Content

I. Heteronuclear NMR and IR Spectra

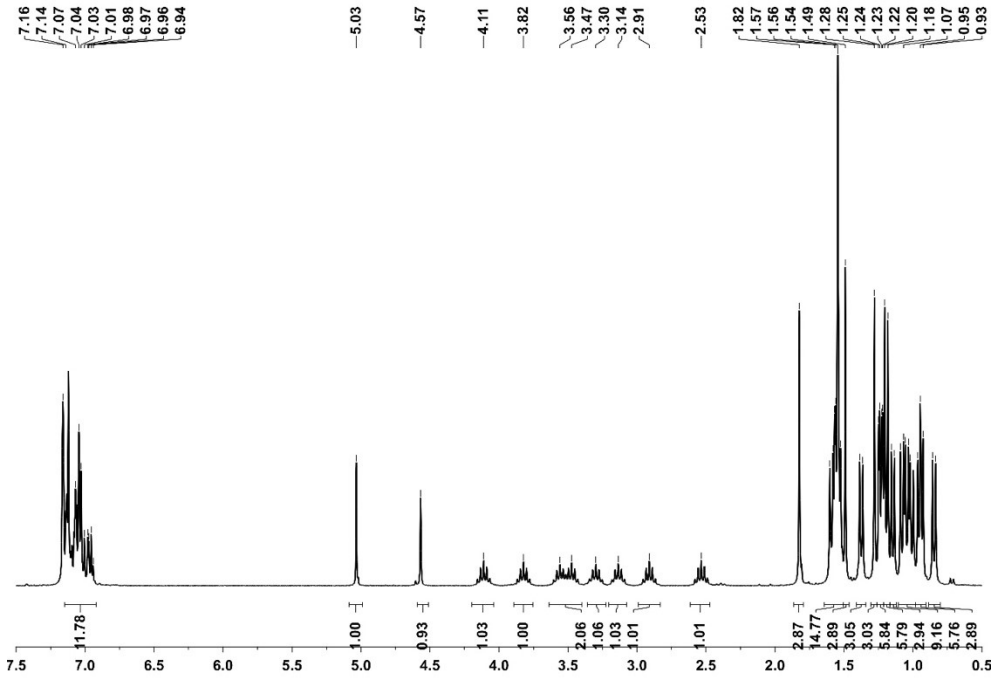

Figure S1: ^{1}H NMR spectrum of {[L(I)Ga]Si[Ga(I)][CH=C(Me)NAr][C(Me)=NAr]} **1** in benzene-d_6 at room temperature.

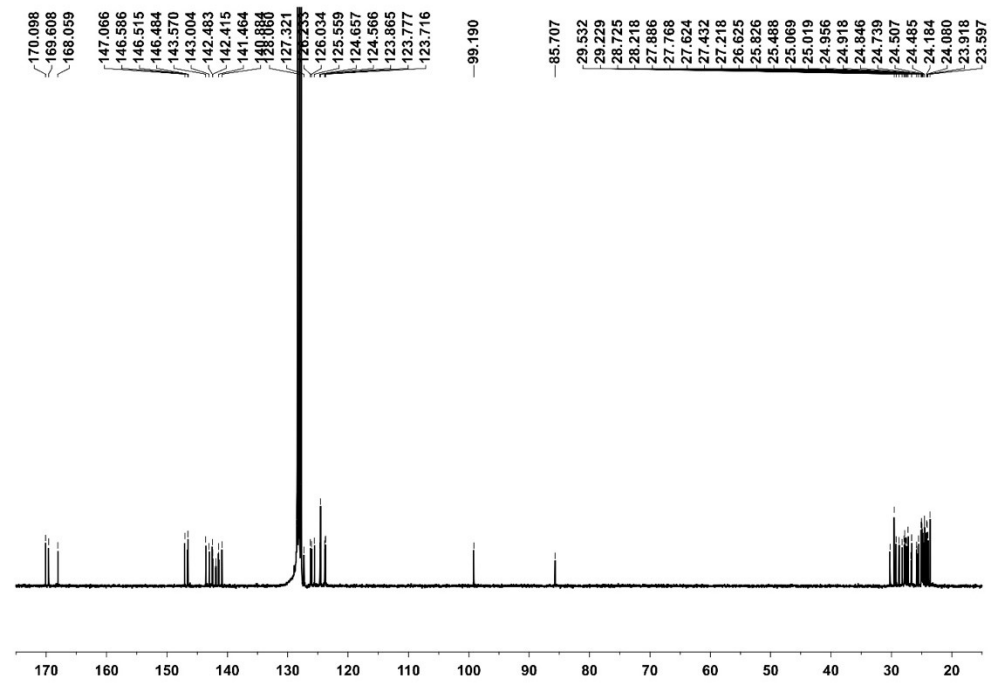

Figure S2: ^{13}C NMR spectrum of {[L(I)Ga]]Si[Ga(I)][CH=C(Me)NAr][C(Me)=NAr]} **1** in benzene-d_6 at room temperature.

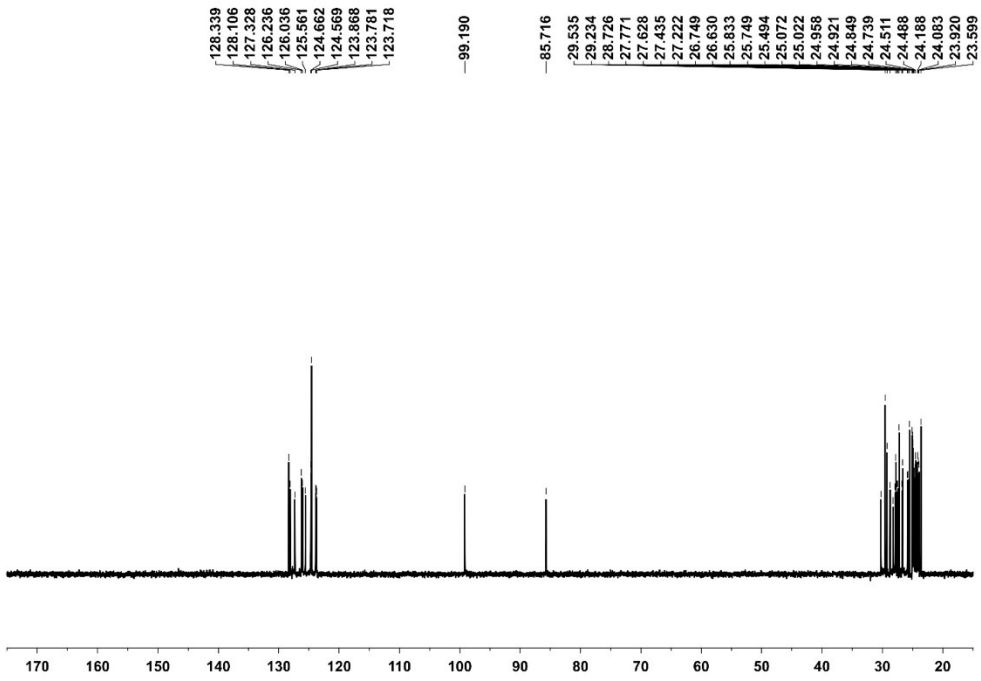

Figure S3: ^{13}C (DEPT135) NMR spectrum of{[L(I)Ga]Si[Ga(I)][CH=C(Me)NAr][C(Me)=NAr]} **1** in benzene-d_6 at room temperature.

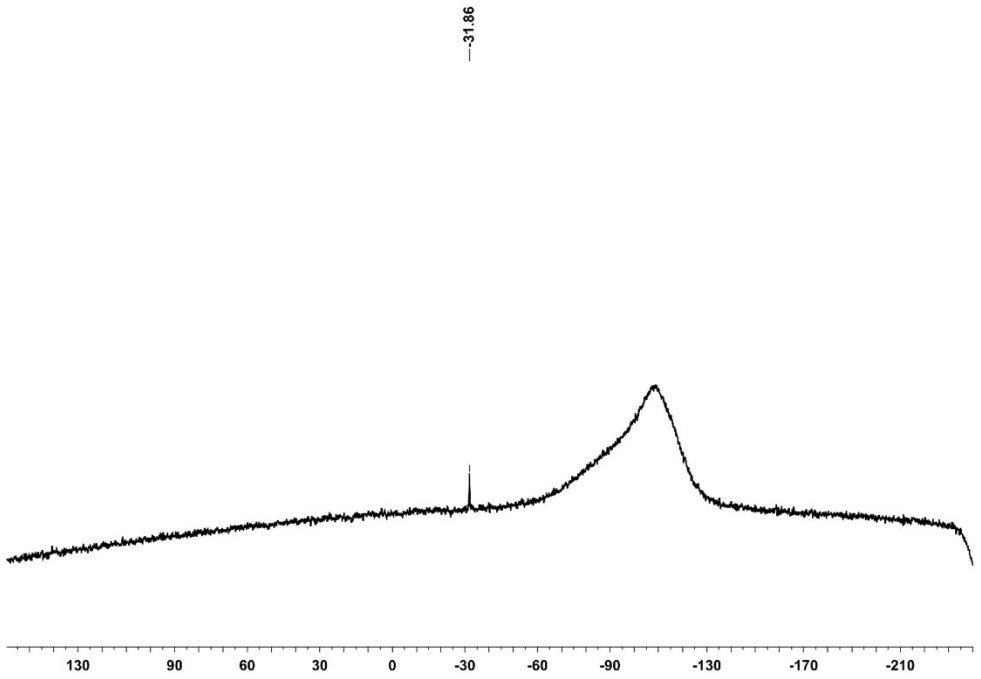

Figure S4: ^{29}Si NMR spectrum of {[L(I)Ga]Si[Ga(I)][CH=C(Me)NAr][C(Me)=NAr]} **1** in benzene-d_6 at room temperature.

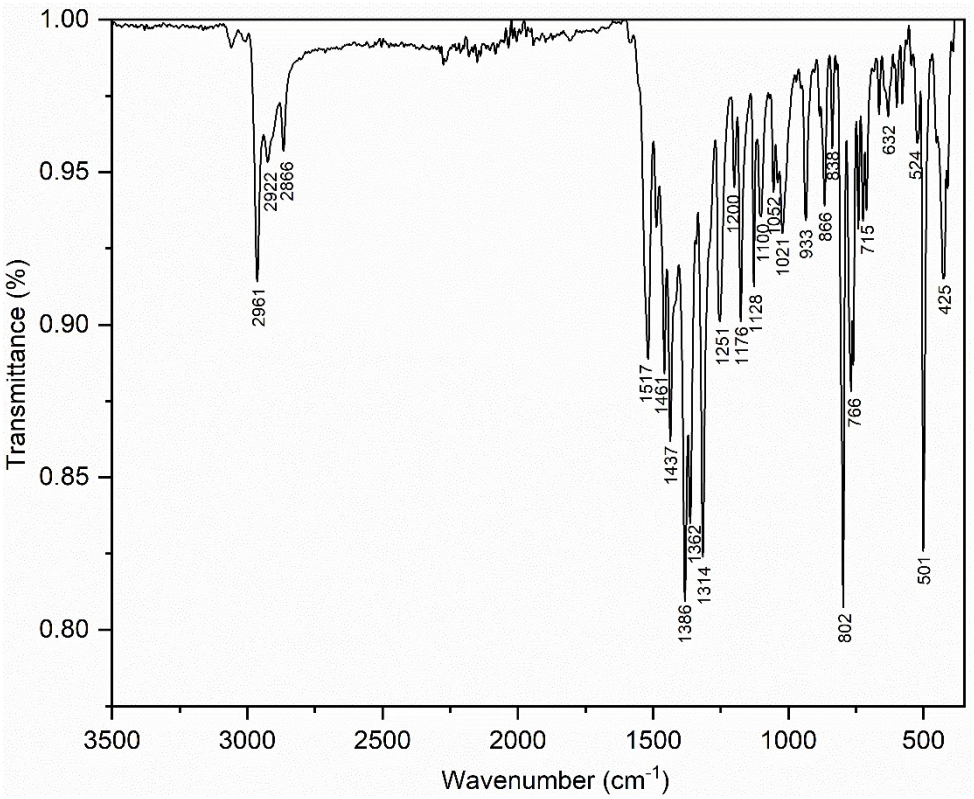

Figure S5: ATR-IR spectrum of {[L(I)Ga]Si[Ga(I)][CH=C(Me)NAr][C(Me)=NAr]} **1**.

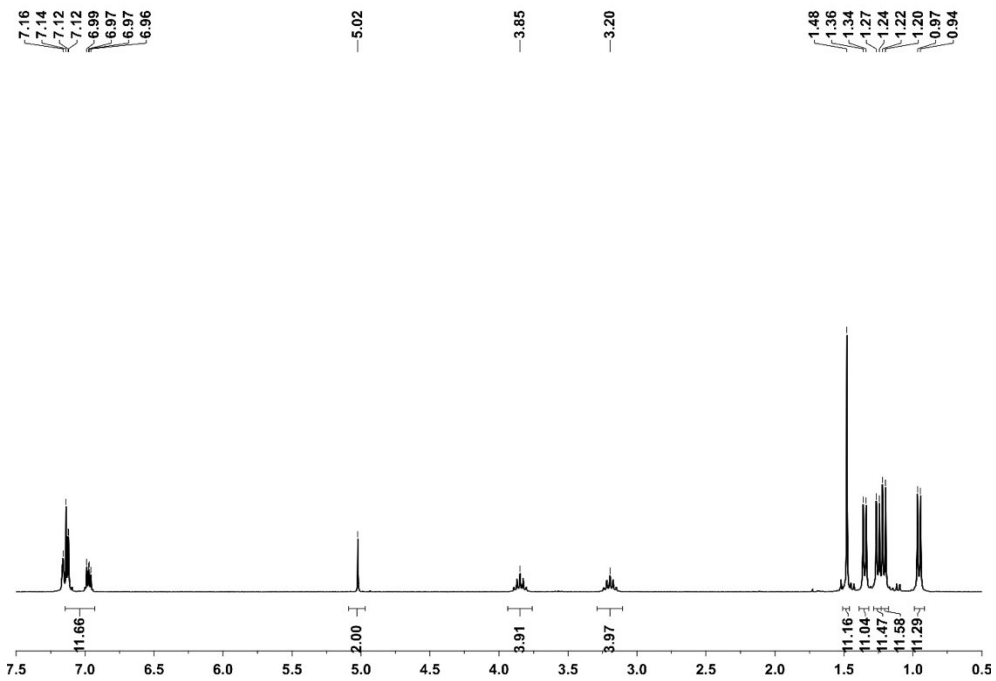

Figure S6: ^{1}H NMR spectrum of $[L(I)Ga]_2SiCO$ **2** in benzene-d_6 at room temperature.

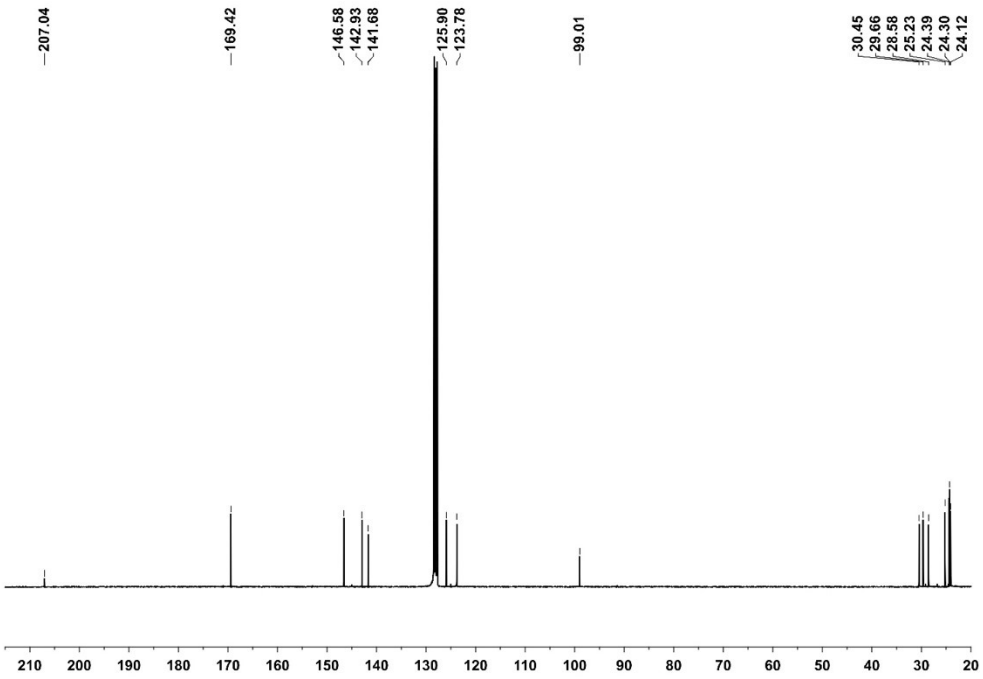

Figure S7: ^{13}C NMR spectrum of $[L(I)Ga]_2SiCO$ **2** in benzene-d_6 at room temperature.

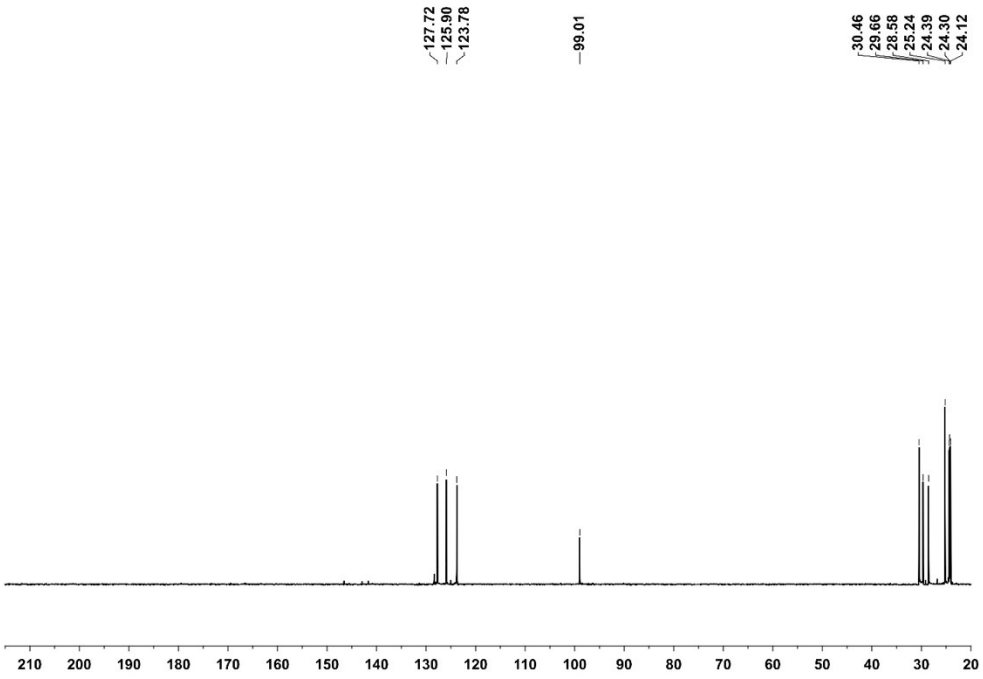

Figure S8: ^{13}C (DEPT135) NMR spectrum of $[L(I)Ga]_2SiCO$ **2** in benzene-d_6 at room temperature.

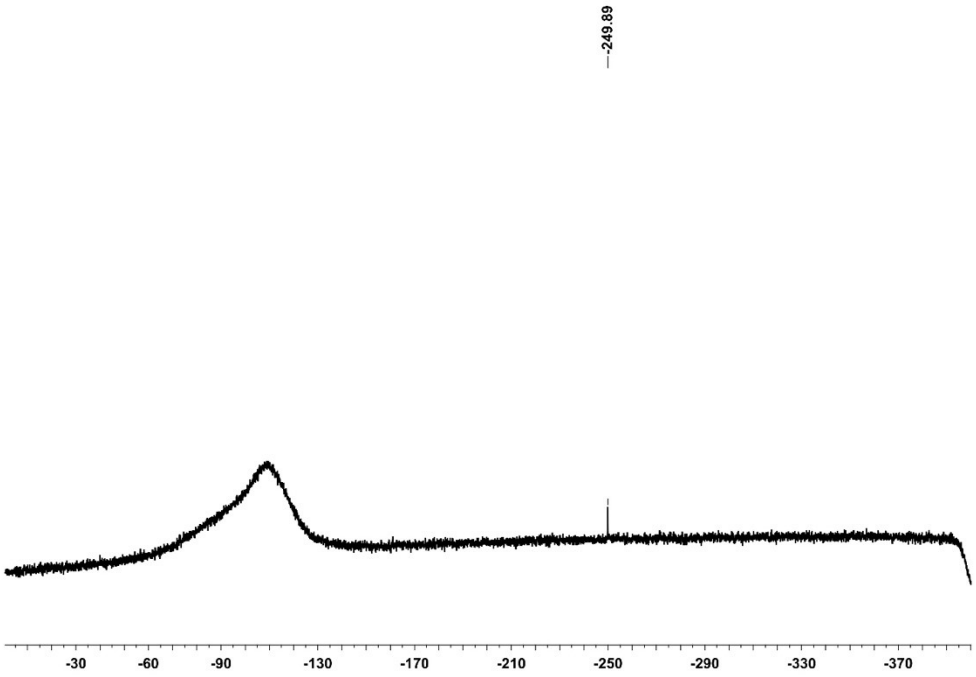

Figure S9: ^{29}Si NMR spectrum of [L(I)Ga]$_2$SiCO **2** in benzene-d_6 at room temperature.

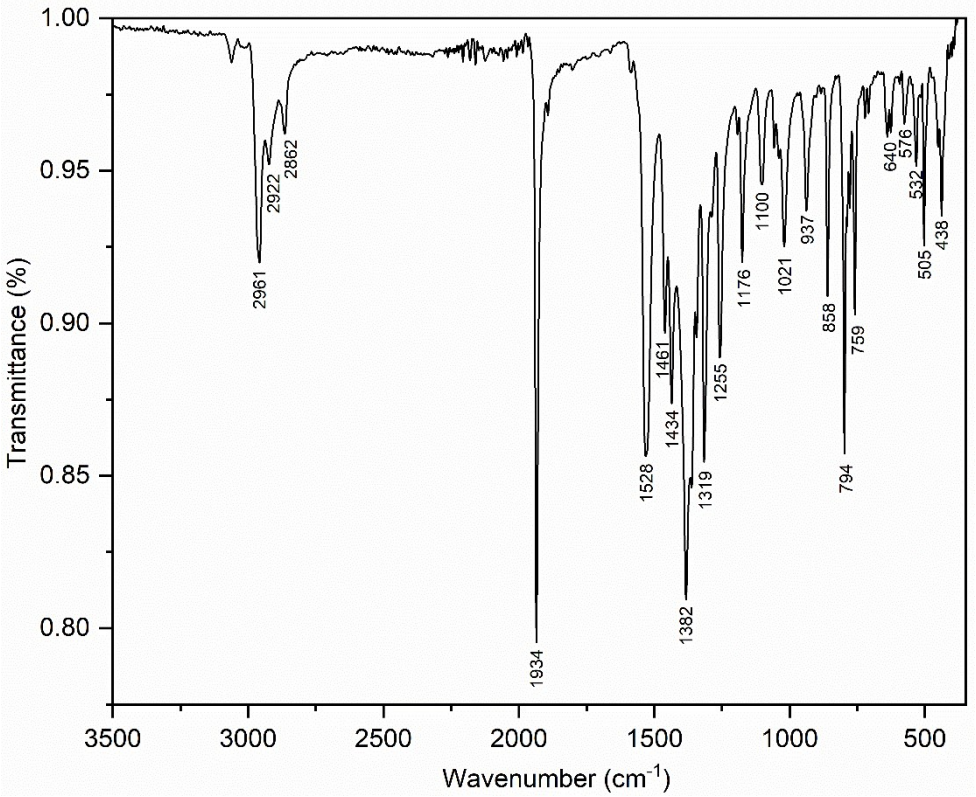

Figure 10: ATR-IR spectrum of [L(I)Ga]$_2$SiCO **2**.

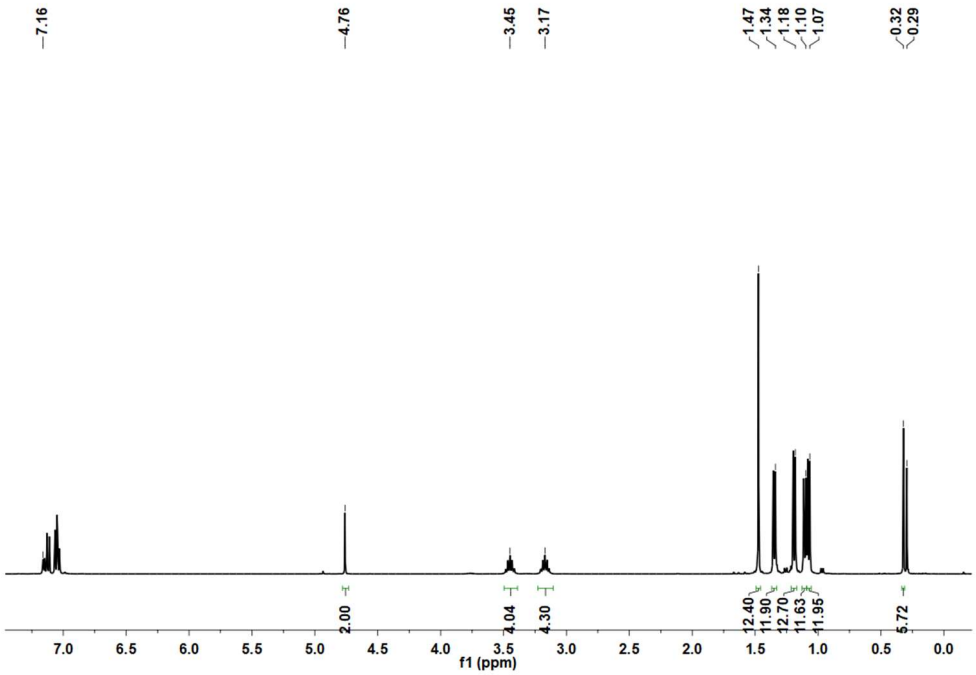

Figure S11: ^{1}H NMR spectrum of [L(Me)Ga]$_2$SiCO **3** in benzene-d_6 at room temperature.

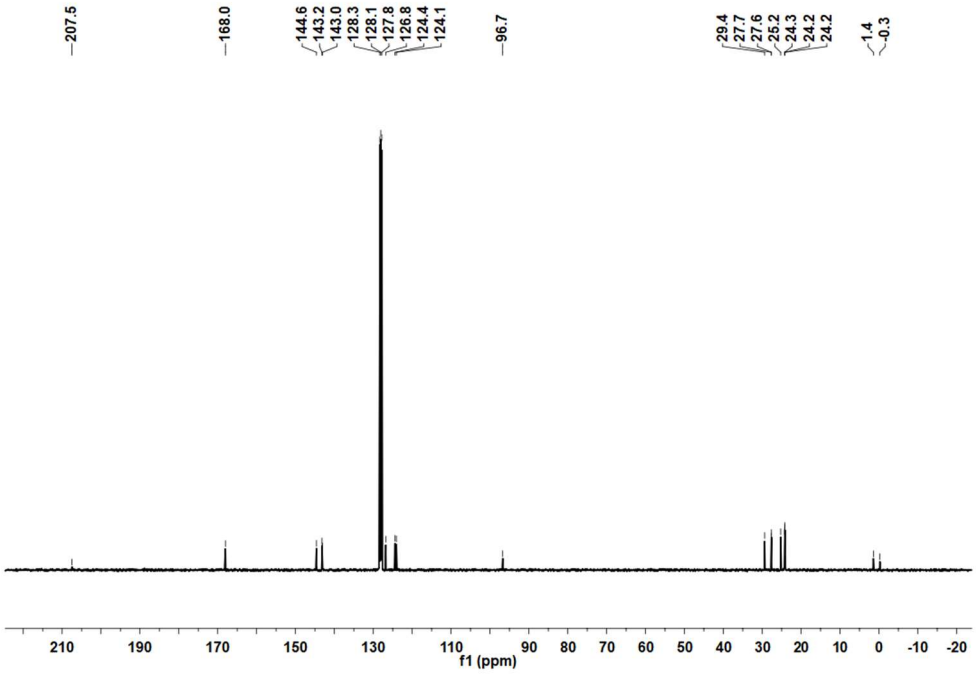

Figure S12: ^{13}C NMR spectrum of [L(Me)Ga]$_2$SiCO **3** in benzene-d_6 at room temperature.

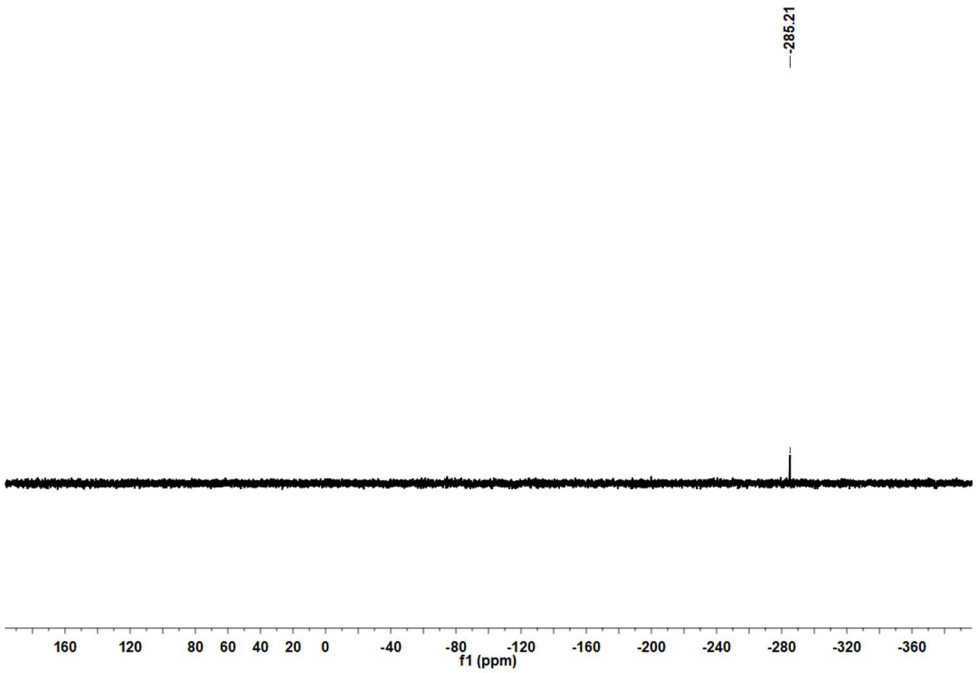

Figure S13: ^{29}Si NMR spectrum of [L(Me)Ga]$_2$SiCO **3** in benzene-d_6 at room temperature.

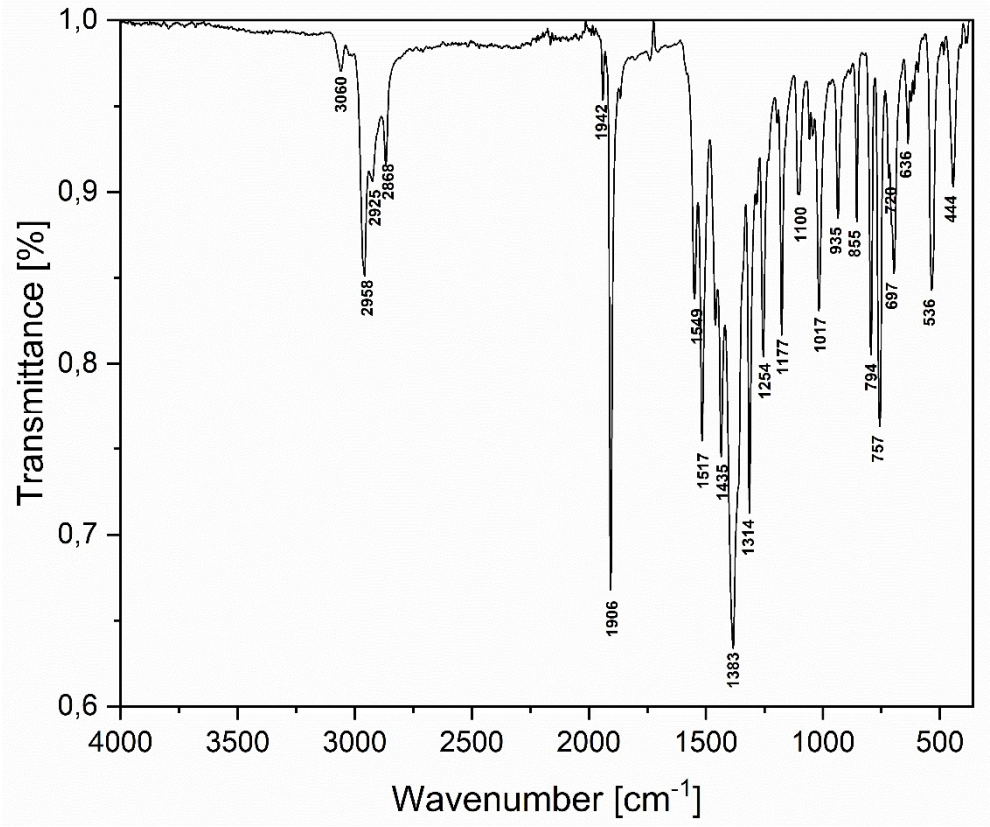

Figure S14: ATR-IR spectrum of [L(Me)Ga]$_2$SiCO **3**.

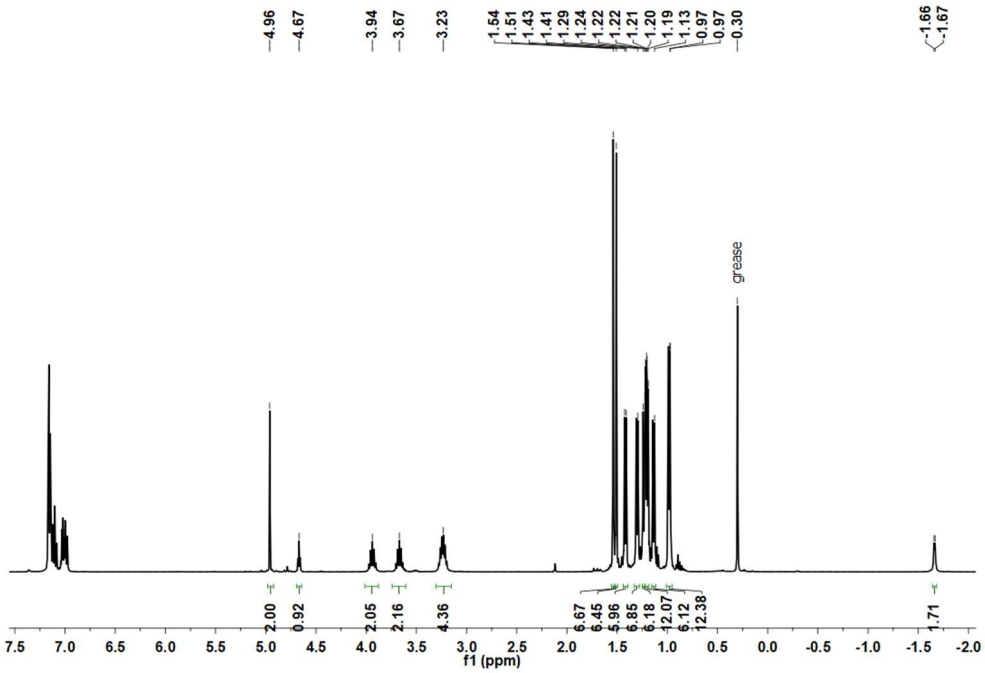

Figure S15: ^{1}H NMR spectrum of $[L(Br)Ga]_2Si(H)NH_2$ **4** in benzene-d_6 at room temperature.

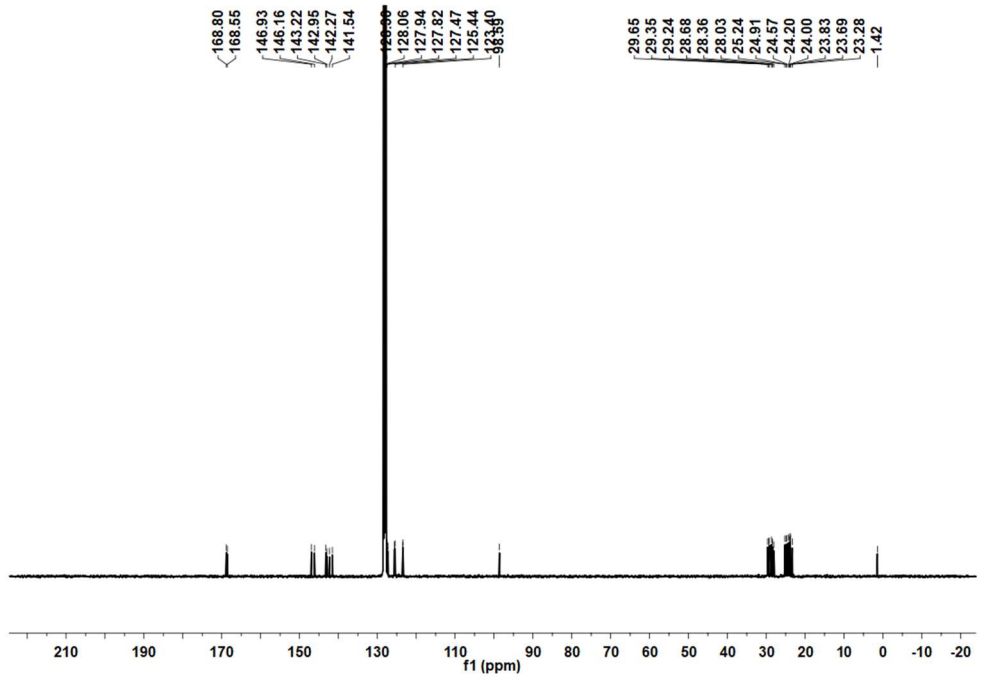

Figure S16: ^{13}C NMR spectrum of $[L(Br)Ga]_2Si(H)NH_2$ **4** in benzene-d_6 at room temperature.

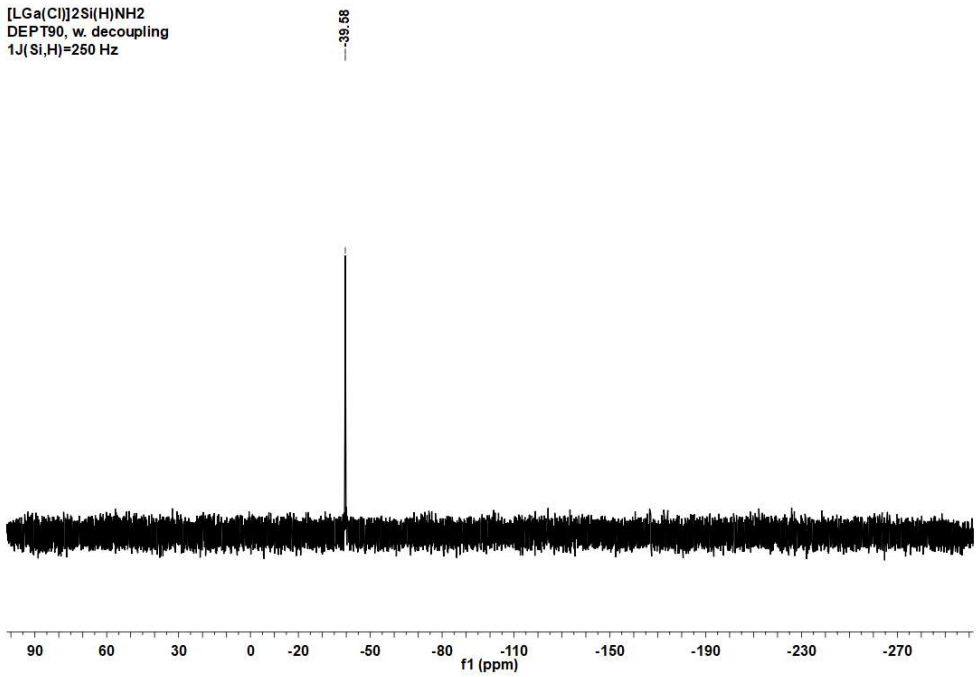

Figure S17: ^{29}Si NMR-DEPT90 (119 MHz) spectrum of $[L(Br)Ga]_2Si(H)NH_2$ **4** in benzene-d_6 at room temperature.

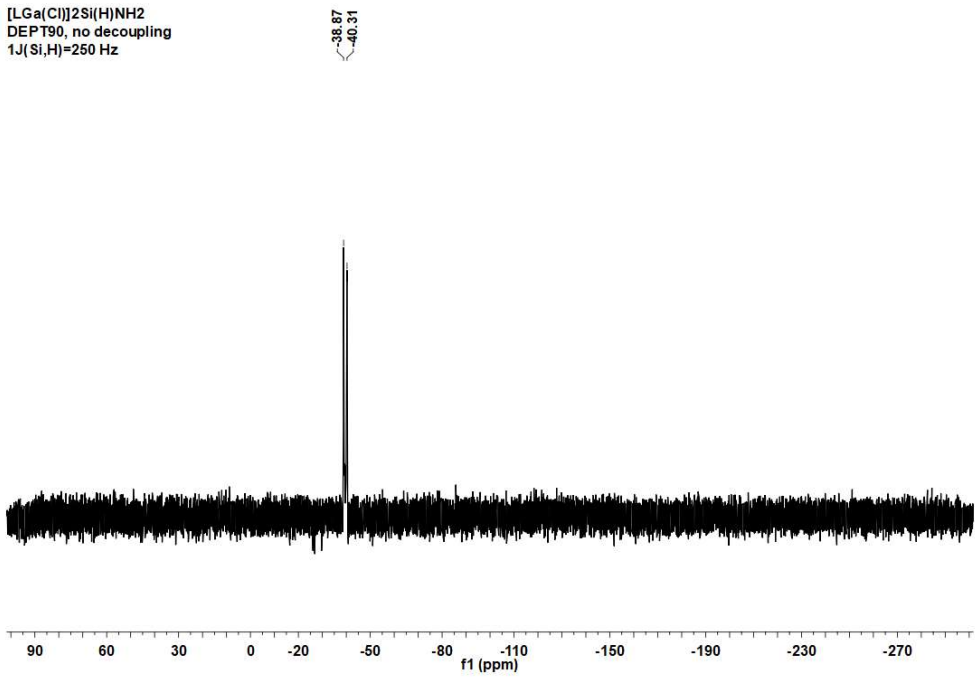

Figure S18: ^{29}Si{^{1}H} NMR DEPT90 (119 MHz) spectrum of $[L(Br)Ga]_2Si(H)NH_2$ **4** in benzene-d_6 at room temperature.

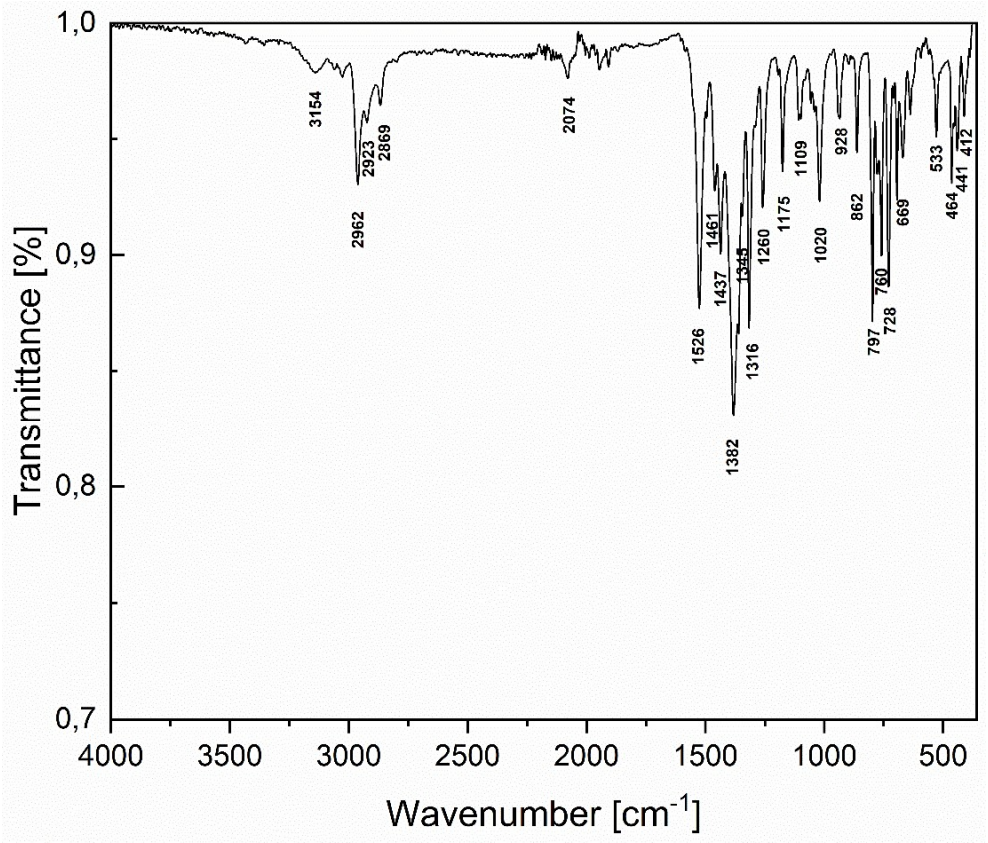

Figure S19: ATR-IR spectrum of $[L(Br)Ga]_2Si(H)NH_2$ **4**.

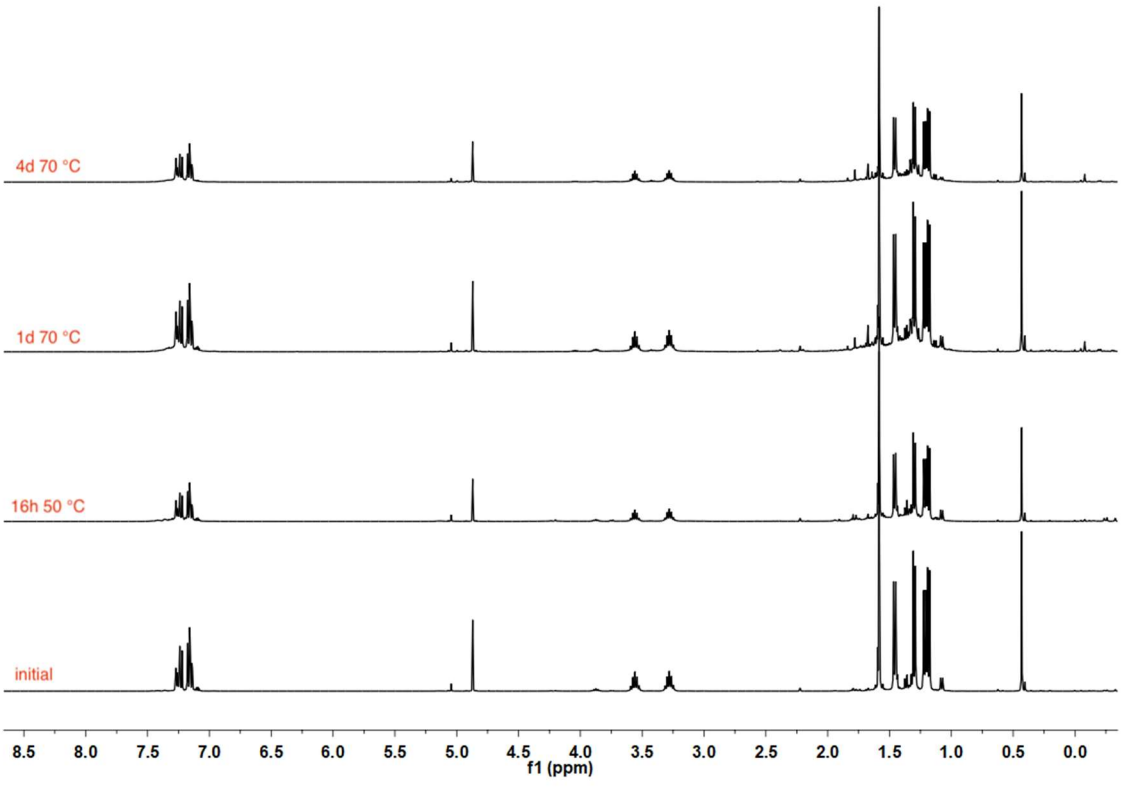

Figure S20: In situ ^1H NMR spectra of the reaction of **3** with NH_3 in benzene-d_6.

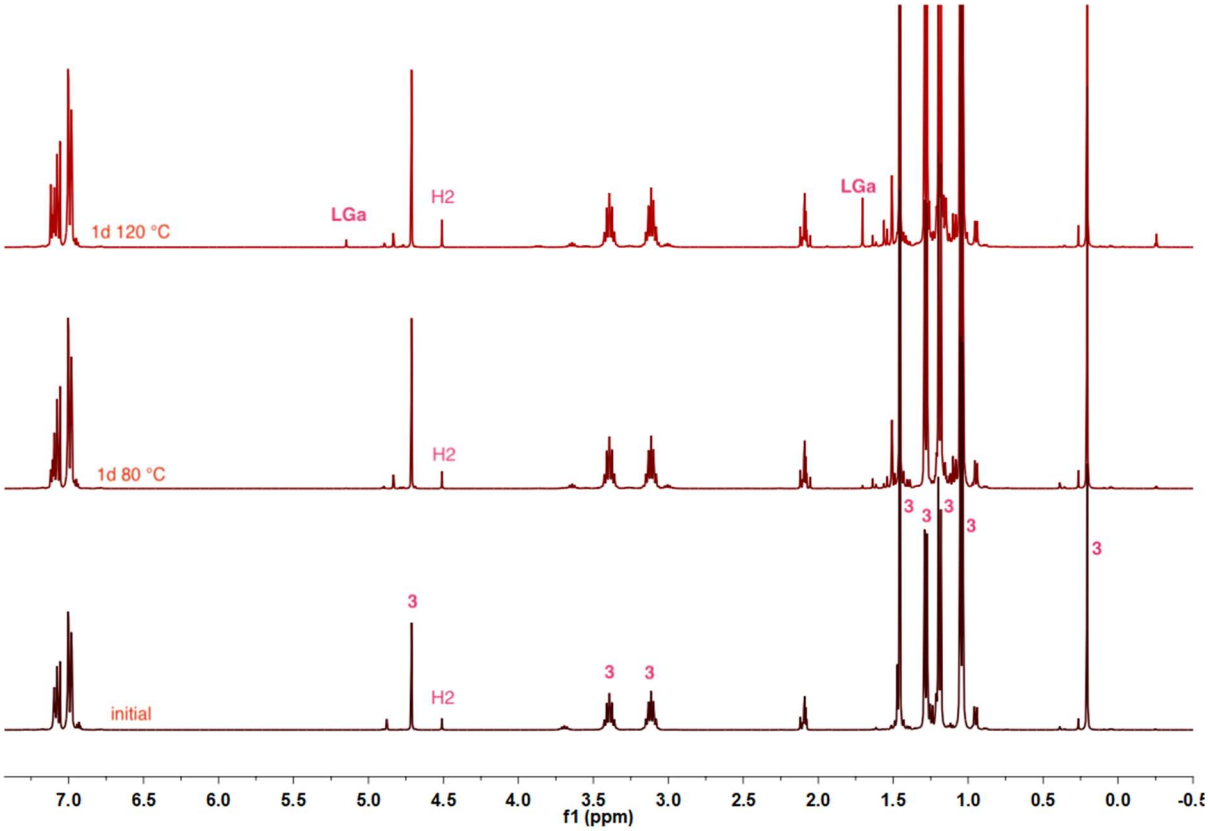

Figure S21: In situ ^{1}H NMR spectra of the reaction of **3** with H_2 in toluene-d_8.

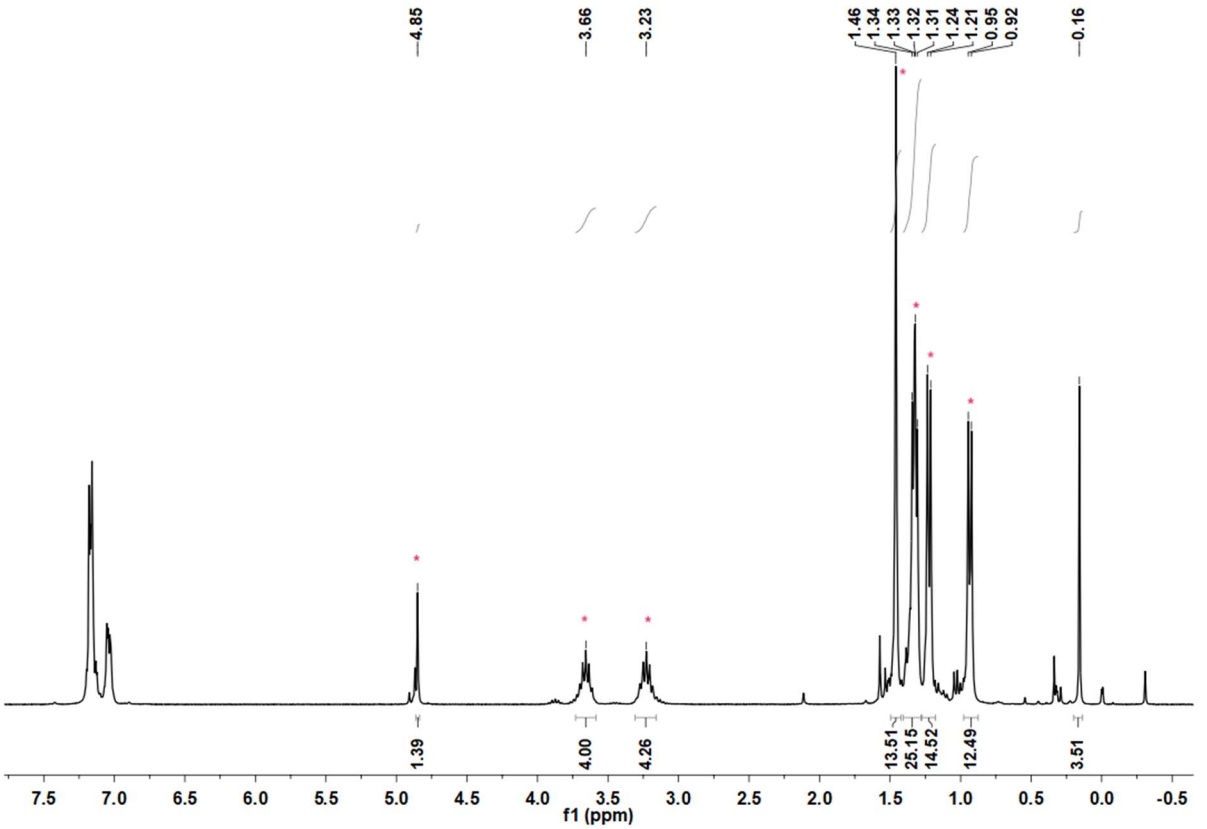

Figure S22: In situ ^{1}H NMR spectrum of the reaction of **I** with $SnCl_4$ in benzene-d_6. Resonances due to $[L(Cl)Ga]_2SiCl_2$ are marked (*).

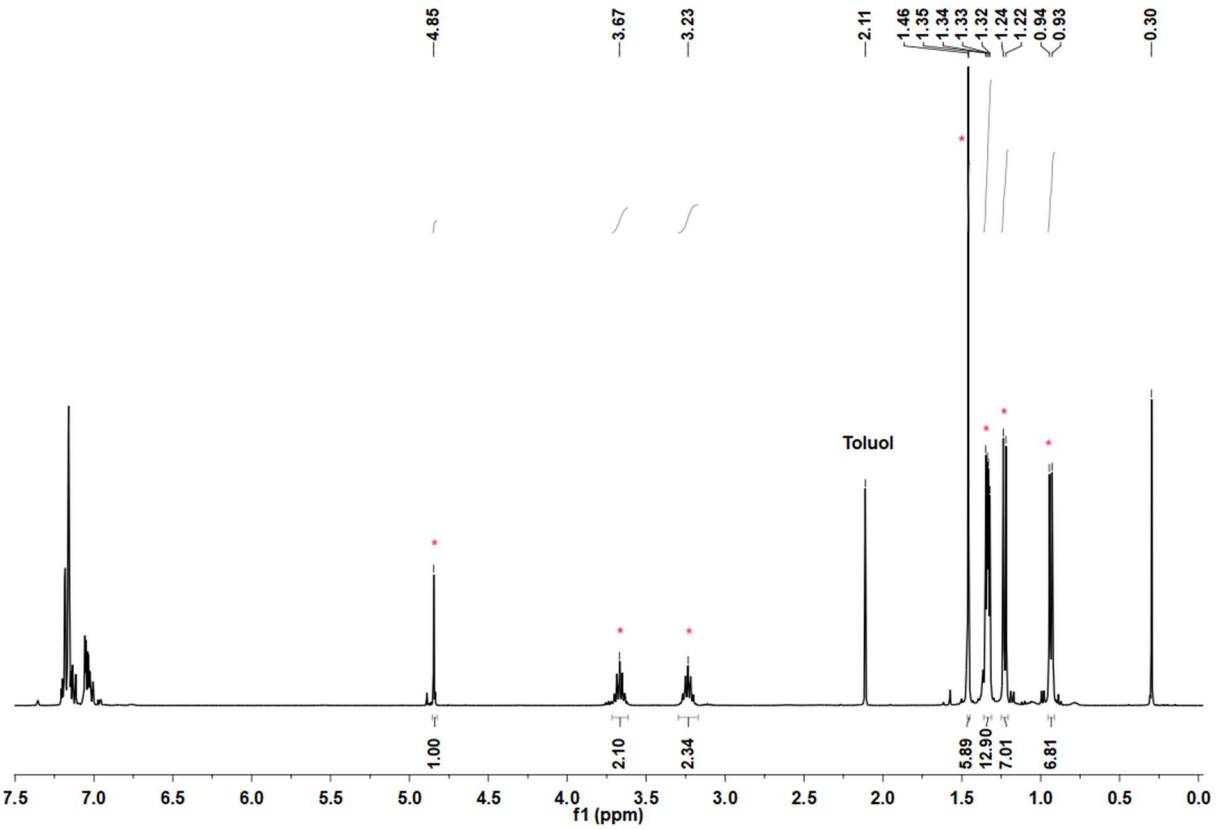

Figure S23: In situ ^{1}H NMR spectrum of the reaction of **3** with $SnCl_4$ in benzene-d_6. Resonances due to $[L(Cl)Ga]_2SiCl_2$ are marked (*).

II. Crystallographic Section

The crystals were mounted on nylon loops in inert oil. Data **1** and **2** were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) those of **3** and **4** on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, microfocus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)[5] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[6,7]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups. An isopropyl group in **3** is disordered over two positions. All corresponding bond lengths and angles were restrained to be equal (SADI), however since the smaller component is only occupied by about 10% its bond length are not very realistic. Forcing this with DFIX restraints results in significantly worse values for the displacement parameters and the other restraints becoming disagreeable. RIGU, SIMU and ISOR restraints were applied to the anisotropic displacement parameters of the smaller component's atoms. In **4** the molecule is disordered over a two-fold rotational axis. The corresponding atoms of the phenyl ring were restrained to lie on a mutual plane (FLAT). The anisotropic displacement parameters of the atoms and those of the bonded isopropyl group were restrained with RIGU. To overcome correlations ISOR restraints (σ 0.01) were applied to the anisotropic displacement parameters of C6 and C6'. Space group *Cc* was tried but the disorder still prevails.

CCDC-2144415 (**1**), -2144416 (**2**), -2144417 (**3**), and -2144418 (**4**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data of {[L(I)Ga]Si[Ga(I)][CHC(Me)NAr][C(Me)NAr]} (**1**), [L(I)Ga]$_2$SiCO (**2**), [L(Me)Ga]$_2$SiCO (**3**) and [L(Br)Ga]$_2$Si(H)NH$_2$ (**4**).

Identification code	**1**	**2**	**3**	**4**
Empirical formula	$C_{64}H_{88}Ga_2I_2N_4Si$	$C_{62}H_{85}Ga_2I_2N_4OSi$	$C_{61}H_{88}Ga_2N_4OSi$	$C_{58}H_{85}Br_2Ga_2N_5Si$
M	1334.71	1323.67	1060.88	1179.65
Crystal size [mm]	0.175 × 0.095 × 0.083	0.120 × 0.100 × 0.080	0.253 × 0.235 × 0.154	0.309 × 0.148 × 0.111
T [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic	monoclinic
Space group	*P*-1	*P*-1	*P*-1	*C*2/*c*
a [Å]	12.1170(4)	10.8429(18)	11.8953(3)	23.796(3)
b [Å]	12.5132(4)	14.778(3)	13.8148(3)	10.9213(12)
c [Å]	22.6085(7)	20.517(4)	19.8705(6)	23.597(3)
α [°]	87.712(2)	84.024(10)	79.3889(14)	90
β [°]	81.221(2)	77.522(9)	84.2512(15)	99.872(3)
γ [°]	68.836(2)	77.605(9)	66.0199(13)	90
V [Å^3]	3158.86(18)	3129.4(10)	2931.32(14)	6041.8(11)
Z	2	2	2	4
D_{calc} [g·cm^{-3}]	1.403	1.405	1.202	1.297
μ(MoK_α [mm^{-1}])	1.889	1.908	1.630	3.117
Transmissions	0.75/0.65	0.75/0.69	0.75/0.64	0.75/0.61
F(000)	1364	1350	1132	2456
Index ranges	-18 ≤ *h* ≤ 16	-13 ≤ *h* ≤ 16	-14 ≤ *h* ≤ 12	-26 ≤ *h* ≤ 30
	-19 ≤ *k* ≤ 17	-22 ≤ *k* ≤ 22	-17 ≤ *k* ≤ 17	-13 ≤ *k* ≤ 13
	-33 ≤ *l* ≤ 33	-31 ≤ *l* ≤ 31	-25 ≤ *l* ≤ 25	-30 ≤ *l* ≤ 30
θ_{max} [°]	33.299	33.447	81.691	80.635
Reflections collected	106341	173539	280503	89420
Independent reflections	20663	21878	12804	6604
R_{int}	0.0329	0.0645	0.0420	0.0540
Refined parameters	678	669	674	450
R_1 [$I > 2\sigma(I)$]	0.0478	0.0353	0.0291	0.0393
wR_2 [all data]	0.1212	0.0680	0.0775	0.0978
GooF	1.099	1.002	1.025	1.370
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	2.026/-1.703	1.305/-1.208	0.749/-0.577	0.334/-0.526

III. Quantum Chemical calculations

Table S2. Computed NBO charges and selected structural data (at the B3LYP-D3BJ level of theory with the 6-311G(d,p)basis set, and def2-TZVP for Ga, Br, I) for $[L(R)Ga]_2Si$:–CO complexes.

R =	F	Cl	Br	I	Me	OMe	NMe_2
Q_{Si}	–0.388	–0.307	–0.295	–0.281	–0.330	–0.334	–0.331
Q_{Ga1}	1.561	1.326	1.246	1.136	1.402	1.546	1.500
Q_{Ga2}	1.555	1.323	1.244	1.137	1.400	1.540	1.484
Q_{R1}	–0.712	–0.544	–0.473	–0.370	–1.203	–0.963	–0.966
Q_{R2}	–0.713	–0.546	–0.476	–0.373	–1.202	–0.959	–0.962
Q_C	0.256	0.263	0.265	0.266	0.242	0.253	0.236
Q_O	–0.424	–0.428	–0.426	–0.425	–0.466	–0.452	–0.463
$Q_C + Q_O$	–0.168	–0.165	–0.161	–0.159	–0.224	–0.199	–0.227
Ga^1-Si-Ga^2-R	25.5	26.6	25.7	25.6	52.1	60.0	63.7
r_{O-H}[a]	2.79	2.42	2.44	2.46	2.35	2.35	2.39
LP_{Si} %s, %p	75.83, 24.06	75.05, 24.84	74.84, 25.05	74.73, 25.15	74.98, 24.90	75.84, 24.04	74.25, 25.63
$LP_{Si} \rightarrow \pi^*_{CO}$	17.64	11.77	13.15	15.21	20.00	20.33	20.18
$\sigma_{Si-Ga} \rightarrow \pi^*_{CO}$	8.76, 18.09	11.16, 13.55	10.70, 13.06	12.56, 13.30	12.09, 14.01	12.10, 15.91	19.32, 8.67

[a] The distance between the carbonyl oxygen and the closest hydrogen of a methyl group (from *i*Pr).

Table S3. Computed Hirshfeld charges (at the B3LYP-D3BJ level of theory with the 6-311G(d,p)basis set, and def2-TZVP for Ga, Br, I) for $[L(R)Ga]_2Si$:–CO complexes.

R =	F	Cl	Br	I	Me	OMe_2nd	NMe_2_2nd
Q_{Si}	–0.049	–0.049	–0.049	–0.049	–0.083	–0.046	–0.061
Q_{Ga1}	0.356	0.311	0.297	0.289	0.290	0.345	0.317
Q_{Ga2}	0.357	0.311	0.297	0.289	0.290	0.345	0.316
Q_{R1}	–0.313	–0.222	–0.196	–0.180	–0.221	–0.284	–0.203
Q_{R2}	–0.309	–0.221	–0.194	–0.177	–0.223	–0.289	–0.204
Q_C	0.101	0.099	0.098	0.098	0.082	0.097	0.087
Q_O	–0.089	–0.087	–0.087	–0.088	–0.105	–0.095	–0.091
$Q_C + Q_O$	0.012	0.012	0.011	0.010	–0.023	0.002	–0.004

Note that the R groups influence the geometry of the complex. For one of the two R groups in each complex the R^1-Ga^1-Si-Ga^2 atoms are roughly on the same plane, but the other R group is on a different plane, as demonstrated by the Ga^1-Si-Ga^2-R angle. This dihedral angle is smaller for the halogens and larger for the other groups. As a result, for the halogens the oxygen is "sandwiched" between two aromatic rings, while for the other R groups the oxygen is close to one aromatic ring and to one methyl from the iPr substituents. This is illustrated by the r_{O-H} distances, which are shorter than the sum of the vdW radii of hydrogen and oxygen. This can also have an effect on the charge of the oxygen.

Comparison of ν_{CO} values to field/inductive and resonance parameters

Table S4. Field parameters (σ_F), resonance parameters (σ_R) and computed ν_{CO} values (cm^{-1}) for the different R groups.

	ν_{CO}	σ_F[a]	σ_I Charton[b]	σ_R[c]	R^-[d]
F	1966	0.45	0.54	-0.39	-0.48
Cl	1959	0.42	0.47	-0.19	-0.23
Br	1958	0.45	0.47	-0.22	-0.2
I	1956	0.42	0.4	-0.24	-0.15
Me	1925	0.01	-0.01	-0.18	-0.18
OMe	1946	0.29	0.3	-0.56	-0.55
NMe_2	1934	0.15	0.17	-0.98	-0.27

[a] σ_F matches the F parameter presented in Table I of reference [8].
[b] From reference [9].
[c] σ_R matches the R parameter presented in Table I of reference [8].
[d] R^- from Table V of reference [8].

Here we show a table with the values of the σ_F field/inductive parameter (Fig. 2 in the main text) and of the σ_R resonance parameter. These match the F and R parameters from table I of reference [8]. The F field parameter is based on pK_a values of substituted bicyclo[2.2.2]octane-1-carboxylic acids or of quinuclidinium cations, in which there is no resonance effect possible. Other field/inductive parameters listed in this reference (σ_I and σ_F values computed from different methods or reference reactions) also give good correlations with ν_{CO}. The R resonance parameter is produced by subtracting the (scaled) field effect F parameters from Hammett's σ_p parameter. R, and also other resonance parameters R^+, R^-, σ_{R+}, σ_{R-}, do not give clear correlations with ν_{CO}.

We chose to list here also two additional parameters from this reference: Charton's σ_I parameter[9] (from Table II) and the R^- parameters (from Table V). Charton's σ_I parameter, derived from pK_a values of substituted guanidinium cations, shows a good correlation with ν_{CO} (Fig. S24A). The R^- parameter is derived from the σ_p^- parameter by subtraction of the field/inductive parameter, such that it describes the conjugation of para substituents on a benzene ring with electron rich centers (phenols). This parameter shows a trend within the halogen series, but not between all groups (Fig. S24).

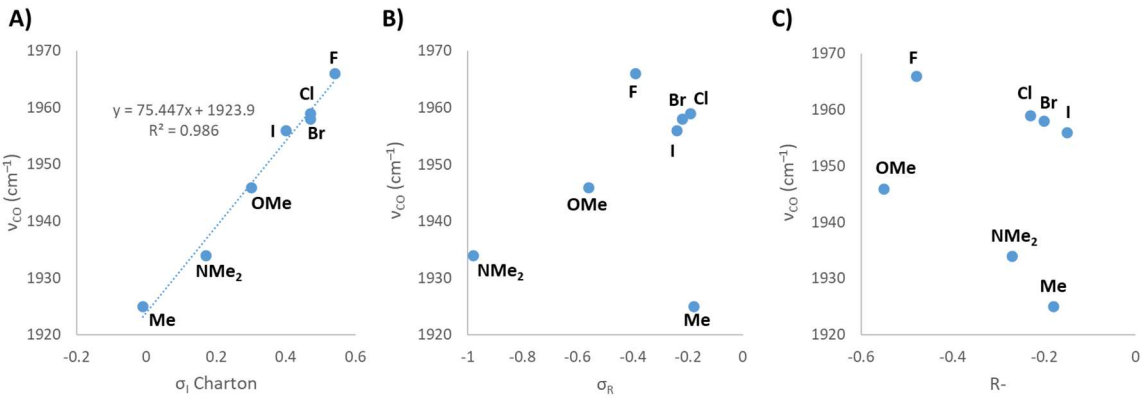

Figure S24. The correlation between ν_{CO} and A) Charton's σ_I parameter, B) the resonance σ_R parameter, and C) the R^- resonance parameter of the various groups.

Selected molecular orbitals

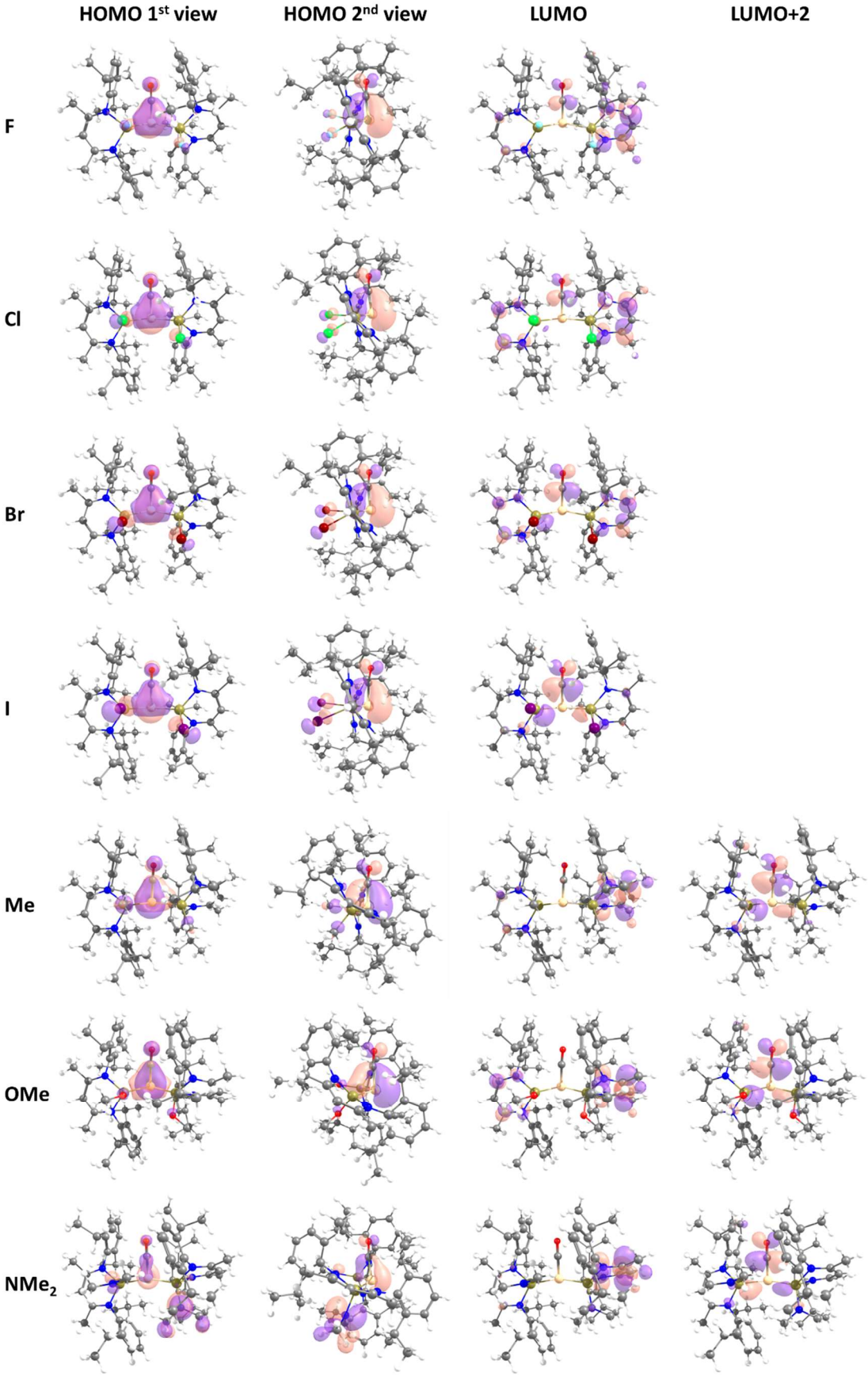

Figure S25: Selected molecular orbitals for the different computed derivatives. Colors by elements: C – grey; H – white; Si – beige; Ga – olive green; N – blue; O – red; F – light blue; Cl – green; Br – dark red; I – purple.

IV. Cartesian Coordinates

X = F
Imaginary frequencies: 0
Electronic Energy = -6932.31843751 a.u.
ZPVE correction = 1.289204 a.u.

Ga	1.977277	-0.250984	-0.483527
Ga	-2.025653	0.282286	-0.535721
Si	-0.049611	-0.042103	0.852570
O	-0.650225	-2.937034	0.779564
N	2.934724	-1.948917	-0.780286
N	3.551735	0.655615	0.331740
N	-3.688045	-0.464404	0.247093
N	-2.734669	2.110686	-0.668767
C	4.264401	-1.999985	-0.893586
C	-0.402036	-1.816735	0.707347
C	5.120174	-0.953465	-0.541730
H	6.174007	-1.131538	-0.700448
C	4.797001	0.247527	0.107494
C	4.912645	-3.278652	-1.369207
H	4.993337	-3.993544	-0.546646
H	5.916407	-3.075849	-1.740702
H	4.324143	-3.755109	-2.151693
C	5.966142	1.098535	0.547963
H	5.712458	1.743022	1.386722
H	6.277889	1.740026	-0.280093
H	6.812396	0.467199	0.817839
C	2.170259	-3.157993	-0.906953
C	1.443495	-3.396036	-2.088130
C	0.649362	-4.543637	-2.146637
H	0.074138	-4.742635	-3.042548
C	0.586832	-5.429575	-1.080428
H	-0.044113	-6.308822	-1.142262
C	1.332990	-5.190215	0.066551
H	1.273466	-5.886239	0.894446
C	2.136836	-4.056321	0.178682
C	1.562692	-2.489948	-3.305868
H	2.128749	-1.604113	-3.022149
C	0.203412	-2.002100	-3.822444
H	-0.412284	-2.831629	-4.183186
H	0.356143	-1.314475	-4.658446
H	-0.363429	-1.466742	-3.062283
C	2.343502	-3.201541	-4.425839
H	1.812089	-4.093551	-4.770558
H	3.337181	-3.513171	-4.094482
H	2.468863	-2.531910	-5.281079
C	2.919972	-3.806163	1.463537
H	3.657425	-3.027212	1.268461
C	2.016634	-3.286419	2.595029
H	1.580686	-2.317978	2.347779
H	2.596314	-3.164336	3.514678
H	1.194945	-3.978514	2.794287
C	3.687593	-5.055527	1.924443
H	3.009777	-5.843011	2.263494
H	4.345458	-4.806365	2.761388
H	4.299537	-5.470083	1.119596
C	3.300702	1.885154	1.027724
C	3.385145	3.109066	0.339427
C	3.080160	4.277662	1.042788
H	3.122991	5.230132	0.528443
C	2.728513	4.238314	2.383936
H	2.500319	5.156724	2.912823
C	2.661441	3.019672	3.050366
H	2.380301	3.000411	4.095362
C	2.930849	1.822457	2.387192
C	3.808930	3.193758	-1.119955
H	4.094628	2.195598	-1.449478
C	2.647499	3.637766	-2.016129
H	1.794837	2.971911	-1.907143
H	2.954250	3.617242	-3.065692
H	2.333058	4.653560	-1.770185
C	5.016998	4.128145	-1.304824
H	4.747665	5.167954	-1.099966
H	5.375762	4.078988	-2.336515
H	5.844262	3.867053	-0.641097
C	2.878612	0.488210	3.117991
H	2.612640	-0.270342	2.379744
C	1.816189	0.437948	4.220631
H	0.839611	0.738829	3.840056
H	2.074460	1.080878	5.066745
H	1.728575	-0.582545	4.601980
C	4.258604	0.105029	3.679158
H	4.606958	0.856181	4.394080
H	5.005250	0.017900	2.889180
H	4.203955	-0.857494	4.195828
C	-4.872083	0.098400	0.013730
C	-5.030361	1.376863	-0.538226
H	-6.049098	1.693833	-0.705045
C	-4.043881	2.339632	-0.783938
C	-6.134120	-0.659883	0.350321
H	-6.984562	0.016903	0.416153
H	-6.036349	-1.211290	1.284514
H	-6.337471	-1.392409	-0.434966
C	-4.517938	3.711233	-1.202661
H	-5.584768	3.823719	-1.017171
H	-4.334763	3.848492	-2.271177
H	-3.975866	4.501175	-0.684033
C	-3.609322	-1.712552	0.952775
C	-3.314617	-1.680633	2.331722
C	-3.209373	-2.894974	3.010306
H	-2.983496	-2.898231	4.068787
C	-3.376230	-4.103548	2.344650
H	-3.283584	-5.037538	2.887044
C	-3.640989	-4.114101	0.983142
H	-3.741753	-5.060852	0.466150
C	-3.758398	-2.925612	0.259238
C	-3.127998	-0.357604	3.061393
H	-2.731803	0.353144	2.334683
C	-4.467238	0.207901	3.563167
H	-5.157142	0.400889	2.741092
H	-4.306828	1.152612	4.090622

H	-4.946884	-0.491104	4.254644
C	-2.113975	-0.438604	4.207705
H	-2.489589	-1.032816	5.045277
H	-1.905816	0.564307	4.588300
H	-1.171027	-0.871482	3.869822
C	-3.981223	-2.978607	-1.244294
H	-4.139089	-1.961738	-1.603668
C	-5.212021	-3.819243	-1.619259
H	-5.063983	-4.875043	-1.376157
H	-5.399868	-3.752280	-2.694147
H	-6.110100	-3.484209	-1.094326
C	-2.726142	-3.508342	-1.954699
H	-2.498869	-4.530721	-1.640840
H	-1.859252	-2.888484	-1.738851
H	-2.874603	-3.501114	-3.037590
C	-1.818411	3.213702	-0.735752
C	-1.421242	3.814830	0.474215
C	-0.583772	4.929602	0.411310
H	-0.262386	5.410209	1.326502
C	-0.157849	5.430070	-0.812377
H	0.482978	6.303891	-0.845135
C	-0.525384	4.795506	-1.991493
H	-0.154148	5.170647	-2.937459
C	-1.345859	3.666125	-1.980305
C	-1.930729	3.293822	1.810498
H	-2.243271	2.260847	1.654772
C	-3.169473	4.072225	2.283794
H	-3.992250	3.990776	1.571947
H	-2.934426	5.132999	2.411595
H	-3.519807	3.682838	3.244071
C	-0.847286	3.278594	2.892159
H	-1.222217	2.778458	3.789055
H	-0.542604	4.287556	3.182715
H	0.040552	2.747653	2.550966
C	-1.683443	2.947051	-3.277608
H	-2.437872	2.190980	-3.059122
C	-0.452659	2.202067	-3.821684
H	-0.026733	1.516874	-3.089765
H	0.331502	2.907435	-4.112985
H	-0.731734	1.617739	-4.702497
C	-2.252699	3.897629	-4.342443
H	-2.573751	3.328666	-5.218885
H	-1.502187	4.619288	-4.676852
H	-3.111061	4.463289	-3.970837
F	-2.103449	-0.304095	-2.250368
F	1.899637	0.550016	-2.111990

X = Cl

Imaginary frequencies: 0

Electronic Energy = -7653.05083418 a.u.

ZPVE correction = 1.288410 a.u.

Ga	1.966481	0.373084	-0.558245
Ga	-2.034290	-0.343554	-0.589363
Si	-0.057841	0.091720	0.769385
O	0.436646	-2.796360	1.135099
N	3.456237	-0.922294	-0.694246
N	3.086989	1.789631	0.286087
N	-3.265000	-1.691007	0.182358
N	-3.366088	1.127343	-0.564092
C	4.694215	-0.463956	-0.909642
C	0.234954	-1.691182	0.886296
C	5.097685	0.849334	-0.651994
H	6.128291	1.076671	-0.881743
C	4.387840	1.859330	0.015193
C	5.742391	-1.397460	-1.467792
H	5.654051	-2.403465	-1.062078
H	6.743947	-1.016107	-1.275370
H	5.604780	-1.470971	-2.549988
C	5.181468	3.074960	0.431888
H	4.825040	3.486761	1.374639
H	5.075978	3.855514	-0.325256
H	6.238519	2.828660	0.520645
C	3.216708	-2.343016	-0.695007
C	2.870096	-3.009901	-1.882784
C	2.611576	-4.382054	-1.813754
H	2.326083	-4.910858	-2.715155
C	2.721030	-5.075670	-0.618195
H	2.517203	-6.139968	-0.586954
C	3.089133	-4.404721	0.541965
H	3.161810	-4.953043	1.472164
C	3.332825	-3.032570	0.530989
C	2.805023	-2.302656	-3.227274
H	3.127639	-1.272121	-3.083104
C	1.373253	-2.252914	-3.776166
H	0.994088	-3.259064	-3.975336
H	1.347854	-1.687043	-4.710630
H	0.690165	-1.763542	-3.084900
C	3.749004	-2.955621	-4.251909
H	3.412078	-3.961034	-4.518898
H	4.769444	-3.041325	-3.871006
H	3.773973	-2.361268	-5.169146
C	3.721351	-2.302048	1.810609
H	3.373129	-1.272597	1.708197
C	3.077958	-2.886725	3.075542
H	1.998773	-2.995022	2.970269
H	3.278803	-2.229108	3.925202
H	3.495592	-3.866434	3.323487
C	5.249650	-2.246791	1.987348
H	5.667341	-3.257534	2.010680
H	5.505469	-1.751145	2.927771
H	5.734835	-1.696454	1.182342
C	2.460160	2.813303	1.076834
C	2.062709	4.025383	0.484387
C	1.468236	4.993600	1.299372
H	1.146977	5.929276	0.858083
C	1.285234	4.777998	2.656413
H	0.829769	5.544423	3.273101
C	1.667106	3.566907	3.222753
H	1.498535	3.397915	4.278339
C	2.241615	2.559917	2.447645
C	2.239615	4.305048	-0.999116
H	2.794433	3.477674	-1.439769
C	0.875819	4.362842	-1.699791
H	0.278339	3.477665	-1.487653

H	1.005511	4.423373	-2.782882
H	0.308537	5.234653	-1.369360
C	3.022131	5.603098	-1.259207
H	2.455703	6.480151	-0.934262
H	3.216636	5.714759	-2.329156
H	3.980057	5.619470	-0.734755
C	2.647943	1.233500	3.070962
H	2.549977	0.476920	2.290878
C	1.735515	0.803576	4.224919
H	0.685848	0.846180	3.930805
H	1.873301	1.429805	5.110726
H	1.964442	-0.224854	4.513933
C	4.119947	1.243221	3.514826
H	4.294487	2.032738	4.251464
H	4.794205	1.406802	2.673434
H	4.385753	0.286649	3.972812
C	-4.575088	-1.603795	-0.057791
C	-5.201093	-0.447609	-0.534676
H	-6.264084	-0.528190	-0.706685
C	-4.665181	0.843549	-0.660301
C	-5.453287	-2.804922	0.198025
H	-6.504954	-2.523885	0.200273
H	-5.207345	-3.291396	1.141122
H	-5.292571	-3.542491	-0.592718
C	-5.656711	1.955581	-0.910768
H	-6.661939	1.639404	-0.637386
H	-5.654864	2.215563	-1.971566
H	-5.399085	2.857886	-0.358139
C	-2.753919	-2.804095	0.937550
C	-2.635610	-2.658961	2.335495
C	-2.131143	-3.730358	3.073254
H	-2.036243	-3.640226	4.148173
C	-1.743188	-4.909321	2.450276
H	-1.345376	-5.728670	3.037990
C	-1.854878	-5.030152	1.073263
H	-1.533459	-5.944799	0.589914
C	-2.359059	-3.988583	0.291810
C	-3.076644	-1.386990	3.043572
H	-3.129787	-0.598455	2.293318
C	-4.486784	-1.543997	3.637715
H	-5.224480	-1.766540	2.865070
H	-4.795688	-0.622697	4.139190
H	-4.509773	-2.355498	4.370894
C	-2.081553	-0.934734	4.119397
H	-2.023165	-1.646141	4.946993
H	-2.395369	0.024080	4.538265
H	-1.081315	-0.811172	3.700654
C	-2.419672	-4.152862	-1.216551
H	-2.912585	-3.276544	-1.636648
C	-3.223113	-5.394633	-1.634507
H	-2.727137	-6.317273	-1.320753
H	-3.324246	-5.427145	-2.722508
H	-4.225351	-5.395161	-1.198880
C	-1.001743	-4.203357	-1.805056
H	-0.456053	-5.078805	-1.443226
H	-0.424649	-3.321096	-1.533461
H	-1.045357	-4.245955	-2.895523
C	-2.947049	2.505116	-0.552955
C	-2.684989	3.109692	0.693736
C	-2.354298	4.465655	0.716308
H	-2.147085	4.948912	1.661679
C	-2.292357	5.205330	-0.456928
H	-2.046603	6.260632	-0.420181
C	-2.517842	4.586260	-1.677134
H	-2.432671	5.161665	-2.590869
C	-2.833142	3.227881	-1.756299
C	-2.819606	2.327119	1.991407
H	-2.591301	1.285865	1.763159
C	-4.259808	2.371293	2.528475
H	-4.967509	1.926772	1.827562
H	-4.569242	3.403227	2.718121
H	-4.331322	1.817382	3.468693
C	-1.822905	2.775739	3.063021
H	-1.863448	2.096986	3.917222
H	-2.044302	3.779690	3.435545
H	-0.803975	2.774697	2.677956
C	-3.015528	2.585543	-3.122620
H	-3.388555	1.571827	-2.977884
C	-1.662554	2.470848	-3.844207
H	-0.936511	1.912189	-3.256273
H	-1.246646	3.462225	-4.046935
H	-1.786600	1.948916	-4.796418
C	-4.022119	3.345814	-4.002026
H	-4.210125	2.785937	-4.921739
H	-3.639148	4.328678	-4.289642
H	-4.978170	3.501712	-3.496607
Cl	1.709658	1.106321	-2.647563
Cl	-1.939281	-0.878337	-2.748740

X = Br

Imaginary frequencies: 0

Electronic Energy = -11880.9651023 a.u.

ZPVE correction = 1.287583 a.u.

Ga	2.000653	0.258646	-0.432471
Ga	-2.057811	-0.236449	-0.441903
Si	-0.040156	0.082484	0.892105
O	0.309148	-2.823617	1.281971
N	3.425999	-1.115186	-0.537617
N	3.178144	1.624378	0.425814
N	-3.339240	-1.534799	0.337084
N	-3.310997	1.306544	-0.351001
C	4.684806	-0.714609	-0.747962
C	0.159990	-1.712488	1.022758
C	5.144393	0.582301	-0.501109
H	6.184996	0.760741	-0.729449
C	4.482247	1.628128	0.160681
C	5.695170	-1.696754	-1.292201
H	5.536635	-2.703778	-0.911829
H	6.710577	-1.377885	-1.061962
H	5.587830	-1.738401	-2.379720
C	5.335491	2.802704	0.577570
H	4.988831	3.244688	1.510044
H	5.284874	3.578315	-0.190429
H	6.375901	2.499473	0.684952

C	3.122262	-2.524315	-0.512167
C	2.748091	-3.201096	-1.686345
C	2.418705	-4.556211	-1.588063
H	2.110401	-5.089209	-2.479413
C	2.488590	-5.228611	-0.377770
H	2.229183	-6.279797	-0.323842
C	2.892515	-4.552660	0.767011
H	2.940082	-5.084101	1.708559
C	3.206059	-3.195310	0.726853
C	2.735265	-2.530278	-3.050325
H	3.087643	-1.506807	-2.927284
C	1.319944	-2.452799	-3.636117
H	0.913334	-3.452031	-3.814992
H	1.334828	-1.915140	-4.587301
H	0.637044	-1.921361	-2.975989
C	3.681690	-3.242688	-4.032581
H	3.318510	-4.244495	-4.277922
H	4.689329	-3.349239	-3.624505
H	3.747359	-2.676794	-4.965740
C	3.643867	-2.466112	1.990371
H	3.379176	-1.415672	1.861545
C	2.950032	-2.968828	3.263724
H	1.865549	-2.983562	3.156506
H	3.206630	-2.317166	4.102613
H	3.278329	-3.977081	3.530330
C	5.171255	-2.529505	2.171845
H	5.505562	-3.569489	2.229280
H	5.466133	-2.025424	3.096196
H	5.699826	-2.048182	1.349795
C	2.604209	2.673702	1.225436
C	2.267959	3.910652	0.646022
C	1.732403	4.903281	1.472528
H	1.459191	5.857974	1.039737
C	1.547888	4.688768	2.829164
H	1.139586	5.474275	3.454814
C	1.868507	3.454763	3.383207
H	1.700050	3.287088	4.438964
C	2.381692	2.423945	2.596541
C	2.448295	4.197987	-0.835088
H	2.945239	3.343134	-1.292096
C	1.083435	4.351443	-1.519219
H	0.434777	3.501464	-1.312574
H	1.204747	4.420885	-2.602659
H	0.574158	5.251121	-1.169029
C	3.308843	5.447191	-1.087750
H	2.802589	6.354230	-0.746178
H	3.499463	5.559613	-2.158328
H	4.270931	5.396041	-0.573490
C	2.720393	1.075435	3.211876
H	2.585036	0.329537	2.427475
C	1.785880	0.685970	4.362698
H	0.740376	0.779550	4.065953
H	1.950842	1.302405	5.250663
H	1.964303	-0.352688	4.649402
C	4.190571	1.011095	3.657257
H	4.402175	1.787818	4.397754
H	4.873127	1.146247	2.817399
H	4.409482	0.040890	4.111120
C	-4.646005	-1.377393	0.111549
C	-5.217562	-0.182042	-0.335257
H	-6.284915	-0.206711	-0.497708
C	-4.623099	1.086667	-0.431680
C	-5.580932	-2.538277	0.351248
H	-6.617098	-2.205295	0.372404
H	-5.349728	-3.058658	1.279752
H	-5.465701	-3.263687	-0.458557
C	-5.568767	2.247998	-0.630908
H	-6.572250	1.982756	-0.302125
H	-5.613033	2.502854	-1.692156
H	-5.236865	3.137285	-0.097876
C	-2.880779	-2.677485	1.083461
C	-2.762130	-2.550664	2.483403
C	-2.307410	-3.648772	3.214192
H	-2.214116	-3.571374	4.290277
C	-1.969418	-4.838891	2.583990
H	-1.609206	-5.679156	3.166366
C	-2.085598	-4.944585	1.206389
H	-1.806808	-5.869759	0.716653
C	-2.541525	-3.876071	0.431600
C	-3.156496	-1.271605	3.205643
H	-3.198524	-0.476067	2.462434
C	-4.561611	-1.395497	3.819479
H	-5.315252	-1.597089	3.056467
H	-4.840428	-0.468702	4.328327
H	-4.594913	-2.208894	4.550106
C	-2.133559	-0.857894	4.270767
H	-2.069506	-1.588299	5.081055
H	-2.424297	0.095477	4.717314
H	-1.139809	-0.740711	3.834878
C	-2.615562	-4.035249	-1.076151
H	-3.057049	-3.131102	-1.494310
C	-3.493143	-5.226545	-1.492076
H	-3.052841	-6.177360	-1.179261
H	-3.598751	-5.252555	-2.579858
H	-4.492447	-5.166720	-1.053996
C	-1.205554	-4.170232	-1.669603
H	-0.712413	-5.077844	-1.311485
H	-0.575343	-3.325036	-1.397704
H	-1.255035	-4.207753	-2.759923
C	-2.823209	2.661945	-0.305838
C	-2.502005	3.210964	0.953355
C	-2.091691	4.543826	1.011602
H	-1.835420	4.981985	1.966578
C	-2.011352	5.318471	-0.137453
H	-1.701757	6.355406	-0.072204
C	-2.303831	4.755841	-1.369984
H	-2.208979	5.356282	-2.266481
C	-2.699374	3.421092	-1.486031
C	-2.659568	2.400174	2.230727
H	-2.472955	1.356926	1.974720
C	-4.093821	2.489267	2.778339
H	-4.823277	2.088868	2.073311
H	-4.360218	3.528404	2.992283
H	-4.181783	1.918670	3.706993
C	-1.640829	2.783240	3.306901
H	-1.699672	2.084062	4.142709

H	-1.824256	3.783792	3.708096
H	-0.625642	2.756690	2.913317
C	-2.956688	2.848436	-2.870788
H	-3.360220	1.842447	-2.757108
C	-1.637827	2.722604	-3.650583
H	-0.909561	2.115769	-3.115148
H	-1.196511	3.707896	-3.827549
H	-1.815484	2.247171	-4.618484
C	-3.966950	3.684152	-3.674788
H	-4.211468	3.174079	-4.610125
H	-3.557356	4.664327	-3.933461
H	-4.895850	3.852455	-3.125254
Br	1.795665	1.036903	-2.676062
Br	-2.040786	-0.764331	-2.763461

X = I

Imaginary frequencies: 0

Electronic Energy = -7328.19810153 a.u.

ZPVE correction = 1.287315 a.u.

I	1.872115	1.045900	-2.759850
I	-2.170110	-0.691793	-2.826215
Ga	2.025854	0.194968	-0.311687
Ga	-2.074190	-0.182856	-0.285449
Si	-0.021910	0.073950	1.012042
O	0.275686	-2.832162	1.442660
N	3.419026	-1.220621	-0.394254
N	3.223002	1.531431	0.573072
N	-3.358178	-1.470669	0.513385
N	-3.287225	1.394811	-0.109289
C	4.684073	-0.840349	-0.606057
C	0.140695	-1.723336	1.166004
C	5.163794	0.450976	-0.365692
H	6.205793	0.611621	-0.600966
C	4.526687	1.507527	0.304487
C	5.679701	-1.837503	-1.149831
H	5.486861	-2.847935	-0.795936
H	6.698371	-1.551030	-0.892754
H	5.593728	-1.850153	-2.240227
C	5.406570	2.660611	0.725125
H	5.083048	3.092936	1.670425
H	5.354601	3.449284	-0.029405
H	6.443535	2.339301	0.809779
C	3.092736	-2.625821	-0.350243
C	2.705720	-3.315895	-1.513049
C	2.345666	-4.661462	-1.393337
H	2.026817	-5.201055	-2.276954
C	2.400870	-5.316921	-0.173466
H	2.117021	-6.360730	-0.102602
C	2.827107	-4.633159	0.957916
H	2.871019	-5.152088	1.906532
C	3.171432	-3.283997	0.896280
C	2.718262	-2.677289	-2.891502
H	3.081529	-1.655570	-2.787694
C	1.312901	-2.599665	-3.499045
H	0.896658	-3.598206	-3.657954
H	1.345079	-2.085401	-4.462477
H	0.627841	-2.044775	-2.860520
C	3.671105	-3.421740	-3.843354
H	3.300904	-4.425140	-4.070916
H	4.671384	-3.528667	-3.418094
H	3.755974	-2.877536	-4.787816
C	3.648491	-2.557613	2.146203
H	3.435274	-1.497945	2.003486
C	2.937518	-3.010662	3.428555
H	1.853043	-2.964210	3.329032
H	3.237700	-2.370262	4.261233
H	3.209088	-4.034239	3.699885
C	5.172059	-2.695417	2.318900
H	5.453210	-3.749670	2.396907
H	5.500553	-2.186791	3.229267
H	5.717192	-2.261178	1.481406
C	2.680564	2.579778	1.398633
C	2.366951	3.837159	0.850519
C	1.875303	4.828526	1.705462
H	1.621190	5.798103	1.294816
C	1.711013	4.595219	3.061116
H	1.338175	5.380260	3.709085
C	2.006212	3.342183	3.584720
H	1.853225	3.158818	4.640143
C	2.474133	2.312230	2.769247
C	2.522482	4.153792	-0.626596
H	2.983740	3.296203	-1.114908
C	1.146236	4.364308	-1.272169
H	0.476840	3.528776	-1.070021
H	1.242104	4.458622	-2.356101
H	0.672286	5.268414	-0.885652
C	3.414070	5.381944	-0.874005
H	2.943633	6.296643	-0.502950
H	3.583637	5.509849	-1.946347
H	4.385662	5.291423	-0.383701
C	2.781799	0.945249	3.358191
H	2.620853	0.217242	2.562222
C	1.844388	0.562680	4.509315
H	0.800160	0.689028	4.220746
H	2.030778	1.161013	5.405291
H	1.996059	-0.484044	4.779628
C	4.252821	0.837534	3.792236
H	4.489171	1.600405	4.539571
H	4.932830	0.964817	2.948949
H	4.450451	-0.142486	4.234132
C	-4.665350	-1.280996	0.309961
C	-5.217738	-0.064175	-0.099701
H	-6.287697	-0.064149	-0.247079
C	-4.603931	1.198706	-0.163915
C	-5.620160	-2.428669	0.533473
H	-6.649675	-2.077217	0.571815
H	-5.390579	-2.974105	1.447850
H	-5.525358	-3.137300	-0.293833
C	-5.539793	2.377382	-0.297559
H	-6.520210	2.131840	0.107748
H	-5.661510	2.622296	-1.355303
H	-5.153821	3.264150	0.201135
C	-2.917123	-2.629506	1.247605
C	-2.796981	-2.520403	2.649179

C	-2.360079	-3.632624	3.369509
H	-2.267036	-3.566854	4.446361
C	-2.041448	-4.822293	2.729340
H	-1.694229	-5.673429	3.303729
C	-2.163485	-4.913453	1.351576
H	-1.903897	-5.839304	0.852737
C	-2.603147	-3.830715	0.587243
C	-3.174660	-1.247292	3.389650
H	-3.225045	-0.443543	2.656225
C	-4.570184	-1.373602	4.024672
H	-5.335870	-1.567831	3.271754
H	-4.839373	-0.450607	4.545361
H	-4.594028	-2.192892	4.749006
C	-2.132371	-0.852841	4.443205
H	-2.048416	-1.601698	5.234389
H	-2.417968	0.087788	4.918503
H	-1.147932	-0.721983	3.990056
C	-2.690555	-3.983655	-0.919389
H	-3.118676	-3.070196	-1.330899
C	-3.595613	-5.154148	-1.334802
H	-3.173205	-6.115933	-1.031036
H	-3.710072	-5.170838	-2.421859
H	-4.589961	-5.075338	-0.888570
C	-1.287811	-4.144387	-1.522626
H	-0.810707	-5.063202	-1.171403
H	-0.638713	-3.313552	-1.249479
H	-1.344056	-4.174966	-2.612666
C	-2.771525	2.739837	-0.025955
C	-2.399718	3.232153	1.243530
C	-1.953239	4.550896	1.342145
H	-1.656991	4.942850	2.305285
C	-1.887938	5.370948	0.224549
H	-1.548795	6.396026	0.321898
C	-2.237373	4.867657	-1.017934
H	-2.159728	5.502823	-1.891818
C	-2.670723	3.548749	-1.175659
C	-2.546463	2.382628	2.496303
H	-2.380064	1.345320	2.204632
C	-3.969794	2.479627	3.070891
H	-4.718016	2.112417	2.367529
H	-4.214001	3.516711	3.318372
H	-4.052546	1.884881	3.984520
C	-1.504215	2.718349	3.565772
H	-1.557247	1.995055	4.380427
H	-1.667678	3.707911	4.001213
H	-0.496686	2.691432	3.153261
C	-2.996690	3.055538	-2.575872
H	-3.400654	2.046105	-2.500297
C	-1.718299	2.973581	-3.425180
H	-0.965920	2.338710	-2.959785
H	-1.283174	3.966963	-3.568701
H	-1.942951	2.551974	-4.408015
C	-4.039824	3.938571	-3.281915
H	-4.333970	3.481201	-4.230162
H	-3.635798	4.929320	-3.506776
H	-4.938512	4.081199	-2.678251

X = Me

Imaginary frequencies: 0

Electronic Energy = -6812.31648633 a.u.

ZPVE correction = 1.358007 a.u.

Ga	1.999921	-0.770115	0.799372
Ga	-1.810620	0.843765	0.803578
Si	0.201262	0.293116	-0.460227
O	-1.003251	-2.189263	-1.475643
N	2.994802	-2.006629	-0.441656
N	3.537153	0.549733	0.852795
N	-2.887328	2.045513	-0.434603
N	-3.404764	-0.374844	1.072799
C	4.303498	-2.161367	-0.262695
C	5.105081	-1.242009	0.432584
H	6.145543	-1.513235	0.535758
C	4.777269	0.068829	0.826920
C	4.986124	-3.388371	-0.821405
H	6.067820	-3.265516	-0.837473
H	4.633924	-3.622605	-1.824772
H	4.742714	-4.249566	-0.191498
C	5.929106	0.958653	1.238010
H	5.853708	1.943855	0.778090
H	6.882689	0.509036	0.966847
H	5.911325	1.111900	2.319817
C	2.292262	-2.799453	-1.408937
C	1.626117	-3.975634	-1.020370
C	0.905686	-4.683999	-1.983332
H	0.376697	-5.583907	-1.692880
C	0.841889	-4.248026	-3.298316
H	0.270192	-4.806296	-4.030656
C	1.507909	-3.088107	-3.670771
H	1.457447	-2.753077	-4.699699
C	2.239206	-2.344586	-2.743718
C	1.643597	-4.477897	0.412475
H	2.317708	-3.837917	0.980734
C	0.245975	-4.374877	1.043020
H	0.269146	-4.688790	2.090170
H	-0.469756	-5.011864	0.519031
H	-0.144442	-3.357404	1.005447
C	2.181557	-5.914255	0.511909
H	3.168885	-6.003512	0.052026
H	1.518299	-6.625592	0.012492
H	2.263537	-6.216682	1.559696
C	2.991525	-1.102957	-3.198725
H	3.325131	-0.575049	-2.305773
C	4.244093	-1.481448	-4.008433
H	4.796194	-0.582873	-4.297983
H	3.970570	-2.020009	-4.920458
H	4.918882	-2.118125	-3.433633
C	2.103739	-0.143097	-3.999925
H	1.272336	0.214634	-3.390657
H	1.697049	-0.616845	-4.896714
H	2.685935	0.722331	-4.324498
C	3.331671	1.950432	1.095307
C	3.250216	2.442713	2.412211
C	3.121616	3.820796	2.604068
H	3.059342	4.211659	3.612751

C	3.080891	4.694510	1.528756
H	2.995741	5.762130	1.695598
C	3.117587	4.191822	0.234842
H	3.049413	4.876044	-0.600548
C	3.217914	2.821632	-0.009052
C	3.263557	1.526878	3.624515
H	3.507908	0.521783	3.282824
C	4.315915	1.932517	4.668117
H	4.081360	2.899095	5.121607
H	5.313030	2.007963	4.228209
H	4.354201	1.192167	5.471798
C	1.863786	1.480511	4.260249
H	1.579616	2.463884	4.644973
H	1.837930	0.770329	5.091611
H	1.108607	1.182853	3.532369
C	3.216046	2.295886	-1.436697
H	2.839206	1.273337	-1.393986
C	4.633170	2.243102	-2.030141
H	5.090189	3.237285	-2.034196
H	4.599678	1.882353	-3.061932
H	5.282477	1.571773	-1.466004
C	2.267916	3.089392	-2.343062
H	1.261440	3.127568	-1.926343
H	2.198966	2.616348	-3.322809
H	2.612825	4.114742	-2.502398
C	-4.149702	2.293212	-0.118005
C	-4.869585	1.532333	0.825334
H	-5.848373	1.910168	1.083404
C	-4.566715	0.249816	1.298615
C	-4.887866	3.438150	-0.772729
H	-4.643419	4.372404	-0.260163
H	-5.964892	3.288096	-0.713181
H	-4.595668	3.556950	-1.815235
C	-5.631939	-0.438494	2.124060
H	-5.349679	-0.381936	3.179672
H	-5.725975	-1.493802	1.875469
H	-6.598442	0.047600	2.000302
C	-2.246952	2.753859	-1.504801
C	-1.691642	4.027177	-1.287626
C	-1.077639	4.676716	-2.362380
H	-0.645698	5.658948	-2.210737
C	-0.995625	4.080189	-3.611478
H	-0.511073	4.597859	-4.431335
C	-1.514300	2.804656	-3.801492
H	-1.424355	2.332497	-4.771319
C	-2.138822	2.119638	-2.759930
C	-1.688253	4.687740	0.081223
H	-2.286725	4.073742	0.754428
C	-0.257138	4.732974	0.638092
H	0.375393	5.381422	0.027416
H	0.205670	3.745688	0.644404
H	-0.246260	5.119235	1.660817
C	-2.298999	6.097842	0.059135
H	-2.361188	6.499336	1.074343
H	-3.303145	6.098301	-0.370562
H	-1.688474	6.786719	-0.530763
C	-2.715183	0.730847	-2.973086
H	-2.649575	0.219932	-2.012263
C	-4.203991	0.798993	-3.353574
H	-4.801655	1.260275	-2.566496
H	-4.599931	-0.204799	-3.526524
H	-4.338709	1.379979	-4.270604
C	-1.937540	-0.108333	-3.991823
H	-2.068724	0.264812	-5.011603
H	-2.293332	-1.139956	-3.969601
H	-0.871894	-0.119007	-3.763212
C	-3.318336	-1.790173	1.315636
C	-2.901563	-2.271235	2.570068
C	-2.816999	-3.651751	2.767187
H	-2.485167	-4.031616	3.726204
C	-3.158355	-4.540175	1.760137
H	-3.087969	-5.608765	1.928286
C	-3.586923	-4.054860	0.530968
H	-3.850133	-4.755354	-0.250470
C	-3.674804	-2.684971	0.280641
C	-2.550417	-1.335937	3.714406
H	-2.846591	-0.328800	3.423545
C	-1.035215	-1.325149	3.950326
H	-0.765088	-0.617893	4.739434
H	-0.501981	-1.043244	3.043010
H	-0.678305	-2.315141	4.246233
C	-3.305493	-1.681081	5.007238
H	-3.111333	-0.921881	5.769967
H	-2.989262	-2.644947	5.414414
H	-4.384173	-1.730107	4.840072
C	-4.181483	-2.187579	-1.067384
H	-3.671598	-1.245549	-1.266677
C	-5.694233	-1.895916	-1.042547
H	-5.945160	-1.062844	-0.388936
H	-6.249563	-2.777501	-0.708655
H	-6.041995	-1.638927	-2.046748
C	-3.879683	-3.148434	-2.226172
H	-4.102178	-2.655227	-3.175882
H	-4.507816	-4.042849	-2.177559
H	-2.835278	-3.454337	-2.237412
C	2.103065	-1.684781	2.574674
H	3.134378	-2.026786	2.705085
H	1.441917	-2.547948	2.622327
H	1.850587	-1.027474	3.403654
C	-1.623140	1.904684	2.491706
H	-0.913307	2.720304	2.351103
H	-1.265342	1.296669	3.321588
H	-2.591814	2.330490	2.767865
C	-0.510976	-1.264553	-0.984243

X = OMe

Imaginary frequencies: 0

Electronic Energy = -6962.85472181 a.u.

ZPVE correction = 1.368464 a.u.

Ga	-1.952166	-0.435681	-0.509652
Ga	1.855949	0.515742	-0.456509
Si	-0.148494	0.335844	0.896311
O	0.627772	-2.365591	1.780155
N	-3.226176	-1.643621	0.435802

N	-3.348929	0.939460	-0.874432
N	3.103100	1.706237	0.580223
N	3.319520	-0.755267	-0.936351
C	-4.520985	-1.661453	0.130280
C	-5.154399	-0.647155	-0.601166
H	-6.204127	-0.798970	-0.804429
C	-4.634664	0.602506	-0.976984
C	-5.368919	-2.829156	0.575384
H	-6.429431	-2.592406	0.506289
H	-5.131213	-3.133841	1.593682
H	-5.162414	-3.688332	-0.069639
C	-5.619548	1.607593	-1.528346
H	-5.495496	2.583290	-1.058581
H	-6.642630	1.266085	-1.381364
H	-5.447887	1.748027	-2.597789
C	-2.688918	-2.554222	1.406613
C	-2.163338	-3.793621	1.003481
C	-1.597078	-4.619921	1.975808
H	-1.175041	-5.572995	1.680118
C	-1.551757	-4.235015	3.307986
H	-1.102035	-4.887604	4.047429
C	-2.072990	-3.005662	3.691040
H	-2.029881	-2.710669	4.732203
C	-2.643241	-2.141790	2.755489
C	-2.171162	-4.234194	-0.449639
H	-2.755513	-3.506328	-1.010779
C	-0.750819	-4.233471	-1.033506
H	-0.768619	-4.551435	-2.079285
H	-0.099287	-4.916764	-0.484679
H	-0.307132	-3.239446	-1.005575
C	-2.837560	-5.607375	-0.629384
H	-3.838929	-5.630346	-0.191587
H	-2.252352	-6.401639	-0.158084
H	-2.922995	-5.848271	-1.692632
C	-3.237153	-0.812908	3.200830
H	-3.356923	-0.194910	2.310967
C	-4.636122	-1.011054	3.809951
H	-5.063273	-0.048744	4.105852
H	-4.585852	-1.648842	4.697311
H	-5.321479	-1.476634	3.099944
C	-2.330189	-0.048351	4.173008
H	-1.355761	0.150342	3.723784
H	-2.177792	-0.595061	5.106995
H	-2.785398	0.911607	4.428551
C	-2.967875	2.308016	-1.108059
C	-2.692517	2.759286	-2.411197
C	-2.422672	4.117580	-2.596568
H	-2.210017	4.482757	-3.594206
C	-2.427875	5.003328	-1.529828
H	-2.231512	6.056401	-1.695799
C	-2.645284	4.530831	-0.241627
H	-2.605670	5.220892	0.591591
C	-2.892999	3.179163	-0.001621
C	-2.654389	1.817532	-3.601848
H	-3.020659	0.848782	-3.268524
C	-3.551438	2.286468	-4.758124
H	-3.182368	3.216030	-5.199851
H	-4.580875	2.461426	-4.435150
H	-3.567667	1.531464	-5.548865
C	-1.207203	1.622760	-4.081466
H	-0.805271	2.563253	-4.472188
H	-1.174680	0.882491	-4.885554
H	-0.555534	1.286571	-3.275198
C	-3.088425	2.671913	1.419854
H	-2.838388	1.610611	1.414267
C	-4.549984	2.792437	1.880012
H	-4.880940	3.834904	1.853010
H	-4.656742	2.429468	2.906339
H	-5.220419	2.205992	1.249639
C	-2.138827	3.348430	2.415868
H	-1.101275	3.275209	2.088274
H	-2.212693	2.863605	3.391168
H	-2.379401	4.405697	2.558076
C	4.380456	1.823598	0.240384
C	5.012133	0.958232	-0.666971
H	6.029469	1.210759	-0.927931
C	4.548994	-0.272362	-1.150365
C	5.220122	2.927241	0.839397
H	5.005772	3.872296	0.333655
H	6.281334	2.710587	0.726835
H	4.989893	3.070349	1.894875
C	5.533285	-1.077666	-1.969168
H	5.343304	-0.890949	-3.029323
H	5.427673	-2.147667	-1.804382
H	6.556701	-0.777690	-1.749046
C	2.536389	2.514619	1.620288
C	2.088784	3.817023	1.342067
C	1.491283	4.545589	2.374530
H	1.133945	5.549156	2.176885
C	1.337014	4.002184	3.641468
H	0.867602	4.581891	4.427966
C	1.766960	2.704705	3.895605
H	1.622894	2.280116	4.880688
C	2.362039	1.936730	2.895524
C	2.198881	4.426664	-0.045615
H	2.836287	3.778091	-0.645654
C	0.823095	4.472351	-0.724932
H	0.123884	5.072358	-0.140510
H	0.403238	3.473771	-0.846514
H	0.899857	4.919215	-1.720089
C	2.842113	5.821999	-0.020691
H	3.013221	6.175168	-1.041229
H	3.799969	5.818117	0.505811
H	2.196373	6.552325	0.474097
C	2.820290	0.512939	3.167926
H	2.704486	-0.035073	2.231603
C	4.312827	0.459294	3.534723
H	4.940994	0.838667	2.728182
H	4.617615	-0.571110	3.736361
H	4.509372	1.054402	4.431224
C	1.981106	-0.212177	4.225253
H	2.161119	0.183252	5.228856
H	2.239567	-1.273241	4.238520
H	0.915192	-0.129077	4.009040
C	3.048757	-2.143200	-1.224128
C	2.602450	-2.535453	-2.498974

C	2.353218	-3.891890	-2.726501
H	2.000509	-4.206347	-3.701485
C	2.556168	-4.836011	-1.733752
H	2.357784	-5.883687	-1.929186
C	3.005732	-4.435397	-0.481159
H	3.155981	-5.179864	0.289223
C	3.257089	-3.092985	-0.197229
C	2.426065	-1.551978	-3.643720
H	2.725267	-0.569969	-3.284843
C	0.960967	-1.448434	-4.085693
H	0.862341	-0.690780	-4.868056
H	0.304758	-1.178540	-3.259579
H	0.612380	-2.401450	-4.497364
C	3.321548	-1.914346	-4.841754
H	3.269290	-1.128162	-5.600210
H	2.994318	-2.846551	-5.310376
H	4.366850	-2.042671	-4.552543
C	3.783847	-2.686653	1.175295
H	3.347433	-1.714419	1.409593
C	5.315094	-2.515169	1.181506
H	5.644297	-1.683010	0.563031
H	5.802633	-3.426768	0.823832
H	5.664806	-2.322759	2.199483
C	3.394532	-3.661516	2.295639
H	3.632163	-3.214899	3.264725
H	3.961645	-4.594412	2.225446
H	2.332273	-3.896826	2.281764
C	0.293266	-1.360105	1.324621
O	1.394607	1.400680	-2.001771
O	-1.550705	-1.213222	-2.118802
C	2.286455	1.991504	-2.909901
H	1.816936	2.037462	-3.900386
H	2.546735	3.019365	-2.619609
H	3.230320	1.438285	-3.014144
C	-2.483151	-1.692552	-3.052833
H	-2.169361	-1.410698	-4.066351
H	-2.546229	-2.789752	-3.024559
H	-3.498520	-1.302900	-2.897228

X = NMe_2

Imaginary frequencies: 0

Electronic Energy = -7001.72573885 a.u.

ZPVE correction = 1.450214 a.u.

Ga	-2.130133	0.331609	0.560306
Ga	2.071390	-0.470898	0.425282
Si	-0.118714	-0.332338	-0.638652
O	0.256026	2.402517	-1.648673
N	-3.456030	1.171438	-0.711277
N	-3.351502	-1.236296	0.887915
N	3.348701	-1.079909	-1.030580
N	3.351742	0.987651	0.995946
C	-4.766293	0.991622	-0.566104
C	-5.328561	-0.032243	0.210021
H	-6.407631	-0.045470	0.261898
C	-4.675259	-1.125188	0.797870
C	-5.736191	1.930216	-1.248205
H	-6.701463	1.448744	-1.399664
H	-5.357038	2.290012	-2.202391
H	-5.889269	2.804438	-0.608638
C	-5.559793	-2.214247	1.362168
H	-5.133875	-3.203828	1.204459
H	-6.551981	-2.173418	0.915191
H	-5.665333	-2.076522	2.441409
C	-2.964357	2.034509	-1.750318
C	-2.692236	3.389729	-1.494875
C	-2.199104	4.175838	-2.538549
H	-1.981612	5.221512	-2.355755
C	-1.964553	3.639759	-3.795460
H	-1.572225	4.264274	-4.589789
C	-2.222754	2.295361	-4.029825
H	-2.033666	1.881285	-5.012403
C	-2.722443	1.470138	-3.022090
C	-2.891986	4.017090	-0.125681
H	-3.236660	3.236741	0.551053
C	-1.563666	4.553548	0.430510
H	-1.704316	4.946870	1.440424
H	-1.174040	5.363813	-0.192286
H	-0.806609	3.772414	0.476104
C	-3.949878	5.132041	-0.157828
H	-4.899869	4.775826	-0.561461
H	-3.621742	5.970194	-0.779220
H	-4.129286	5.515033	0.850792
C	-3.047252	0.013685	-3.321689
H	-3.135810	-0.501484	-2.365732
C	-4.404680	-0.109550	-4.035916
H	-4.644308	-1.160760	-4.219501
H	-4.383576	0.408215	-4.999475
H	-5.213107	0.319400	-3.442273
C	-1.949610	-0.692886	-4.126049
H	-1.000445	-0.684348	-3.588806
H	-1.799914	-0.234172	-5.106865
H	-2.228318	-1.735233	-4.297294
C	-2.765941	-2.468722	1.337839
C	-2.626111	-2.735557	2.712382
C	-2.037225	-3.942989	3.096832
H	-1.915995	-4.160547	4.151324
C	-1.599463	-4.861374	2.154971
H	-1.141758	-5.791203	2.472596
C	-1.736004	-4.580716	0.801030
H	-1.382075	-5.298597	0.073442
C	-2.312494	-3.387211	0.365322
C	-3.079707	-1.756299	3.783405
H	-3.623177	-0.951113	3.291423
C	-4.021057	-2.410781	4.807522
H	-3.496962	-3.153540	5.414835
H	-4.860939	-2.915076	4.324065
H	-4.421405	-1.653948	5.487674
C	-1.872758	-1.120771	4.487982
H	-1.261397	-1.879321	4.984296
H	-2.205100	-0.404753	5.244626
H	-1.250689	-0.589889	3.770930
C	-2.493225	-3.110762	-1.120990
H	-2.461388	-2.028529	-1.248026
C	-3.868432	-3.589126	-1.616758

H	-3.981900	-4.666540	-1.463940
H	-3.976075	-3.384528	-2.685766
H	-4.684726	-3.084227	-1.099485
C	-1.374991	-3.695050	-1.988071
H	-0.397046	-3.331606	-1.675942
H	-1.514324	-3.394509	-3.027177
H	-1.362013	-4.788123	-1.964851
C	4.663869	-0.982118	-0.877873
C	5.268767	-0.188340	0.109158
H	6.345756	-0.252021	0.169950
C	4.668399	0.775373	0.928344
C	5.597285	-1.760639	-1.777369
H	5.775225	-2.747636	-1.341959
H	6.557575	-1.253555	-1.865079
H	5.175717	-1.911237	-2.769215
C	5.609535	1.589637	1.789378
H	5.714857	1.095558	2.759028
H	5.237418	2.594957	1.972215
H	6.596494	1.648597	1.332293
C	2.797087	-1.769731	-2.163131
C	2.612303	-3.162828	-2.135128
C	2.017087	-3.775929	-3.241956
H	1.860979	-4.848308	-3.232126
C	1.615226	-3.036948	-4.343206
H	1.148783	-3.529028	-5.188986
C	1.806035	-1.659633	-4.357661
H	1.482015	-1.089042	-5.217847
C	2.392694	-1.001855	-3.277352
C	3.029797	-4.018368	-0.949635
H	3.502748	-3.366624	-0.216373
C	1.809233	-4.653374	-0.270072
H	1.301497	-5.349145	-0.943861
H	1.093254	-3.893908	0.035825
H	2.113505	-5.208929	0.621108
C	4.040144	-5.104556	-1.355109
H	4.400624	-5.635893	-0.469730
H	4.902144	-4.684300	-1.876968
H	3.581883	-5.842198	-2.019617
C	2.610730	0.504083	-3.306763
H	2.478887	0.861329	-2.283884
C	4.048603	0.864736	-3.720763
H	4.786246	0.476657	-3.019689
H	4.166925	1.951306	-3.756729
H	4.274032	0.464451	-4.713569
C	1.612892	1.251784	-4.197974
H	1.801411	1.059410	-5.258250
H	1.707747	2.327097	-4.036024
H	0.582443	0.976816	-3.975856
C	2.854751	2.149616	1.686377
C	2.604659	2.105566	3.070558
C	2.054747	3.233605	3.686013
H	1.843218	3.205834	4.748398
C	1.773162	4.379612	2.961518
H	1.334544	5.241513	3.451116
C	2.063690	4.425098	1.602901
H	1.854335	5.330927	1.050945
C	2.614194	3.327445	0.939604
C	2.942502	0.895048	3.926387
H	3.411566	0.152911	3.284154
C	1.684247	0.249089	4.518031
H	1.947890	-0.644986	5.089221
H	0.995458	-0.044210	3.730331
H	1.163800	0.936749	5.190112
C	3.932226	1.256245	5.047665
H	4.252600	0.352056	5.573097
H	3.471265	1.920302	5.783852
H	4.819851	1.760947	4.661265
C	2.986651	3.432449	-0.536618
H	2.718923	2.484811	-1.005901
C	4.501631	3.627701	-0.742693
H	5.079445	2.754219	-0.450553
H	4.860146	4.489416	-0.172128
H	4.708150	3.814273	-1.800292
C	2.250081	4.557935	-1.276149
H	2.407200	4.448450	-2.351781
H	2.639723	5.539133	-0.988092
H	1.177740	4.539620	-1.095001
C	0.106186	1.365592	-1.160167
C	3.321617	-2.309956	2.339657
H	3.362518	-2.166505	3.433463
H	3.419864	-3.395993	2.166516
H	4.203367	-1.830675	1.910959
C	-3.348510	1.729232	2.806053
H	-3.519773	2.820569	2.783501
H	-4.220078	1.254931	2.350243
H	-3.329095	1.439915	3.870214
N	2.104904	-1.782592	1.766890
N	-2.131038	1.356642	2.123637
C	-0.958602	1.966677	2.704663
H	-1.025350	3.063630	2.724506
H	-0.798148	1.643238	3.744257
H	-0.063848	1.708417	2.136720
C	0.926000	-2.406782	2.319113
H	0.019717	-2.024210	1.847173
H	0.928315	-3.495689	2.176374
H	0.827577	-2.232621	3.400950

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