Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Metal–metal cooperativity boosts Lewis basicity and reduction properties of the bis(gallanediyl) $^{Cy}L_2Ga_2$

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Content

I. Spectroscopic Characterization

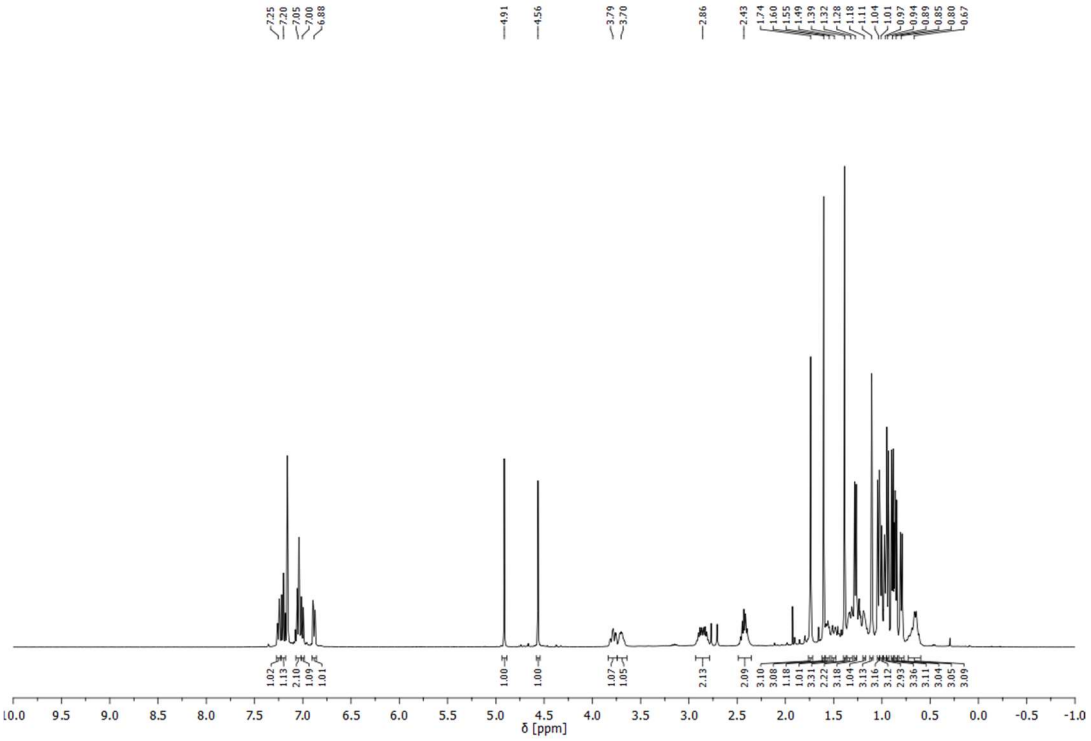


Figure S1. ^{1}H NMR spectrum (400.1 MHz, C_6D_6) of $^{Cy}L_2Ga_2$–$B(C_6F_5)_3$ (**1**–**B**).

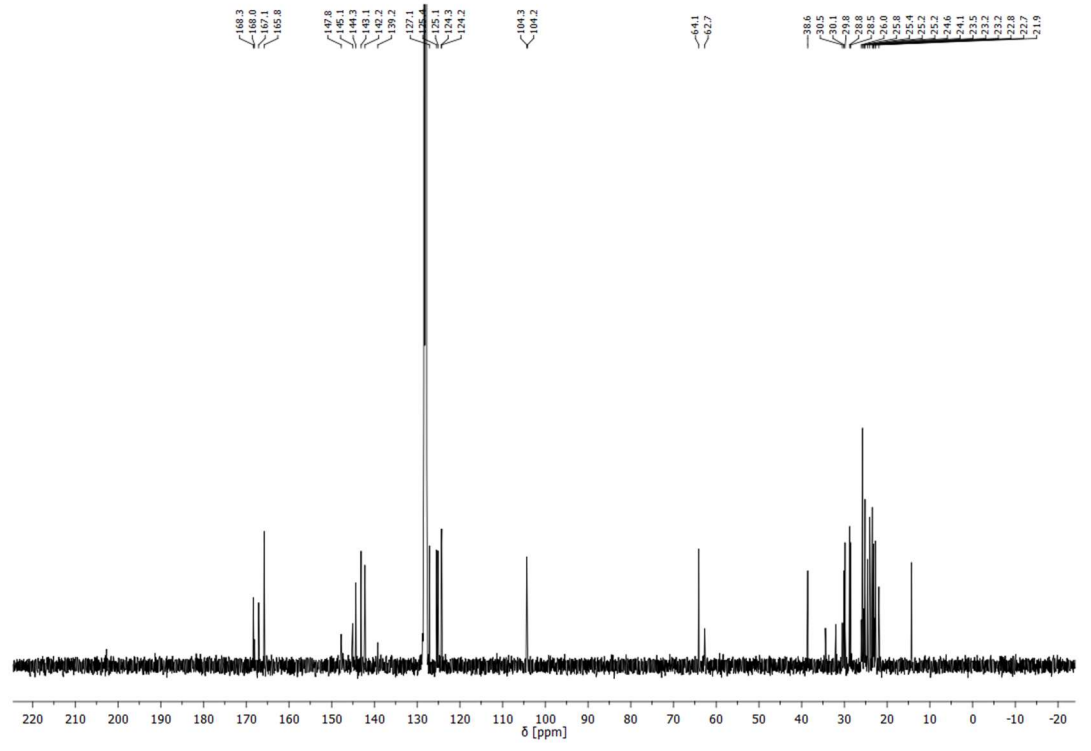


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, C_6D_6) of $^{Cy}L_2Ga_2$–$B(C_6F_5)_3$ (**1**–**B**).

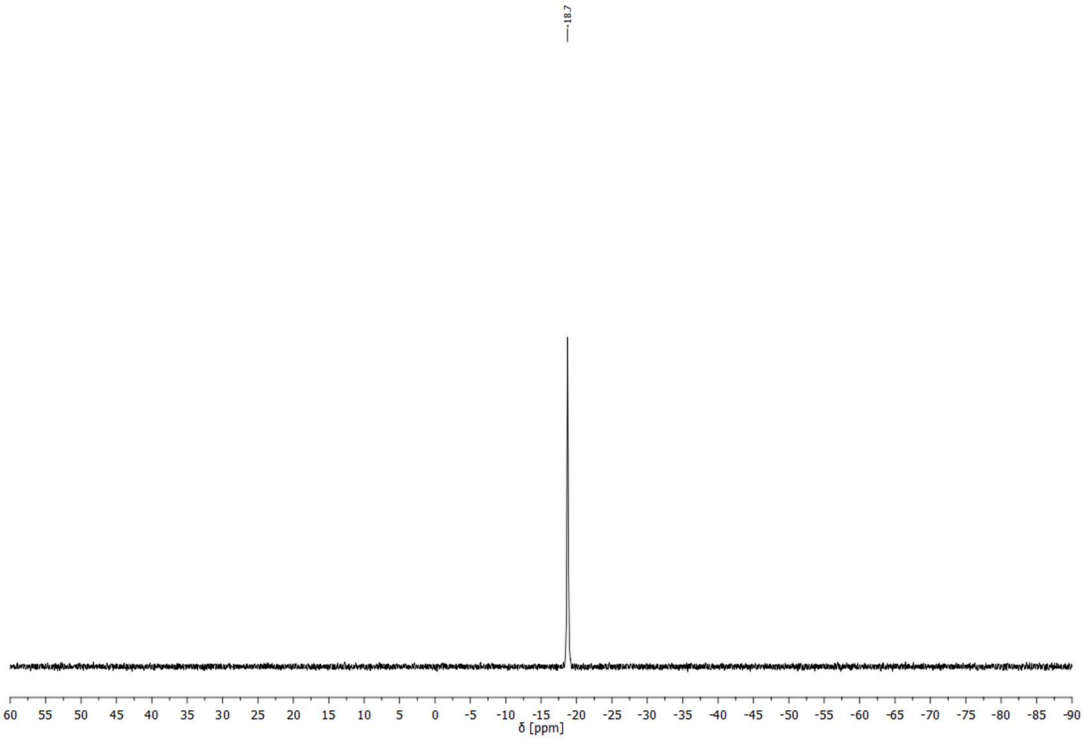


Figure S3. ^{11}B NMR spectrum (128.4 MHz, C_6D_6) of $^{Cy}L_2Ga_2–B(C_6F_5)_3$ (**1**–**B**).

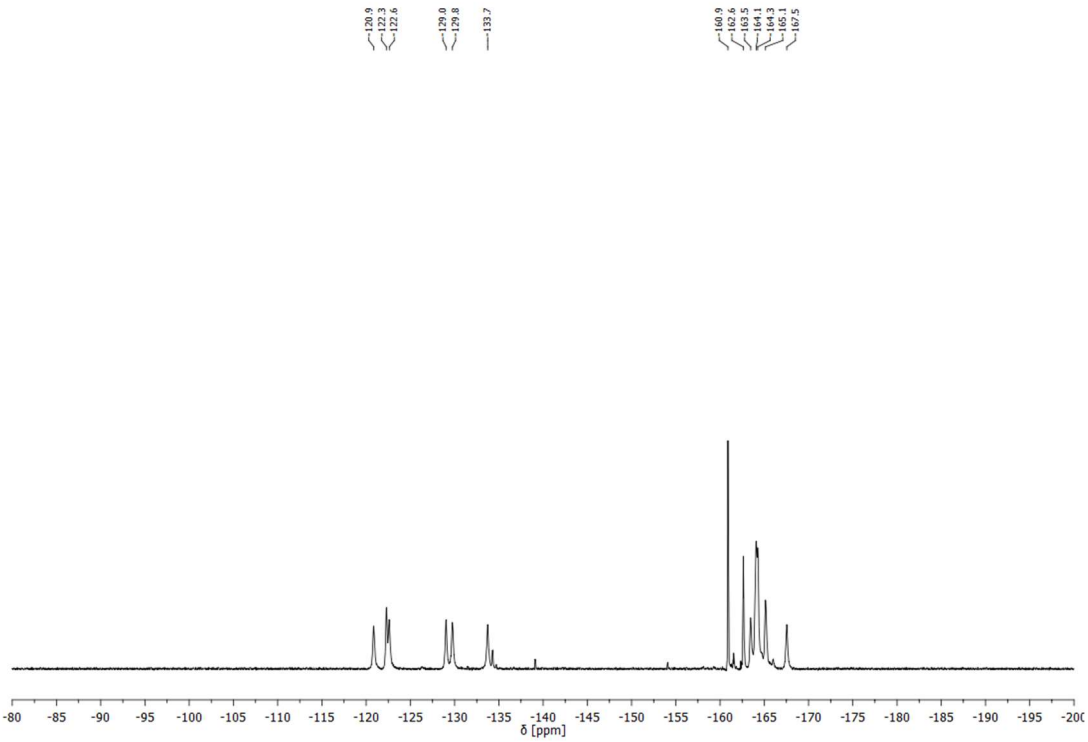


Figure S4. ^{19}F NMR spectrum (376.5 MHz, C_6D_6) of $^{Cy}L_2Ga_2–B(C_6F_5)_3$ (**1**–**B**).

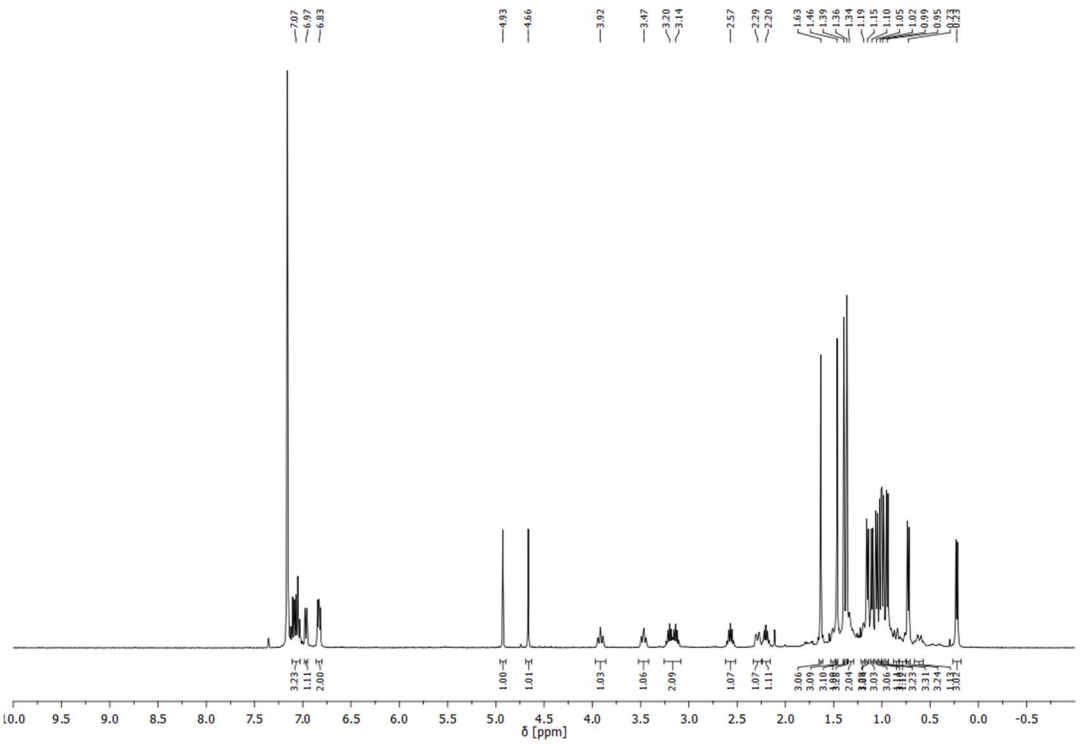


Figure S5. ^{1}H NMR spectrum (400.1 MHz, C_6D_6) of $^{Cy}L_2Ga_2$–Al(C_6F_5)$_3$ (**1**–**Al**).

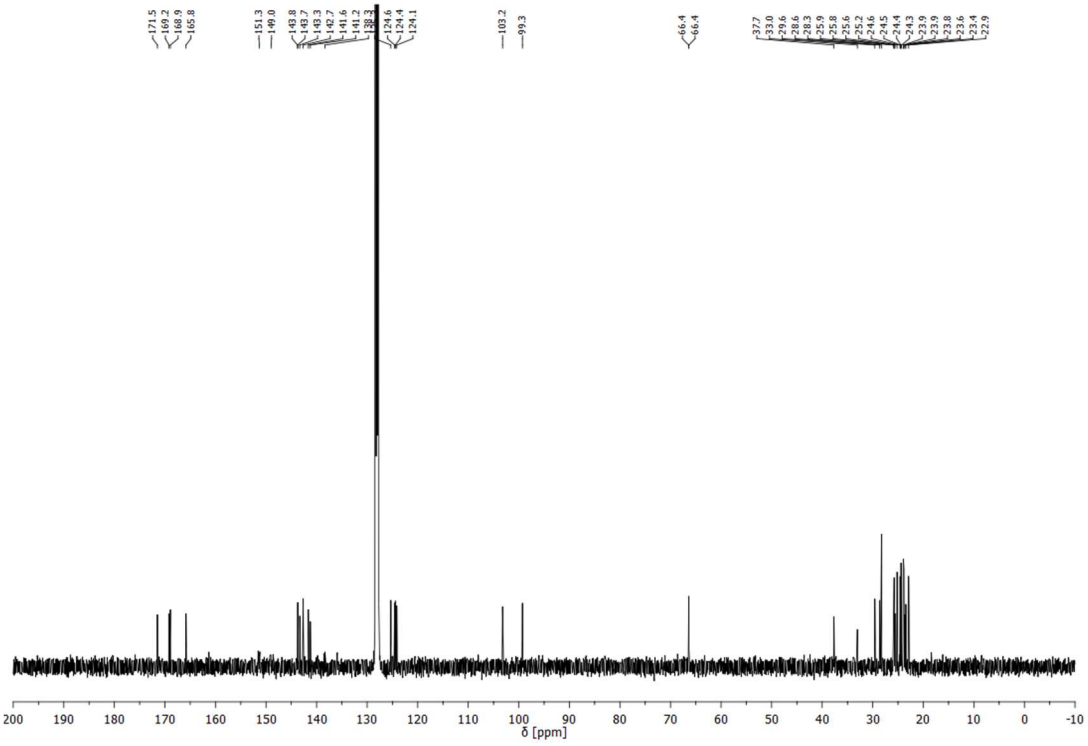


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, C_6D_6) of $^{Cy}L_2Ga_2$–Al(C_6F_5)$_3$ (**1**–**Al**).

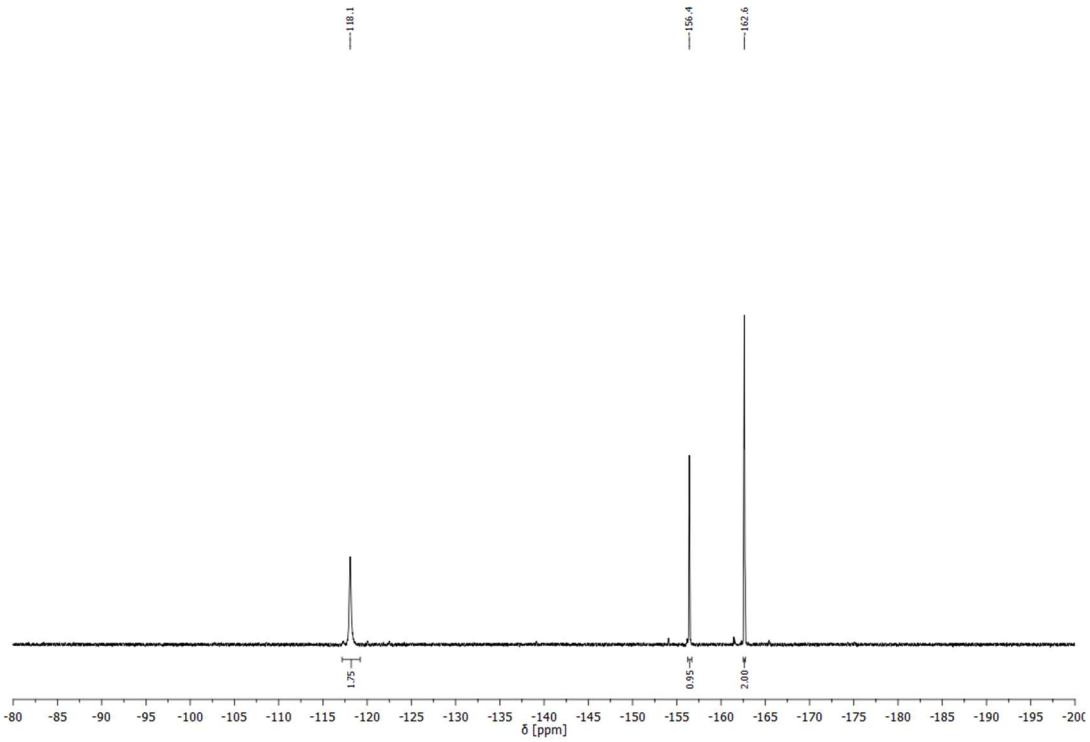


Figure S7. ^{19}F NMR spectrum (376.5 MHz, C_6D_6) of $^{Cy}L_2Ga_2$–Al$(C_6F_5)_3$ (**1**–**Al**).

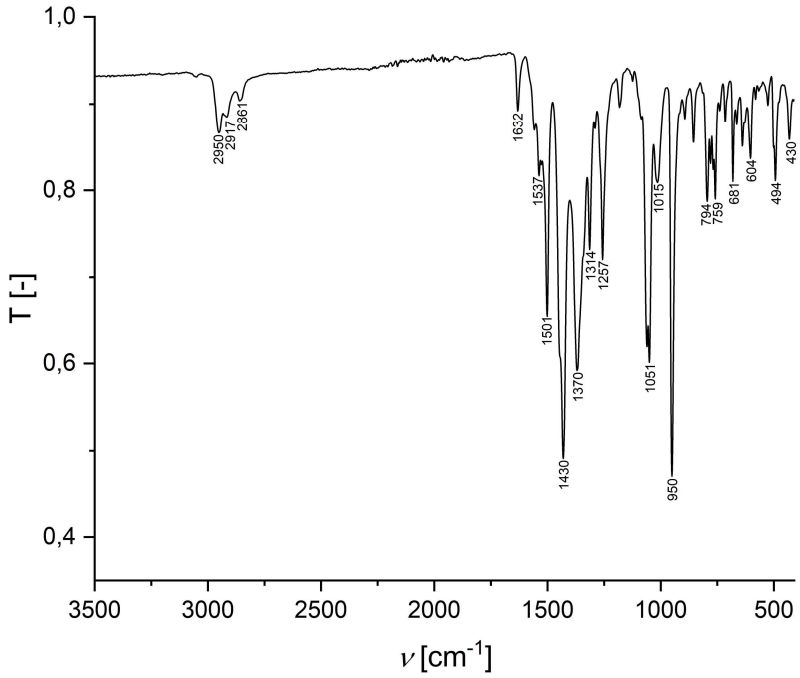


Figure S8. IR spectrum (neat) of $^{Cy}L_2Ga_2$–Al$(C_6F_5)_3$ (**1**–**Al**).

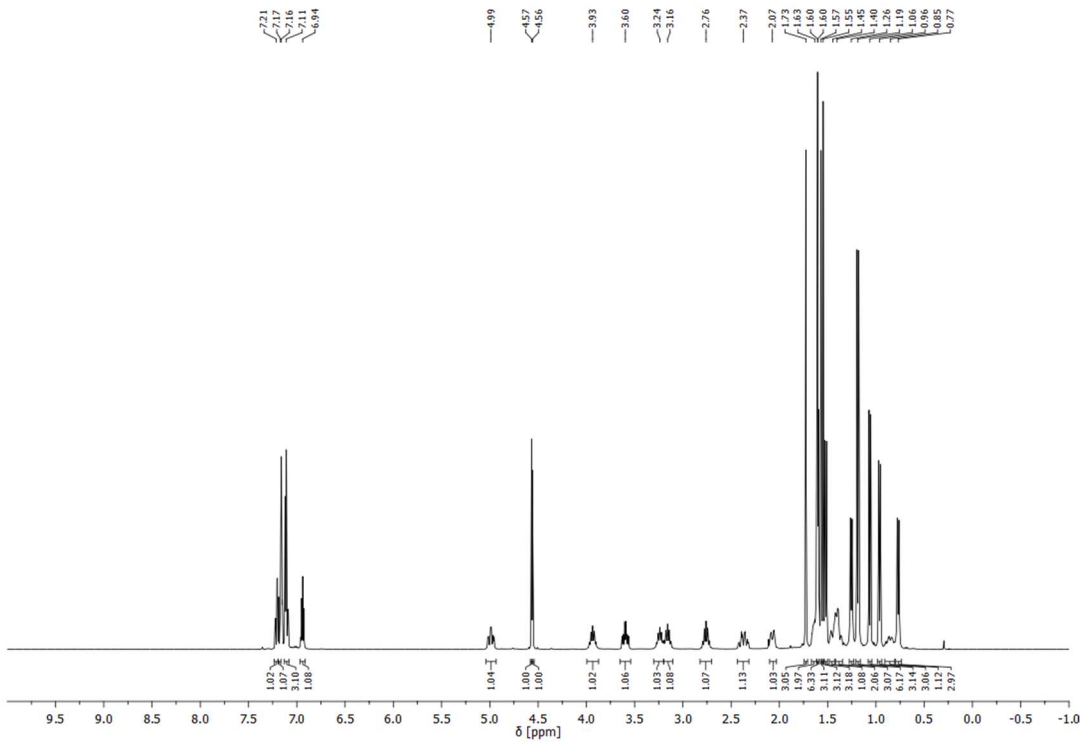


Figure S9. ^{1}H NMR spectrum (400.1 MHz, C_6D_6) of $^{Cy}L_2Ga_2Cl_2$ (**1–Cl₂**).

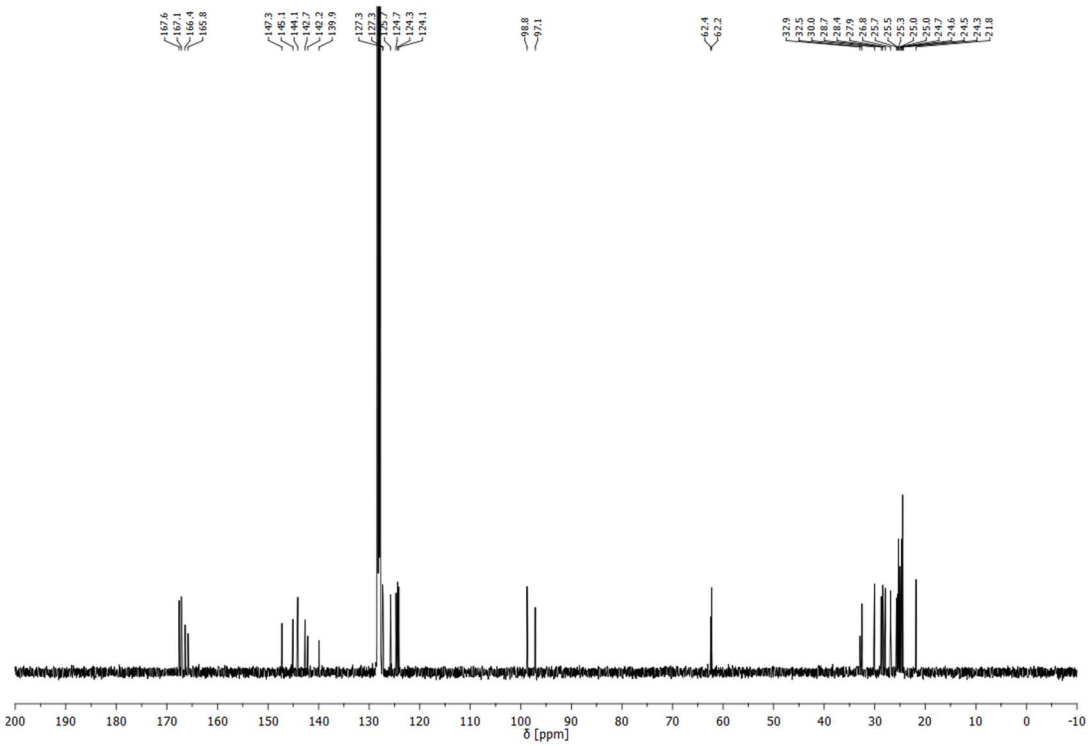


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, C_6D_6) of $^{Cy}L_2Ga_2Cl_2$ (**1–Cl₂**).

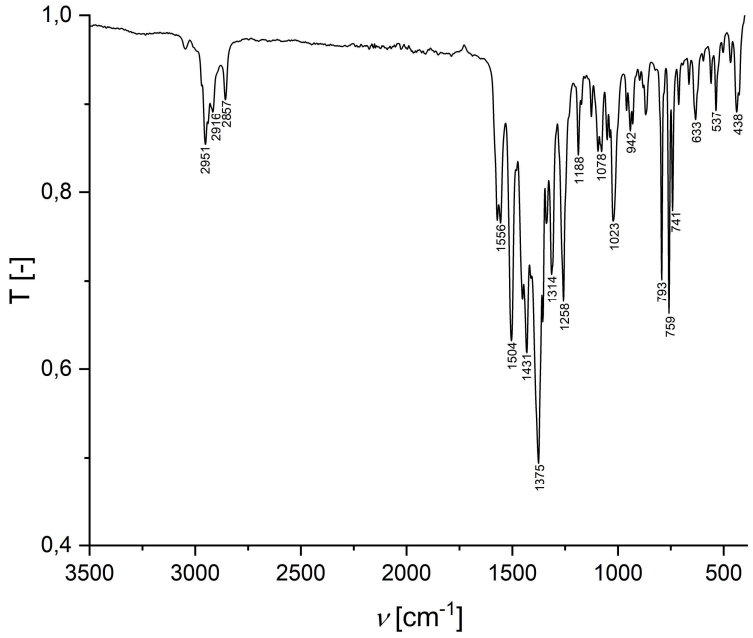


Figure S11. IR spectrum (neat) of $^{Cy}L_2Ga_2Cl_2$ (**1–Cl₂**).

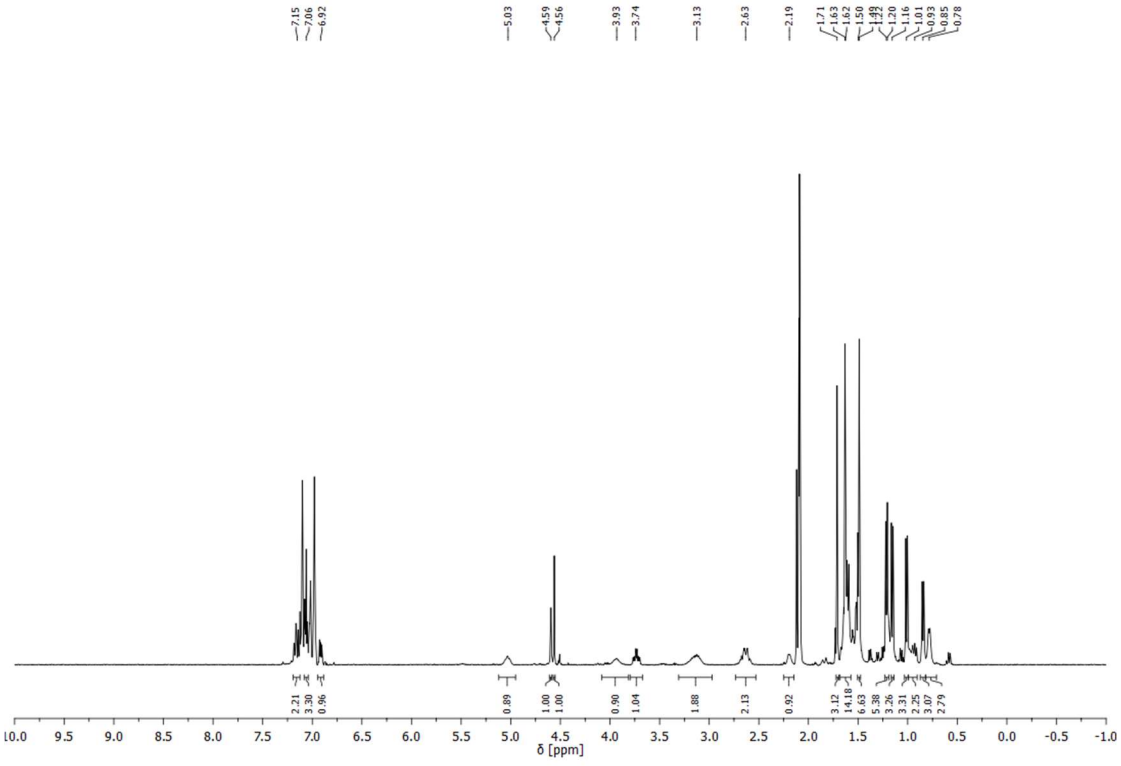


Figure S12. ^{1}H NMR spectrum (400.1 MHz, toluene-d_8) of $^{Cy}L_2Ga_2I_2$ (**1–I₂**).

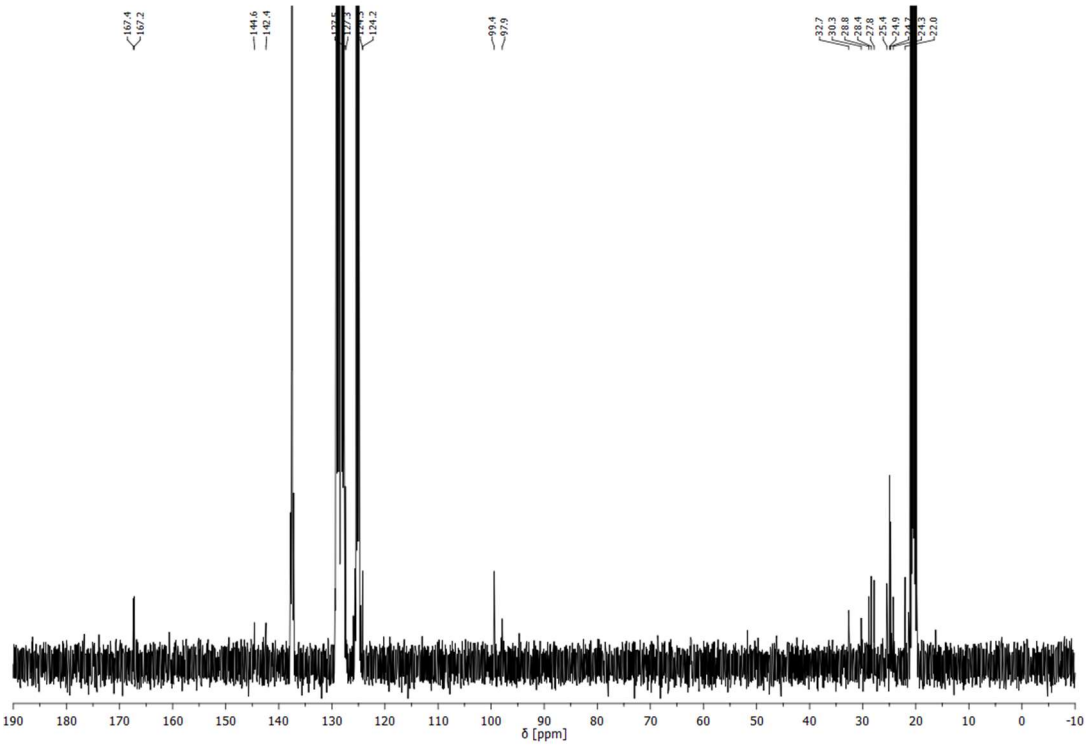


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, toluene-d_8) of $^{Cy}L_2Ga_2I_2$ (**1–I₂**).

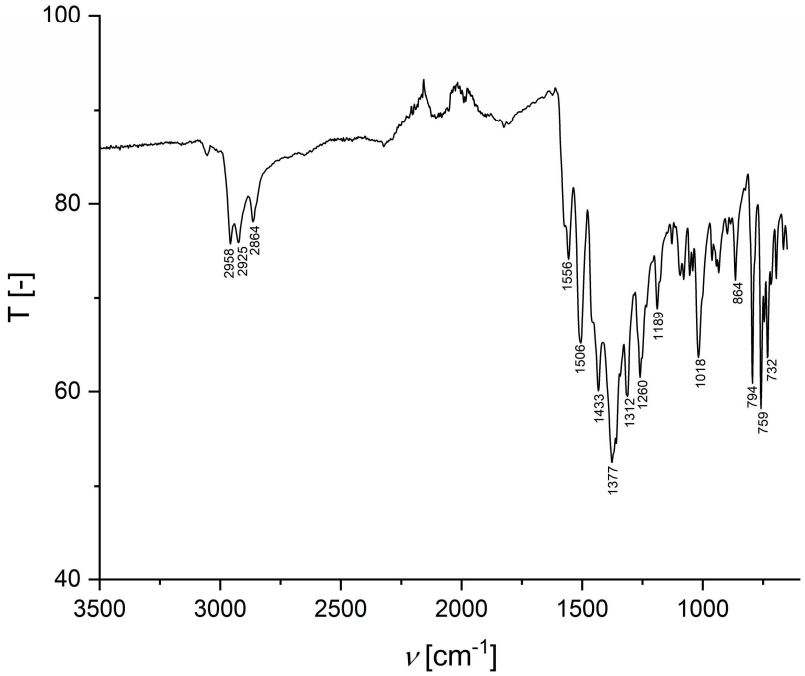


Figure S14. IR spectrum (neat) of $^{Cy}L_2Ga_2I_2$ (**1–I₂**).

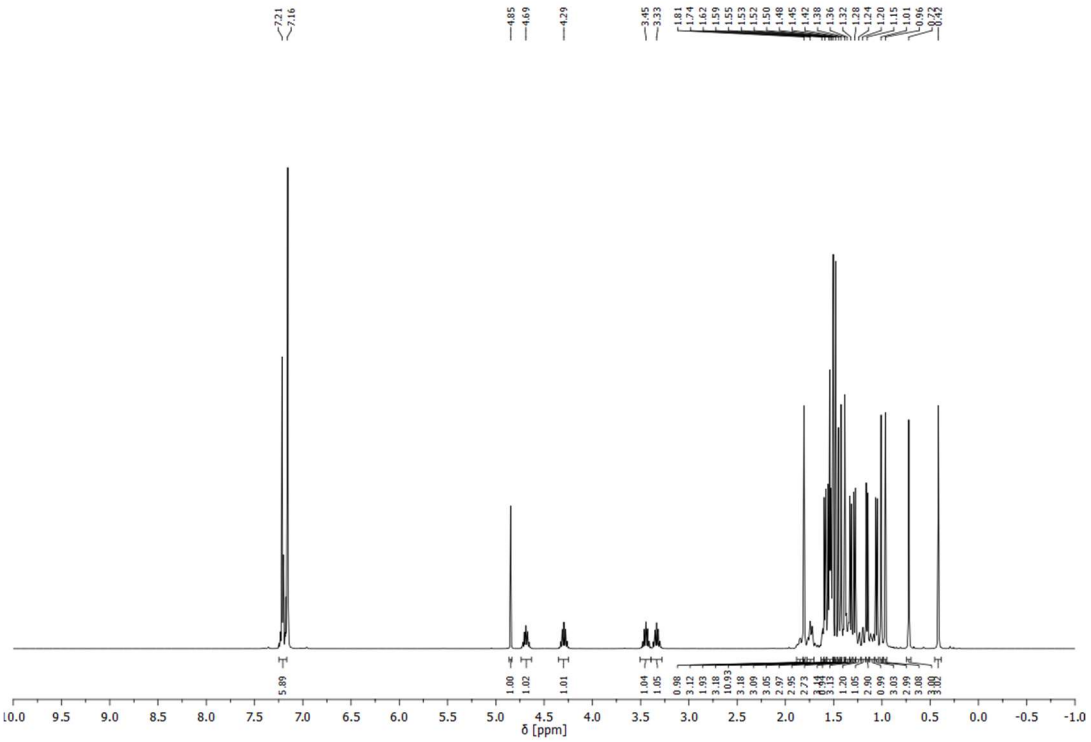


Figure S15. ^{1}H NMR spectrum (400.1 MHz, C_6D_6) of LGa(TEMPO)$_2$ (**2–(TEMPO)$_2$**).

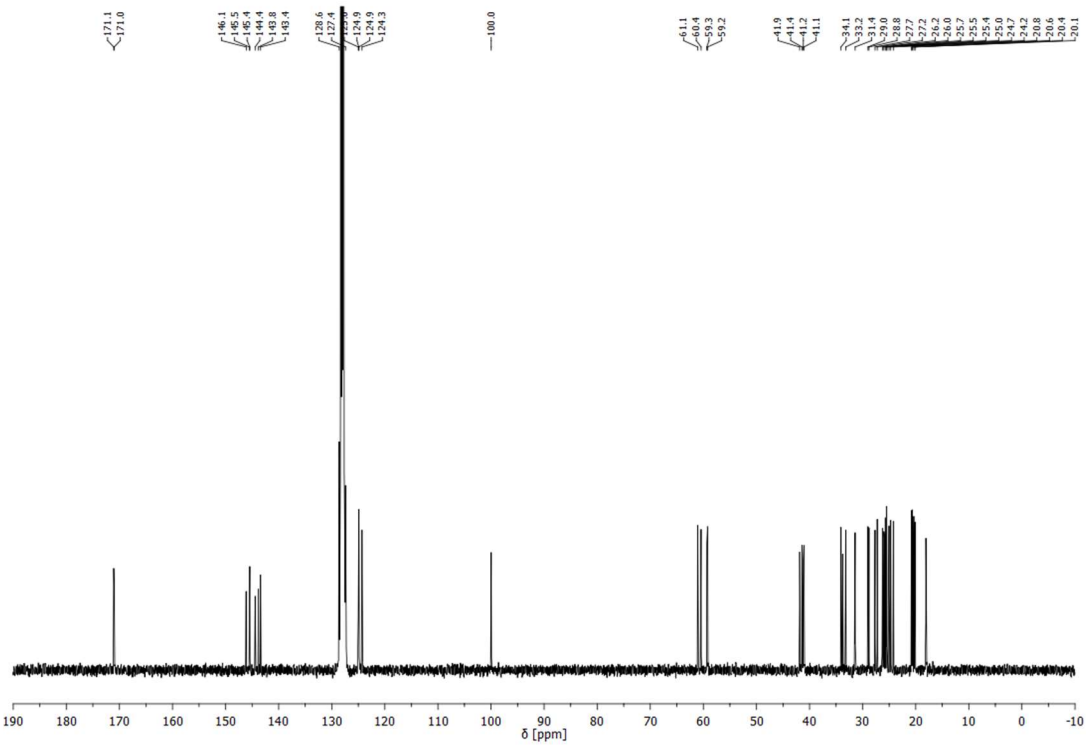


Figure S16. ^{13}C{^{1}H} NMR spectrum (100.6 MHz, C_6D_6) of LGa(TEMPO)$_2$ (**2–(TEMPO)$_2$**).

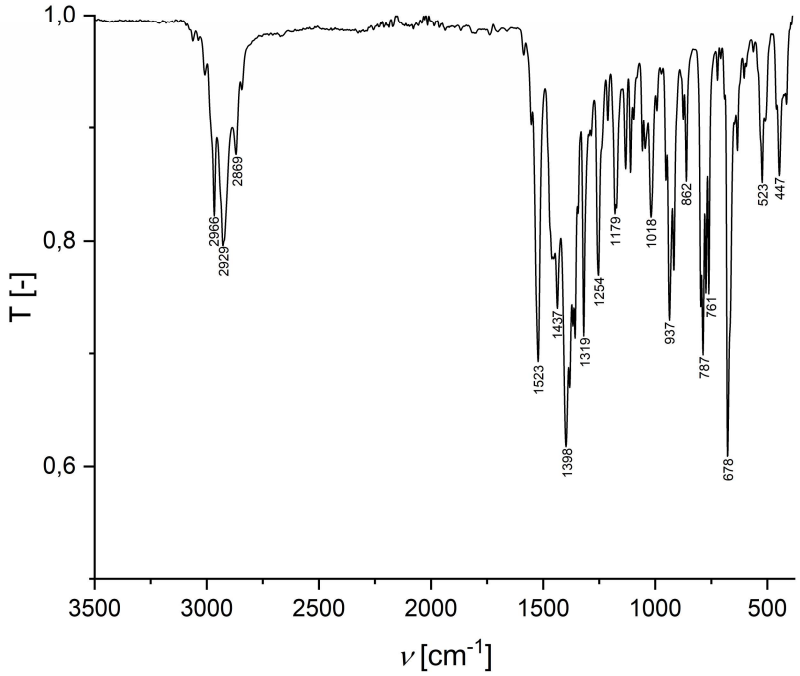


Figure S17. IR spectrum (neat) of LGa(TEMPO)$_2$ (**2–(TEMPO)$_2$**).

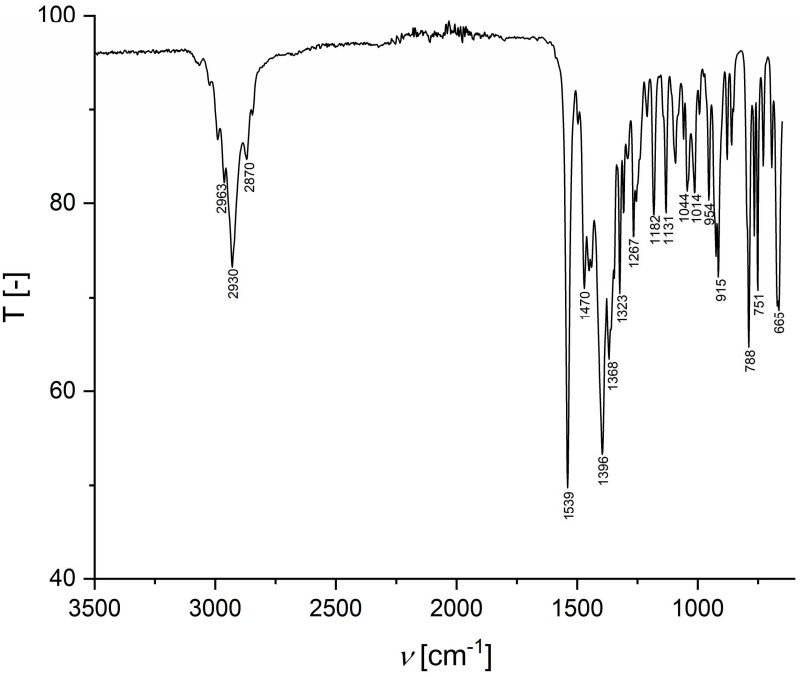


Figure S18. IR spectrum (neat) of $^{Cy}L_2Ga_2(TEMPO)_2$ (**1–(TEMPO)$_4$**).

Cross-over experiment between $^{Cy}L_2Ga_2$ (1) and LGa–B(C_6F_5)$_3$ (2–B(C_6F_5)$_3$). $^{Cy}L_2Ga_2$ **1** (5 mg, 0.00681 mmol) and LGa–B(C_6F_5)$_3$ **2**–**B** (7 mg, 0.00681 mmol) were dissolved in C_6D_6 (0.5 mL) at ambient temperature affording a bright yellow solution, which was subjected to ^{1}H NMR spectroscopic analysis.

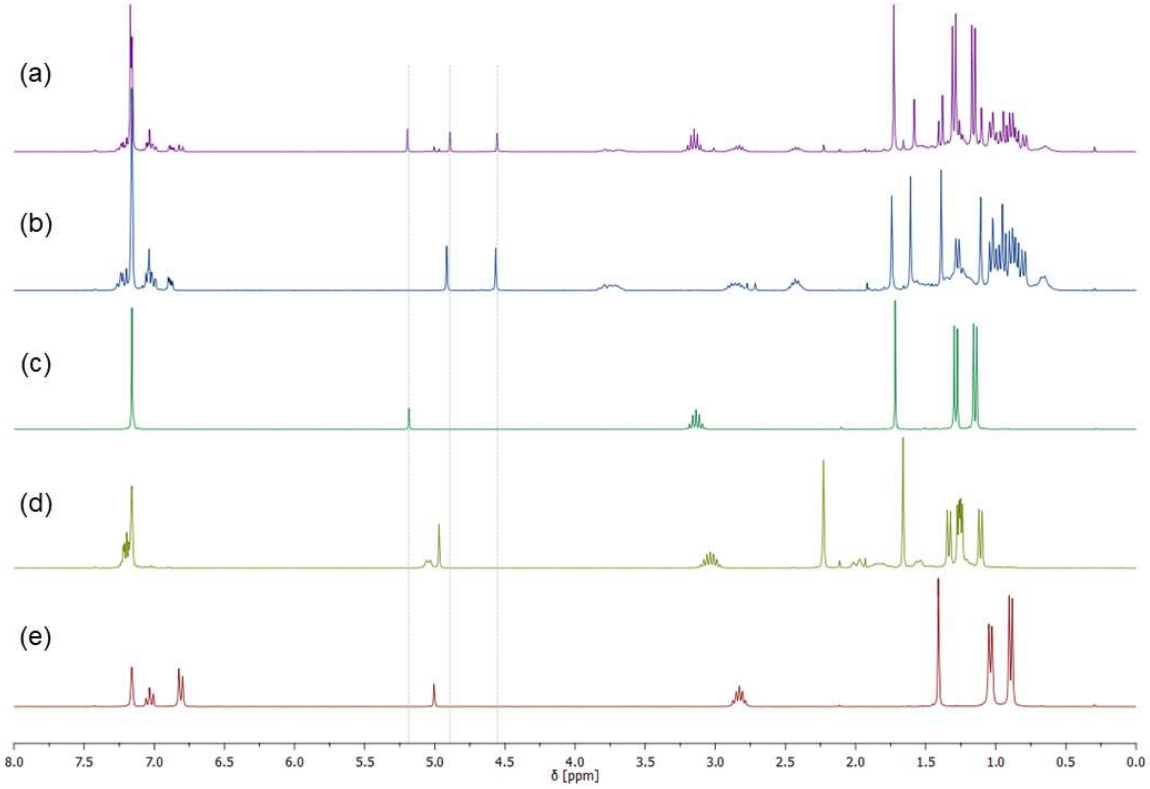


Figure S19. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the cross-over experiment between $^{Cy}L_2Ga_2$ **1** and LGa–B(C_6F_5)$_3$ **2**–**B**, (b) $^{Cy}L_2Ga_2$–B(C_6F_5)$_3$ **1**–**B**, (c) LGa **2**, (d) $^{Cy}L_2Ga_2$ **1**, and (e) LGa–B(C_6F_5)$_3$ **2**–**B**. Grey dashed lines are drawn for simplified assignment *via* the corresponding *γ*-C*H* resonances.

Cross-over experiment between $^{Cy}L_2Ga_2$ (1) and LGa–Al(C_6F_5)$_3$ (2–Al). $^{Cy}L_2Ga_2$ **1** (5 mg, 0.00681 mmol) and LGa–Al(C_6F_5)$_3$ **2**–**Al** (8 mg, 0.00681 mmol) were dissolved in C_6D_6 (0.5 mL) at ambient temperature affording a bright yellow solution, which was subjected to ^{1}H NMR spectroscopic analysis.

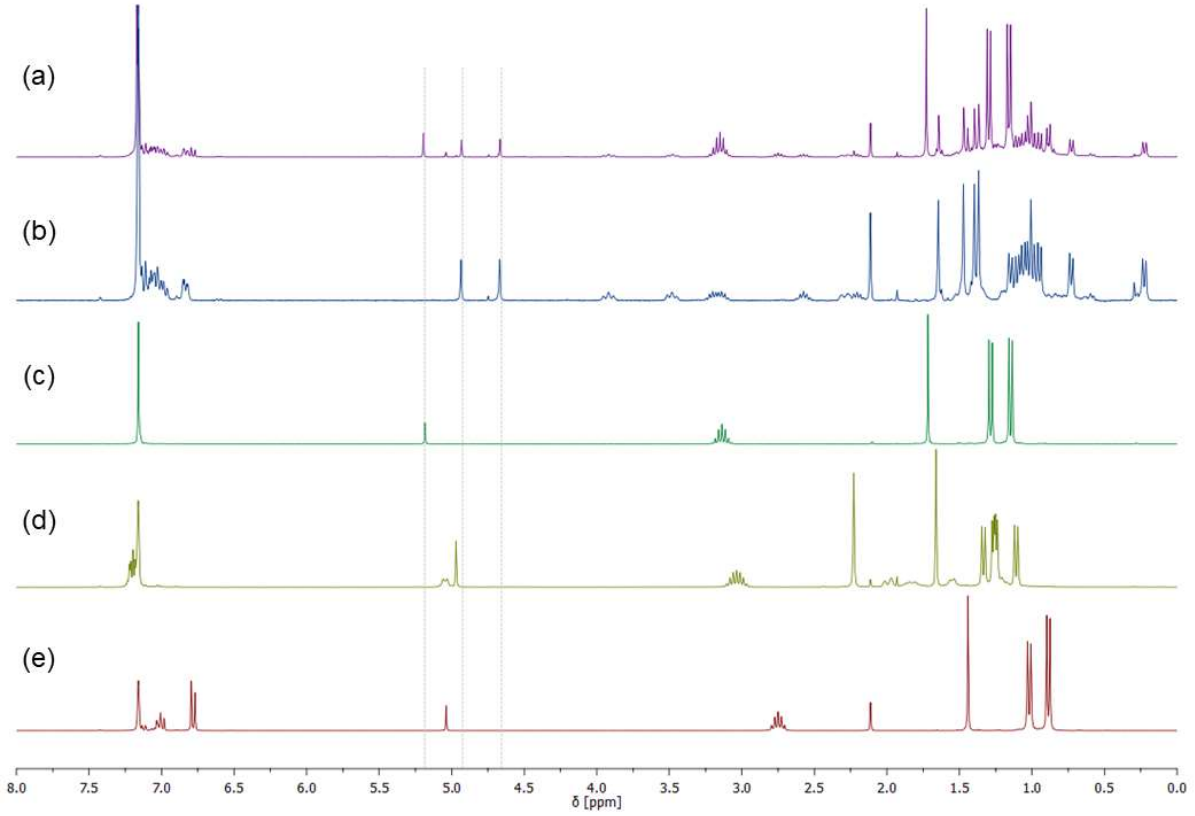


Figure S20. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the cross-over experiment between $^{Cy}L_2Ga_2$ **1** and LGa–Al(C_6F_5)$_3$ **2**–**Al**, (b) $^{Cy}L_2Ga_2$–Al(C_6F_5)$_3$ **1**–**Al**, (c) LGa **2**, (d) $^{Cy}L_2Ga_2$ **1**, and (e) LGa–Al(C_6F_5)$_3$ **2**–**Al**. Grey dashed lines are drawn for simplified assignment *via* the corresponding *γ*-C*H* resonances.

Cross-over experiment between $^{Cy}L_2Ga_2$ (1) and $LGaCl_2$ (2–Cl_2). $^{Cy}L_2Ga_2$ **1** (5 mg, 0.00681 mmol) and $LGaCl_2$ **2–Cl_2** (4 mg, 0.00681 mmol) were dissolved in C_6D_6 (0.5 mL) at ambient temperature and heated to 90 °C, while monitoring the reaction progress *via* ^{1}H NMR spectroscopy. Full conversion of $^{Cy}L_2Ga_2$ **1** of was achieved after 2 days.

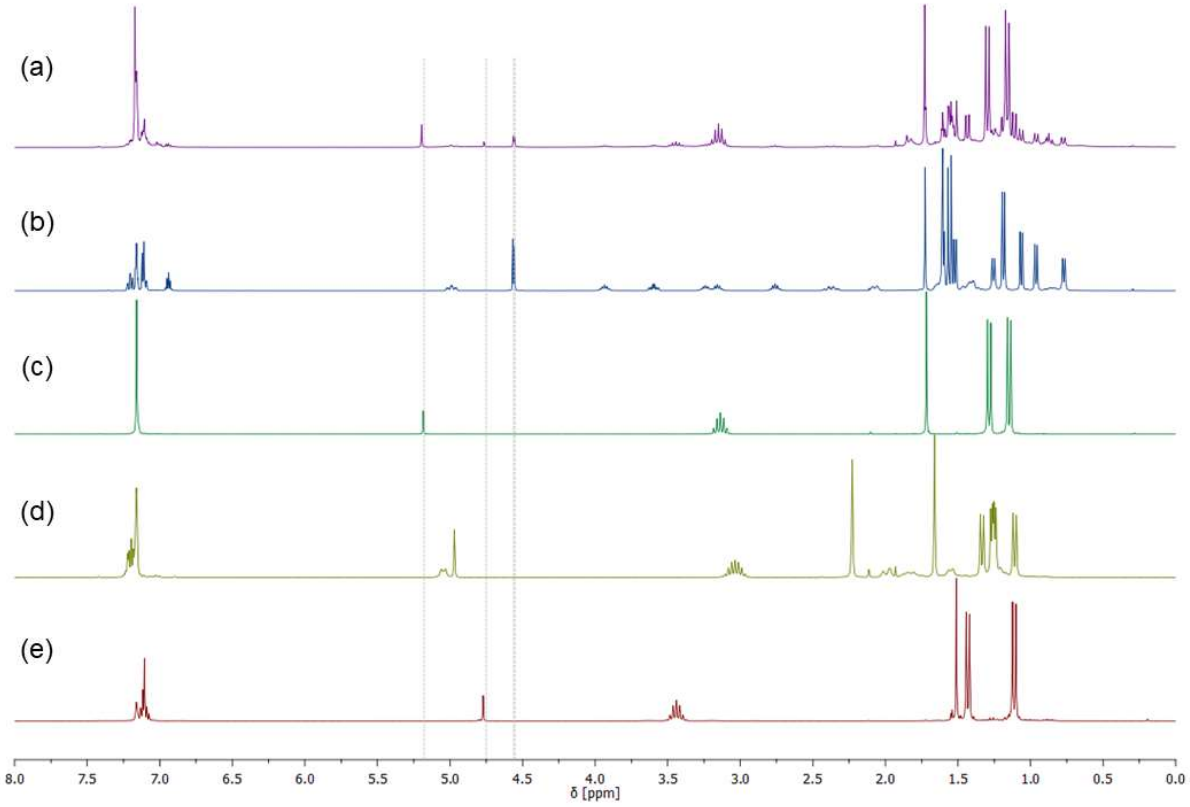


Figure S21. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the cross-over experiment between $^{Cy}L_2Ga_2$ **1** and $LGaCl_2$ **2–Cl_2**, (b) $^{Cy}L_2Ga_2Cl_2$ **1–Cl_2**, (c) LGa **2**, (d) $^{Cy}L_2Ga_2$ **1**, and (e) $LGaCl_2$ **2–Cl_2**. Grey dashed lines are drawn for simplified assignment *via* the corresponding *γ*-C*H* resonances.

Cross-over experiment between $^{Cy}L_2Ga_2$ (1) and $LGaI_2$ (2–I_2). $^{Cy}L_2Ga_2$ **1** (5 mg, 0.00681 mmol) and $LGaI_2$ **2–I_2** (5 mg, 0.00681 mmol) were dissolved in C_6D_6 (0.5 mL) at ambient temperature and heated to 70 °C, while monitoring the reaction progress *via* ^{1}H NMR spectroscopy. Full conversion of $^{Cy}L_2Ga_2$ **1** was achieved after 5 days.

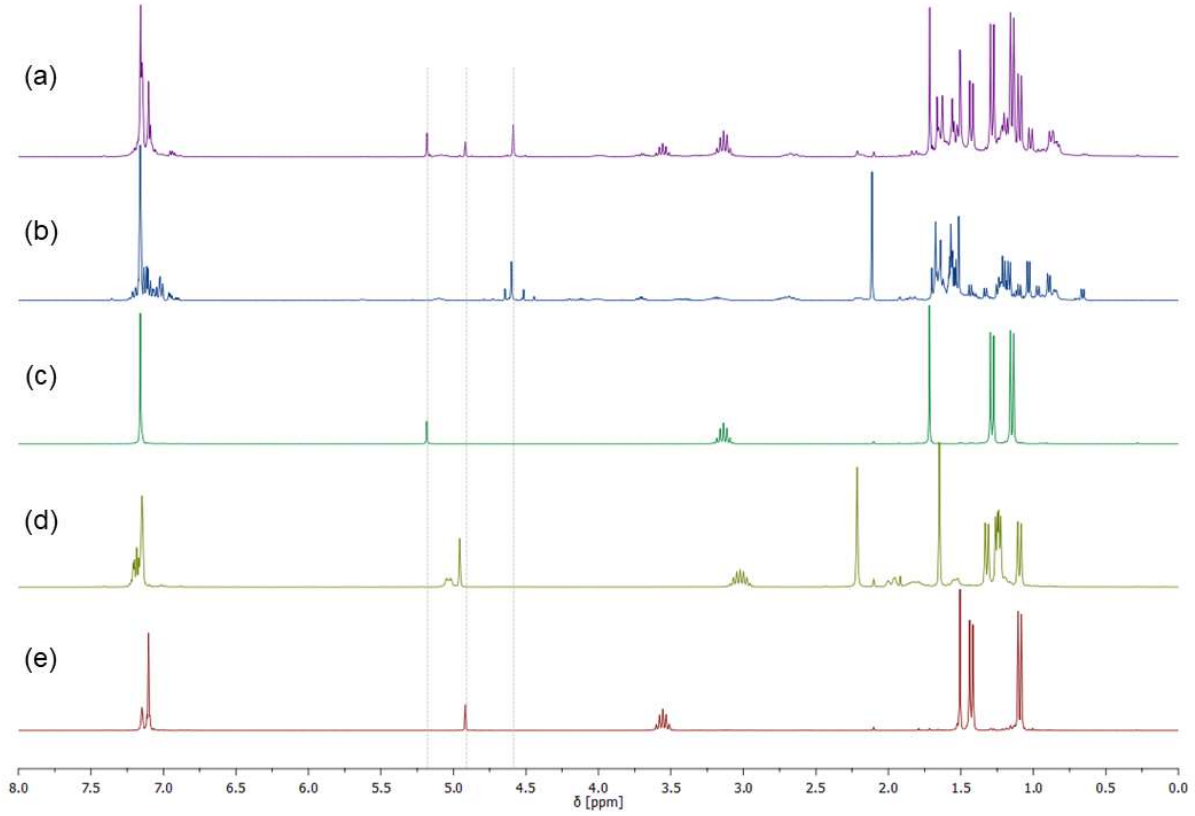


Figure S22. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the cross-over experiment between $^{Cy}L_2Ga_2$ **1** and $LGaI_2$ **2–I_2**, (b) $^{Cy}L_2Ga_2I_2$ **1–I_2**, (c) LGa **2**, (d) $^{Cy}L_2Ga_2$ **1**, and (e) $LGaI_2$ **2–I_2**. Grey dashed lines are drawn for simplified assignment *via* the corresponding *γ*-C*H* resonances.

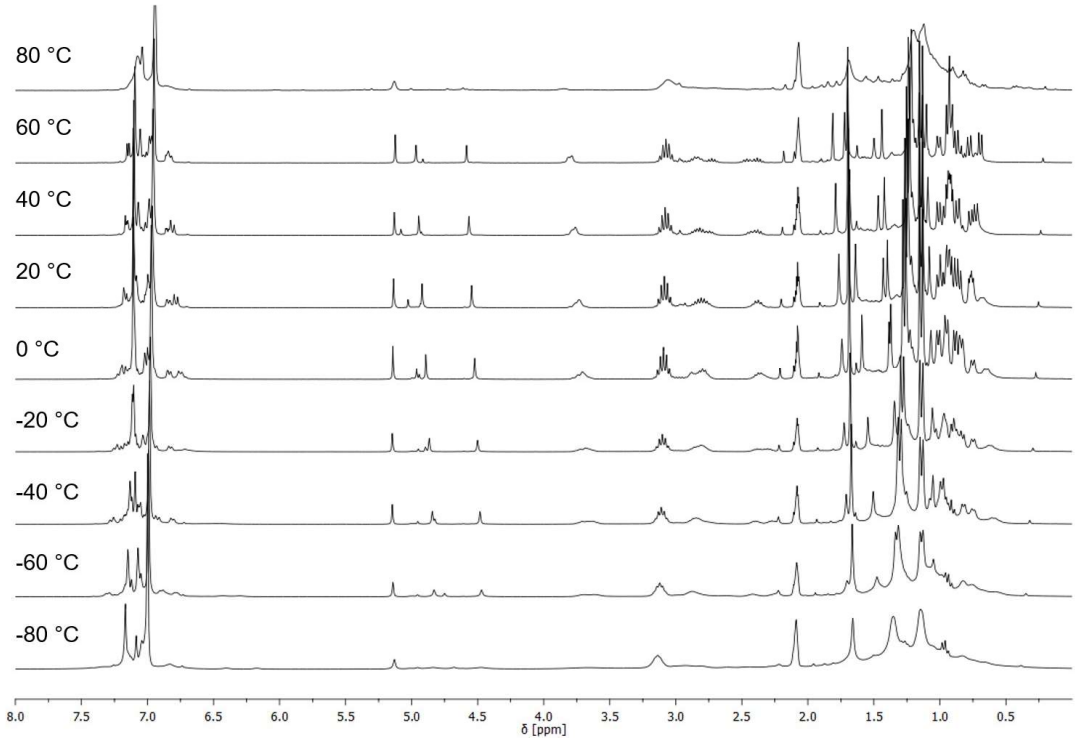


Figure S23. Variable-temperature ^{1}H NMR spectra (300.1 MHz, Tol-d_8) of the reaction mixture containing $^{Cy}L_2Ga_2$ **1** and LGa–B(C_6F_5)$_3$ **2**–**B**.

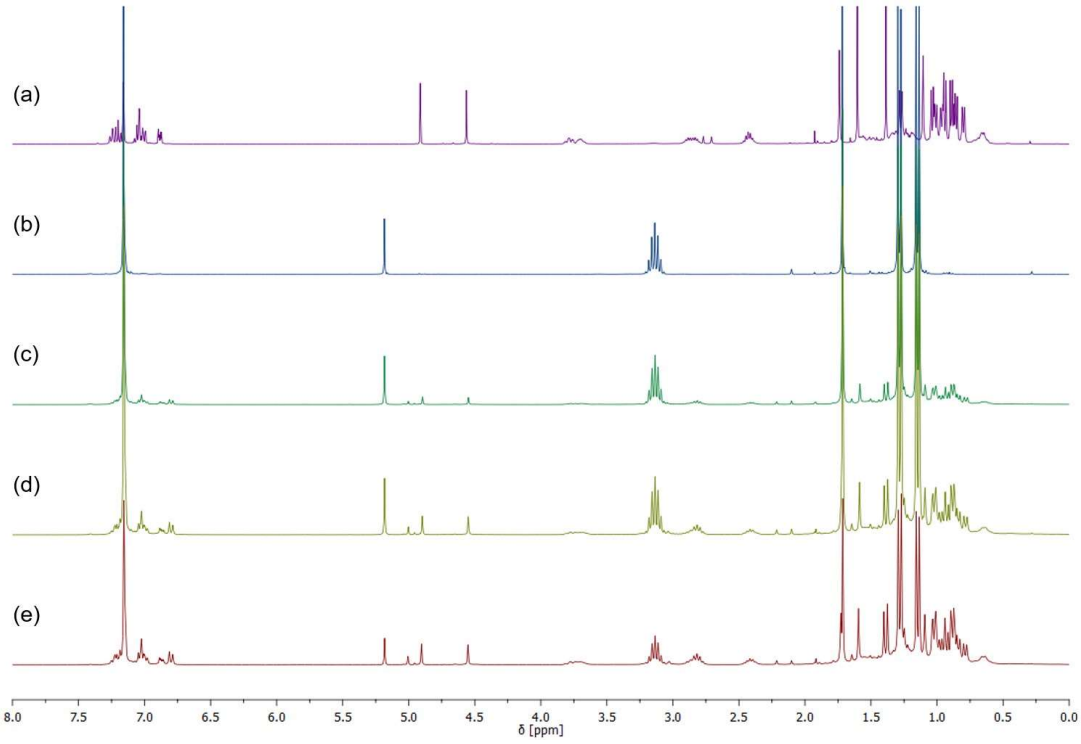


Figure S24. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) $^{Cy}L_2Ga_2$–B(C_6F_5)$_3$ **1**–**B**, (b) LGa **2**, (c) $^{Cy}L_2Ga_2$ **1** and LGa–B(C_6F_5)$_3$ **2**–**B** + 3 eq of LGa **2**, (d) $^{Cy}L_2Ga_2$ **1** and LGa–B(C_6F_5)$_3$ **2**–**B** + 1 eq of LGa **2**, and (e) $^{Cy}L_2Ga_2$ **1** and LGa–B(C_6F_5)$_3$ **2**–**B**.

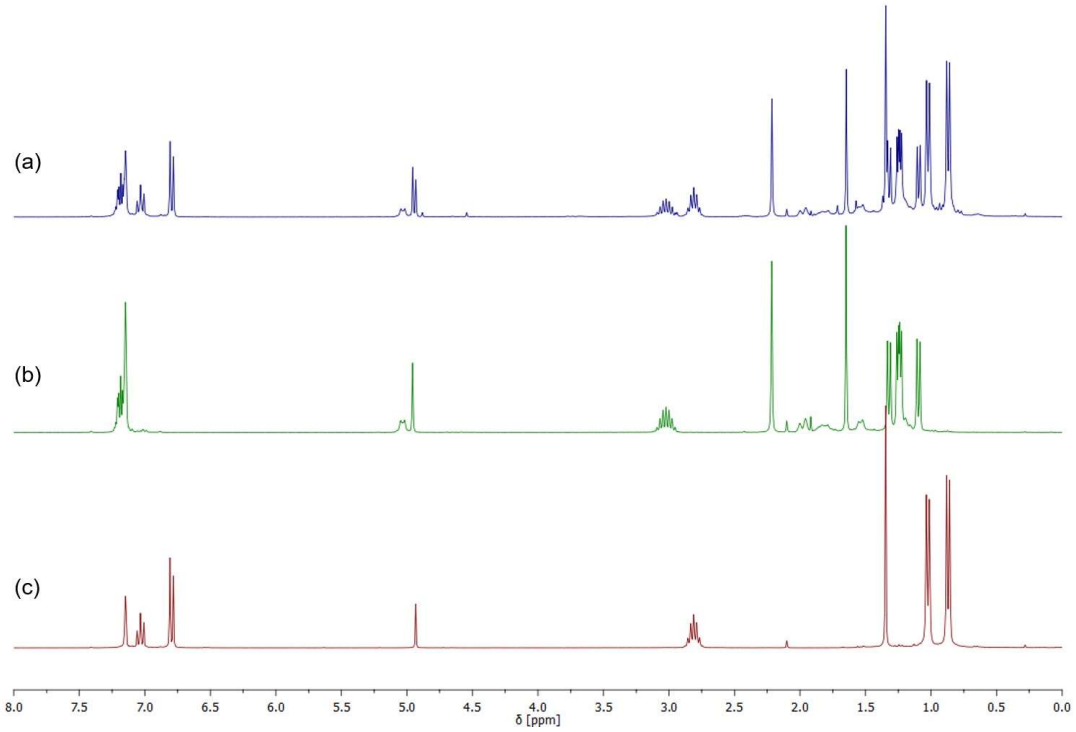


Figure S25. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the reaction mixture containing $^{Cy}L_2Ga_2$ **1** and LAl–B(C_6F_5)$_3$, (b) $^{Cy}L_2Ga_2$ **1**, and (c) LAl–B(C_6F_5)$_3$.

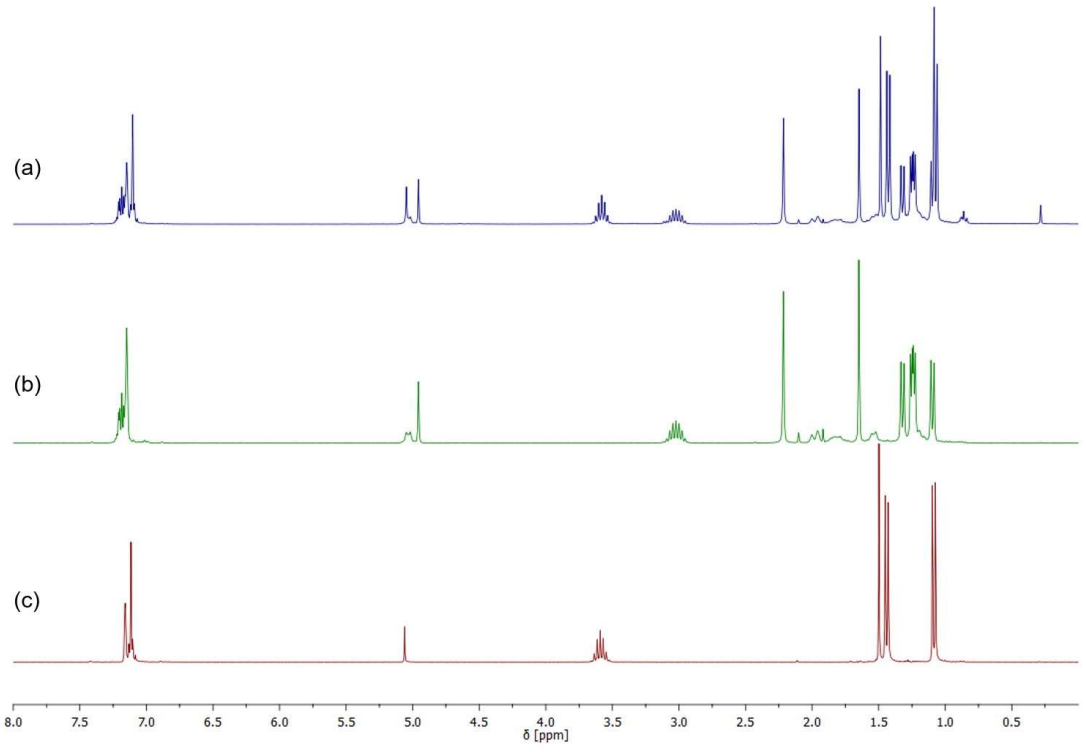


Figure S26. Stacked plot of ^{1}H NMR spectra (300.1 MHz, C_6D_6) of (a) the reaction mixture containing $^{Cy}L_2Ga_2$ **1** and LAlI$_2$, (b) $^{Cy}L_2Ga_2$ **1**, and (c) LAlI$_2$.

II. Single-Crystal X-ray Diffraction

Table S1. Crystallographic details of **1–Al**, **1–Cl_2** and **1–I_2**.

	1–Al	**1–Cl_2**	**1–I_2**
Empirical formula	$C_{70.86}H_{70.86}AlF_{15}Ga_2N_4$	$C_{40}H_{58}Cl_2Ga_2N_4$	$C_{40}H_{58}Ga_2I_2N_4$•0.25 C_6H_{14}
M [g mol^{-1}]	1429.94	805.24	1009.68
Crystal size [mm]	0.337 x 0.230 x 0.154	0.206 x 0.136 x 0.095	0.102 x 0.094 x 0.088
T [K]	100(2)	100(2)	133(2)
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	$P2_1/c$
a [Å]	13.4212(7)	8.8180(9)	9.3956(2)
b [Å]	13.8477(7)	14.0432(15)	19.7798(4)
c [Å]	17.6750(9)	16.3175(18)	24.2518(5)
α [°]	93.742(3)	88.348(4)	90
β [°]	90.471(3)	82.154(4)	91.776(1)
γ [°]	94.259(3)	79.180(4)	90
V [Å^3]	3268.6(3)	1966.1(4)	4504.86(16)
Z	2	2	4
D_{calcd} [g cm^{-3}]	1.453	1.360	1.489
μ(K_α [mm^{-1}])	0.926 (Mo)	1.539 (Mo)	2.598 (Mo)
Transmissions	0.75/0.58	0.75/0.68	0.75/0.58
F(000)	1468	844	2026
Index ranges	-17 ≤ h ≤ 17	-13 ≤ h ≤ 13	-12 ≤ h ≤ 11
	-18 ≤ k ≤ 18	-21 ≤ k ≤ 21	-19 ≤ k ≤ 25
	-23 ≤ l ≤ 23	-25 ≤ l ≤ 25	-30 ≤ l ≤ 31
θ_{max} [°]	28.706	33.619	27.484
Reflections collected	115956	132428	23816
Independent reflections	16571	15414	10228
R_{int}	0.0667	0.0311	0.0311
Refined parameters	947	466	503
R_1 [$I > 2\sigma(I)$]	0.0619	0.0248	0.0447
wR_2 [all data]	0.1539	0.631	0.1213
GooF	1.152	1.026	1.099
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.504/-0.917	0.934/-0.685	2.080/-1.529

Table S2. Crystallographic details of **1–(TEMPO)$_4$**, **2–(TEMPO)$_2$** and **S1**.

	1–(TEMPO)$_4$	**2–(TEMPO)$_2$**	**S1**
Empirical formula	$C_{76}H_{130}Ga_2N_8O_4$	$C_{50}H_{80}GaN_4O_2$	$C_{40}H_{58}Cl_4Ga_2N_4$
M [g mol^{-1}]	1359.32	838.90	876.14
Crystal size [mm]	0.46 x 0.14 x 0.12	0.298 x 0.152 x 0.090	0.189 x 0.094 x 0.081
T [K]	120(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	orthorhombic
Space group	$C2$	P-1	$P2_12_12_1$
a [Å]	20.896(3)	11.361(10)	10.2640(19)
b [Å]	11.169(1)	11.781(11)	18.797(3)
c [Å]	16.882(2)	19.831(17)	22.810(4)
α [°]	90	92.67(3)	90
β [°]	108.583(4)	94.81(3)	90
γ [°]	90	115.886(18)	90
V [Å^3]	3734.6(8)	2369(4)	4400.9(14)
Z	2	2	4
D_{calcd} [g cm^{-3}]	1.209	1.176	1.322
μ(K_α [mm^{-1}])	0.773 (Mo)	0.622 (Mo)	1.498 (Mo)
Transmissions	0.7466; 0.4358	0.75/0.64	0.75/0.64
F(000)	1472	910	1824
Index ranges	$-28 \le h \le 28$	$-17 \le h \le 17$	$-15 \le h \le 15$
	$-15 \le h \le 15$	$-18 \le k \le 18$	$-28 \le k \le 29$
	$-23 \le h \le 23$	$-30 \le l \le 30$	$-35 \le l \le 35$
θ_{max} [°]	28.999	33.192	33.336
Reflections collected	26209	193835	164660
Independent reflections	26209	17973	16960
R_{int}	0.0782	0.0632	0.0719
Refined parameters	462	532	463
R_1 [$I > 2\sigma(I)$]	0.0810	0.0366	0.0312
wR_2 [all data]	0.2049	0.0964	0.0680
GooF	1.029	1.063	1.057
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	4.223/–1.558	1.543/-0.576	0.756/-0.421

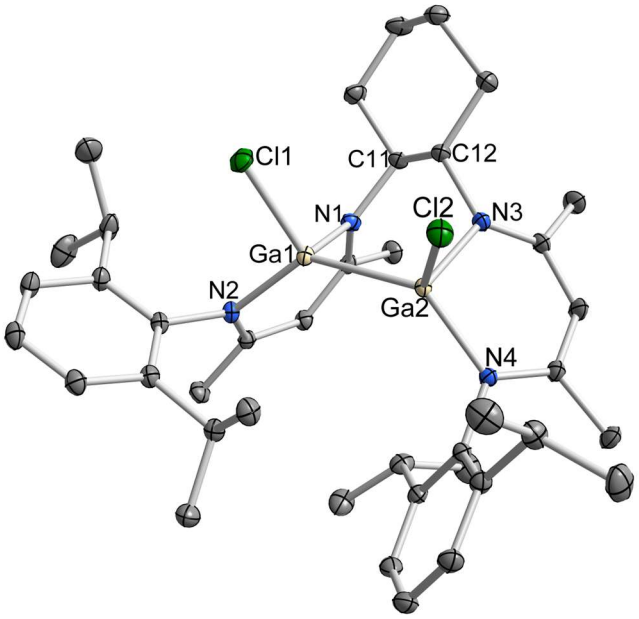


Figure S27. Molecular structure of **1**–$\mathbf{Cl_2}$ in the solid-state. Hydrogen atoms, the minor components of the disordered Cl atom and cyclohexylene group were omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

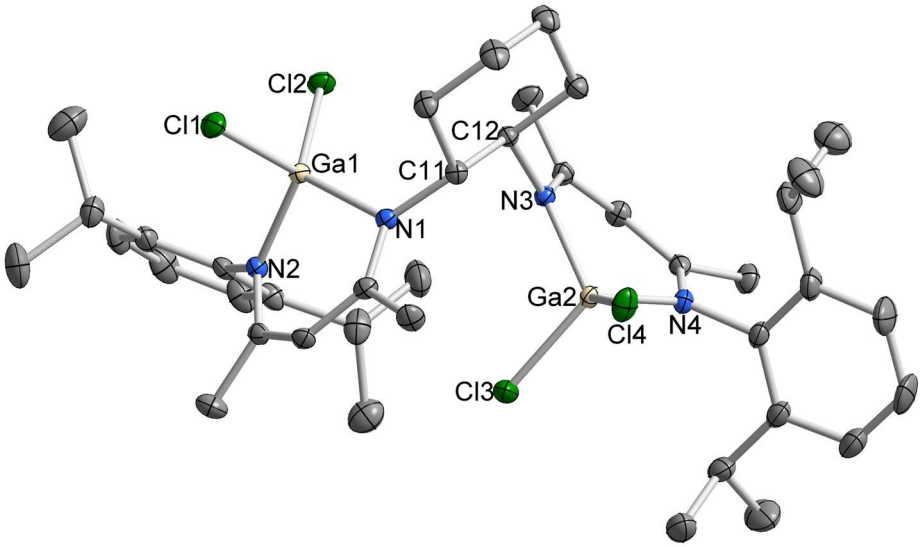


Figure S28. Molecular structure of $^{Cy}L_2Ga_2Cl_4$ (**S1**) in the solid-state. Hydrogen atoms were omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

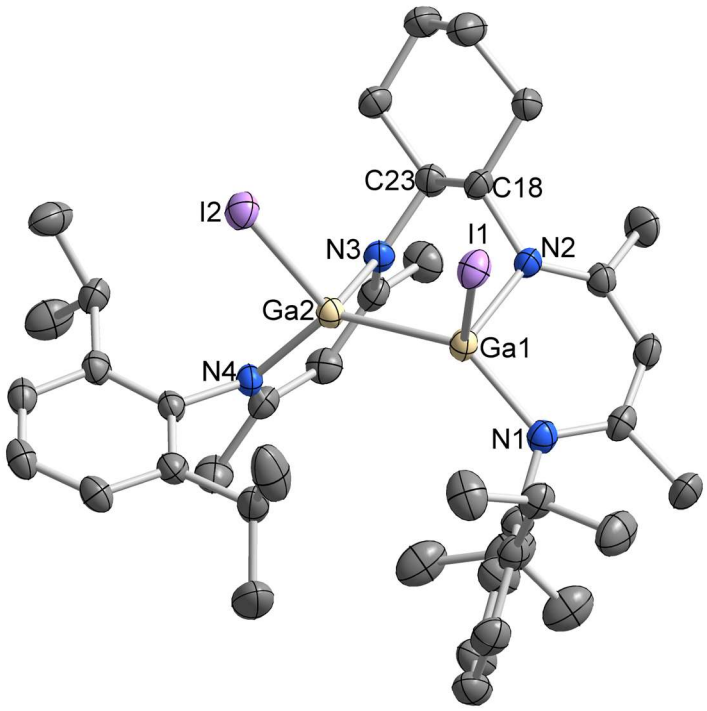


Figure S29. Molecular structure of **1–I_2** in the solid-state. Hydrogen atoms, the minor component of the disordered *i*-Pr group, and the co-crystallized molecule of *n*-hexane were omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

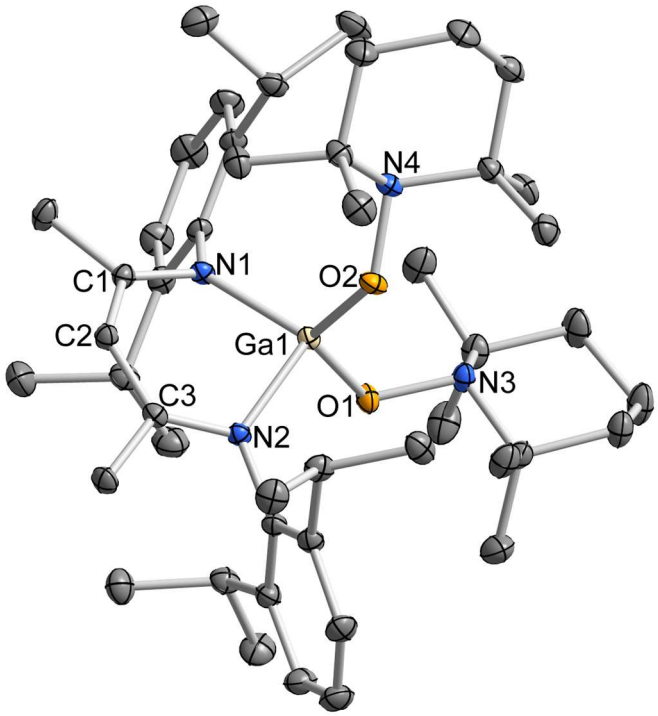


Figure S30. Molecular structure of **2–$(TEMPO)_2$** in the solid-state. Hydrogen atoms and a co-crystallized molecule of benzene were omitted for clarity. Displacement ellipsoids are drawn at 50% probability level.

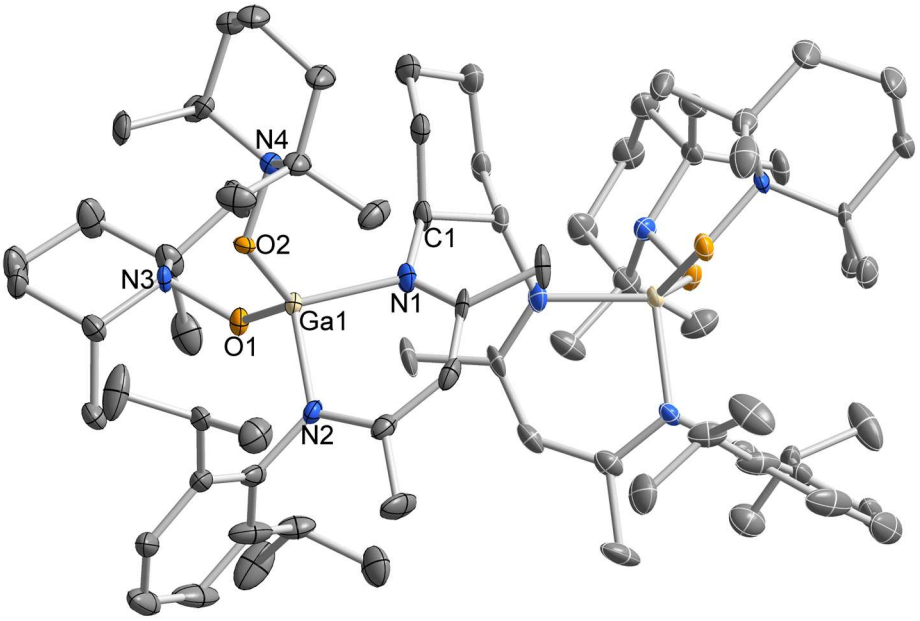


Figure S31. Molecular structure of **1–(TEMPO)$_4$** in the solid-state. Hydrogen atoms and the minor components of the disordered *i*-Pr groups were omitted for clarity. Displacement ellipsoids are drawn at 50% probability level. The symmetry generated part is depicted with pale inner lines.

III. Computational Details

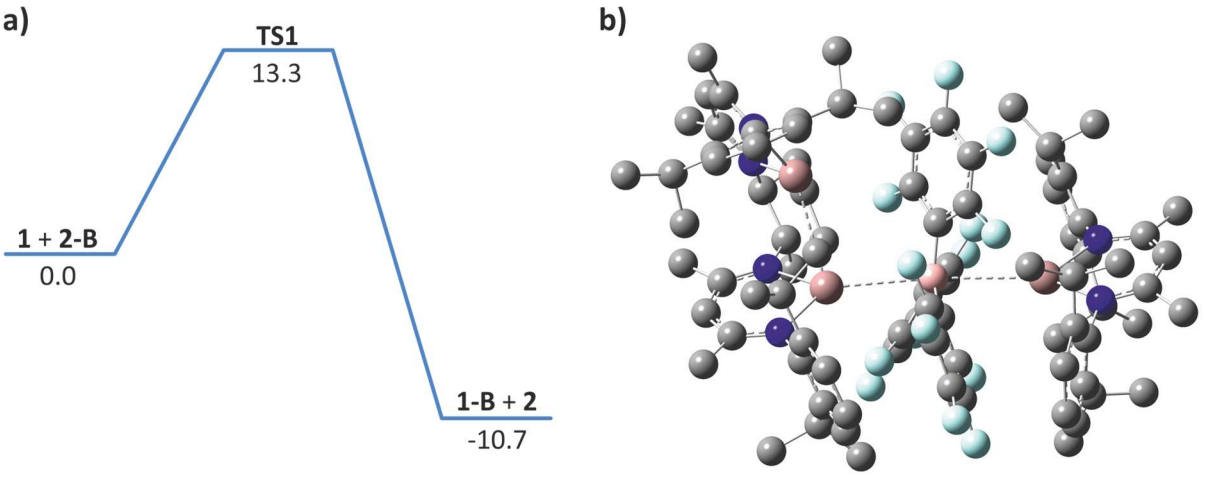
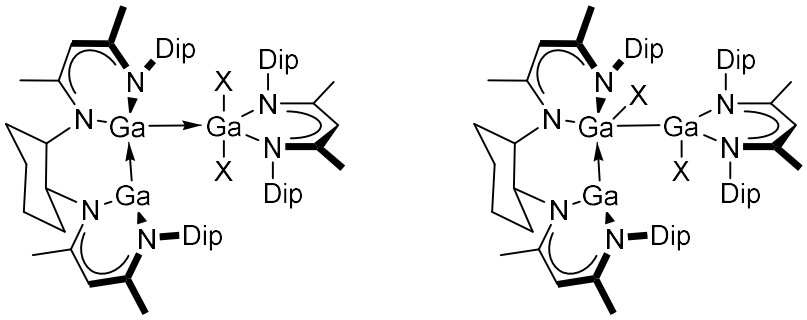


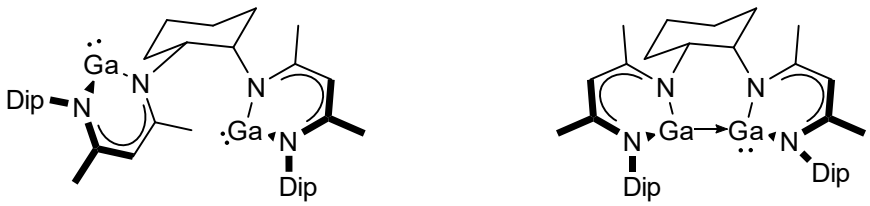
Figure S32. a) Potential-energy surface for the reaction of **1** with **2–B** and b) related transition state structure (hydrogen atoms are omitted for clarity calculated at the BP86(D3-BJ)/def2SVP level of theory.



Int1-X
X = Cl: -0.7 kJ mol^{-1}
X = I : 13.9 kJ mol^{-1}

Int2-X
X = Cl: -39.9 kJ mol^{-1}
X = I : -18.4 kJ mol^{-1}

Figure S33. Local minima on the potential-energy surface *en route* **1** + **2–X$_2$**→ **1–X$_2$** + **2** calculated at the BP86(D3-BJ)/def2SVP level of theory.



1 (0.0 kJ mol^{-1}) **1'** (7.1 kJ mol^{-1})

Figure S34. Bimetallic complex **1** and its isomer **1'** comprising an intramolecular donor-acceptor interaction along with corresponding relative energies.[1]

IV. XYZ coordinates

1

Sum of electronic and thermal Free Energies = -5626.209873

0 1

Ga	2.344403	1.206800	-0.657716
Ga	-2.522113	1.376318	0.543129
N	2.862115	-0.498893	0.417025
N	1.027173	1.729055	0.921459
N	-1.137385	1.792869	-1.001370
N	-2.907798	-0.443544	-0.397220
C	3.801849	-1.320930	-0.283576
C	3.346331	-2.204422	-1.298276
C	4.302129	-2.954760	-2.013376
H	3.963827	-3.644999	-2.802783
C	5.670119	-2.836050	-1.738969
H	6.402180	-3.431411	-2.306961
C	6.106720	-1.949779	-0.742303
H	7.184286	-1.852099	-0.539374
C	5.191101	-1.178476	-0.002864
C	1.865100	-2.333595	-1.638092
H	1.301901	-1.718285	-0.906406
C	1.363287	-3.782799	-1.508067
H	1.545006	-4.185758	-0.490678
H	1.866567	-4.457774	-2.232262
H	0.272340	-3.836513	-1.704101
C	1.573732	-1.761068	-3.037810
H	1.891415	-0.699560	-3.101631
H	0.487727	-1.806534	-3.258095
H	2.114553	-2.324978	-3.827260
C	5.675447	-0.161052	1.027495
H	4.842509	0.017422	1.738778
C	6.883374	-0.646846	1.845344
H	6.689101	-1.633766	2.314369
H	7.119105	0.076835	2.652926
H	7.796644	-0.744982	1.221367
C	5.971739	1.186312	0.337129
H	5.078611	1.563226	-0.207994
H	6.788714	1.075981	-0.406943
H	6.274971	1.957301	1.076685
C	2.438952	-0.875969	1.638439
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C	0.050126	1.708042	3.210401
H	-1.019974	1.724717	2.900191
H	0.337022	2.752781	3.448107
H	0.127037	1.106598	4.134261
C	2.914815	-2.200221	2.201090
H	2.692181	-3.023762	1.491849
H	2.435328	-2.422000	3.172459
H	4.016065	-2.204907	2.335854
C	-1.143325	4.285978	-0.952420
H	-2.001325	4.269381	-0.241187
C	-0.283679	5.536244	-0.721490
H	0.511992	5.580135	-1.499763
H	-0.897584	6.453216	-0.847897
C	0.370924	5.511130	0.667987
H	1.034330	6.391578	0.803804
H	-0.421212	5.590410	1.446993
C	1.160687	4.213375	0.886131
H	1.600206	4.179619	1.905588
H	2.017075	4.156549	0.174838
C	0.277334	2.967494	0.674865
H	-0.585108	3.036855	1.374275
C	-0.328461	2.991948	-0.756748
H	0.533610	3.020541	-1.459348
C	-1.041671	1.158584	-2.179241
C	-1.677625	-0.079737	-2.452711
H	-1.478875	-0.504689	-3.445228
C	-2.486055	-0.862924	-1.605473
C	-2.900789	-2.234586	-2.102712
H	-3.989099	-2.272339	-2.315235
H	-2.712572	-3.005432	-1.328513
H	-2.354226	-2.506665	-3.024861
C	-0.196759	1.733180	-3.303337
H	0.882444	1.726269	-3.028417
H	-0.473958	2.783800	-3.525281
H	-0.315649	1.136820	-4.226133
C	-3.764891	-1.279998	0.382317
C	-3.229731	-1.953289	1.517367
C	-4.095162	-2.764440	2.277960
H	-3.702696	-3.305292	3.151467
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H	-6.109389	-3.533012	2.552354
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H	-7.048000	-2.251391	0.627474
C	-5.150903	-1.353011	0.068104
C	-1.755817	-1.798727	1.888319
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H	-0.930584	-2.350397	-0.074680
H	-1.089350	-3.725853	1.069881
H	0.218965	-2.508049	1.278659
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H	-0.415489	-1.808319	3.598564
H	-1.600607	-3.142613	3.630172
H	-2.125883	-1.472737	4.032882
C	-5.745632	-0.482583	-1.036554
H	-4.935315	-0.246089	-1.756162
C	-6.214708	0.860387	-0.438048
H	-5.381172	1.379432	0.082836
H	-7.021247	0.698250	0.307877
H	-6.602488	1.536832	-1.228897
C	-6.874167	-1.170020	-1.822013
H	-6.554117	-2.154936	-2.221536
H	-7.189497	-0.538359	-2.678117
H	-7.774804	-1.338965	-1.194880
H	-1.584083	4.287152	-1.971830

2–Cl_2

Sum of electronic and thermal Free Energies = -4083.275153

0 1

Ga	-0.005821	-0.627218	-0.551573
N	-1.471430	-0.107161	0.623919
N	1.466797	-0.232771	0.655087
C	-1.287651	-0.157374	1.958167
C	-0.025408	-0.349764	2.571712

H	-0.042054	-0.428560	3.666305
C	1.259617	-0.292844	1.985971
C	-2.487088	0.012432	2.860863
H	-3.109206	0.871195	2.540682
H	-2.178292	0.154098	3.912236
H	-3.139088	-0.882877	2.800156
C	2.462366	-0.275217	2.899270
H	3.103403	-1.158004	2.697724
H	2.160910	-0.281838	3.962169
H	3.095832	0.613272	2.706488
C	-2.758110	0.238650	0.074877
C	-3.767247	-0.750460	-0.067940
C	-5.021527	-0.346599	-0.570109
H	-5.819581	-1.097140	-0.683176
C	-5.265190	0.981604	-0.936600
H	-6.253230	1.275980	-1.323873
C	-4.240479	1.933000	-0.832375
H	-4.430524	2.968577	-1.149714
C	-2.969671	1.584732	-0.336682
C	-3.531737	-2.224325	0.248847
H	-2.511777	-2.326521	0.672418
C	-4.539935	-2.775973	1.275588
H	-4.550700	-2.184112	2.214354
H	-4.290785	-3.825049	1.538001
H	-5.574996	-2.771810	0.873586
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H	-4.575021	-3.025878	-1.515572
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H	-2.828429	-2.687741	-1.782264
C	-1.856749	2.625344	-0.236715
H	-0.900932	2.085227	-0.395770
C	-1.790283	3.269699	1.162008
H	-2.749598	3.767040	1.418974
H	-0.988412	4.036795	1.197599
H	-1.567789	2.524466	1.950923
C	-1.945715	3.693151	-1.336968
H	-1.998137	3.225711	-2.340507
H	-1.047913	4.341998	-1.311087
H	-2.828731	4.354575	-1.210965
C	2.757802	0.134425	0.134557
C	3.035025	1.517459	-0.045774
C	4.304607	1.882107	-0.532992
H	4.542605	2.948321	-0.672141
C	5.264951	0.911703	-0.850858
H	6.252499	1.216498	-1.231264
C	4.959754	-0.446508	-0.697207
H	5.710284	-1.206533	-0.965881
C	3.705669	-0.864166	-0.207471
C	2.004251	2.593640	0.284346
H	1.036553	2.081681	0.461892
C	1.800234	3.565736	-0.889885
H	1.021889	4.314834	-0.637205
H	1.476175	3.020321	-1.797840
H	2.728143	4.126268	-1.128632
C	2.367814	3.348464	1.578344
H	3.340234	3.875150	1.474774
H	2.447142	2.663547	2.446451
H	1.594534	4.107657	1.819407
C	3.396028	-2.351662	-0.088793
H	2.385706	-2.453307	0.356824
C	3.340852	-3.002579	-1.484987
H	2.610585	-2.484714	-2.137181
H	3.027928	-4.064144	-1.407948
H	4.333582	-2.970056	-1.982504
C	4.394535	-3.083243	0.828041
H	5.423775	-3.064983	0.411328
H	4.103163	-4.147266	0.949021
H	4.439026	-2.625567	1.838453
Cl	0.117312	0.521062	-2.400719
Cl	-0.111606	-2.804418	-0.861382

2–I_2

Sum of electronic and thermal Free Energies = -3758.750100

0 1

Ga	-0.016088	-0.444663	-0.216154
N	-1.491686	0.199539	0.910817
N	1.459257	0.005803	0.989507
C	-1.320190	0.130728	2.246665
C	-0.075123	-0.137906	2.870058
H	-0.114931	-0.251977	3.961042
C	1.223965	-0.097830	2.314035
C	-2.512649	0.361142	3.145379
H	-3.096222	1.243123	2.816342
H	-2.198909	0.499041	4.195790
H	-3.202349	-0.506013	3.093094
C	2.406529	-0.169001	3.251417
H	2.940680	-1.130133	3.095531
H	2.090028	-0.104412	4.308096
H	3.141413	0.631529	3.038490
C	-2.755899	0.621141	0.356712
C	-3.832780	-0.297783	0.225929
C	-5.061810	0.183569	-0.270367
H	-5.906382	-0.515761	-0.372219
C	-5.224311	1.520893	-0.645131
H	-6.193660	1.875521	-1.029000
C	-4.140300	2.403358	-0.548900
H	-4.265112	3.448632	-0.866193
C	-2.892207	1.977201	-0.056257
C	-3.706288	-1.783350	0.543281
H	-2.694279	-1.962642	0.961031
C	-4.743342	-2.264794	1.576183
H	-4.705735	-1.676419	2.516264
H	-4.564325	-3.329082	1.834271
H	-5.778835	-2.188327	1.182720
C	-3.818282	-2.608128	-0.755153
H	-4.831744	-2.513489	-1.199805
H	-3.628632	-3.682511	-0.553401
H	-3.079347	-2.273237	-1.509224
C	-1.733350	2.962590	0.052669
H	-0.801063	2.378180	-0.092164
C	-1.660960	3.601215	1.453884
H	-2.609422	4.123032	1.701818
H	-0.840354	4.346987	1.500581
H	-1.467283	2.847211	2.242193
C	-1.762631	4.034432	-1.047147
H	-1.843561	3.572052	-2.051503
H	-0.830851	4.632310	-1.022919
H	-2.607758	4.743112	-0.919161
C	2.756063	0.406726	0.506458
C	3.016757	1.800390	0.382638

C	4.289290	2.204881	-0.062957
H	4.511027	3.278921	-0.156815
C	5.274405	1.265092	-0.394991
H	6.263714	1.600998	-0.743203
C	4.990429	-0.101599	-0.293922
H	5.760005	-0.839377	-0.570287
C	3.733891	-0.558281	0.153006
C	1.966544	2.844589	0.746542
H	0.985572	2.327395	0.761627
C	1.880307	3.968612	-0.297760
H	1.069085	4.676696	-0.032739
H	1.668594	3.558154	-1.305595
H	2.818240	4.559569	-0.352105
C	2.206306	3.415246	2.158862
H	3.201423	3.904245	2.225244
H	2.165411	2.625535	2.934741
H	1.435703	4.172752	2.412317
C	3.458163	-2.053567	0.208371
H	2.455386	-2.195691	0.660380
C	3.403062	-2.635891	-1.217538
H	2.660913	-2.097620	-1.840928
H	3.110021	-3.705597	-1.193484
H	4.391198	-2.556542	-1.718917
C	4.474687	-2.809641	1.083271
H	5.498876	-2.768317	0.655928
H	4.191950	-3.879589	1.165956
H	4.526585	-2.389314	2.109313
I	0.229351	0.716040	-2.439817
I	-0.190502	-3.003512	-0.287655

2

Sum of electronic and thermal Free Energies = -3162.925059

0 1

Ga	-0.003033	-0.203043	-1.018400
N	-1.448068	-0.135590	0.528499
N	1.431285	-0.216790	0.531796
C	-1.285813	-0.246372	1.856830
C	-0.018902	-0.361962	2.474128
H	-0.022559	-0.452463	3.568532
C	1.252006	-0.304136	1.861672
C	-2.506498	-0.250102	2.757485
H	-3.193069	0.582083	2.503568
H	-2.220483	-0.174035	3.822999
H	-3.090156	-1.184032	2.618124
C	2.470997	-0.318315	2.761406
H	3.164185	-1.134867	2.473001
H	2.190348	-0.440238	3.823946
H	3.047049	0.623666	2.649439
C	-2.753827	0.071421	-0.011537
C	-3.623213	-1.033428	-0.222161
C	-4.892979	-0.787285	-0.778693
H	-5.583842	-1.628452	-0.943872
C	-5.287194	0.509951	-1.136265
H	-6.286018	0.683817	-1.566388
C	-4.399274	1.582493	-0.969233
H	-4.706497	2.591871	-1.281460
C	-3.117596	1.386901	-0.418654
C	-3.153122	-2.457062	0.064388
H	-2.327852	-2.394946	0.803518
C	-4.247884	-3.354473	0.664088
H	-4.702243	-2.897222	1.567702
H	-3.826611	-4.339891	0.952069
H	-5.066588	-3.550629	-0.059910
C	-2.557219	-3.075842	-1.217632
H	-3.327903	-3.151756	-2.013500
H	-2.157518	-4.093329	-1.022064
H	-1.729682	-2.450561	-1.616863
C	-2.136263	2.546110	-0.253397
H	-1.116353	2.115588	-0.376575
C	-2.190954	3.148694	1.164328
H	-3.205778	3.542115	1.386444
H	-1.468865	3.986603	1.262194
H	-1.937397	2.397996	1.937885
C	-2.294945	3.634134	-1.325039
H	-2.277349	3.201411	-2.345942
H	-1.466730	4.368518	-1.249321
H	-3.242967	4.200840	-1.207906
C	2.752908	-0.049481	0.010004
C	3.255008	1.267612	-0.182625
C	4.516767	1.421628	-0.788617
H	4.918959	2.434122	-0.950550
C	5.266752	0.307561	-1.192165
H	6.250588	0.447163	-1.666976
C	4.760981	-0.984455	-0.990248
H	5.354830	-1.855455	-1.309076
C	3.504406	-1.188599	-0.387437
C	2.426496	2.486664	0.216296
H	1.622618	2.132654	0.894383
C	1.738421	3.099792	-1.020004
H	1.087820	3.952611	-0.733031
H	1.109442	2.346936	-1.543059
H	2.488448	3.466976	-1.752216
C	3.245166	3.540373	0.982248
H	4.026644	4.003646	0.343717
H	3.752134	3.098384	1.864850
H	2.586696	4.359475	1.339318
C	2.946216	-2.596667	-0.202392
H	2.103955	-2.522749	0.516882
C	2.365336	-3.125480	-1.529537
H	1.578306	-2.445237	-1.920384
H	1.916252	-4.132342	-1.395932
H	3.155692	-3.199280	-2.306410
C	3.977617	-3.573711	0.388609
H	4.818610	-3.762255	-0.311563
H	3.505068	-4.554859	0.603038
H	4.409961	-3.186662	1.334630

2–Al(C6F5)3 (2-Al)

Sum of electronic and thermal Free Energies = -5587.176296

0 1

Ga	-0.026837	0.834865	0.826287
Al	0.082340	-1.028522	-0.839090
F	-2.184666	-3.427185	-0.901134
F	-4.790886	-3.296788	-1.644578
F	-5.797683	-0.984243	-2.728964
F	-4.187903	1.205077	-3.051347
F	-1.597770	1.128658	-2.161405
F	-0.085673	-0.498489	-4.050500
F	1.863030	0.162565	-5.813186
F	4.467127	0.351929	-4.979490

F	5.122127	-0.151960	-2.368812
F	3.159457	-0.757146	-0.570855
F	0.918242	-3.933685	-1.484171
F	1.688485	-6.036594	0.083470
F	1.801053	-5.736775	2.805024
F	1.140603	-3.332931	3.959930
F	0.361117	-1.251692	2.432663
N	-1.519525	1.552355	1.879917
N	1.333245	1.929809	1.731580
C	-1.380886	2.260869	3.021251
C	-0.144733	2.778382	3.458451
H	-0.175531	3.382738	4.374405
C	1.105234	2.716354	2.802084
C	-2.604606	2.521680	3.868035
H	-3.473579	2.822395	3.251505
H	-2.408208	3.295458	4.632395
H	-2.896221	1.584144	4.387238
C	2.219295	3.592455	3.324072
H	2.987189	2.989741	3.849127
H	1.829151	4.349774	4.028179
H	2.740749	4.099331	2.487487
C	-2.829033	1.323234	1.322862
C	-3.318744	2.272471	0.378860
C	-4.594569	2.052084	-0.172208
H	-4.999703	2.766145	-0.902214
C	-5.338101	0.908649	0.156240
H	-6.317407	0.737287	-0.316080
C	-4.819353	-0.031162	1.054297
H	-5.400994	-0.935935	1.290585
C	-3.564348	0.161692	1.667038
C	-2.484341	3.489255	-0.025306
H	-1.420292	3.163230	-0.009591
C	-2.789072	3.994535	-1.444332
H	-3.783281	4.486069	-1.498938
H	-2.766813	3.174648	-2.184834
H	-2.038712	4.755901	-1.742431
C	-2.612704	4.649082	0.984479
H	-3.673489	4.961580	1.086013
H	-2.029988	5.527903	0.637875
H	-2.235391	4.381220	1.989120
C	-3.040301	-0.861261	2.669640
H	-2.084966	-0.472717	3.078325
C	-2.726369	-2.201446	1.984296
H	-3.634942	-2.654519	1.535419
H	-2.305633	-2.927733	2.709896
H	-1.992047	-2.075619	1.169552
C	-4.016082	-1.059384	3.846163
H	-4.274263	-0.098625	4.337471
H	-3.572410	-1.730180	4.610866
H	-4.966506	-1.523384	3.508838
C	2.617598	1.929497	1.084413
C	2.719806	2.533508	-0.201303
C	3.981164	2.548914	-0.825499
H	4.089347	3.009640	-1.817684
C	5.101617	1.976029	-0.207416
H	6.078257	1.999655	-0.713003
C	4.966025	1.334260	1.028678
H	5.838956	0.838122	1.480525
C	3.724705	1.278397	1.690750
C	1.500880	3.154721	-0.881481
H	0.626491	2.488317	-0.664651
C	1.162042	4.540170	-0.299409
H	0.928549	4.489386	0.782371
H	0.280866	4.975998	-0.813833
H	2.016676	5.235694	-0.434696
C	1.601690	3.196810	-2.411504
H	2.345924	3.944692	-2.757068
H	0.622322	3.477762	-2.847951
H	1.885175	2.208576	-2.822104
C	3.578551	0.439280	2.957740
H	2.563762	0.615321	3.369299
C	3.665704	-1.060709	2.604721
H	2.992943	-1.316873	1.766235
H	3.390640	-1.686003	3.478862
H	4.694919	-1.335357	2.291787
C	4.608229	0.797559	4.045227
H	5.642650	0.566072	3.715676
H	4.417900	0.210565	4.967412
H	4.582475	1.874077	4.314235
C	-1.797900	-1.148997	-1.505170
C	-2.642755	-2.260964	-1.411287
C	-3.992641	-2.229495	-1.804778
C	-4.510048	-1.048134	-2.363175
C	-3.684778	0.079981	-2.514244
C	-2.363056	0.004409	-2.058777
C	1.459730	-0.625051	-2.230506
C	1.177392	-0.395215	-3.585326
C	2.168334	-0.057707	-4.526043
C	3.506207	0.039784	-4.100938
C	3.839153	-0.214391	-2.757867
C	2.807025	-0.527195	-1.859484
C	0.610122	-2.521242	0.399499
C	0.960020	-3.763834	-0.143287
C	1.359202	-4.862222	0.637381
C	1.415638	-4.711628	2.036538
C	1.067172	-3.483610	2.627142
C	0.677050	-2.428138	1.790706

2–B(C_6F_5)$_3$ (2-B)

Sum of electronic and thermal Free Energies = -5369.593090

0 1

Ga	-0.041348	0.865370	0.446443
F	-1.418210	0.513721	-2.176229
F	0.282672	-0.269614	2.528943
F	-5.385955	-2.055271	-2.147984
F	1.077290	-3.864985	-0.525018
F	-1.688779	-3.510299	0.382767
F	2.944974	-0.720710	-0.028720
F	-3.926511	0.053874	-3.113660
F	1.215907	-1.782061	4.536892
F	2.037923	-5.360034	1.511573
F	-4.224059	-3.816720	-0.375856
F	-0.306371	-1.783675	-3.367743
N	1.255019	2.286591	0.904225
F	4.881239	-0.895366	-1.883092
N	-1.591625	1.827331	1.207550
F	2.113319	-4.349167	4.059807
F	1.616655	-1.866978	-5.193149
F	4.242827	-1.425208	-4.507641
C	2.549354	2.178184	0.288417

C	-3.622866	0.423468	1.483421
C	0.684833	-1.556785	2.217778
C	-2.192390	-2.564740	-0.440607
C	-2.908846	1.425064	0.778309
C	3.600327	-1.067661	-2.242388
B	0.099704	-1.118926	-0.378145
C	0.626051	-2.005690	0.895095
C	3.598924	1.555676	2.568188
H	2.578305	1.820413	2.912202
C	-1.478569	2.862717	2.070288
C	1.377065	2.602211	-1.953441
H	0.554566	1.972545	-1.530508
C	0.969053	3.366707	1.658701
C	-2.083377	-0.587927	-1.730251
C	2.629649	2.326562	-1.124149
C	2.565053	-0.981417	-1.300295
C	-1.428670	-1.451490	-0.834236
C	-4.885421	0.042648	0.984222
H	-5.449625	-0.751727	1.497530
C	-3.110113	-0.175768	2.791298
H	-2.170884	0.352181	3.054230
C	3.896276	2.224975	-1.728837
H	3.987662	2.332801	-2.818967
C	1.167899	-2.303276	3.301251
C	-0.275011	3.555829	2.297056
H	-0.340045	4.418695	2.972407
C	4.611859	2.354012	3.411346
H	4.542865	3.447317	3.233594
H	5.655187	2.050977	3.184184
H	4.445260	2.170967	4.492924
C	-3.523379	-2.773892	-0.848513
C	-5.443791	0.672839	-0.134374
H	-6.431694	0.361081	-0.505876
C	3.773468	0.043269	2.819639
H	3.066626	-0.552770	2.216325
H	3.605287	-0.195911	3.889843
H	4.797207	-0.288712	2.547234
C	-3.376562	-0.786223	-2.220473
C	0.937094	-1.492064	-2.936292
C	1.636807	-3.603163	3.056277
C	-4.118464	-1.882118	-1.750269
C	1.104666	-3.316352	0.702785
C	5.042954	1.973378	-0.962657
H	6.023551	1.890816	-1.454906
C	-3.451111	2.072953	-0.369695
C	-4.738351	1.691580	-0.791703
H	-5.184282	2.175219	-1.672038
C	-2.673241	3.165968	-1.106126
H	-1.594742	2.928950	-0.984131
C	1.936716	-1.566012	-3.925903
C	-4.122124	0.052544	3.933898
H	-4.428593	1.115540	4.013485
H	-3.685871	-0.256811	4.906343
H	-5.044667	-0.545145	3.779574
C	-2.702187	3.321562	2.831037
H	-3.607083	3.338625	2.194744
H	-2.544888	4.321343	3.275049
H	-2.906614	2.606047	3.655139
C	2.005656	4.454283	1.823639
H	2.514617	4.659895	0.861294
H	2.797019	4.150500	2.537303
H	1.539173	5.382971	2.199936
C	-2.899973	4.559165	-0.482026
H	-2.539340	4.620500	0.561612
H	-3.979213	4.820829	-0.489263
H	-2.357382	5.333151	-1.064040
C	1.499069	2.175562	-3.421198
H	1.862875	1.134007	-3.508796
H	2.190884	2.834907	-3.986421
H	0.508562	2.231728	-3.915014
C	4.935199	1.789099	0.420853
H	5.836180	1.549402	1.006473
C	1.601456	-4.115791	1.745524
C	-2.767053	-1.668951	2.670828
H	-1.940257	-1.844113	1.962989
H	-3.634996	-2.263418	2.316438
H	-2.455768	-2.076226	3.655109
C	3.692172	1.874703	1.076251
C	3.279549	-1.348027	-3.580124
C	1.198720	-1.168444	-1.587854
C	-2.968937	3.217427	-2.613850
H	-2.867369	2.223733	-3.085280
H	-2.265042	3.916093	-3.111844
H	-3.992622	3.595717	-2.818588
C	0.926477	4.071372	-1.836864
H	0.679189	4.350184	-0.793993
H	0.024436	4.252827	-2.456380
H	1.729292	4.750203	-2.193221

1-B

Sum of electronic and thermal Free Energies = -7832.881965

0 1

Ga	-0.400984	-0.006973	-0.842613
Ga	1.988475	-0.910210	-0.323041
B	-1.819602	-0.240274	0.836801
F	-2.094366	0.940070	3.657686
F	-0.611198	0.295183	5.766992
F	1.253122	-1.710226	5.635576
F	1.597477	-3.072223	3.237591
F	0.158724	-2.417399	1.109864
F	-2.937435	-0.859139	-1.861144
F	-4.681213	-2.783000	-2.473584
F	-5.636926	-4.482388	-0.522225
F	-4.791773	-4.155886	2.077126
F	-3.091945	-2.212685	2.727616
F	-4.736578	0.664909	0.368794
F	-5.632054	3.155580	0.775524
F	-3.929216	5.154722	1.573491
F	-1.271043	4.574719	2.028743
F	-0.345034	2.082686	1.574155
N	-0.044262	-1.376320	-2.319661
N	-0.267112	1.562241	-2.108820
N	2.191305	-2.822133	-1.060345
N	3.917012	-0.727171	0.162021
C	0.573852	-1.081982	-3.465770
C	0.779895	0.251789	-3.893552
H	1.286713	0.362426	-4.860701
C	0.334157	1.458784	-3.313434
C	1.161185	-2.151079	-4.367872
H	0.521777	-3.047840	-4.446958

H	2.147492	-2.469118	-3.967110
H	1.328727	-1.751610	-5.385104
C	0.551318	2.710402	-4.138516
H	0.836576	2.453160	-5.174629
H	1.357377	3.329467	-3.696874
H	-0.354414	3.345624	-4.156208
C	3.397638	-3.410230	-1.191607
C	4.588515	-2.932948	-0.591900
H	5.457336	-3.597992	-0.683333
C	4.840238	-1.710556	0.052473
C	3.571004	-4.655413	-2.048054
H	3.264047	-4.445009	-3.094842
H	2.961594	-5.512821	-1.704588
H	4.630174	-4.968490	-2.063802
C	6.238762	-1.477679	0.585577
H	6.805149	-0.777599	-0.062524
H	6.798366	-2.429631	0.642995
H	6.205349	-1.010132	1.588809
C	-0.254275	-2.734274	-1.811595
H	-0.705708	-2.578447	-0.812006
C	1.027684	-3.580849	-1.579142
H	1.312549	-4.007394	-2.563496
C	0.632010	-4.775254	-0.672219
H	1.522388	-5.389618	-0.431232
H	0.263532	-4.382404	0.294073
C	-0.447561	-5.637014	-1.345189
H	-0.731784	-6.474150	-0.673312
H	-0.026338	-6.102758	-2.266188
C	-1.681781	-4.801839	-1.715380
H	-2.168085	-4.439840	-0.783152
H	-2.437492	-5.420166	-2.243361
C	-1.293164	-3.587954	-2.571557
H	-2.173968	-2.962369	-2.806509
H	-0.886742	-3.939912	-3.544636
C	-0.764026	2.862782	-1.727258
C	0.130212	3.819714	-1.177165
C	-0.381035	5.085706	-0.825782
H	0.292733	5.830956	-0.376129
C	-1.723929	5.409007	-1.037953
H	-2.109026	6.397797	-0.745915
C	-2.586946	4.461282	-1.606876
H	-3.641563	4.726308	-1.764203
C	-2.137286	3.175860	-1.963348
C	1.622491	3.548245	-1.000717
H	1.856006	2.596730	-1.517809
C	2.031396	3.367141	0.470615
H	1.684853	2.397539	0.866730
H	1.604116	4.165318	1.111746
H	3.132150	3.399298	0.561519
C	2.484751	4.655265	-1.642317
H	2.191994	4.869320	-2.691240
H	3.554402	4.357951	-1.631263
H	2.406475	5.608281	-1.078538
C	-3.098474	2.159378	-2.581720
H	-2.952816	1.217101	-2.019145
C	-2.806893	1.852124	-4.067754
H	-3.584138	1.166334	-4.463687
H	-1.832360	1.356537	-4.227983
H	-2.836093	2.780705	-4.676995
C	-4.581369	2.542649	-2.455195
H	-4.834971	3.411032	-3.100304
H	-4.882634	2.788941	-1.422101
H	-5.210980	1.692785	-2.787239
C	4.397383	0.576733	0.534881
C	4.175197	1.080233	1.843084
C	4.810048	2.289034	2.196472
H	4.674897	2.692431	3.209652
C	5.589003	2.999625	1.275109
H	6.073186	3.941760	1.575327
C	5.718971	2.532771	-0.041264
H	6.297933	3.120368	-0.768303
C	5.128587	1.318551	-0.438492
C	3.285883	0.341451	2.841478
H	2.452998	-0.112186	2.253108
C	4.035723	-0.810402	3.540223
H	4.365862	-1.583313	2.819376
H	3.382896	-1.308281	4.283713
H	4.930609	-0.425520	4.073629
C	2.643204	1.284838	3.870099
H	2.071741	2.097215	3.378556
H	3.400840	1.744066	4.538750
H	1.946410	0.726213	4.521771
C	5.245131	0.812099	-1.876899
H	5.355647	-0.292353	-1.840375
C	6.465643	1.359976	-2.631753
H	6.555689	0.866464	-3.621069
H	7.408917	1.184456	-2.074429
H	6.380544	2.450742	-2.820658
C	3.948594	1.097782	-2.658693
H	3.984707	0.653206	-3.674563
H	3.782142	2.189271	-2.763535
H	3.052918	0.679693	-2.152074
C	-0.978587	-0.618538	2.201231
C	-1.160746	-0.011153	3.464452
C	-0.431018	-0.365430	4.613373
C	0.514093	-1.401916	4.557662
C	0.700874	-2.074438	3.344489
C	-0.047443	-1.664651	2.233093
C	-2.875614	-1.433307	0.462532
C	-3.370926	-1.642330	-0.836412
C	-4.295565	-2.632082	-1.193893
C	-4.772520	-3.508830	-0.206885
C	-4.326996	-3.346056	1.114012
C	-3.410266	-2.320826	1.421067
C	-2.477654	1.244964	0.945914
C	-3.829108	1.585228	0.766509
C	-4.332338	2.879915	0.994901
C	-3.469900	3.906768	1.402459
C	-2.112316	3.616021	1.608180
C	-1.662103	2.319717	1.348185

1-Al

Sum of electronic and thermal Free Energies = -8050.472952

0 1

Ga	-0.178870	0.266592	-1.035147
Ga	2.138744	-0.788383	-0.568562
Al	-1.833280	-0.260075	0.804354
F	-2.322243	-0.005827	3.958274
F	-1.190752	-1.259078	6.073429
F	0.856650	-3.049564	5.687869

F	1.737710	-3.592474	3.134876
F	0.633695	-2.350298	1.025899
F	-3.294146	-0.547962	-1.984080
F	-4.991946	-2.391779	-2.982431
F	-5.806346	-4.506222	-1.421838
F	-4.892761	-4.738673	1.154764
F	-3.185450	-2.908232	2.166372
F	-4.837207	1.036349	0.405248
F	-5.686682	3.568420	0.877391
F	-4.002511	5.395968	2.040006
F	-1.451411	4.664111	2.748523
F	-0.591185	2.124191	2.265922
N	0.121718	-0.945808	-2.623918
N	0.046990	1.927840	-2.110993
N	2.280748	-2.606333	-1.501980
N	4.028889	-0.792830	0.065272
C	0.787404	-0.569805	-3.718317
C	1.123782	0.786879	-3.972877
H	1.686811	0.968028	-4.898056
C	0.727726	1.949326	-3.272045
C	1.290032	-1.575966	-4.735504
H	0.581332	-2.408554	-4.894103
H	2.252902	-2.007543	-4.387373
H	1.477917	-1.086458	-5.709161
C	1.094592	3.288095	-3.876152
H	1.431474	3.177818	-4.923041
H	1.914707	3.754009	-3.290639
H	0.242962	3.994415	-3.836677
C	3.463064	-3.231536	-1.674499
C	4.658413	-2.876099	-1.003697
H	5.508187	-3.550664	-1.171711
C	4.923782	-1.777869	-0.166065
C	3.591088	-4.391061	-2.649745
H	3.286686	-4.073409	-3.669641
H	2.952148	-5.254646	-2.381785
H	4.637892	-4.740050	-2.701375
C	6.298834	-1.683861	0.459563
H	6.894409	-0.867265	0.002235
H	6.853089	-2.632835	0.339849
H	6.220075	-1.438767	1.537397
C	-0.148168	-2.325075	-2.211460
H	-0.549694	-2.219669	-1.175945
C	1.084559	-3.257574	-2.081162
H	1.338464	-3.614864	-3.101233
C	0.629454	-4.491839	-1.261766
H	1.485941	-5.171865	-1.080862
H	0.299280	-4.143817	-0.262861
C	-0.509096	-5.236299	-1.975442
H	-0.825956	-6.109805	-1.367667
H	-0.132312	-5.645685	-2.941267
C	-1.702274	-4.307608	-2.240877
H	-2.147941	-4.005974	-1.268633
H	-2.501516	-4.834800	-2.802430
C	-1.268446	-3.041880	-2.993037
H	-2.114513	-2.340553	-3.121758
H	-0.919579	-3.312093	-4.013987
C	-0.517410	3.134354	-1.568824
C	0.279355	3.996780	-0.774272
C	-0.326947	5.141637	-0.219768
H	0.267781	5.814933	0.415594
C	-1.679051	5.422458	-0.448301
H	-2.143940	6.306520	0.013932
C	-2.452559	4.559234	-1.238866
H	-3.517238	4.783464	-1.397398
C	-1.894873	3.403197	-1.816262
C	1.741504	3.678175	-0.491925
H	2.071570	2.934790	-1.243578
C	1.903452	3.007158	0.879717
H	1.368365	2.037971	0.911586
H	1.486094	3.639188	1.689674
H	2.971268	2.817302	1.091834
C	2.662579	4.902946	-0.618617
H	2.546064	5.408948	-1.599868
H	3.722735	4.593438	-0.506163
H	2.459458	5.655165	0.172085
C	-2.721412	2.476872	-2.705156
H	-2.417204	1.440382	-2.450164
C	-2.412302	2.685436	-4.204037
H	-3.068721	2.036968	-4.820935
H	-1.367862	2.432224	-4.464401
H	-2.599409	3.739515	-4.500413
C	-4.236602	2.584104	-2.483664
H	-4.637313	3.553117	-2.850042
H	-4.520392	2.474497	-1.422775
H	-4.752307	1.780354	-3.046328
C	4.491524	0.404125	0.712930
C	4.168529	0.651724	2.071284
C	4.724685	1.793188	2.686148
H	4.502416	1.995002	3.744412
C	5.527409	2.686326	1.967580
H	5.945836	3.574799	2.465201
C	5.772017	2.466001	0.602927
H	6.374826	3.192067	0.038024
C	5.264706	1.327516	-0.049793
C	3.242816	-0.268558	2.858396
H	2.649595	-0.848162	2.117248
C	4.034134	-1.290428	3.697986
H	4.665508	-1.941278	3.059921
H	3.346684	-1.947327	4.267230
H	4.697322	-0.772921	4.422994
C	2.246636	0.519259	3.724776
H	1.674997	1.254748	3.127779
H	2.753948	1.060666	4.549951
H	1.519392	-0.171149	4.191145
C	5.491533	1.107625	-1.545298
H	5.553643	0.013553	-1.722938
C	6.796717	1.725049	-2.070843
H	6.962547	1.428526	-3.126816
H	7.675664	1.394879	-1.479485
H	6.769843	2.834661	-2.047030
C	4.279334	1.617881	-2.348849
H	4.389053	1.393802	-3.430141
H	4.164840	2.714972	-2.229719
H	3.330531	1.148895	-2.010779
C	-0.881210	-1.091043	2.395723
C	-1.307194	-0.860828	3.712955
C	-0.753628	-1.512119	4.831752
C	0.286285	-2.441465	4.638828
C	0.735681	-2.717552	3.337384
C	0.143962	-2.025119	2.272879

C	-3.152960	-1.642400	0.134026
C	-3.675627	-1.563931	-1.161293
C	-4.567649	-2.495993	-1.711423
C	-4.972954	-3.585294	-0.920753
C	-4.493611	-3.706502	0.395784
C	-3.598695	-2.737588	0.890300
C	-2.668906	1.493308	1.297603
C	-3.971955	1.898233	0.994610
C	-4.448131	3.197303	1.245655
C	-3.588888	4.135077	1.842200
C	-2.280246	3.763109	2.194717
C	-1.862956	2.455680	1.914658

1-Cl_2

Sum of electronic and thermal Free Energies = -6546.584080

0 1

Ga	1.104367	0.357266	-0.363113
Ga	-1.247529	0.779038	-0.720002
Cl	2.304229	0.776233	-2.213970
Cl	-1.962351	1.066008	-2.820024
N	1.404450	1.817504	0.997637
N	2.135940	-1.005372	0.601386
N	-1.146643	2.665995	-0.057662
N	-2.792272	0.234326	0.370991
C	1.634520	1.501939	2.274402
C	1.963936	0.188088	2.712128
H	2.092987	0.070241	3.796109
C	2.305896	-0.941239	1.935064
C	1.566491	2.574922	3.345306
H	0.573830	3.071896	3.346122
H	2.330228	3.362985	3.180602
H	1.735412	2.139690	4.346846
C	2.914441	-2.132946	2.637118
H	2.500826	-3.079823	2.237486
H	2.738939	-2.082362	3.727664
H	4.009370	-2.168514	2.468523
C	-2.065718	3.211962	0.735117
C	-3.239800	2.511930	1.135805
H	-3.966765	3.105954	1.705393
C	-3.573420	1.150931	0.985091
C	-1.942209	4.629705	1.267214
H	-2.608575	4.771535	2.138300
H	-2.233744	5.369541	0.493529
H	-0.907449	4.866562	1.579229
C	-4.875511	0.683786	1.598763
H	-4.715281	-0.182812	2.270677
H	-5.568069	0.336547	0.805815
H	-5.364265	1.496667	2.165865
C	1.234177	3.205688	0.551659
H	0.937981	3.850339	1.406940
C	0.106443	3.287772	-0.516364
H	0.451496	2.634305	-1.352237
C	1.350960	5.076534	-1.779444
H	1.631368	4.346559	-2.570721
H	1.266094	6.068297	-2.271384
C	2.439452	5.097411	-0.696070
H	3.418074	5.396467	-1.127569
H	2.183499	5.869067	0.066945
C	0.000505	4.678555	-1.166678
H	-0.290073	5.453464	-0.429628
H	-0.798594	4.637440	-1.935958
C	2.570304	3.722550	-0.029220
H	3.328547	3.737380	0.782759
H	2.916766	2.976580	-0.776053
C	2.758655	-2.027566	-0.190219
C	4.159171	-1.967252	-0.441940
C	4.719809	-2.935242	-1.297348
H	5.800612	-2.902545	-1.507701
C	3.929467	-3.921346	-1.902958
H	4.389157	-4.660715	-2.577400
C	2.552068	-3.958280	-1.652098
H	1.931203	-4.731856	-2.130819
C	1.943147	-3.021970	-0.794281
C	5.059182	-0.878400	0.141156
H	4.442901	-0.250835	0.817008
C	6.219407	-1.470834	0.966538
H	5.864682	-2.164556	1.756933
H	6.801752	-0.663295	1.457434
H	6.921669	-2.041019	0.322641
C	5.603653	0.047414	-0.965275
H	6.257878	-0.512562	-1.666857
H	6.208614	0.866967	-0.522467
H	4.774053	0.491603	-1.548348
C	0.442242	-3.094741	-0.535496
H	0.202173	-2.341778	0.244038
C	0.029819	-4.472379	0.013471
H	0.214307	-5.276898	-0.729034
H	-1.050771	-4.479389	0.257984
H	0.597492	-4.730927	0.931731
C	-0.374464	-2.730154	-1.790006
H	-0.240380	-3.487480	-2.591217
H	-0.071475	-1.748806	-2.208161
H	-1.455239	-2.680632	-1.543041
C	-3.109873	-1.160854	0.492160
C	-2.491634	-1.896687	1.547099
C	-2.858965	-3.245779	1.713938
H	-2.411759	-3.832915	2.528032
C	-3.775712	-3.864537	0.850246
H	-4.046321	-4.921369	1.001030
C	-4.322222	-3.142944	-0.215467
H	-5.017768	-3.640105	-0.909804
C	-4.005151	-1.783224	-0.418441
C	-1.443716	-1.251148	2.458230
H	-0.789604	-0.632400	1.800209
C	-0.548976	-2.283751	3.157282
H	-1.114898	-2.877649	3.905561
H	0.262398	-1.761869	3.698760
H	-0.087137	-2.988701	2.439071
C	-2.037418	-0.299363	3.517329
H	-2.763462	-0.834238	4.165867
H	-2.543936	0.575357	3.069635
H	-1.224444	0.090163	4.165431
C	-4.615049	-1.046393	-1.607128
H	-4.269493	0.006659	-1.569632
C	-4.104243	-1.639745	-2.934989
H	-4.405176	-2.703671	-3.044241
H	-3.001788	-1.572609	-3.002035
H	-4.520265	-1.074789	-3.794487
C	-6.156059	-1.055872	-1.569170
H	-6.561699	-2.083966	-1.679248

H	-6.566449	-0.446082	-2.400574
H	-6.555293	-0.645017	-0.618694

1-I_2

Sum of electronic and thermal Free Energies = -6222.061856

0 1

Ga	1.079118	0.242318	0.112436
Ga	-1.311973	0.619619	-0.128505
I	2.297498	1.075628	-2.028021
I	-2.063983	1.579878	-2.429117
N	1.334571	1.416686	1.736723
N	2.178801	-1.242109	0.794031
N	-1.283701	2.318981	0.925893
N	-2.832487	-0.210481	0.805178
C	1.586308	0.860953	2.925936
C	1.969409	-0.498283	3.096664
H	2.106058	-0.822880	4.136623
C	2.346935	-1.440381	2.114280
C	1.477603	1.693810	4.190044
H	0.460390	2.126041	4.294452
H	2.196889	2.538688	4.184653
H	1.682723	1.076247	5.083066
C	2.988561	-2.729514	2.572850
H	2.651168	-3.582109	1.951547
H	2.754906	-2.929070	3.635184
H	4.091137	-2.676038	2.474422
C	-2.224690	2.651309	1.804461
C	-3.366792	1.832244	2.040691
H	-4.114980	2.260284	2.720961
C	-3.643459	0.521789	1.604648
C	-2.162765	3.933025	2.616820
H	-2.813426	3.853334	3.507613
H	-2.515090	4.797345	2.016876
H	-1.134516	4.160457	2.955603
C	-4.914993	-0.122641	2.112268
H	-4.706044	-1.098191	2.594837
H	-5.599734	-0.335881	1.267287
H	-5.434454	0.533958	2.833518
C	1.080961	2.855992	1.588603
H	0.773252	3.291439	2.562975
C	-0.078309	3.089925	0.581487
H	0.272004	2.638624	-0.378386
C	1.035760	5.157275	-0.319194
H	1.331575	4.612738	-1.243213
H	0.886865	6.219678	-0.605008
C	2.148993	5.027463	0.730826
H	3.099080	5.460732	0.352924
H	1.872166	5.617602	1.635475
C	-0.275942	4.572341	0.222640
H	-0.589684	5.169138	1.102338
H	-1.089517	4.634302	-0.530046
C	2.371437	3.558447	1.110816
H	3.145018	3.456656	1.901809
H	2.748323	3.000982	0.226103
C	2.833240	-2.055849	-0.189175
C	4.236604	-1.922347	-0.396560
C	4.816035	-2.631978	-1.465972
H	5.897703	-2.533975	-1.649533
C	4.044373	-3.438119	-2.313221
H	4.519026	-3.970427	-3.152293
C	2.667563	-3.562454	-2.089364
H	2.062341	-4.200258	-2.752702
C	2.039242	-2.883306	-1.028389
C	5.125960	-1.026498	0.466033
H	4.500572	-0.597701	1.275530
C	6.271942	-1.826617	1.119886
H	5.905052	-2.717362	1.670897
H	6.837140	-1.190041	1.832283
H	6.992321	-2.190559	0.357479
C	5.695570	0.159662	-0.336362
H	6.346523	-0.193035	-1.164181
H	6.308151	0.813347	0.320053
H	4.882819	0.765131	-0.782572
C	0.542029	-3.059999	-0.798422
H	0.275757	-2.494599	0.119326
C	0.188800	-4.536833	-0.542362
H	0.407992	-5.164453	-1.431574
H	-0.890181	-4.638804	-0.311488
H	0.768600	-4.951864	0.308446
C	-0.297777	-2.481826	-1.952418
H	-0.141411	-3.052761	-2.891976
H	-0.039565	-1.423918	-2.163539
H	-1.376950	-2.531659	-1.699040
C	-3.081970	-1.617038	0.647569
C	-2.417478	-2.513971	1.536995
C	-2.721397	-3.885565	1.441626
H	-2.235581	-4.597407	2.123266
C	-3.623399	-4.367969	0.481268
H	-3.845399	-5.445262	0.426931
C	-4.216351	-3.480345	-0.421615
H	-4.899646	-3.865538	-1.194728
C	-3.960738	-2.094055	-0.361651
C	-1.388281	-2.010364	2.552467
H	-0.777248	-1.238327	2.028263
C	-0.431744	-3.114578	3.021993
H	-0.955613	-3.879071	3.633436
H	0.357037	-2.671952	3.658569
H	0.057271	-3.630672	2.172931
C	-2.010548	-1.323995	3.785939
H	-2.696442	-2.016500	4.318662
H	-2.569066	-0.405681	3.527435
H	-1.206820	-1.029479	4.493020
C	-4.617134	-1.174776	-1.386642
H	-4.297537	-0.135382	-1.166098
C	-4.127904	-1.509964	-2.809222
H	-4.433079	-2.535231	-3.109533
H	-3.025762	-1.437112	-2.883301
H	-4.554147	-0.795027	-3.542529
C	-6.156315	-1.231237	-1.324863
H	-6.539038	-2.235901	-1.603801
H	-6.597137	-0.498246	-2.031775
H	-6.545902	-1.000150	-0.312065

LAl

Sum of electronic and thermal Free Energies = -1480.417279

0 1

Al	-0.010082	-0.290894	-1.044005
N	-1.422917	-0.192222	0.419331
N	1.394712	-0.275521	0.427008
C	-1.286047	-0.319791	1.754972

C	-0.027756	-0.456830	2.381257
H	-0.033639	-0.564136	3.473929
C	1.237862	-0.380479	1.763381
C	-2.514881	-0.307345	2.639995
H	-3.162653	0.562077	2.409382
H	-2.236775	-0.280306	3.709874
H	-3.136087	-1.209062	2.460766
C	2.462782	-0.389136	2.650962
H	3.168393	-1.187333	2.343213
H	2.191042	-0.534228	3.712896
H	3.020993	0.564697	2.551350
C	-2.737907	0.058014	-0.108323
C	-3.640873	-1.018500	-0.314327
C	-4.918432	-0.725973	-0.830573
H	-5.636290	-1.544649	-0.993526
C	-5.285660	0.588217	-1.149875
H	-6.290862	0.798534	-1.547685
C	-4.363626	1.632650	-0.988583
H	-4.651254	2.655156	-1.274268
C	-3.072618	1.391224	-0.479552
C	-3.212713	-2.462330	-0.065032
H	-2.342026	-2.440274	0.622746
C	-4.306898	-3.316464	0.597048
H	-4.686394	-2.847999	1.529239
H	-3.911613	-4.321047	0.853872
H	-5.175742	-3.471731	-0.076567
C	-2.724348	-3.095084	-1.385116
H	-3.544759	-3.128929	-2.132844
H	-2.362311	-4.131855	-1.219498
H	-1.893279	-2.503605	-1.827301
C	-2.047388	2.516086	-0.339057
H	-1.057051	2.064128	-0.587275
C	-1.947835	3.045191	1.104973
H	-2.925072	3.448685	1.445844
H	-1.199395	3.862992	1.168465
H	-1.635139	2.254466	1.814013
C	-2.265915	3.665688	-1.332259
H	-2.351089	3.291689	-2.372620
H	-1.410881	4.371222	-1.291157
H	-3.181202	4.250118	-1.098835
C	2.724836	-0.068121	-0.085575
C	3.193725	1.263818	-0.251583
C	4.464998	1.458121	-0.825913
H	4.843087	2.483035	-0.967041
C	5.252672	0.369418	-1.225486
H	6.243095	0.540530	-1.675669
C	4.775394	-0.937351	-1.053881
H	5.397203	-1.788651	-1.372791
C	3.511021	-1.182413	-0.482824
C	2.332689	2.462436	0.141030
H	1.478919	2.078124	0.736585
C	1.743662	3.137459	-1.113701
H	1.074774	3.978762	-0.834737
H	1.155666	2.411164	-1.715831
H	2.547483	3.538373	-1.766867
C	3.090695	3.471563	1.021891
H	3.927363	3.953006	0.473104
H	3.517934	2.985125	1.923229
H	2.410177	4.280739	1.359895
C	2.994499	-2.610324	-0.331592
H	2.096530	-2.567654	0.319670
C	2.542446	-3.168749	-1.696033
H	1.758531	-2.523797	-2.148223
H	2.128518	-4.193623	-1.588141
H	3.393501	-3.213815	-2.408358
C	4.017375	-3.538476	0.348090
H	4.921372	-3.686730	-0.279423
H	3.574639	-4.540402	0.527191
H	4.352241	-3.132085	1.325209

LAl-I_2

Sum of electronic and thermal Free Energies = -2076.289460

0 1

Al	-0.016048	-0.468966	-0.188553
N	-1.460448	0.180763	0.886229
N	1.436974	-0.007955	0.956093
C	-1.308152	0.128534	2.229526
C	-0.065165	-0.131159	2.859954
H	-0.101447	-0.235704	3.952029
C	1.227759	-0.099498	2.290686
C	-2.506115	0.364326	3.116738
H	-3.082511	1.248945	2.781905
H	-2.201308	0.500666	4.169967
H	-3.200425	-0.498690	3.057916
C	2.421022	-0.164187	3.212383
H	2.967658	-1.115370	3.040141
H	2.116219	-0.114170	4.273238
H	3.142313	0.648538	2.998596
C	-2.731876	0.600849	0.331821
C	-3.809055	-0.318899	0.209466
C	-5.041128	0.159285	-0.283082
H	-5.884647	-0.542010	-0.379366
C	-5.208255	1.495261	-0.658975
H	-6.179892	1.847838	-1.038894
C	-4.125423	2.379288	-0.567805
H	-4.253795	3.424067	-0.884965
C	-2.873840	1.956368	-0.080812
C	-3.685542	-1.803595	0.532548
H	-2.675047	-1.983648	0.952966
C	-4.724749	-2.280966	1.565127
H	-4.688035	-1.690385	2.503935
H	-4.546566	-3.344613	1.826329
H	-5.759776	-2.205103	1.170431
C	-3.796519	-2.631774	-0.763927
H	-4.809476	-2.537433	-1.209761
H	-3.607564	-3.705761	-0.559478
H	-3.056813	-2.298693	-1.518162
C	-1.719884	2.948539	0.019888
H	-0.784761	2.370120	-0.130807
C	-1.643235	3.590209	1.419464
H	-2.594418	4.104181	1.673326
H	-0.828982	4.343264	1.459382
H	-1.437288	2.839471	2.207872
C	-1.762993	4.017932	-1.082079
H	-1.845492	3.552484	-2.084917
H	-0.836221	4.623464	-1.063973
H	-2.612894	4.720341	-0.951563
C	2.738919	0.393047	0.469564
C	3.002914	1.786254	0.351952
C	4.275541	2.190784	-0.093739

H	4.498265	3.265113	-0.182802
C	5.259136	1.251708	-0.431075
H	6.248194	1.587593	-0.779966
C	4.973793	-0.114491	-0.331628
H	5.742489	-0.852704	-0.609071
C	3.717772	-0.571397	0.117430
C	1.959281	2.835452	0.720227
H	0.979046	2.319276	0.767945
C	1.850515	3.937349	-0.345638
H	1.052689	4.657766	-0.073525
H	1.607433	3.505859	-1.337485
H	2.791137	4.518726	-0.440127
C	2.231249	3.434491	2.114784
H	3.224816	3.930008	2.147589
H	2.214404	2.659314	2.906285
H	1.462981	4.192786	2.373068
C	3.449846	-2.067968	0.179011
H	2.452068	-2.213883	0.640250
C	3.385417	-2.655013	-1.244591
H	2.635036	-2.122915	-1.863541
H	3.098612	-3.726294	-1.214717
H	4.368808	-2.571664	-1.754583
C	4.476709	-2.817207	1.047736
H	5.497064	-2.774789	0.611519
H	4.197719	-3.887591	1.136972
H	4.536391	-2.393018	2.071830
I	0.200147	0.628512	-2.430225
I	-0.186575	-3.006618	-0.258842

LAl–B(C_6F_5)$_3$

Sum of electronic and thermal Free Energies = -3687.109230

0 1

Al	-0.045570	0.896246	0.530303
F	-1.424711	0.548616	-2.183170
F	0.249551	-0.125881	2.424050
F	-5.373451	-2.051324	-2.133684
F	1.153581	-3.850044	-0.435098
F	-1.648171	-3.478286	0.376124
F	2.967185	-0.720249	-0.031910
F	-3.932366	0.067242	-3.109890
F	1.137888	-1.549212	4.541951
F	2.076575	-5.244750	1.693417
F	-4.188685	-3.800852	-0.362409
F	-0.293704	-1.730414	-3.380151
N	1.225549	2.277547	0.936402
F	4.900367	-0.890977	-1.886950
N	-1.578152	1.824650	1.218966
F	2.070473	-4.131458	4.194422
F	1.628486	-1.813833	-5.205653
F	4.259476	-1.393842	-4.519036
C	2.519338	2.173278	0.305891
C	-3.615835	0.421314	1.486597
C	0.664999	-1.450054	2.197872
C	-2.165623	-2.533859	-0.442941
C	-2.899492	1.422778	0.783688
C	3.617715	-1.053359	-2.249250
B	0.114958	-1.057208	-0.386940
C	0.636011	-1.943578	0.895418
C	3.605060	1.550490	2.570975
H	2.585955	1.800918	2.930710
C	-1.486410	2.858031	2.094380
C	1.317807	2.607110	-1.915647
H	0.501359	1.972977	-1.483527
C	0.956974	3.360690	1.698584
C	-2.077057	-0.560368	-1.735531
C	2.581509	2.327927	-1.106014
C	2.582776	-0.967530	-1.307191
C	-1.410574	-1.414873	-0.838651
C	-4.878952	0.043849	0.985872
H	-5.443544	-0.752517	1.495418
C	-3.110360	-0.182761	2.795649
H	-2.177306	0.349938	3.071091
C	3.840384	2.234345	-1.728083
H	3.916364	2.345779	-2.818935
C	1.123317	-2.128243	3.332022
C	-0.286267	3.550196	2.339657
H	-0.353818	4.408593	3.020395
C	4.619782	2.359023	3.402545
H	4.536582	3.451869	3.228728
H	5.663069	2.068419	3.159810
H	4.470471	2.171282	4.485831
C	-3.497665	-2.753158	-0.841268
C	-5.437042	0.679556	-0.129236
H	-6.424829	0.369698	-0.502463
C	3.805571	0.039965	2.815033
H	3.101767	-0.565411	2.217401
H	3.655217	-0.204618	3.886709
H	4.830825	-0.274931	2.528853
C	-3.370885	-0.769710	-2.219331
C	0.952406	-1.451150	-2.945098
C	1.610382	-3.432601	3.150178
C	-4.103688	-1.869420	-1.743728
C	1.137415	-3.253589	0.767757
C	4.997558	1.985912	-0.977400
H	5.972192	1.908983	-1.482071
C	-3.442732	2.078180	-0.359131
C	-4.731275	1.701207	-0.781191
H	-5.177333	2.189827	-1.658522
C	-2.666375	3.173581	-1.093417
H	-1.588328	2.929342	-0.984296
C	1.951422	-1.524492	-3.935617
C	-4.132641	0.033016	3.931649
H	-4.448758	1.093074	4.013453
H	-3.700915	-0.276868	4.905917
H	-5.048931	-0.571651	3.768369
C	-2.720453	3.308991	2.839584
H	-3.613487	3.339625	2.187299
H	-2.567214	4.300722	3.302431
H	-2.943842	2.580996	3.647661
C	1.997119	4.442389	1.861385
H	2.514984	4.636319	0.901426
H	2.781068	4.140158	2.583978
H	1.533199	5.376547	2.227139
C	-2.879225	4.563744	-0.457767
H	-2.499529	4.619978	0.579440
H	-3.957750	4.828103	-0.444843
H	-2.345422	5.339469	-1.045503
C	1.418497	2.187150	-3.386819
H	1.787790	1.148726	-3.484655
H	2.096420	2.854781	-3.959174

H	0.419680	2.238251	-3.863758
C	4.908259	1.798162	0.407012
H	5.817931	1.561528	0.980211
C	1.617050	-3.998211	1.859319
C	-2.758596	-1.673556	2.669710
H	-1.923672	-1.841406	1.969535
H	-3.619580	-2.269106	2.300944
H	-2.457397	-2.086018	3.655051
C	3.673399	1.874870	1.078817
C	3.296099	-1.317956	-3.589941
C	1.213789	-1.138478	-1.593343
C	-2.976606	3.237754	-2.597820
H	-2.890602	2.245779	-3.075872
H	-2.270186	3.931729	-3.098751
H	-3.997967	3.629004	-2.789332
C	0.874144	4.077373	-1.787361
H	0.633861	4.352502	-0.741782
H	-0.029634	4.267109	-2.401498
H	1.678536	4.753741	-2.144650

TS1

Sum of electronic and thermal Free Energies = -10995.797844

0 1

Ga	1.95401000	0.55870400	-1.38757500
Ga	3.69397900	-1.39948300	0.53154500
B	-0.86309400	-0.02658400	-0.41924700
N	3.32997600	-0.67673500	-2.47303800
N	3.07603100	2.23150500	-1.99650500
N	4.49428300	-2.90155100	-0.77190900
N	5.41851600	-1.50639700	1.70447300
C	4.44317800	-0.29122200	-3.10543000
C	4.86909200	1.05895700	-3.16337200
H	5.82195800	1.22885200	-3.68198400
C	4.25861000	2.21898200	-2.64456100
C	5.38258500	-1.29400400	-3.75194700
H	4.84597500	-2.04775900	-4.35815500
H	5.94916300	-1.83267200	-2.96335800
H	6.11375900	-0.78068300	-4.40350600
C	5.02488100	3.51941000	-2.81065000
H	5.80389900	3.42394100	-3.58978100
H	5.52649100	3.78403600	-1.85557300
H	4.35926500	4.36744900	-3.05851900
C	5.61276100	-3.60088100	-0.52286300
C	6.39175900	-3.47254700	0.65874800
H	7.21182100	-4.19651700	0.75776700
C	6.33501800	-2.49569500	1.67237500
C	6.14989300	-4.59613700	-1.54257600
H	6.42390800	-4.07788400	-2.48622300
H	5.40900200	-5.37490800	-1.81006300
H	7.05704700	-5.09751500	-1.15966200
C	7.39793700	-2.55401900	2.75455600
H	8.18830700	-1.79342300	2.58631000
H	7.87968900	-3.54969000	2.77848200
H	6.96102400	-2.33426800	3.74857300
C	2.80977400	-2.05112700	-2.46454200
H	1.99646100	-2.00891100	-1.71007900
C	3.72711600	-3.21640300	-1.98935600
H	4.42585300	-3.46318200	-2.81491400
C	2.82616800	-4.45890900	-1.77256100
H	3.44291700	-5.30307300	-1.40179800
H	2.10165200	-4.22946900	-0.96536500
C	2.09137600	-4.85673300	-3.06089800
H	1.44756600	-5.74191900	-2.87238500
H	2.83776800	-5.16836600	-3.82789400
C	1.25430000	-3.69135400	-3.60482000
H	0.44234000	-3.46688800	-2.88198900
H	0.75737700	-3.96631100	-4.55914300
C	2.10860900	-2.42993700	-3.78735300
H	1.48246800	-1.57295900	-4.11074000
H	2.86074600	-2.59117900	-4.59233700
C	2.52109300	3.49460300	-1.60247300
C	2.94481300	4.10445700	-0.39030100
C	2.37312600	5.34170100	-0.03706000
H	2.68335900	5.83205600	0.89757300
C	1.41082600	5.95427400	-0.85058800
H	0.96563900	6.91408900	-0.54885100
C	0.99807500	5.33387100	-2.03866400
H	0.23079500	5.81676500	-2.66203400
C	1.54478800	4.10066300	-2.44367400
C	3.99773400	3.44317000	0.49447200
H	4.58097800	2.75748100	-0.15055000
C	3.36535400	2.56302600	1.58554800
H	2.78195500	1.73100400	1.14448900
H	2.67344900	3.14897300	2.22405600
H	4.15118400	2.11941100	2.22706100
C	4.98786400	4.44736800	1.10660000
H	5.43480100	5.11047700	0.33639300
H	5.80565700	3.90180900	1.62076200
H	4.50344300	5.09422100	1.86809000
C	1.16135000	3.46428900	-3.77826200
H	1.25388700	2.36754800	-3.64867900
C	2.14488600	3.86323500	-4.89967100
H	1.81877700	3.43048200	-5.86874200
H	3.17137100	3.49972400	-4.70478200
H	2.18564200	4.96743500	-5.01449300
C	-0.27876600	3.76378000	-4.21915700
H	-0.40742000	4.82523300	-4.52009100
H	-1.01383600	3.54672600	-3.42415200
H	-0.54160800	3.13845400	-5.09625900
C	5.66380200	-0.36916000	2.53749600
C	4.84041400	-0.10809100	3.66850900
C	5.14350000	1.01777700	4.46180600
H	4.52920200	1.23535100	5.34660600
C	6.20183500	1.87608800	4.13797500
H	6.41826000	2.74843900	4.77390800
C	6.96330500	1.64098700	2.98420000
H	7.77015400	2.33943900	2.71767600
C	6.70544800	0.53038600	2.15945500
C	3.65483800	-1.01071700	4.00715600
H	3.16829300	-1.26472100	3.03375900
C	4.09448900	-2.34072100	4.64887600
H	4.78695300	-2.90011100	3.99046200
H	3.21269900	-2.98676900	4.83486700
H	4.60623800	-2.16060600	5.61810300
C	2.58995700	-0.30848300	4.86103900
H	2.23845500	0.62936700	4.38482200
H	2.96953800	-0.06122600	5.87492700
H	1.71498200	-0.96884700	5.00601100
C	7.46667100	0.32946600	0.84947300
H	7.58850200	-0.76024300	0.68322600

C	8.87376500	0.94543400	0.84602700
H	9.41160300	0.66487500	-0.08288900
H	9.47789600	0.59919300	1.71016500
H	8.84110600	2.05497500	0.87782700
C	6.63612000	0.85817300	-0.33518100
H	7.12221100	0.62375800	-1.30380800
H	6.51527500	1.95892200	-0.27047500
H	5.61905300	0.41529100	-0.35994700
C	-0.46876700	-0.85866100	0.89029200
C	-0.84528500	-0.48694900	2.20031500
C	-0.50260100	-1.20278400	3.35515100
C	0.28425200	-2.35873700	3.23837800
C	0.68424100	-2.78332800	1.96607700
C	0.27344200	-2.05511500	0.84114800
C	-1.21487400	-0.82861300	-1.75775400
C	-0.96851900	-0.32037400	-3.04912800
C	-1.26483000	-1.00017700	-4.23847900
C	-1.86904300	-2.26430500	-4.17024300
C	-2.13813800	-2.82563900	-2.91211400
C	-1.80701900	-2.11212700	-1.75006100
C	-1.07658800	1.55307800	-0.32967100
C	-1.95025400	2.27707300	-1.16993900
C	-2.09700700	3.67066800	-1.11529700
C	-1.41369900	4.40795600	-0.14015400
C	-0.55433400	3.73631000	0.73966200
C	-0.39299000	2.35146300	0.61474600
N	-5.16771100	-1.81584100	1.12804100
N	-5.13519200	1.07959100	1.60760500
C	-6.28812300	-1.72056300	1.87303500
C	-6.73289600	-0.52968400	2.48168600
H	-7.65037400	-0.61653900	3.07950800
C	-6.25531500	0.78733500	2.28868200
C	-7.18204300	-2.93754400	2.02179900
H	-7.70300200	-3.14341700	1.06320900
H	-7.94545600	-2.77614900	2.80557700
H	-6.59966900	-3.84945400	2.25554900
C	-7.16310800	1.89493400	2.79838400
H	-6.63339600	2.84868800	2.96163200
H	-7.66784800	1.58532600	3.73400500
H	-7.95363600	2.09121500	2.04368700
C	-4.94503700	-3.05505200	0.44331400
C	-5.57590800	-3.26199100	-0.81335500
C	-5.41560500	-4.50883100	-1.44639500
H	-5.89709200	-4.68996200	-2.41960600
C	-4.63890400	-5.51553300	-0.86079800
H	-4.52684500	-6.48881400	-1.36340600
C	-3.95971700	-5.26613900	0.33989700
H	-3.30735200	-6.04722300	0.75489200
C	-4.08021300	-4.03244100	1.00884000
C	-6.33686300	-2.13178900	-1.50316100
H	-6.61236500	-1.38679800	-0.72841000
C	-5.40587300	-1.42020000	-2.50852000
H	-5.05737200	-2.12598900	-3.29189600
H	-4.50122700	-1.01329400	-2.00640100
H	-5.92405600	-0.57478900	-3.00767200
C	-7.63812400	-2.59154800	-2.18019400
H	-7.44350900	-3.26653700	-3.04007900
H	-8.19963800	-1.71808500	-2.57200100
H	-8.29765900	-3.13245700	-1.47045100
C	-3.24446300	-3.71527700	2.25151400
H	-2.84836600	-2.68453900	2.09150500
C	-2.03853300	-4.65431200	2.40537200
H	-2.35786100	-5.69461500	2.62732800
H	-1.40292100	-4.33056600	3.25227600
H	-1.41036900	-4.67464600	1.49266800
C	-4.05202700	-3.68977600	3.56502100
H	-4.84232400	-2.91635500	3.55827800
H	-3.37946900	-3.46606300	4.41958300
H	-4.52713700	-4.67555900	3.75589600
C	-4.84783200	2.45672500	1.33698400
C	-5.29537800	3.00615400	0.09934200
C	-5.12972900	4.38943300	-0.10176600
H	-5.48270800	4.84749300	-1.03605500
C	-4.48899400	5.19091100	0.85476400
H	-4.35995900	6.26795300	0.67009800
C	-3.96542400	4.61100400	2.01733000
H	-3.41457700	5.23818400	2.73508400
C	-4.13031300	3.23667700	2.28566400
C	-5.89961000	2.10979400	-0.98861800
H	-5.28450200	1.17778600	-0.98867300
C	-7.35722200	1.68270100	-0.72076300
H	-7.45338200	1.03936200	0.17327100
H	-7.74647200	1.10292500	-1.58390900
H	-8.01092800	2.57110100	-0.58978600
C	-5.78615700	2.70809200	-2.39890100
H	-6.46568900	3.57697700	-2.53099700
H	-6.08100300	1.94886900	-3.15223100
C	-3.57777400	2.62691900	3.57494300
H	-3.53782700	1.53010700	3.42070600
C	-2.15058700	3.10898900	3.89041900
H	-1.47356000	3.00091200	3.02597400
H	-1.72626600	2.51265400	4.72379300
H	-2.13439500	4.17448500	4.20283100
C	-4.48635700	2.89049500	4.79481500
H	-4.64186800	3.98051600	4.94382100
H	-4.01613400	2.48701300	5.71603100
H	-5.48009600	2.41662900	4.69430900
Ga	-3.83483600	-0.26945100	0.59327700
H	-4.75523600	3.03421700	-2.62565200
F	0.48449100	1.78747800	1.46942700
F	0.09148800	4.41690700	1.69955900
F	-1.56852700	5.73414800	-0.06308500
F	-2.87023000	4.31645300	-2.00677300
F	-2.70853800	1.64131100	-2.09055800
F	-0.35851000	0.87510000	-3.20491400
F	-0.94357600	-0.46706500	-5.42752500
F	-2.14933700	-2.94697100	-5.28779000
F	-2.68926900	-4.04444800	-2.84077400
F	-2.09636100	-2.72509000	-0.58702800
F	-1.64964300	0.57818000	2.40445400
F	-0.92467200	-0.80015900	4.56396300
F	0.62152100	-3.06401600	4.33078600
F	1.41354900	-3.90406100	1.82621600
F	0.60825800	-2.59991000	-0.34926600

Int1-Cl

Sum of electronic and thermal Free Energies = -9709.485285

0 1

Ga	-0.21460800	-0.41455800	-0.92921500
Ga	-2.44131100	0.73133000	-0.05697800

N	-0.93748000	0.66560700	-2.52142100
N	-0.71343100	-2.16447900	-1.81593800
N	-2.92315800	2.38649300	-1.20973500
N	-4.26447800	0.62761800	0.80167900
C	-1.73461900	0.19385900	-3.48308700
C	-2.05116000	-1.17969600	-3.60523100
H	-2.72794500	-1.43920900	-4.42911400
C	-1.54760300	-2.26887900	-2.87480800
C	-2.43409300	1.07938600	-4.50235500
H	-1.84253400	1.96033000	-4.80316000
H	-3.40000900	1.43693000	-4.08575600
H	-2.66728200	0.49265800	-5.41053700
C	-1.96286400	-3.64601500	-3.35530000
H	-2.59723400	-3.56872500	-4.25701100
H	-2.52410900	-4.18732600	-2.56809500
H	-1.07963100	-4.27340000	-3.58745100
C	-4.16440800	2.90557900	-1.23410000
C	-5.17709100	2.59456300	-0.29252200
H	-6.08346500	3.21099500	-0.36124200
C	-5.24026200	1.55004600	0.64672700
C	-4.58419700	3.87100000	-2.33191500
H	-4.48944300	3.38054900	-3.32409400
H	-3.96367300	4.78619500	-2.37108200
H	-5.63968100	4.17081700	-2.20328000
C	-6.51628000	1.42526700	1.45610200
H	-7.18241000	0.64594100	1.03087400
H	-7.06850200	2.38374900	1.46245200
H	-6.30267300	1.11615300	2.49691700
C	-0.66813700	2.08939300	-2.31629300
H	-0.12205400	2.14181500	-1.34144600
C	-1.92778400	2.97097100	-2.13992000
H	-2.40467400	3.09108500	-3.13259500
C	-1.44620800	4.36563300	-1.69371500
H	-2.30427100	5.02519800	-1.45477100
H	-0.87515000	4.25125200	-0.75488000
C	-0.53708000	5.00574300	-2.74843300
H	-0.22320300	6.01361400	-2.40412400
H	-1.10552900	5.15312200	-3.69667600
C	0.69132700	4.12318500	-2.99654300
H	1.29985400	4.10209600	-2.07015000
H	1.33935000	4.55347100	-3.78884800
C	0.30064600	2.68747900	-3.35818100
H	1.19335800	2.03112000	-3.38450800
H	-0.16189600	2.66361500	-4.36828400
C	-0.10679900	-3.39721500	-1.39228200
C	-0.81713500	-4.28206400	-0.54141600
C	-0.27443100	-5.56201600	-0.32145900
H	-0.81311800	-6.27464900	0.32169000
C	0.94750400	-5.93550800	-0.89966600
H	1.35697000	-6.94156300	-0.71604200
C	1.66791400	-5.02018600	-1.68065500
H	2.64444800	-5.30868400	-2.09583600
C	1.15343500	-3.73631300	-1.95214200
C	-2.11247600	-3.84219900	0.12830400
H	-2.51202100	-2.99053800	-0.45816000
C	-1.83738400	-3.30577600	1.54452000
H	-1.10683900	-2.47157200	1.54558200
H	-1.42897700	-4.10674100	2.19610000
H	-2.77562200	-2.93823900	1.99997700
C	-3.19101200	-4.93670900	0.15265600
H	-3.38677600	-5.35220200	-0.85877800
H	-4.13984200	-4.52198000	0.54895200
H	-2.90505600	-5.78332600	0.81192700
C	1.89427900	-2.75229100	-2.85367800
H	1.68414500	-1.72889900	-2.47261200
C	1.40598700	-2.80448100	-4.31612100
H	2.00380100	-2.10382700	-4.93564500
H	0.34433800	-2.51072100	-4.42414600
H	1.53112800	-3.82492900	-4.73828400
C	3.41286800	-2.92762700	-2.79325500
H	3.75155200	-3.85490800	-3.30369200
H	3.76558700	-2.96095500	-1.74879600
H	3.91323000	-2.07205800	-3.28874000
C	-4.60558400	-0.58319200	1.49766100
C	-4.12433800	-0.82670500	2.81084900
C	-4.57695900	-1.98519300	3.47663800
H	-4.22523000	-2.18754100	4.49810600
C	-5.44673200	-2.88914000	2.85643300
H	-5.78526900	-3.78735700	3.39569900
C	-5.86273700	-2.66489400	1.53578100
H	-6.52448100	-3.39450700	1.04700400
C	-5.45136500	-1.51887700	0.83070900
C	-3.16756500	0.13795600	3.50368200
H	-2.49781400	0.55159300	2.71475600
C	-3.93697300	1.30769100	4.15015600
H	-4.49645800	1.90436200	3.40312700
H	-3.24115400	1.99573900	4.67309800
H	-4.66417800	0.92617100	4.89789300
C	-2.25807000	-0.54889400	4.53285800
H	-1.73244100	-1.41736400	4.09141300
H	-2.82487600	-0.88182900	5.42850600
H	-1.47615300	0.15683200	4.87514200
C	-5.86900100	-1.29546500	-0.62292900
H	-6.03517200	-0.20746900	-0.76787500
C	-7.17571500	-2.00394400	-1.01058900
H	-7.48273800	-1.70481100	-2.03375200
H	-8.00412000	-1.75201800	-0.31655600
H	-7.06182100	-3.10832500	-1.01712900
C	-4.72913000	-1.69423600	-1.57770400
H	-4.97863500	-1.44868700	-2.63024600
H	-4.52178100	-2.78178700	-1.51482800
H	-3.78129700	-1.16824700	-1.33738900
N	2.11827700	2.05994000	1.37280100
N	3.53142800	-0.53538900	1.28678900
C	2.80957400	2.15062300	2.53363000
C	3.56020200	1.10252600	3.09020800
H	4.01051800	1.31202100	4.06870100
C	4.00705600	-0.07640800	2.45812100
C	2.88292600	3.47272300	3.28017200
H	3.55983100	4.17951300	2.76015600
H	3.27673500	3.30824900	4.30028100
H	1.90594700	3.98168900	3.34591800
C	5.10298300	-0.82933700	3.18905600
H	4.65417700	-1.66060000	3.77128700
H	5.62642400	-0.16191200	3.89802300
H	5.84020800	-1.28277300	2.50213600
C	1.68619400	3.33015000	0.86727900
C	2.61801500	4.11948000	0.13692300
C	2.30110300	5.47218900	-0.10491000
H	3.01597600	6.10134000	-0.65842200

C	1.10832900	6.03117600	0.37015700
H	0.89154100	7.09818700	0.20389100
C	0.17910200	5.22450900	1.04467700
H	-0.76753900	5.66846000	1.38496500
C	0.42852900	3.85719800	1.28278000
C	3.95958200	3.55428400	-0.32914300
H	3.91132900	2.45765800	-0.18602900
C	4.19599300	3.79675100	-1.82974500
H	4.22867100	4.87821700	-2.08261500
H	3.40922600	3.30703500	-2.43340400
H	5.16688900	3.35390600	-2.13322700
C	5.14355500	4.09006200	0.50035500
H	5.19061400	5.20021000	0.47850000
H	6.09996000	3.70417100	0.09051400
H	5.08927000	3.76748800	1.55826900
C	-0.61632100	2.98464400	1.98504100
H	-0.58628600	1.98980100	1.47510500
C	-2.04378200	3.54890800	1.86516400
H	-2.18719400	4.43261700	2.52191700
H	-2.77903600	2.78816000	2.19176000
H	-2.30639100	3.84048500	0.83243300
C	-0.31924900	2.70409600	3.47209100
H	0.55945800	2.04967100	3.61039100
H	-1.17992500	2.17311800	3.92260700
H	-0.17996100	3.65321200	4.03215700
C	4.23504900	-1.65035200	0.71038600
C	5.30459100	-1.40039300	-0.19512900
C	6.04736800	-2.50031800	-0.66761500
H	6.88192700	-2.32479600	-1.36369200
C	5.73768900	-3.81030300	-0.27567200
H	6.31811500	-4.65782300	-0.67329700
C	4.69392800	-4.03575700	0.63140000
H	4.46899200	-5.06253200	0.95956000
C	3.94911200	-2.96593100	1.16826800
C	5.71868300	0.01962000	-0.56962800
H	4.85220000	0.67232700	-0.35045800
C	6.90394200	0.49647000	0.29382200
H	6.64713500	0.51969500	1.37109400
H	7.20737600	1.52383700	0.00125000
H	7.78658200	-0.16710500	0.16887500
C	6.02814900	0.17458600	-2.06622900
H	6.91016700	-0.42370300	-2.37973700
H	6.25197200	1.23632400	-2.29958300
C	2.93025200	-3.22608500	2.27277100
H	2.63886200	-2.24978700	2.70841000
C	1.64726200	-3.84406600	1.71556400
H	1.21232100	-3.21014800	0.92171800
H	0.88594600	-3.94816200	2.51352100
H	1.84214300	-4.84376900	1.28204100
C	3.50342700	-4.11028300	3.39751300
H	3.67043400	-5.15361500	3.05480800
H	2.79042500	-4.15501300	4.24705600
H	4.47307400	-3.73085100	3.78138900
Ga	1.76580700	0.22092900	0.56118100
H	5.15287900	-0.12455800	-2.67457000
Cl	0.53467800	-0.52986300	2.48647200
Cl	2.63954500	0.68489500	-1.70221700

Int2-Cl

Sum of electronic and thermal Free Energies = -9709.500207

0 1			
Ga	0.67429800	-0.12417700	-1.40103500
Ga	-2.46451700	0.31750000	0.07737100
N	-0.91490900	0.58786400	-2.44215200
N	0.51709600	-2.02390500	-2.01764000
N	-3.44259000	1.77767900	-1.23160300
N	-4.41503300	-0.29467400	0.70606200
C	-1.52987000	-0.13870200	-3.38669400
C	-1.22071200	-1.49065700	-3.65624500
H	-1.80998900	-1.94813400	-4.46022900
C	-0.32107300	-2.36450000	-3.02329000
C	-2.68579900	0.40442400	-4.20539200
H	-2.47020100	1.38971400	-4.65745400
H	-3.58011500	0.51060200	-3.55704600
H	-2.93641400	-0.30048500	-5.01820100
C	-0.33789800	-3.79231300	-3.53383300
H	-0.77732500	-3.82766400	-4.54774600
H	-0.95461500	-4.43362500	-2.87222700
H	0.67196500	-4.23936200	-3.55524300
C	-4.76981600	1.95758600	-1.33572000
C	-5.72907800	1.37826900	-0.46605000
H	-6.75948400	1.73328100	-0.60441100
C	-5.58412800	0.32138200	0.45458300
C	-5.36191900	2.79617600	-2.46331600
H	-5.10604900	2.34849200	-3.44771400
H	-4.98333700	3.83628600	-2.48250800
H	-6.46384500	2.82937900	-2.38778800
C	-6.85261200	-0.18098100	1.12426100
H	-7.23234300	-1.09527000	0.62182200
H	-7.64870100	0.58664100	1.08420600
H	-6.66609900	-0.46128900	2.17876700
C	-1.13051000	2.03928200	-2.27973800
H	-0.61103700	2.29714800	-1.32585500
C	-2.58887200	2.56379200	-2.12885000
H	-3.03580500	2.57657400	-3.14326200
C	-2.47629700	4.04124800	-1.69154500
H	-3.47383700	4.43920200	-1.41864000
H	-1.86681800	4.08814100	-0.77062600
C	-1.82339300	4.89310700	-2.78424200
H	-1.75273500	5.95041800	-2.45056400
H	-2.46967600	4.88837900	-3.69280700
C	-0.43124900	4.34974000	-3.12325100
H	0.23336600	4.53837300	-2.25677300
H	0.01220400	4.89435300	-3.98398000
C	-0.44282600	2.84458700	-3.41045800
H	0.58616900	2.45616600	-3.53717700
H	-0.97422100	2.64590900	-4.36728600
C	1.26300000	-3.11391400	-1.43484500
C	0.56358100	-4.00886900	-0.57396100
C	1.25296400	-5.12723500	-0.06814400
H	0.72909200	-5.82125900	0.60629600
C	2.58751300	-5.36342000	-0.40718800
H	3.11820700	-6.23712100	0.00304800
C	3.24799600	-4.49550000	-1.28566900
H	4.28687800	-4.71428800	-1.56144400
C	2.60977400	-3.36647400	-1.84064600
C	-0.91209400	-3.81958100	-0.22428500
H	-1.34487700	-3.11485100	-0.96062100
C	-1.12160900	-3.17358100	1.15178400
H	-0.60197900	-2.20214600	1.24635000

H	-0.75866600	-3.83259900	1.96719900
H	-2.19883400	-2.99199000	1.32039200
C	-1.70912000	-5.13388000	-0.31538900
H	-1.57390400	-5.64618500	-1.29128700
H	-2.78882000	-4.92880100	-0.17079600
H	-1.41285300	-5.84906300	0.48022400
C	3.35177400	-2.50543300	-2.87438100
H	3.40184200	-1.47755200	-2.45321600
C	2.65281000	-2.38497400	-4.24737500
H	3.30010500	-1.79690200	-4.92942000
H	1.68506900	-1.85802400	-4.20580200
H	2.50400800	-3.38505800	-4.70749400
C	4.78878600	-2.98050800	-3.14105300
H	4.79769400	-3.96283500	-3.66107400
H	5.38672100	-3.07152400	-2.21798000
H	5.30285800	-2.25390700	-3.80262900
C	-4.45565000	-1.57509700	1.33526800
C	-4.00470400	-1.73998300	2.67425900
C	-4.08134000	-3.02603500	3.24673000
H	-3.74361200	-3.17597900	4.28205900
C	-4.56111800	-4.12054800	2.51618200
H	-4.61052100	-5.11640100	2.98343600
C	-4.95339800	-3.95247100	1.17976900
H	-5.30523100	-4.82379800	0.60800300
C	-4.90002500	-2.68941400	0.56129200
C	-3.44365600	-0.55911900	3.46297400
H	-2.82749900	0.03051400	2.74501400
C	-4.56229700	0.36058700	3.99089400
H	-5.16177000	0.79687800	3.16874400
H	-4.13385000	1.20091900	4.57634100
H	-5.24957500	-0.20180700	4.65823800
C	-2.50793300	-0.97970300	4.60413800
H	-1.71401200	-1.66361600	4.24548700
H	-3.06040500	-1.47417400	5.43183900
H	-2.00490100	-0.08758200	5.02835800
C	-5.25835900	-2.51233700	-0.91577800
H	-5.75912700	-1.52865500	-1.02782900
C	-6.23033000	-3.57614900	-1.44822100
H	-6.54278900	-3.32580900	-2.48300700
H	-7.14370800	-3.64995800	-0.82236400
H	-5.76273400	-4.58275400	-1.48615400
C	-3.99052200	-2.45219300	-1.79088800
H	-4.24251900	-2.19930500	-2.84148100
H	-3.45861300	-3.42452700	-1.79115300
H	-3.27206400	-1.68691300	-1.42907600
N	1.45219800	2.46817800	1.52944600
N	3.28269000	0.16070800	1.59203400
C	2.16167300	2.79441500	2.63708800
C	3.13257600	1.96444500	3.22231300
H	3.59742400	2.35367200	4.13666600
C	3.74727600	0.82098000	2.66986600
C	1.99078500	4.16243300	3.27347600
H	2.39940100	4.95844000	2.61979500
H	2.52274100	4.20044800	4.24167800
H	0.92804300	4.41749000	3.43244100
C	5.02610900	0.36803000	3.34586400
H	4.84335500	-0.54316200	3.94901100
H	5.40790900	1.15742600	4.01853200
H	5.80965700	0.10558900	2.61049700
C	0.75870700	3.58208600	0.94497800
C	1.49917300	4.44781600	0.09582500
C	0.94628600	5.70783400	-0.21427500
H	1.51338700	6.40398000	-0.85233400
C	-0.29585200	6.09577700	0.30348400
H	-0.69842500	7.09676400	0.08296200
C	-1.04436300	5.19435500	1.07647400
H	-2.04079800	5.49160000	1.43406300
C	-0.55393400	3.91091800	1.39151900
C	2.89458700	4.07574300	-0.40736900
H	3.05677600	3.00543200	-0.16563900
C	3.02595600	4.22415100	-1.93257500
H	2.86813300	5.27179800	-2.26584400
H	2.31135000	3.56688000	-2.46130400
H	4.04401300	3.92159600	-2.25362900
C	3.98870900	4.88916800	0.31501700
H	3.80884300	5.98066200	0.21385800
H	4.98491900	4.67060100	-0.12012200
H	4.04083100	4.64718400	1.39442600
C	-1.40833900	2.91576100	2.17988200
H	-1.16971800	1.90837500	1.76360100
C	-2.91690600	3.14921400	1.98463400
H	-3.26792900	4.05884700	2.51632700
H	-3.48498100	2.29484700	2.40116300
H	-3.19465600	3.23969300	0.91730100
C	-1.09059500	2.83526300	3.68605200
H	-0.08537700	2.41976300	3.88218800
H	-1.81599300	2.15412300	4.17587400
H	-1.18253000	3.83125800	4.17061800
C	4.10286800	-0.92126800	1.11443900
C	5.01482200	-0.66101200	0.05334000
C	5.93817300	-1.66848400	-0.28292600
H	6.67640100	-1.47636300	-1.07443800
C	5.93677000	-2.90728800	0.37468300
H	6.66342100	-3.68396700	0.08780900
C	5.01151900	-3.15427100	1.39422300
H	5.01247200	-4.12893500	1.90576800
C	4.09883200	-2.16373300	1.80657400
C	5.06229300	0.70323700	-0.63231200
H	4.01394300	1.06200900	-0.71355000
C	5.85375200	1.73720600	0.19585500
H	5.35286600	1.99209800	1.14903200
H	5.96378400	2.67928800	-0.37955500
H	6.87409800	1.36315900	0.42608800
C	5.62354300	0.64664100	-2.06067100
H	6.71401700	0.43372500	-2.07086400
H	5.47219600	1.62448300	-2.56067400
C	3.17658900	-2.43455100	2.99179300
H	2.71979000	-1.47268400	3.29950500
C	2.01865000	-3.34873800	2.57538900
H	1.49890500	-2.94429400	1.69036200
H	1.27561000	-3.44003900	3.39384300
H	2.38574300	-4.36167900	2.31315900
C	3.91663200	-3.03186700	4.20410300
H	4.27452700	-4.06281300	3.99872700
H	3.23286400	-3.09092800	5.07618900
H	4.80080700	-2.43171800	4.50414600
Ga	1.40849400	0.54331300	0.91931300
H	5.10831000	-0.11819600	-2.67174300
Cl	0.28464600	-0.28786300	2.71042900
Cl	2.28787500	0.79759800	-2.75773200

Int1-I

Sum of electronic and thermal Free Energies = - -9384.95469

0 1

Ga	-0.33338000	-0.32684700	-1.01662100
Ga	-2.54726500	0.83567900	-0.13508000
N	-0.95878600	0.83977100	-2.59077400
N	-0.84154800	-2.05670600	-1.95819000
N	-2.95055200	2.54207500	-1.24024300
N	-4.41601400	0.72795200	0.62982700
C	-1.73372100	0.41357800	-3.59092100
C	-2.02905800	-0.95331700	-3.79809900
H	-2.66547500	-1.16976300	-4.66510800
C	-1.59034500	-2.08275500	-3.08701900
C	-2.43742100	1.35154400	-4.55742900
H	-1.84020700	2.23771400	-4.83027600
H	-3.38758900	1.70329200	-4.10116000
H	-2.69933500	0.81076300	-5.48573000
C	-2.01000600	-3.42204400	-3.66349900
H	-2.56918700	-3.28057200	-4.60605900
H	-2.64912700	-3.97314300	-2.94687600
H	-1.13777400	-4.07605700	-3.85570100
C	-4.17328300	3.10332100	-1.28458300
C	-5.23768300	2.76484200	-0.41473700
H	-6.12830200	3.40197400	-0.49641900
C	-5.37191800	1.66862000	0.45488600
C	-4.51363800	4.15219300	-2.33259000
H	-4.40137500	3.72319500	-3.35109400
H	-3.85819100	5.04267500	-2.28980800
H	-5.56105200	4.48514300	-2.22108800
C	-6.71036400	1.51411700	1.15243800
H	-7.36084200	0.80270200	0.60202400
H	-7.23408300	2.48737500	1.20207400
H	-6.59530100	1.10520300	2.17299000
C	-0.67209900	2.25201400	-2.33276300
H	-0.09752900	2.25441000	-1.37339600
C	-1.91038100	3.15079600	-2.09980600
H	-2.35934800	3.35882800	-3.09144700
C	-1.39186500	4.49128000	-1.53888800
H	-2.23363000	5.15250600	-1.25074700
H	-0.83442700	4.28196900	-0.60835500
C	-0.45550300	5.19423700	-2.52770100
H	-0.09661000	6.14635100	-2.08334500
H	-1.01851300	5.46272700	-3.45211700
C	0.72941800	4.28725400	-2.87982900
H	1.35194100	4.14529300	-1.97188000
H	1.38249900	4.76292900	-3.64143100
C	0.26038000	2.91527200	-3.37081000
H	1.12269000	2.23916900	-3.53071500
H	-0.26168100	3.02687100	-4.34503600
C	-0.33212800	-3.34694600	-1.55823100
C	-1.12354500	-4.21935500	-0.76692400
C	-0.67896700	-5.54604200	-0.59815800
H	-1.28280800	-6.24144500	0.00558800
C	0.51233600	-5.99285200	-1.18275900
H	0.83617500	-7.03670500	-1.04494300
C	1.30968600	-5.10119300	-1.91397000
H	2.26318600	-5.44501400	-2.34113600
C	0.90682100	-3.76749600	-2.11903800
C	-2.42495300	-3.77306100	-0.11009100
H	-2.65143800	-2.75058500	-0.47700400
C	-2.26794500	-3.68839300	1.41816100
H	-1.45487000	-2.99237200	1.70205000
H	-2.03760100	-4.68587700	1.84982300
H	-3.20490100	-3.32100500	1.88030300
C	-3.61123400	-4.68707800	-0.47189900
H	-3.75320300	-4.78903500	-1.56828400
H	-4.54732600	-4.28109300	-0.04004700
H	-3.47313700	-5.70943000	-0.06170700
C	1.75309900	-2.81577800	-2.95566400
H	1.54556700	-1.78736800	-2.59149700
C	1.38699800	-2.83665400	-4.45331200
H	2.06830700	-2.16106700	-5.01113200
H	0.35419400	-2.48689500	-4.64463900
H	1.49445200	-3.85858400	-4.87729400
C	3.25570800	-3.04313900	-2.76674400
H	3.60400900	-3.98842500	-3.23578600
H	3.51935200	-3.07150600	-1.69506600
H	3.82250800	-2.20867900	-3.22610700
C	-4.83458500	-0.50725200	1.23953600
C	-4.50686900	-0.80006800	2.59050600
C	-5.03818100	-1.97933200	3.15392500
H	-4.80386400	-2.22847700	4.19797000
C	-5.85578400	-2.83959700	2.41175100
H	-6.26184700	-3.75108700	2.87706000
C	-6.14121300	-2.55050900	1.07003300
H	-6.77690600	-3.23763500	0.49360900
C	-5.63529600	-1.39001500	0.45553600
C	-3.64176400	0.13883500	3.42778700
H	-2.80586500	0.47330900	2.76940700
C	-4.42271700	1.38427100	3.89529000
H	-4.78044000	2.00505200	3.05222400
H	-3.77670300	2.02750000	4.52784700
H	-5.30342300	1.08728600	4.50365200
C	-3.00104400	-0.55181500	4.64007600
H	-2.47748500	-1.48389900	4.35092600
H	-3.75418600	-0.78960700	5.42189200
H	-2.24497100	0.11692700	5.09760200
C	-5.93469000	-1.07904000	-1.01212000
H	-6.11245000	0.01367000	-1.09743200
C	-7.19195300	-1.77848900	-1.55051000
H	-7.41694500	-1.42032500	-2.57599700
H	-8.08030300	-1.58041600	-0.91580900
H	-7.05729100	-2.87872400	-1.61404200
C	-4.72189300	-1.39120300	-1.90554400
H	-4.89375800	-1.05827400	-2.94908600
H	-4.50490300	-2.47715000	-1.91972900
H	-3.79941700	-0.88377100	-1.55217700
N	1.98823000	1.96188300	1.48697300
N	3.33261400	-0.69235700	1.38104400
C	2.59816200	1.96700200	2.69754200
C	3.24306500	0.85487300	3.26247600
H	3.60177100	0.99214800	4.29043000
C	3.69169700	-0.31897500	2.62267100
C	2.68852500	3.25067700	3.50752600
H	3.44286000	3.93242000	3.06730600
H	2.99836600	3.01992100	4.54353300
H	1.74275200	3.81778600	3.52948400
C	4.63086400	-1.17408500	3.45170300
H	4.01655900	-1.84929800	4.08431900
H	5.23734900	-0.54473200	4.12951600

H	5.29988500	-1.80465200	2.84106200
C	1.60028400	3.27383800	1.04269600
C	2.57336400	4.08234500	0.38946700
C	2.29187400	5.45282700	0.21291200
H	3.03494600	6.09359400	-0.28575800
C	1.09926100	6.01409900	0.68608600
H	0.91124900	7.09325700	0.57082200
C	0.13654700	5.19597000	1.29404500
H	-0.80874800	5.64211700	1.63557000
C	0.34737900	3.81154300	1.46151200
C	3.91728500	3.51388800	-0.06380900
H	3.77499900	2.42041200	-0.17000800
C	4.34054300	4.04360700	-1.44379400
H	4.61448500	5.12030200	-1.41625100
H	3.53885800	3.90117600	-2.19378700
H	5.22821700	3.48335400	-1.80163400
C	5.04873400	3.73617700	0.96078400
H	5.13155700	4.80509100	1.25419600
H	6.01984500	3.43398200	0.51682700
H	4.90972900	3.12856900	1.87538600
C	-0.73917700	2.94155800	2.09913200
H	-0.68686300	1.94664000	1.59361300
C	-2.15551000	3.51249400	1.90156700
H	-2.34082500	4.38168700	2.56708200
H	-2.90929600	2.74629700	2.16733600
H	-2.35333800	3.82778100	0.86227400
C	-0.53805700	2.66565700	3.60285500
H	0.34332100	2.03265900	3.80759300
H	-1.41461600	2.11155600	3.99386100
H	-0.45413700	3.61843700	4.16864300
C	4.07356200	-1.77470200	0.78209300
C	5.22261300	-1.46477500	-0.00249600
C	5.95637200	-2.53127200	-0.55818000
H	6.83998200	-2.31013300	-1.17493700
C	5.59107500	-3.86539800	-0.32997700
H	6.17131800	-4.68279700	-0.78637800
C	4.49817500	-4.15276900	0.49603900
H	4.23525400	-5.20039800	0.71053300
C	3.73780200	-3.12288100	1.08751000
C	5.74506600	-0.03491500	-0.12706600
H	4.86938400	0.63834300	-0.03785100
C	6.71081400	0.29728700	1.03047800
H	6.20662100	0.27418600	2.01463900
H	7.13351000	1.31517300	0.89888300
H	7.55670300	-0.42226500	1.06193500
C	6.42236000	0.25247000	-1.47540700
H	7.39477400	-0.27614100	-1.57277500
H	6.63163000	1.33834200	-1.56923100
C	2.66580500	-3.47948400	2.11003700
H	2.31797800	-2.53937400	2.58252000
C	1.43806100	-4.11211500	1.45388600
H	1.01910800	-3.45320800	0.67202300
H	0.64019900	-4.28859300	2.20272300
H	1.69303900	-5.08000500	0.98000400
C	3.21130500	-4.40410100	3.21659100
H	3.42849300	-5.42169500	2.82773800
H	2.45642200	-4.51470700	4.02297200
H	4.14621000	-4.01678400	3.66956300
Ga	1.64685900	0.16909400	0.55263200
H	5.77084800	-0.03951500	-2.32218100
I	0.04211600	-0.81935200	2.66941300
I	2.81257400	0.65683600	-2.04455000

Int2-l

Sum of electronic and thermal Free Energies = -9384.966977

0 1

Ga	0.59872900	-0.09234200	-1.37101300
Ga	-2.65488000	0.46832300	-0.00121100
N	-0.88851800	0.83363400	-2.41387700
N	0.35255300	-1.93090600	-2.15450500
N	-3.44819900	2.06727400	-1.25086700
N	-4.68990900	-0.07859800	0.40588700
C	-1.48243800	0.22847600	-3.45387000
C	-1.21730200	-1.10321500	-3.84542900
H	-1.77366700	-1.43885800	-4.72897200
C	-0.42648800	-2.10005600	-3.24982600
C	-2.57434300	0.90016500	-4.26484700
H	-2.29278500	1.90768800	-4.62103000
H	-3.48660700	0.99747600	-3.64084700
H	-2.82696600	0.28155300	-5.14432000
C	-0.51350400	-3.46483000	-3.90826900
H	-0.85449600	-3.35743400	-4.95463700
H	-1.24559200	-4.10602100	-3.37611600
H	0.45068500	-4.00257200	-3.88981800
C	-4.74890000	2.35204100	-1.43764600
C	-5.81021600	1.76743000	-0.70350900
H	-6.80311100	2.19967800	-0.88772100
C	-5.80034200	0.62488800	0.12009100
C	-5.19262200	3.32781900	-2.52237000
H	-4.89631900	2.94797600	-3.52383000
H	-4.74209600	4.33383600	-2.42071200
H	-6.29206800	3.43829800	-2.51960000
C	-7.14782500	0.14258300	0.63232000
H	-7.53432900	-0.69162600	0.01009300
H	-7.89231700	0.96094000	0.60577700
H	-7.07045500	-0.24906000	1.66431400
C	-1.04850100	2.27984100	-2.13915800
H	-0.55051600	2.43598200	-1.15328700
C	-2.48540900	2.87151700	-2.00774400
H	-2.86334900	3.00959400	-3.04051400
C	-2.32065300	4.29357000	-1.42253300
H	-3.30880000	4.70811800	-1.14037100
H	-1.73891900	4.22479100	-0.48480000
C	-1.59505900	5.21178400	-2.40908900
H	-1.47735700	6.22644500	-1.97225600
H	-2.21403300	5.32993200	-3.32886000
C	-0.22594800	4.62356200	-2.76409000
H	0.42241100	4.69925000	-1.86855300
H	0.26928200	5.21519900	-3.56337400
C	-0.30306600	3.15193700	-3.18276600
H	0.71315500	2.74077500	-3.32965500
H	-0.82081000	3.06425200	-4.16272100
C	0.94063900	-3.14704000	-1.63304400
C	0.08070400	-4.06257200	-0.95773300
C	0.60449700	-5.30499600	-0.55378300
H	-0.04680400	-6.01617700	-0.02475700
C	1.93711200	-5.64237900	-0.80570800
H	2.33569200	-6.61437800	-0.47446400
C	2.76319900	-4.74478700	-1.49186400
H	3.80124300	-5.03208200	-1.70279600

C	2.28910000	-3.49623300	-1.94742100
C	-1.38838600	-3.75068700	-0.68475100
H	-1.70857700	-2.97149200	-1.40333400
C	-1.59304300	-3.14910900	0.71096800
H	-0.99684200	-2.22858300	0.85239700
H	-1.29795600	-3.86200300	1.50796600
H	-2.65542600	-2.88291500	0.86672900
C	-2.30358500	-4.96971200	-0.88983700
H	-2.15258200	-5.44852600	-1.88051600
H	-3.36376000	-4.66030000	-0.80424400
H	-2.13888900	-5.74551900	-0.11326600
C	3.19549700	-2.61417400	-2.81054200
H	3.23227900	-1.61665000	-2.32211700
C	2.67411200	-2.39547400	-4.24787200
H	3.41522200	-1.79748700	-4.81636700
H	1.72316800	-1.83657700	-4.29290900
H	2.54924900	-3.36680700	-4.77275600
C	4.63868500	-3.12560300	-2.91564000
H	4.69945700	-4.05221800	-3.52670600
H	5.08574100	-3.32693400	-1.92737400
H	5.26486300	-2.35948700	-3.41687300
C	-4.86212800	-1.40412200	0.90565800
C	-4.56617600	-1.71337400	2.26269800
C	-4.75704100	-3.04258700	2.69311700
H	-4.53690300	-3.30976100	3.73607300
C	-5.21477000	-4.03472100	1.81641400
H	-5.35774800	-5.06512300	2.17740300
C	-5.47474100	-3.71932000	0.47488700
H	-5.82269700	-4.50949800	-0.20642400
C	-5.29489800	-2.41041900	-0.00984100
C	-4.04112200	-0.64081800	3.21656200
H	-3.23609400	-0.10217200	2.66182700
C	-5.11658200	0.39476500	3.60213300
H	-5.48592300	0.96048900	2.72658700
H	-4.69982000	1.12957100	4.32237700
H	-5.98357300	-0.09978900	4.08992800
C	-3.39858800	-1.21766200	4.48481300
H	-2.63415700	-1.98367500	4.24681800
H	-4.15614900	-1.67388700	5.15803300
H	-2.89356700	-0.41010300	5.05256800
C	-5.52054900	-2.07138500	-1.48555400
H	-5.96990400	-1.05829200	-1.53426600
C	-6.49046100	-3.02726000	-2.19665200
H	-6.70607500	-2.66111400	-3.22160200
H	-7.45436600	-3.11553200	-1.65405500
H	-6.06472700	-4.04770400	-2.30057100
C	-4.18855900	-1.98532000	-2.25669400
H	-4.34993600	-1.60306900	-3.28563800
H	-3.70570900	-2.97940500	-2.33490700
H	-3.46375600	-1.30646700	-1.76012700
N	1.47755500	2.24511600	1.72993000
N	3.15422500	-0.21330000	1.73368400
C	2.15509700	2.44267100	2.88651400
C	2.99834000	1.48433900	3.47953100
H	3.41119200	1.76562300	4.45618100
C	3.55699800	0.32370200	2.90436000
C	2.08957800	3.78684000	3.58974400
H	2.62379300	4.56104000	3.00427000
H	2.56334100	3.71751700	4.58599400
H	1.05425600	4.15295800	3.70395400
C	4.68048300	-0.32118900	3.69162700
H	4.29168300	-1.21132700	4.22739900
H	5.08272200	0.38283800	4.44250700
H	5.50412400	-0.67421000	3.04470800
C	0.87164000	3.44336700	1.20706300
C	1.68684700	4.31481800	0.43226800
C	1.23515300	5.63378600	0.22019600
H	1.86146100	6.33150500	-0.35583000
C	0.01327800	6.07343300	0.74616300
H	-0.30902200	7.11599000	0.59823400
C	-0.81516500	5.17262200	1.42994600
H	-1.79614600	5.51114700	1.79463900
C	-0.42274700	3.83718700	1.65620600
C	3.04497000	3.86786800	-0.10907100
H	3.00434000	2.76252400	-0.21269500
C	3.34637600	4.44233500	-1.50300600
H	3.53266500	5.53713600	-1.47121400
H	2.52411800	4.24577400	-2.21634500
H	4.25788600	3.96248300	-1.91336100
C	4.20308000	4.20914300	0.85157600
H	4.18673900	5.28585300	1.12587800
H	5.17517400	4.00434500	0.35953800
H	4.17377900	3.60820900	1.77991700
C	-1.36104300	2.87263300	2.38263700
H	-1.13508800	1.85569100	1.99148600
C	-2.84722500	3.14999300	2.09439400
H	-3.20493000	4.07685900	2.59095300
H	-3.46239400	2.31801700	2.49088600
H	-3.06224100	3.23367300	1.01209900
C	-1.14428500	2.81106900	3.90741100
H	-0.16342900	2.37859600	4.17741400
H	-1.91312000	2.15303800	4.36233300
H	-1.23983800	3.81934900	4.36583900
C	3.96910300	-1.29276400	1.22512000
C	5.04131300	-0.97438800	0.34212400
C	5.93916600	-1.99905400	-0.01157200
H	6.78452000	-1.76605400	-0.67482800
C	5.77751700	-3.30818300	0.46326500
H	6.48838500	-4.09548100	0.16629700
C	4.71232700	-3.60705100	1.31736300
H	4.58963900	-4.63247100	1.69802100
C	3.81275600	-2.60857200	1.74184100
C	5.30753300	0.45698900	-0.11655200
H	4.32191700	0.96090800	-0.20837500
C	6.14557800	1.22924600	0.92541000
H	5.58742000	1.41826800	1.86169100
H	6.45097000	2.21482200	0.51882400
H	7.07018200	0.66803700	1.17846100
C	5.99900500	0.52902000	-1.48725600
H	7.06447600	0.21985100	-1.42805800
H	5.97967100	1.57154400	-1.86551300
C	2.75576400	-2.96048000	2.77944400
H	2.32527500	-2.01385400	3.16338900
C	1.60503700	-3.73976300	2.13504700
H	1.18916300	-3.19199800	1.27014000
H	0.78115500	-3.89978600	2.86009400
H	1.95217500	-4.72548100	1.76644500
C	3.32656200	-3.74112500	3.97841200
H	3.63549300	-4.76894800	3.69313000
H	2.55275600	-3.83871000	4.76790300

H	4.21185400	-3.24321900	4.42573900
Ga	1.32112000	0.34440400	1.02996000
H	5.48931900	-0.10688800	-2.23682600
I	-0.11398900	-0.61172500	3.04221600
I	2.62400100	0.99194600	-2.74192300