π-back donation (E_π).

Molecule	E_σ	E_π	Molecule	E_σ	E_π
1-B1	-76.0	-3.4	**2-B1**	-70.8	-3.4
1-B2	-74.7	-3.6	**2-B2**	-70.1	-3.7
1-B3	-73.5	-3.4	**2-B3**	-68.7	-3.6
1-B4	-78.1	-3.8	**2-B4**	-73.5	-4.0
1-B5	-85.6	-5.4	**2-B5**	-83.6	-5.8
1-B6	-100.5	-7.0	**2-B6**	-96.8	-7.5

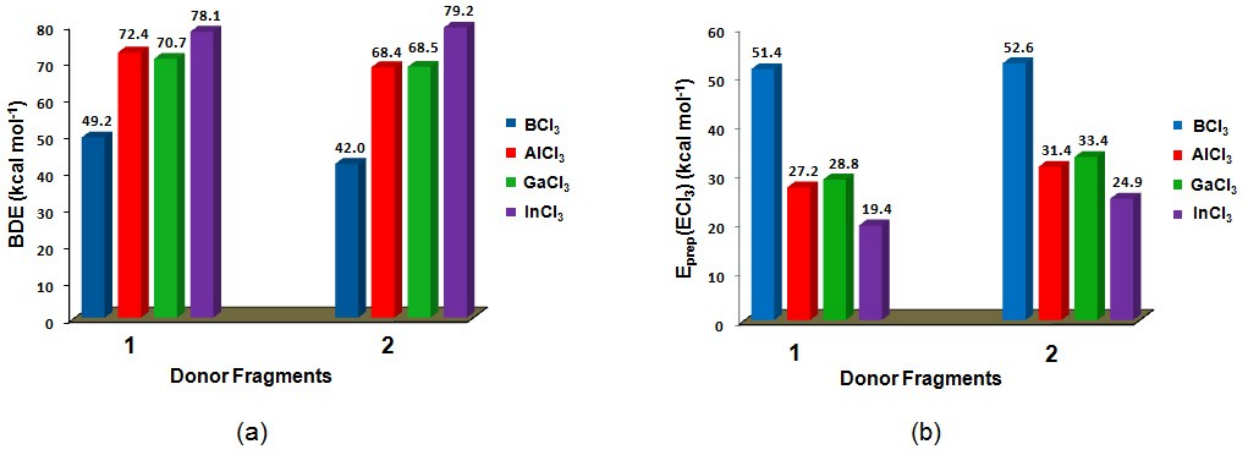

Fig S1: Bar diagrams representing the variation of (a) bond dissociation energies (BDE) and (b) preparation energies ($E_{prep}(ECl_3)$) of group 13 halides as a function of different donor fragments.

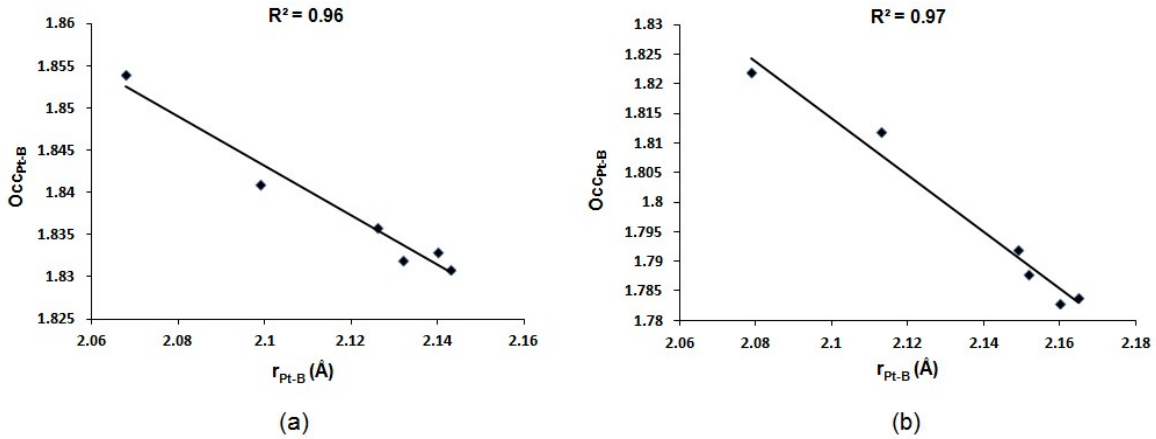

Fig. S2: Correlation plots between Pt-B bond lengths (r_{Pt-B}) and the respective occupancies (Occ_{Pt-B}) for (a) **1**-**Bn** and (b) **2**-**Bn** complexes where **Bn** = **B1**-**B6**.

Cartesian coordinates of all the complexes along with their total energies (T. E. in hartrees) including zero point vibrational correction.

BCl_3, T. E. = -1405.554827

B	0.000000000	0.000000000	-0.000159000
Cl	0.000000000	0.000000000	1.743108000
Cl	0.000000000	1.510000000	-0.871531000
Cl	0.000000000	-1.510000000	-0.871531000

$AlCl_3$, T. E. = -1623.220468

Cl	0.000000000	0.000000000	2.071860000
Cl	0.000000000	1.794940000	-1.035778000
Cl	0.000000000	-1.794940000	-1.035778000
Al	0.000000000	0.000000000	-0.000397000

$GaCl_3$, T. E. = -3305.582396

Cl	0.000000000	0.000000000	-2.132197000
Cl	0.000000000	1.846723000	1.065997000
Cl	0.000000000	-1.846723000	1.065997000
Ga	0.000000000	0.000000000	0.000112000

$InCl_3$, T. E. = -1382.636034

Cl	0.000000000	0.000000000	2.293212000
Cl	0.000000000	1.984485000	-1.147068000
Cl	0.000000000	-1.984485000	-1.147068000
In	0.000000000	0.000000000	0.000321000

B1, T. E. = -406.924805

B	0.000000000	0.000000000	-1.172579000
C	0.000000000	-1.517511000	-0.747299000
H	-0.950268000	-2.048490000	-0.829982000
H	0.807327000	-2.140819000	-1.130589000
C	-1.314203000	0.758755000	-0.747299000

H	-1.298910000	1.847202000	-0.829982000
H	-2.257667000	0.371244000	-1.130589000
C	1.314203000	0.758755000	-0.747299000
H	1.450340000	1.769575000	-1.130589000
H	2.249178000	0.201288000	-0.829982000
C	0.000000000	0.000000000	1.110483000
H	0.000000000	0.000000000	2.197372000
O	0.983674000	0.901760000	0.680655000
O	0.289110000	-1.302767000	0.680655000
O	-1.272784000	0.401007000	0.680655000

B2, T. E. = -658.443935

B	0.000000000	0.000000000	-1.298727000
C	1.224775000	-0.959259000	-0.950496000
H	1.056640000	-2.022459000	-1.132623000
H	2.186776000	-0.671640000	-1.376523000
C	-1.443130000	-0.581057000	-0.950496000
H	-2.279821000	0.096152000	-1.132623000
H	-1.675045000	-1.557983000	-1.376523000
C	0.218355000	1.540315000	-0.950496000
H	-0.511731000	2.229623000	-1.376523000
H	1.223181000	1.926307000	-1.132623000
H	0.000000000	0.000000000	2.624776000
O	0.000000000	1.523056000	0.504828000
O	1.319006000	-0.761528000	0.504828000
O	-1.319006000	-0.761528000	0.504828000
Si	0.000000000	0.000000000	1.170668000

B3, T. E. = -697.739602

B	0.000000000	0.000000000	-1.635741000
C	1.215646000	-0.969350000	-1.288921000
H	1.035386000	-2.032276000	-1.464770000
H	2.178259000	-0.695147000	-1.723719000
C	-1.447305000	-0.568105000	-1.288921000
H	-2.277696000	0.119467000	-1.464770000
H	-1.691144000	-1.538854000	-1.723719000

C	0.231659000	1.537455000	-1.288921000
H	-0.487115000	2.234001000	-1.723719000
H	1.242310000	1.912809000	-1.464770000
O	0.000000000	1.521864000	0.161517000
O	1.317973000	-0.760932000	0.161517000
O	-1.317973000	-0.760932000	0.161517000
Si	0.000000000	0.000000000	0.846008000
C	0.000000000	0.000000000	2.674636000
H	-0.803799000	0.630197000	3.058806000
H	-0.143867000	-1.011208000	3.058806000
H	0.947666000	0.381012000	3.058806000

B4, T. E. = -1118.107262

B	0.000000000	0.000000000	-1.906365000
C	-1.220432000	0.965986000	-1.552135000
H	-1.046453000	2.029257000	-1.724781000
H	-2.184283000	0.684262000	-1.976602000
C	1.446784000	0.573932000	-1.552135000
H	2.280615000	-0.108373000	-1.724781000
H	1.684730000	1.549514000	-1.976602000
C	-0.226352000	-1.539918000	-1.552135000
H	0.499553000	-2.233776000	-1.976602000
H	-1.234162000	-1.920884000	-1.724781000
O	0.000000000	-1.525499000	-0.093024000
O	-1.321121000	0.762749000	-0.093024000
O	1.321121000	0.762749000	-0.093024000
Si	0.000000000	0.000000000	0.536375000
Cl	0.000000000	0.000000000	2.546925000

B5, T. E. = -407.062270

B	-0.000893000	0.001339000	-1.036223000
C	-1.202023000	0.792411000	0.600848000
H	-1.246014000	1.796440000	1.023231000
H	-2.143324000	0.270057000	0.786162000
C	1.289275000	0.643179000	0.599063000
H	1.310812000	1.719149000	0.786667000

H	2.180861000	0.176259000	1.017952000
C	-0.085441000	-1.438460000	0.597607000
H	-0.933389000	-1.978998000	1.018357000
H	0.837417000	-1.993468000	0.781245000
C	0.000771000	-0.001233000	1.159652000
H	0.001301000	-0.002365000	2.250935000
O	1.310492000	0.402872000	-0.843343000
O	-0.308830000	-1.335088000	-0.844093000
O	-1.003999000	0.936072000	-0.840870000

B6, T. E. = -1375.922367

B	0.000059000	-0.000010000	-1.008954000
C	1.427860000	-0.363083000	1.053994000
H	1.816711000	-1.187367000	1.651365000
H	2.093692000	0.494520000	1.143485000
C	-1.029117000	-1.054914000	1.054577000
H	-0.621865000	-2.061412000	1.145227000
H	-1.937702000	-0.976230000	1.651155000
C	-0.399496000	1.417907000	1.054755000
H	0.121435000	2.165658000	1.652345000
H	-1.475002000	1.567282000	1.143682000
C	-0.000023000	-0.000576000	1.498774000
H	0.000388000	-0.000839000	2.595471000
S	-1.626987000	-0.796163000	-0.706771000
S	1.503543000	-1.010710000	-0.706256000
S	0.123864000	1.807025000	-0.706383000

1, T. E. = -728.574258

Pt	0.000005000	0.000020000	0.000000000
C	-2.022106000	0.000003000	0.000010000
C	-4.191586000	0.491140000	-0.464656000
C	-4.191571000	-0.491178000	0.464705000
H	-5.003377000	1.006221000	-0.951602000
H	-5.003346000	-1.006267000	0.951671000
C	-2.436550000	1.796931000	-1.677666000
H	-2.870475000	1.606026000	-2.659674000

H	-2.744203000	2.784071000	-1.330521000
H	-1.351050000	1.752020000	-1.738488000
C	-2.436495000	-1.796984000	1.677636000
H	-2.870494000	-1.606184000	2.659631000
H	-2.744052000	-2.784121000	1.330401000
H	-1.351001000	-1.751993000	1.738527000
N	-2.867026000	0.776330000	-0.735935000
N	-2.867003000	-0.776347000	0.735959000
C	2.022102000	-0.000006000	0.000003000
C	4.191582000	0.491089000	0.464715000
C	4.191566000	-0.491161000	-0.464719000
H	5.003373000	1.006144000	0.951688000
H	5.003340000	-1.006248000	-0.951687000
N	2.866997000	-0.776283000	-0.736025000
N	2.867023000	0.776265000	0.736008000
C	2.436480000	-1.796966000	-1.677647000
H	2.871439000	-1.606860000	-2.659348000
H	2.742991000	-2.784216000	-1.329799000
H	1.351068000	-1.751200000	-1.739440000
C	2.436538000	1.796964000	1.677629000
H	2.871277000	1.606698000	2.659397000
H	2.743310000	2.784178000	1.329911000
H	1.351107000	1.751399000	1.739221000

2, T. E. = -1317.766007

C	1.951949000	-0.762749000	0.414819000
N	-2.822861000	0.117663000	0.048736000
C	2.712662000	-1.712315000	1.334164000
N	2.823085000	0.114511000	-0.049563000
C	4.094540000	-1.050852000	1.532940000
H	4.133563000	-0.558341000	2.508400000
H	4.910170000	-1.776702000	1.499481000
C	4.241348000	0.003911000	0.422245000
C	2.438613000	1.160656000	-0.954766000
C	1.462264000	3.328877000	-1.312991000
H	0.999272000	4.226493000	-0.918436000
C	1.847513000	2.313374000	-0.445676000
C	1.666495000	3.192423000	-2.684535000

H	1.362889000	3.984412000	-3.359668000
C	2.251606000	2.034260000	-3.187348000
H	2.398702000	1.917162000	-4.255010000
C	2.639746000	1.014107000	-2.322679000
C	1.973653000	-1.887295000	2.661333000
H	2.556594000	-2.527223000	3.331137000
H	0.994624000	-2.342990000	2.499030000
H	1.818985000	-0.923750000	3.153939000
C	2.815499000	-3.070346000	0.624955000
H	3.378797000	-3.770568000	1.248577000
H	3.322746000	-2.988212000	-0.339608000
H	1.819255000	-3.480808000	0.446397000
C	4.723261000	1.348012000	0.961034000
H	5.712330000	1.222336000	1.407880000
H	4.044168000	1.724279000	1.729587000
H	4.801883000	2.094981000	0.167686000
C	5.148149000	-0.458517000	-0.718310000
H	6.159883000	-0.609915000	-0.334969000
H	5.200703000	0.289106000	-1.512873000
H	4.798511000	-1.399801000	-1.147092000
C	-1.953370000	-0.760247000	-0.417462000
C	-2.716680000	-1.709002000	-1.335493000
C	-4.098387000	-1.046325000	-1.531300000
H	-4.138632000	-0.552845000	-2.506229000
H	-4.914577000	-1.771518000	-1.497137000
C	-4.242354000	0.007530000	-0.419407000
C	-2.436144000	1.161714000	0.955429000
C	-2.628309000	1.008839000	2.323977000
C	-2.237524000	2.026324000	3.190513000
H	-2.377484000	1.904301000	4.258590000
C	-1.658681000	3.188193000	2.688876000
H	-1.352819000	3.978086000	3.365453000
C	-1.463758000	3.331164000	1.316671000
H	-1.005948000	4.231868000	0.923058000
C	-1.851720000	2.318269000	0.447447000
C	-5.145683000	-0.455742000	0.723574000
H	-4.795468000	-1.397931000	1.149874000
H	-6.158928000	-0.605565000	0.343639000
H	-5.194465000	0.290823000	1.519395000
C	-4.726042000	1.351934000	-0.955778000

H	-5.716361000	1.226367000	-1.399873000
H	-4.049300000	1.728862000	-1.726060000
H	-4.802549000	2.098302000	-0.161660000
C	-2.819274000	-3.067045000	-0.626227000
H	-3.385055000	-3.766434000	-1.248529000
H	-3.323835000	-2.984523000	0.339705000
H	-1.823073000	-3.478739000	-0.450347000
C	-1.980367000	-1.884560000	-2.664066000
H	-2.564806000	-2.524430000	-3.332616000
H	-1.001211000	-2.340614000	-2.503483000
H	-1.826291000	-0.921210000	-3.157196000
H	-3.052665000	0.087072000	2.705883000
H	-1.683321000	2.402401000	-0.620653000
H	1.672124000	2.392486000	0.621688000
H	3.068696000	0.095115000	-2.706063000
Pt	-0.000547000	-0.799296000	-0.002151000

1-BCl_3, T. E. = -2134.207539

Pt	0.001330000	0.012130000	-0.620833000
B	0.064045000	-0.032629000	1.413856000
Cl	1.796480000	-0.038904000	2.202591000
Cl	-0.824564000	1.477337000	2.140749000
Cl	-0.802850000	-1.587737000	2.067082000
C	2.022365000	0.017059000	-0.757866000
C	4.166016000	0.697849000	-0.678976000
C	4.168850000	-0.657113000	-0.704522000
H	4.976244000	1.406613000	-0.643159000
H	4.981987000	-1.363338000	-0.696064000
N	2.844320000	1.089427000	-0.731322000
N	2.848804000	-1.052024000	-0.771512000
C	2.372323000	2.457743000	-0.572423000
H	1.588667000	2.659424000	-1.299998000
H	1.973657000	2.589165000	0.434700000
H	3.204879000	3.139584000	-0.734053000
C	2.383383000	-2.427722000	-0.664602000
H	1.599263000	-2.605067000	-1.398021000
H	3.219035000	-3.098650000	-0.853807000
H	1.987108000	-2.600139000	0.337355000

C	-2.061169000	0.013165000	-0.596777000
C	-4.215995000	-0.657273000	-0.616313000
C	-4.212375000	0.695453000	-0.589637000
H	-5.028513000	-1.364498000	-0.629914000
H	-5.021086000	1.407036000	-0.574658000
N	-2.894776000	-1.054634000	-0.628575000
N	-2.889078000	1.085871000	-0.586282000
C	-2.480973000	-2.449898000	-0.682926000
H	-2.819789000	-2.972300000	0.210777000
H	-2.902870000	-2.919276000	-1.571742000
H	-1.395397000	-2.484131000	-0.722874000
C	-2.467812000	2.479976000	-0.586245000
H	-2.888570000	2.986122000	-1.455220000
H	-2.803195000	2.968636000	0.327579000
H	-1.382062000	2.510090000	-0.626830000

1-$AlCl_3$, T. E. = -2351.910140

Pt	0.000758000	-0.698417000	-0.513276000
Cl	1.836521000	1.512110000	1.960330000
Cl	-0.198093000	3.013112000	-0.436657000
Cl	-1.626245000	1.325401000	2.252380000
C	2.031877000	-0.667660000	-0.452272000
C	4.191071000	-0.092373000	-0.742478000
C	4.139695000	-0.981664000	0.277989000
H	5.023637000	0.417077000	-1.198074000
H	4.919519000	-1.401030000	0.891183000
N	2.894428000	0.077724000	-1.182049000
N	2.815012000	-1.329942000	0.430605000
C	2.502022000	1.032378000	-2.210412000
H	1.523362000	0.750867000	-2.592671000
H	2.444540000	2.035124000	-1.785413000
H	3.232773000	1.012501000	-3.017614000
C	2.297537000	-2.170839000	1.500665000
H	1.543689000	-2.847141000	1.102634000
H	3.118039000	-2.748561000	1.922054000
H	1.853138000	-1.543879000	2.274856000
C	-2.033030000	-0.647428000	-0.433857000
C	-4.138782000	-0.974930000	0.298777000

C	-4.197498000	-0.088446000	-0.723549000
H	-4.914607000	-1.394758000	0.916716000
H	-5.033207000	0.415663000	-1.179480000
N	-2.811414000	-1.312172000	0.452422000
N	-2.901852000	0.094247000	-1.161009000
C	-2.292095000	-2.176310000	1.503689000
H	-1.820223000	-1.569648000	2.276888000
H	-3.118296000	-2.740422000	1.932362000
H	-1.562285000	-2.865552000	1.083168000
C	-2.534849000	0.989365000	-2.250239000
H	-3.076855000	0.708778000	-3.153023000
H	-2.769923000	2.017865000	-1.978952000
H	-1.463656000	0.902461000	-2.415675000
Al	0.005016000	1.217311000	0.797998000

1-$GaCl_3$, T. E. = -4034.269337

Pt	-0.018441000	-0.973218000	0.244124000
Cl	-1.843173000	2.112982000	-1.335111000
Cl	0.243358000	2.639084000	1.514595000
Cl	1.716069000	1.965673000	-1.665403000
C	-2.046846000	-0.882848000	0.203343000
C	-4.180843000	-0.434798000	0.767900000
C	-4.173763000	-0.815226000	-0.532182000
H	-4.990509000	-0.143828000	1.415609000
H	-4.974623000	-0.917051000	-1.245090000
N	-2.872388000	-0.487758000	1.200361000
N	-2.862930000	-1.096103000	-0.853549000
C	-2.417544000	-0.122724000	2.536904000
H	-1.886711000	-0.959164000	2.988834000
H	-1.754923000	0.740652000	2.478887000
H	-3.285955000	0.124855000	3.143677000
C	-2.400995000	-1.417622000	-2.196210000
H	-1.506951000	-2.032895000	-2.126866000
H	-3.182645000	-1.965067000	-2.720139000
H	-2.169040000	-0.497039000	-2.733463000
C	2.016937000	-0.892506000	0.213299000
C	4.132847000	-0.902152000	-0.561229000
C	4.168003000	-0.441006000	0.711543000

H	4.919276000	-1.056359000	-1.280931000
H	4.991409000	-0.121562000	1.328175000
N	2.813218000	-1.182914000	-0.842453000
N	2.866325000	-0.445123000	1.168475000
C	2.324065000	-1.609854000	-2.146258000
H	2.001144000	-0.741575000	-2.721328000
H	3.126735000	-2.124067000	-2.671925000
H	1.486673000	-2.290381000	-2.009731000
C	2.481375000	-0.032551000	2.512232000
H	2.894587000	-0.725994000	3.244808000
H	2.850602000	0.973807000	2.705006000
H	1.395768000	-0.030370000	2.573339000
Ga	0.016718000	1.331176000	-0.319864000

1-$InCl_3$, T. E. = -2111.334729

Pt	-0.000731000	-1.108032000	0.352288000
Cl	-1.931306000	1.939057000	-1.600963000
Cl	0.028453000	2.782522000	1.528869000
Cl	1.905425000	1.932345000	-1.645376000
C	-2.030730000	-1.004741000	0.282366000
C	-4.182284000	-0.475451000	0.696627000
C	-4.129747000	-1.029565000	-0.537757000
H	-5.011987000	-0.095574000	1.268890000
H	-4.904804000	-1.224274000	-1.259997000
N	-2.891675000	-0.473960000	1.183555000
N	-2.810396000	-1.353455000	-0.768680000
C	-2.508363000	0.115010000	2.460322000
H	-1.478631000	-0.162278000	2.672793000
H	-2.580401000	1.201472000	2.402782000
H	-3.162854000	-0.259276000	3.246256000
C	-2.294563000	-1.853745000	-2.035447000
H	-1.477870000	-2.545692000	-1.842901000
H	-3.093505000	-2.371909000	-2.562536000
H	-1.933505000	-1.020473000	-2.640215000
C	2.029286000	-1.004611000	0.279888000
C	4.127953000	-1.026683000	-0.541123000
C	4.182144000	-0.483482000	0.698046000
H	4.902371000	-1.216648000	-1.265313000

H	5.012897000	-0.110783000	1.273524000
N	2.807941000	-1.345946000	-0.774452000
N	2.891619000	-0.482771000	1.185128000
C	2.292375000	-1.838676000	-2.044419000
H	1.937243000	-1.001552000	-2.647297000
H	3.090006000	-2.359138000	-2.571274000
H	1.471832000	-2.527186000	-1.856271000
C	2.511574000	0.089743000	2.470414000
H	3.155698000	-0.309302000	3.252808000
H	2.601656000	1.175566000	2.432431000
H	1.476269000	-0.174237000	2.672521000
In	0.000827000	1.285250000	-0.347144000

1-B1, T. E. = -1135.588737

Pt	0.012565000	-0.881073000	0.044741000
C	2.039071000	-0.911320000	0.023049000
C	4.167495000	-0.852776000	-0.734717000
C	4.216221000	-0.796460000	0.617208000
H	4.953069000	-0.850869000	-1.471822000
H	5.051789000	-0.737809000	1.294602000
C	2.321472000	-0.920474000	-2.439844000
H	1.853557000	0.042579000	-2.648715000
H	3.149010000	-1.082355000	-3.127805000
H	1.583608000	-1.710754000	-2.562933000
C	2.525350000	-0.738218000	2.459432000
H	3.025648000	-1.513082000	3.039897000
H	2.799413000	0.243522000	2.847531000
H	1.447118000	-0.865566000	2.523346000
N	2.832966000	-0.934369000	-1.076829000
N	2.909266000	-0.842427000	1.059954000
C	-2.026451000	-0.873094000	0.022236000
C	-4.199256000	-0.844469000	0.649773000
C	-4.169368000	-0.886818000	-0.702247000
H	-5.026002000	-0.812236000	1.339714000
H	-4.964625000	-0.900250000	-1.429056000
N	-2.837716000	-0.907627000	-1.065795000
N	-2.884938000	-0.841174000	1.072724000
C	-2.375415000	-0.944699000	-2.445425000

H	-2.597909000	-1.914194000	-2.891991000
H	-2.866060000	-0.156923000	-3.016850000
H	-1.300008000	-0.777369000	-2.444538000
C	-2.487994000	-0.785769000	2.471816000
H	-2.959343000	0.070381000	2.954377000
H	-2.784283000	-1.702262000	2.982515000
H	-1.406592000	-0.674095000	2.512549000
B	0.021054000	1.244399000	-0.018460000
C	-0.765484000	1.901972000	1.245390000
H	-1.839864000	1.676215000	1.269803000
H	-0.347776000	1.644801000	2.227489000
C	-0.736795000	1.845544000	-1.327280000
H	-0.249364000	1.623271000	-2.286731000
H	-1.787647000	1.543463000	-1.411081000
C	1.492742000	1.944401000	-0.010647000
H	2.138635000	1.661790000	-0.851608000
H	2.064312000	1.774935000	0.912293000
C	-0.046758000	3.753610000	-0.072433000
H	-0.081152000	4.842475000	-0.096263000
O	1.298841000	3.389794000	-0.123934000
O	-0.648621000	3.356911000	1.124236000
O	-0.751085000	3.304122000	-1.191609000

1-B2, T. E. = -1387.107028

Pt	0.016338000	-0.960047000	-0.022065000
C	2.046089000	-1.026056000	-0.012086000
C	4.215042000	-1.019967000	-0.648259000
C	4.189850000	-1.080488000	0.703622000
H	5.039493000	-1.001531000	-1.341414000
H	4.987816000	-1.122299000	1.426245000
C	2.497521000	-0.884144000	-2.459706000
H	2.959548000	-0.003251000	-2.906000000
H	2.800756000	-1.774050000	-3.011505000
H	1.414918000	-0.781504000	-2.491770000
C	2.395963000	-1.052426000	2.450461000
H	3.061332000	-1.648322000	3.073513000
H	2.381996000	-0.022256000	2.810464000
H	1.388939000	-1.460694000	2.491031000

N	2.899640000	-0.995171000	-1.065698000
N	2.859675000	-1.096509000	1.071850000
C	-2.022430000	-1.009591000	-0.011383000
C	-4.183191000	-1.120245000	-0.673061000
C	-4.173854000	-1.122565000	0.679769000
H	-4.998168000	-1.157344000	-1.376737000
H	-4.978855000	-1.164630000	1.394628000
N	-2.849422000	-1.058955000	1.064536000
N	-2.864197000	-1.056759000	-1.075517000
C	-2.414703000	-1.055183000	2.453699000
H	-2.913894000	-0.250831000	2.993818000
H	-2.650088000	-2.011454000	2.921538000
H	-1.339440000	-0.891406000	2.471406000
C	-2.448881000	-1.020900000	-2.469897000
H	-2.766297000	-1.932751000	-2.975863000
H	-2.887919000	-0.155009000	-2.965693000
H	-1.364158000	-0.942821000	-2.496200000
B	0.013076000	1.179888000	0.003909000
C	-0.722142000	1.715898000	1.373074000
H	-1.764053000	1.385095000	1.452334000
H	-0.207637000	1.409353000	2.293140000
C	-0.840622000	1.751959000	-1.281154000
H	-0.420927000	1.452402000	-2.250126000
H	-1.891638000	1.440216000	-1.266944000
C	1.531536000	1.821146000	-0.058261000
H	2.070197000	1.556284000	-0.976129000
H	2.160849000	1.516937000	0.787197000
H	-0.122813000	5.292419000	0.063006000
O	1.490842000	3.294713000	-0.022402000
O	-0.765589000	3.191797000	1.396818000
O	-0.859567000	3.228574000	-1.279221000
Si	-0.069008000	3.828436000	0.040921000

1-B3, T. E. = -1426.399890

Pt	0.069880000	-1.143749000	-0.011571000
C	-1.966121000	-1.290018000	-0.001910000
C	-4.120417000	-1.495141000	-0.662799000
C	-4.111216000	-1.489866000	0.690094000

H	-4.932732000	-1.569470000	-1.366625000
H	-4.913626000	-1.561569000	1.405521000
C	-2.391708000	-1.326576000	-2.459750000
H	-2.669470000	-2.251580000	-2.965132000
H	-2.867367000	-0.480823000	-2.956585000
H	-1.311484000	-1.201215000	-2.485366000
C	-2.356475000	-1.336566000	2.463113000
H	-2.894956000	-0.555724000	2.999957000
H	-2.542242000	-2.301436000	2.935572000
H	-1.291025000	-1.118001000	2.478859000
N	-2.805200000	-1.378488000	-1.065522000
N	-2.790705000	-1.368094000	1.074251000
C	2.099178000	-1.108405000	-0.001965000
C	4.261077000	-1.020468000	-0.656562000
C	4.248811000	-1.051388000	0.696493000
H	5.078383000	-0.977259000	-1.357020000
H	5.053013000	-1.034106000	1.413151000
N	2.923348000	-1.117768000	1.076475000
N	2.942742000	-1.061485000	-1.062979000
C	2.474360000	-1.052697000	2.458963000
H	3.117261000	-1.676100000	3.079008000
H	2.508860000	-0.022258000	2.816724000
H	1.450271000	-1.414872000	2.506874000
C	2.520330000	-1.024227000	-2.455269000
H	3.122259000	-0.293465000	-2.994478000
H	2.637679000	-2.005383000	-2.916572000
H	1.473667000	-0.727822000	-2.485424000
B	-0.022622000	0.997534000	-0.012005000
C	-0.917737000	1.522943000	-1.287037000
H	-0.502144000	1.233683000	-2.261477000
H	-1.953620000	1.164764000	-1.254221000
C	1.464124000	1.704499000	-0.100202000
H	2.118247000	1.432382000	0.737780000
H	2.001288000	1.453233000	-1.023595000
C	-0.760919000	1.510170000	1.362813000
H	-0.220531000	1.229466000	2.276793000
H	-1.785894000	1.132509000	1.459766000
O	-0.866850000	2.979816000	1.377750000
O	-0.999275000	2.994144000	-1.292714000
O	1.358893000	3.171777000	-0.073772000

Si	-0.220935000	3.657343000	0.010667000
C	-0.368897000	5.495559000	0.026667000
H	0.146508000	5.922388000	0.889488000
H	0.068845000	5.928873000	-0.874968000
H	-1.415429000	5.803782000	0.073614000

1-B4, T. E. = -1846.778691

Pt	-1.318164000	0.073877000	-0.010477000
C	-1.205691000	2.114037000	-0.000971000
C	-1.108058000	4.266360000	0.688711000
C	-1.112882000	4.274952000	-0.663933000
H	-1.063930000	5.071624000	1.403065000
H	-1.070924000	5.089113000	-1.368263000
C	-1.208555000	2.513708000	2.465496000
H	-0.375026000	2.957810000	3.009388000
H	-2.148657000	2.820710000	2.924365000
H	-1.123021000	1.429731000	2.492126000
C	-1.187682000	2.541659000	-2.461121000
H	-2.059412000	2.957740000	-2.965976000
H	-0.278925000	2.885574000	-2.955398000
H	-1.227168000	1.455050000	-2.491642000
N	-1.169806000	2.942107000	1.074479000
N	-1.179646000	2.955963000	-1.065618000
C	-1.522825000	-1.948033000	-0.000681000
C	-1.691675000	-4.088338000	0.705840000
C	-1.682711000	-4.107542000	-0.647527000
H	-1.760517000	-4.886928000	1.425632000
H	-1.745247000	-4.925700000	-1.345632000
N	-1.587425000	-2.793612000	-1.059038000
N	-1.606913000	-2.762818000	1.081056000
C	-1.499113000	-2.389588000	-2.454150000
H	-0.645739000	-2.877641000	-2.925666000
H	-2.412302000	-2.662357000	-2.982960000
H	-1.363439000	-1.310777000	-2.484249000
C	-1.480760000	-2.315888000	2.460274000
H	-2.134682000	-2.912333000	3.094864000
H	-0.448224000	-2.422715000	2.797069000
H	-1.768622000	-1.268612000	2.511782000

B	0.807849000	-0.085008000	-0.010884000
C	1.434718000	0.749840000	-1.285736000
H	1.106192000	0.368619000	-2.259582000
H	1.206327000	1.820043000	-1.249793000
C	1.339006000	-1.647675000	-0.110700000
H	1.007466000	-2.272108000	0.726195000
H	1.032769000	-2.145102000	-1.037362000
C	1.410950000	0.577999000	1.369076000
H	1.078192000	0.066396000	2.279931000
H	1.168626000	1.640345000	1.472355000
O	2.894708000	0.509206000	1.383471000
O	2.917398000	0.664218000	-1.297977000
O	2.820621000	-1.720380000	-0.092886000
Si	3.413033000	-0.198846000	0.001217000
Cl	5.462222000	-0.276284000	0.014108000

1-B5, T. E. = -1135.702588

Pt	0.072804000	-0.870344000	0.134661000
C	-1.954309000	-0.929063000	0.157349000
C	-4.099882000	-0.774845000	0.843439000
C	-4.115124000	-1.060691000	-0.480999000
H	-4.902525000	-0.616859000	1.544173000
H	-4.934195000	-1.197455000	-1.166961000
C	-2.291102000	-0.403294000	2.555882000
H	-1.468954000	0.305331000	2.471076000
H	-3.105115000	0.040333000	3.127569000
H	-1.958869000	-1.316559000	3.050521000
C	-2.345099000	-1.380803000	-2.243143000
H	-3.215627000	-1.425767000	-2.895652000
H	-1.701427000	-0.551211000	-2.530706000
H	-1.797129000	-2.320510000	-2.307491000
N	-2.771811000	-0.701123000	1.213118000
N	-2.797013000	-1.157790000	-0.877036000
C	2.106138000	-0.749283000	0.158591000
C	4.195660000	-0.155253000	0.771921000
C	4.295202000	-0.828990000	-0.398498000
H	4.950553000	0.295605000	1.394385000
H	5.151298000	-1.083545000	-1.001077000

N	3.009094000	-1.189713000	-0.751989000
N	2.856690000	-0.127673000	1.099319000
C	2.676239000	-1.892180000	-1.980855000
H	2.960601000	-1.289233000	-2.843459000
H	3.197382000	-2.849059000	-2.017891000
H	1.601049000	-2.056016000	-1.995080000
C	2.293742000	0.559648000	2.253858000
H	1.875403000	-0.163906000	2.954154000
H	3.089203000	1.117129000	2.746154000
H	1.509258000	1.236023000	1.915828000
B	-0.099312000	1.184879000	-0.256025000
C	-0.525642000	3.250998000	0.837995000
H	-1.443320000	3.702159000	1.234047000
H	0.321401000	3.635401000	1.427154000
C	-1.374065000	2.797453000	-1.438216000
H	-2.382802000	2.965538000	-1.032462000
H	-1.378310000	3.110340000	-2.489315000
C	1.043830000	3.105044000	-1.059241000
H	1.828191000	3.733599000	-0.619740000
H	1.150542000	3.150527000	-2.153134000
C	-0.342696000	3.604164000	-0.641973000
H	-0.453184000	4.678693000	-0.815368000
O	-1.036266000	1.418554000	-1.370963000
O	1.213112000	1.772890000	-0.597939000
O	-0.618302000	1.838378000	0.966315000

1-B6, T. E. = -2104.596027

Pt	-0.016171000	-1.066287000	0.003846000
C	2.004921000	-1.210855000	0.021425000
C	4.159769000	-1.300071000	-0.626440000
C	4.144457000	-1.203012000	0.725567000
H	4.979359000	-1.365791000	-1.322184000
H	4.948228000	-1.168749000	1.441711000
C	2.402387000	-1.256998000	-2.420203000
H	2.106997000	-0.233556000	-2.657944000
H	3.222220000	-1.567251000	-3.065497000
H	1.553097000	-1.922288000	-2.561816000
C	2.336973000	-0.954336000	2.461024000

H	3.190216000	-0.952435000	3.136445000
H	1.816243000	0.002608000	2.514197000
H	1.654623000	-1.756333000	2.738970000
N	2.843159000	-1.319872000	-1.034410000
N	2.818542000	-1.162041000	1.101400000
C	-2.068852000	-1.046948000	0.016260000
C	-4.228675000	-1.089657000	-0.638621000
C	-4.216426000	-1.058898000	0.714233000
H	-5.046214000	-1.112721000	-1.339823000
H	-5.020451000	-1.048803000	1.431254000
N	-2.890363000	-1.043899000	1.095329000
N	-2.910758000	-1.093092000	-1.044698000
C	-2.457674000	-1.034499000	2.485477000
H	-2.808257000	-0.127748000	2.976657000
H	-2.852297000	-1.913034000	2.996445000
H	-1.370288000	-1.051688000	2.505803000
C	-2.502728000	-1.130204000	-2.440963000
H	-2.865068000	-2.048101000	-2.904822000
H	-2.902142000	-0.262995000	-2.964727000
H	-1.416263000	-1.099348000	-2.479888000
B	0.069779000	1.000035000	-0.039663000
C	-1.063924000	3.447818000	-0.985800000
H	-1.056339000	4.070216000	-1.882649000
H	-2.032387000	3.573191000	-0.495603000
C	1.440467000	3.471745000	-0.539494000
H	1.493633000	3.613046000	-1.621667000
H	2.207937000	4.097211000	-0.079184000
C	-0.194068000	3.452048000	1.412102000
H	-0.979893000	4.065772000	1.856778000
H	0.717491000	3.594436000	1.997528000
C	0.055049000	3.891460000	-0.036392000
H	0.042786000	4.989474000	-0.034069000
S	-0.752245000	1.704905000	1.576631000
S	-0.912551000	1.704978000	-1.562857000
S	1.879490000	1.731483000	-0.138775000

2-BCl_3, T. E. = -2723.387794

C	1.983953000	-0.656963000	-0.536337000
N	-2.802446000	0.494481000	-0.454184000
C	2.816750000	-1.811106000	-1.078197000
N	2.783239000	0.369016000	-0.389627000
C	4.256229000	-1.436875000	-0.691609000
H	4.514376000	-1.934967000	0.246760000
H	4.982410000	-1.746140000	-1.446359000
C	4.266453000	0.085503000	-0.483213000
C	2.365993000	1.713917000	-0.087863000
C	1.720558000	3.397309000	1.496717000
H	1.427654000	3.674248000	2.503044000
C	1.995461000	2.065043000	1.206499000
C	1.827068000	4.370437000	0.506824000
H	1.623349000	5.409180000	0.742486000
C	2.162593000	4.005399000	-0.792123000
H	2.218800000	4.754181000	-1.574298000
C	2.423720000	2.672547000	-1.095611000
C	2.431613000	-3.194211000	-0.571871000
H	3.108127000	-3.934299000	-1.010339000
H	1.409345000	-3.446087000	-0.857922000
H	2.502188000	-3.259349000	0.513677000
C	2.593103000	-1.772141000	-2.604504000
H	3.209451000	-2.539988000	-3.079113000
H	2.852668000	-0.805018000	-3.039876000
H	1.545630000	-1.979457000	-2.839238000
C	4.919147000	0.479418000	0.839433000
H	5.957760000	0.140378000	0.837108000
H	4.401872000	0.008205000	1.678262000
H	4.914613000	1.562034000	0.984468000
C	4.926809000	0.840657000	-1.635509000
H	5.967054000	0.516007000	-1.707526000
H	4.928371000	1.917693000	-1.462790000
H	4.443620000	0.637630000	-2.592605000
C	-2.111627000	-0.615801000	-0.462148000
C	-3.055025000	-1.746431000	-0.863551000
C	-4.265167000	-1.011683000	-1.473795000
H	-4.147521000	-0.944659000	-2.559476000
H	-5.207013000	-1.525194000	-1.271873000
C	-4.249300000	0.402964000	-0.879811000
C	-2.285633000	1.781135000	-0.070240000

C	-2.494762000	2.241098000	1.223590000
C	-2.094545000	3.531230000	1.560998000
H	-2.251538000	3.894401000	2.570094000
C	-1.495762000	4.347657000	0.608474000
H	-1.187978000	5.352783000	0.873833000
C	-1.271183000	3.869597000	-0.680174000
H	-0.785625000	4.498028000	-1.417451000
C	-1.664952000	2.582306000	-1.024086000
C	-5.170500000	0.590712000	0.326007000
H	-4.930291000	-0.093124000	1.140082000
H	-6.201961000	0.409229000	0.016823000
H	-5.111550000	1.612317000	0.706477000
C	-4.559295000	1.465313000	-1.929902000
H	-5.566897000	1.290814000	-2.314401000
H	-3.861096000	1.408014000	-2.767690000
H	-4.525039000	2.473199000	-1.511545000
C	-3.478275000	-2.540275000	0.384201000
H	-4.201050000	-3.302457000	0.078993000
H	-3.948596000	-1.907246000	1.136509000
H	-2.627993000	-3.033344000	0.846805000
C	-2.385344000	-2.691927000	-1.860315000
H	-3.106039000	-3.439798000	-2.203504000
H	-1.543677000	-3.208233000	-1.392805000
H	-2.015773000	-2.150390000	-2.735701000
H	-2.958320000	1.590880000	1.955024000
H	-1.507964000	2.197187000	-2.026219000
H	1.934812000	1.298632000	1.969606000
H	2.681626000	2.376651000	-2.106048000
B	0.045676000	-1.519032000	1.516044000
Pt	-0.041753000	-0.656654000	-0.332286000
Cl	-1.265303000	-0.768779000	2.662795000
Cl	-0.240159000	-3.390506000	1.470531000
Cl	1.715843000	-1.299025000	2.417864000

2-$AlCl_3$, T. E. = -2941.095477

C	2.041659000	-0.580865000	-0.568183000
N	-2.812740000	0.479473000	-0.440609000
C	2.921854000	-1.745274000	-0.999791000

N	2.818076000	0.446810000	-0.347901000
C	4.332226000	-1.336213000	-0.540786000
H	4.547629000	-1.809350000	0.420987000
H	5.105113000	-1.646014000	-1.247130000
C	4.306598000	0.189439000	-0.362718000
C	2.355325000	1.789912000	-0.112988000
C	1.697689000	3.537261000	1.392959000
H	1.439784000	3.865952000	2.393110000
C	2.034347000	2.205289000	1.174725000
C	1.693855000	4.443421000	0.336524000
H	1.439300000	5.482321000	0.515141000
C	1.989331000	4.012287000	-0.952478000
H	1.964191000	4.709604000	-1.782193000
C	2.315135000	2.679260000	-1.182603000
C	2.510423000	-3.096567000	-0.430290000
H	3.201225000	-3.864242000	-0.791412000
H	1.500678000	-3.366980000	-0.743940000
H	2.541468000	-3.098557000	0.660232000
C	2.793682000	-1.795802000	-2.535484000
H	3.452981000	-2.574184000	-2.927871000
H	3.063455000	-0.848365000	-3.006872000
H	1.767478000	-2.037780000	-2.824679000
C	4.902384000	0.622140000	0.973865000
H	5.946731000	0.303607000	1.013437000
H	4.365601000	0.155655000	1.802807000
H	4.873199000	1.706931000	1.097076000
C	4.983291000	0.941308000	-1.507512000
H	6.042242000	0.674607000	-1.520606000
H	4.913796000	2.021994000	-1.372023000
H	4.557257000	0.681345000	-2.478015000
C	-2.031636000	-0.523662000	-0.737495000
C	-2.880551000	-1.636208000	-1.337403000
C	-4.258066000	-0.979751000	-1.564246000
H	-4.360776000	-0.687324000	-2.612819000
H	-5.082359000	-1.653499000	-1.325178000
C	-4.289678000	0.277156000	-0.684181000
C	-2.356154000	1.761103000	0.028161000
C	-2.571272000	2.158156000	1.341984000
C	-2.222119000	3.450171000	1.727657000
H	-2.380669000	3.760794000	2.753925000

C	-1.674445000	4.334629000	0.805660000
H	-1.407552000	5.340433000	1.110313000
C	-1.451286000	3.923015000	-0.505622000
H	-1.011537000	4.604763000	-1.224161000
C	-1.788113000	2.633485000	-0.896974000
C	-5.004820000	0.055112000	0.648573000
H	-4.520702000	-0.726913000	1.236442000
H	-6.036981000	-0.242284000	0.451598000
H	-5.031650000	0.970158000	1.242558000
C	-4.879739000	1.479063000	-1.412075000
H	-5.913971000	1.251562000	-1.680475000
H	-4.327564000	1.694328000	-2.329806000
H	-4.880332000	2.373199000	-0.785140000
C	-2.953925000	-2.818817000	-0.364165000
H	-3.653801000	-3.561916000	-0.755378000
H	-3.291725000	-2.516851000	0.630019000
H	-1.978326000	-3.290814000	-0.256505000
C	-2.255118000	-2.107392000	-2.653472000
H	-2.901729000	-2.855988000	-3.120007000
H	-1.275369000	-2.558787000	-2.477171000
H	-2.134076000	-1.279062000	-3.357095000
H	-2.985395000	1.460921000	2.056778000
H	-1.634872000	2.300684000	-1.918358000
H	2.055972000	1.488275000	1.986689000
H	2.549394000	2.328681000	-2.181819000
Pt	0.005533000	-0.541505000	-0.599835000
Cl	-1.718452000	-0.861920000	2.767044000
Cl	-0.171338000	-3.708329000	1.664803000
Cl	1.770033000	-1.092853000	2.705220000
Al	-0.039725000	-1.520051000	1.525713000

2-$GaCl_3$, T. E. = -4623.457568

C	2.044558000	-0.473258000	-0.680730000
N	-2.802130000	0.604600000	-0.486861000
C	2.914628000	-1.627218000	-1.155627000
N	2.827781000	0.528722000	-0.386425000
C	4.324675000	-1.257524000	-0.661660000
H	4.526944000	-1.782544000	0.275609000

H	5.101311000	-1.537186000	-1.376433000
C	4.313858000	0.256972000	-0.403285000
C	2.371578000	1.857864000	-0.073102000
C	1.702692000	3.507210000	1.534637000
H	1.432931000	3.771904000	2.550656000
C	2.033431000	2.189884000	1.234646000
C	1.721077000	4.480444000	0.539542000
H	1.471390000	5.507695000	0.781611000
C	2.031914000	4.132394000	-0.770609000
H	2.023032000	4.882790000	-1.553053000
C	2.353255000	2.815005000	-1.082988000
C	2.476678000	-2.995694000	-0.648504000
H	3.159762000	-3.757994000	-1.034537000
H	1.466895000	-3.237745000	-0.985186000
H	2.496705000	-3.045502000	0.441401000
C	2.804771000	-1.609841000	-2.693071000
H	3.453891000	-2.383461000	-3.110823000
H	3.099308000	-0.648710000	-3.119713000
H	1.777872000	-1.818906000	-3.004934000
C	4.906726000	0.614803000	0.956305000
H	5.948508000	0.286626000	0.982892000
H	4.364017000	0.110997000	1.758937000
H	4.886034000	1.692101000	1.134597000
C	5.002710000	1.061608000	-1.504169000
H	6.057980000	0.781885000	-1.530983000
H	4.947425000	2.133877000	-1.308503000
H	4.574224000	0.862428000	-2.487982000
C	-2.024870000	-0.372779000	-0.865374000
C	-2.878506000	-1.448434000	-1.521015000
C	-4.265810000	-0.788586000	-1.671312000
H	-4.399755000	-0.436113000	-2.697492000
H	-5.079092000	-1.481649000	-1.450426000
C	-4.282492000	0.414062000	-0.717552000
C	-2.333546000	1.852606000	0.054771000
C	-2.515694000	2.163535000	1.396635000
C	-2.154185000	3.427775000	1.855808000
H	-2.287943000	3.671173000	2.903490000
C	-1.625202000	4.369271000	0.980572000
H	-1.348811000	5.352789000	1.343559000
C	-1.430906000	4.041940000	-0.358887000

H	-1.002822000	4.766358000	-1.041983000
C	-1.782660000	2.781767000	-0.824884000
C	-4.974837000	0.111590000	0.611042000
H	-4.487007000	-0.710524000	1.137699000
H	-6.012957000	-0.164532000	0.413908000
H	-4.982894000	0.986873000	1.262927000
C	-4.883666000	1.656762000	-1.363224000
H	-5.922413000	1.445561000	-1.626914000
H	-4.346253000	1.923801000	-2.276038000
H	-4.872106000	2.512748000	-0.685355000
C	-2.919212000	-2.694781000	-0.628745000
H	-3.620281000	-3.418221000	-1.053193000
H	-3.238406000	-2.464171000	0.390648000
H	-1.937462000	-3.164174000	-0.573139000
C	-2.279016000	-1.820835000	-2.879974000
H	-2.928642000	-2.542329000	-3.383311000
H	-1.291251000	-2.273246000	-2.757816000
H	-2.182668000	-0.943883000	-3.526124000
H	-2.911233000	1.420671000	2.075520000
H	-1.655288000	2.517048000	-1.869490000
H	2.039323000	1.420848000	1.998419000
H	2.600239000	2.529419000	-2.099704000
Pt	0.009776000	-0.400789000	-0.740372000
Cl	-1.796902000	-0.971721000	2.698737000
Cl	-0.209635000	-3.804783000	1.420869000
Cl	1.785138000	-1.192759000	2.638487000
Ga	-0.064855000	-1.543232000	1.358717000

2-$InCl_3$, T. E. = -2700.528260

C	2.049591000	-0.359131000	-0.795127000
N	-2.799139000	0.731053000	-0.540163000
C	2.895092000	-1.508392000	-1.321803000
N	2.851635000	0.596309000	-0.412655000
C	4.312240000	-1.196750000	-0.805291000
H	4.504724000	-1.783789000	0.096535000
H	5.084508000	-1.444374000	-1.536446000
C	4.331065000	0.298523000	-0.451398000
C	2.414072000	1.909376000	-0.016446000

C	1.803334000	3.473600000	1.695005000
H	1.576623000	3.688783000	2.733028000
C	2.138137000	2.176452000	1.320314000
C	1.762351000	4.490350000	0.745274000
H	1.507875000	5.500974000	1.044894000
C	2.023012000	4.208423000	-0.591822000
H	1.971498000	4.994912000	-1.336226000
C	2.345648000	2.911630000	-0.978955000
C	2.417990000	-2.884037000	-0.867860000
H	3.073625000	-3.651850000	-1.288460000
H	1.398560000	-3.083459000	-1.205606000
H	2.449316000	-2.982059000	0.219625000
C	2.789378000	-1.425340000	-2.856289000
H	3.424769000	-2.192341000	-3.306022000
H	3.102717000	-0.452380000	-3.240411000
H	1.759174000	-1.601531000	-3.177833000
C	4.943432000	0.561129000	0.920796000
H	5.978905000	0.213031000	0.914518000
H	4.400639000	0.019216000	1.697903000
H	4.946162000	1.625706000	1.164474000
C	5.018450000	1.160083000	-1.509331000
H	6.073034000	0.880748000	-1.557163000
H	4.964933000	2.220435000	-1.255336000
H	4.583243000	1.014764000	-2.499745000
C	-2.009436000	-0.198642000	-1.004034000
C	-2.850998000	-1.242538000	-1.721655000
C	-4.252825000	-0.602456000	-1.804357000
H	-4.407720000	-0.182122000	-2.801581000
H	-5.049170000	-1.326044000	-1.622733000
C	-4.278594000	0.530555000	-0.767510000
C	-2.335581000	1.936906000	0.093464000
C	-2.496759000	2.132462000	1.459678000
C	-2.117016000	3.349653000	2.019960000
H	-2.231586000	3.503291000	3.086835000
C	-1.591490000	4.358203000	1.220634000
H	-1.298955000	5.304043000	1.662717000
C	-1.422913000	4.146899000	-0.145349000
H	-0.998781000	4.924498000	-0.769829000
C	-1.793830000	2.934679000	-0.713143000
C	-4.950236000	0.120095000	0.542581000

H	-4.449028000	-0.734665000	1.000187000
H	-5.988279000	-0.150113000	0.336815000
H	-4.958175000	0.942193000	1.260397000
C	-4.906621000	1.806445000	-1.314671000
H	-5.944842000	1.598576000	-1.582660000
H	-4.383384000	2.149259000	-2.210225000
H	-4.900120000	2.609767000	-0.574986000
C	-2.843460000	-2.547962000	-0.915413000
H	-3.542985000	-3.256687000	-1.365987000
H	-3.137380000	-2.396311000	0.126994000
H	-1.851670000	-3.002240000	-0.924024000
C	-2.267436000	-1.507768000	-3.112530000
H	-2.912106000	-2.204009000	-3.656005000
H	-1.270472000	-1.949901000	-3.037165000
H	-2.196170000	-0.586176000	-3.696561000
H	-2.883825000	1.335278000	2.079190000
H	-1.683697000	2.758514000	-1.778200000
H	2.190223000	1.374018000	2.047162000
H	2.556331000	2.675143000	-2.016607000
Pt	0.020902000	-0.232737000	-0.888887000
Cl	-1.952901000	-1.081201000	2.706273000
Cl	-0.246524000	-3.935224000	1.220617000
Cl	1.870788000	-1.259678000	2.627616000
In	-0.094472000	-1.530450000	1.257071000

2-B1, T. E. = -1724.768074

C	2.035587000	-0.608738000	-0.597730000
N	-2.947497000	0.244412000	-0.516989000
C	2.865534000	-1.812611000	-1.027193000
N	2.859183000	0.402043000	-0.433594000
C	4.305066000	-1.434913000	-0.639371000
H	4.546750000	-1.881098000	0.329458000
H	5.041707000	-1.792806000	-1.361972000
C	4.334647000	0.097502000	-0.517519000
C	2.427999000	1.772723000	-0.377315000
C	2.248920000	3.894418000	0.739128000
H	2.374565000	4.494435000	1.632878000
C	2.594163000	2.545168000	0.767168000

C	1.749218000	4.468171000	-0.424513000
H	1.491681000	5.521491000	-0.442418000
C	1.567703000	3.685796000	-1.562732000
H	1.168370000	4.124432000	-2.470425000
C	1.906226000	2.338743000	-1.539579000
C	2.428125000	-3.142571000	-0.424048000
H	3.063195000	-3.943781000	-0.813280000
H	1.391184000	-3.361163000	-0.688402000
H	2.509165000	-3.142166000	0.663358000
C	2.681715000	-1.894030000	-2.557319000
H	3.329311000	-2.678701000	-2.957163000
H	2.930561000	-0.956997000	-3.059362000
H	1.646680000	-2.142870000	-2.803305000
C	5.048583000	0.539686000	0.757418000
H	6.058911000	0.123759000	0.751561000
H	4.529969000	0.165310000	1.643423000
H	5.135725000	1.625580000	0.823432000
C	4.948826000	0.800662000	-1.726848000
H	6.009738000	0.547961000	-1.784668000
H	4.866437000	1.885965000	-1.632331000
H	4.475810000	0.498345000	-2.662094000
C	-2.018691000	-0.638859000	-0.793501000
C	-2.659937000	-1.757249000	-1.608951000
C	-4.046713000	-1.210610000	-1.997860000
H	-4.025041000	-0.849048000	-3.029481000
H	-4.824688000	-1.973622000	-1.933735000
C	-4.335271000	-0.034058000	-1.053237000
C	-2.691344000	1.494052000	0.148277000
C	-3.317724000	1.798333000	1.352930000
C	-3.090660000	3.031206000	1.955012000
H	-3.568255000	3.257822000	2.901112000
C	-2.244230000	3.958074000	1.355304000
H	-2.069379000	4.919032000	1.825694000
C	-1.618404000	3.646214000	0.151812000
H	-0.957189000	4.361972000	-0.319838000
C	-1.839942000	2.414668000	-0.455154000
C	-5.300507000	-0.415678000	0.070124000
H	-4.876935000	-1.180974000	0.724063000
H	-6.214722000	-0.813550000	-0.374879000
H	-5.583585000	0.447094000	0.673513000

C	-4.852148000	1.189522000	-1.803043000
H	-5.791138000	0.930032000	-2.297225000
H	-4.139233000	1.508917000	-2.567005000
H	-5.042599000	2.027767000	-1.129761000
C	-2.748036000	-3.016100000	-0.736426000
H	-3.240148000	-3.814815000	-1.298048000
H	-3.318315000	-2.838637000	0.178335000
H	-1.748767000	-3.351669000	-0.452842000
C	-1.822658000	-2.069694000	-2.853211000
H	-2.359636000	-2.782894000	-3.485302000
H	-0.861284000	-2.507467000	-2.576226000
H	-1.635470000	-1.168296000	-3.443929000
H	-3.942224000	1.065172000	1.844963000
H	-1.357220000	2.160270000	-1.392632000
H	2.986780000	2.103362000	1.673668000
H	1.786500000	1.716399000	-2.420789000
B	0.106599000	-1.047908000	1.538766000
C	-0.278518000	-2.593052000	1.874098000
H	-1.340338000	-2.812878000	1.707145000
H	0.302728000	-3.365739000	1.364708000
C	-0.970374000	-0.204174000	2.410600000
H	-0.799610000	0.879654000	2.452082000
H	-2.003622000	-0.369365000	2.089070000
C	1.539484000	-0.754670000	2.258986000
H	1.854432000	0.289845000	2.169048000
H	2.380001000	-1.377326000	1.922205000
C	0.151607000	-1.591625000	3.992006000
H	0.168419000	-1.830405000	5.055334000
O	1.382085000	-1.004713000	3.689206000
O	-0.029261000	-2.793419000	3.305781000
O	-0.907043000	-0.706317000	3.788221000
Pt	0.027952000	-0.563413000	-0.553298000

2-B2, T. E. = -1976.285182

C	2.035405000	-0.392621000	-0.795317000
N	-2.960395000	0.340952000	-0.567509000
C	2.880424000	-1.466574000	-1.470123000
N	2.835724000	0.601054000	-0.478832000

C	4.320409000	-1.121799000	-1.057406000
H	4.602483000	-1.726699000	-0.190788000
H	5.043985000	-1.320654000	-1.850860000
C	4.314388000	0.364670000	-0.661163000
C	2.366278000	1.920731000	-0.155250000
C	2.152394000	3.786850000	1.345741000
H	2.287930000	4.214585000	2.332342000
C	2.543507000	2.471277000	1.110042000
C	1.591646000	4.547333000	0.325185000
H	1.298452000	5.574431000	0.512509000
C	1.397069000	3.984715000	-0.934515000
H	0.950422000	4.568639000	-1.731452000
C	1.785895000	2.672863000	-1.175440000
C	2.491745000	-2.900179000	-1.125787000
H	3.130113000	-3.593180000	-1.681457000
H	1.451797000	-3.088661000	-1.401701000
H	2.605294000	-3.111168000	-0.061949000
C	2.649070000	-1.260136000	-2.981937000
H	3.300553000	-1.935737000	-3.542383000
H	2.859968000	-0.238581000	-3.303166000
H	1.612649000	-1.486511000	-3.242100000
C	5.060768000	0.590176000	0.651668000
H	6.081998000	0.218784000	0.538274000
H	4.587186000	0.039918000	1.468656000
H	5.117020000	1.647785000	0.915254000
C	4.868172000	1.295397000	-1.738720000
H	5.932782000	1.092564000	-1.872813000
H	4.759913000	2.341718000	-1.443986000
H	4.371752000	1.154671000	-2.699672000
C	-2.013238000	-0.469758000	-0.973596000
C	-2.602702000	-1.370132000	-2.056641000
C	-3.930358000	-0.691070000	-2.438620000
H	-3.788071000	-0.092416000	-3.342737000
H	-4.721914000	-1.414110000	-2.643833000
C	-4.298041000	0.234505000	-1.270861000
C	-2.765761000	1.384078000	0.403848000
C	-3.491152000	1.377823000	1.591555000
C	-3.321746000	2.409200000	2.507908000
H	-3.876784000	2.392893000	3.438522000
C	-2.430289000	3.443254000	2.239337000

H	-2.297263000	4.245912000	2.955608000
C	-1.702771000	3.439010000	1.052978000
H	-1.002418000	4.236800000	0.840316000
C	-1.867132000	2.410117000	0.131089000
C	-5.369148000	-0.372725000	-0.363552000
H	-5.016991000	-1.283955000	0.123464000
H	-6.238584000	-0.626674000	-0.973384000
H	-5.703661000	0.330014000	0.399691000
C	-4.731185000	1.617143000	-1.748688000
H	-5.622389000	1.513223000	-2.371875000
H	-3.945977000	2.085747000	-2.346730000
H	-4.975048000	2.276117000	-0.912950000
C	-2.806558000	-2.774290000	-1.469287000
H	-3.298072000	-3.409079000	-2.211561000
H	-3.422969000	-2.761018000	-0.567483000
H	-1.844165000	-3.221855000	-1.215117000
C	-1.670064000	-1.473668000	-3.266817000
H	-2.183166000	-1.998136000	-4.078437000
H	-0.763993000	-2.030144000	-3.017967000
H	-1.380574000	-0.485054000	-3.635309000
H	-4.145803000	0.548925000	1.825888000
H	-1.300003000	2.396708000	-0.793504000
H	2.978988000	1.881187000	1.905772000
H	1.656234000	2.223695000	-2.155003000
B	0.182307000	-1.274828000	1.294939000
C	-0.248237000	-2.860062000	1.258583000
H	-1.281316000	-2.988419000	0.919058000
H	0.384933000	-3.499394000	0.636905000
C	-0.902833000	-0.521643000	2.266240000
H	-0.764365000	0.563474000	2.344622000
H	-1.929022000	-0.699722000	1.929065000
C	1.675265000	-1.109952000	1.975472000
H	1.944638000	-0.056506000	2.108712000
H	2.489673000	-1.579236000	1.411158000
H	0.265206000	-2.878123000	5.084105000
O	1.721361000	-1.718387000	3.315451000
O	-0.198385000	-3.436333000	2.620287000
O	-0.835564000	-1.050173000	3.646172000
Pt	0.039302000	-0.427726000	-0.687007000
Si	0.235544000	-2.302007000	3.737407000

2-B3, T. E. = -2015.579354

C	-2.024791000	-0.309192000	-0.930366000
N	2.967002000	-0.720562000	-0.257988000
C	-2.876545000	0.124487000	-2.119130000
N	-2.820993000	-0.906491000	-0.071703000
C	-4.316755000	0.089927000	-1.580380000
H	-4.611010000	1.095111000	-1.265860000
H	-5.036189000	-0.246730000	-2.330107000
C	-4.300619000	-0.843876000	-0.358777000
C	-2.352361000	-1.749667000	0.994463000
C	-2.138562000	-2.297626000	3.325617000
H	-2.265277000	-2.023323000	4.366376000
C	-2.518319000	-1.400440000	2.330405000
C	-1.605096000	-3.536659000	2.988690000
H	-1.322803000	-4.235504000	3.768336000
C	-1.420214000	-3.872932000	1.649654000
H	-0.993131000	-4.832506000	1.380513000
C	-1.793021000	-2.979750000	0.652672000
C	-2.502895000	1.475642000	-2.718829000
H	-3.147453000	1.683609000	-3.577876000
H	-1.464617000	1.468583000	-3.057295000
H	-2.619138000	2.288932000	-2.001993000
C	-2.640444000	-0.957576000	-3.193924000
H	-3.295260000	-0.765002000	-4.047855000
H	-2.846079000	-1.964489000	-2.826134000
H	-1.605133000	-0.931163000	-3.541175000
C	-5.047962000	-0.228824000	0.821820000
H	-6.074766000	-0.018608000	0.512780000
H	-4.583746000	0.712137000	1.127497000
H	-5.087933000	-0.904704000	1.677813000
C	-4.842388000	-2.243958000	-0.642818000
H	-5.908076000	-2.174341000	-0.871057000
H	-4.727123000	-2.891741000	0.229271000
H	-4.343233000	-2.715653000	-1.490322000
C	2.027933000	-0.347311000	-1.094534000
C	2.644234000	-0.281470000	-2.489985000
C	4.005229000	-0.987982000	-2.345933000

H	3.926080000	-2.016269000	-2.709146000
H	4.791015000	-0.495695000	-2.921664000
C	4.333237000	-1.004227000	-0.847034000
C	2.741908000	-0.991644000	1.137064000
C	3.415614000	-0.266340000	2.115620000
C	3.216341000	-0.570106000	3.457497000
H	3.729049000	0.007729000	4.217628000
C	2.348899000	-1.595158000	3.821472000
H	2.193770000	-1.830400000	4.868230000
C	1.675039000	-2.313190000	2.838107000
H	0.998588000	-3.111760000	3.113658000
C	1.869107000	-2.014430000	1.493526000
C	5.344622000	0.077450000	-0.463754000
H	4.949293000	1.079697000	-0.640889000
H	6.240209000	-0.050247000	-1.075426000
H	5.651785000	-0.001684000	0.579132000
C	4.817575000	-2.373309000	-0.380898000
H	5.731489000	-2.627831000	-0.922370000
H	4.069393000	-3.141994000	-0.589051000
H	5.040562000	-2.381927000	0.687763000
C	2.787008000	1.189963000	-2.903230000
H	3.290277000	1.245944000	-3.872299000
H	3.370196000	1.766311000	-2.181318000
H	1.804937000	1.657047000	-2.995638000
C	1.759451000	-0.999086000	-3.512689000
H	2.279784000	-1.050376000	-4.473640000
H	0.817595000	-0.466072000	-3.657778000
H	1.532383000	-2.021617000	-3.196741000
H	4.050670000	0.564395000	1.838861000
H	1.347613000	-2.566089000	0.718801000
H	-2.938470000	-0.438936000	2.595555000
H	-1.671933000	-3.231663000	-0.395924000
B	-0.164710000	1.684775000	0.163812000
C	0.246600000	2.910171000	-0.848974000
H	1.291342000	2.832274000	-1.169348000
H	-0.366687000	2.995255000	-1.750799000
C	0.923804000	1.705903000	1.386137000
H	0.771768000	0.923231000	2.140201000
H	1.947489000	1.606860000	1.011079000
C	-1.655090000	1.957239000	0.811972000

H	-1.915671000	1.187992000	1.547174000
H	-2.472964000	1.988613000	0.081734000
O	-1.702248000	3.242008000	1.523390000
O	0.131183000	4.206739000	-0.152612000
O	0.882768000	2.994926000	2.104218000
Pt	-0.024791000	-0.215403000	-0.864069000
Si	-0.241229000	4.019329000	1.449611000
C	-0.289952000	5.639280000	2.330070000
H	0.674943000	6.146679000	2.266998000
H	-1.044624000	6.298577000	1.896234000
H	-0.529704000	5.502448000	3.386507000

2-B4, T. E. = -2435.957681

C	-2.016801000	-0.636049000	-0.884049000
N	2.986457000	-0.863710000	-0.114234000
C	-2.834909000	-0.478591000	-2.160834000
N	-2.837701000	-1.020040000	0.067197000
C	-4.286482000	-0.379478000	-1.663749000
H	-4.571152000	0.673894000	-1.587435000
H	-4.994964000	-0.866467000	-2.337370000
C	-4.309818000	-1.017001000	-0.264144000
C	-2.396904000	-1.596559000	1.308805000
C	-2.236594000	-1.593379000	3.707678000
H	-2.394262000	-1.091710000	4.655285000
C	-2.603998000	-0.955497000	2.525802000
C	-1.677664000	-2.865544000	3.674682000
H	-1.405459000	-3.362207000	4.599170000
C	-1.460249000	-3.498075000	2.452569000
H	-1.018763000	-4.487677000	2.419606000
C	-1.818522000	-2.863899000	1.269776000
C	-2.435550000	0.700613000	-3.041008000
H	-3.075259000	0.723001000	-3.928280000
H	-1.397409000	0.604081000	-3.366986000
H	-2.543838000	1.653764000	-2.521972000
C	-2.586596000	-1.777666000	-2.955296000
H	-3.216355000	-1.779785000	-3.848812000
H	-2.813948000	-2.673267000	-2.374574000
H	-1.542767000	-1.837455000	-3.270645000

C	-5.083128000	-0.149781000	0.726525000
H	-6.093530000	-0.000184000	0.338484000
H	-4.613681000	0.830677000	0.837883000
H	-5.169251000	-0.621601000	1.706907000
C	-4.857080000	-2.443180000	-0.241301000
H	-5.916000000	-2.422858000	-0.508031000
H	-4.770297000	-2.879907000	0.756305000
H	-4.340954000	-3.094026000	-0.947986000
C	2.040005000	-0.698246000	-1.005955000
C	2.649655000	-0.915894000	-2.388696000
C	4.045464000	-1.505438000	-2.107690000
H	4.020269000	-2.590482000	-2.240243000
H	4.805601000	-1.108776000	-2.783008000
C	4.369559000	-1.182243000	-0.642762000
C	2.756240000	-0.877128000	1.306472000
C	3.394305000	0.037370000	2.140232000
C	3.180139000	-0.016555000	3.513006000
H	3.663497000	0.709375000	4.156799000
C	2.337473000	-0.983298000	4.053414000
H	2.172324000	-1.023151000	5.124213000
C	1.702683000	-1.894245000	3.214425000
H	1.044732000	-2.648829000	3.626366000
C	1.910193000	-1.844407000	1.839511000
C	5.303551000	0.022699000	-0.510231000
H	4.840506000	0.935139000	-0.891627000
H	6.206857000	-0.172038000	-1.092410000
H	5.613435000	0.188447000	0.521663000
C	4.943119000	-2.385228000	0.098044000
H	5.878010000	-2.682287000	-0.382941000
H	4.253282000	-3.231864000	0.060275000
H	5.157242000	-2.154138000	1.143425000
C	2.715071000	0.425143000	-3.131243000
H	3.184061000	0.276333000	-4.107586000
H	3.296490000	1.170457000	-2.583583000
H	1.710776000	0.823746000	-3.285730000
C	1.798142000	-1.894660000	-3.205093000
H	2.330388000	-2.159028000	-4.123584000
H	0.841370000	-1.447502000	-3.481715000
H	1.605685000	-2.817807000	-2.650537000
H	4.012458000	0.820347000	1.721801000

H	1.420182000	-2.550585000	1.177450000
H	-3.045350000	0.031770000	2.557404000
H	-1.670629000	-3.347710000	0.309378000
B	-0.140628000	1.527717000	-0.211947000
C	0.269277000	2.526433000	-1.453812000
H	1.322444000	2.418797000	-1.733485000
H	-0.330145000	2.417925000	-2.360396000
C	0.951919000	1.804966000	0.980776000
H	0.794877000	1.213856000	1.890144000
H	1.973511000	1.628061000	0.636081000
C	-1.634214000	1.931830000	0.364947000
H	-1.909685000	1.315978000	1.224761000
H	-2.441765000	1.851318000	-0.371175000
O	-1.680391000	3.332174000	0.849930000
O	0.108343000	3.949111000	-1.044519000
O	0.932461000	3.231269000	1.405590000
Pt	-0.012527000	-0.534823000	-0.813237000
Si	-0.223322000	4.019003000	0.556545000
Cl	-0.280006000	5.981157000	1.149046000

2-B5, T. E. = -1724.889912

C	2.045738000	-0.569828000	-0.706249000
N	-2.812614000	0.385965000	-0.446953000
C	2.952144000	-1.754377000	-1.007765000
N	2.812642000	0.454422000	-0.428720000
C	4.311041000	-1.352959000	-0.405817000
H	4.425873000	-1.823595000	0.574195000
H	5.152262000	-1.669389000	-1.026964000
C	4.279087000	0.175487000	-0.236943000
C	2.325547000	1.783614000	-0.177718000
C	1.395656000	3.401476000	1.329674000
H	0.952793000	3.646352000	2.288463000
C	1.765159000	2.089304000	1.060504000
C	1.575629000	4.396695000	0.370531000
H	1.283580000	5.418529000	0.587769000
C	2.101333000	4.074400000	-0.875134000
H	2.220630000	4.839816000	-1.633860000
C	2.477670000	2.762031000	-1.153762000

C	2.446034000	-3.075193000	-0.439335000
H	3.159624000	-3.869633000	-0.681415000
H	1.472140000	-3.329988000	-0.859425000
H	2.325107000	-3.013283000	0.642171000
C	3.007916000	-1.855219000	-2.543290000
H	3.674563000	-2.672413000	-2.831858000
H	3.375233000	-0.934173000	-3.002326000
H	2.013577000	-2.062113000	-2.947528000
C	4.687020000	0.598806000	1.172530000
H	5.700241000	0.242097000	1.372663000
H	4.008262000	0.161052000	1.908607000
H	4.678600000	1.685050000	1.287714000
C	5.124652000	0.908833000	-1.276265000
H	6.171676000	0.627335000	-1.142887000
H	5.053741000	1.991657000	-1.157672000
H	4.829630000	0.647528000	-2.294616000
C	-2.017003000	-0.582439000	-0.822748000
C	-2.881135000	-1.722927000	-1.346668000
C	-4.288929000	-1.106883000	-1.480478000
H	-4.472184000	-0.818253000	-2.519584000
H	-5.076218000	-1.804430000	-1.187395000
C	-4.294100000	0.150186000	-0.598899000
C	-2.370749000	1.661018000	0.047543000
C	-2.492086000	1.976643000	1.395684000
C	-2.210917000	3.272980000	1.819589000
H	-2.303632000	3.523252000	2.870582000
C	-1.804048000	4.239094000	0.905424000
H	-1.584675000	5.246647000	1.241770000
C	-1.646245000	3.903271000	-0.436422000
H	-1.298117000	4.644184000	-1.147258000
C	-1.931918000	2.613724000	-0.868218000
C	-4.942518000	-0.077779000	0.767121000
H	-4.430014000	-0.859052000	1.330583000
H	-5.981442000	-0.382016000	0.620757000
H	-4.945286000	0.836637000	1.362653000
C	-4.951699000	1.337440000	-1.295620000
H	-5.993811000	1.088296000	-1.509604000
H	-4.452399000	1.561916000	-2.240994000
H	-4.937522000	2.233489000	-0.671290000
C	-2.852310000	-2.878387000	-0.337361000

H	-3.491934000	-3.687265000	-0.703306000
H	-3.216765000	-2.565409000	0.643553000
H	-1.836063000	-3.243538000	-0.195446000
C	-2.349551000	-2.215773000	-2.694078000
H	-3.027319000	-2.969643000	-3.105766000
H	-1.360165000	-2.663584000	-2.577335000
H	-2.274166000	-1.397341000	-3.415701000
H	-2.772002000	1.204474000	2.099090000
H	-1.833394000	2.339426000	-1.913143000
H	1.621693000	1.286185000	1.774977000
H	2.886483000	2.496363000	-2.122400000
B	0.025932000	-1.268154000	1.209175000
O	-1.066226000	-0.627658000	1.962182000
O	-0.157344000	-2.727214000	1.228327000
O	1.320762000	-0.945764000	1.860706000
C	-1.231550000	-1.267372000	3.218010000
C	0.087099000	-3.235919000	2.527459000
C	1.235977000	-1.182299000	3.257249000
H	-1.399087000	-0.501624000	3.986291000
H	-2.113700000	-1.926274000	3.201629000
H	1.072619000	-3.727279000	2.571742000
H	-0.673577000	-3.992224000	2.760234000
H	2.162634000	-1.665769000	3.591944000
H	1.137399000	-0.230491000	3.803502000
C	0.027722000	-2.082368000	3.534578000
H	0.024033000	-2.445491000	4.566549000
Pt	0.021534000	-0.550187000	-0.778773000

2-B6, T. E. = -2693.774978

C	1.916731000	-0.101293000	-1.001788000
N	-2.849004000	0.905374000	-0.438368000
C	2.700938000	-0.928929000	-2.014270000
N	2.743647000	0.781789000	-0.497272000
C	4.164988000	-0.734410000	-1.588963000
H	4.458460000	-1.564807000	-0.941149000
H	4.847231000	-0.715194000	-2.441676000
C	4.212685000	0.578311000	-0.792982000
C	2.368312000	1.909699000	0.317582000

C	1.928280000	2.894757000	2.460853000
H	1.763146000	2.784916000	3.526759000
C	2.163883000	1.763590000	1.685323000
C	1.914533000	4.158884000	1.878611000
H	1.743815000	5.037135000	2.491426000
C	2.095633000	4.292703000	0.506070000
H	2.060728000	5.272342000	0.042557000
C	2.312231000	3.166172000	-0.280331000
C	2.323669000	-2.401753000	-2.089653000
H	2.975779000	-2.899176000	-2.814887000
H	1.287827000	-2.527690000	-2.408190000
H	2.429079000	-2.889145000	-1.120967000
C	2.395095000	-0.276095000	-3.378280000
H	2.985638000	-0.768598000	-4.155324000
H	2.626193000	0.790974000	-3.393643000
H	1.336919000	-0.395525000	-3.625394000
C	4.960035000	0.422624000	0.529328000
H	5.986502000	0.111583000	0.320873000
H	4.482246000	-0.337654000	1.151249000
H	4.995818000	1.362614000	1.084704000
C	4.805318000	1.739587000	-1.589416000
H	5.844798000	1.500017000	-1.824474000
H	4.801536000	2.665030000	-1.011605000
H	4.278801000	1.909457000	-2.529801000
C	-2.162728000	-0.160503000	-0.769914000
C	-3.121016000	-1.120165000	-1.471886000
C	-4.320581000	-0.227607000	-1.850339000
H	-4.201532000	0.141287000	-2.873379000
H	-5.268757000	-0.766001000	-1.797933000
C	-4.289094000	0.962545000	-0.881232000
C	-2.318637000	1.999777000	0.327290000
C	-2.500568000	2.014667000	1.704705000
C	-2.051350000	3.108977000	2.438683000
H	-2.183600000	3.122645000	3.514372000
C	-1.434320000	4.176093000	1.794999000
H	-1.088352000	5.028361000	2.368814000
C	-1.243684000	4.143951000	0.415679000
H	-0.747556000	4.966908000	-0.085283000
C	-1.685861000	3.054122000	-0.323466000
C	-5.224576000	0.824351000	0.320602000

H	-5.003608000	-0.062582000	0.914390000
H	-6.254591000	0.753978000	-0.035550000
H	-5.155738000	1.698742000	0.971337000
C	-4.567476000	2.281866000	-1.596149000
H	-5.572520000	2.240846000	-2.022728000
H	-3.858554000	2.444697000	-2.410801000
H	-4.523025000	3.133094000	-0.913923000
C	-3.563665000	-2.222605000	-0.494067000
H	-4.268563000	-2.879465000	-1.013186000
H	-4.061531000	-1.811753000	0.384045000
H	-2.714096000	-2.810017000	-0.153283000
C	-2.461514000	-1.757389000	-2.693928000
H	-3.186003000	-2.381229000	-3.225570000
H	-1.619110000	-2.383667000	-2.391536000
H	-2.092488000	-0.997103000	-3.388220000
H	-2.974067000	1.170326000	2.190968000
H	-1.548187000	3.014153000	-1.398846000
H	2.192937000	0.770286000	2.117955000
H	2.447308000	3.257768000	-1.352489000
B	0.105912000	-1.696156000	0.703849000
C	-1.111549000	-2.997015000	2.931295000
C	0.311022000	-4.465049000	1.405062000
C	1.431982000	-2.824274000	2.984782000
H	-1.305611000	-2.835124000	3.993407000
H	-1.923937000	-3.607379000	2.527164000
H	1.341664000	-4.784142000	1.228036000
H	-0.319111000	-5.356641000	1.422430000
H	2.311876000	-3.427635000	3.216673000
H	1.239021000	-2.166674000	3.835695000
C	0.222410000	-3.735407000	2.750513000
H	0.259520000	-4.508401000	3.529827000
Pt	-0.088063000	-0.197643000	-0.724284000
S	-1.160367000	-1.336933000	2.133807000
S	-0.266416000	-3.458378000	-0.021844000
S	1.878270000	-1.795681000	1.526366000