Electronic Supplementary Information

Binding of Base-Stabilized Borylenes with Transition Metals and Formation of Metal Only Lewis Pairs

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Contents:

Table S1: SMD(benzene)-M06-2X-D3/6-311+G* calculated reaction free energies (ΔG°, in kcal mol^{-1}) for the formation of $Fe(CO)_4L$ and $Ni(CO)_3L$ complexes.

L	$\Delta G_{Fe(CO)_4L}$	$\Delta G_{Ni(CO)_3L}$
b	-7.4	-1.1
c	-9.6	-4.1
d	-14.0	-9.3
e	-14.0	-7.0
f	12.5	10.6
g	10.0	4.5
h	-4.2	4.4
i	1.6	-1.8

Table S2: SMD(benzene)-M06-2X-D3/6-311+G* calculated M–L (M=Fe and Ni, L=**a-i**) bond lengths (in Å) and their corresponding Wiberg Bond Indices (WBI) given within parentheses for $Fe(CO)_4L$ and $Ni(CO)_3L$ complexes, respectively.

Ligands	Fe-L	Ni-L
a	1.884(1.033)	1.902(0.866)
b	2.315(0.816)	2.313(0.623)
c	2.080(0.755)	2.065(0.612)
d	2.063(0.779)	2.040(0.625)
e	2.022(0.802)	2.029(0.636)
f	2.124(0.551)	2.281(0.253)
g	2.119(0.675)	2.225(0.349)
h	2.096(0.691)	2.118(0.451)
i	1.991(0.928)	2.079(0.600)

Table S3: SMD(benzene)-M06-2X-D3/6-311+G* calculated reaction free energies (ΔG in kcal mol^{-1}) and HOMO-LUMO gaps (ΔE_{H-L} in eV) of (1) Fe,and (2) Ni based MOLPs.

Molecules	ΔG^o	ΔE_{H-L}	Molecules	ΔG^o	ΔE_{H-L}
1a−$GaCl_3$	-13.6	6.95	**2a−$GaCl_3$**	0.0	7.71
1b−$GaCl_3$	-23.2	7.20	**2b−$GaCl_3$**	-12.6	7.22
1c−$GaCl_3$	-24.6	7.05	**2c−$GaCl_3$**	-17.1	7.28
1d−$GaCl_3$	-27.5	6.79	**2d−$GaCl_3$**	-18.0	6.86
1e−$GaCl_3$	-32.3	7.03	**2e−$GaCl_3$**	-17.3	7.31
1f−$GaCl_3$	-12.1	5.77	**2f−$GaCl_3$**	-15.9	5.24
1g−$GaCl_3$	-14.4	5.26	**2g−$GaCl_3$**	-21.2	5.33
1h−$GaCl_3$	-23.0	6.26	**2h−$GaCl_3$**	-24.9	5.71
1i−$GaCl_3$	-32.6	5.57	**2i−$GaCl_3$**	-22.1	5.42

Table S4: SMD(benzene)-M06-2X-D3/6-311+G* calculated energies of the lone pair orbital (E_{LP}) of free ligands (L) and metal centers (in eV) in $Fe(CO)_4L$, and $Ni(CO)_3L$ respectively.

Ligands (L)	E_{LP}		
	Free ligands	$Fe(CO)_4L$	$Ni(CO)_3L$
a	-12.26	-7.91	-8.22
b	-7.48	-7.20	-6.99
c	-7.67	-6.74	-6.83
d	-6.97	-6.68	-6.58
e	-7.78	-6.82	-6.72
f	-5.39	-6.12	-5.72
g	-5.49	-6.57	-5.74
h	-5.59	-6.43	-5.47
i	-5.48	-5.82	-5.68

Table S5: SMD(benzene)-M06-2X-D3/6-311+G* calculated sum of the angles around Ga (Σ_{ClGaCl}) and Ga Pyramidalization (360^o- Σ_{ClGaCl}) at the Ga center of the Fe and Ni based MOLPs employing different ligands (L=**a-i**).

Ligands (L)	**Σ_{ClGaCl}**		**Ga Pyramidalization (360^o- Σ_{ClGaCl})**	
	Fe	Ni	Fe	Ni
a	329.8	342.2	30.2	17.7
b	320.6	335.8	39.4	24.2
c	321.9	331.8	38.0	28.1
d	317.7	329.7	42.2	30.3
e	319.6	332.0	40.4	27.9
f	314.1	324.3	45.9	35.6
g	317.2	325.7	42.8	34.3
h	315.2	326.8	44.7	33.1
i	313.3	328.9	46.7	31.0

Table S6: SMD(benzene)-M06-2X-D3/6-311+G* natural charges of the donor atoms (q_E) in free ligands L (L=**a-i**), metal complexes $Fe(CO)_4L$ and $Ni(CO)_3L$ their corresponding $GaCl_3$ adducts ($[L(CO)_4Fe\rightarrow GaCl_3]$ and $[L(CO)_3Ni\rightarrow GaCl_3]$ respectively.

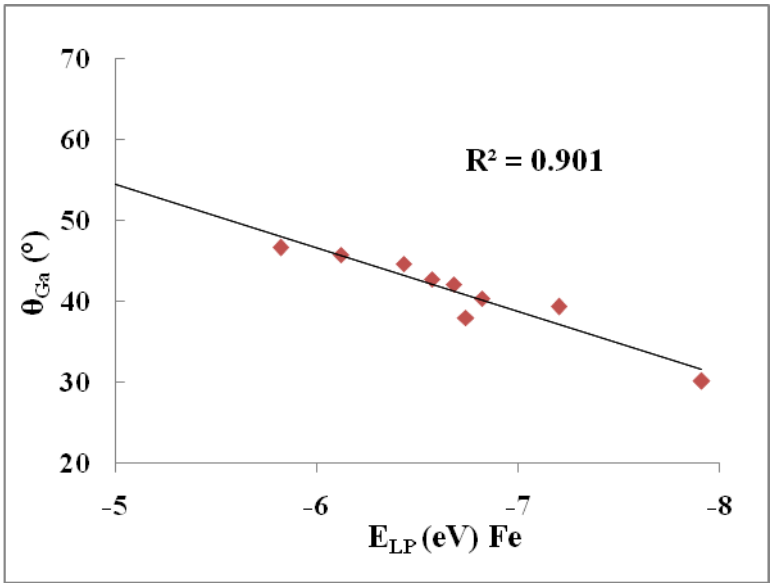
Ligands (L)	**Donor atom (E)**	**q_E (L)**	**Fe**		**Ni**	
			q_E [$Fe(CO)_4L$]	**q_E [$Fe(CO)_4L\rightarrow GaCl_3$]**	**q_E [$Ni(CO)_3L$]**	**q_E [$Ni(CO)_3L\rightarrow GaCl_3$]**
a	**C**	0.489	0.895	0.917	0.726	0.776
b	**P**	0.737	1.290	1.289	1.060	1.126
c	**C_c**	0.071	0.447	0.441	0.312	0.333
d	**C_c**	0.102	0.503	0.628	0.335	0.355
e	**C_c**	0.341	0.720	0.748	0.570	0.602
f	**B**	0.938	0.990	1.317	0.982	0.937
g	**B**	0.179	0.510	0.712	0.205	0.240
h	**B**	0.855	0.949	1.161	0.814	0.862
i	**B**	0.118	0.341	0.699	0.308	0.421

Table S7: SMD(benzene)-M06-2X-D3/6-311+G* valence population of the donor atoms (Val_E) in free ligands L (**L**=**a-i**), metal complexes $Fe(CO)_4L$ and $Ni(CO)_3L$, and their corresponding $GaCl_3$ adducts $[L(CO)_4Fe{\rightarrow}GaCl_3]$ and $[L(CO)_3Ni{\rightarrow}GaCl_3]$ respectively.

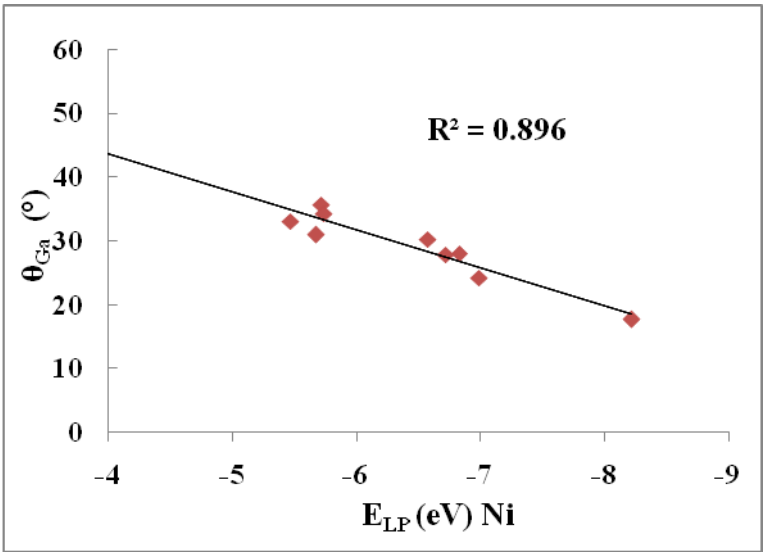
Ligands (L)	**Donor atom (E)**	**Val_E (L)**	**Fe**		**Ni**	
			Val_E $[Fe(CO)_4L]$	**Val_E $[Fe(CO)_4L{\rightarrow}Gacl_3]$**	**Val_E $[Ni(CO)_3L]$**	**Val_E $[Ni(CO)_3L{\rightarrow}GaCl_3]$**
a	**C**	3.457	3.032	3.029	3.197	3.158
b	**P**	4.212	3.661	3.664	3.888	3.826
c	**C_c**	3.893	3.500	3.504	3.635	3.618
d	**C_c**	3.870	3.444	3.316	3.613	3.595
e	**C_c**	3.620	3.221	3.189	3.371	3.343
f	**B**	2.035	1.957	1.595	1.977	2.015
g	**B**	2.806	2.435	2.220	2.762	2.719
h	**B**	2.126	2.003	1.778	2.143	2.096
i	**B**	2.865	2.613	2.237	2.650	2.538

Table S8: Calculated important AIM parameters such as electron density at the BCP (ρ_b), laplacian of electron density ($\nabla^2\rho_b$), local energy density H_b(r) and delocalization index (DI) of the L–M (L = **a-i**, M = Fe, Ni) bonds for all the MOLPs. All the tabulated values are in a.u.

L–M	**AIM Parameters**	**Ligands (L)**								
		a	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**
L–Fe	ρ_b	0.105	0.071	0.078	0.083	0.089	0.079	0.077	0.084	0.102
	$\nabla^2\rho_b$	0.574	0.218	0.311	0.309	0.366	0.076	0.112	0.096	0.067
	H_b(r)	-0.026	-0.016	-0.015	-0.018	-0.043	-0.027	-0.023	-0.028	-0.041
	DI	0.837	0.622	0.577	0.623	0.631	0.509	0.619	0.627	0.913
L–Ni	ρ_b	0.107	0.072	0.083	0.088	0.089	0.055	0.059	0.075	0.080
	$\nabla^2\rho_b$	0.482	0.170	0.286	0.305	0.330	0.086	0.077	0.080	0.095
	H_b(r)	-0.026	-0.020	-0.019	-0.021	-0.020	-0.017	-0.019	-0.028	-0.030
	DI	0.853	0.615	0.587	0.633	0.621	0.257	0.385	0.470	0.623



(a)



(b)

Fig. S1: Correlation plot between the pyramidalization angle at the Ga center (Θ_{Ga} in degree) of the MOLPs of (a) Fe and (b) Ni and the energies of the lone pair orbitals concentrated at Fe and Ni respectively.

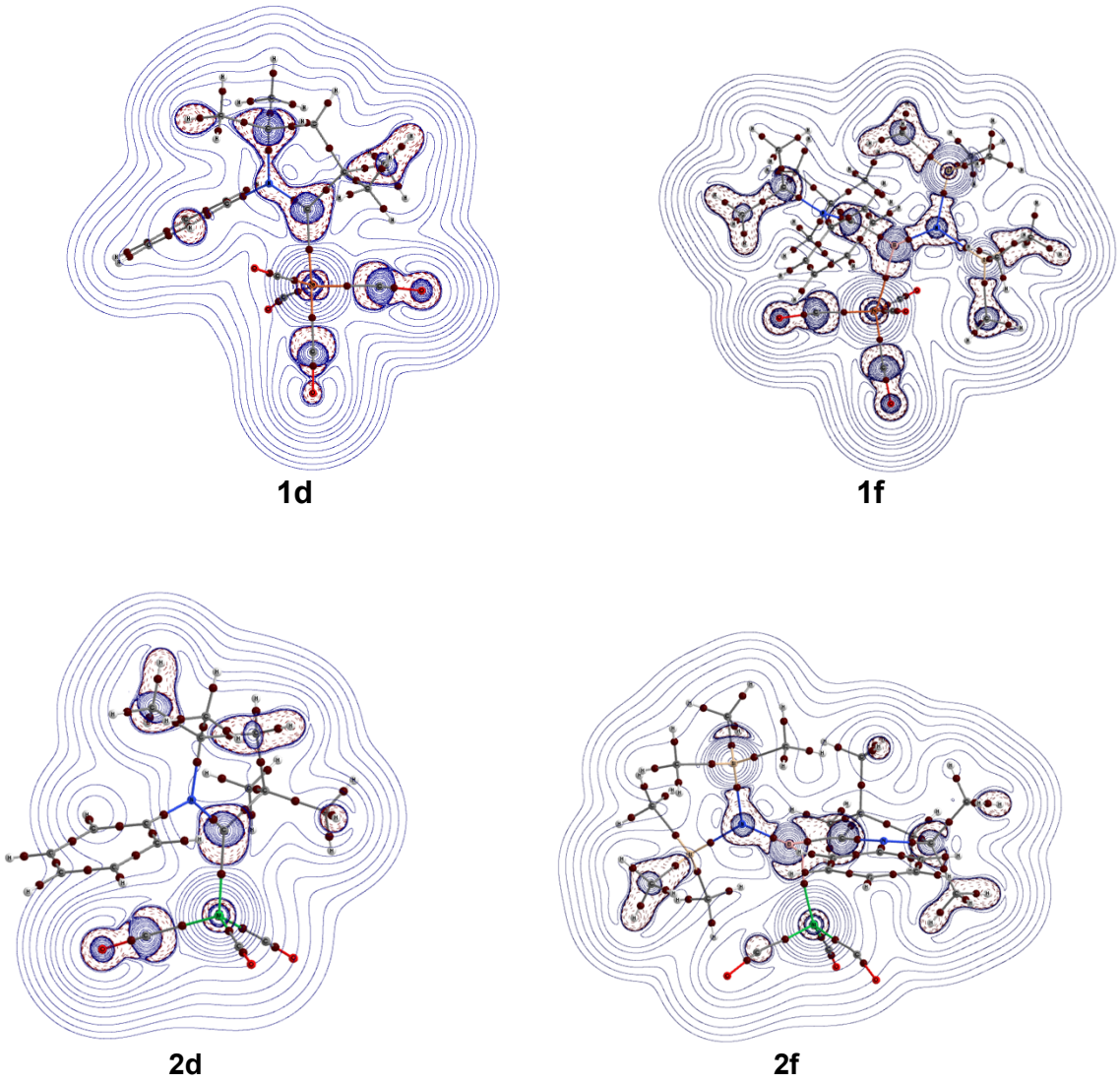
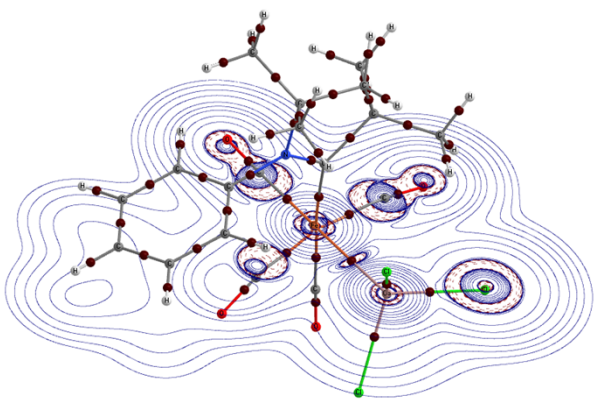
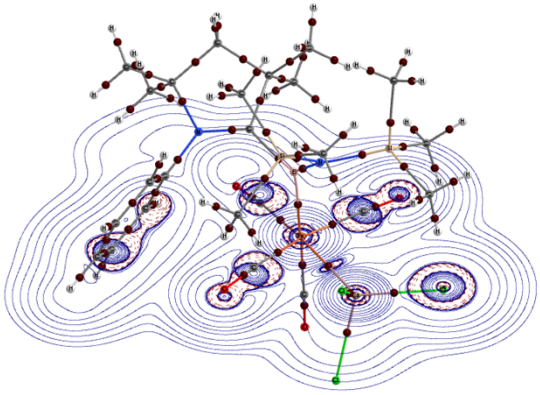


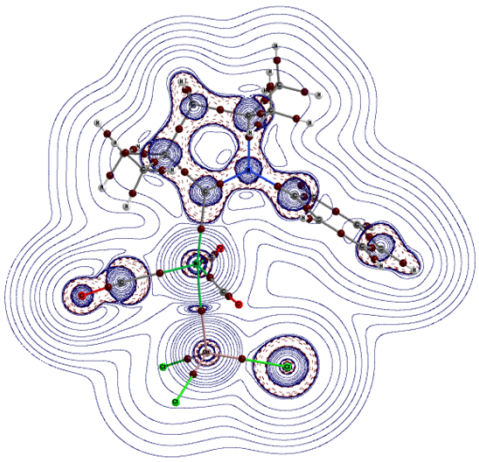
Fig. S2: Contour plots of Laplacian of the electron density ($\nabla^2\rho_b$) in the L–M–CO (M = Fe and Ni) plane showing the bonding of the ligands L (L= **d** and **f** as representative cases) to the metal complex. Regions of charge depletion ($\nabla^2\rho_b > 0$) are denoted by solid blue lines while regions of charge concentration ($\nabla^2\rho_b < 0$) are denoted by dashed red lines. Brown spheres denote bond critical points (BCPs).



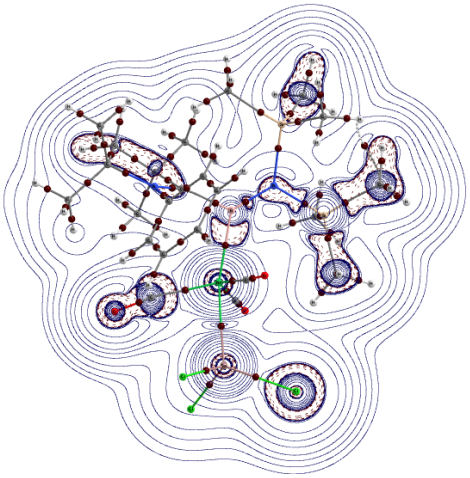
1d–$GaCl_3$



1f–$GaCl_3$



2d–$GaCl_3$



2f–$GaCl_3$

Fig. S3: Contour plots of Laplacian of the electron density ($\nabla^2\rho_b$) in the M–Ga–Cl (M = Fe and Ni) plane showing the bonding of the $Fe(CO)_4L$ and $Ni(CO)_3L$ (L= **d** and **f** as representative cases) complexes respectively to $GaCl_3$. Regions of charge depletion ($\nabla^2\rho_b > 0$) are denoted by solid blue lines while regions of charge concentration ($\nabla^2\rho_b < 0$) are denoted by dashed red lines. Brown spheres denote bond critical points (BCPs).

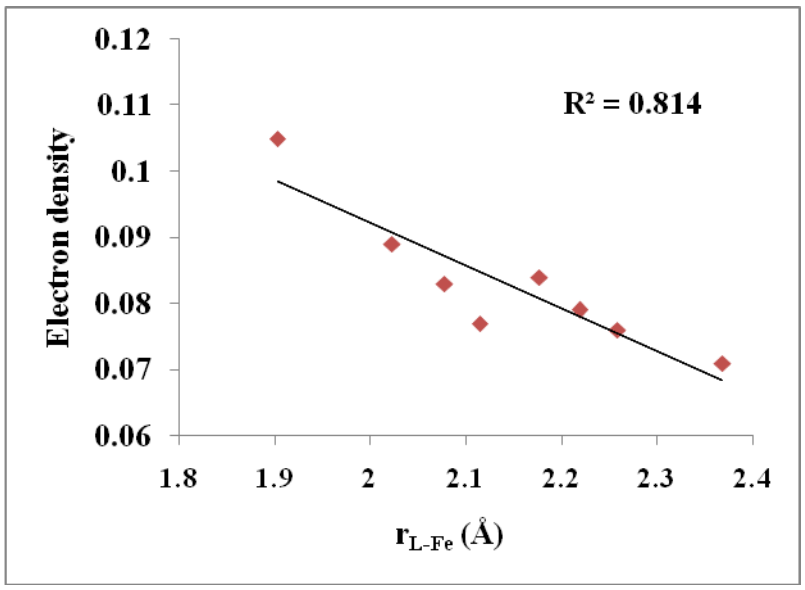


Fig. S4: Correlation plot between the L–Fe (L = **a-i**) bond distances and electron density at the bond critical point of the L–Fe bonds of $Fe(CO)_4L$ (Omitting the point corresponding to L = **1c**).

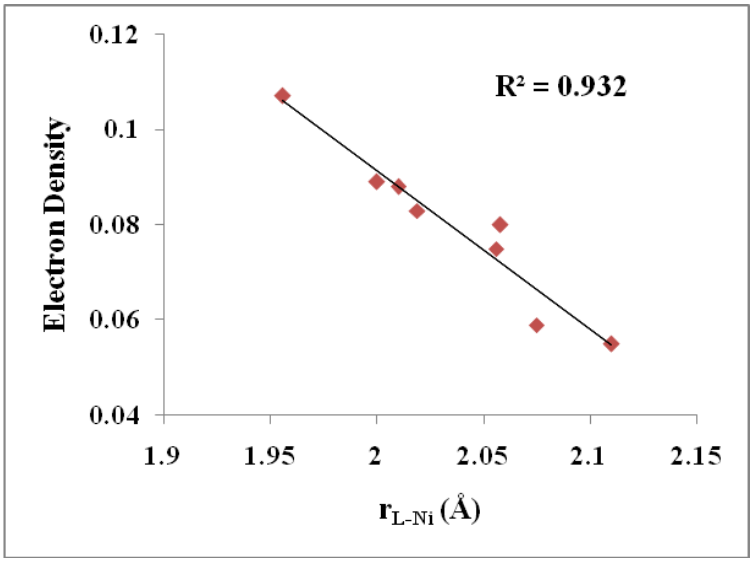


Fig. S5: Correlation plot between the L–Ni (L = **a-i**) bond distances and electron density at the bond critical point of the L-Ni bonds of $Ni(CO)_3L$ (Omitting the point corresponding to L = **1b**).

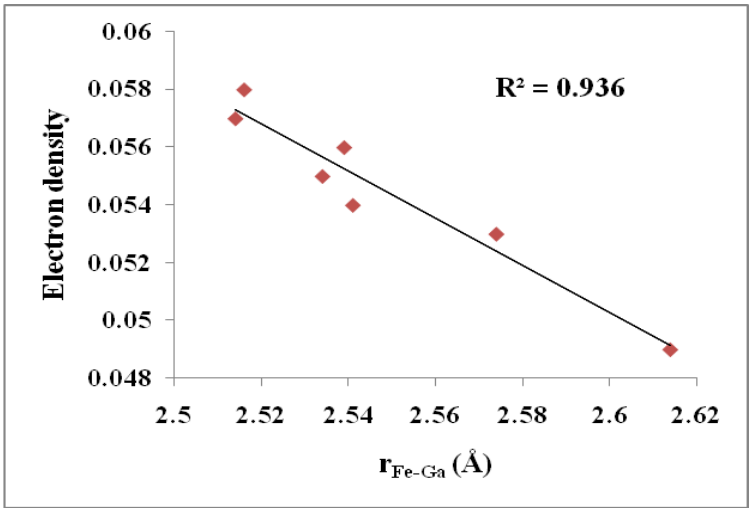


Fig. S6: Correlation plot between the Fe–Ga bond distances and electron density at the bond critical point of the Fe–Ga bond for the Fe MOLPs (Omitting the points corresponding to **1c**−$GaCl_3$and **1d**−$GaCl_3$).

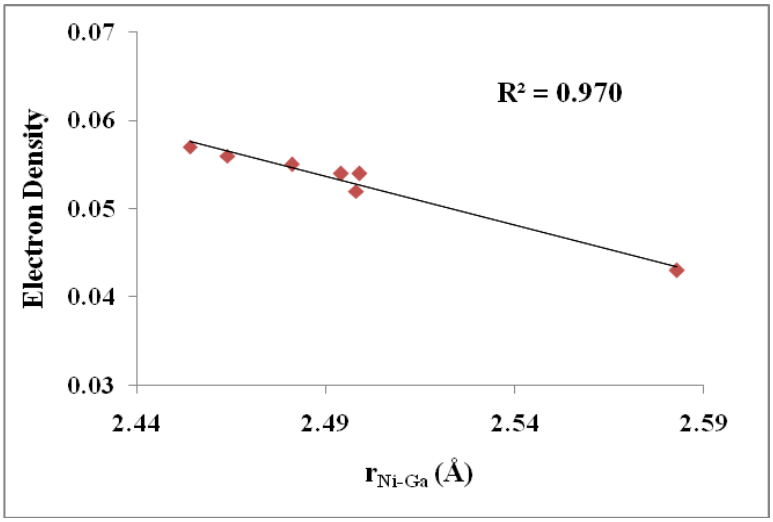


Fig. S7: Correlation plot between the Ni–Ga bond distances and electron density at the bond critical point of the Ni–Ga bond for the Ni MOLPs (Omitting the point corresponding to **1d**−$GaCl_3$).

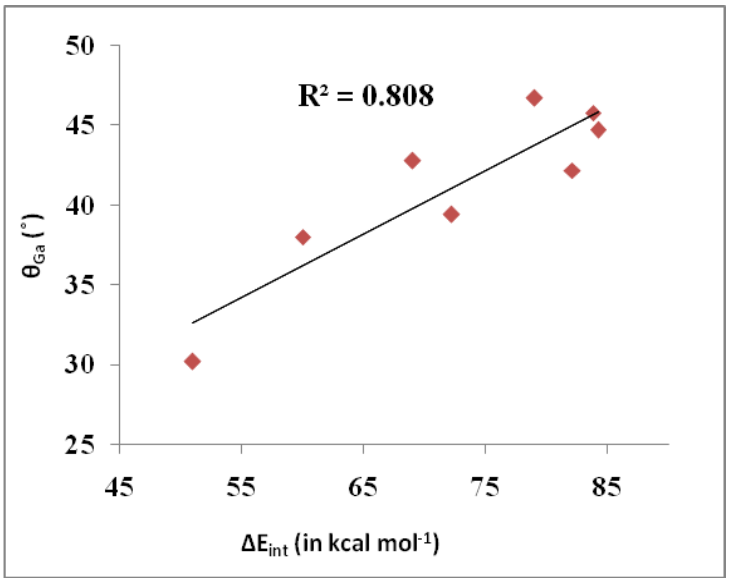


Fig. S8: Correlation plot between the calculated interaction energy (ΔE_{int}) values and the gallium pyramidalization at Ga center (θ_{Ga}) of the Fe–Ga bond for the Fe MOLPs (Omitting the point corresponding to **1e**–$GaCl_3$).

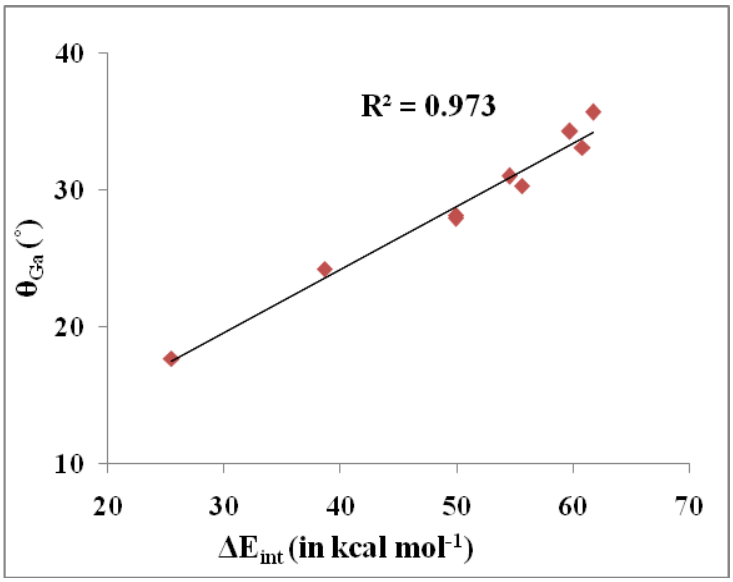


Fig. S9: Correlation plot between the calculated interaction energy (ΔE_{int}) values and the gallium pyramidalization at Ga center (θ_{Ga}) of the Ni–Ga bond for the Ni MOLPs.

Cartesian coordinates of the optimized geometries of the free ligands L (L=**a-i**) considered in this study are given along with their total energies (TE) and Gibbs free enthalpies (H) in hartrees including zero point vibrational correction.

a (TE = -113.300301, H=-113.296996)

6	0.000000000	0.000000000	-0.641163000
8	0.000000000	0.000000000	0.480872000

b (TE = -460.927074, H = -460.919573)

15	0.000000000	0.000000000	0.608972000
6	0.000000000	1.620474000	-0.280669000
1	0.000000000	1.494671000	-1.367441000
1	-0.880514000	2.201407000	0.003298000
1	0.880514000	2.201407000	0.003298000
6	-1.403371000	-0.810237000	-0.280669000
1	-1.294423000	-0.747336000	-1.367441000
1	-1.466217000	-1.863251000	0.003298000
1	-2.346732000	-0.338156000	0.003298000
6	1.403371000	-0.810237000	-0.280669000
1	2.346732000	-0.338156000	0.003298000
1	1.466217000	-1.863251000	0.003298000
1	1.294423000	-0.747336000	-1.367441000

c (TE = -304.624940, H = -304.617031)

6	-0.000119000	0.983982000	0.000000000
7	-0.000018000	0.129104000	1.058362000
7	-0.000018000	0.129104000	-1.058362000
6	0.000083000	-1.200115000	0.675954000
1	0.000150000	-2.012593000	1.385190000
6	0.000083000	-1.200115000	-0.675954000
1	0.000150000	-2.012593000	-1.385190000
6	-0.000018000	0.556657000	-2.445419000
1	0.889854000	0.187280000	-2.957886000
1	-0.889668000	0.186896000	-2.957991000
1	-0.000250000	1.643493000	-2.465200000
6	-0.000018000	0.556657000	2.445419000
1	-0.889668000	0.186896000	2.957991000
1	0.889854000	0.187280000	2.957886000
1	-0.000250000	1.643493000	2.465200000

d (TE = -599.211189, H = -599.195828)

6	2.291320000	0.845463000	0.297965000
6	0.818102000	1.209199000	0.057664000
6	0.980478000	-1.217068000	0.052533000
6	2.404417000	-0.677182000	0.038960000
1	2.954589000	1.429699000	-0.344900000
1	2.559213000	1.069772000	1.334433000
7	0.196702000	-0.171732000	0.061326000
6	-1.236690000	-0.294857000	0.023383000
6	-1.894508000	-0.343101000	-1.200967000
6	-1.953970000	-0.361345000	1.213040000
6	-3.281052000	-0.453864000	-1.233146000
1	-1.315782000	-0.313881000	-2.117736000
6	-3.339668000	-0.472999000	1.175741000
1	-1.421241000	-0.343474000	2.157293000
6	-4.005099000	-0.513636000	-0.046239000
1	-3.793867000	-0.501069000	-2.187258000
1	-3.898598000	-0.534708000	2.102729000
1	-5.085297000	-0.602784000	-0.073332000
6	3.239688000	-1.378563000	1.109850000
1	3.292655000	-2.452590000	0.917840000
1	4.259188000	-0.979738000	1.124173000
1	2.808352000	-1.237946000	2.105002000
6	2.992199000	-0.985253000	-1.345044000
1	4.027044000	-0.633907000	-1.400591000
1	2.983517000	-2.060099000	-1.538939000
1	2.428083000	-0.498791000	-2.145053000
6	0.576803000	1.878901000	-1.294239000
1	-0.487167000	2.056441000	-1.468383000
1	1.082080000	2.847650000	-1.318341000
1	0.965585000	1.272908000	-2.115292000
6	0.235982000	2.065733000	1.176876000
1	-0.819521000	2.293325000	1.010467000
1	0.337470000	1.569278000	2.144932000
1	0.778771000	3.013486000	1.225409000

e (TE = -556.610951, H = -556.598626)

6	2.880251000	-0.025844000	-0.253756000
6	1.176398000	-1.393325000	-0.999516000
6	1.592063000	0.511311000	0.366486000
1	3.669890000	-0.216852000	0.472078000
1	3.258413000	0.623158000	-1.047622000

8	2.499662000	-1.285103000	-0.857919000
7	0.626813000	-0.328270000	-0.411879000
6	1.414802000	2.003994000	0.130309000
1	0.480936000	2.368627000	0.563170000
1	2.233883000	2.548814000	0.607462000
1	1.425854000	2.239645000	-0.935932000
6	1.475409000	0.167215000	1.849868000
1	2.206658000	0.738024000	2.427948000
1	0.480875000	0.410505000	2.230941000
1	1.657724000	-0.897306000	2.017937000
6	-0.786915000	-0.198067000	-0.250493000
6	-1.462165000	0.873403000	-0.829786000
6	-1.484953000	-1.146940000	0.492460000
6	-2.836328000	0.999348000	-0.654316000
1	-0.915319000	1.589282000	-1.432258000
6	-2.860086000	-1.021759000	0.656629000
1	-0.943183000	-1.981343000	0.923636000
6	-3.536575000	0.054169000	0.089352000
1	-3.361136000	1.830467000	-1.111663000
1	-3.402440000	-1.766596000	1.227988000
1	-4.608548000	0.151251000	0.219395000

f (TE = -1497.127421, H = -1497.094361)

6	3.148767000	-1.122182000	0.405437000
6	0.834690000	-0.923922000	-0.194119000
6	1.169711000	-2.395950000	-0.379448000
6	2.431278000	-2.491965000	0.490072000
1	2.122799000	-2.674390000	1.523636000
1	3.095644000	-3.307888000	0.190623000
7	2.082157000	-0.229817000	-0.150035000
6	4.361885000	-1.230821000	-0.526720000
1	4.837283000	-0.273905000	-0.737596000
1	5.113808000	-1.878729000	-0.067242000
1	4.079470000	-1.674074000	-1.482614000
6	3.564467000	-0.713770000	1.825844000
1	4.106284000	-1.541617000	2.292251000
1	4.209822000	0.162385000	1.870565000
1	2.674166000	-0.513141000	2.428441000
6	0.078353000	-3.344661000	0.105873000
1	-0.849834000	-3.203588000	-0.459220000
1	0.385231000	-4.386380000	-0.029306000
1	-0.142179000	-3.188319000	1.164515000
6	1.468008000	-2.686441000	-1.859038000
1	1.970014000	-3.652527000	-1.980794000

1	0.538138000	-2.716201000	-2.432749000
1	2.097439000	-1.912424000	-2.301340000
6	2.169528000	1.145311000	-0.217751000
6	1.037652000	1.931118000	-0.532469000
6	3.372265000	1.855580000	0.009718000
6	1.106434000	3.317364000	-0.609128000
1	0.091284000	1.463741000	-0.763080000
6	3.423589000	3.238641000	-0.065872000
1	4.285411000	1.333638000	0.243102000
6	2.294248000	3.995138000	-0.370930000
1	0.206081000	3.870398000	-0.858023000
1	4.372465000	3.732048000	0.118918000
1	2.342744000	5.076245000	-0.423604000
5	-0.493966000	-0.497742000	-0.028075000
7	-1.828679000	-0.189474000	0.068453000
14	-2.779910000	0.111352000	-1.416343000
14	-2.411732000	0.159119000	1.727761000
6	-4.236955000	-1.065167000	-1.482188000
1	-4.612505000	-1.131545000	-2.508624000
1	-3.943152000	-2.075071000	-1.180097000
1	-5.074114000	-0.757253000	-0.852490000
6	-3.358258000	1.893888000	-1.410527000
1	-3.977114000	2.146055000	-0.545257000
1	-2.511220000	2.586513000	-1.425479000
1	-3.958092000	2.099667000	-2.303214000
6	-4.278951000	0.018252000	1.783214000
1	-4.798304000	0.719515000	1.125734000
1	-4.616903000	-0.992363000	1.538526000
1	-4.617382000	0.232096000	2.802777000
6	-1.854489000	1.890520000	2.156089000
1	-2.212440000	2.201250000	3.142524000
1	-0.761869000	1.954631000	2.164342000
1	-2.216590000	2.621986000	1.427033000
6	-1.683673000	-1.089728000	2.910853000
1	-0.591335000	-1.057950000	2.922223000
1	-2.031813000	-0.887500000	3.929209000
1	-1.990993000	-2.108221000	2.656837000
6	-1.688246000	-0.194816000	-2.898963000
1	-1.386816000	-1.243227000	-2.971144000
1	-2.243023000	0.048286000	-3.811722000
1	-0.775738000	0.406696000	-2.895741000

g (TE = -1548.527581, H = -1548.489728)

6	-4.061588000	-0.338551000	-0.515361000

6	-1.739073000	-0.878137000	-0.229714000
6	-2.430492000	-2.224483000	-0.401816000
6	-3.806313000	-1.798964000	-0.962805000
1	-3.778363000	-1.842752000	-2.055097000
1	-4.604393000	-2.466965000	-0.627390000
7	-2.747331000	0.041882000	0.059317000
6	-5.141490000	-0.218796000	0.559498000
1	-5.206417000	0.810248000	0.925159000
1	-6.121090000	-0.491816000	0.157135000
1	-4.924070000	-0.869544000	1.409143000
6	-4.443165000	0.526559000	-1.719403000
1	-5.366626000	0.148995000	-2.167991000
1	-4.611781000	1.567677000	-1.432711000
1	-3.661539000	0.496479000	-2.483011000
6	-1.689576000	-3.167114000	-1.344133000
1	-0.700376000	-3.420330000	-0.949012000
1	-2.243394000	-4.102993000	-1.468594000
1	-1.551393000	-2.714436000	-2.328564000
6	-2.586418000	-2.887947000	0.975483000
1	-3.219125000	-3.778639000	0.903125000
1	-1.615154000	-3.194930000	1.372385000
1	-3.040642000	-2.203771000	1.696113000
6	-2.390820000	1.391226000	0.338534000
6	-1.948443000	2.247531000	-0.672462000
6	-2.403796000	1.839279000	1.658458000
6	-1.537172000	3.539779000	-0.365591000
1	-1.910214000	1.884964000	-1.693322000
6	-1.987838000	3.131672000	1.966078000
1	-2.728670000	1.155662000	2.436159000
6	-1.554578000	3.983440000	0.954335000
1	-1.194051000	4.198228000	-1.156559000
1	-1.997698000	3.470732000	2.996212000
1	-1.228207000	4.989492000	1.194254000
5	-0.341429000	-0.632106000	-0.268045000
15	1.238461000	0.142399000	-0.018051000
7	2.220778000	-0.490613000	1.255071000
7	2.274767000	0.266251000	-1.347519000
6	1.678094000	-1.409450000	2.271080000
1	2.464856000	-1.487501000	3.025830000
6	3.245891000	0.471329000	1.714072000
1	3.540351000	1.019834000	0.813089000
6	2.347749000	1.571981000	-2.028255000
1	1.913743000	2.295107000	-1.331291000
6	2.886646000	-0.883744000	-2.041665000
1	3.156581000	-0.522458000	-3.037933000
6	4.504532000	-0.230816000	2.225780000

1	5.316181000	0.495357000	2.320806000
1	4.363137000	-0.676902000	3.213524000
1	4.829323000	-1.014021000	1.539004000
6	2.736734000	1.485966000	2.740329000
1	3.491394000	2.256484000	2.922196000
1	1.826645000	1.979161000	2.387896000
1	2.522013000	1.005767000	3.699307000
6	1.484294000	-2.808725000	1.691128000
1	1.144730000	-3.500380000	2.467356000
1	0.730728000	-2.806812000	0.899339000
1	2.419706000	-3.190546000	1.275686000
6	0.407387000	-0.942649000	2.999167000
1	0.472410000	0.102812000	3.304286000
1	-0.475417000	-1.050111000	2.367317000
1	0.255572000	-1.549049000	3.897694000
6	1.505070000	1.600037000	-3.304745000
1	1.510402000	2.597938000	-3.752277000
1	1.884512000	0.902153000	-4.056939000
1	0.471319000	1.326523000	-3.080547000
6	3.791234000	1.998532000	-2.296117000
1	4.294164000	1.331264000	-3.001683000
1	3.812836000	3.002987000	-2.727207000
1	4.371384000	2.015877000	-1.370434000
6	1.925091000	-2.050474000	-2.241328000
1	0.994217000	-1.721496000	-2.708783000
1	2.389308000	-2.808246000	-2.878743000
1	1.678415000	-2.526748000	-1.288520000
6	4.167286000	-1.348786000	-1.348434000
1	4.847990000	-0.511216000	-1.177789000
1	3.927077000	-1.796138000	-0.382452000
1	4.686880000	-2.096189000	-1.955941000

h (TE = -1454.494934, H = -1454.465087)

6	2.501750000	-1.929400000	-1.698417000
6	0.706856000	-0.850805000	-0.794409000
6	2.578980000	-1.995110000	-0.161524000
1	2.574800000	-2.913717000	-2.167763000
1	3.287401000	-1.279944000	-2.103077000
8	1.225743000	-1.368734000	-1.996328000
7	1.728025000	-0.815957000	0.204658000
6	4.010954000	-1.920402000	0.340963000
1	4.049054000	-1.931743000	1.432797000
1	4.559701000	-2.794349000	-0.020492000
1	4.529743000	-1.027664000	-0.011794000

6	1.893492000	-3.256949000	0.358001000
1	2.455077000	-4.146779000	0.061300000
1	1.833683000	-3.232100000	1.448733000
1	0.879831000	-3.343582000	-0.038273000
6	2.405370000	0.440540000	0.342018000
6	2.553249000	1.335616000	-0.722096000
6	2.918283000	0.784471000	1.593510000
6	3.205524000	2.549229000	-0.531914000
1	2.145384000	1.075644000	-1.693766000
6	3.579710000	1.994314000	1.778129000
1	2.777242000	0.096281000	2.420072000
6	3.723874000	2.883644000	0.717200000
1	3.312904000	3.235638000	-1.365252000
1	3.968726000	2.249455000	2.758115000
1	4.230930000	3.830946000	0.862547000
5	-0.626871000	-0.506731000	-0.525712000
7	-1.872266000	-0.035684000	-0.209040000
14	-3.047743000	-1.147955000	0.554875000
14	-2.146716000	1.721770000	-0.444419000
6	-2.178894000	-2.766224000	0.890211000
1	-2.843560000	-3.437297000	1.444531000
1	-1.890475000	-3.275499000	-0.032965000
1	-1.274033000	-2.624055000	1.487326000
6	-4.501126000	-1.426291000	-0.593383000
1	-4.166164000	-1.590078000	-1.621797000
1	-5.055444000	-2.319418000	-0.286990000
1	-5.207968000	-0.593585000	-0.598949000
6	-3.616492000	-0.386475000	2.169389000
1	-2.773534000	-0.214145000	2.844586000
1	-4.142022000	0.563320000	2.038667000
1	-4.309059000	-1.064801000	2.678515000
6	-3.967567000	2.006180000	-0.782502000
1	-4.618992000	1.734297000	0.051851000
1	-4.133741000	3.070803000	-0.978830000
1	-4.302694000	1.459876000	-1.668631000
6	-1.598481000	2.616638000	1.101263000
1	-1.738213000	3.697980000	1.004771000
1	-2.150650000	2.289676000	1.986669000
1	-0.534701000	2.438288000	1.289382000
6	-1.147100000	2.289098000	-1.915782000
1	-0.074483000	2.254795000	-1.710361000
1	-1.336831000	1.672263000	-2.799002000
1	-1.401666000	3.322655000	-2.172401000

i (TE = -1505.908926, H = -1505.874580)

6	-3.929462000	-1.235734000	-0.665326000
6	-1.624783000	-1.143643000	-0.967618000
6	-3.502244000	-1.991862000	-1.923751000
1	-3.732057000	-1.414022000	-2.824834000
1	-3.932421000	-2.990485000	-2.001647000
7	-2.725207000	-0.377905000	-0.555671000
6	-4.072388000	-2.181608000	0.527667000
1	-4.264862000	-1.623689000	1.447242000
1	-4.907780000	-2.869417000	0.372498000
1	-3.162871000	-2.773401000	0.665797000
6	-5.183144000	-0.404347000	-0.873526000
1	-6.037137000	-1.053302000	-1.084581000
1	-5.419801000	0.173235000	0.023566000
1	-5.058325000	0.288732000	-1.708092000
6	-2.554530000	0.548857000	0.515109000
6	-2.903783000	1.882634000	0.312521000
6	-2.009873000	0.156272000	1.740832000
6	-2.702493000	2.820166000	1.321563000
1	-3.310048000	2.175677000	-0.649381000
6	-1.799639000	1.096942000	2.743810000
1	-1.747307000	-0.884016000	1.894702000
6	-2.141412000	2.431100000	2.534550000
1	-2.970177000	3.857718000	1.153572000
1	-1.374149000	0.785201000	3.691403000
1	-1.974030000	3.163978000	3.316032000
5	-0.266523000	-0.967628000	-0.557312000
15	1.486097000	-0.585481000	-0.673661000
7	2.407191000	-0.899655000	0.726386000
7	1.683903000	1.067994000	-1.014017000
6	3.110592000	-2.187742000	0.855320000
1	3.550956000	-2.185045000	1.856477000
6	2.118373000	-0.162401000	1.966523000
1	1.492586000	0.685194000	1.674224000
6	0.732796000	2.093007000	-0.542002000
1	0.097459000	1.602349000	0.201195000
6	2.604957000	1.467098000	-2.093552000
1	2.543898000	2.556549000	-2.156797000
6	3.396592000	0.413630000	2.574902000
1	3.163265000	1.045464000	3.436813000
1	4.073753000	-0.372578000	2.921081000
1	3.929835000	1.016214000	1.836521000
6	1.330692000	-0.985636000	2.987270000
1	1.054470000	-0.365760000	3.845025000
1	0.418246000	-1.384959000	2.538945000

1	1.919854000	-1.824947000	3.368593000
6	4.261247000	-2.298845000	-0.141126000
1	4.806562000	-3.235672000	0.004301000
1	3.888853000	-2.290116000	-1.169671000
1	4.959552000	-1.467953000	-0.018640000
6	2.190286000	-3.408654000	0.755966000
1	1.333908000	-3.321332000	1.427034000
1	1.804602000	-3.524070000	-0.260709000
1	2.736697000	-4.321688000	1.011415000
6	-0.185354000	2.602240000	-1.653445000
1	-0.883558000	3.344952000	-1.258587000
1	0.381649000	3.082555000	-2.456689000
1	-0.763608000	1.777850000	-2.079599000
6	1.451136000	3.244414000	0.163963000
1	2.066516000	3.833146000	-0.522238000
1	0.721272000	3.925206000	0.611124000
1	2.099197000	2.866380000	0.958640000
6	2.207279000	0.897442000	-3.456684000
1	1.165706000	1.125022000	-3.692507000
1	2.840449000	1.309840000	-4.247757000
1	2.322191000	-0.190135000	-3.468686000
6	4.048674000	1.106910000	-1.755541000
1	4.332412000	1.509892000	-0.780731000
1	4.179639000	0.022618000	-1.724487000
1	4.733087000	1.502134000	-2.511751000
8	-2.082457000	-2.128930000	-1.801097000

Cartesian coordinates of the optimized geometries of the $Fe(CO)_4L$ and $Ni(CO)_3L$ complexes for the ligands L (L=**a-i**).are given along with their total energies (TE) and Gibbs free enthalpies (H) in hartrees including zero point vibrational correction.

1a (TE = -1830.178393, H = -1830.164927)

26	0.000058000	0.002829000	-0.004168000
6	1.883884000	0.001091000	-0.003897000
6	0.000954000	1.743678000	-0.592300000
6	-0.000642000	-1.388870000	-1.203161000
6	-1.883743000	0.002769000	-0.004132000
6	-0.000356000	-0.353269000	1.796503000
8	3.011492000	0.000009000	-0.001505000
8	-0.000650000	-0.577957000	2.908896000
8	-0.001230000	-2.257312000	-1.933907000
8	-3.011349000	0.002318000	-0.001808000

8	0.001476000	2.819699000	-0.952890000

1b (TE = -2177.820165, H = -2177.801708)

15	0.008720000	-0.007727000	0.530555000
6	0.062355000	1.629293000	-0.279221000
1	0.043741000	1.533333000	-1.367360000
1	-0.793480000	2.228081000	0.039537000
1	0.971354000	2.159171000	0.012835000
6	-1.439442000	-0.803116000	-0.249742000
1	-1.351161000	-0.810084000	-1.338663000
1	-1.532887000	-1.830948000	0.107621000
1	-2.350438000	-0.268201000	0.026822000
6	1.420456000	-0.887269000	-0.226243000
1	2.356869000	-0.436185000	0.108628000
1	1.419233000	-1.932916000	0.088356000
1	1.376645000	-0.847180000	-1.317198000
26	-0.017181000	0.023073000	2.845098000
6	0.128796000	-1.781444000	2.802573000
6	1.494715000	1.018633000	2.809696000
6	-1.630935000	0.840631000	2.747660000
6	-0.076573000	0.037630000	4.684689000
8	0.225037000	-2.918172000	2.748404000
8	-2.643644000	1.362842000	2.668361000
8	2.448659000	1.644965000	2.771069000
8	-0.120844000	0.045594000	5.817102000

1c (TE =-2021.522342, H = -2021.503736)

6	-1.149362000	0.060446000	-0.026826000
7	-1.973269000	-1.021418000	-0.058757000
7	-2.007182000	1.112709000	-0.008576000
6	-3.302651000	-0.649155000	-0.087356000
1	-4.100447000	-1.372642000	-0.116996000
6	-3.324084000	0.700054000	-0.054686000
1	-4.144607000	1.398015000	-0.048777000
6	-1.627155000	2.515150000	0.073242000
1	-1.251631000	2.869261000	-0.886386000
1	-2.508212000	3.094007000	0.344811000
1	-0.868109000	2.647652000	0.841620000
6	-1.565452000	-2.420733000	-0.058681000
1	-2.299722000	-2.996693000	0.503410000
1	-1.510868000	-2.804255000	-1.078415000
1	-0.592950000	-2.518435000	0.416177000

26	0.928923000	0.003543000	0.025196000
6	1.211443000	1.727845000	-0.483299000
6	0.699213000	-0.450772000	1.769994000
6	0.880398000	-1.133267000	-1.390857000
6	2.745877000	-0.246707000	0.193902000
8	1.506411000	2.772342000	-0.839076000
8	0.492486000	-0.742003000	2.856222000
8	0.837217000	-1.819176000	-2.303342000
8	3.861180000	-0.419315000	0.314720000

1d (TE = -2316.118607, H = -2316.092451)

6	-1.033722000	2.978953000	0.383429000
6	-2.073454000	1.866368000	0.209829000
6	0.117803000	0.894094000	-0.100386000
6	0.306166000	2.414167000	-0.130644000
1	-1.324871000	3.889805000	-0.143794000
1	-0.940863000	3.227115000	1.444228000
7	-1.170535000	0.672317000	0.008217000
6	-1.781229000	-0.630846000	-0.040269000
6	-2.318026000	-1.081890000	-1.240236000
6	-1.842902000	-1.414591000	1.106988000
6	-2.925687000	-2.332210000	-1.292192000
1	-2.230189000	-0.469400000	-2.130894000
6	-2.444468000	-2.665983000	1.046265000
1	-1.411549000	-1.050716000	2.032266000
6	-2.988324000	-3.124580000	-0.151108000
1	-3.332232000	-2.692474000	-2.230122000
1	-2.482970000	-3.284787000	1.935274000
1	-3.453368000	-4.102798000	-0.194833000
6	1.459877000	2.919343000	0.736193000
1	2.434912000	2.616638000	0.356152000
1	1.436041000	4.013333000	0.757820000
1	1.374644000	2.563218000	1.765645000
6	0.545561000	2.812386000	-1.597850000
1	0.628811000	3.900485000	-1.666864000
1	1.465687000	2.381960000	-1.992974000
1	-0.274016000	2.494638000	-2.246075000
6	-2.990723000	2.071001000	-0.994234000
1	-3.701649000	1.249428000	-1.100337000
1	-3.567432000	2.987168000	-0.847063000
1	-2.429913000	2.171346000	-1.925089000
6	-2.909180000	1.666282000	1.470778000
1	-3.642578000	0.865530000	1.354473000
1	-2.273937000	1.438448000	2.330481000

1	-3.451305000	2.590348000	1.686936000
26	1.621166000	-0.514620000	0.012406000
6	1.319061000	-0.331482000	1.780169000
6	0.789747000	-1.779312000	-1.014394000
6	2.824583000	0.473817000	-0.933269000
8	1.087020000	-0.187734000	2.893943000
8	0.393888000	-2.618903000	-1.676313000
8	3.639321000	1.003533000	-1.534399000
6	2.956902000	-1.725573000	0.386983000
8	3.773309000	-2.468778000	0.651566000

1e (TE = -2273.516345, H = -2273.492926)

6	0.998403000	-3.042790000	0.229429000
6	2.075595000	-1.970814000	0.017366000
6	-0.103976000	-1.049714000	-0.050171000
1	1.070599000	-3.872169000	-0.472581000
1	0.982602000	-3.425643000	1.251665000
7	1.191312000	-0.765879000	-0.014808000
6	1.734614000	0.559174000	-0.008852000
6	2.263965000	1.099170000	-1.176549000
6	1.733750000	1.290108000	1.175205000
6	2.804146000	2.380787000	-1.154276000
1	2.217644000	0.534283000	-2.100421000
6	2.264692000	2.574625000	1.187999000
1	1.305981000	0.854997000	2.071598000
6	2.804979000	3.117776000	0.025435000
1	3.205826000	2.809213000	-2.065236000
1	2.253449000	3.150679000	2.105999000
1	3.217483000	4.120186000	0.037002000
6	2.801637000	-2.149585000	-1.312404000
1	3.530866000	-1.354922000	-1.479233000
1	3.342078000	-3.099449000	-1.305391000
1	2.095121000	-2.163531000	-2.146064000
6	3.055384000	-1.892881000	1.179968000
1	3.780374000	-1.089611000	1.032606000
1	2.532378000	-1.721472000	2.123415000
1	3.606893000	-2.832923000	1.259746000
26	-1.760667000	0.109687000	-0.025944000
6	-1.578078000	0.128905000	1.768465000
6	-1.025438000	1.445815000	-1.033242000
6	-2.648574000	-1.269765000	-0.837433000
8	-1.429688000	0.112774000	2.902869000
8	-0.660340000	2.319386000	-1.670000000
8	-3.198739000	-2.126880000	-1.348789000

6	-3.333967000	1.078695000	0.060871000
8	-4.302904000	1.665698000	0.120721000
8	-0.256569000	-2.370651000	-0.000524000

1f (TE = -3213.999584, H = -3213.957507)

6	-3.192296000	-1.480559000	0.533628000
6	-0.972892000	-0.613264000	0.782869000
6	-1.413171000	-1.018577000	2.202484000
6	-2.636540000	-1.914964000	1.903127000
1	-2.326824000	-2.962625000	1.851833000
1	-3.393525000	-1.833851000	2.685217000
7	-1.978470000	-0.823600000	-0.056698000
6	-4.382652000	-0.526357000	0.638535000
1	-4.773890000	-0.272916000	-0.348295000
1	-5.186403000	-1.022300000	1.188199000
1	-4.132509000	0.397847000	1.157997000
6	-3.582492000	-2.678210000	-0.329318000
1	-4.379640000	-3.233800000	0.170887000
1	-3.955130000	-2.362323000	-1.306397000
1	-2.740207000	-3.356246000	-0.483427000
6	-0.305689000	-1.762725000	2.952977000
1	0.591258000	-1.143863000	3.047166000
1	-0.646793000	-2.001141000	3.963979000
1	-0.034648000	-2.700553000	2.470377000
6	-1.845927000	0.169618000	3.079776000
1	-2.223524000	-0.233098000	4.023920000
1	-1.017028000	0.837890000	3.305286000
1	-2.642048000	0.756999000	2.627618000
6	-1.904001000	-0.494420000	-1.450953000
6	-1.048743000	-1.202531000	-2.289197000
6	-2.668939000	0.557550000	-1.953018000
6	-0.969653000	-0.871814000	-3.637906000
1	-0.452738000	-2.008957000	-1.883693000
6	-2.585830000	0.880846000	-3.302423000
1	-3.297455000	1.137866000	-1.289723000
6	-1.741112000	0.166550000	-4.146700000
1	-0.301409000	-1.425658000	-4.287776000
1	-3.171187000	1.707161000	-3.689033000
1	-1.674237000	0.429165000	-5.196250000
5	0.393243000	0.008451000	0.376068000
7	1.599404000	-0.661274000	0.049656000
26	-0.028792000	2.084915000	0.524941000
6	0.283596000	1.932824000	-1.218382000
6	0.959383000	1.739555000	1.952774000

6	-1.776670000	2.306580000	0.762601000
8	0.509487000	1.851808000	-2.341974000
8	1.610887000	1.481683000	2.870273000
8	-2.890112000	2.574057000	0.864509000
14	3.098219000	0.187211000	-0.528870000
14	1.828100000	-2.443233000	0.155327000
6	3.185267000	-0.047612000	-2.397259000
1	3.905903000	-0.814266000	-2.691680000
1	2.212240000	-0.319556000	-2.813259000
1	3.489024000	0.886938000	-2.877831000
6	3.379608000	2.009735000	-0.188085000
1	2.761083000	2.686855000	-0.773838000
1	3.301938000	2.288080000	0.863268000
1	4.422116000	2.180792000	-0.488585000
6	4.585675000	-0.585236000	0.335333000
1	5.487379000	-0.168936000	-0.127708000
1	4.605376000	-0.278698000	1.386213000
1	4.689355000	-1.668900000	0.307685000
6	2.729405000	-2.858424000	1.760105000
1	2.124896000	-3.489698000	2.416120000
1	3.653440000	-3.407942000	1.555215000
1	3.000628000	-1.963699000	2.324684000
6	2.821201000	-3.082246000	-1.310439000
1	2.850801000	-4.174920000	-1.222219000
1	2.327786000	-2.854717000	-2.260171000
1	3.853978000	-2.741814000	-1.382005000
6	0.262782000	-3.495694000	0.038760000
1	-0.666357000	-3.056791000	0.389141000
1	0.102756000	-3.838629000	-0.987025000
1	0.437164000	-4.397296000	0.637254000
6	0.433266000	3.812950000	0.558571000
8	0.767780000	4.903768000	0.584668000

1g (TE = -3265.403971, H =-3265.403971)

6	-3.705571000	0.168436000	1.635547000
6	-1.416335000	0.384372000	0.974044000
6	-1.516469000	1.009858000	2.393685000
6	-2.877164000	0.488147000	2.877918000
1	-2.732110000	-0.433167000	3.450254000
1	-3.383320000	1.208414000	3.523423000
7	-2.598197000	-0.106873000	0.636570000
6	-4.554505000	1.321142000	1.100855000
1	-5.067301000	1.020344000	0.183454000
1	-5.316237000	1.588073000	1.837128000

1	-3.962842000	2.206468000	0.874637000
6	-4.612547000	-1.023773000	1.926512000
1	-5.218913000	-0.759492000	2.797157000
1	-5.297736000	-1.248748000	1.109378000
1	-4.040298000	-1.916929000	2.186521000
6	-0.399036000	0.559401000	3.338238000
1	0.562829000	0.998864000	3.069966000
1	-0.654329000	0.895638000	4.347506000
1	-0.279270000	-0.524292000	3.357734000
6	-1.523728000	2.549470000	2.392964000
1	-1.669664000	2.874601000	3.426865000
1	-0.584707000	2.966473000	2.038635000
1	-2.329703000	2.974419000	1.798968000
6	-2.936137000	-0.658510000	-0.652200000
6	-3.575258000	-1.896847000	-0.743064000
6	-2.656495000	0.059173000	-1.812009000
6	-3.948502000	-2.395287000	-1.985332000
1	-3.750144000	-2.493678000	0.138967000
6	-3.012368000	-0.458235000	-3.053581000
1	-2.155328000	1.013820000	-1.753418000
6	-3.669877000	-1.679180000	-3.144900000
1	-4.437191000	-3.361195000	-2.043529000
1	-2.778209000	0.107836000	-3.947766000
1	-3.953293000	-2.076005000	-4.112992000
5	-0.078621000	0.464556000	0.177077000
15	1.239989000	-0.838816000	0.716121000
26	0.353343000	2.295414000	-0.798402000
6	0.948011000	3.748541000	-1.697349000
8	1.340705000	4.653360000	-2.265953000
7	0.920351000	-2.360544000	0.010403000
7	2.837265000	-0.322947000	0.368290000
6	3.515383000	-0.570550000	-0.916159000
6	4.648775000	-1.598065000	-0.820762000
6	4.013173000	0.681217000	-1.658891000
1	2.751747000	-1.005800000	-1.557024000
1	4.338273000	-2.485800000	-0.266367000
1	4.956590000	-1.905088000	-1.824932000
1	5.530849000	-1.181778000	-0.329406000
1	3.319912000	1.514467000	-1.545610000
1	4.999224000	1.004346000	-1.323310000
1	4.094581000	0.453084000	-2.725811000
6	3.614640000	0.067144000	1.570875000
6	4.682016000	1.128144000	1.304695000
6	4.226512000	-1.105369000	2.346683000
1	2.885238000	0.531420000	2.239341000
1	4.297551000	1.958105000	0.714730000

1	5.022209000	1.528846000	2.263432000
1	5.558483000	0.715307000	0.800741000
1	3.476643000	-1.869929000	2.550456000
1	5.056700000	-1.572160000	1.814555000
1	4.610107000	-0.749828000	3.308236000
6	0.816005000	-2.617246000	-1.442374000
6	-0.570843000	-3.063522000	-1.888955000
6	1.873787000	-3.613454000	-1.922075000
1	-1.304701000	-2.304205000	-1.636809000
1	-0.585951000	-3.198896000	-2.973945000
1	-0.876009000	-4.011307000	-1.435049000
1	2.875467000	-3.316788000	-1.613923000
1	1.686391000	-4.619264000	-1.534391000
1	1.857859000	-3.680934000	-3.013500000
6	0.553916000	-3.490068000	0.884540000
6	-0.828392000	-3.292930000	1.511137000
6	1.596920000	-3.788775000	1.955369000
1	0.501560000	-4.368216000	0.235654000
1	-1.576411000	-3.108037000	0.737861000
1	-1.133107000	-4.170417000	2.089918000
1	-0.816147000	-2.431820000	2.187709000
1	2.592185000	-3.882325000	1.514578000
1	1.622774000	-2.999028000	2.709781000
1	1.356107000	-4.725479000	2.465820000
1	0.996342000	-1.662609000	-1.933973000
6	-1.300307000	2.959113000	-0.695368000
6	0.745577000	1.181575000	-2.132573000
6	1.437937000	2.570272000	0.588320000
8	0.962734000	0.475467000	-3.012843000
8	-2.355912000	3.414951000	-0.695110000
8	2.056101000	2.814818000	1.524907000

1h (TE =-3171.391122, H = -3171.351643)

6	-2.240910000	-1.767759000	-2.319631000
6	-0.817745000	-0.814917000	-0.828999000
6	-2.953560000	-1.771900000	-0.953171000
1	-2.715177000	-1.100837000	-3.038738000
1	-2.131292000	-2.764186000	-2.747514000
8	-0.910456000	-1.254196000	-2.069094000
7	-1.935141000	-1.019512000	-0.155588000
6	-3.113714000	-3.169285000	-0.362931000
1	-3.504905000	-3.109582000	0.655480000
1	-3.823230000	-3.744646000	-0.962455000
1	-2.164737000	-3.706590000	-0.337614000

6	-4.304719000	-1.071931000	-1.035812000
1	-4.917484000	-1.593886000	-1.775645000
1	-4.834937000	-1.115025000	-0.083511000
1	-4.202290000	-0.034155000	-1.353874000
6	-2.094521000	-0.650862000	1.218117000
6	-1.224522000	-1.169234000	2.172742000
6	-3.088436000	0.255756000	1.580637000
6	-1.360055000	-0.789070000	3.503741000
1	-0.441530000	-1.853295000	1.869252000
6	-3.229901000	0.611495000	2.915929000
1	-3.712314000	0.710812000	0.822284000
6	-2.369833000	0.090129000	3.877840000
1	-0.675127000	-1.183698000	4.245438000
1	-3.994676000	1.325112000	3.199497000
1	-2.474722000	0.385302000	4.915539000
5	0.435760000	0.063837000	-0.350816000
7	1.618039000	-0.604748000	0.084647000
26	-0.104377000	2.049293000	-0.748570000
6	-0.262312000	3.821248000	-1.050957000
6	-1.507883000	1.633665000	-1.752918000
6	-0.421573000	2.201038000	0.989461000
6	1.521554000	1.967631000	-1.455502000
8	-0.345046000	4.942816000	-1.235570000
8	-2.427708000	1.389064000	-2.402789000
8	2.575010000	1.892173000	-1.910816000
8	-0.641368000	2.344356000	2.107824000
14	2.011880000	-2.192146000	-0.648499000
14	2.916903000	0.134684000	1.080098000
6	3.509907000	-3.013395000	0.134321000
1	3.774061000	-3.855513000	-0.516342000
1	4.403500000	-2.394548000	0.223519000
1	3.284714000	-3.432877000	1.117720000
6	2.362076000	-1.900257000	-2.464024000
1	2.499880000	-2.845267000	-2.999954000
1	1.544317000	-1.359542000	-2.948330000
1	3.270137000	-1.307059000	-2.604043000
6	0.639013000	-3.471382000	-0.474838000
1	-0.101589000	-3.417724000	-1.273365000
1	1.104611000	-4.460333000	-0.548899000
1	0.124460000	-3.443184000	0.488533000
6	4.511215000	0.297211000	0.088579000
1	4.631289000	1.326535000	-0.257879000
1	5.378895000	0.061141000	0.713969000
1	4.560712000	-0.339847000	-0.796810000
6	3.154679000	-1.009496000	2.568030000
1	3.236657000	-0.408578000	3.479327000

1	2.301387000	-1.680322000	2.706841000
1	4.054049000	-1.625505000	2.508783000
6	2.568208000	1.812372000	1.821379000
1	2.381103000	2.608620000	1.101911000
1	1.751298000	1.797846000	2.544510000
1	3.479434000	2.074304000	2.375071000

1i (TE = -3222.794920, H =-3222.750529)

6	1.238630000	-0.206822000	0.725326000
6	2.219770000	-0.268730000	2.760231000
1	1.516159000	0.094281000	3.514707000
1	2.932175000	-0.955246000	3.214931000
7	1.980168000	0.904392000	0.786309000
6	2.207569000	1.785610000	-0.322908000
6	2.604599000	3.104033000	-0.096983000
6	2.072038000	1.324754000	-1.632227000
6	2.884449000	3.942328000	-1.169449000
1	2.665717000	3.501957000	0.903171000
6	2.335431000	2.177985000	-2.697597000
1	1.762711000	0.306232000	-1.833182000
6	2.750868000	3.486275000	-2.475604000
1	3.188511000	4.964639000	-0.975400000
1	2.224227000	1.802944000	-3.708738000
1	2.964045000	4.142900000	-3.311057000
5	0.199080000	-0.834999000	-0.270796000
15	-1.672235000	-0.155081000	-0.296079000
7	-1.598321000	1.509593000	-0.755647000
7	-2.234723000	-0.270459000	1.331282000
6	-2.252767000	1.858054000	-2.036228000
1	-2.206736000	2.947046000	-2.110610000
6	-1.384303000	2.620171000	0.174245000
1	-0.788383000	2.213210000	0.999269000
6	-1.452739000	-0.021777000	2.553243000
1	-0.517475000	0.438965000	2.228097000
6	-3.473681000	-1.058414000	1.536605000
1	-3.669310000	-1.038582000	2.611769000
6	-2.702778000	3.162417000	0.738370000
1	-2.523701000	3.930235000	1.498417000
1	-3.288964000	3.627682000	-0.060073000
1	-3.300268000	2.362912000	1.176375000
6	-0.592757000	3.775145000	-0.457971000
1	-0.092015000	4.364467000	0.315070000
1	0.161014000	3.406113000	-1.153330000
1	-1.247763000	4.461561000	-1.000976000

6	-3.727913000	1.460266000	-2.135923000
1	-4.180468000	1.922626000	-3.018498000
1	-3.837193000	0.378145000	-2.235855000
1	-4.289703000	1.781370000	-1.256216000
6	-1.465382000	1.291807000	-3.216150000
1	-0.431271000	1.641115000	-3.188088000
1	-1.455285000	0.198196000	-3.186797000
1	-1.911486000	1.596095000	-4.167718000
6	-1.106579000	-1.306300000	3.314002000
1	-0.419572000	-1.089862000	4.137846000
1	-1.996264000	-1.761378000	3.758004000
1	-0.635084000	-2.040108000	2.661127000
6	-2.127967000	0.984238000	3.490724000
1	-3.126366000	0.653328000	3.789851000
1	-1.540160000	1.103847000	4.406298000
1	-2.224917000	1.963134000	3.021348000
6	-3.324883000	-2.523574000	1.119557000
1	-2.474648000	-2.996175000	1.613613000
1	-4.225737000	-3.090047000	1.374377000
1	-3.176606000	-2.601925000	0.038814000
6	-4.684608000	-0.427978000	0.855444000
1	-4.812963000	0.612930000	1.161793000
1	-4.582217000	-0.459003000	-0.230690000
1	-5.593508000	-0.976243000	1.119708000
8	1.466387000	-0.984458000	1.777960000
26	0.586029000	-2.557954000	-1.190165000
6	1.144145000	-3.666828000	-2.530933000
6	2.287200000	-2.096157000	-0.873028000
6	0.219147000	-3.547450000	0.217062000
6	-1.045038000	-2.478688000	-2.073494000
8	1.511049000	-4.355206000	-3.360207000
8	0.025705000	-4.195790000	1.139056000
8	3.380304000	-1.799492000	-0.684973000
8	-1.980549000	-2.564635000	-2.715393000
6	2.880781000	0.882301000	1.998738000
6	2.827067000	2.131983000	2.878680000
1	3.105339000	1.842042000	3.896017000
1	3.536033000	2.897594000	2.567748000
1	1.820094000	2.554458000	2.916779000
6	4.307439000	0.557725000	1.572279000
1	4.357880000	-0.402607000	1.057985000
1	4.700595000	1.327924000	0.905724000
1	4.948944000	0.517802000	2.456259000

2a (TE = -1961.465971, H = -1961.452936)

28	-0.273584000	-0.140454000	-0.000008000
6	0.363755000	0.740048000	-1.560717000
6	0.386784000	-1.922613000	-0.001440000
6	0.362170000	0.740870000	1.560782000
6	-2.175808000	-0.129968000	0.001225000
8	0.755284000	1.241903000	-2.492930000
8	0.797446000	-2.974106000	-0.002535000
8	0.750763000	1.245275000	2.492847000
8	-3.304472000	-0.115882000	0.002777000

2b (TE = -2309.099600, -2309.082043)

15	-0.665271000	0.396263000	-0.856185000
6	-0.707118000	2.031503000	-1.684517000
1	-0.680370000	1.940700000	-2.773755000
1	-1.614239000	2.566781000	-1.394977000
1	0.148825000	2.626204000	-1.357127000
6	-2.025254000	-0.497225000	-1.703068000
1	-1.922657000	-0.465549000	-2.791098000
1	-2.032433000	-1.540300000	-1.378136000
1	-2.984163000	-0.055556000	-1.423460000
6	0.815786000	-0.370139000	-1.619608000
1	1.713842000	0.151120000	-1.279673000
1	0.894391000	-1.410644000	-1.296427000
1	0.780703000	-0.339284000	-2.712033000
28	-0.665918000	0.406822000	1.456925000
6	0.970796000	1.202858000	1.846550000
6	-2.135960000	1.419079000	1.980514000
6	-0.802110000	-1.394448000	1.905701000
8	-0.899782000	-2.510116000	2.087745000
8	-3.048374000	2.039030000	2.245586000
8	1.978383000	1.706203000	1.984541000

2c (TE = -2152.803078, H = -2152.785139)

28	-1.003645000	0.000670000	-0.004394000
6	-1.713291000	1.665133000	-0.450744000
6	-1.555525000	-1.278198000	-1.247124000
6	-1.591680000	-0.480684000	1.691889000
8	-2.183609000	2.669850000	-0.698522000
8	-1.889176000	-2.065126000	-1.995605000
8	-1.938429000	-0.779307000	2.731986000

6	1.061066000	0.038397000	0.010337000
6	3.227240000	-0.640187000	0.005540000
6	3.227931000	0.712271000	-0.011554000
7	1.902310000	1.101968000	-0.006057000
7	1.900605000	-1.026903000	0.024028000
6	1.455802000	-2.410923000	0.002749000
1	0.544403000	-2.502676000	0.590301000
1	1.258725000	-2.733235000	-1.021150000
1	2.229756000	-3.042861000	0.436805000
6	1.456912000	2.485942000	-0.033718000
1	0.989949000	2.713841000	-0.992335000
1	0.741212000	2.659951000	0.768552000
1	2.319075000	3.135654000	0.108393000
1	4.038064000	-1.349854000	0.015703000
1	4.039450000	1.421126000	-0.016156000

2d (TE = -2447.400441, H = -2447.375049)

6	-0.025027000	3.158798000	-0.296066000
6	1.288602000	2.404453000	-0.040356000
6	-0.500049000	0.780799000	-0.042539000
6	-1.168777000	2.149364000	-0.038780000
1	-0.105375000	4.043933000	0.338799000
1	-0.054858000	3.496136000	-1.335591000
7	0.793069000	0.980332000	-0.041858000
6	1.736645000	-0.105268000	-0.004585000
6	2.180901000	-0.592369000	1.219207000
6	2.170094000	-0.674872000	-1.196707000
6	3.069580000	-1.662444000	1.248156000
1	1.804538000	-0.154934000	2.137854000
6	3.056459000	-1.745400000	-1.161483000
1	1.793848000	-0.292602000	-2.139371000
6	3.509128000	-2.237498000	0.059843000
1	3.406986000	-2.053819000	2.201086000
1	3.386524000	-2.199950000	-2.088576000
1	4.196321000	-3.075596000	0.085159000
6	-2.241238000	2.235525000	-1.125348000
1	-3.071444000	1.557025000	-0.921748000
1	-2.639950000	3.253319000	-1.175372000
1	-1.833287000	1.982922000	-2.107933000
6	-1.815818000	2.349682000	1.338798000
1	-2.308463000	3.325413000	1.379171000
1	-2.565752000	1.579902000	1.533470000
1	-1.078615000	2.308398000	2.144635000
6	1.915142000	2.730503000	1.314171000

1	2.804755000	2.124198000	1.498933000
1	2.220662000	3.779556000	1.329016000
1	1.208878000	2.570733000	2.131589000
6	2.307416000	2.613348000	-1.155126000
1	3.224653000	2.046508000	-0.980520000
1	1.895454000	2.322670000	-2.124430000
1	2.572068000	3.672541000	-1.204581000
28	-1.398487000	-1.050649000	-0.028924000
6	-3.247295000	-0.904884000	0.226018000
6	-1.021289000	-1.861993000	-1.654800000
6	-0.735229000	-2.078336000	1.382517000
8	-0.374464000	-2.707761000	2.256946000
8	-0.771795000	-2.332215000	-2.659406000
8	-4.369522000	-0.845892000	0.397930000

2e (TE = -2404.794192, H = -2404.771622)

6	0.729245000	-3.150534000	0.193942000
6	1.828574000	-2.108747000	-0.041098000
6	-0.320802000	-1.117196000	0.021513000
1	0.753239000	-3.975678000	-0.516355000
1	0.736614000	-3.540172000	1.214192000
7	0.985374000	-0.882323000	0.067523000
6	1.534066000	0.438763000	0.028204000
6	1.679491000	1.090070000	-1.193167000
6	1.893371000	1.068300000	1.215371000
6	2.190536000	2.382869000	-1.224500000
1	1.369294000	0.589533000	-2.104301000
6	2.402878000	2.362178000	1.178336000
1	1.748488000	0.551340000	2.157733000
6	2.552818000	3.018143000	-0.039933000
1	2.293487000	2.897636000	-2.172917000
1	2.670918000	2.861271000	2.102467000
1	2.943590000	4.029040000	-0.065708000
6	2.427913000	-2.203993000	-1.441720000
1	3.111784000	-1.373982000	-1.632632000
1	2.993784000	-3.133600000	-1.542037000
1	1.644561000	-2.193723000	-2.203935000
6	2.909416000	-2.145810000	1.029071000
1	3.650070000	-1.359704000	0.866905000
1	2.480937000	-2.022943000	2.025883000
1	3.428706000	-3.106878000	0.995222000
28	-1.822842000	0.246617000	0.015667000
6	-3.400445000	-0.779677000	0.033731000
6	-1.643794000	1.288421000	1.545147000

6	-1.732884000	1.332497000	-1.490856000
8	-1.680263000	2.013414000	-2.399341000
8	-1.500449000	1.911787000	2.484217000
8	-4.303135000	-1.466334000	0.040459000
8	-0.514379000	-2.434223000	0.009651000

2f (TE = -3345.289649, H = -3345.247168)

6	2.851008000	-0.475743000	1.702107000
6	0.581906000	-0.348427000	0.895870000
6	0.490570000	-0.392254000	2.431582000
6	1.908213000	0.045618000	2.810243000
1	1.941313000	1.139041000	2.832683000
1	2.210110000	-0.317282000	3.796483000
7	1.894104000	-0.770289000	0.580775000
6	3.582288000	-1.734330000	2.191789000
1	4.206394000	-2.203858000	1.433690000
1	4.233451000	-1.462704000	3.026891000
1	2.881843000	-2.487781000	2.551260000
6	3.853006000	0.637329000	1.366821000
1	4.419154000	0.878287000	2.271263000
1	4.571602000	0.377396000	0.590572000
1	3.326628000	1.543353000	1.061631000
6	-0.567825000	0.498611000	3.071951000
1	-1.574587000	0.220961000	2.744064000
1	-0.537850000	0.385287000	4.159840000
1	-0.410836000	1.552314000	2.840895000
6	0.207189000	-1.842443000	2.863176000
1	0.368576000	-1.961383000	3.939513000
1	-0.832260000	-2.106970000	2.651870000
1	0.840567000	-2.560767000	2.343553000
6	2.277133000	-1.122226000	-0.707190000
6	1.337564000	-1.148643000	-1.758413000
6	3.609735000	-1.429547000	-1.053671000
6	1.706281000	-1.457603000	-3.062067000
1	0.294107000	-0.934787000	-1.578070000
6	3.966179000	-1.735800000	-2.358742000
1	4.390184000	-1.426581000	-0.311566000
6	3.024662000	-1.750982000	-3.383678000
1	0.942007000	-1.459258000	-3.832676000
1	5.005613000	-1.961244000	-2.572882000
1	3.312051000	-1.985052000	-4.401753000
5	-0.654597000	-0.124271000	0.190366000
7	-1.975084000	-0.470609000	-0.061543000
14	-2.389278000	-2.221700000	-0.078412000

14	-3.296425000	0.718808000	-0.296164000
6	-3.274763000	-2.693767000	1.516464000
1	-2.855635000	-3.612189000	1.937993000
1	-3.197952000	-1.918071000	2.281970000
1	-4.339551000	-2.875385000	1.345977000
6	-3.491345000	-2.538200000	-1.564498000
1	-4.469289000	-2.055125000	-1.524034000
1	-3.000174000	-2.220455000	-2.489408000
1	-3.671620000	-3.615375000	-1.651709000
6	-4.828457000	0.065919000	0.576249000
1	-5.176354000	-0.916777000	0.254428000
1	-4.687095000	0.033264000	1.660893000
1	-5.648952000	0.766864000	0.385240000
6	-3.649243000	0.909977000	-2.130429000
1	-4.455950000	0.243563000	-2.448263000
1	-3.959690000	1.931910000	-2.368218000
1	-2.775200000	0.682366000	-2.744376000
6	-2.950991000	2.360056000	0.546112000
1	-2.442068000	3.097909000	-0.073626000
1	-3.915846000	2.791527000	0.835944000
1	-2.368191000	2.235866000	1.462717000
6	-0.866407000	-3.279792000	-0.322069000
1	-0.028143000	-3.021423000	0.326374000
1	-1.136808000	-4.321358000	-0.114325000
1	-0.509464000	-3.243530000	-1.354112000
28	0.437004000	1.831122000	-0.246437000
6	2.115884000	1.836671000	-1.219365000
6	0.476817000	3.161837000	1.060690000
6	-0.580229000	2.322097000	-1.705310000
8	0.479823000	4.026546000	1.796752000
8	2.981758000	2.060192000	-1.912309000
8	-1.014275000	2.730014000	-2.674269000

2g (TE = -3396.700124, H = -3396.653252)

6	-3.746068000	1.162425000	0.728100000
6	-1.507954000	0.278410000	0.839489000
6	-2.046854000	0.225539000	2.276041000
6	-3.564144000	0.398072000	2.052778000
1	-4.025247000	-0.589799000	1.964132000
1	-4.044800000	0.915483000	2.886540000
7	-2.425118000	0.935762000	0.086332000
6	-3.996986000	2.660308000	0.918138000
1	-4.001875000	3.175207000	-0.046199000
1	-4.973684000	2.818856000	1.382700000

1	-3.240843000	3.126466000	1.551051000
6	-4.878473000	0.575182000	-0.113229000
1	-5.818780000	0.644585000	0.440408000
1	-5.003152000	1.119074000	-1.052754000
1	-4.698972000	-0.476359000	-0.340544000
6	-1.725513000	-1.053934000	3.044120000
1	-0.645481000	-1.212099000	3.114948000
1	-2.118848000	-0.978774000	4.062682000
1	-2.164985000	-1.933398000	2.572269000
6	-1.445597000	1.409861000	3.055136000
1	-1.959246000	1.522594000	4.014325000
1	-0.387049000	1.232569000	3.259718000
1	-1.527537000	2.354126000	2.513133000
6	-2.142657000	1.348405000	-1.247213000
6	-2.474673000	0.538601000	-2.331370000
6	-1.498875000	2.565446000	-1.455628000
6	-2.152881000	0.949571000	-3.621496000
1	-2.968901000	-0.411000000	-2.156831000
6	-1.174300000	2.971997000	-2.744835000
1	-1.261009000	3.181110000	-0.595294000
6	-1.499438000	2.160842000	-3.828897000
1	-2.403646000	0.316373000	-4.465161000
1	-0.668071000	3.918203000	-2.903021000
1	-1.243331000	2.472119000	-4.835462000
5	-0.199595000	-0.260333000	0.430993000
15	1.437747000	0.177938000	-0.206189000
7	2.236340000	1.556285000	0.521446000
7	2.600818000	-1.048187000	-0.157675000
6	3.236247000	-1.526079000	1.089168000
1	3.521533000	-2.565580000	0.898308000
6	2.279934000	-1.529104000	2.277542000
1	1.364224000	-2.074854000	2.060322000
1	2.766041000	-1.999989000	3.135849000
1	2.014186000	-0.507236000	2.564661000
6	4.498808000	-0.748687000	1.483321000
1	5.202219000	-0.635826000	0.658229000
1	4.226966000	0.244709000	1.843505000
1	5.016952000	-1.270175000	2.293910000
28	-1.047100000	-2.208971000	-0.229021000
6	-2.856983000	-2.549700000	-0.005091000
6	-0.516754000	-2.090653000	-2.017947000
6	-0.205630000	-3.544552000	0.751238000
8	-0.177620000	-2.004786000	-3.098164000
8	-3.915372000	-2.941157000	0.151112000
8	0.245607000	-4.380403000	1.375267000
6	3.453875000	1.958041000	-0.211683000

6	4.407478000	2.810533000	0.624693000
6	3.233187000	2.591232000	-1.595759000
1	3.975430000	1.015530000	-0.387660000
1	4.607675000	2.358955000	1.597411000
1	5.359341000	2.903146000	0.094137000
1	4.033193000	3.822403000	0.788725000
1	2.447929000	2.069116000	-2.150023000
1	2.967236000	3.647923000	-1.538426000
1	4.155033000	2.520024000	-2.181144000
6	1.387652000	2.559896000	1.182281000
6	1.186041000	3.876677000	0.424568000
6	1.838446000	2.829630000	2.621871000
1	0.399850000	2.100312000	1.248755000
1	0.900173000	3.700846000	-0.612456000
1	0.388595000	4.451002000	0.907079000
1	2.078049000	4.505986000	0.430740000
1	1.997307000	1.891167000	3.158097000
1	2.766653000	3.402333000	2.661349000
1	1.075660000	3.403334000	3.158432000
6	3.012917000	-1.684095000	-1.426701000
6	2.694573000	-3.181375000	-1.469714000
6	4.486035000	-1.467136000	-1.781086000
1	2.412274000	-1.197534000	-2.199930000
1	1.673964000	-3.380552000	-1.142861000
1	2.802405000	-3.554057000	-2.491900000
1	3.374217000	-3.766154000	-0.843728000
1	4.750451000	-0.407349000	-1.792663000
1	5.147270000	-1.985508000	-1.081592000
1	4.687538000	-1.871919000	-2.776776000

2h (TE = -3302.666399, H = -3302.627139)

6	2.344352000	-1.019961000	-2.536445000
6	0.795042000	-0.381503000	-1.015434000
6	3.064044000	-0.087974000	-1.555920000
1	2.891581000	-1.934948000	-2.754913000
1	2.110293000	-0.496811000	-3.470073000
8	1.117723000	-1.367464000	-1.895047000
7	1.853933000	0.501385000	-0.921552000
6	3.865111000	0.956699000	-2.323627000
1	4.366301000	1.660994000	-1.659404000
1	4.636077000	0.454849000	-2.915118000
1	3.220796000	1.522048000	-2.999658000
6	3.945178000	-0.873970000	-0.561703000
1	4.293599000	-1.806464000	-1.009787000

1	4.834030000	-0.309265000	-0.275368000
1	3.396355000	-1.122782000	0.348527000
6	1.874617000	1.551598000	0.013277000
6	0.694657000	2.246427000	0.308109000
6	3.043307000	1.894755000	0.705392000
6	0.684002000	3.240164000	1.280455000
1	-0.209039000	2.037249000	-0.247210000
6	3.023273000	2.899620000	1.663621000
1	3.968588000	1.370072000	0.521180000
6	1.844789000	3.573388000	1.967793000
1	-0.242598000	3.763620000	1.491295000
1	3.939219000	3.140319000	2.191868000
1	1.833309000	4.347614000	2.725957000
5	-0.487358000	-0.413163000	-0.220595000
7	-1.785833000	0.086157000	-0.426669000
14	-2.900610000	0.519885000	0.897655000
14	-2.215286000	0.516775000	-2.109864000
6	-2.098635000	0.474749000	2.588049000
1	-2.787742000	0.974668000	3.279490000
1	-1.903202000	-0.518152000	2.992796000
1	-1.162211000	1.039378000	2.603840000
6	-4.450517000	-0.543432000	0.869934000
1	-4.293453000	-1.476367000	0.324673000
1	-4.742752000	-0.812444000	1.889916000
1	-5.299402000	-0.027901000	0.413085000
6	-3.326351000	2.339675000	0.657671000
1	-2.431160000	2.956628000	0.790445000
1	-3.765665000	2.599494000	-0.306926000
1	-4.040932000	2.650896000	1.427477000
6	-4.082377000	0.471041000	-2.309097000
1	-4.647305000	1.157816000	-1.677454000
1	-4.321754000	0.725644000	-3.347440000
1	-4.468529000	-0.537645000	-2.134345000
6	-1.528453000	2.203745000	-2.559309000
1	-1.839974000	2.468121000	-3.575688000
1	-1.869676000	3.003445000	-1.896450000
1	-0.433354000	2.205108000	-2.552906000
6	-1.536510000	-0.741575000	-3.319477000
1	-0.490046000	-0.567853000	-3.573936000
1	-1.619334000	-1.765575000	-2.945729000
1	-2.112677000	-0.685309000	-4.249415000
28	0.405664000	-1.680485000	1.223237000
6	-1.216130000	-2.510512000	1.475636000
6	1.547598000	-2.958772000	0.477788000
6	1.107068000	-0.616086000	2.586915000
8	-2.255141000	-2.976094000	1.443475000

8	1.489227000	0.066380000	3.410609000
8	2.146703000	-3.759304000	-0.062260000

2i (TE = -3354.088386, H = -3354.044303)

6	-3.323866000	1.411676000	-1.030663000
6	-1.259283000	0.295327000	-1.000701000
6	-2.796445000	1.142312000	-2.448567000
1	-2.486571000	2.059750000	-2.953691000
1	-3.505235000	0.600634000	-3.073817000
7	-2.106848000	1.036182000	-0.258697000
6	-4.495445000	0.505944000	-0.660922000
1	-4.792387000	0.658866000	0.378927000
1	-5.356432000	0.736237000	-1.293608000
1	-4.243545000	-0.546793000	-0.798766000
6	-3.684303000	2.876234000	-0.825559000
1	-4.508152000	3.147794000	-1.490411000
1	-4.012088000	3.058505000	0.200184000
1	-2.835408000	3.525432000	-1.047301000
6	-2.079924000	1.066957000	1.171725000
6	-1.752563000	2.252317000	1.826975000
6	-2.423746000	-0.070321000	1.902048000
6	-1.756030000	2.295831000	3.217953000
1	-1.499883000	3.131108000	1.243129000
6	-2.426355000	-0.020110000	3.291339000
1	-2.677845000	-0.983703000	1.376041000
6	-2.090848000	1.160122000	3.949420000
1	-1.498182000	3.217198000	3.727749000
1	-2.685629000	-0.906700000	3.858953000
1	-2.089107000	1.194021000	5.033194000
5	-0.086722000	-0.545001000	-0.523380000
15	1.738530000	-0.038153000	-0.632200000
7	2.483411000	-0.259027000	0.902483000
7	1.777034000	1.623082000	-1.043455000
6	3.439054000	-1.368583000	1.090688000
1	3.700624000	-1.353964000	2.151936000
6	1.891361000	0.287142000	2.137155000
1	1.208838000	1.079524000	1.820930000
6	1.002139000	2.658140000	-0.354351000
1	0.320606000	2.124428000	0.307402000
6	2.768325000	2.100435000	-2.025373000
1	2.616968000	3.180108000	-2.105462000
6	2.951431000	0.939658000	3.030673000
1	2.470446000	1.571192000	3.783304000
1	3.549037000	0.199852000	3.569742000

1	3.633032000	1.559460000	2.444285000
6	1.070988000	-0.732583000	2.926422000
1	0.613053000	-0.261337000	3.800756000
1	0.274200000	-1.144681000	2.305951000
1	1.694557000	-1.557822000	3.283544000
6	4.729747000	-1.158134000	0.305323000
1	5.456517000	-1.936790000	0.554268000
1	4.542698000	-1.216559000	-0.770161000
1	5.172814000	-0.185663000	0.529783000
6	2.854899000	-2.748226000	0.781016000
1	1.895750000	-2.901998000	1.277755000
1	2.700583000	-2.861265000	-0.294592000
1	3.541869000	-3.537475000	1.101683000
6	0.134399000	3.465724000	-1.323407000
1	-0.527829000	4.138946000	-0.769914000
1	0.731619000	4.089375000	-1.993978000
1	-0.476584000	2.800739000	-1.937963000
6	1.857360000	3.584868000	0.511933000
1	2.539147000	4.187048000	-0.096422000
1	1.226850000	4.279111000	1.076932000
1	2.455323000	3.011789000	1.222333000
6	2.522960000	1.501889000	-3.409396000
1	1.499344000	1.698895000	-3.737883000
1	3.213191000	1.926576000	-4.144287000
1	2.669078000	0.418740000	-3.396870000
6	4.212353000	1.881884000	-1.577100000
1	4.367408000	2.247404000	-0.559190000
1	4.466381000	0.820910000	-1.598188000
1	4.907064000	2.402962000	-2.242819000
8	-1.627853000	0.314778000	-2.284199000
28	-0.805666000	-2.496043000	-0.524822000
6	-0.884134000	-3.236078000	1.170848000
6	-2.416006000	-2.525465000	-1.469124000
6	0.461765000	-3.138053000	-1.719427000
8	-3.314429000	-2.510117000	-2.169135000
8	-0.955250000	-3.630075000	2.236109000
8	1.212533000	-3.407142000	-2.528329000

Cartesian coordinates of the optimized geometries of the Fe and Ni based MOLPs for the ligands L (L=**a-i**).are given along with their total energies (TE) and Gibbs free enthalpies (H) in hartrees including zero point vibrational correction.

1a-$GaCl_3$ (TE = 5135.810450, H = -5135.789706)

26	-0.017246000	-0.029775000	0.176520000
6	1.861183000	0.032065000	-0.161465000
6	-0.066097000	1.879838000	0.340018000
6	-0.075438000	-1.864099000	-0.379264000
6	-1.915908000	0.009311000	-0.006967000
6	0.070436000	-0.389990000	2.042777000
8	2.968316000	0.065925000	-0.342082000
8	0.136122000	-0.605992000	3.141285000
8	-0.170629000	-2.944885000	-0.662279000
8	-3.035308000	0.023360000	-0.078266000
8	-0.147730000	2.989936000	0.475090000
31	0.042179000	0.453461000	-2.351603000
17	-1.985485000	0.650415000	-3.209207000
17	1.142731000	-1.216826000	-3.319680000
17	1.193411000	2.332123000	-2.643112000

1b-$GaCl_3$ (TE = -5483.468118, H = -5483.442289)

15	-1.877954000	-1.214104000	-0.051522000
6	-3.596840000	-1.076252000	0.564062000
1	-4.055581000	-2.065791000	0.621697000
1	-3.611840000	-0.629855000	1.561248000
1	-4.198994000	-0.458171000	-0.104823000
6	-1.204323000	-2.553385000	0.987748000
1	-1.880098000	-3.411286000	0.948466000
1	-0.220279000	-2.862799000	0.636589000
1	-1.116527000	-2.226589000	2.025696000
6	-2.102205000	-1.968974000	-1.695458000
1	-2.633902000	-1.279557000	-2.355023000
1	-1.134694000	-2.212018000	-2.136030000
1	-2.687431000	-2.886573000	-1.601992000
26	-0.776215000	0.883279000	-0.013991000
6	-0.387745000	0.696907000	-1.836300000
6	-2.413279000	1.784263000	-0.136397000
6	-0.720442000	0.691043000	1.847235000
6	0.239546000	2.474613000	0.090337000
8	-0.177769000	0.588617000	-2.938871000

8	-0.750945000	0.579565000	2.968445000
8	-3.379587000	2.358556000	-0.192081000
8	0.785509000	3.453033000	0.171815000
31	1.480834000	-0.279228000	0.048843000
17	2.036838000	-1.072745000	2.060298000
17	1.536907000	-2.042058000	-1.349433000
17	3.089695000	1.103481000	-0.650581000

1c-$GaCl_3$ (TE = -5327.174125, H = -5327.148345)

6	1.834123000	-0.385121000	0.153747000
7	1.932729000	-1.558808000	0.826842000
7	2.892806000	-0.413266000	-0.702257000
6	3.006984000	-2.302996000	0.390056000
1	3.234053000	-3.271459000	0.802901000
6	3.612244000	-1.584082000	-0.576140000
1	4.474555000	-1.793103000	-1.187081000
6	3.277673000	0.573490000	-1.703685000
1	4.362580000	0.669353000	-1.698216000
1	2.949447000	0.255577000	-2.693650000
1	2.850264000	1.545444000	-1.480049000
6	1.078578000	-2.048841000	1.902174000
1	1.156459000	-3.133693000	1.928123000
1	1.401394000	-1.643882000	2.861760000
1	0.036693000	-1.803490000	1.722114000
26	0.377926000	1.109354000	0.256020000
6	1.706266000	2.400805000	0.574506000
6	0.300709000	1.017592000	-1.613370000
6	0.042572000	0.760202000	2.077797000
6	-1.079495000	2.328717000	0.271574000
8	2.496848000	3.169020000	0.802373000
8	0.281255000	0.946298000	-2.740397000
8	-0.142102000	0.636130000	3.182026000
8	-1.938312000	3.053799000	0.309167000
31	-1.484698000	-0.554582000	-0.247983000
17	-0.639115000	-2.419875000	-1.163119000
17	-2.981862000	0.298513000	-1.678175000
17	-2.632204000	-1.153459000	1.583509000

1d-$GaCl_3$ (TE = -5621.774752, H = -5621.741491)

6	-1.227089000	3.116042000	0.028142000
6	-2.160093000	1.917146000	0.176370000
6	0.075141000	1.072506000	-0.186424000

6	0.119782000	2.578865000	-0.495782000
1	-1.648115000	3.875547000	-0.633833000
1	-1.071592000	3.574765000	1.007371000
7	-1.161829000	0.779172000	0.123389000
6	-1.679317000	-0.545225000	0.344954000
6	-2.003114000	-1.336370000	-0.754768000
6	-1.889862000	-1.001339000	1.642079000
6	-2.513935000	-2.613260000	-0.552323000
1	-1.862714000	-0.945479000	-1.757078000
6	-2.408851000	-2.277164000	1.834722000
1	-1.610579000	-0.379046000	2.482951000
6	-2.715016000	-3.083782000	0.743015000
1	-2.758589000	-3.236096000	-1.404959000
1	-2.555132000	-2.645265000	2.843375000
1	-3.109415000	-4.081059000	0.900453000
6	1.242665000	3.375833000	0.172504000
6	0.216547000	2.716404000	-2.027467000
1	0.144191000	3.772744000	-2.298096000
1	1.165593000	2.346682000	-2.421788000
1	-0.585985000	2.182224000	-2.542276000
6	-3.155635000	1.767694000	-0.972736000
1	-3.746478000	0.854805000	-0.872480000
1	-3.848182000	2.612241000	-0.954710000
1	-2.661873000	1.758740000	-1.946182000
6	-2.897626000	1.939437000	1.510779000
1	-3.595000000	1.106192000	1.613468000
1	-2.195834000	1.928036000	2.347007000
1	-3.474538000	2.865985000	1.567395000
26	1.631340000	-0.277510000	-0.459175000
6	0.841919000	-1.728130000	0.495835000
6	0.965239000	-0.688087000	-2.155199000
6	2.859493000	1.038995000	-1.036343000
8	0.577861000	-2.702094000	0.995789000
8	0.579974000	-0.911625000	-3.190265000
8	3.704619000	1.662090000	-1.446319000
6	3.161727000	-1.401039000	-0.452951000
8	4.068508000	-2.067518000	-0.462650000
31	2.368239000	0.336233000	1.867622000
17	3.118423000	-1.469466000	2.977238000
17	4.003098000	1.864179000	1.998398000
17	0.652915000	1.141139000	3.104499000
1	2.236609000	3.179761000	-0.220256000
1	1.047073000	4.438908000	0.002317000
1	1.262152000	3.214979000	1.250899000

1e-$GaCl_3$ (TE = -5579.178651, H = -5579.147764)

6	1.040647000	2.896857000	1.018687000
6	2.343709000	2.252808000	0.537287000
6	0.645452000	0.654583000	0.839933000
1	1.163943000	3.529507000	1.895463000
1	0.520488000	3.437144000	0.226241000
7	1.832764000	0.860979000	0.306663000
6	2.639180000	-0.147143000	-0.311365000
6	3.301595000	-1.076464000	0.486481000
6	2.755225000	-0.181199000	-1.697676000
6	4.070926000	-2.067981000	-0.112802000
1	3.218723000	-1.009769000	1.566218000
6	3.536075000	-1.168810000	-2.288118000
1	2.207210000	0.535299000	-2.298688000
6	4.187893000	-2.112679000	-1.499451000
1	4.582225000	-2.798845000	0.502987000
1	3.619290000	-1.209574000	-3.367823000
1	4.787572000	-2.885723000	-1.966143000
6	3.410530000	2.208751000	1.626567000
1	4.269458000	1.613185000	1.309097000
1	3.764183000	3.220148000	1.839025000
1	3.011620000	1.783026000	2.551401000
6	2.864725000	2.896461000	-0.737459000
1	3.786978000	2.420311000	-1.075712000
1	2.120645000	2.848276000	-1.533924000
1	3.086485000	3.948054000	-0.538721000
26	-0.584821000	-0.948694000	0.928562000
6	0.061558000	-1.677305000	-0.693889000
6	0.488411000	-1.931821000	2.110249000
6	-1.556486000	0.017975000	2.249659000
8	0.363488000	-2.177567000	-1.656555000
8	1.106194000	-2.540441000	2.828376000
8	-2.112403000	0.547866000	3.070238000
6	-2.036996000	-2.167398000	0.833188000
8	-2.914307000	-2.871165000	0.805475000
31	-1.917023000	0.390062000	-0.734452000
17	-3.025245000	-0.940427000	-2.159873000
17	-3.387788000	1.813830000	0.151809000
17	-0.528274000	1.646211000	-2.008894000
8	0.201081000	1.779177000	1.388699000

1f-$GaCl_3$ (TE = -6519.631072, H = -6519.582103)

6	-4.240231000	-0.409394000	-1.196259000
6	-1.968346000	0.269678000	-0.844346000
6	-2.386387000	0.881997000	-2.196359000
6	-3.917396000	0.721596000	-2.176533000
1	-4.371927000	1.650668000	-1.821348000
1	-4.312028000	0.517611000	-3.173708000
7	-2.952179000	-0.457398000	-0.390198000
6	-4.509789000	-1.750878000	-1.872681000
1	-4.703960000	-2.536525000	-1.140958000
1	-5.406451000	-1.651568000	-2.488360000
1	-3.690288000	-2.065752000	-2.518612000
6	-5.404140000	-0.053029000	-0.277472000
1	-6.285851000	0.129286000	-0.896472000
1	-5.641097000	-0.861818000	0.416076000
1	-5.202487000	0.855058000	0.295632000
6	-2.003132000	2.351160000	-2.364167000
1	-0.937867000	2.471474000	-2.547472000
1	-2.531980000	2.741361000	-3.238592000
1	-2.280011000	2.955411000	-1.503242000
6	-1.752348000	0.101299000	-3.363251000
1	-2.040124000	0.592226000	-4.296299000
1	-0.661961000	0.110105000	-3.308244000
1	-2.091217000	-0.931633000	-3.417587000
6	-2.959697000	-1.223050000	0.834445000
6	-3.205763000	-0.571051000	2.034264000
6	-2.830203000	-2.610614000	0.790328000
6	-3.274656000	-1.306611000	3.212964000
1	-3.345388000	0.502590000	2.042595000
6	-2.902299000	-3.337249000	1.971974000
1	-2.676825000	-3.121109000	-0.150485000
6	-3.118327000	-2.686750000	3.183699000
1	-3.445204000	-0.794986000	4.153031000
1	-2.782872000	-4.413959000	1.943984000
1	-3.164422000	-3.257082000	4.104005000
5	-0.424977000	0.475379000	-0.357626000
7	-0.071614000	1.773752000	0.136435000
26	0.732475000	-1.404989000	-0.579353000
6	0.237695000	-1.607993000	1.165090000
6	1.633500000	-0.816366000	-2.059447000
6	-0.576464000	-2.236443000	-1.516102000
8	-0.036126000	-1.792809000	2.252112000
8	2.168222000	-0.615752000	-3.037769000
8	-1.288192000	-2.870436000	-2.132026000
14	-0.972963000	2.473640000	1.525593000

14	1.111778000	2.907966000	-0.618580000
6	-2.752144000	2.903293000	1.038754000
1	-2.788337000	3.855290000	0.500519000
1	-3.268211000	2.164163000	0.422365000
1	-3.348063000	3.040429000	1.948157000
6	-0.976010000	1.369038000	3.044594000
1	-0.898633000	0.300148000	2.865871000
1	-0.123336000	1.638806000	3.670697000
1	-1.881546000	1.549936000	3.634428000
6	-0.214422000	4.058822000	2.182942000
1	-0.934375000	4.436419000	2.920516000
1	0.706433000	3.852572000	2.731535000
1	-0.028541000	4.869001000	1.478804000
6	2.596699000	3.441792000	0.383972000
1	3.060421000	4.261950000	-0.179221000
1	2.377996000	3.813203000	1.383654000
1	3.343945000	2.654141000	0.475954000
6	0.139729000	4.479448000	-1.072012000
1	0.701437000	5.366490000	-0.762404000
1	0.013353000	4.552490000	-2.156291000
1	-0.854569000	4.559890000	-0.629883000
6	1.817168000	2.281459000	-2.234885000
1	1.114701000	1.805965000	-2.922333000
1	2.204781000	3.170500000	-2.747360000
1	2.671759000	1.623266000	-2.084955000
6	1.716036000	-2.982357000	-0.585634000
8	2.244670000	-3.973680000	-0.677050000
31	2.714920000	-0.594007000	0.774469000
17	3.628977000	-2.343178000	1.883904000
17	4.404933000	0.225721000	-0.464322000
17	2.317432000	0.856637000	2.443518000

1g-$GaCl_3$ (TE = -6571.037870, H = -6570.983227)

6	-3.638355000	-2.511018000	-0.915612000
6	-1.841467000	-0.917488000	-1.037335000
6	-2.557643000	-0.856161000	-2.406275000
6	-3.879748000	-1.591160000	-2.114864000
1	-4.648387000	-0.856645000	-1.858032000
1	-4.225379000	-2.144540000	-2.990014000
7	-2.396462000	-1.876019000	-0.330256000
6	-3.400664000	-3.968025000	-1.310759000
1	-3.274888000	-4.605958000	-0.435485000
1	-4.283187000	-4.325336000	-1.846142000
1	-2.536862000	-4.090819000	-1.963827000

6	-4.770719000	-2.440663000	0.104673000
1	-5.694009000	-2.772764000	-0.376002000
1	-4.583438000	-3.090715000	0.961642000
1	-4.923898000	-1.422265000	0.467461000
6	-2.859608000	0.541131000	-2.936925000
1	-1.966264000	1.018431000	-3.338367000
1	-3.570184000	0.441833000	-3.762470000
1	-3.320018000	1.181185000	-2.181973000
6	-1.724149000	-1.583533000	-3.477517000
1	-2.219808000	-1.454801000	-4.442881000
1	-0.719588000	-1.161261000	-3.562214000
1	-1.638032000	-2.652091000	-3.292997000
6	-1.985086000	-2.262616000	0.992480000
6	-2.196476000	-1.361197000	2.024030000
6	-1.464787000	-3.531320000	1.240682000
6	-1.901090000	-1.728361000	3.331713000
1	-2.589133000	-0.385027000	1.774039000
6	-1.168634000	-3.888646000	2.551336000
1	-1.281338000	-4.224939000	0.430674000
6	-1.393214000	-2.995079000	3.595641000
1	-2.063293000	-1.022208000	4.138596000
1	-0.748531000	-4.866800000	2.754334000
1	-1.154324000	-3.282716000	4.612825000
5	-0.566189000	-0.084784000	-0.655983000
15	-0.478122000	1.599052000	0.325749000
26	1.350819000	-1.273182000	-0.785685000
6	2.856310000	-2.341469000	-1.094253000
8	3.694436000	-3.010578000	-1.440097000
7	-0.122670000	2.846698000	-0.786652000
7	-1.958708000	1.934702000	1.157897000
6	-3.122171000	2.538572000	0.488353000
6	-3.524675000	3.923828000	1.001753000
6	-4.331268000	1.596923000	0.408187000
1	-2.807942000	2.695757000	-0.541028000
1	-2.662177000	4.590532000	1.049519000
1	-4.255937000	4.365684000	0.318503000
1	-3.984472000	3.895407000	1.990134000
1	-4.012440000	0.607581000	0.066200000
1	-4.845883000	1.480799000	1.362717000
1	-5.062167000	1.981016000	-0.310871000
6	-1.856744000	1.899614000	2.644795000
6	-3.162685000	1.566142000	3.377389000
6	-1.246147000	3.155531000	3.271001000
1	-1.156546000	1.084784000	2.857345000
1	-3.660730000	0.665331000	3.020775000
1	-2.928454000	1.413809000	4.433944000

1	-3.884660000	2.382330000	3.334956000
1	-0.251130000	3.339796000	2.872751000
1	-1.861310000	4.042179000	3.107623000
1	-1.144265000	3.014749000	4.350887000
6	-0.894605000	3.134253000	-2.009759000
6	-0.103012000	2.949920000	-3.301529000
6	-1.548604000	4.523352000	-1.996816000
1	0.295256000	1.938863000	-3.386701000
1	-0.750913000	3.136328000	-4.163883000
1	0.733326000	3.649860000	-3.369909000
1	-1.962202000	4.766799000	-1.017869000
1	-0.848158000	5.315028000	-2.272764000
1	-2.361921000	4.552800000	-2.728333000
6	1.013663000	3.778142000	-0.571040000
6	2.340648000	3.138884000	-0.952048000
6	1.065675000	4.349655000	0.837878000
1	0.830720000	4.615284000	-1.249029000
1	2.358478000	2.812601000	-1.992251000
1	3.178990000	3.821670000	-0.788761000
1	2.509341000	2.272763000	-0.318459000
1	0.099195000	4.768848000	1.128288000
1	1.359724000	3.584900000	1.558155000
1	1.814448000	5.144525000	0.885204000
1	-1.693318000	2.406468000	-2.018703000
6	0.408595000	-2.685335000	-1.438476000
6	1.119293000	-1.467839000	1.020213000
6	1.780191000	-0.193548000	-2.196715000
8	0.953357000	-1.574723000	2.138602000
8	-0.052949000	-3.661904000	-1.785320000
8	2.055418000	0.413104000	-3.114957000
31	3.306983000	-0.128250000	0.517441000
17	2.992872000	1.345524000	2.163047000
17	4.828861000	0.636988000	-0.936925000
17	4.344536000	-1.830290000	1.600894000

1h-$GaCl_3$ (TE = -6477.039679, H = -6476.992596)

6	2.862340000	-2.006416000	-2.467153000
6	1.727299000	-0.604107000	-1.080701000
6	3.758975000	-1.765621000	-1.240694000
1	2.469854000	-3.022154000	-2.518283000
1	3.338804000	-1.744045000	-3.409613000
8	1.726388000	-1.113827000	-2.293491000
7	2.797955000	-0.965186000	-0.407221000
6	4.979513000	-0.913933000	-1.571245000

1	5.507137000	-0.619283000	-0.661656000
1	5.670738000	-1.496686000	-2.184357000
1	4.707418000	-0.016890000	-2.129746000
6	4.173744000	-3.053689000	-0.544612000
1	4.774742000	-3.651555000	-1.233812000
1	4.787857000	-2.841444000	0.332637000
1	3.314344000	-3.649951000	-0.239279000
6	3.050086000	-0.638668000	0.969589000
6	3.723926000	0.533369000	1.291154000
6	2.644455000	-1.530326000	1.960258000
6	3.994991000	0.815664000	2.626665000
1	4.018718000	1.215734000	0.501714000
6	2.919544000	-1.239674000	3.291491000
1	2.117596000	-2.439600000	1.692433000
6	3.597270000	-0.069654000	3.623247000
1	4.512457000	1.731933000	2.886671000
1	2.595339000	-1.922630000	4.067690000
1	3.805660000	0.157335000	4.662292000
5	0.443042000	0.134642000	-0.381870000
7	0.509274000	1.540368000	-0.246504000
26	-1.005493000	-1.465776000	-0.101617000
6	-2.401615000	-2.678209000	0.068094000
6	0.203278000	-2.787601000	-0.327762000
6	-0.863937000	-1.326706000	1.721930000
6	-1.335483000	-1.099010000	-1.860167000
8	-3.178837000	-3.482739000	0.209033000
8	0.894178000	-3.672465000	-0.499272000
8	-1.530112000	-0.914701000	-2.961959000
8	-0.776930000	-1.393632000	2.848676000
14	1.018595000	2.457877000	-1.713227000
14	0.262516000	2.529584000	1.235917000
6	0.287864000	4.180238000	-1.759363000
1	0.661402000	4.653557000	-2.675117000
1	-0.799812000	4.131079000	-1.845342000
1	0.538713000	4.844917000	-0.933530000
6	0.391858000	1.642364000	-3.275724000
1	0.703768000	2.265546000	-4.121965000
1	0.761788000	0.636295000	-3.471699000
1	-0.700144000	1.617317000	-3.281951000
6	2.894787000	2.556617000	-1.784709000
1	3.361245000	1.568787000	-1.767716000
1	3.203563000	3.038172000	-2.718734000
1	3.313880000	3.141298000	-0.962256000
6	-1.223934000	3.658309000	1.289541000
1	-2.164204000	3.117857000	1.391493000
1	-1.109716000	4.284304000	2.183543000

1	-1.313266000	4.323155000	0.430487000
6	1.794288000	3.623021000	1.396829000
1	1.703208000	4.175108000	2.339291000
1	2.711995000	3.034745000	1.462123000
1	1.928854000	4.370379000	0.613458000
6	0.268903000	1.457324000	2.764574000
1	-0.724812000	1.092603000	3.024827000
1	0.956406000	0.611584000	2.700090000
1	0.607040000	2.079119000	3.601291000
31	-2.900973000	0.182461000	-0.002568000
17	-4.783826000	-0.746809000	-0.841091000
17	-2.714371000	2.037400000	-1.262992000
17	-3.436622000	0.785663000	2.097636000

1i-$GaCl_3$ (TE = -6528.456536, H = -6528.404603)

6	1.051285000	-0.222428000	0.628804000
6	2.237323000	-0.967665000	2.420426000
1	1.896531000	-1.092347000	3.446645000
1	2.972898000	-1.734910000	2.174941000
7	1.946419000	0.717531000	0.853747000
6	2.295383000	1.819721000	-0.002440000
6	2.128239000	3.125794000	0.456873000
6	2.892585000	1.567291000	-1.230806000
6	2.590481000	4.181464000	-0.318969000
1	1.624047000	3.315578000	1.396515000
6	3.321400000	2.632805000	-2.016683000
1	3.047072000	0.552555000	-1.574998000
6	3.188371000	3.936456000	-1.554031000
1	2.463791000	5.198968000	0.033076000
1	3.767909000	2.427885000	-2.982552000
1	3.537124000	4.764218000	-2.160550000
5	0.036424000	-0.569012000	-0.536074000
15	-1.907550000	-0.190902000	-0.308169000
7	-2.125860000	1.466221000	-0.679150000
7	-2.075992000	-0.457070000	1.389358000
6	-3.188003000	1.835793000	-1.649898000
1	-2.985634000	2.872072000	-1.923629000
6	-1.085987000	2.498053000	-0.501849000
1	-0.377631000	2.092639000	0.223721000
6	-1.606756000	0.489913000	2.411283000
1	-0.773299000	1.039772000	1.959393000
6	-3.191257000	-1.338700000	1.825679000
1	-3.232949000	-1.247775000	2.912580000
6	-1.622664000	3.801254000	0.091790000

1	-0.790388000	4.489845000	0.266966000
1	-2.315914000	4.309234000	-0.583182000
1	-2.132108000	3.637132000	1.042089000
6	-0.334696000	2.746534000	-1.803304000
1	0.447822000	3.496543000	-1.683359000
1	0.126920000	1.826079000	-2.159537000
1	-1.001126000	3.098870000	-2.594972000
6	-4.577048000	1.804725000	-1.022801000
1	-5.315038000	2.221707000	-1.714220000
1	-4.880720000	0.782203000	-0.794984000
1	-4.605492000	2.389456000	-0.099490000
6	-3.147717000	1.020103000	-2.940815000
1	-2.136013000	0.982257000	-3.353826000
1	-3.490399000	-0.002615000	-2.772341000
1	-3.803219000	1.469544000	-3.692065000
6	-1.075702000	-0.212462000	3.667037000
1	-0.515302000	0.492483000	4.287528000
1	-1.885345000	-0.593341000	4.293539000
1	-0.430755000	-1.051767000	3.407877000
6	-2.683018000	1.507619000	2.803621000
1	-3.484828000	1.023244000	3.368745000
1	-2.265040000	2.293373000	3.440441000
1	-3.121853000	1.966607000	1.917979000
6	-2.895687000	-2.799011000	1.507253000
1	-1.965691000	-3.117318000	1.979730000
1	-3.703552000	-3.443206000	1.865836000
1	-2.808162000	-2.948312000	0.426780000
6	-4.566823000	-0.942086000	1.290401000
1	-4.766013000	0.120741000	1.437892000
1	-4.652162000	-1.167110000	0.224840000
1	-5.344359000	-1.509377000	1.810236000
8	1.099130000	-1.171265000	1.551253000
26	0.665225000	-2.173672000	-1.762759000
6	1.239535000	-3.650702000	-2.762656000
6	2.335526000	-1.927453000	-1.072176000
6	0.068938000	-3.221987000	-0.401340000
6	-0.902433000	-1.965158000	-2.762143000
8	1.615861000	-4.593396000	-3.250166000
8	-0.179663000	-3.969508000	0.408430000
8	3.341123000	-1.784402000	-0.564700000
8	-1.830348000	-1.881516000	-3.398208000
6	2.733047000	0.451934000	2.112176000
6	2.344394000	1.432125000	3.215429000
1	2.743689000	1.072107000	4.166727000
1	2.765524000	2.421810000	3.038980000
1	1.259177000	1.514155000	3.309168000

6	4.227979000	0.496687000	1.833080000
1	4.502691000	-0.166828000	1.012159000
1	4.550289000	1.509959000	1.587141000
1	4.766935000	0.180764000	2.729768000
31	1.590770000	-0.992633000	-3.814183000
17	1.011172000	-2.237936000	-5.607524000
17	3.853651000	-0.968233000	-3.779748000
17	1.001648000	1.065334000	-4.449232000

2a-$GaCl_3$ (TE = -5267.077050, H = -5267.056869)

28	-0.418137000	-0.281577000	0.193950000
6	-0.420275000	-0.306284000	2.150370000
6	1.479929000	-0.369770000	-0.171552000
6	-1.431800000	-1.882359000	-0.194282000
6	-1.304611000	1.399793000	-0.144623000
8	2.595099000	-0.437914000	-0.274073000
8	-1.826084000	2.389844000	-0.227398000
8	-2.039633000	-2.818910000	-0.304491000
8	-0.425323000	-0.323202000	3.269975000
31	-0.423495000	-0.243709000	-2.389361000
17	0.547301000	-2.120681000	-2.959931000
17	0.721329000	1.549599000	-2.901256000
17	-2.541312000	-0.142495000	-2.931927000

2b-$GaCl_3$ (TE = -5614.729866, H = -5614.705070)

15	-0.884062000	0.113721000	-2.290640000
6	-0.457321000	1.725615000	-3.036006000
1	-0.454254000	1.666457000	-4.127078000
1	-1.183149000	2.480762000	-2.727397000
1	0.531788000	2.042172000	-2.698049000
6	-2.478660000	-0.310842000	-3.073904000
1	-2.406004000	-0.264641000	-4.163125000
1	-2.777390000	-1.321172000	-2.786448000
1	-3.252995000	0.384198000	-2.742847000
6	0.294226000	-1.043879000	-3.069990000
1	1.314530000	-0.798718000	-2.768260000
1	0.077570000	-2.066015000	-2.752732000
1	0.230425000	-0.993448000	-4.159598000
28	-0.892324000	0.084396000	0.021737000
31	-0.912803000	0.038596000	2.519828000
17	-1.260132000	-2.057700000	3.117221000
17	1.058898000	0.774432000	3.185745000

17	-2.546331000	1.368343000	3.179406000
6	0.561583000	-1.112061000	0.313378000
6	-0.562240000	1.932507000	0.359214000
6	-2.658732000	-0.547255000	0.315698000
8	1.432711000	-1.821518000	0.374342000
8	-3.718851000	-0.918673000	0.384185000
8	-0.365936000	3.036229000	0.454105000

2c-$GaCl_3$ (TE = -5458.440700, H = -5458.415544)

6	2.516261000	0.010727000	-0.005374000
7	3.200399000	-1.154318000	0.053730000
7	3.474545000	0.963721000	-0.011949000
6	4.562801000	-0.935123000	0.074445000
1	5.274852000	-1.742635000	0.119353000
6	4.736086000	0.405556000	0.035574000
1	5.630785000	1.005674000	0.042629000
6	3.218454000	2.397160000	-0.069842000
1	4.167039000	2.923876000	0.013444000
1	2.751430000	2.658321000	-1.019300000
1	2.576694000	2.696520000	0.757969000
6	2.604901000	-2.485139000	0.032862000
1	2.606723000	-2.882758000	-0.982868000
1	3.180703000	-3.144519000	0.680535000
1	1.581334000	-2.434880000	0.399109000
28	0.503907000	0.172687000	-0.029251000
31	-1.980060000	-0.099778000	0.027854000
17	-2.381721000	-2.257472000	0.363242000
17	-2.815194000	1.143857000	1.663024000
17	-2.820977000	0.581557000	-1.908763000
6	0.011944000	2.069760000	-0.344014000
6	0.195252000	-0.839369000	-1.597165000
8	-0.294990000	3.137130000	-0.517066000
8	0.158045000	-1.455965000	-2.538876000
6	0.216092000	-0.323096000	1.764156000
8	0.197090000	-0.642072000	2.844314000

2d-$GaCl_3$ (TE = -5753.041033, H = -5753.009075)

6	-3.955582000	-1.807294000	-0.291788000
6	-4.028757000	-0.289954000	-0.055139000
6	-1.715642000	-0.923408000	-0.049971000
6	-2.487883000	-2.228221000	-0.040207000
1	-4.650581000	-2.342628000	0.358111000

1	-4.231966000	-2.030215000	-1.325404000
7	-2.559630000	0.064713000	-0.055230000
6	-2.143630000	1.446727000	-0.020121000
6	-1.956702000	2.075721000	1.205123000
6	-1.900427000	2.115311000	-1.214477000
6	-1.500542000	3.389477000	1.232467000
1	-2.149614000	1.534860000	2.125156000
6	-1.444394000	3.428199000	-1.178080000
1	-2.054472000	1.606080000	-2.159278000
6	-1.242090000	4.063494000	0.043344000
1	-1.333390000	3.879451000	2.184511000
1	-1.233703000	3.948767000	-2.104832000
1	-0.869866000	5.080830000	0.068405000
6	-1.982503000	-3.172744000	-1.132622000
1	-0.972179000	-3.529216000	-0.925642000
1	-2.634402000	-4.048310000	-1.194243000
1	-1.979155000	-2.687545000	-2.112605000
6	-2.292730000	-2.871680000	1.340881000
1	-2.852402000	-3.809179000	1.392177000
1	-1.240279000	-3.097720000	1.529489000
1	-2.645851000	-2.222505000	2.146143000
6	-4.636220000	0.079540000	1.295324000
1	-4.596571000	1.156586000	1.471176000
1	-5.686466000	-0.219828000	1.308100000
1	-4.129120000	-0.429393000	2.117814000
6	-4.742463000	0.446800000	-1.181588000
1	-4.756936000	1.526239000	-1.017359000
1	-4.272968000	0.243466000	-2.146879000
1	-5.777752000	0.101240000	-1.230601000
28	0.277227000	-0.664103000	-0.012679000
31	2.625081000	0.195556000	-0.004114000
17	3.721819000	-0.613179000	-1.764945000
17	2.535534000	2.412862000	-0.052939000
17	3.685032000	-0.521868000	1.818417000
6	0.469564000	-0.079589000	-1.771022000
6	1.217357000	-2.512954000	0.072052000
6	0.434319000	-0.006670000	1.732102000
8	0.449141000	0.231317000	-2.854858000
8	1.803765000	-3.469700000	0.106136000
8	0.406421000	0.335794000	2.805995000

2e-$GaCl_3$ (TE = -5710.432747, H = -5710.402835)

6	3.258766000	-2.782593000	0.210748000
6	3.924103000	-1.414624000	-0.004248000

6	1.575305000	-1.248397000	0.025822000
1	3.559823000	-3.532744000	-0.518130000
1	3.402617000	-3.167659000	1.221401000
7	2.696868000	-0.559069000	0.051124000
6	2.740707000	0.874602000	0.018422000
6	2.709402000	1.537529000	-1.204434000
6	2.789644000	1.581524000	1.215131000
6	2.711344000	2.928033000	-1.226083000
1	2.668306000	0.965102000	-2.124933000
6	2.791296000	2.971836000	1.185584000
1	2.807725000	1.043077000	2.156620000
6	2.750045000	3.643307000	-0.032783000
1	2.670589000	3.450445000	-2.174642000
1	2.813165000	3.528731000	2.114932000
1	2.739938000	4.726930000	-0.052236000
6	4.574838000	-1.292917000	-1.378063000
1	4.939016000	-0.278435000	-1.552116000
1	5.429159000	-1.971007000	-1.440874000
1	3.870578000	-1.554770000	-2.171805000
6	4.893448000	-1.054792000	1.111400000
1	5.312969000	-0.057734000	0.962767000
1	4.402064000	-1.087909000	2.086036000
1	5.720538000	-1.768459000	1.121499000
28	-0.308378000	-0.574803000	0.001038000
31	-2.685122000	0.181424000	0.007400000
17	-3.657158000	-0.569700000	1.853240000
17	-2.693694000	2.398838000	-0.051035000
17	-3.690942000	-0.662742000	-1.779799000
6	-0.338525000	0.472337000	1.600445000
6	-1.200779000	-2.276212000	0.041530000
6	-0.379759000	0.364374000	-1.669219000
8	-0.287746000	1.046154000	2.567358000
8	-1.615371000	-3.320575000	0.065290000
8	-0.362089000	0.873042000	-2.673000000
8	1.836496000	-2.544185000	0.041442000

2f-$GaCl_3$ (TE = -6650.928086, H = -6650.879625)

6	2.263697000	3.213615000	-0.963566000
6	1.678872000	0.905060000	-0.818344000
6	2.192957000	1.091440000	-2.249699000
6	2.890840000	2.466069000	-2.157456000
1	3.959869000	2.323886000	-1.974636000
1	2.785385000	3.033892000	-3.083363000
7	1.664627000	2.061620000	-0.197737000

6	1.202343000	4.232459000	-1.374198000
1	0.800807000	4.760292000	-0.507875000
1	1.665053000	4.978916000	-2.023706000
1	0.375878000	3.777796000	-1.920092000
6	3.315056000	3.894389000	-0.093023000
1	3.839192000	4.643992000	-0.690511000
1	2.859718000	4.402533000	0.759724000
1	4.052461000	3.180352000	0.280537000
6	3.141850000	-0.028839000	-2.684274000
1	2.648196000	-1.004078000	-2.647171000
1	3.453190000	0.146471000	-3.717135000
1	4.042741000	-0.070659000	-2.073796000
6	1.031936000	1.131808000	-3.260043000
1	1.450081000	1.288295000	-4.257630000
1	0.475704000	0.193389000	-3.272027000
1	0.335538000	1.945663000	-3.066298000
6	1.189574000	2.220046000	1.151698000
6	1.902416000	1.651350000	2.202104000
6	0.011143000	2.923781000	1.394978000
6	1.439820000	1.796043000	3.505645000
1	2.815954000	1.108184000	1.999526000
6	-0.446661000	3.059192000	2.700831000
1	-0.564301000	3.339016000	0.577724000
6	0.267873000	2.501095000	3.756256000
1	1.994530000	1.349332000	4.322826000
1	-1.376223000	3.584025000	2.885349000
1	-0.098720000	2.601728000	4.771066000
5	1.113813000	-0.451368000	-0.286613000
7	1.868845000	-1.549399000	0.176835000
14	3.621012000	-1.538800000	0.591205000
14	1.094437000	-3.190872000	0.150604000
6	3.812795000	-2.004529000	2.400195000
1	4.773817000	-1.636170000	2.773357000
1	3.027339000	-1.536888000	3.003999000
1	3.784034000	-3.075024000	2.600114000
6	4.548839000	-2.713234000	-0.545735000
1	4.137577000	-3.720283000	-0.613949000
1	4.603627000	-2.317371000	-1.563873000
1	5.579111000	-2.813989000	-0.186139000
6	2.028615000	-4.449837000	1.191695000
1	3.098802000	-4.563159000	1.025267000
1	1.861318000	-4.285036000	2.259414000
1	1.572368000	-5.418297000	0.954519000
6	1.149636000	-3.744605000	-1.641023000
1	0.486432000	-4.598433000	-1.811911000
1	0.851752000	-2.955898000	-2.335159000

1	2.161025000	-4.054989000	-1.920936000
6	-0.623362000	-3.309142000	0.876732000
1	-1.442289000	-2.872086000	0.311370000
1	-0.839241000	-4.381611000	0.952686000
1	-0.671298000	-2.917589000	1.895783000
6	4.511436000	0.125566000	0.428848000
1	4.004698000	0.925107000	-0.103607000
1	4.779269000	0.509721000	1.416793000
1	5.456741000	-0.052665000	-0.095324000
28	-0.974215000	-0.200671000	-0.462229000
6	-1.391815000	-1.399104000	-1.822506000
6	-0.961569000	-0.229128000	1.349477000
6	-1.482986000	1.536368000	-1.268198000
31	-3.401933000	-0.224998000	0.050658000
17	-4.082207000	-1.995395000	1.219277000
17	-3.857014000	1.625784000	1.245608000
17	-4.594654000	-0.107175000	-1.837179000
8	-1.616483000	-2.110352000	-2.672457000
8	-0.871094000	-0.280996000	2.478271000
8	-1.923144000	2.459877000	-1.744839000

2g-$GaCl_3$ (TE = -6702.346478, H = -6702.293178)

6	-1.475620000	-4.010869000	-0.624116000
6	-1.133197000	-1.655531000	-0.851907000
6	-1.501214000	-2.150094000	-2.258042000
6	-2.053732000	-3.561753000	-1.972164000
1	-3.144025000	-3.516537000	-1.897049000
1	-1.803389000	-4.262126000	-2.771013000
7	-1.116994000	-2.680378000	-0.018995000
6	-0.227209000	-4.884373000	-0.742249000
1	0.165345000	-5.144917000	0.242748000
1	-0.485517000	-5.815422000	-1.251587000
1	0.567669000	-4.398193000	-1.309795000
6	-2.521347000	-4.714913000	0.233267000
1	-2.862830000	-5.609522000	-0.293051000
1	-2.115678000	-5.028790000	1.197006000
1	-3.388293000	-4.072963000	0.406370000
6	-2.552102000	-1.264822000	-2.920134000
1	-2.146960000	-0.285632000	-3.182499000
1	-2.901517000	-1.745462000	-3.838060000
1	-3.409226000	-1.116067000	-2.265959000
6	-0.267775000	-2.209808000	-3.173209000
1	-0.586470000	-2.564427000	-4.156944000
1	0.186029000	-1.226520000	-3.305388000

1	0.493095000	-2.897988000	-2.808398000
6	-0.672460000	-2.623430000	1.351714000
6	-1.595728000	-2.474460000	2.382521000
6	0.680037000	-2.796564000	1.639162000
6	-1.155892000	-2.446829000	3.701941000
1	-2.650939000	-2.403039000	2.152393000
6	1.113403000	-2.770754000	2.959727000
1	1.392174000	-2.954732000	0.839699000
6	0.197853000	-2.586388000	3.990741000
1	-1.875949000	-2.323518000	4.502809000
1	2.169298000	-2.883369000	3.175818000
1	0.539242000	-2.557220000	5.018951000
5	-0.737736000	-0.213318000	-0.502622000
15	-1.836258000	1.269704000	-0.562295000
7	-3.396938000	0.980380000	0.057881000
7	-1.156236000	2.667307000	0.116814000
6	-1.072177000	2.801606000	1.587599000
6	-2.255647000	3.545353000	2.218420000
6	0.236251000	3.426567000	2.073821000
1	-1.104207000	1.772834000	1.965860000
1	-3.206600000	3.145396000	1.872123000
1	-2.218855000	3.437442000	3.307047000
1	-2.229381000	4.613268000	1.998100000
1	1.115841000	3.004553000	1.589844000
1	0.248040000	4.506377000	1.910768000
1	0.332206000	3.262436000	3.150260000
6	-0.775224000	3.777556000	-0.790091000
6	0.739827000	4.021227000	-0.896549000
6	-1.464665000	5.115222000	-0.503136000
1	-1.114503000	3.445437000	-1.776010000
1	1.313212000	3.105274000	-0.769447000
1	0.979347000	4.440503000	-1.877745000
1	1.100432000	4.728605000	-0.148513000
1	-2.546784000	5.025534000	-0.419224000
1	-1.082030000	5.575925000	0.409689000
1	-1.243491000	5.805791000	-1.321997000
6	-3.651372000	-0.010037000	1.120363000
6	-4.523238000	-1.170168000	0.635538000
6	-4.225739000	0.592570000	2.403852000
1	-4.078830000	-1.663126000	-0.233812000
1	-4.651364000	-1.914680000	1.426266000
1	-5.526125000	-0.831701000	0.361383000
1	-3.518129000	1.280321000	2.866182000
1	-5.163751000	1.127619000	2.232398000
1	-4.435937000	-0.202032000	3.126049000
6	-4.580644000	1.609347000	-0.572849000

6	-4.997815000	0.957685000	-1.892670000
6	-4.400220000	3.107050000	-0.798485000
1	-5.400546000	1.483752000	0.140555000
1	-5.219774000	-0.103746000	-1.780307000
1	-5.895823000	1.445713000	-2.281915000
1	-4.208638000	1.070437000	-2.641572000
1	-4.158118000	3.629973000	0.125072000
1	-3.604985000	3.301239000	-1.524711000
1	-5.321360000	3.534755000	-1.201955000
1	-2.669417000	-0.409266000	1.372529000
6	2.200542000	-1.621100000	-1.153885000
6	1.301102000	0.321733000	1.227474000
6	1.332355000	1.057259000	-2.150235000
8	1.200386000	0.436804000	2.349974000
8	2.775372000	-2.530416000	-1.492387000
8	1.254299000	1.577032000	-3.149374000
31	3.659866000	0.721313000	-0.189895000
17	3.914596000	2.739510000	0.711076000
17	4.565533000	-0.795753000	1.198714000
17	4.768166000	0.641438000	-2.128102000
28	1.320277000	0.045583000	-0.566186000

2h-$GaCl_3$ (TE = -6608.316393, H = -6608.270520)

6	-1.939210000	2.539376000	-2.503213000
6	-1.587333000	1.025857000	-0.848865000
6	-1.932993000	3.317218000	-1.174843000
1	-1.074241000	2.763045000	-3.127596000
1	-2.856077000	2.674344000	-3.075470000
8	-1.857356000	1.138338000	-2.135363000
7	-1.531145000	2.203605000	-0.255295000
6	-3.315443000	3.815686000	-0.767934000
1	-3.287424000	4.238292000	0.239107000
1	-3.639592000	4.601820000	-1.453724000
1	-4.054208000	3.012612000	-0.787431000
6	-0.936822000	4.468355000	-1.213682000
1	-1.225665000	5.145795000	-2.021168000
1	-0.951046000	5.039457000	-0.284596000
1	0.078957000	4.124721000	-1.411879000
6	-1.233196000	2.360942000	1.136369000
6	-2.026868000	1.723073000	2.085744000
6	-0.115065000	3.100258000	1.521172000
6	-1.709815000	1.844129000	3.435141000
1	-2.881775000	1.136703000	1.769182000
6	0.180606000	3.230237000	2.872378000

1	0.540056000	3.535018000	0.776456000
6	-0.615655000	2.606764000	3.828914000
1	-2.321910000	1.342713000	4.175834000
1	1.057657000	3.791047000	3.172988000
1	-0.369015000	2.698102000	4.880297000
5	-1.147881000	-0.375424000	-0.219639000
7	-2.073766000	-1.394404000	0.064630000
6	1.229065000	1.172574000	-1.464547000
6	1.178078000	0.091438000	1.525506000
6	1.000737000	-1.879758000	-1.141203000
8	1.381853000	2.015836000	-2.203360000
8	0.955326000	-2.861160000	-1.701842000
8	1.330129000	0.284228000	2.629705000
14	-3.620895000	-1.430443000	-0.859868000
14	-1.692748000	-2.827639000	1.090034000
6	-4.811449000	-2.725298000	-0.215465000
1	-5.631695000	-2.779251000	-0.940580000
1	-4.401092000	-3.733617000	-0.133728000
1	-5.252994000	-2.454056000	0.745697000
6	-3.199657000	-1.846350000	-2.634365000
1	-4.097112000	-1.839475000	-3.261876000
1	-2.491343000	-1.133775000	-3.064116000
1	-2.752478000	-2.841350000	-2.716729000
6	-4.521425000	0.219132000	-0.768798000
1	-4.307181000	0.857933000	-1.627467000
1	-5.599087000	0.025617000	-0.779177000
1	-4.316328000	0.779626000	0.146440000
6	-1.646745000	-4.374778000	0.024425000
1	-0.615990000	-4.629318000	-0.236892000
1	-2.057224000	-5.230465000	0.569986000
1	-2.202664000	-4.286499000	-0.911601000
6	-3.026960000	-2.927168000	2.417337000
1	-2.573639000	-3.270213000	3.352600000
1	-3.469402000	-1.946903000	2.620781000
1	-3.837942000	-3.617849000	2.183233000
6	-0.089476000	-2.715161000	2.039091000
1	0.829695000	-2.642847000	1.456957000
1	-0.102815000	-1.910914000	2.778314000
1	-0.022409000	-3.652612000	2.605578000
28	0.904773000	-0.262458000	-0.260394000
31	3.355829000	-0.380935000	-0.251806000
17	4.071277000	-2.005646000	1.096676000
17	4.128493000	-0.744497000	-2.315829000
17	4.160498000	1.590665000	0.456566000

2i-$GaCl_3$ (TE = -6659.732752, H = -6659.681401)

6	-0.960965000	-1.382675000	-1.008890000
6	-1.168252000	-3.022288000	-2.565353000
1	-2.091240000	-3.085152000	-3.141952000
1	-0.334944000	-3.395553000	-3.159159000
7	-1.222375000	-2.479485000	-0.317867000
6	-1.213035000	-2.535649000	1.116158000
6	-2.417818000	-2.548549000	1.814245000
6	0.005589000	-2.612391000	1.787438000
6	-2.398518000	-2.624472000	3.203170000
1	-3.356302000	-2.513909000	1.271329000
6	0.015108000	-2.684305000	3.176029000
1	0.934218000	-2.616585000	1.225511000
6	-1.184759000	-2.688797000	3.881555000
1	-3.332479000	-2.633201000	3.753241000
1	0.961049000	-2.736695000	3.702217000
1	-1.173185000	-2.742376000	4.964190000
5	-0.589780000	0.012967000	-0.428422000
15	-1.764235000	1.496213000	-0.535420000
7	-2.000166000	2.190168000	1.008680000
7	-3.228123000	0.925449000	-1.198843000
6	-1.368627000	3.487967000	1.337734000
1	-1.621084000	3.676338000	2.383509000
6	-2.498265000	1.400236000	2.152413000
1	-3.023569000	0.545424000	1.723673000
6	-4.051520000	-0.128033000	-0.591469000
1	-3.404790000	-0.617503000	0.139605000
6	-3.885711000	1.731474000	-2.252242000
1	-4.807182000	1.200328000	-2.500757000
6	-3.527328000	2.181486000	2.976517000
1	-4.119380000	1.489735000	3.581976000
1	-3.059227000	2.885952000	3.668084000
1	-4.208400000	2.741926000	2.332094000
6	-1.389268000	0.847368000	3.041432000
1	-1.811916000	0.314577000	3.897547000
1	-0.766716000	0.141740000	2.487117000
1	-0.752656000	1.646983000	3.430298000
6	-1.943875000	4.635258000	0.514604000
1	-1.544152000	5.589518000	0.867964000
1	-1.666606000	4.535750000	-0.538462000
1	-3.032571000	4.667526000	0.587931000
6	0.155901000	3.479113000	1.234330000
1	0.597644000	2.655161000	1.796006000
1	0.471385000	3.396637000	0.191870000
1	0.572776000	4.411767000	1.624274000

6	-4.451006000	-1.197381000	-1.610893000
1	-4.947502000	-2.031011000	-1.105662000
1	-5.153276000	-0.820604000	-2.358022000
1	-3.572840000	-1.574760000	-2.139824000
6	-5.284511000	0.404998000	0.140397000
1	-6.004926000	0.835507000	-0.561223000
1	-5.794178000	-0.401306000	0.676980000
1	-5.013003000	1.178511000	0.860113000
6	-3.036849000	1.790571000	-3.519262000
1	-2.795325000	0.784832000	-3.871246000
1	-3.570341000	2.317872000	-4.314859000
1	-2.098165000	2.320908000	-3.338638000
6	-4.278131000	3.132076000	-1.785212000
1	-4.806575000	3.099060000	-0.829702000
1	-3.393305000	3.758717000	-1.662391000
1	-4.926242000	3.615374000	-2.521876000
8	-0.918619000	-1.615478000	-2.305193000
6	1.701247000	0.235428000	1.560144000
6	1.969545000	-1.340546000	-1.264791000
6	1.580493000	1.678702000	-1.422876000
8	2.205091000	-2.241068000	-1.907578000
8	1.834406000	0.235845000	2.683114000
8	1.596258000	2.528272000	-2.163426000
6	-1.279398000	-3.698717000	-1.182549000
6	-2.598511000	-4.435193000	-0.995028000
1	-2.656526000	-5.263050000	-1.705473000
1	-2.667985000	-4.854833000	0.010843000
1	-3.450391000	-3.776494000	-1.165612000
6	-0.102956000	-4.620248000	-0.881943000
1	0.852912000	-4.107292000	-0.991712000
1	-0.170885000	-5.022419000	0.130797000
1	-0.117239000	-5.462437000	-1.577646000
28	1.455805000	0.178322000	-0.267684000
31	3.916751000	0.404995000	-0.146472000
17	4.446252000	2.281931000	0.919354000
17	4.784254000	0.454908000	-2.195968000
17	4.720776000	-1.374306000	0.944447000