

Supplementary Information to

**Why is a Dicationic Digallene so Reactive towards Activation of
Strong Covalent Bonds? Scope and Mechanistic Investigations**

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1 General Remarks

All manipulations were carried out under exclusion of moisture and air through usage of a *MBraun* glovebox filled with nitrogen ($O_2/H_2O < 1$ ppm) and standard Schlenk technique. All glassware used in reactions have been stored overnight in an oven at 180 °C and were additionally dried with a heat gun prior to usage.

Ortho-difluorobenzene (*o*DFB) was dried over CaH_2 for two days, distilled and degassed prior to use. and stored under an atmosphere of argon or nitrogen in sealed vessels and over 4 Å molecular sieves. The water content of the solvents was below 8 ppm, as determined by Carl Fischer titration.

$Li[pf]$,^[1] $Ag[pf]$ (synthesis in SO_2 , instead of CH_2Cl_2 or perfluorohexane, under ambient conditions),^[1,2] $[Ga(PhF)_2][pf]$,^[3] $[Ga(dcpe)]_2[pf]_2$ ^[4] ($dcpe$ = *bis*(dicyclohexylphosphino)ethane; $[pf]^- = [Al(OR^F)_4]^-$, $R^F = C(CF_3)_3$) and *trans*- β -deutero-styrene^[5] were prepared according to literature protocols. Note that, in the fluorobenzene complex of Ga^+ , the number of fluorobenzene molecules coordinated to Ga^+ can vary, depending on the vacuum applied when drying the product. Thus, the formula $[Ga(PhF)_2][pf]$ is used for the sake of simplicity instead of $[Ga(PhF)_x][pf]$ ($1 < x < 3$). The exact ratio x was determined *via* ^{19}F NMR spectroscopy.

1.1 Single Crystal X-Ray Diffraction

Crystals were obtained by layering a concentrated *o*DFB solution with *n*-pentane. Single crystal X-ray diffraction data were collected from shock-cooled single crystals at 100(2) K on a Bruker *D8 VENTURE* dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker *PHOTON III* detector. Crystals were selected under perfluoropolyether oil, mounted on 0.1 to 0.2 mm diameter CryoLoops and quench-cooled using an *Oxford Cryostream 800* open flow N_2 cooling device.^[6] Data were collected at 100 K using monochromated Mo K_α radiation ($\lambda = 0.71073$ Å).

All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.^[7] The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL-2018/3^[8] employing shelXle.^[9] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered

moieties were refined using bond lengths restraints and displacement parameter restraints. Some parts of the disorder model were introduced by the program DSR.^[10] Graphical representations were prepared using Olex2-1.3.^[11]

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.^[12] CCDC numbers 2488257–2488261 and 2490061 contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.^[13]

1.2 NMR Spectroscopy

^1H -, ^2D -, ^{13}C -, ^{19}F -, ^{27}Al -, ^{31}P -, ^{71}Ga -, and 2D NMR spectra were detected on an *Avance DPX 200* (200 MHz), *Avance III HD* (300 MHz) and *Avance II+ 400* (400 MHz) NMR spectrometer from *Bruker*. NMR spectra were analyzed using *Bruker TopSpin 3.2*. ^1H NMR chemical shifts are given with respect to tetramethylsilane (TMS). The ^1H NMR spectrum was calibrated using the solvent signal as secondary standard. The chemical shifts of *o*DFB and 3FB were determined experimentally by adding TMS to the aromatic solvents. The most intensive signal of the downfield multiplet of these solvents appear at 6.96 and 6.86 ppm, respectively, when the signal of TMS is at 0.00 ppm (**Figure S 1** and **Figure S 2**).

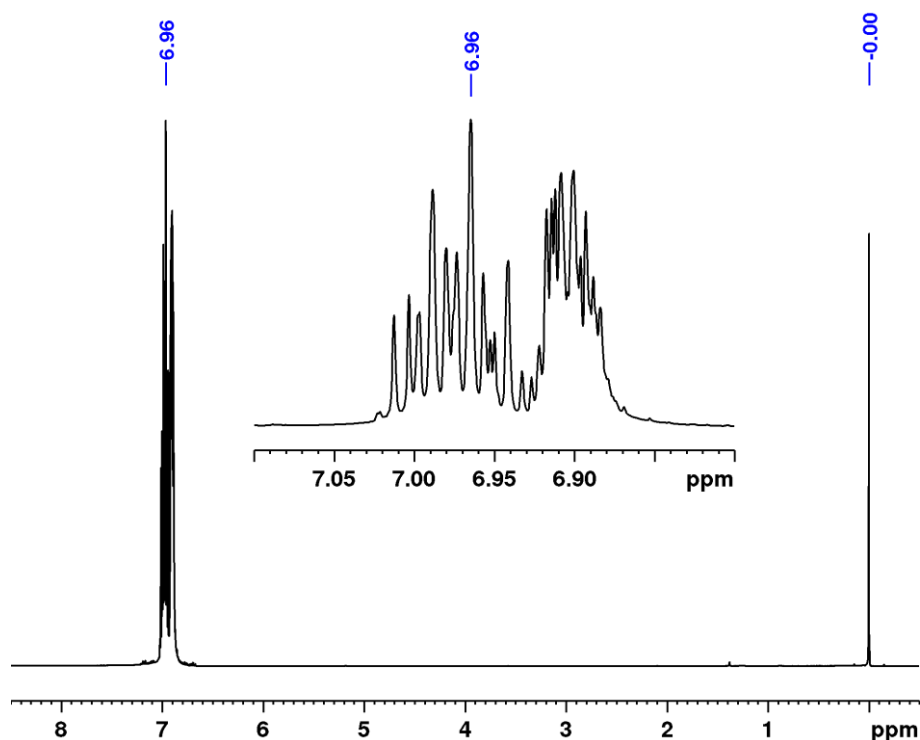


Figure S 1: ^1H NMR spectrum (400.17 MHz, *o*DFB, 298 K) of TMS in *o*DFB.

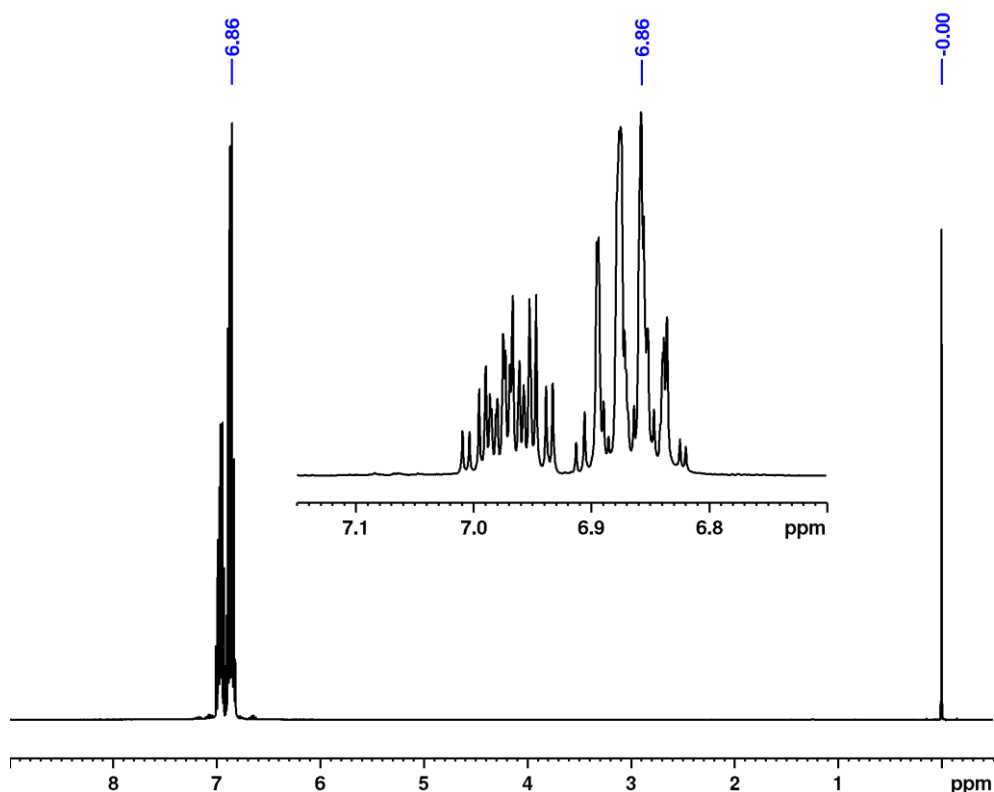


Figure S 2: ^1H NMR spectrum (400.17 MHz, 3FB, 298 K) of TMS in 3FB.

Heteronuclear spectra were calibrated according to the IUPAC Ξ -table.^[14] The ^{19}F and ^{27}Al NMR spectra show signals at ca. -75 ppm and 35 ppm, respectively, indicating the presence of non-decomposed $[\text{Al}(\text{OR}^{\text{F}})_4]^-$ anion. The broad resonance between 50 and 100 ppm in the ^{27}Al NMR spectra is caused by the probe head. Note that ^{71}Ga spectra without a detected signal, due to the quadrupolar relaxation of ^{71}Ga , are not shown here.

1.3 IR Spectroscopy

IR spectra FT-IR spectra were recorded on a FT-IR Bruker Alpha, equipped with a Quick Snap Platinum ATR (diamond or ZnSe crystal) unit inside a glove box under an atmosphere of nitrogen at room temperature (rt). The spectra were recorded with a resolution of 2 cm^{-1} and 64 scans. For measurements and data processing, the software *OPUS 7.5* (Bruker Optic GmbH) was used. All spectra were ATR corrected and base line corrections (5 cycles) were employed. By setting the most intense peak to 100 %, the other IR bands were given the following intensity assignment: very weak (vw) < 20 %, weak (w) < 40 %; medium (m) < 60 %, strong (s) < 80 % and very strong (vs) for ≥ 80 %.

1.4 Quantum Chemical Calculations

Quantum chemical calculations were performed with *Turbomole* (version 7.5.1).^[15,16] Structures were optimized using density functional theory (DFT),^[15] internal coordinates, resolution of identity-approximation (RI),^[17,18] D3(BJ)-dispersion correction^[19] and a fine integration gridsize (gridsize = m5). Calculations were performed on the RI-BP86^[20](D3BJ)/def2-TZVPP^[21] level of theory. Thermal and entropic contributions to the Gibbs energy were calculated without scaling factor at standard conditions (298.15 K, 0.1 MPa) with the FREEH module. Every species presented herein were checked in terms of reasonable geometry and electronic occupation with the EIGER module. Vibrational analyses were performed with the AOFORCE module, in order to detect imaginary frequencies.^[22] To counteract imaginary frequencies, the convergence criteria for geometry optimization were modified from the default 10^{-7} H (energy) and 10^{-4} a.u. (gradient) to 10^{-8} H and 10^{-5} a.u., respectively. The coordinates of the herein investigated compounds are listed in section 6.

Due to the size of the dcpe-complexes, the geometry of the herein investigated molecules was optimized at the RI-BP86(D3BJ)/def2-TZVPP level of theory. However, in order to obtain more reliable electronic energy values, the thereby optimized structures were further analysed employing a double-hybrid functional^[23] using the ORCA program (version 4.2.1).^[24] Single point calculations at the DSD-PBEP86^[25]-D3(BJ) level of theory were performed, with the RIJCOSX^[26] approximation, the def2-QZVPP^[21] orbital basis set and the def2-QZVPP/C^[27] auxiliary basis set. The DSD-PBEP86 double-hybrid functional is known to yield accurate thermochemistry results for various types of reactions involving main group elements.^[28] The results from the vibrational analysis were taken from the respective gas phase calculations at the RI-BP86(D3BJ)/def2-TZVPP level.

For each molecular species, the standard enthalpy H° at 298.15 K and 0.1 MPa was calculated from the electronic energy obtained by the double-hybrid energy E_{DH} and the sum of translational, rotational, and vibrational energy including zero-point energy E_{vrt} (FREEH energy) using the following equation:

$$H^\circ = E_{\text{DH}} + E_{\text{vrt}} + R \cdot T \quad (1)$$

E_{DH} : electronic double-hybrid energy

E_{vrt} : sum of translational, rotational, and vibrational energy including zero-point energy

R: universal gas constant ($8.314 \text{ J K}^{-1} \text{ mol}^{-1}$)

T: temperature in Kelvin (298.15 K)

The Gibbs free energy G° follows from the standard enthalpy H° and the standard entropy S° :

$$G^\circ = H^\circ - S^\circ \cdot T \quad (2)$$

Solvation effects were incorporated using the conductor like screening model (COSMO).^[29] A dielectric constant of 13.38 D for *o*DFB^[30] and of 22.1 D for 3FB^[31] was assumed at 298 K. Single point calculations were performed on the optimized gas phase structures and the results from the vibrational analysis were taken from the respective gas phase calculations.

In order to find transition state structures, relaxed potential energy surface scans along selected bond lengths or bond angles were performed with the ORCA program on the RI-BP86(D3BJ)/def2-SVP^[17,21] level of theory. The geometry of the most energy-rich species was chosen as the starting geometry for the transition state structure search in *Turbomole* at the RI-BP86(D3BJ)/def2-TZVPP level of theory. The transition states thus obtained display one imaginary frequency and were distorted along the reaction coordinate to make sure that the transition state describes the desired transformation.

The calculated energies, entropies and vibrations of all the species presented herein are summarized in section 6.

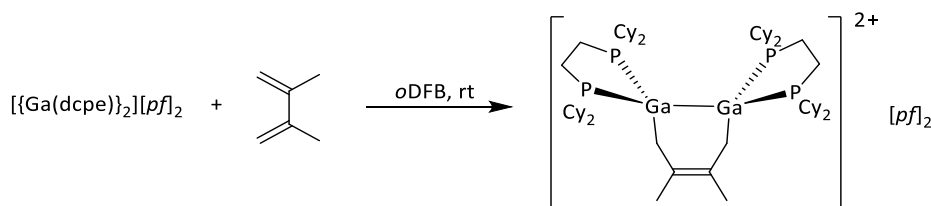
2 Syntheses

2.1 NMR Investigations of [2+2] Cycloaddition Reactions with $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$

2.1.1 Reactions with *trans*- β -deutero-styrene, *cis*- β -methyl-styrene, *cis*-3-hexene and ethynylcyclopropane

$[\text{Ga}(\text{PhF})_x][pf]$ (for $x = 2.0$: 50 mg, 40.7 μmol , 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol , 1.0 eq.) were mixed in oDFB (ca. 0.6 ml). A stock solution of *trans*- β -deutero-styrene, *cis*- β -methyl-styrene, *cis*-3-hexene or ethynylcyclopropane in oDFB (0.09 mL, $c = 0.225$ M, 20.2 μmol , 0.5 eq.) was added, respectively. The reaction solutions remained red with *trans*- β -deutero-styrene, *cis*- β -methyl-styrene and *cis*-3-hexene. Only the reaction solution with ethynylcyclopropane turned colourless with minutes, indicating the complete consumption of the dicationic digallene. The reaction mixtures were analyzed *via* multinuclear NMR spectroscopy (see section 4).

2.2 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][pf]_2$

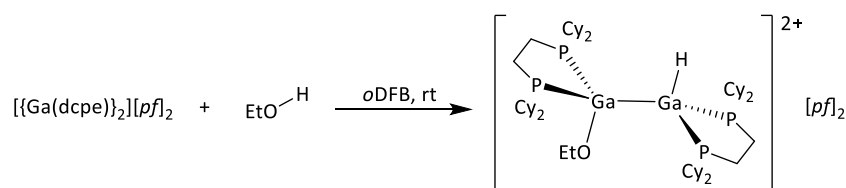


Scheme S 1: Synthesis $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][pf]_2$.

$[\text{Ga}(\text{PhF})_x][pf]$ (for $x = 2.0$: 50 mg, 40.7 μmol , 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol , 1.0 eq.) were mixed in oDFB (ca. 0.8 ml). A stock solution of 2,3-dimethylbutadiene in oDFB (0.06 mL, $c = 0.43$ M, 25.8 μmol , 0.63 eq.) was added. The initially red reaction solution turned pink within minutes and was stirred overnight at rt. Layering the then colourless solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10^{-3} mbar) yielded white crystals of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][pf]_2$ (13.0 mg, 4.33 μmol , 21 %).

Note that a co-crystallized 2,3-dimethylbutadiene molecule is found in the crystals which have directly been picked from the mother liquor (section 3.1). However, this molecule is probably removed when drying the product in *vacuo*, since no traces of 2,3-dimethylbutadiene are found in the NMR and IR spectra of the thoroughly dried product.

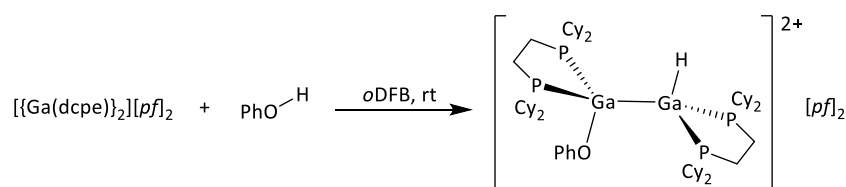
2.3 [H{Ga(dcpe)}₂(OEt)][pf]₂



Scheme S 2: Synthesis of [H{Ga(dcpe)}₂(OEt)][pf]₂.

[Ga(PhF)_x][pf] (for x = 2.0: 50 mg, 40.7 μmol, 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.8 ml). A stock solution of ethanol in oDFB (0.08 mL, c = 0.26 M, 20.8 μmol, 0.5 eq.) was added. The initially red reaction solution immediately turned colourless. Layering the solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10⁻³ mbar) yielded colorless crystals of [H{Ga(dcpe)}₂(OEt)][pf]₂ (16.5 mg, 5.57 μmol, 27 %).

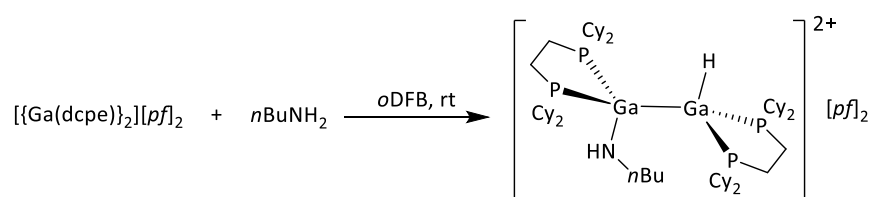
2.4 [H{Ga(dcpe)}₂(OPh)][pf]₂



Scheme S 3: Synthesis of [H{Ga(dcpe)}₂(OPh)][pf]₂.

[Ga(PhF)_x][pf] (for x = 2.0: 50 mg, 40.7 μmol, 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.8 ml). A stock solution of phenol in oDFB (0.09 mL, c = 0.225 M, 20.3 μmol, 0.5 eq.) was added. The initially red reaction solution immediately turned colourless. Layering the solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10⁻³ mbar) yielded colorless crystals of [H{Ga(dcpe)}₂(OPh)][pf]₂ (45.0 mg, 14.9 μmol, 73 %).

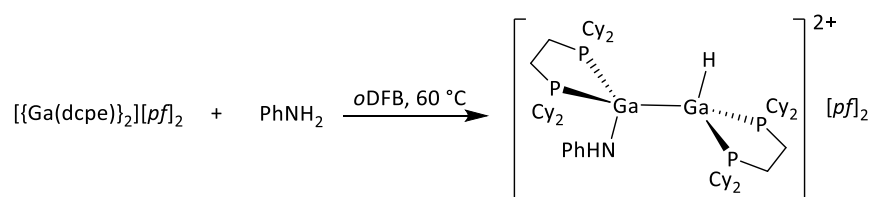
2.5 [H{Ga(dcpe)}₂(NHC₄H₉)][pf]₂



Scheme S 4: Synthesis of [H{Ga(dcpe)}₂(NHC₄H₉)][pf]₂.

[Ga(PhF)_x][pf] (for x = 1.0: 40 mg, 32.5 μmol, 1.0 eq.) and dcpe (13.5 mg, 31.9 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.5 ml) upon which a stock solution of *n*butylamine in oDFB (0.16 mL, c = 0.10 M, 16.0 μmol, 0.5 eq.) was added. The initially red solution mixture turned colorless within 30 minutes. Layering the reaction solution with *n*-pentane (ca. 8 mL) yielded colorless crystals, which were not suitable for scXRD (21.3 mg, 7.12 μmol, 45 %).

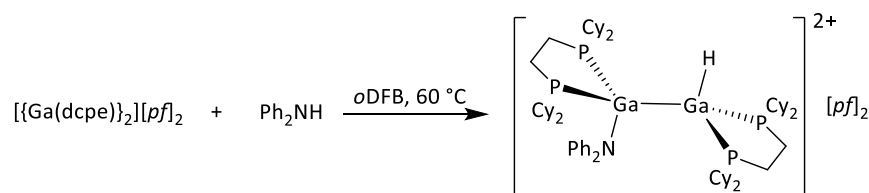
2.6 [H{Ga(dcpe)}₂(NHPH)][pf]₂



Scheme S 5: Synthesis of [H{Ga(dcpe)}₂(NHPH)][pf]₂.

[Ga(PhF)_x][pf] (for x = 1.0: 40 mg, 32.5 μmol, 1.0 eq.) and dcpe (13.5 mg, 31.9 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.5 ml) upon which a stock solution of aniline in oDFB (0.16 mL, c = 0.1 M, 16.0 μmol, 0.5 eq.) was added. The initially red solution mixture turned colorless within 30 minutes. Layering the then colourless solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10⁻³ mbar) yielded colorless crystals of [H{Ga(dcpe)}₂(NHPH)][pf]₂ (11.8 mg, 3.92 μmol, 25 %).

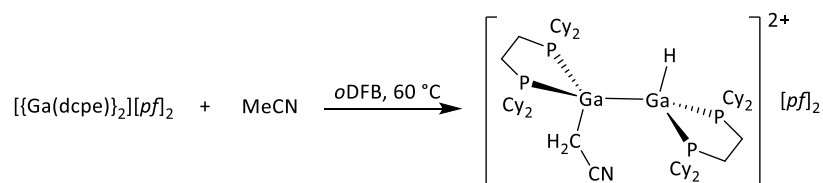
2.7 [H{Ga(dcpe)}₂(NPh₂)][pf]₂



Scheme S 6: Synthesis of [H{Ga(dcpe)}₂(NPh₂)][pf]₂.

[Ga(PhF)_x][pf] (for x = 1.0: 40 mg, 32.5 μmol, 1.0 eq.) and dcpe (13.5 mg, 31.9 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.5 ml) upon which a stock solution of diphenylamine in oDFB (0.16 mL, c = 0.1 M, 16.0 μmol, 0.5 eq.) was added. The reaction mixture was stirred for 24 hours at 60 °C. Layering the then colourless solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10⁻³ mbar) yielded colorless crystals of [H{Ga(dcpe)}₂(NPh₂)][pf]₂ (37.0 mg, 12.0 μmol, 75 %).

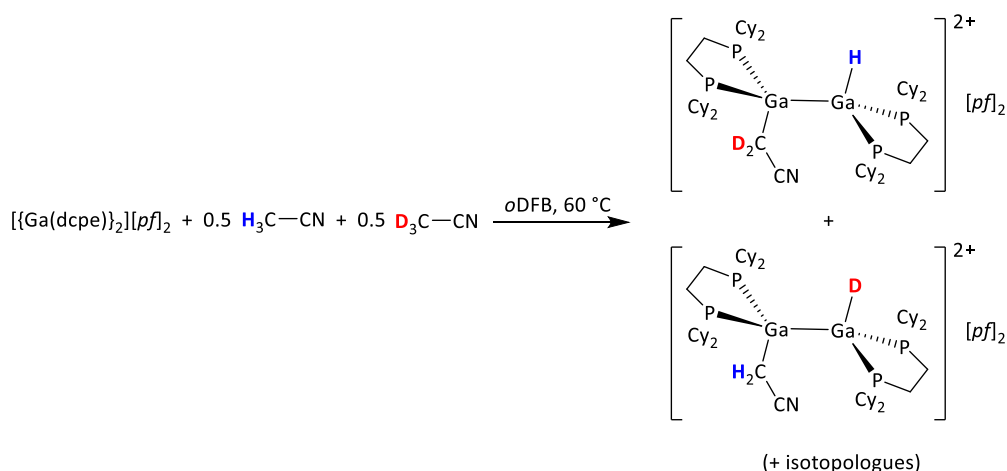
2.8 [H{Ga(dcpe)}₂(CH₂CN)][pf]₂



Scheme S 7: Synthesis of [H{Ga(dcpe)}₂(CH₂CN)][pf]₂.

[Ga(PhF)_x][pf] (for x = 2.0: 50 mg, 40.7 μmol, 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.8 ml). A stock solution of acetonitrile in oDFB (0.08 mL, c = 0.225 M, 20.2 μmol, 0.5 eq.) was added. The red reaction solution was stirred for 4 days at 60 °C. Layering the then colourless solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10⁻³ mbar) yielded white crystals of [H{Ga(dcpe)}₂(CH₂CN)][pf]₂ (33.8 mg, 11.4 μmol, 56 %).

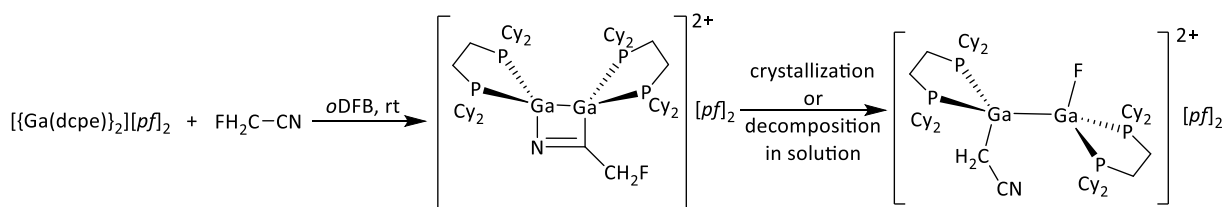
2.9 Reaction between H₃C–CN and D₃C–CN with [{Ga(dcpe)}₂][pf]₂



Scheme S 8: Reaction of [{Ga(dcpe)}₂][pf]₂ with an equimolar solution of acetonitrile and acetonitrile-*d*₃.

[Ga(PhF)_x][pf] (for *x* = 2.0: 50 mg, 45.0 μmol, 1.0 eq.) and dcpe (17.2 mg, 45.0 μmol, 1.0 eq.) were mixed in *o*DFB (ca. 0.6 ml). Two stock solutions of acetonitrile and of acetonitrile-*d*₃ in *o*DFB (0.05 mL, *c* = 0.225 M, 11.2 μmol, 0.25 eq., respectively) were added. The red reaction solution was stirred for 4 days at 60 °C. The then colourless reaction mixture was analyzed *via* multinuclear NMR spectroscopy (see section 4.9).

2.10 [{Ga(dcpe)}₂(NCCH₂F)][pf]₂ and [F{Ga(dcpe)}₂(CH₂CN)][pf]₂

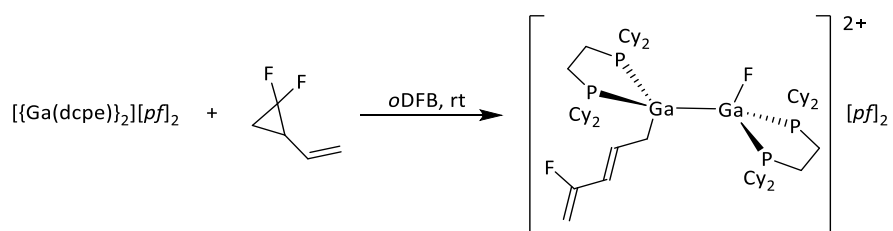


Scheme S 9: Synthesis of [H{Ga(dcpe)}₂(CH₂CN)][pf]₂.

[Ga(PhF)_x][pf] (for *x* = 2.0: 50 mg, 40.7 μmol, 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol, 1.0 eq.) were mixed in *o*DFB (ca. 0.8 ml). A stock solution of monofluoroacetonitrile in *o*DFB (0.09 mL, *c* = 0.225 M, 20.2 μmol, 0.50 eq.) was added. The initially red reaction solution immediately turned yellow. NMR spectroscopy confirms that the CH₂F moiety is intact in the freshly prepared solution, while the ¹³C NMR shift of 215 ppm and the AA'BB' spin system in the ³¹P{¹H} NMR spectrum strongly suggest that the [2+2] cycloaddition product is present in solution (see section 4.10).

Layering the solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10^{−3} mbar) yielded white crystals of the C–F activation product [F{Ga(dcpe)}₂(CH₂CN)][pf]₂ (34.9 mg, 11.7 μmol, 58 %), as suggested by NMR and IR spectroscopy (see section 4.12). Unfortunately, the crystals were not suitable for sc-XRD

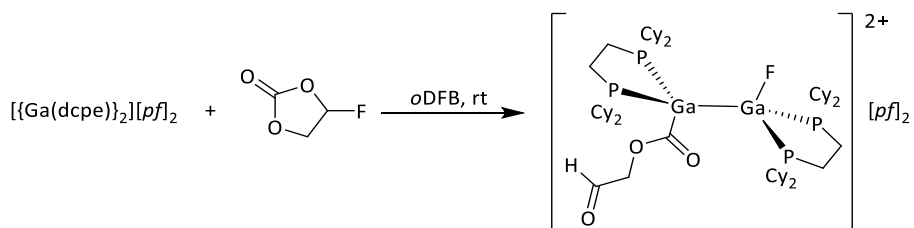
2.11 [F{Ga(dcpe)}₂(C₅H₆F)][pf]₂



Scheme S 10: Synthesis of [F{Ga(dcpe)}₂(C₅H₆F)][pf]₂.

[Ga(PhF)_x][pf] (for x = 1.3: 60 mg, 51.6 μmol, 1.0 eq.) and dcpe (21.8 mg, 51.6 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.6 ml). A stock solution of 1,1-difluoro-2-vinylcyclopropane in oDFB (0.08 mL, c = 0.43 M, 34.4 μmol, 0.7 eq.) was added. The colourless reaction solution was analyzed *via* NMR spectroscopy and the structure of the main product was determined unambiguously. Layering the reaction solution with *n*-pentane (ca. 8 mL) did not yield crystals suitable for sc-XRD (the yield was not determined).

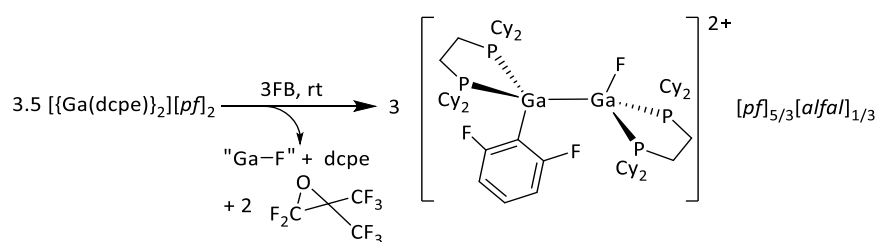
2.12 [F{Ga(dcpe)}₂(COOCH₂CHO)][pf]₂



Scheme S 11: Synthesis of [F{Ga(dcpe)}₂(COOCH₂CHO)][pf]₂.

[Ga(PhF)_x][pf] (for x = 2.0: 50 mg, 40.7 μmol, 1.0 eq.) and dcpe (17.2 mg, 40.7 μmol, 1.0 eq.) were mixed in oDFB (ca. 0.6 ml). A stock solution of FEC in oDFB (0.1 mL, c = 0.225 M, 22.5 μmol, 0.55 eq.) was added. The colourless reaction solution was analyzed *via* NMR spectroscopy and the structure of the main product was determined unambiguously. Layering the reaction solution with *n*-pentane (ca. 8 mL) did not yield crystals suitable for sc-XRD (the yield was not determined).

2.13 $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfal}]_{1/3}$



Scheme S 12: Synthesis of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfal}]_{1/3}$.

$[\text{Ga}(\text{PhF})_x][\text{pf}]$ (for $x = 1.0$: 40 mg, 32.5 μmol , 1.0 eq.) and dcpe (13.5 mg, 31.9 μmol , 1.0 eq.) were mixed in 3FB (ca. 0.8 ml). The red reaction solution was stirred for 4 days at 40 °C. The reaction is best performed under the exclusion of light. This observation may indicate that the formation of the encounter complex is impeded by the irradiation of light, in analogy to the well-known displacement of arene ligands in transition metal complexes.^[32]

Layering the then colourless solution with *n*-pentane (ca. 8 mL), filtration and drying the filter residue in *vacuo* (1×10^{-3} mbar) yielded colorless crystals of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfal}]_{1/3}$ (33.5 mg, 10.4 μmol , 76 %).

3 Crystal Structures

Table S 1: Crystal data and summary of the data collection and refinement for $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$ * C_6H_{10} and $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$.

CCDC	-	2488257
Empirical formula	$\text{C}_{96}\text{H}_{116}\text{Al}_2\text{F}_{72}\text{Ga}_2\text{O}_8\text{P}_4$	$\text{C}_{86}\text{H}_{102}\text{Al}_2\text{F}_{72}\text{Ga}_2\text{O}_9\text{P}_4$
Formula weight	3083.16	2964.95
Temperature [K]	100(2)	100(2)
Crystal system	triclinic	triclinic
Space group (number)	$P\bar{1}$ (2)	$P\bar{1}$ (2)
a [Å]	14.919(4)	17.168(4)
b [Å]	14.959(4)	17.984(5)
c [Å]	29.752(9)	22.621(8)
α [°]	97.393(8)	69.090(8)
β [°]	102.118(11)	67.933(9)
γ [°]	98.894(11)	63.812(8)
Volume [Å ³]	6324(3)	5653(3)
Z	2	2
ρ_{calc} [gcm ⁻³]	1.619	1.742
μ [mm ⁻¹]	0.647	0.720
$F(000)$	3104	2972
Crystal size [mm ³]	0.168×0.254×0.309	0.202×0.248×0.4413
Crystal colour	yellow	colourless
Crystal shape	block	plate
Radiation	MoK_α ($\lambda=0.71073$ Å)	MoK_α ($\lambda=0.71073$ Å)
2 θ range [°]	2.79 to 55.50 (0.76 Å)	2.59 to 54.37 (0.78 Å)
	$-19 \leq h \leq 18$	$-22 \leq h \leq 22$
Index ranges	$-19 \leq k \leq 19$	$-23 \leq k \leq 23$
	$0 \leq l \leq 38$	$-29 \leq l \leq 29$
Reflections collected	27494	217054
	27494	25055
Independent reflections	$R_{\text{int}} = 0.1315$	$R_{\text{int}} = 0.0603$
	$R_{\text{sigma}} = 0.1554$	$R_{\text{sigma}} = 0.0370$
Completeness to $\theta = 25.242^\circ$	93.9 %	100.0 %
Data / Restraints / Parameters	27494 / 47512 / 2867	25055 / 48279 / 2726
Absorption correction $T_{\text{min}}/T_{\text{max}}$ (method)	0.6174 / 0.7456 (multi-scan)	0.6821 / 0.7455 (multi-scan)
Goodness-of-fit on F^2	1.761	0.874
Final R indexes [$\geq 2\sigma(I)$]	$R_1 = 0.1462$ $wR_2 = 0.4157$	$R_1 = 0.0676$ $wR_2 = 0.1788$
Final R indexes [all data]	$R_1 = 0.1895$ $wR_2 = 0.4303$	$R_1 = 0.0952$ $wR_2 = 0.2133$
Largest peak/hole [eÅ ⁻³]	2.30/−1.63	2.27/−0.99

Table S 2: Crystal data and summary of the data collection and refinement for [H{Ga(dcpe)}₂(OPh)][*pf*]₂, [H{Ga(dcpe)}₂(NHPH)][*pf*]₂ and [H{Ga(dcpe)}₂(NPh₂)] [*pf*]₂.

CCDC	2488258	2488259	2488260
Empirical formula	C ₉₀ H ₁₀₂ Al ₂ F ₇₂ Ga ₂ O ₉ P ₄	C ₉₀ H ₁₀₃ Al ₂ F ₇₂ Ga ₂ NO ₈ P ₄	C ₉₆ H ₁₀₇ Al ₂ F ₇₂ Ga ₂ NO ₈ P ₄
Formula weight	3012.99	3012.01	3088.10
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	orthorhombic	monoclinic	triclinic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)	<i>Cc</i> (9)	<i>P</i> $\bar{1}$ (2)
<i>a</i> [Å]	15.677(2)	18.260(3)	15.468(5)
<i>b</i> [Å]	23.421(4)	29.497(5)	18.034(4)
<i>c</i> [Å]	31.572(5)	22.081(4)	22.835(5)
α [°]	90	90	81.311(12)
β [°]	90	96.514(9)	72.120(5)
γ [°]	90	90	86.298(8)
Volume [Å ³]	11592(3)	11816(4)	5992(2)
<i>Z</i>	4	4	2
ρ_{calc} [gcm ⁻³]	1.726	1.693	1.712
μ [mm ⁻¹]	0.704	0.690	0.683
<i>F</i> (000)	6040	6040	3100
Crystal size [mm ³]	0.118×0.134×0.419	0.200×0.210×0.369	0.214×0.263×0.44
Crystal colour	colourless	colourless	colourless
Crystal shape	block	plate	block
Radiation	MoK α (λ =0.71073 Å)	MoK α (λ =0.71073 Å)	MoK α (λ =0.71073 Å)
2 θ range [°]	2.90 to 55.07 (0.77 Å)	2.64 to 56.76 (0.75 Å)	2.77 to 55.18 (0.77 Å)
	−20 ≤ <i>h</i> ≤ 20	−24 ≤ <i>h</i> ≤ 24	−20 ≤ <i>h</i> ≤ 20
Index ranges	−30 ≤ <i>k</i> ≤ 30	−39 ≤ <i>k</i> ≤ 39	−23 ≤ <i>k</i> ≤ 23
	−41 ≤ <i>l</i> ≤ 41	−29 ≤ <i>l</i> ≤ 29	−29 ≤ <i>l</i> ≤ 29
Reflections collected	553135	473329	412837
	26698	29446	27702
Independent reflections	<i>R</i> _{int} = 0.0617 <i>R</i> _{sigma} = 0.0237	<i>R</i> _{int} = 0.0467 <i>R</i> _{sigma} = 0.0233	<i>R</i> _{int} = 0.0503 <i>R</i> _{sigma} = 0.0211
Completeness to θ = 25.242°	99.9 %	100.0 %	100.0 %
Data / Restraints / Parameters	26698 / 33678 / 2379	29446 / 33743 / 2382	27702 / 24108 / 2160
Absorption correction	0.6901 / 0.7456	0.6743 / 0.7457	0.6343 / 0.7456
<i>T</i> _{min} / <i>T</i> _{max} (method)	(multi-scan)	(multi-scan)	(multi-scan)
Goodness-of-fit on <i>F</i> ²	1.018	1.039	1.060
Final <i>R</i> indexes	<i>R</i> ₁ = 0.0487	<i>R</i> ₁ = 0.0291	<i>R</i> ₁ = 0.0447
[<i>I</i> ≥ 2σ(<i>I</i>)]	<i>wR</i> ₂ = 0.1271	<i>wR</i> ₂ = 0.0786	<i>wR</i> ₂ = 0.1171
Final <i>R</i> indexes	<i>R</i> ₁ = 0.0527	<i>R</i> ₁ = 0.0302	<i>R</i> ₁ = 0.0526
[all data]	<i>wR</i> ₂ = 0.1314	<i>wR</i> ₂ = 0.0798	<i>wR</i> ₂ = 0.1255
Largest peak/hole [eÅ ⁻³]	0.81/−0.52	0.68/−0.58	2.58/−0.57
Flack <i>X</i> parameter	0.017(9)	0.047(5)	–

Table S 3: Crystal data and summary of the data collection and refinement for $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$ and $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfa}]_{1/3}$.

CCDC	2488261	2490061
Empirical formula	$\text{C}_{86}\text{H}_{99}\text{Al}_2\text{F}_{72}\text{Ga}_2\text{NO}_8\text{P}_4$	$\text{C}_{278}\text{H}_{297}\text{Al}_7\text{F}_{244}\text{Ga}_6\text{O}_{26}\text{P}_{12}$
Formula weight	2959.94	9668.99
Temperature [K]	100(2)	100(2)
Crystal system	monoclinic	triclinic
Space group (number)	$P2_1$ (4)	$P\bar{1}$ (2)
a [Å]	13.550(4)	18.462(5)
b [Å]	27.099(5)	27.562(6)
c [Å]	15.504(4)	37.435(9)
α [°]	90	86.961(6)
β [°]	91.200(7)	88.862(7)
γ [°]	90	75.387(10)
Volume [Å ³]	5692(3)	18406(8)
Z	2	2
ρ_{calc} [gcm ⁻³]	1.727	1.745
μ [mm ⁻¹]	0.715	0.684
$F(000)$	2964	9652
Crystal size [mm ³]	0.319×0.366×0.477	0.210×0.322×0.389
Crystal colour	colourless	colourless
Crystal shape	block	block
Radiation	MoK_α ($\lambda=0.71073$ Å)	MoK_α ($\lambda=0.71073$ Å)
2θ range [°]	2.63 to 55.26 (0.77 Å)	2.53 to 55.26 (0.77 Å)
Index ranges	$-17 \leq h \leq 17$ $-35 \leq k \leq 35$ $-20 \leq l \leq 20$	$-24 \leq h \leq 24$ $-35 \leq k \leq 35$ $-48 \leq l \leq 48$
Reflections collected	218575 26263	1009603 85023
Independent reflections	$R_{\text{int}} = 0.0611$ $R_{\text{sigma}} = 0.0402$	$R_{\text{int}} = 0.0663$ $R_{\text{sigma}} = 0.0343$
Completeness to $\theta = 25.242^\circ$	99.8 %	99.9 %
Data / Restraints / Parameters	26263 / 44139 / 3022	85023 / 328226 / 8698
Absorption correction $T_{\text{min}}/T_{\text{max}}$ (method)	0.6500 / 0.7084 (multi-scan)	0.6849 / 0.7456 (multi-scan)
Goodness-of-fit on F^2	1.044	1.100
Final R indexes [$\geq 2\sigma(I)$]	$R_1 = 0.0889$ $wR_2 = 0.2511$	$R_1 = 0.0990$ $wR_2 = 0.2598$
Final R indexes [all data]	$R_1 = 0.1063$ $wR_2 = 0.2781$	$R_1 = 0.1243$ $wR_2 = 0.2809$
Largest peak/hole [eÅ ⁻³]	1.00/−0.64	1.45/−1.09
Flack X parameter	0.12(2)	

3.1 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2 \cdot \text{C}_6\text{H}_{10}$

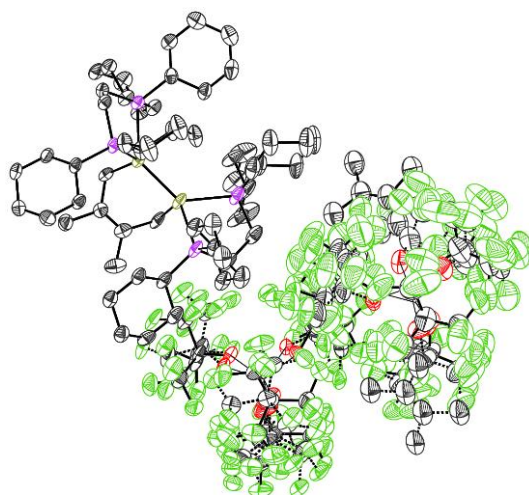


Figure S 3: Molecular structure of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2 \cdot \text{C}_6\text{H}_{10}$. Hydrogen atoms are omitted for clarity. The disordered anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

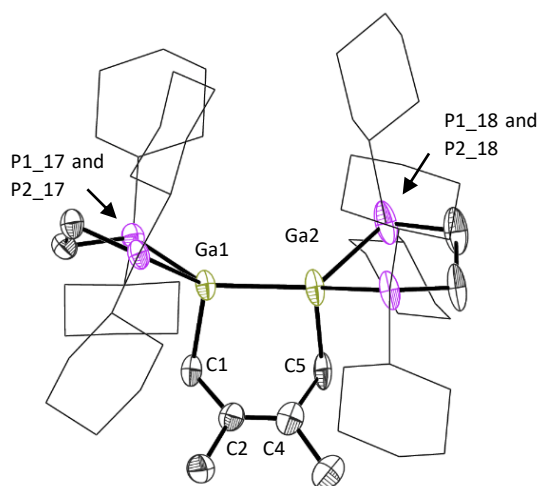


Figure S 4: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})]^{2+}$ in $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2 \cdot \text{C}_6\text{H}_{10}$. Hydrogen atoms are omitted and the cyclohexyl groups are depicted in wireframe for simplicity. Thermal ellipsoids are set at 50 % probability level.

Table S 4: Selected bond lengths in $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2 \cdot \text{C}_6\text{H}_{10}$.

Atom–Atom	Bond Length [pm]
Ga1–C1	201.5(6)
Ga1–P1_17	242.18(19)
Ga1–P2_17	243.6(2)
Ga1–Ga2	243.90(11)
Ga2–C5	203.9(7)
Ga2–P2_18	242.2(2)
Ga2–P1_18	244.0(2)
C2–C1	1.500(9)
C2–C4	1.314(11)
C4–C5	1.510(10)

It has to be noted that the compound crystallizes in a superstructure, as previously observed for cycloaddition products of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ with an alkene and an alkyne. Thus, the scXRD data were not uploaded in the CCDC data base and only allow to show atom connectivities. The bond lengths in **Table S 4** are only shown to underline the good agreement with the computed values and with the Ga–Ga and Ga–P bond lengths in the other crystalline compounds presented herein. Interestingly, the determined C1–C2 and C4–C5 bond lengths are not only in good agreement with the calculated distances (ca. 150 pm) but are also significantly longer than the C2–C4 distance (calculated bond length: 136 pm). This strongly implies that the cycloaddition leads to the formation of a C=C double bond between C2 and C4 and a concomitant formation of C1–C2 and C4–C5 single bonds, which is expected for the product of a hetero-Diels-Alder reaction.

3.2 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$

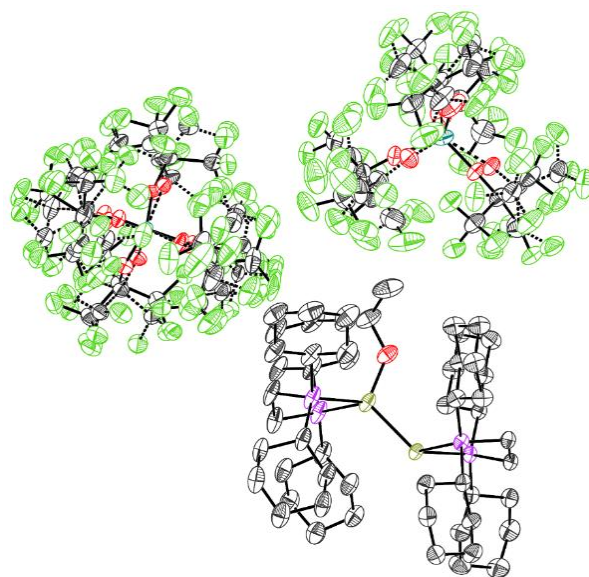


Figure S 5: Molecular structure of the asymmetric unit of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. Disordered anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

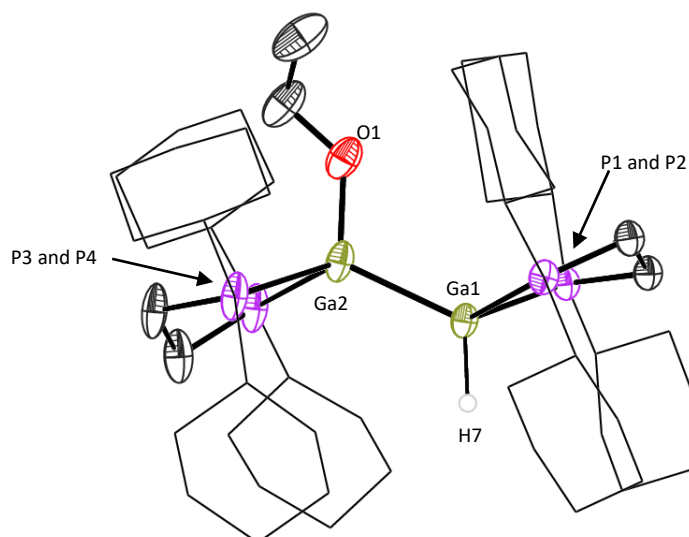


Figure S 6: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})]^{2+}$ in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$. Hydrogen atoms are omitted (except for the hydrogen atom bound to Ga) and the cyclohexyl groups are depicted in wireframe for simplicity. Thermal ellipsoids are set at 50 % probability level.

Table S 5: Selected bond lengths in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$.

Atom–Atom	Bond Length [pm]
Ga1–P2	241.57(12)
Ga1–P1	241.70(11)
Ga1–Ga2	243.35(9)
Ga1–H7	147(4)
Ga2–O1	181.5(4)
Ga2–P3	247.82(13)
Ga2–P4	247.88(13)

3.3 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$

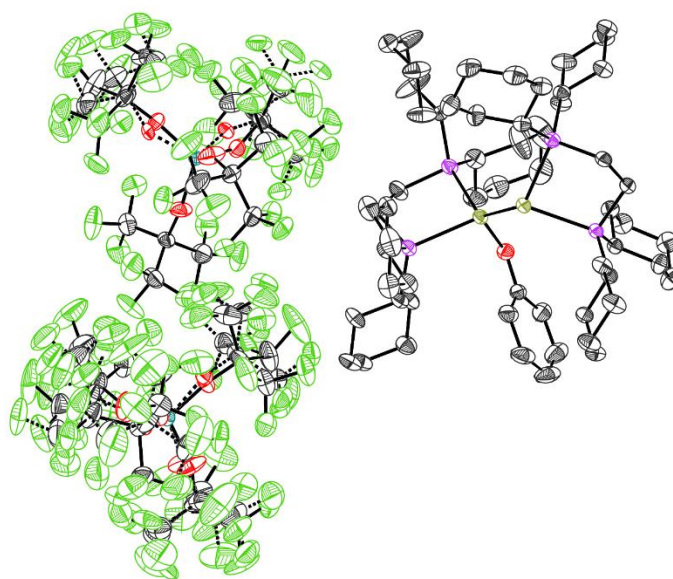


Figure S 7: Molecular structure of the asymmetric unit of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. Disordered anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

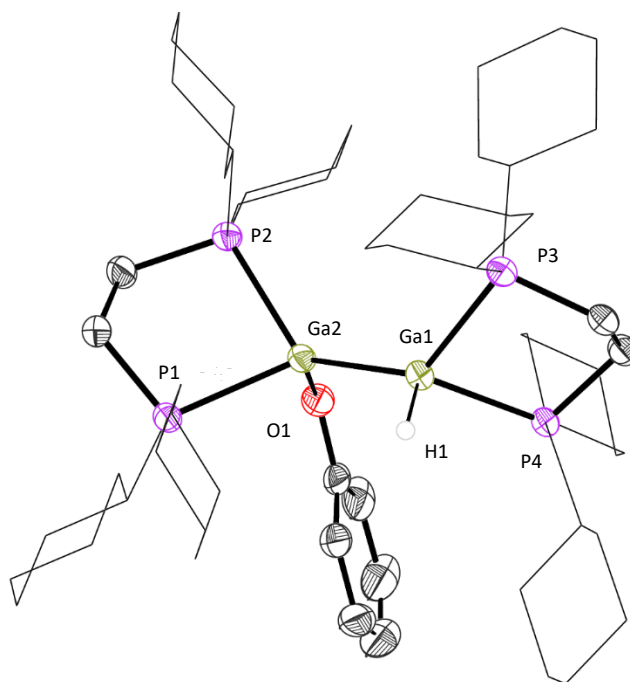


Figure S 8: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})]^{2+}$ in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$. Hydrogen atoms are omitted (except for the hydrogen atom bound to Ga) and the cyclohexyl groups are depicted in wireframe for simplicity. Thermal ellipsoids are set at 50 % probability level.

Table S 6: Selected bond lengths in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$.

Atom–Atom	Bond Length [pm]
Ga1–P3	241.81(13)
Ga1–P4	242.64(12)
Ga1–Ga2	246.28(7)
Ga1–H1	143(6)
Ga2–O1	185.9(4)
Ga2–P2	242.83(13)
Ga2–P1	247.39(12)

3.4 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPH})][\text{pf}]_2$

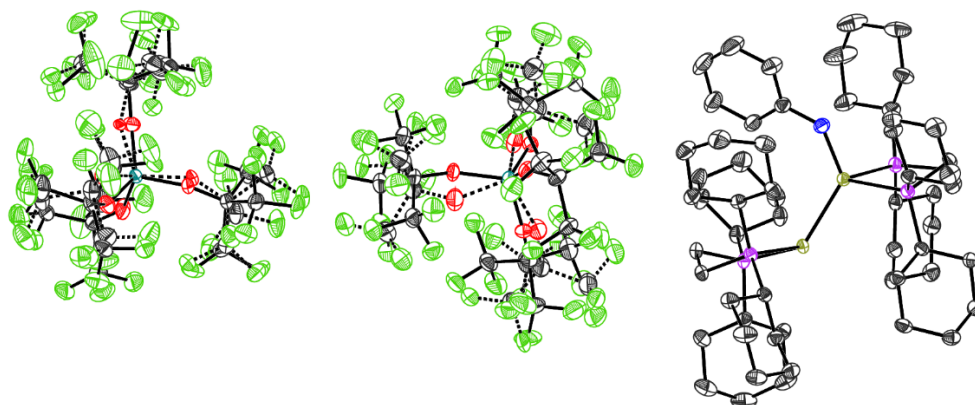


Figure S 9: Molecular structure of the asymmetric unit of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPH})][\text{pf}]_2$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. Disordered anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

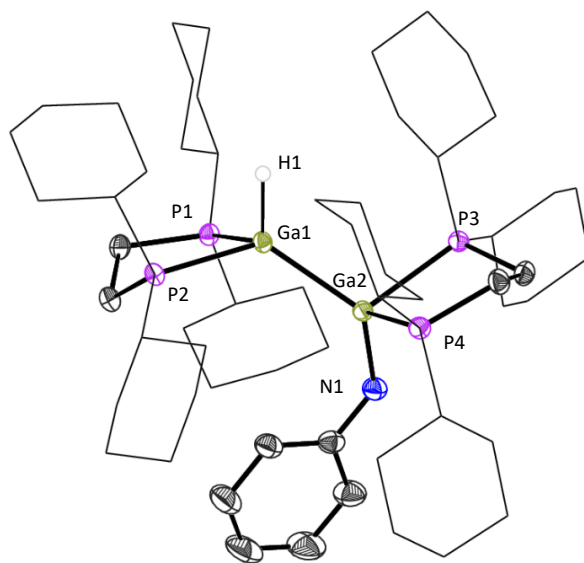


Figure S 10: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPh})]^{2+}$ in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPh})][\text{pf}]_2$. Hydrogen atoms are omitted (except for the hydrogen atom bound to Ga) and the cyclohexyl groups are depicted in wireframe for simplicity. Thermal ellipsoids are set at 50 % probability level.

Table S 7: Selected bond lengths in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPh})][\text{pf}]_2$.

Atom–Atom	Bond Length [pm]
Ga1–P2	240.78(8)
Ga1–P1	241.16(8)
Ga1–Ga2	243.21(5)
Ga1–H1	149(6)
Ga2–N1	187.1(2)
Ga2–P3	242.68(8)
Ga2–P4	246.97(8)

3.5 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$

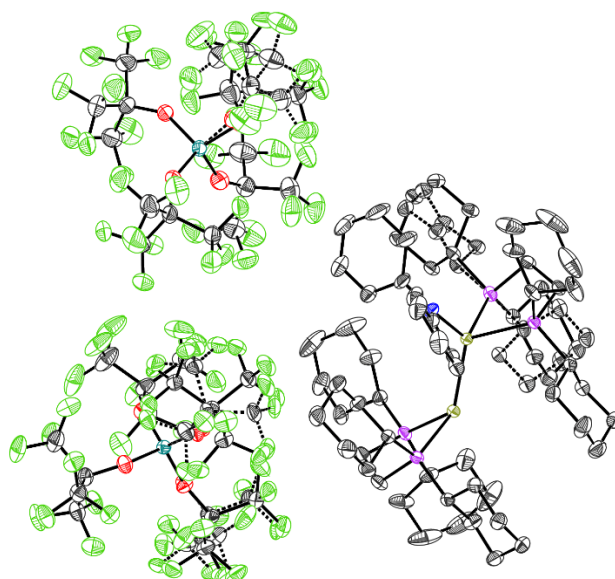


Figure S 11: Molecular structure of the asymmetric unit of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. Disordered anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

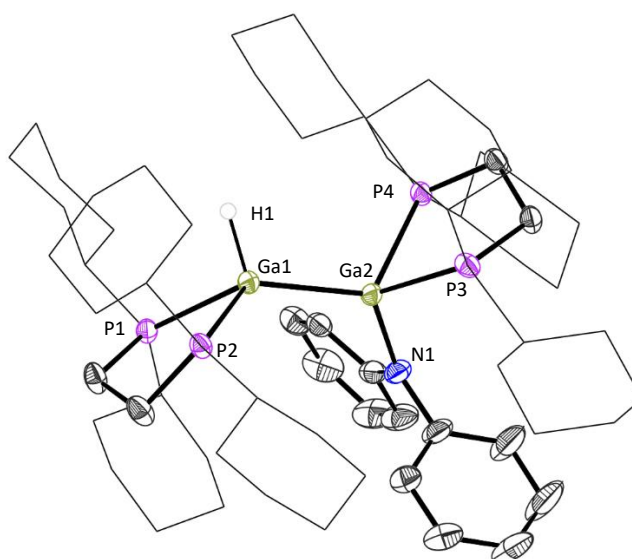


Figure S 12: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)]^{2+}$ in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$. Hydrogen atoms are omitted (except for the hydrogen atom bound to Ga) and the cyclohexyl groups are depicted in wireframe for simplicity. Thermal ellipsoids are set at 50 % probability level.

Table S 8: Selected bond lengths in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$.

Atom–Atom	Bond Length [pm]
Ga1–P2	244.37(7)
Ga1–P1	245.72(8)
Ga1–Ga2	248.53(6)
Ga1–H1	144(3)
Ga2–N1	191.9(2)
Ga2–P3	247.32(9)
Ga2–P4	250.50(7)

3.6 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$

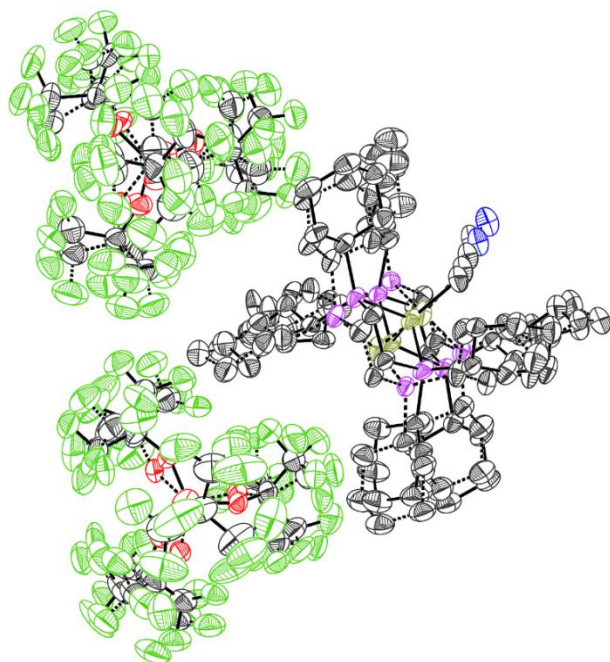


Figure S 13: Molecular structure of the asymmetric unit of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. Disordered ligand and anion fragments are shown. Thermal ellipsoids are set at 50 % probability level.

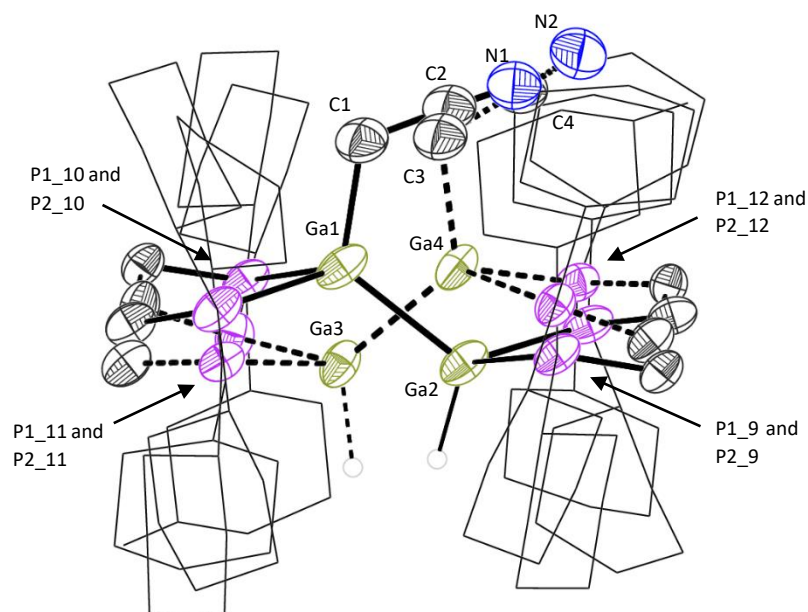


Figure S 14: Molecular structure of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})]^{2+}$ in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$. Hydrogen atoms are omitted (except for the hydrogen atoms bound to Ga) and the cyclohexyl groups are depicted in wireframe for simplicity. Disordered ligand fragments are also shown. Thermal ellipsoids are set at 50 % probability level.

Table S 9: Selected bond lengths in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$.

Atom–Atom	Bond Length [pm]
Ga1–C1	205.4(16)
Ga1–Ga2	244.64(18)
Ga1–P2_10	243.7(4)
Ga1–P1_10	246.4(5)
Ga2–P2_9	241.5(4)
Ga2–P1_9	243.5(5)
Ga4–C3	208(2)
Ga4–Ga3	244.1(3)
Ga3–P2_11	241.7(5)
Ga3–P1_11	242.6(4)
Ga4–P2_12	242.0(5)
Ga4–P1_12	244.8(5)

It has to be noted that the quality of the scXRD data only allow to show atom connectivities, and not to discuss bond lengths. The bond lengths in **Table S 9** are only shown to underline the good agreement with the computed values and with the Ga–Ga, Ga–P and Ga–C bond lengths in the other crystalline compounds presented herein. Since the Ga–H distance cannot be determined reliably, the bond distance is not included in **Table S 9**. However, the Ga–H signal in the ^1H NMR spectrum as well as the Ga–H band in the IR spectrum unequivocally confirm the presence of this proton in the reaction product.

3.7 $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$

A structural model for the crystals obtained upon layering a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{FH}_2\text{C–CN}$ in oDFB with *n*-pentane is shown in **Figure S 15**. Unfortunately, the quality of the scXRD data ($R_1 = 0.1241$; $wR_2 = 0.4161$; reflection/parameter ration = 4.78) does not allow to upload the structural model in the CCDC database. The handling of the data (space group: $P2_1/n$) is complicated by the fact that the whole cation is disordered on a special position, i.e. the surface centre of the unit cell (**Figure S 16** and **Figure S 17**).

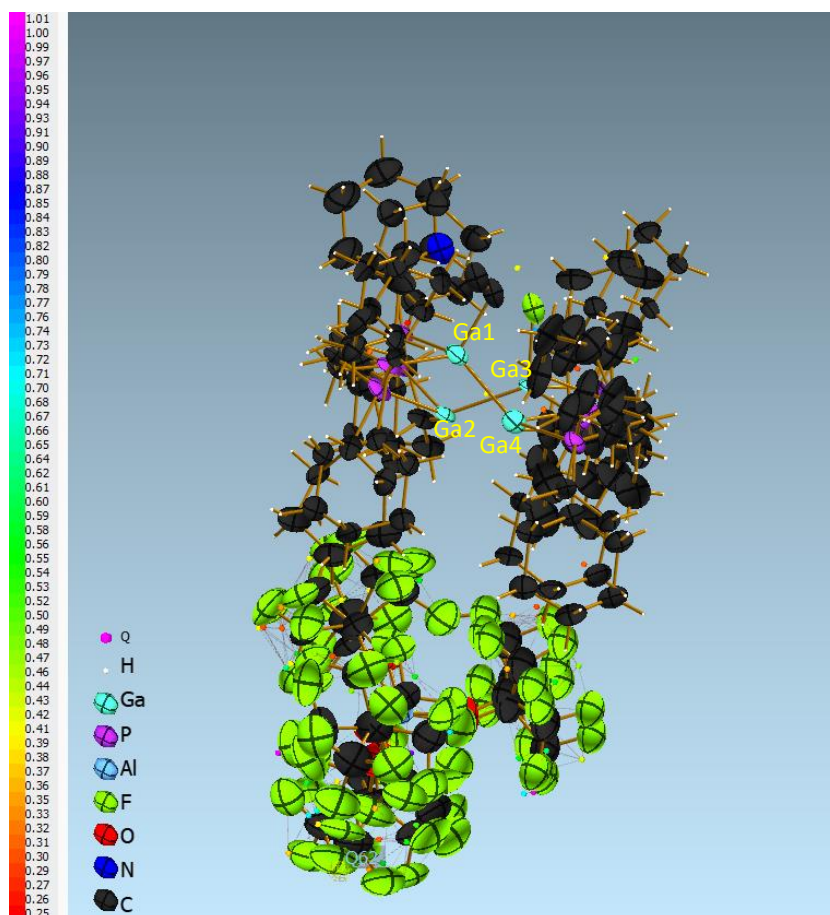


Figure S 15: Structural model for the crystals obtained upon layering a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{FH}_2\text{C}-\text{CN}$ in *o*DFB with *n*-pentane.

However, it is reasonable to assume that the positions of the heavy, electron rich gallium atoms within the unit cell can be determined reliably, as well as the Ga–Ga distances. The main question that arises when assigning the disordered fragments is, whether Ga1 is bound to Ga4 or to Ga3. The bond distances Ga1–Ga3 and Ga2–Ga4 are unreasonably short (213.6 and 191.1 pm), considering that the Ga–Ga bond length typically ranges from 235–255 pm^[33] in elemental gallium and organometallic gallium compounds. Thus, in the structural model presented in **Figure S 15**, Ga1 has to be bound to Ga4 and Ga2 has to be bound to Ga3 (bond lengths: 242.2 and 243.8 pm). This is an important finding, since the “zigzag” arrangement of the central “ P_2GaGaP_2 ”-unit is not consistent with the structure of a [2+2] cycloaddition product.

As a consequence, the scXRD data of the crystalline product of the reaction between $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$ and $\text{FH}_2\text{C}-\text{CN}$ are more in line with the *anti*-periplanar C–F activation product, which is also confirmed by NMR spectroscopy (section 4.12).

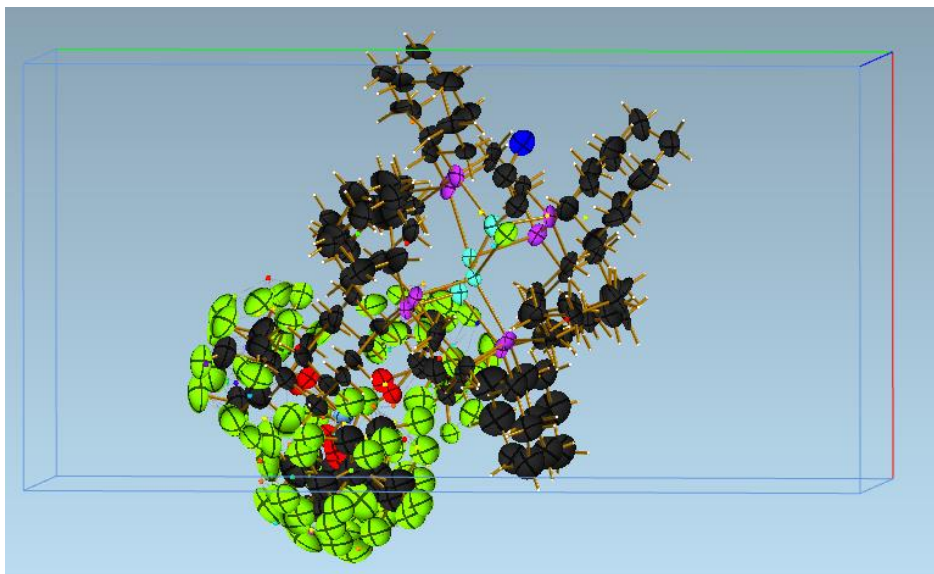


Figure S 16: Structural model, and unit cell, for the crystals obtained upon layering a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{FH}_2\text{C-CN}$ in *o*DFB with *n*-pentane.

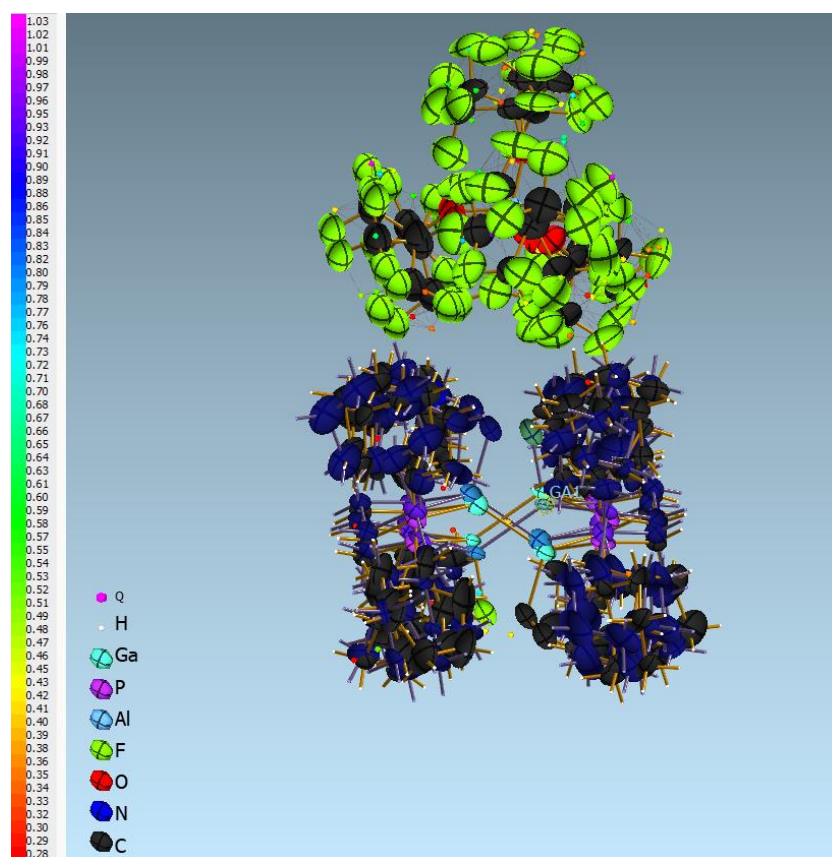


Figure S 17: Structural model for the crystals obtained upon layering a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{FH}_2\text{C-CN}$ in *o*DFB with *n*-pentane. The disordered and symmetry-generated cation fragments are shown.

3.8 $[F\{Ga(dcpe)\}_2(C_6F_2H_3)][pf]_{5/3}[alfal]_{1/3}$

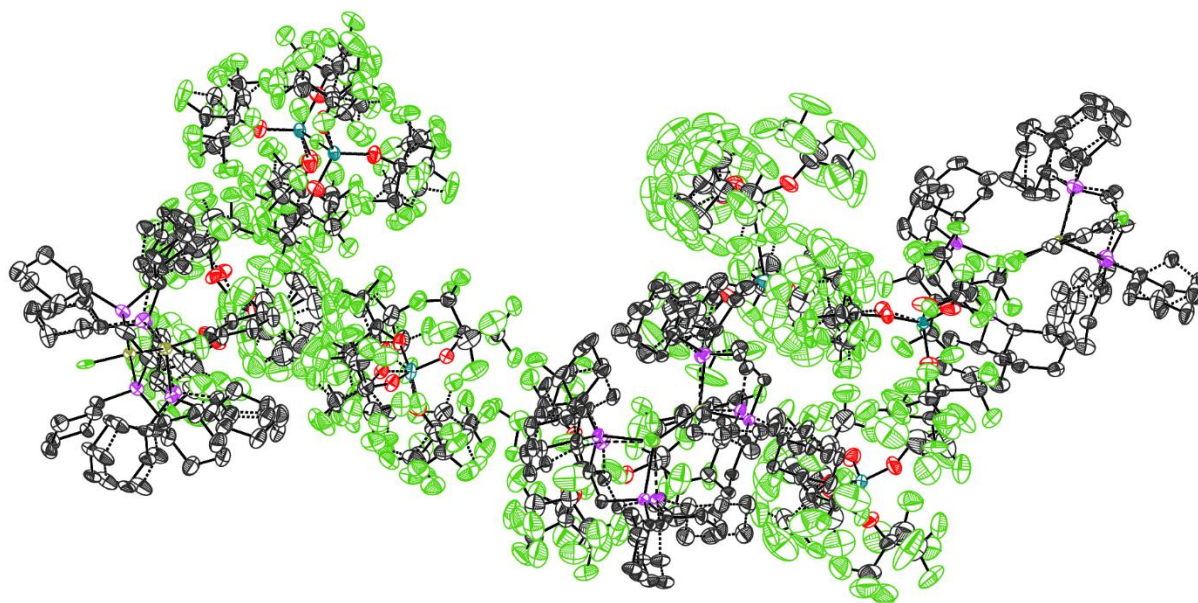


Figure S 18: Molecular structure of the asymmetric unit of $[F\{Ga(dcpe)\}_2(C_6F_2H_3)][pf]_{5/3}[alfal]_{1/3}$ in the solid state from scXRD. Hydrogen atoms are omitted for the sake of clarity. The three crystallographically independent $[F\{Ga(dcpe)\}_2(C_6F_2H_3)]^{2+}$ units are shown, as well as disordered ligand and anion fragments. The second $[Al\{O(CF_3)_3\}_3]$ fragments of the two $[alfal]^-$ anions are symmetry-generated (by an inversion operation). Thermal ellipsoids are set at 50 % probability level

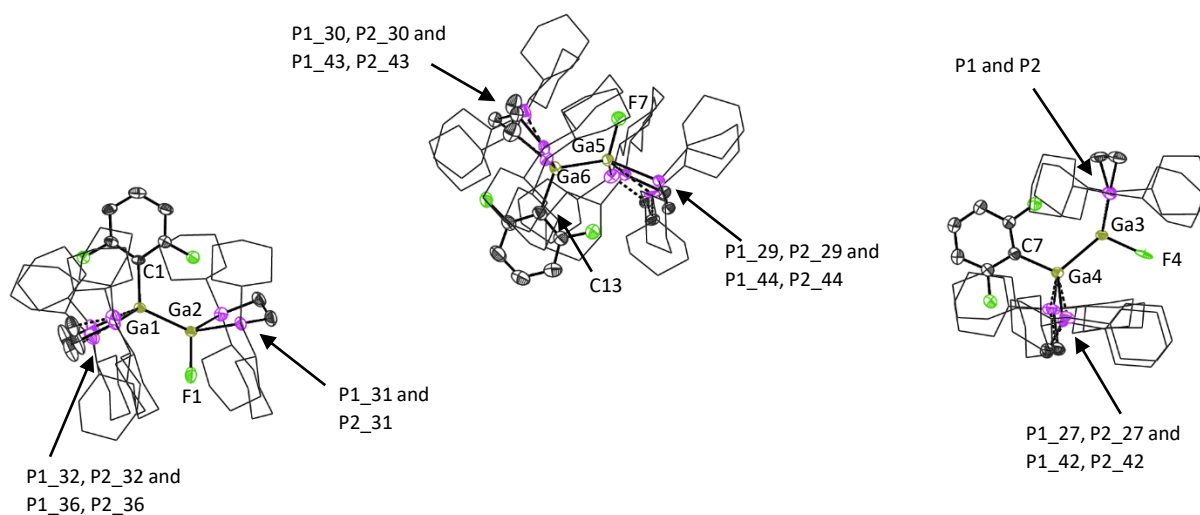


Figure S 19: Molecular structure of the three crystallographically independent $[F\{Ga(dcpe)\}_2(C_6F_2H_3)]^{2+}$ fragments in $[F\{Ga(dcpe)\}_2(C_6F_2H_3)][pf]_{5/3}[alfal]_{1/3}$. Hydrogen atoms are omitted and the cyclohexyl groups are depicted in wireframe for simplicity. Disordered ligand fragments are also shown. Thermal ellipsoids are set at 50 % probability level.

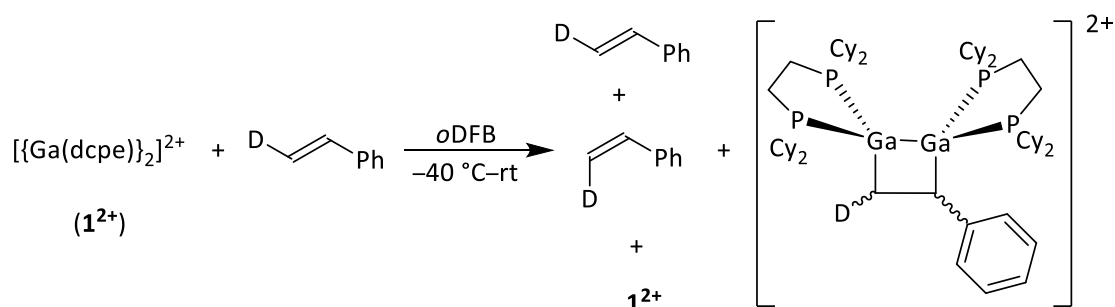
Table S 10: Selected bond lengths in $[F\{Ga(dcpe)\}_2(C_6F_5H_3)][pf]_{5/3}[alfa]_{1/3}$.

Atom–Atom	Bond Length [pm]
Ga1–C1	200.8(5)
Ga1–P1_32	243.4(3)
Ga1–P2_32	244.2(3)
Ga1–Ga2	245.83(9)
Ga1–P2_36	247(3)
Ga1–P1_36	254(3)
Ga2–F1	185.0(4)
Ga2–P1_31	245.00(16)
Ga2–P2_31	246.28(16)
Ga3–F4	195.0(4)
Ga3–P1	243.37(15)
Ga3–Ga4	245.41(10)
Ga3–P2	247.51(16)
Ga4–C7	199.6(5)
Ga4–P2_42	236.8(15)
Ga4–P1_42	240.5(13)
Ga4–P2_27	241.6(10)
Ga4–P1_27	251.1(11)
Ga5–F7	180.9(4)
Ga5–P1_44	239.6(15)
Ga5–P2_29	242.87(18)
Ga5–Ga6	244.38(9)
Ga5–P2_44	245(2)
Ga5–P1_29	247.6(2)
Ga6–C13	201.0(6)
Ga6–P2_43	230(2)
Ga6–P1_30	241.22(17)
Ga6–P2_30	245.6(2)
Ga6–P1_43	266.2(15)

4 NMR Spectroscopy

4.1 NMR Investigations of [2+2] Cycloaddition Reactions with $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$

4.1.1 Reaction with *trans*- β -deutero-styrene



Scheme S 13: Reaction of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ (1^{2+}) and *trans*- β -deutero-styrene in *o*DFB at different temperatures. The $[\text{pf}]^-$ anions are omitted for clarity. Note that the [2+2] cycloaddition products are only formed very slowly below $0\text{ }^\circ\text{C}$.

The NMR spectra in **Figure S 20–Figure S 26** show that *trans*- β -deutero-styrene is converted to a 1:1 mixture of the *trans* and *cis* isomers in the presence of 1^{2+} in an *o*DFB solution, already at 233 K (**Figure S 22**). At this temperature, only the isomerization takes place and no [2+2] cycloaddition products are formed (**Figure S 24**). However, at rt, the formation of the stereoisomeric [2+2] cycloaddition products is indicated by a broad signal at ca. 2.1 ppm in the ^2D NMR spectrum (**Figure S 20** and **Figure S 21**) and by the AA'BB' spin system in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (**Figure S 26**).

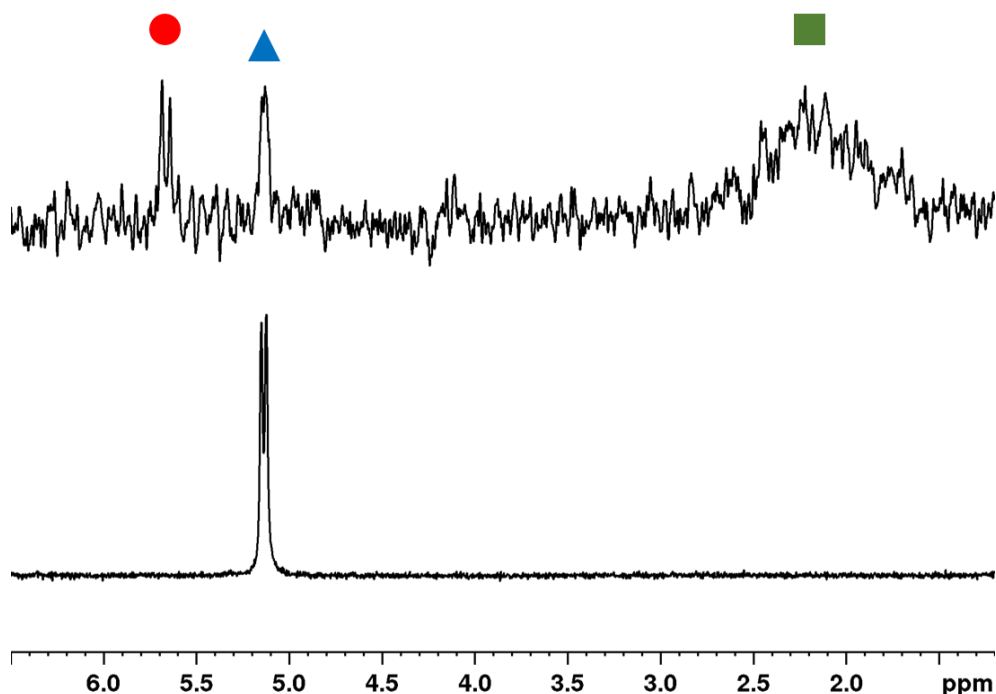


Figure S 20: ^2D NMR spectrum of *trans*- β -deutero-styrene in *o*DFB (61.43 MHz, 298 K, bottom) and of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in *o*DFB (61.43 MHz, 298 K, top). The ^2D NMR signals of the olefinic deuterium atoms of *trans*- β -deutero-styrene (blue triangle), of *cis*- β -deutero-styrene (red point) and of the deuterium atoms in the stereoisomeric [2+2] cycloaddition products (green square) are shown.

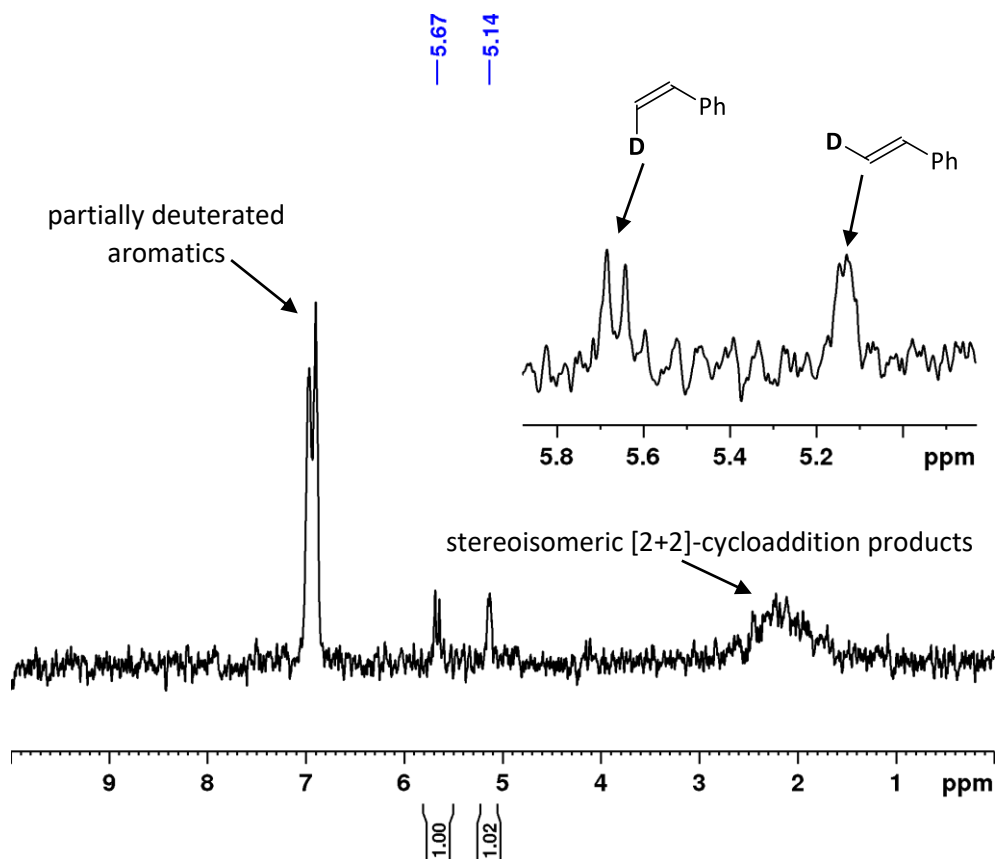


Figure S 21: ^2D NMR spectrum of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in *o*DFB (61.43 MHz, 298 K), with integrated signal intensities for the olefinic deuterium atoms for both products.

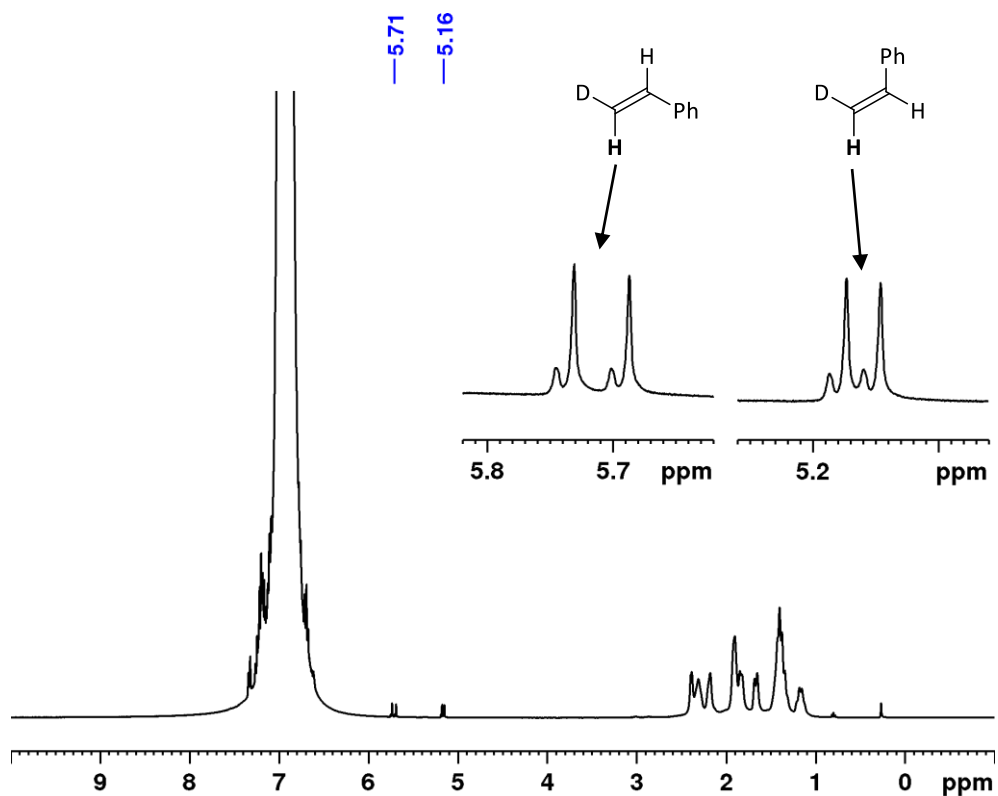


Figure S 22: ^1H NMR spectrum (400.17 MHz, 233 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in *o*DFB, measured directly after mixing the components at low temperatures.

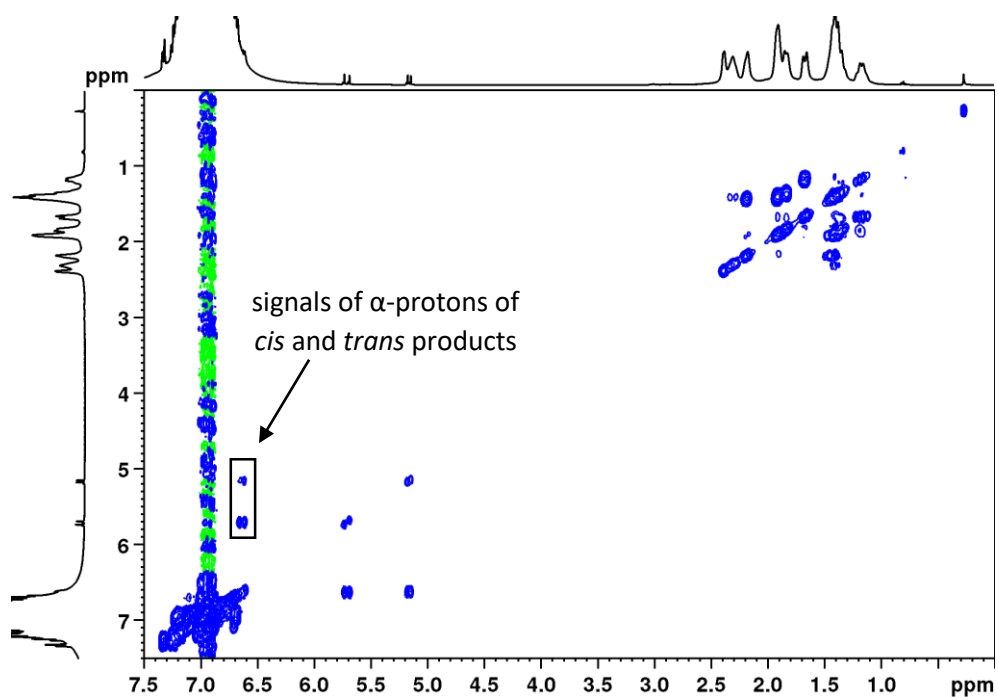


Figure S 23: ^1H -COSY NMR spectrum (400.17 MHz, 233 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in oDFB, measured directly after mixing the components at low temperatures.

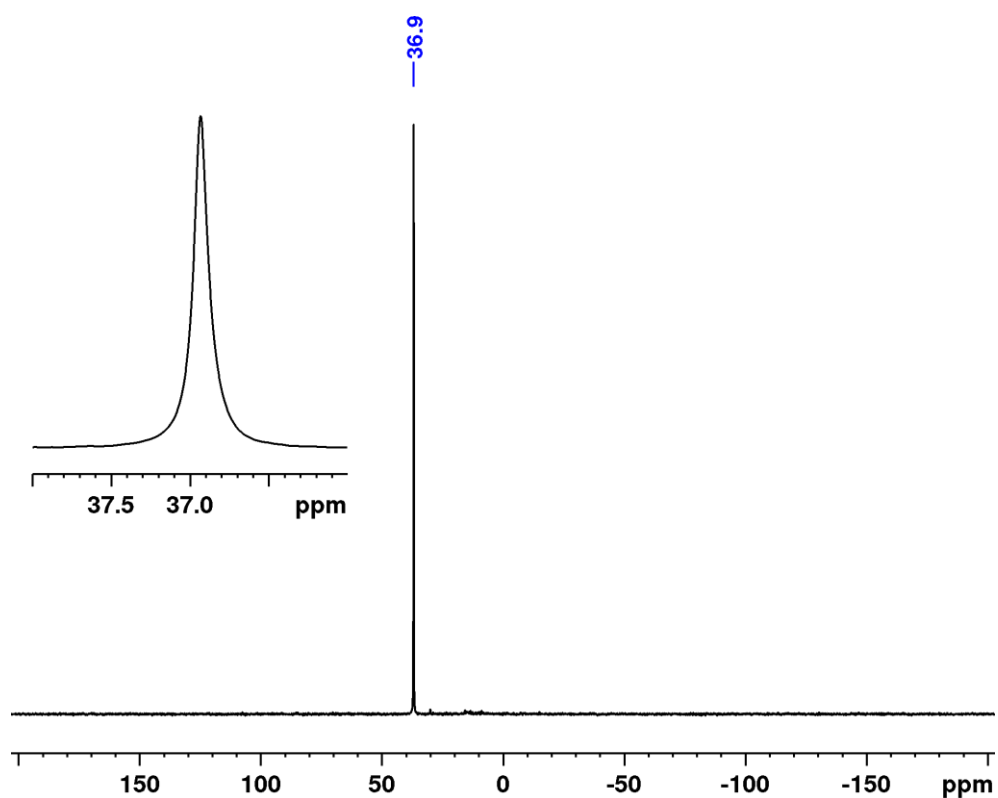


Figure S 24: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, 233 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in oDFB, measured directly after mixing the components at low temperatures.

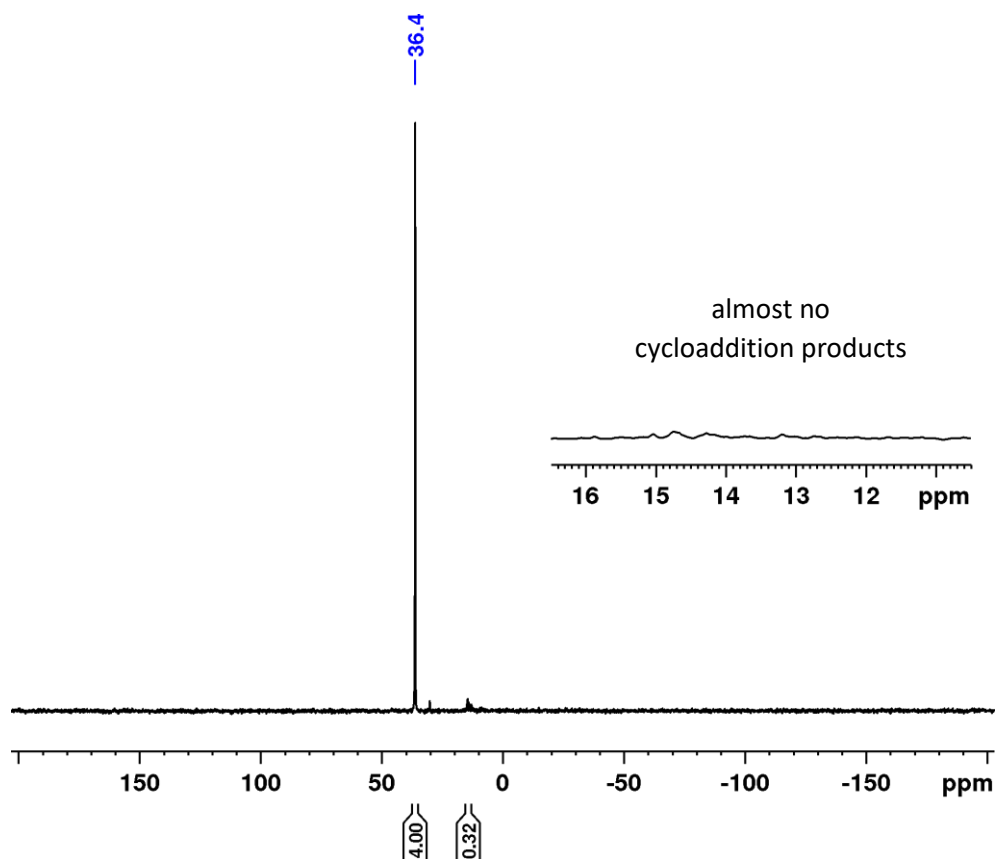


Figure S 25: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, 263 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in oDFB, measured directly after allowing the sample to warm up to 263 K.

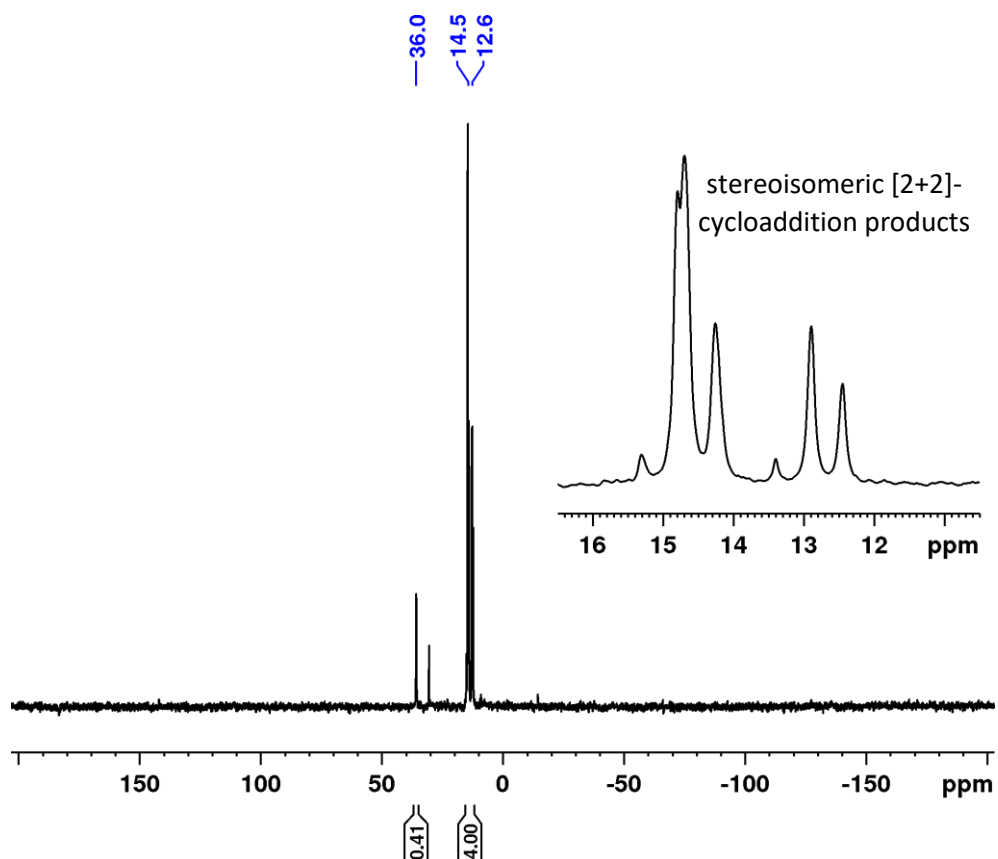
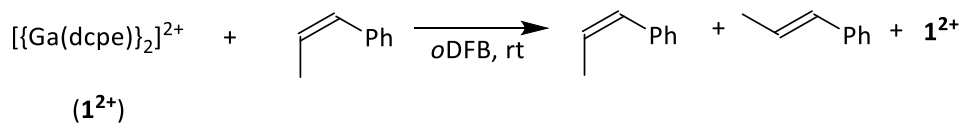


Figure S 26: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *trans*- β -deutero-styrene in oDFB, measured 1 d after mixing the components.

4.1.2 Reaction with *cis*- β -methyl-styrene



Scheme S 14: Reaction of [Ga(dcpe)]₂[pf]₂ (**1**)[pf]₂ and *cis*- β -methyl-styrene in oDFB at rt. The [pf][−] anions are omitted for clarity.

The NMR spectra in **Figure S 27**–**Figure S 29** show that *cis*- β -methyl-styrene is converted to a $\approx$ 99:1 mixture of the *trans* and *cis* isomers in the presence of **1**²⁺ in an oDFB solution. No [2+2] cycloaddition product can be detected in the ³¹P{¹H} NMR spectrum.

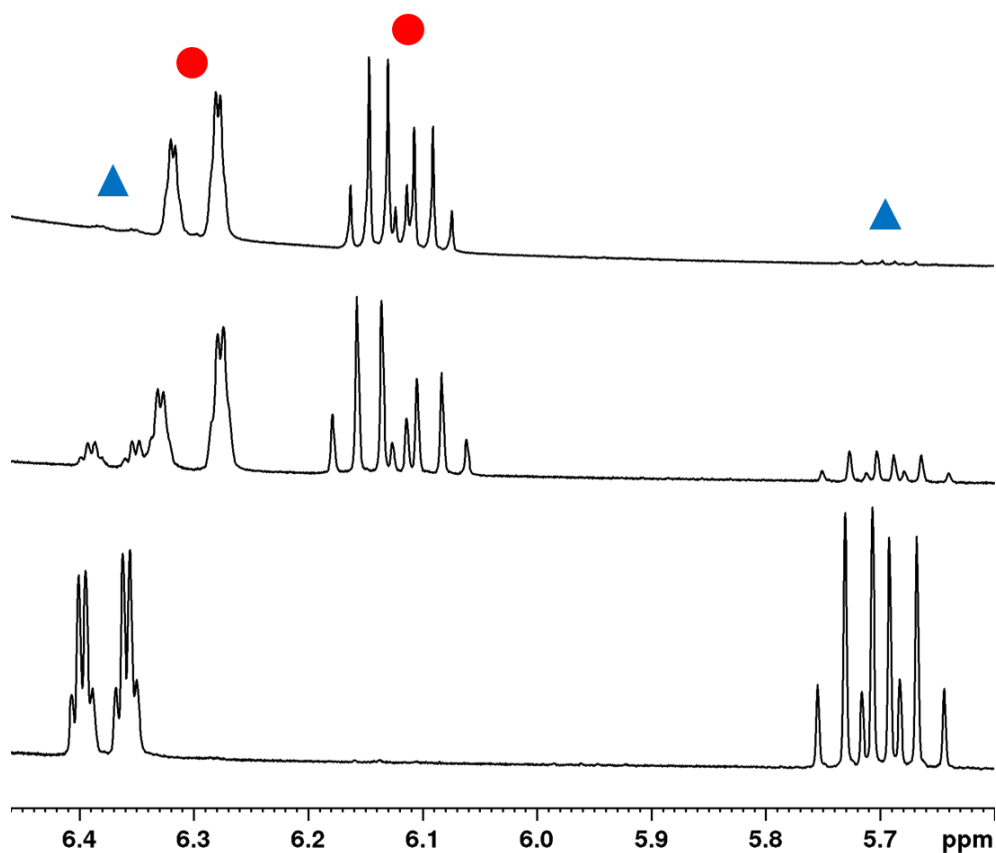


Figure S 27: ¹H NMR spectrum of *cis*- β -methyl-styrene in oDFB (300.18 MHz, 298 K, bottom) and of a mixture of [Ga(dcpe)]₂[pf]₂ and *cis*- β -methyl-styrene in oDFB, 3 h (300.18 MHz, 298 K, middle) and 1 d (400.17 MHz, 298 K, top) after mixing the components. The ¹H NMR signals of the olefinic protons of *cis*- β -methyl-styrene (blue triangles) and of *trans*- β -methyl-styrene (red points) are shown.

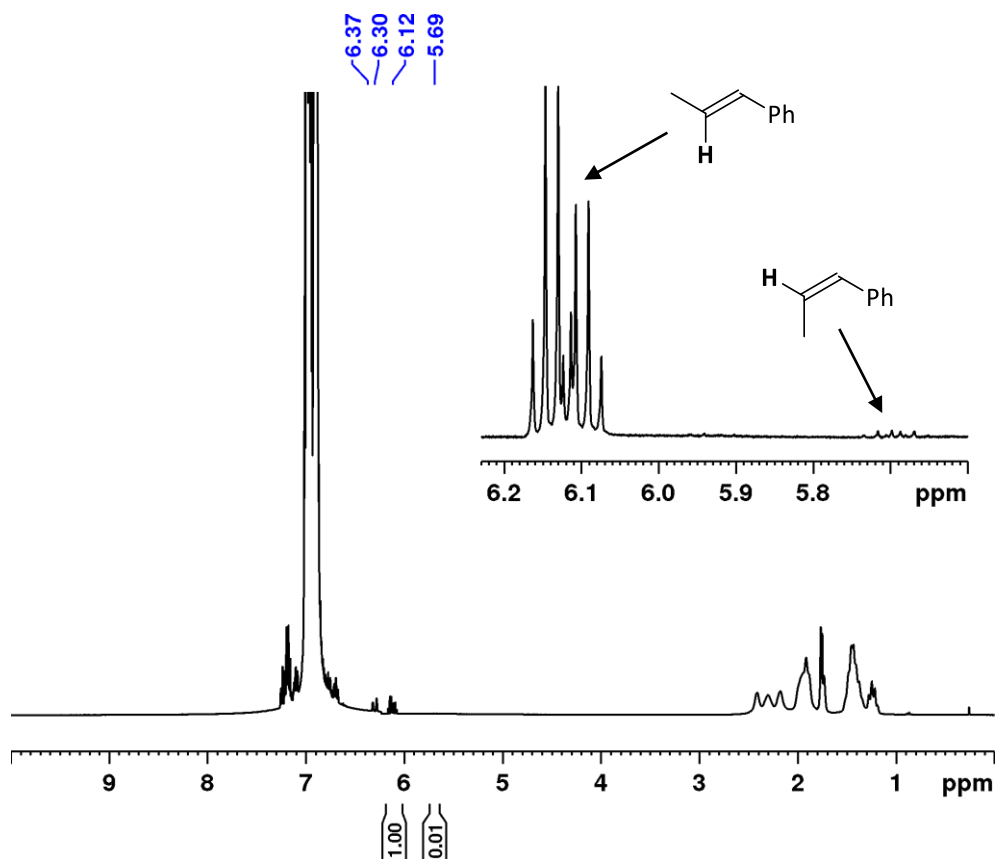


Figure S 28: ^1H NMR spectrum of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *cis*- β -methyl-styrene in *o*DFB, 1 d (400.17 MHz, 298 K) after mixing the components, with integrated signal intensities for the olefinic protons in β position for both products.

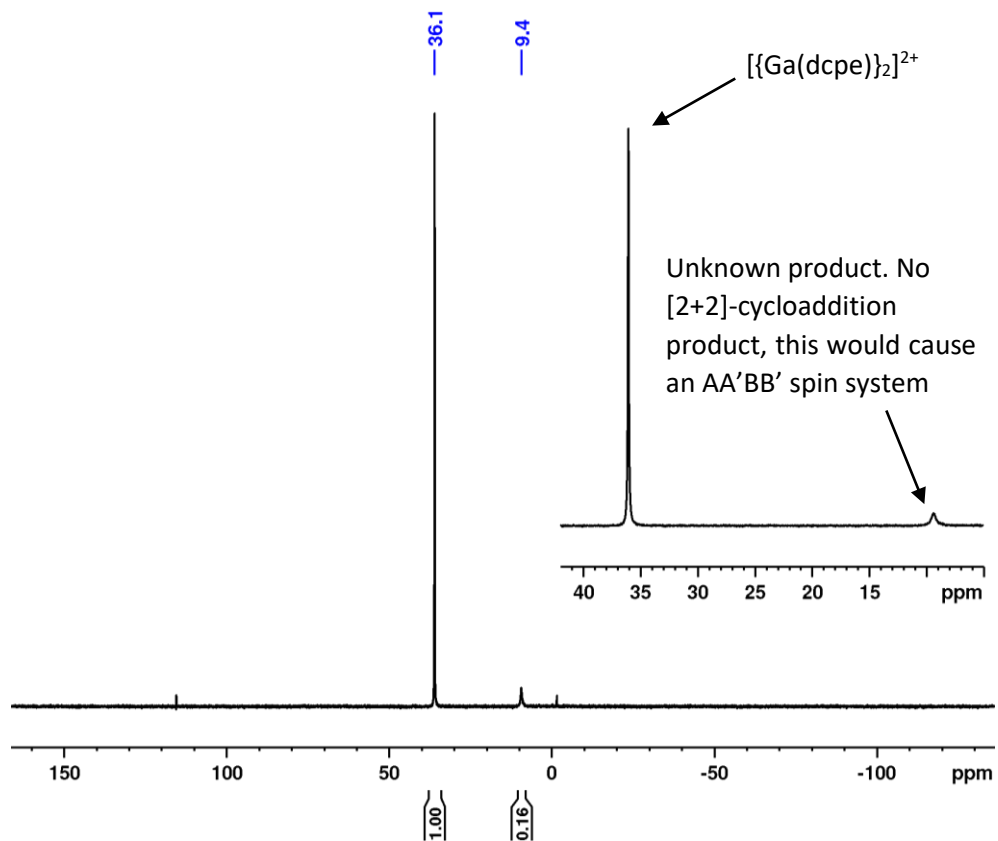
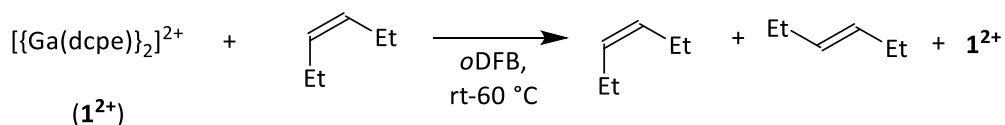


Figure S 29: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and *cis*- β -methyl-styrene in *o*DFB, 1 d (161.99 MHz, 298 K) after mixing the components.

4.1.3 Reaction with *cis*-3-hexene



Scheme S 15: Reaction of $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ (1^{2+}) and *cis*-3-hexene in *o*DFB at rt–60 °C. The $[\text{pf}]^-$ anions are omitted for clarity.

The NMR spectra in **Figure S 30–Figure S 32** show that *cis*-3-hexene is converted to a $\approx 3:1$ mixture of the *trans* and *cis* isomers in the presence of 1^{2+} in an *o*DFB solution. No [2+2] cycloaddition product can be detected in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum.

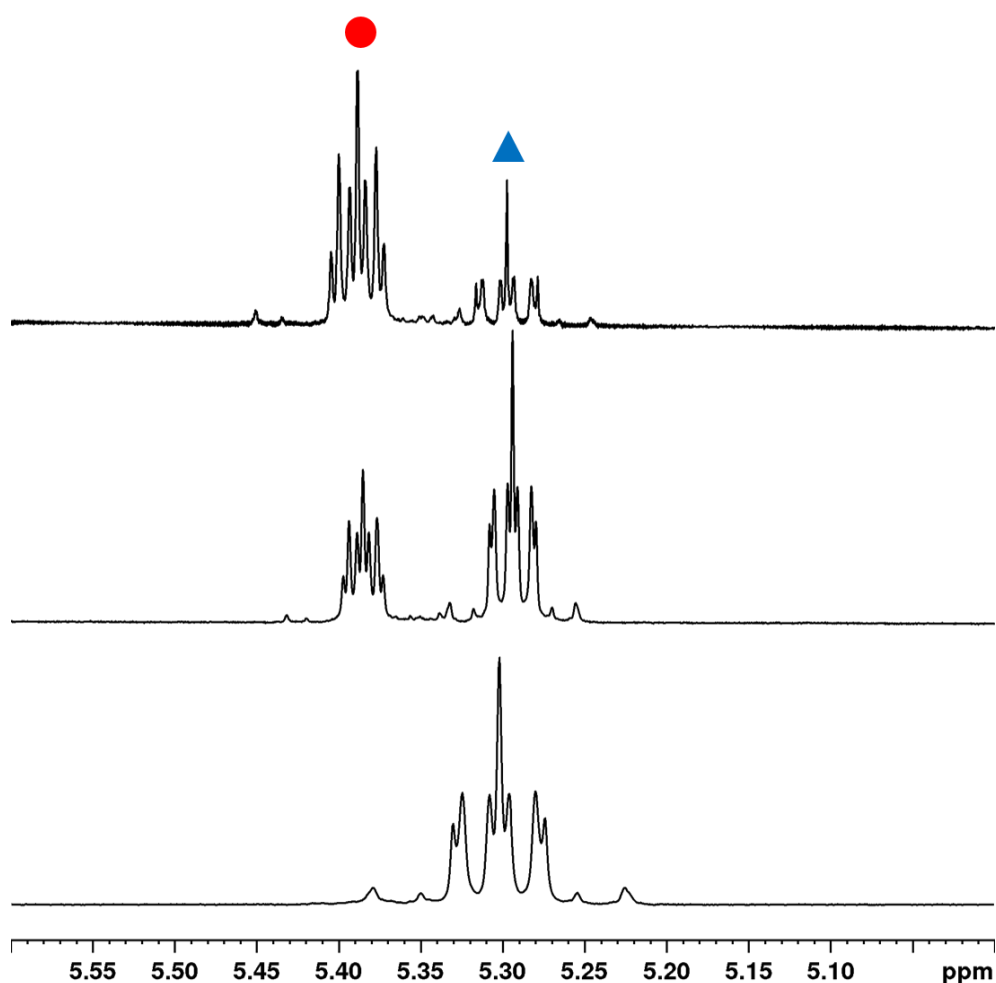


Figure S 30: ^1H NMR spectrum of *cis*-3-hexene in *o*DFB (200.13 MHz, 298 K, bottom) and of a mixture of $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ and *cis*-3-hexene in *o*DFB, after 18 h at 60 °C (400.17 MHz, 298 K, middle) and 8 weeks (300.18 MHz, 298 K, top) after mixing the components. The ^1H NMR signals of the olefinic protons of *cis*-3-hexene (blue triangle) and of *trans*-3-hexene (red point) are shown.

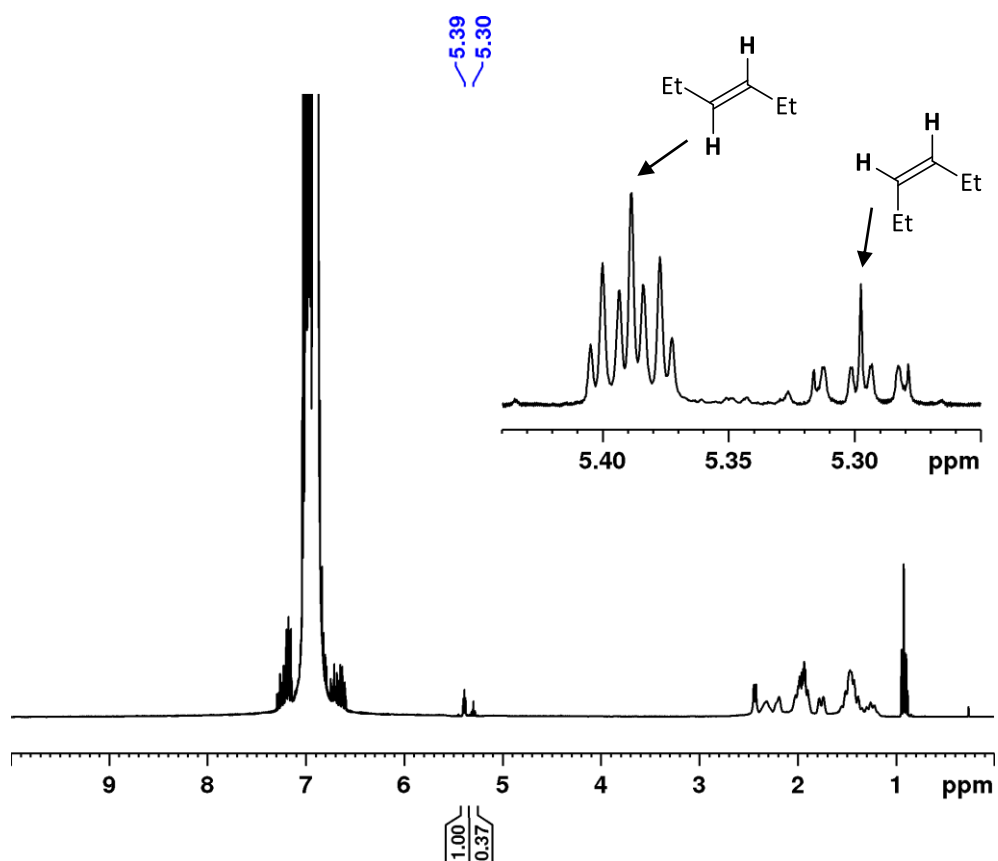


Figure S 31: ^1H NMR spectrum of a mixture of $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ and *cis*-3-hexene in *o*DFB, 8 weeks (400.17 MHz, 298 K) after mixing the components, with integrated signal intensities for the olefinic protons for both products.

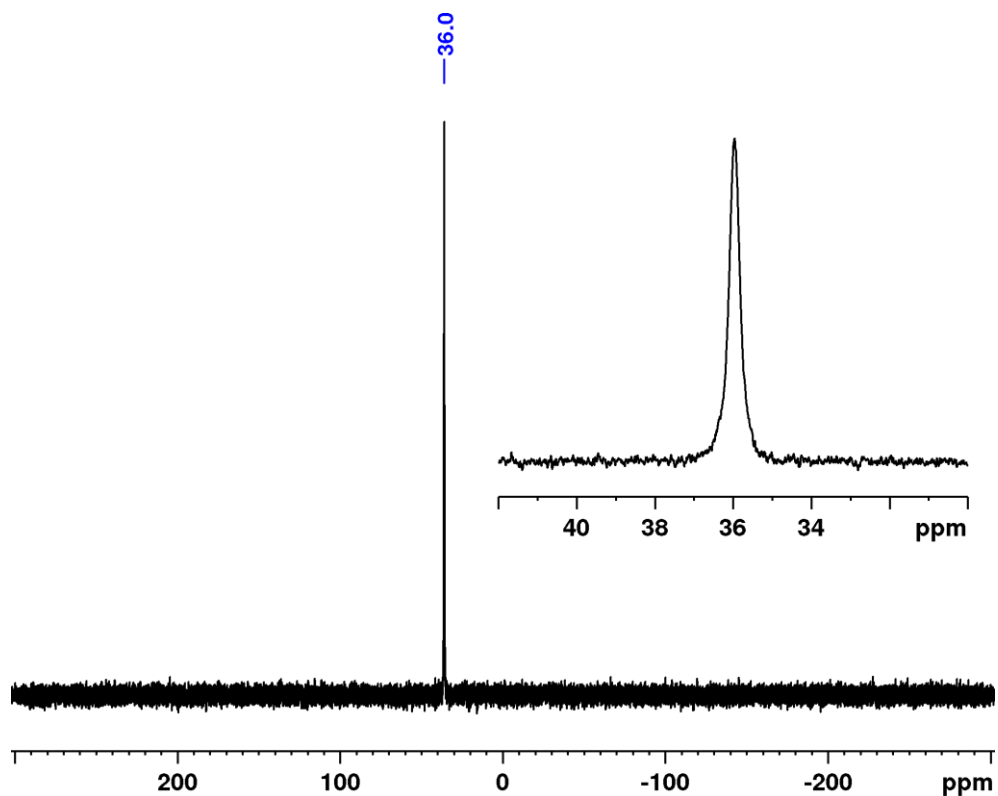
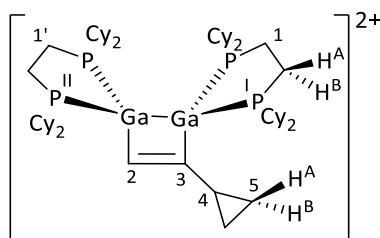


Figure S 32: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of a mixture of $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ and *cis*-3-hexene in *o*DFB (121.52 MHz, 298 K), 1 d after mixing the components (the mixture was heated at 60 °C for 18 h).

4.1.4 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$



^1H NMR [400.17 MHz, *o*D₂F₆, calibrated at $\delta(\text{C}_6\text{F}_5\text{H}) = 6.96$ ppm, 298 K]: $\delta = 7.26$ (t, 1 H, C^2H , $^3J_{\text{H,P}} = 16.7$ Hz), 2.53 and 2.38 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^{1'}\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{B}}$), 2.46–2.15 (m, 8 H, CH protons of the Cy groups), 2.06–1.28 (m, 80 H, CH_2 protons of the Cy groups), 1.72 (m, 1 H, C^4H), 1.01 and 0.81 (m, 4 H, $\text{C}^5\text{H}^{\text{A}}$ and $\text{C}^5\text{H}^{\text{B}}$) ppm.

^{13}C NMR [100.62 MHz, *o*D₂F₆, 298 K]: $\delta = 190.5$ (1 C, C^3), 152.2 (1 C, C^2), 33.4–31.7 (8 C, CH carbon atoms of the Cy groups), 29.2–25.0 (40 C, CH_2 carbon atoms of the Cy groups), 20.0 (1 C, C^4), 15.8 (4 C, C^1), 12.6 (2 C, C^5) ppm.

^{19}F NMR [376.54 MHz, *o*D₂F₆, 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.8 (m, PhF), -139.5 (m, $\text{C}_6\text{F}_5\text{H}$) ppm.

^{27}Al NMR [78.22 MHz, *o*D₂F₆, 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [161.99 MHz, *o*D₂F₆, 298 K]: $\delta = 12.57$ (m, 2 P, P^{II}), 12.52 (m, 2 P, P^{I}) ppm.

^{71}Ga NMR [91.55 MHz, *o*D₂F₆, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

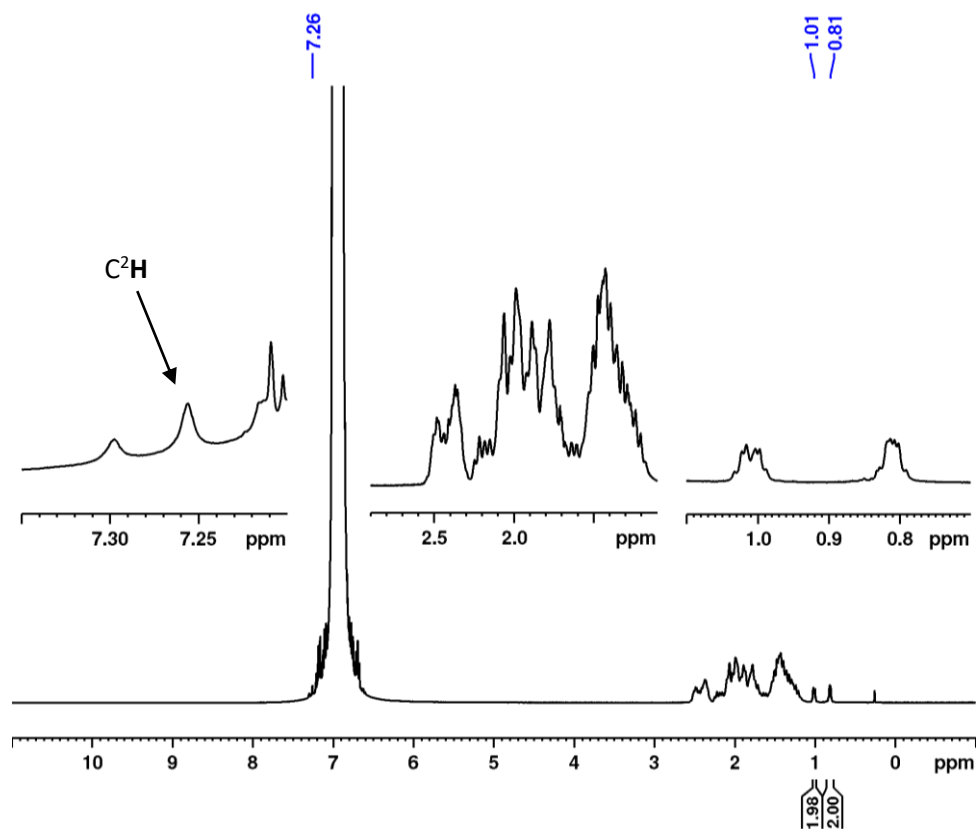


Figure S 33: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$.

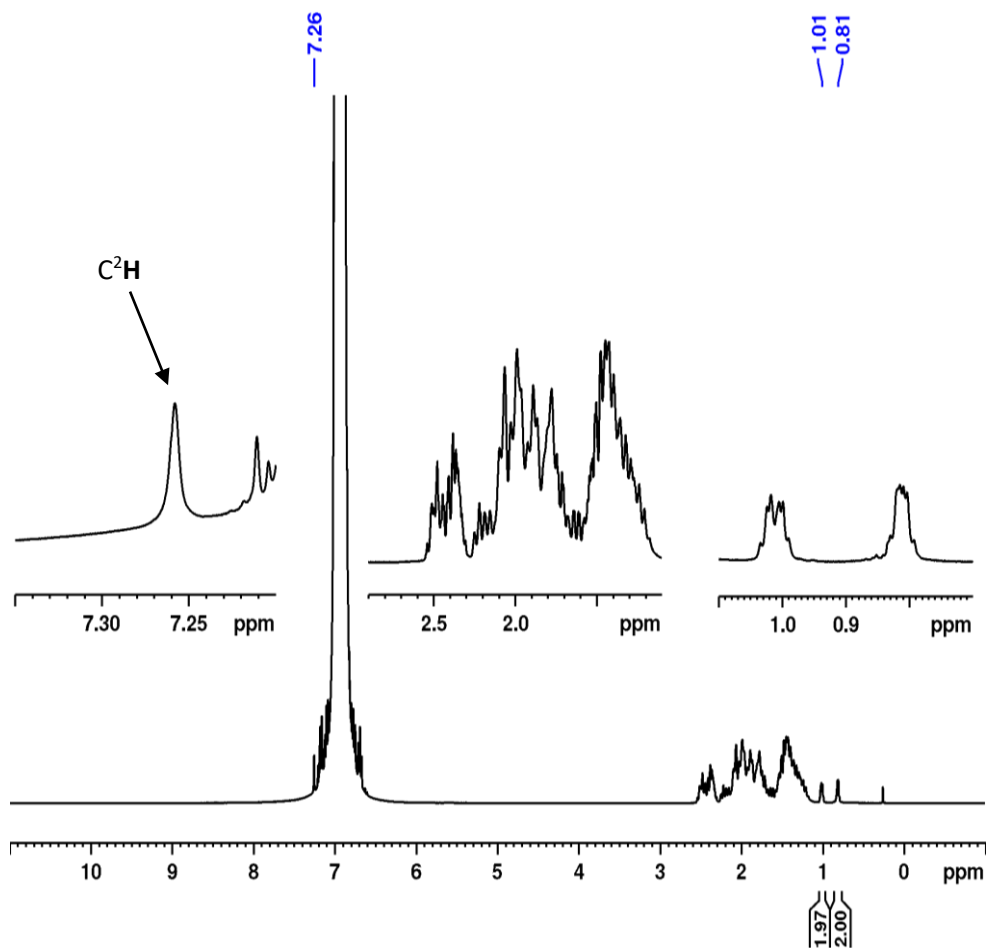


Figure S 34: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (400.17 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$.

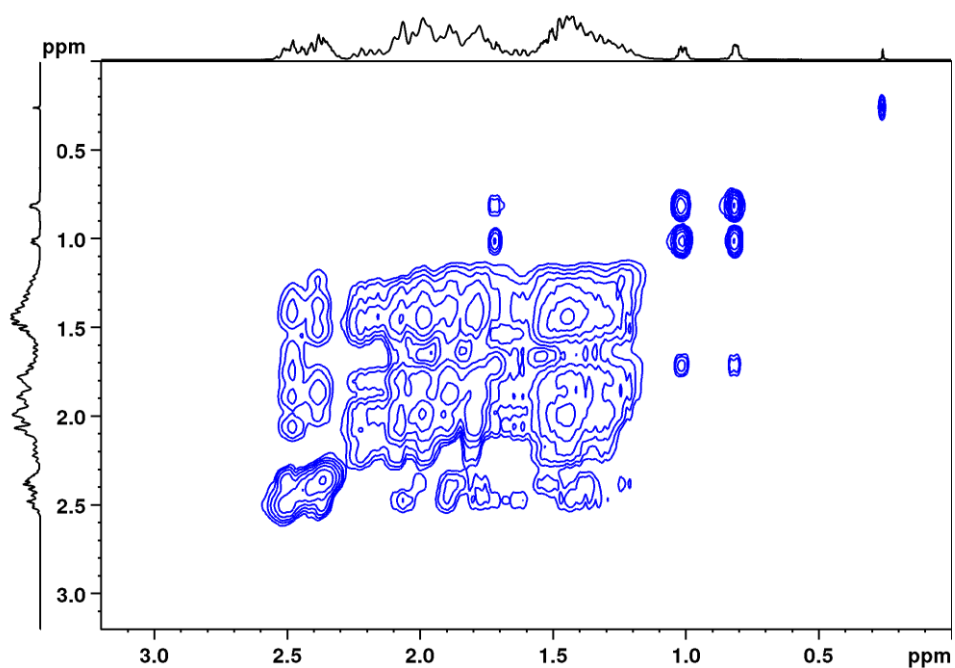


Figure S 35: ^1H -TOCSY NMR spectrum (400.17 MHz, oDFB, 298 K, mixing time: 0.12 s) of $\{[\text{Ga}(\text{dcpe})_2(\text{C}_5\text{H}_6)]_2[\text{pf}]_2\}$.

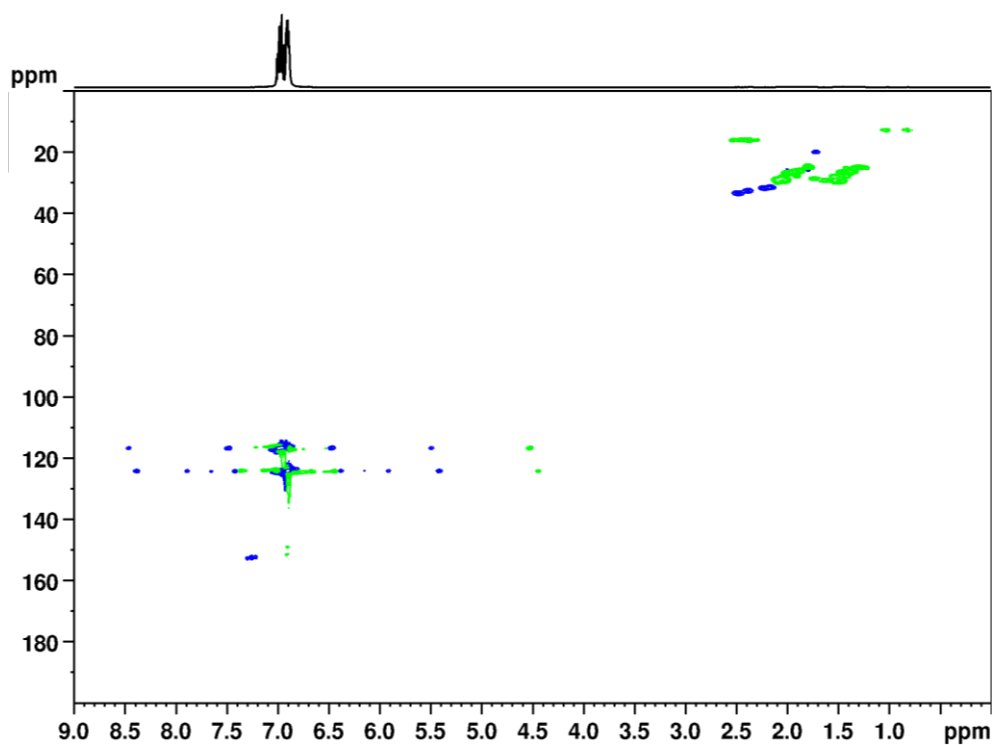


Figure S 36: Edited $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of $\{[\text{Ga}(\text{dcpe})_2(\text{C}_5\text{H}_6)]_2[\text{pf}]_2\}$.

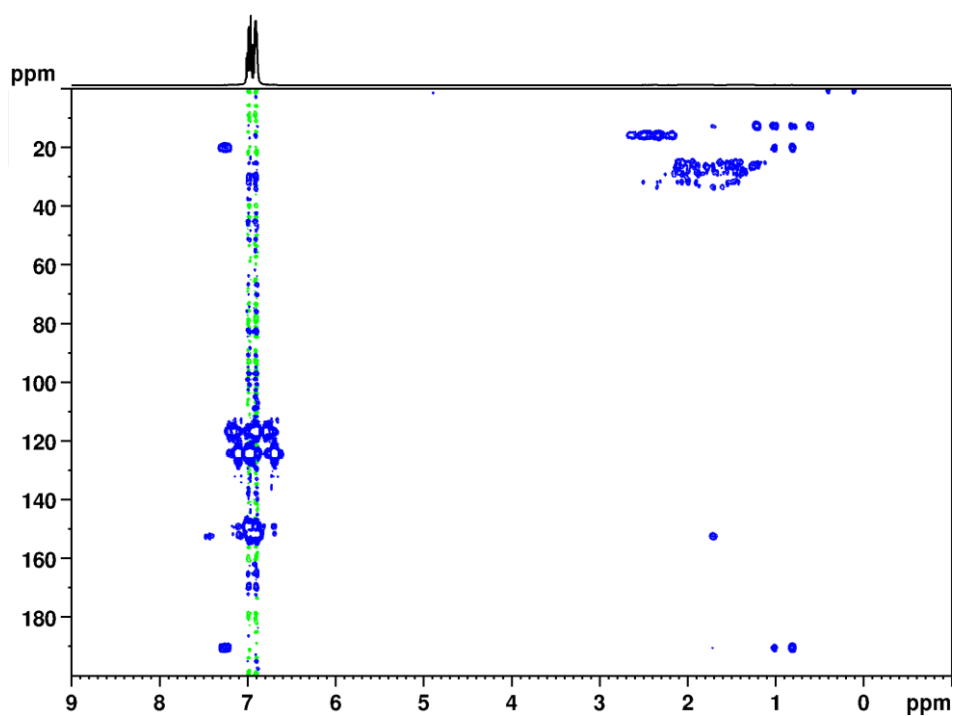


Figure S 37: ^1H , ^{13}C -HMBC NMR spectrum (400.17 MHz, *o*D₂F₆, 298 K, optimized for $J = 8$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$.

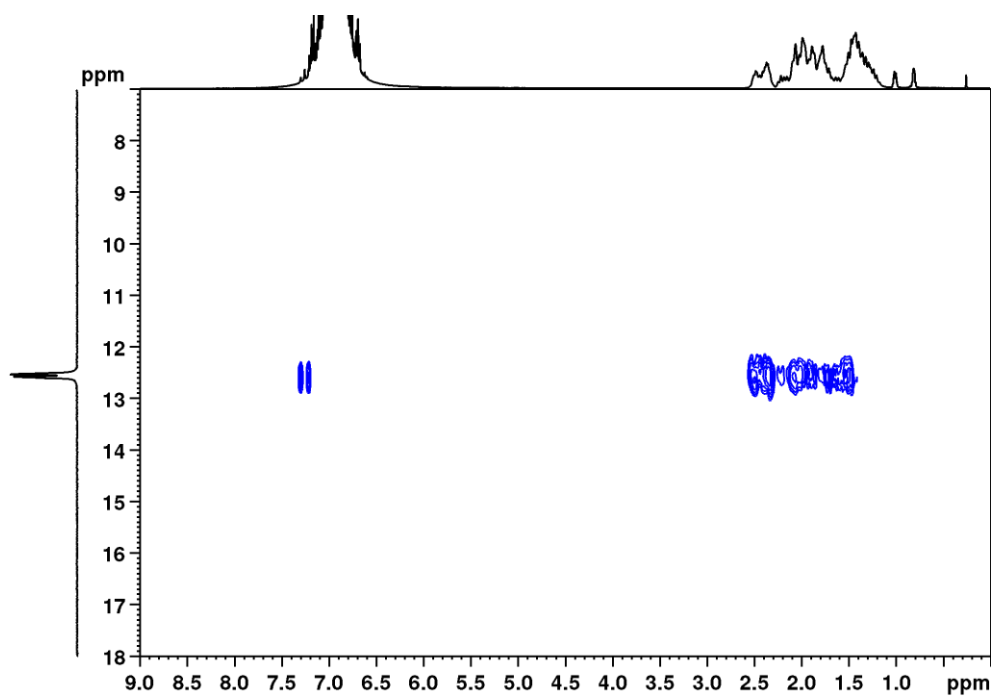


Figure S 38: ^1H , ^{31}P -HMBC NMR spectrum (400.17 MHz, *o*D₂F₆, 298 K, optimized for $J = 15$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$.

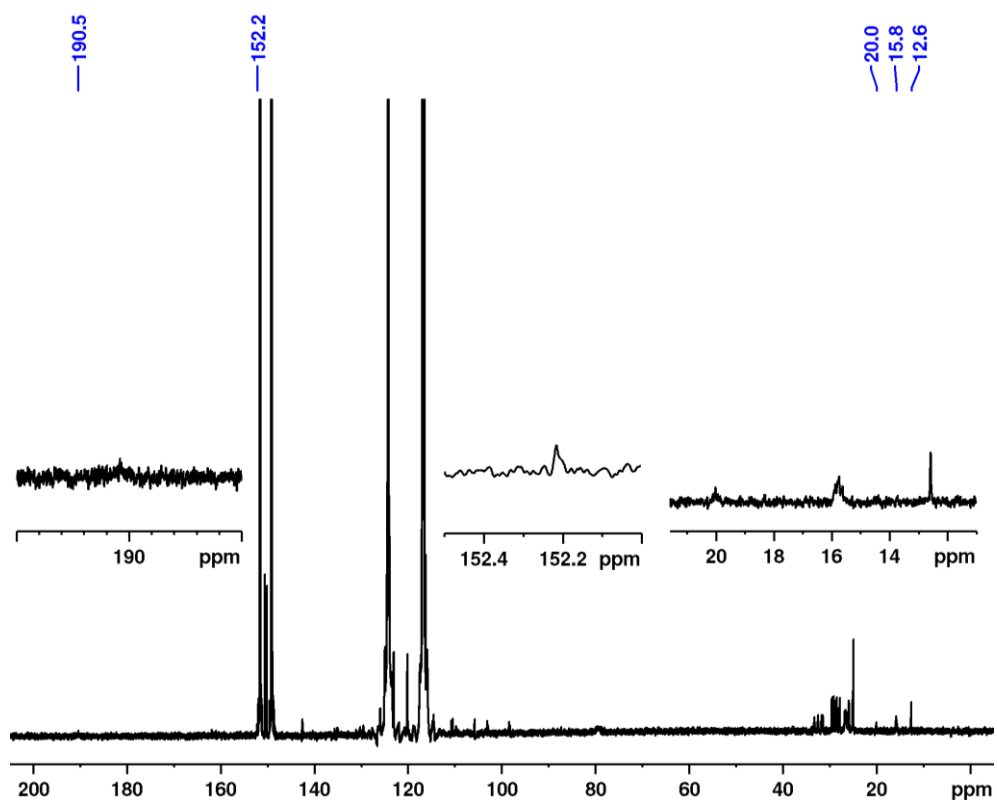


Figure S 39: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, *o*DfB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_5\text{H}_6)][\text{pf}]_2$.

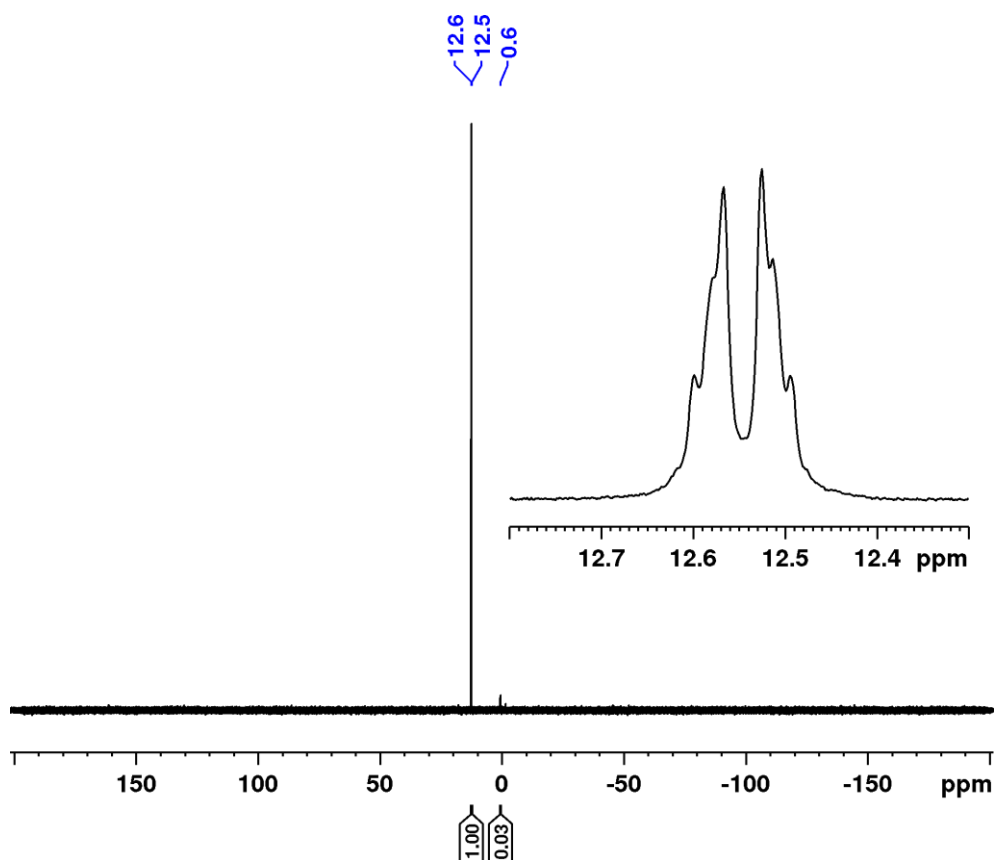
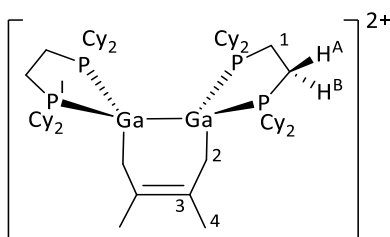


Figure S 40: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, *o*DfB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and ethynylcyclopropane in *o*DfB.

4.2 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$



^1H NMR [300.18 MHz, *o*D₂F₆, calibrated at $\delta(\text{C}_6\text{F}_5\text{H}) = 6.96$ ppm, 298 K]: $\delta = 2.22$ (m, 8 H, C^1H^A and C^1H^B), 2.32 and 2.12 (m, 8 H, CH protons of the Cy groups), 2.01–1.26 (m, 80 H, CH_2 protons of the Cy groups), 1.81 (s, 6 H, C^4H_3), 1.64 (s, 4 H, C^2H_2) ppm.

^{13}C NMR [75.48 MHz, *o*D₂F₆, 298 K]: $\delta = 132.3$ (2 C, C^3), 33.1 and 31.6 (8 C, CH carbon atoms of the Cy groups), 29.1–25.0 (40 C, CH_2 carbon atoms of the Cy groups), 22.4 (2 C, C^2), 19.9 (2 C, C^4), 15.5 (4 C, C^1) ppm.

^{19}F NMR [282.45 MHz, *o*D₂F₆, 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.8 (m, PhF), -139.5 (m, $\text{C}_6\text{F}_5\text{H}$) ppm.

^{27}Al NMR [78.22 MHz, *o*D₂F₆, 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [121.52 MHz, *o*D₂F₆, 298 K]: $\delta = 14.0$ (minor impurity), 5.7 (s, 4 P, P^I) ppm.

^{71}Ga NMR [91.55 MHz, *o*D₂F₆, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

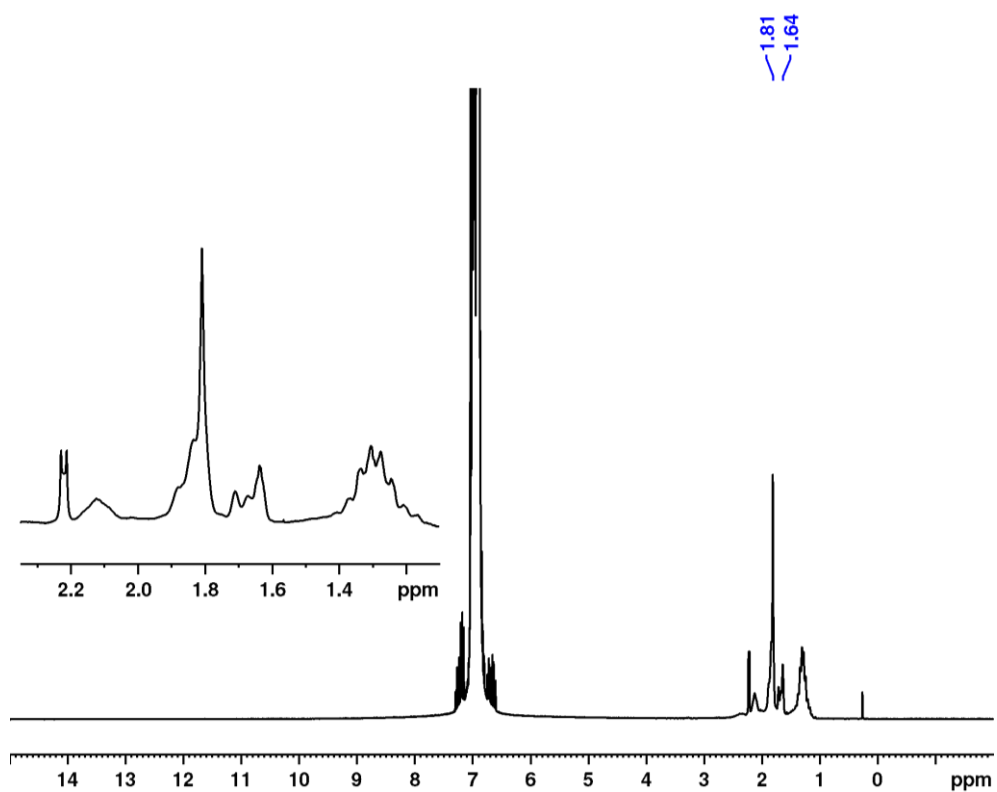


Figure S 41: ^1H NMR spectrum (300.18 MHz, *o*DFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

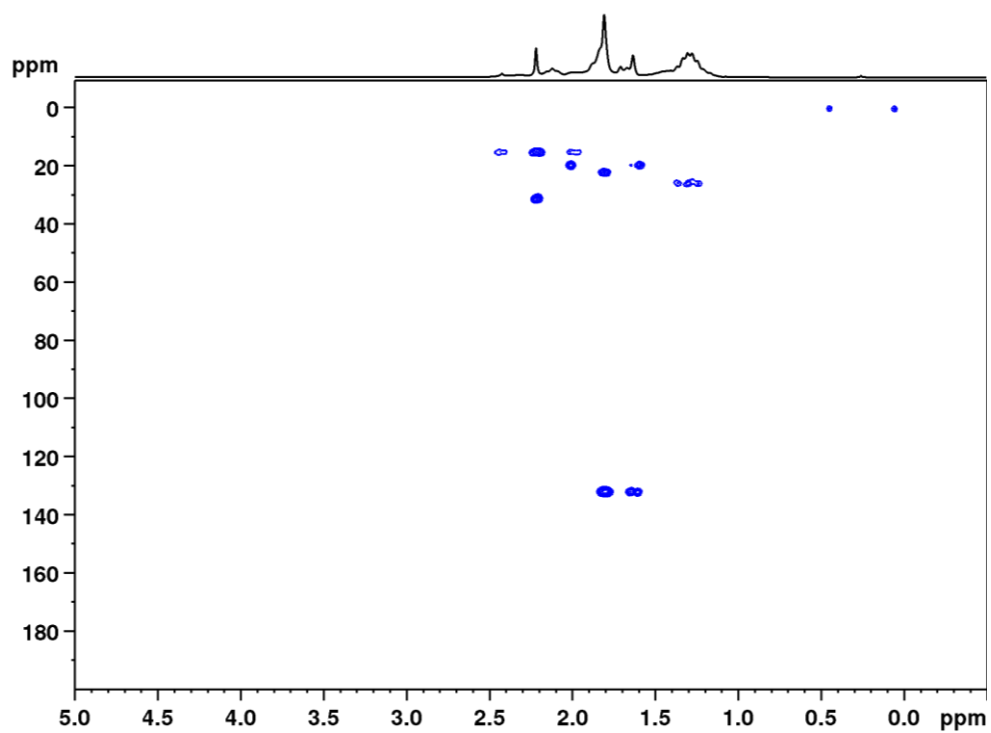


Figure S 42: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for $J = 8$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

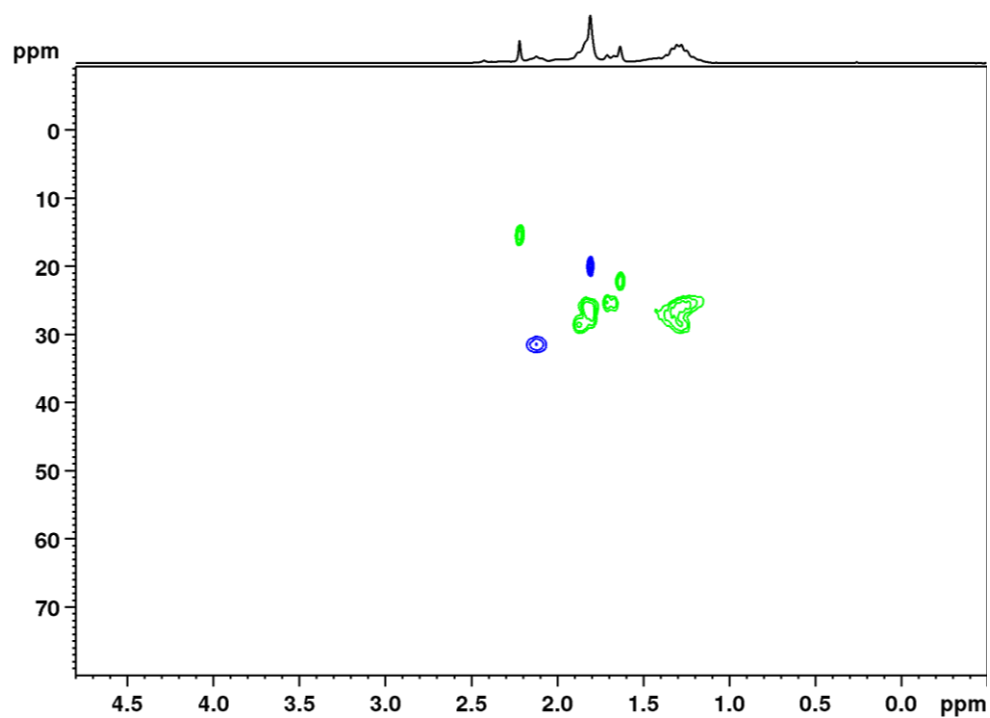


Figure S 43: Edited $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

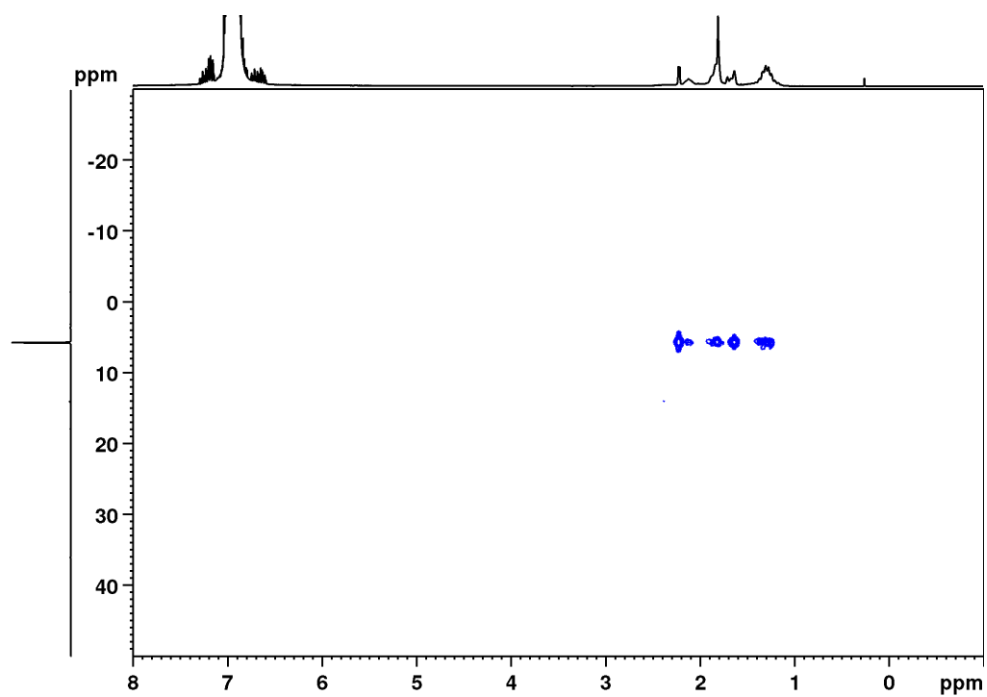


Figure S 44: $^1\text{H},^{31}\text{P}$ -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

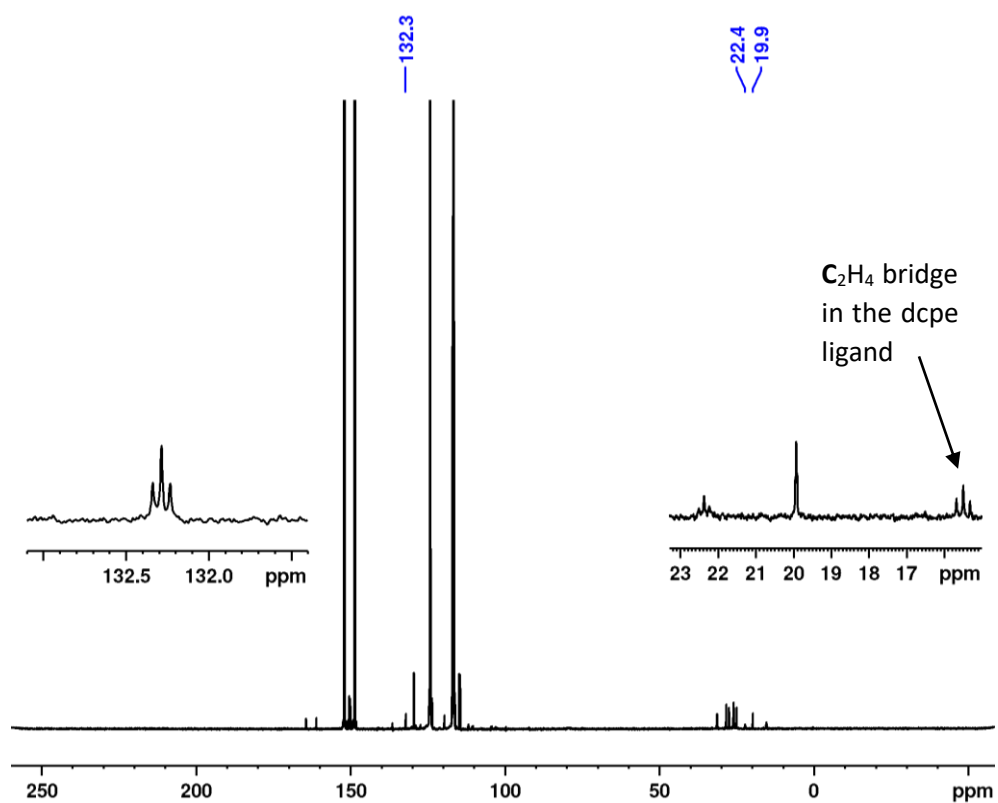


Figure S 45: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (75.48 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

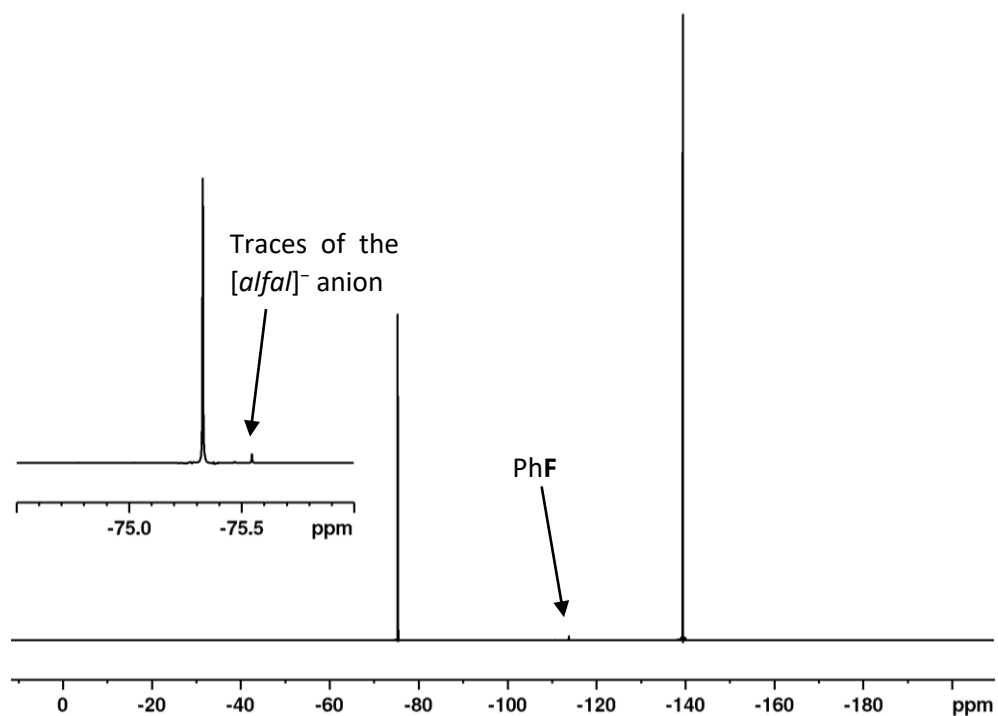


Figure S 46: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

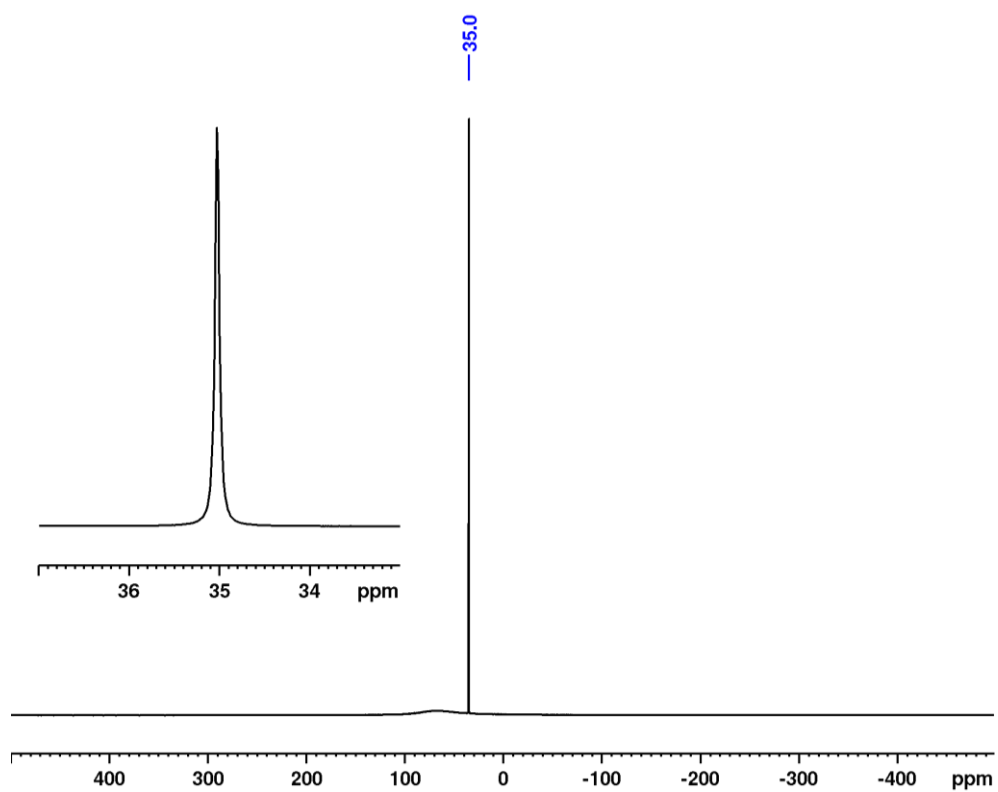


Figure S 47: ^{27}Al NMR spectrum (78.22 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

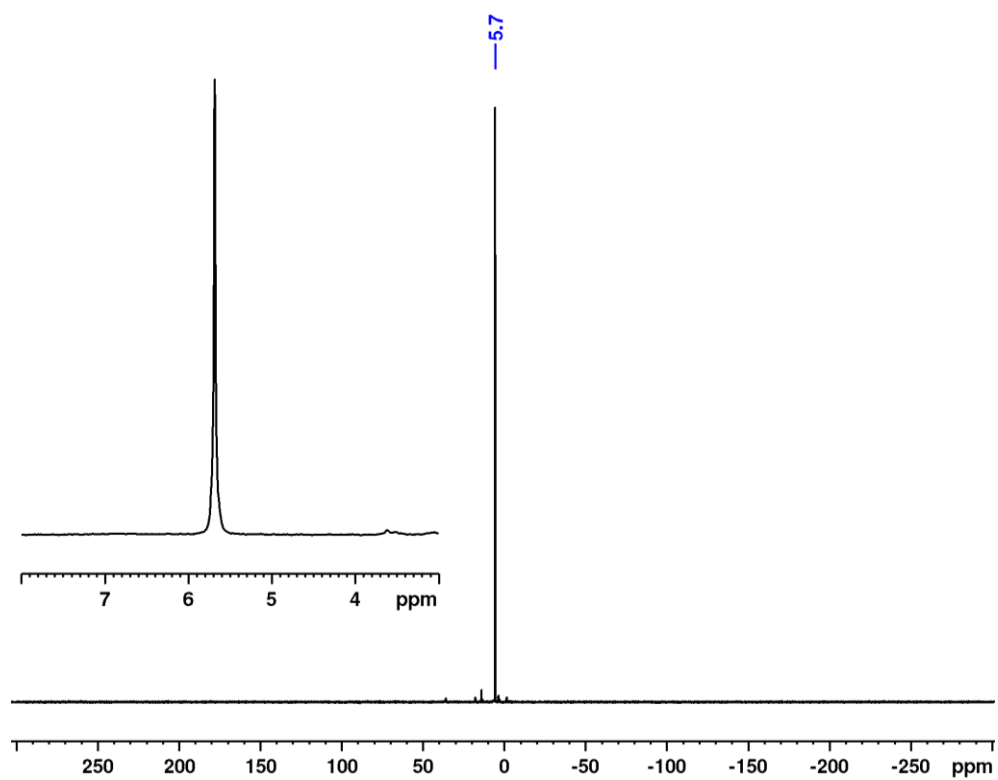
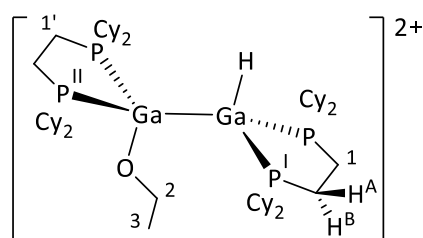


Figure S 48: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

4.3 $[H\{Ga(dcpe)\}_2(OEt)][pf]_2$



^1H NMR [400.17 MHz, *o*DfB, calibrated at $oC_6F_2H_4$ = 6.96 ppm, 298 K]: δ = 4.53 (t, 1 H, GaH, $^2J_{H,P}$ = 19.6 Hz), 3.91 (q, 2 H, C^2H_2 , $^3J_{H,H}$ = 6.8 Hz), 2.45–2.22 (m, 8 H, CH protons of the Cy groups), 2.13–1.29 (m, 80 H, CH_2 protons of the Cy groups), 2.45–2.19 (m, 8 H, C^1H^A , C^1H^B , $C^{1'}H^A$ and $C^{1'}H^B$), 1.36 (t, 2 H, C^3H_3 , $^3J_{H,H}$ = 6.8 Hz) ppm.

^{13}C NMR [100.62 MHz, *o*DfB, 298 K]: δ = 64.0 (1 C, C^2), 20.2 (1 C, C^3) 33.1–31.5 (8 C, CH carbon atoms of the Cy groups), 29.3–25.1 (40 C, CH_2 carbon atoms of the Cy groups), 16.8 and 15.2 (4 C, C^1 and $C^{1'}$) ppm.

^{19}F NMR [376.54 MHz, *o*DfB, 298 K]: δ = –75.3 (s, 36 F, $[Al(OC(CF_3)_3)_4]^-$), –113.9 (m, PhF), –139.5 (m, $oC_6F_2H_4$) ppm.

^{27}Al NMR [104.27 MHz, *o*DfB, 298 K]: δ = 35.0 (s, 1 Al, $[Al(OC(CF_3)_3)_4]^-$) ppm.

^{31}P NMR [161.99 MHz, *o*DfB, 298 K]: δ = 27.6 and –2.0 (unknown impurity), 21.4 (m, 2 P, P^I), 9.4 (m, 2 P, P^{II}), –1.5 (unknown impurity) ppm.

^{71}Ga NMR [122.04 MHz, *o*DfB, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

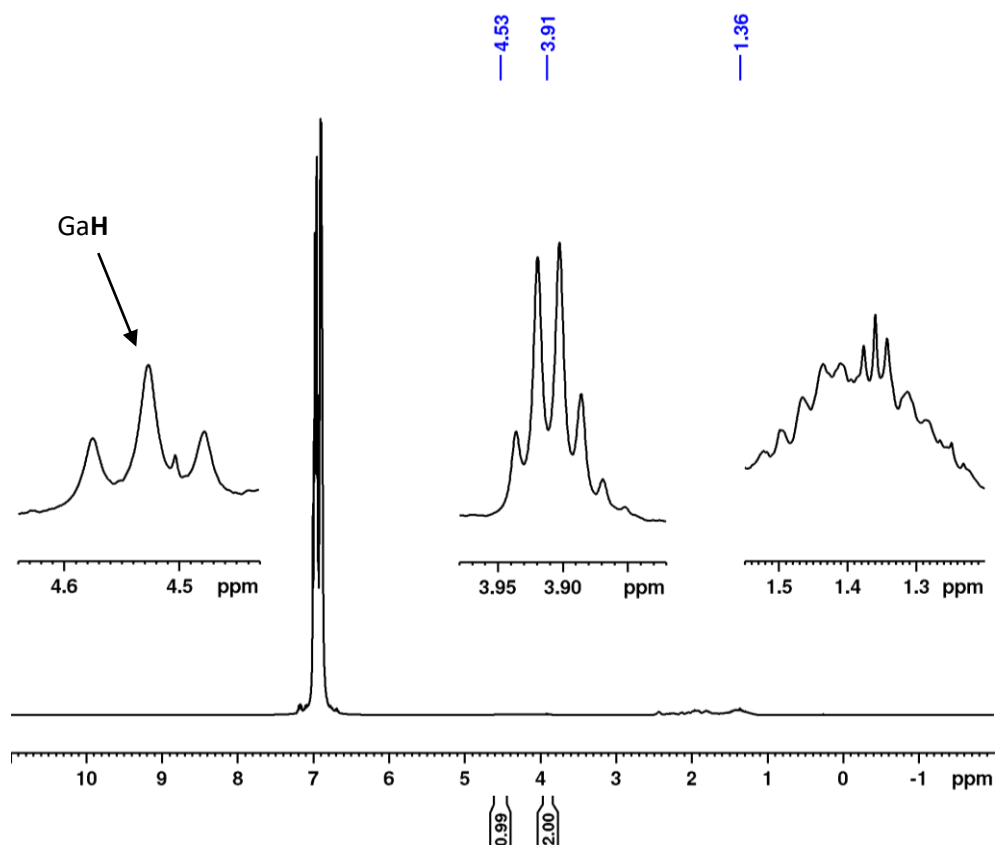


Figure S 49: ^1H NMR spectrum (400.17 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in *o*DFB.

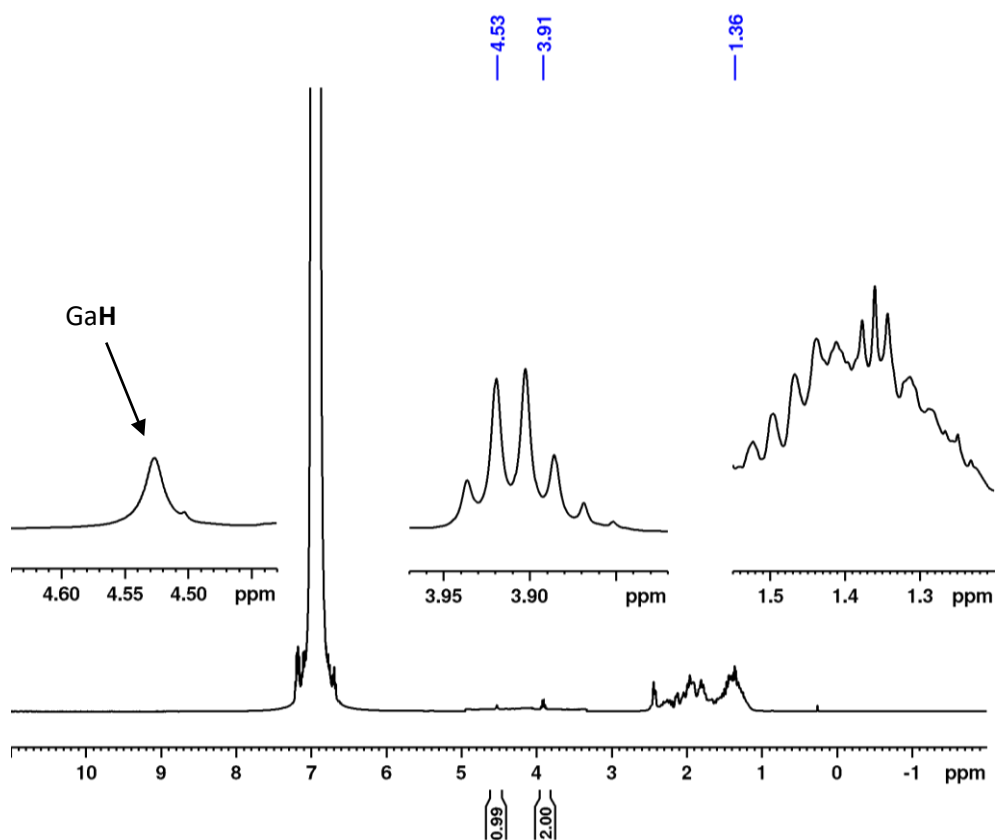


Figure S 50: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (400.17 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in *o*DFB.

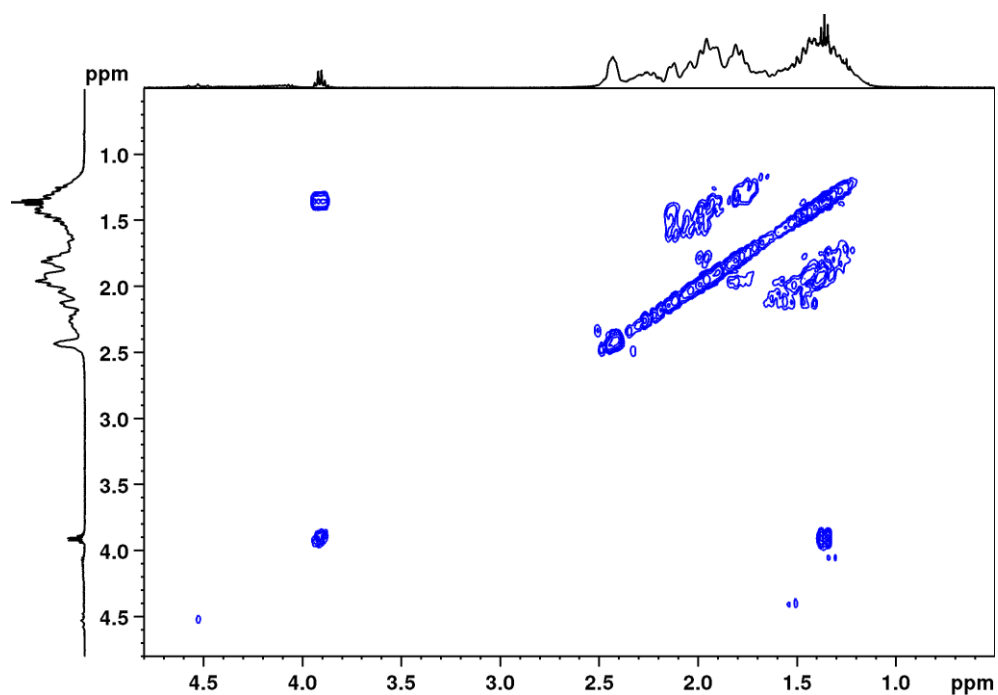


Figure S 51: ^1H -COSY NMR spectrum (400.17 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in *o*DFB.

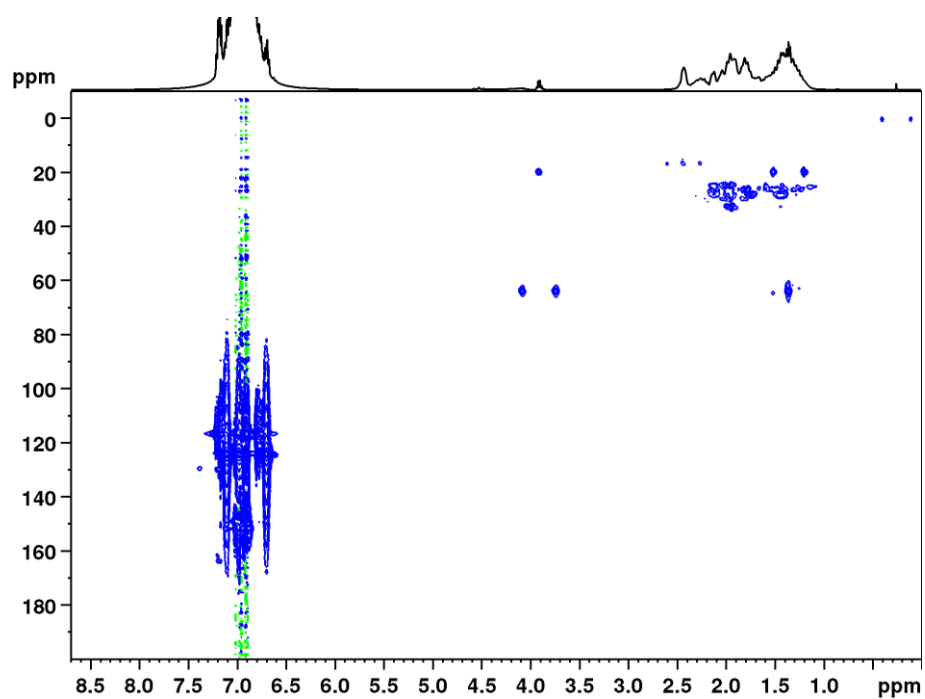


Figure S 52: ^1H , ^{13}C -HMBC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in *o*DFB.

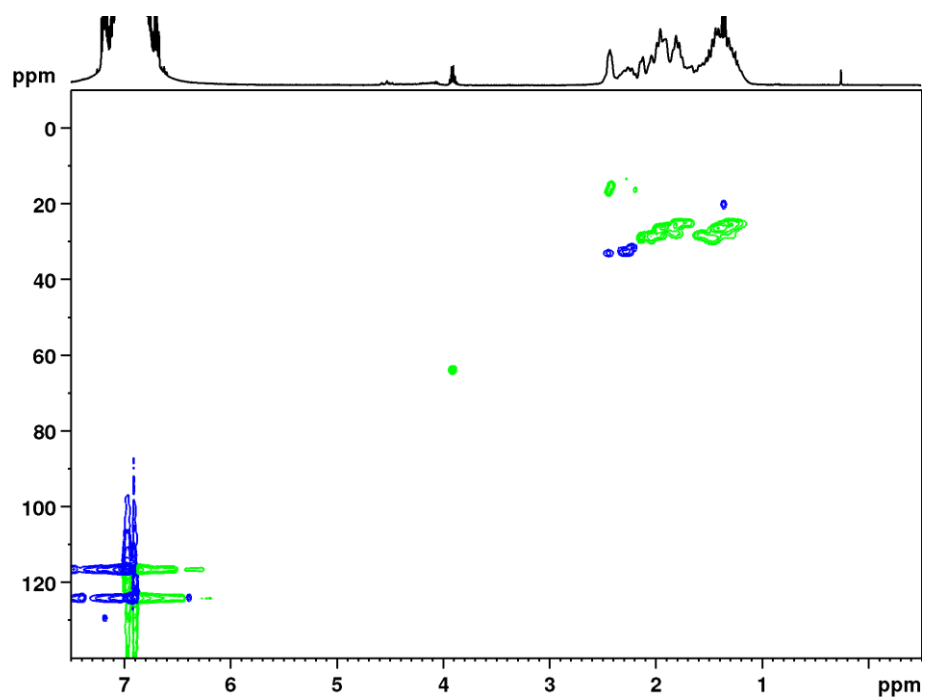


Figure S 53: Edited ^1H , ^{13}C -HSQC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and HOEt in oDFB.

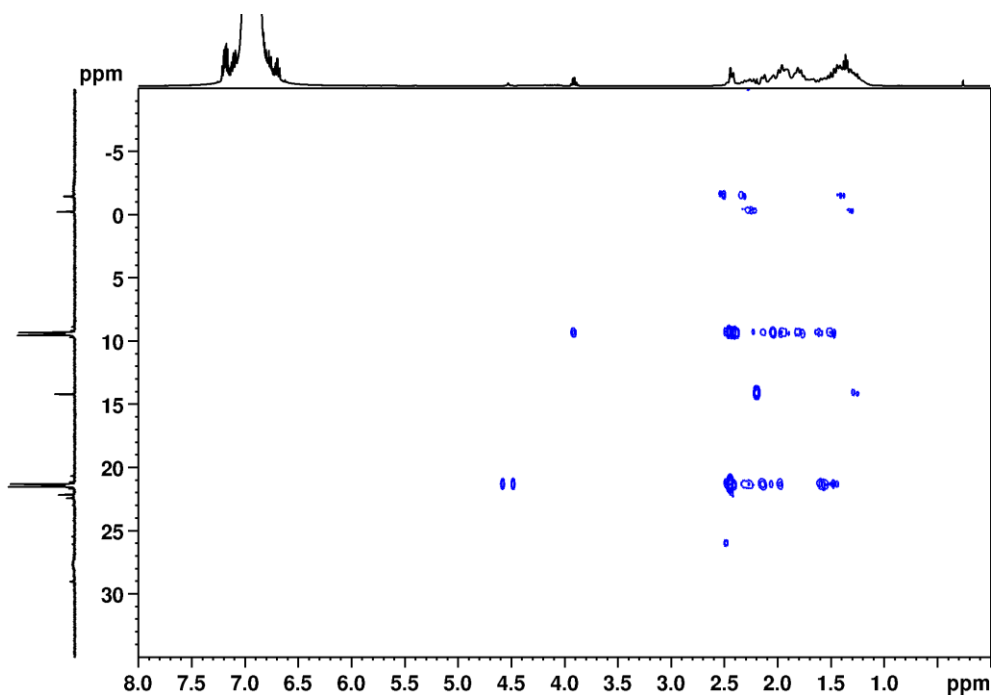


Figure S 54: ^1H , ^{31}P -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and HOEt in oDFB.

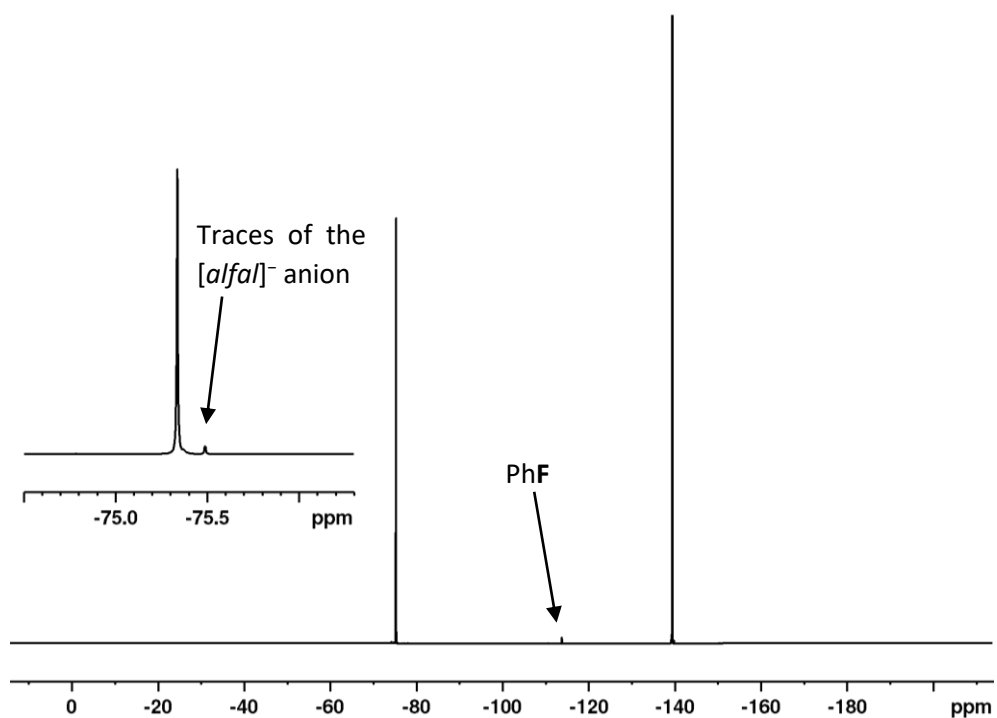


Figure S 55: ^{19}F NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in oDFB.

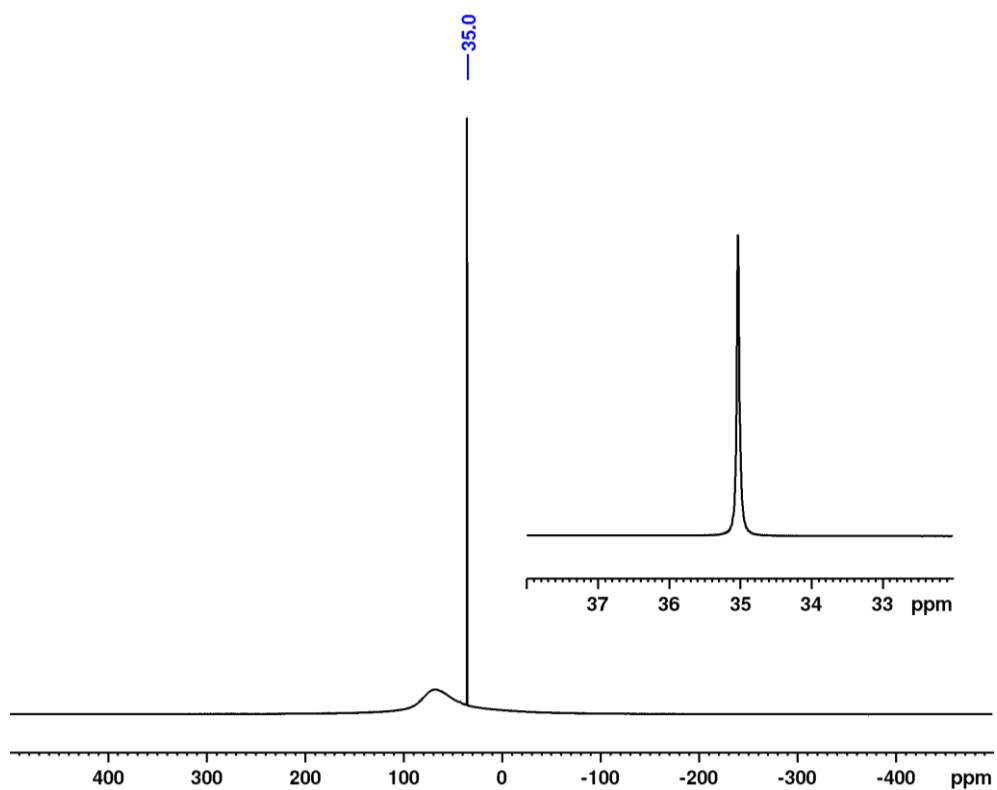


Figure S 56: ^{27}Al NMR spectrum (104.27 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in oDFB.

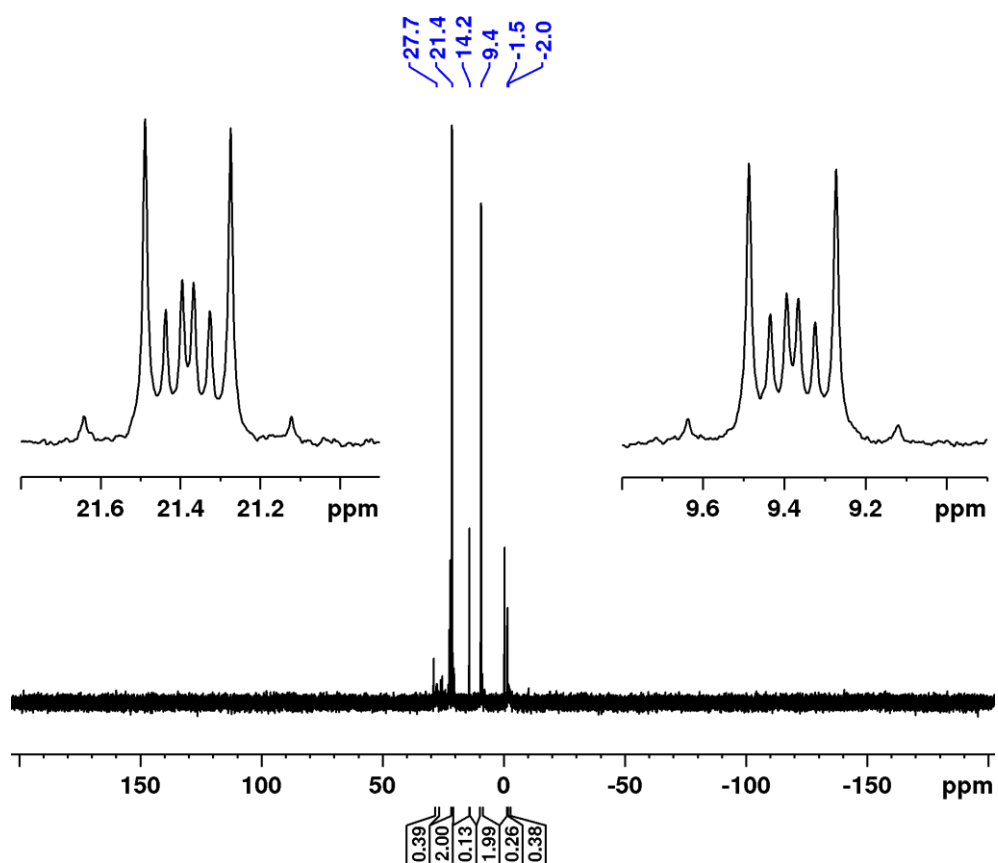
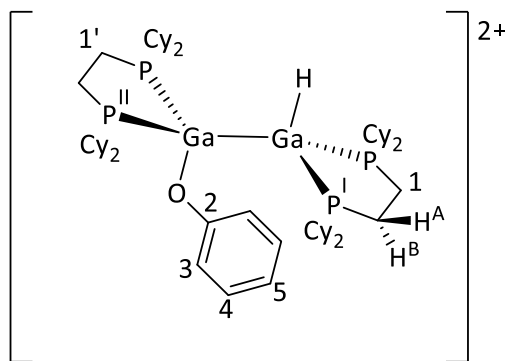


Figure S 57: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HOEt in *o*DFB.

4.4 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$



^1H NMR [300.18 MHz, *o*D₂F₆, calibrated at $\text{oC}_6\text{F}_2\text{H}_4 = 6.96$ ppm, 298 K]: $\delta = 7.32$ (m, 2 H, C^4H), ca. 6.92 (m, 1 H, C^5H), 6.77 (m, 2 H, C^3H), 4.78 (t, 1 H, GaH , $^2J_{\text{H,P}} = 20.6$ Hz), 2.54–2.44 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{A}}$, $\text{C}^{1'}\text{H}^{\text{B}}$), 2.50–2.16 (m, 8 H, CH protons of the Cy groups), 2.21–1.12 (m, 80 H, CH_2 protons of the Cy groups) ppm.

^{13}C NMR [75.48 MHz, *o*D₂F₆, 298 K]: $\delta = 160.8$ (1 C, C^2), 130.0 (2 C, C^4), 119.7 (1 C, C^5), 118.0 (2 C, C^3), 33.1–31.5 (8 C, CH carbon atoms of the Cy groups), 29.1–25.0 (40 C, CH_2 carbon atoms on the Cy groups), 16.9–15.1 (4 C, C^1 and $\text{C}^{1'}$) ppm.

^{19}F NMR [282.45 MHz, *o*D₂F₆, 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.9 (m, PhF), -139.5 (m, $\text{oC}_6\text{F}_2\text{H}_4$) ppm.

^{27}Al NMR [78.22 MHz, *o*D₂F₆, 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [121.51 MHz, *o*D₂F₆, 298 K]: $\delta = 20.7$ (m, 2 P, P^{I}), 10.5 (m, 2 P, P^{II}) ppm.

^{71}Ga NMR [91.54 MHz, *o*D₂F₆, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

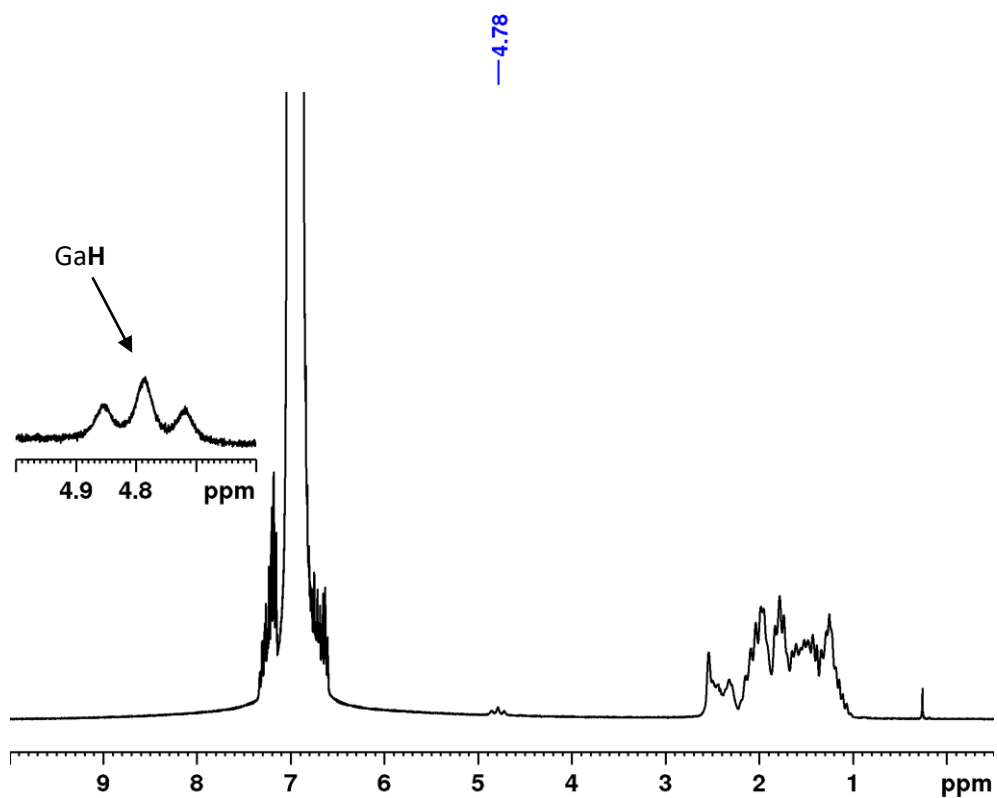


Figure S 58: ^1H NMR spectrum (300.18 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and PhOH in *o*DFB.

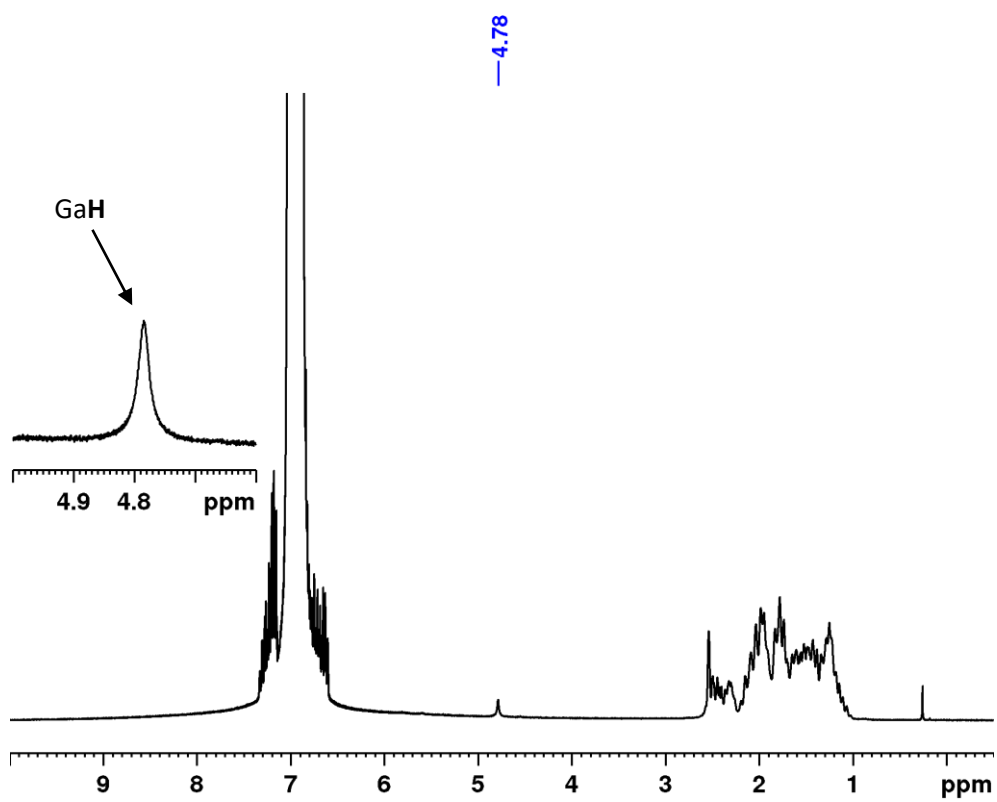


Figure S 59: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and PhOH in *o*DFB.

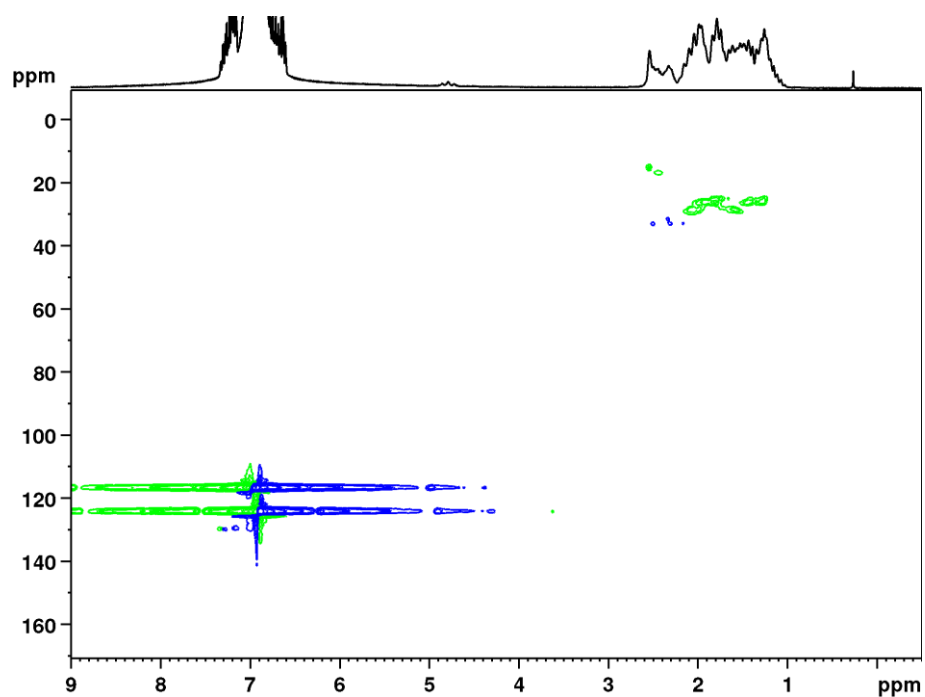


Figure S 60: Edited ^1H , ^{13}C -HSQC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and PhOH in oDFB.

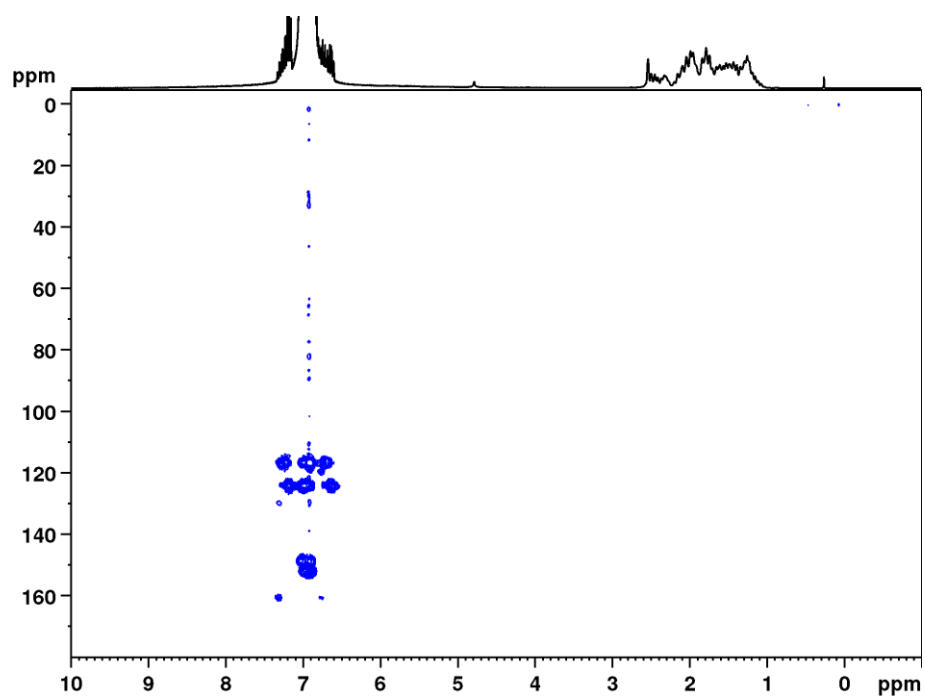


Figure S 61: ^1H , ^{13}C -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and PhOH in oDFB.

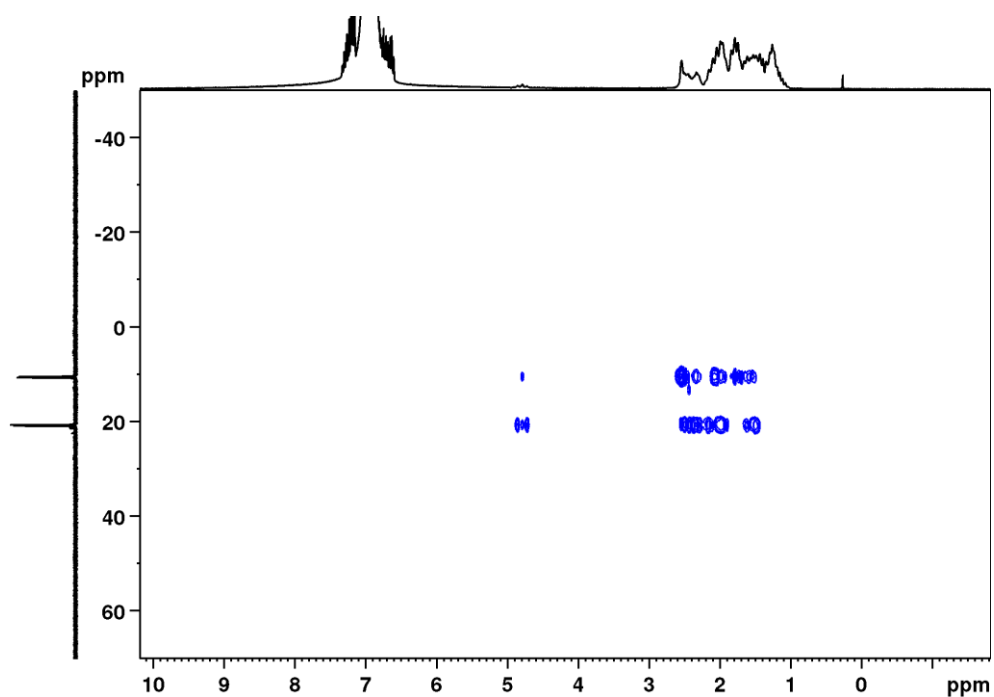


Figure S 62: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and PhOH in oDFB.

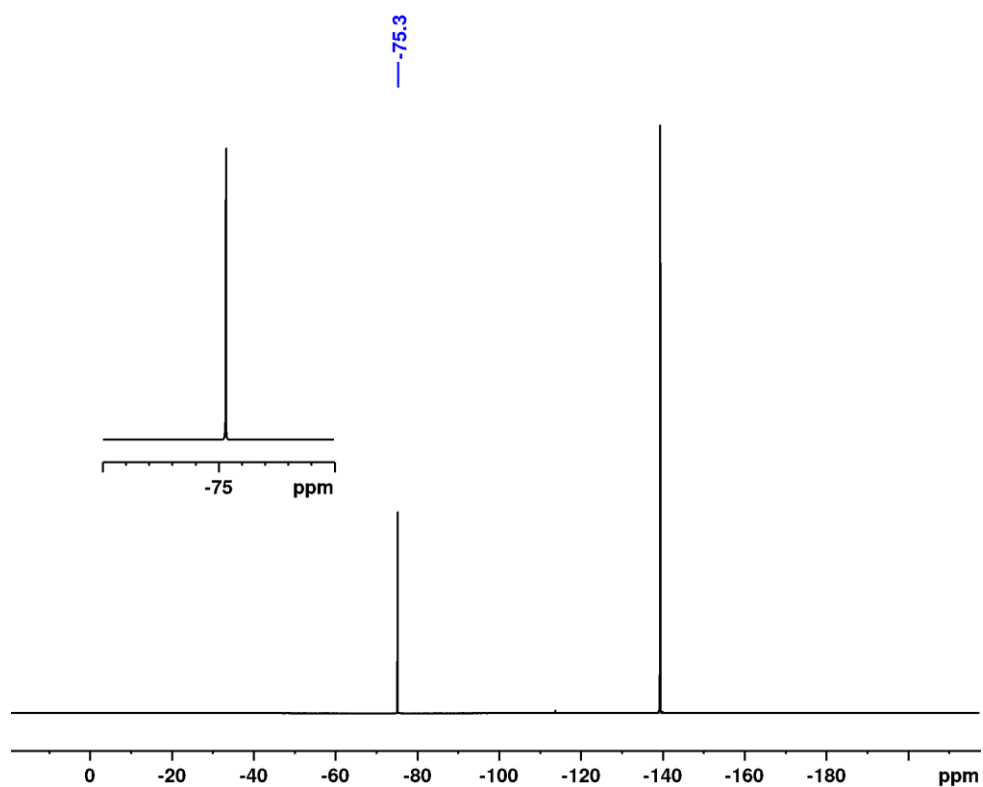


Figure S 63: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and PhOH in oDFB.

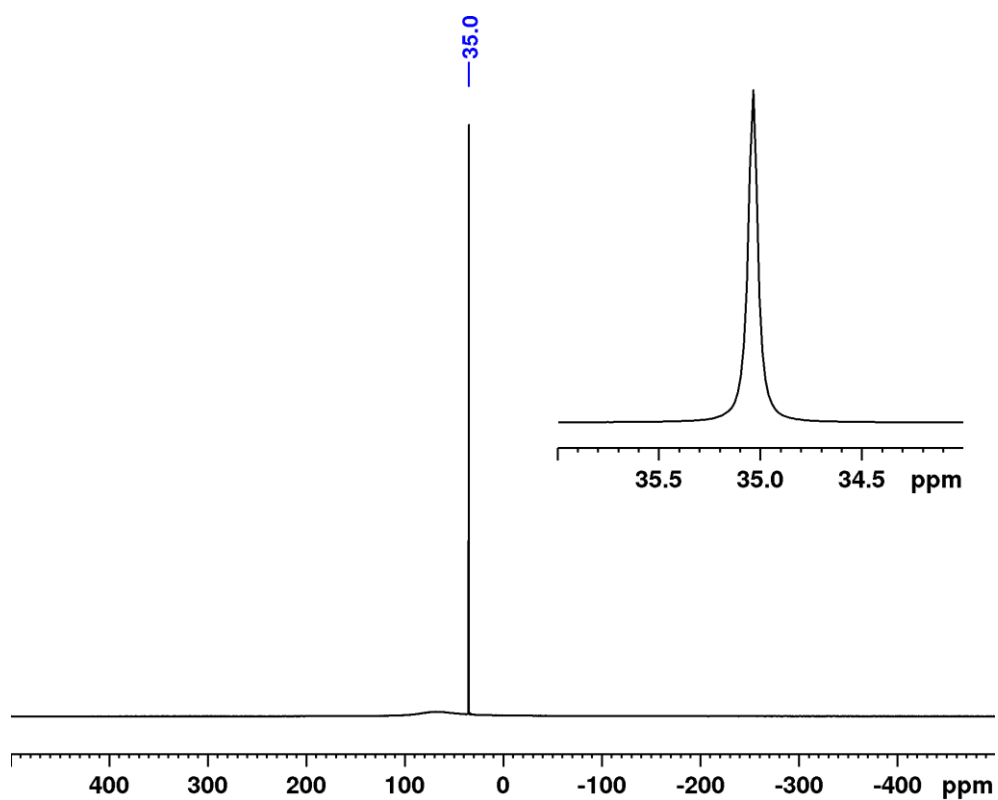


Figure S 64: ^{27}Al NMR spectrum (78.22 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{PF}_6]_2$ and PhOH in oDFB.

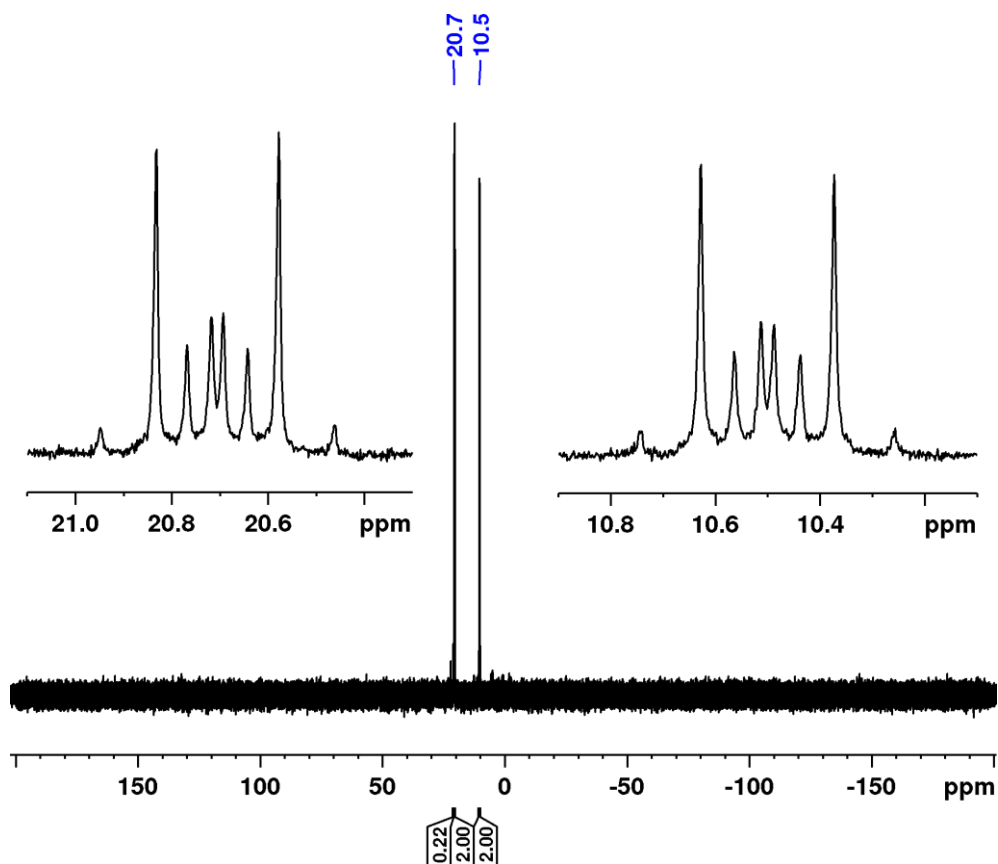


Figure S 65: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.51 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{PF}_6]_2$ and PhOH in oDFB, 5 h after mixing the components.

4.4.1 Observed Intermediates during the Formation of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2\text{OPh}]^{2+}$

During the H–O bond activation with HOPh, one intermediate is observed in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum, when no more $\mathbf{1}^{2+}$ is present in solution. While the concentration of the dimer increases, the intermediate is consumed after ca. 1 h (*cf.* **Figure S 66** and **Figure S 65**). It is characterized by a singlet in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum ($\delta(^{31}\text{P}) = 13.4$ ppm) and $J_{\text{H,P}}$ coupling constants of ca. 27 Hz. The ^1H signal of the corresponding GaH proton at ca. 5.25 ppm is remarkably broad, so that it cannot be determined whether the ^1H signal has a triplet or quintet splitting pattern in the non-decoupled ^1H NMR spectrum. In summary, the fact that this compound produces a singlet in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum and is directly converted to the final Ga^{II} addition product suggests that this intermediate has a symmetric, but dimeric structure. A plausible structure is presented in **Figure S 66**.

Nevertheless, taking into account that the ^{31}P NMR and ^1H NMR shift of the P–Ga–H units in the intermediates observed during the reactions with HOPh, H_2NPh and HNPh_2 (sections 4.4.1, 4.6.1 and 4.7.1) is very similar, it cannot be ruled out that the OPh group acts as a bridging ligand with its aromatic π -system or that the OPh group is only weakly associated.

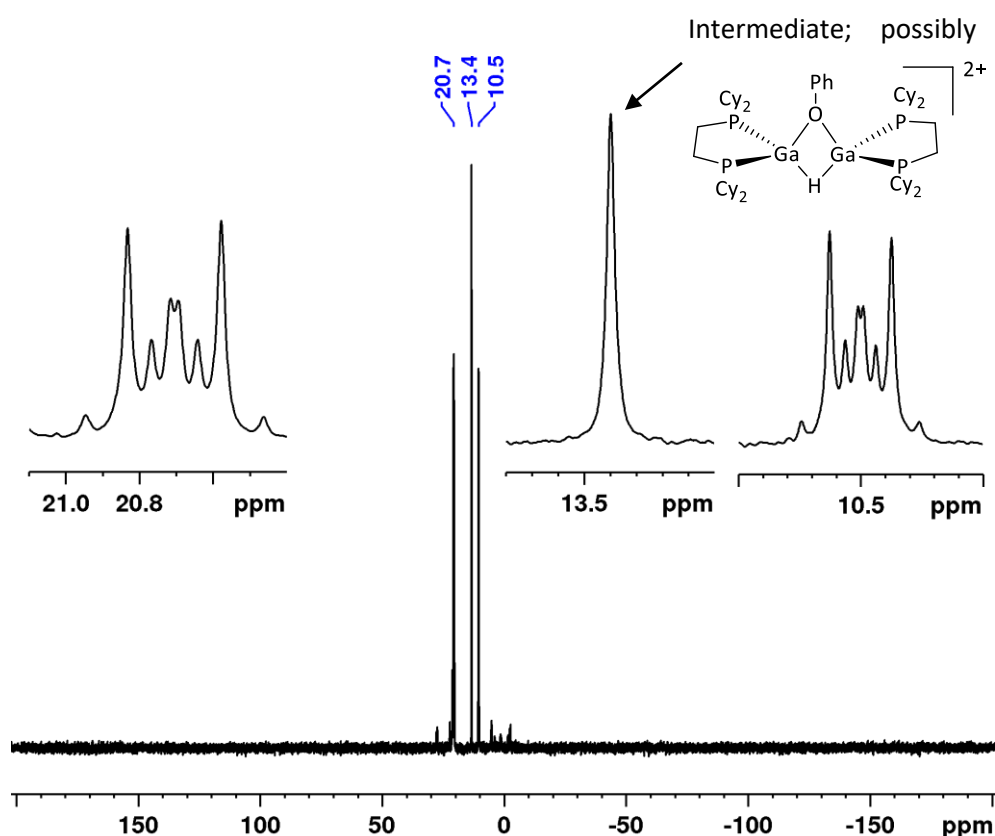


Figure S 66: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.51 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and PhOH in oDFB, 30 minutes after mixing the components.

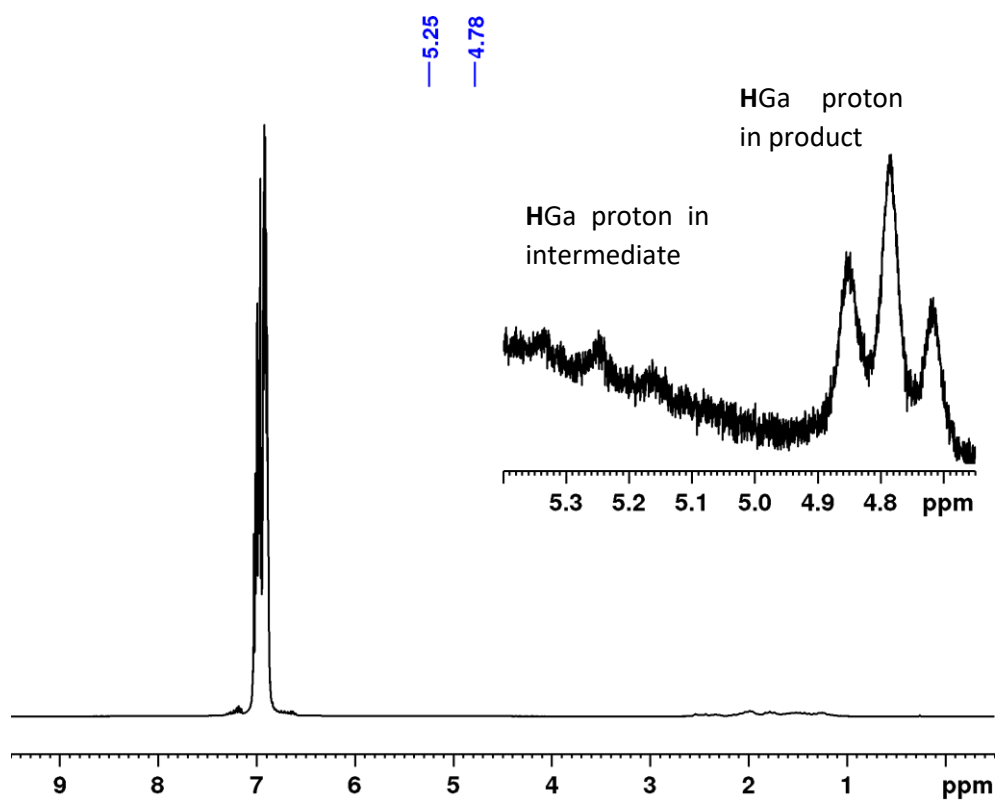


Figure S 67: ^1H NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and PhOH in oDFB, 30 minutes after mixing the components.

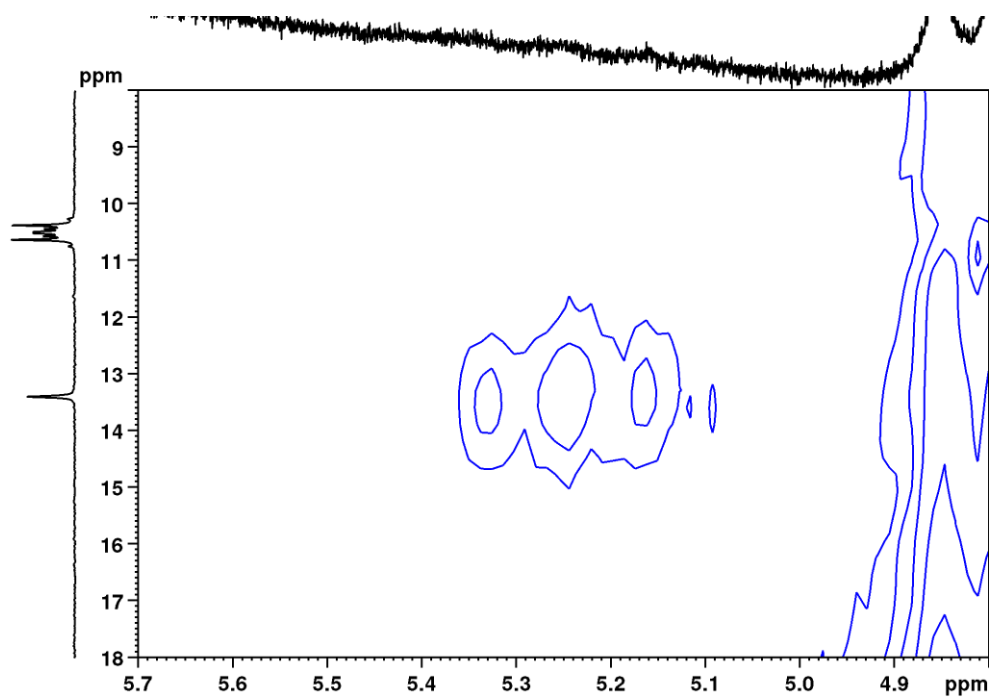
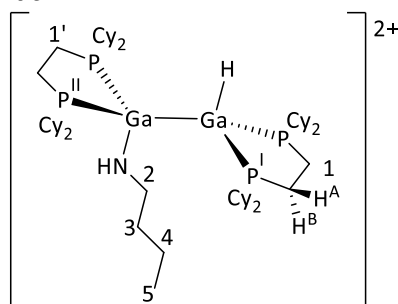


Figure S 68: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and PhOH in oDFB, 2 h after mixing the components.

4.5 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NH}n\text{Bu})][\text{pf}]_2$



^1H NMR [400.17 MHz, *o*D F_2B , calibrated at $\text{oC}_6\text{F}_2\text{H}_4 = 6.96$ ppm, 298 K]: $\delta = 4.55$ (t, 1 H, GaH, $^2J_{\text{H,P}} = 19.6$ Hz), 3.05 (m, 2 H, C^2H_2 , $^3J_{\text{H,H}} = 7.0$ Hz), 2.49–2.37 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{A}}$, $\text{C}^{1'}\text{H}^{\text{B}}$), 2.41–2.15 (m, 8 H, CH protons of the Cy groups), 2.21–1.18 (m, 80 H, CH_2 protons of the Cy groups), 1.66–1.60 (m, 2 H, C^3H_2), 1.47–1.40 (m, 2 H, C^4H_2), 0.97 (t, 3 H, C^5H_3 , $^3J_{\text{H,H}} = 7.5$ Hz), 0.29 (m, 1 H, N–H, $^3J_{\text{H,H}} = 6.9$ Hz)

^{13}C NMR [100.62 MHz, *o*D F_2B , 298 K]: $\delta = 50.3$ (1 C, C^2), 38.0 (1 C, C^3), 20.1 (1 C, C^4), 35.0–30.7 (8 C, CH carbon atoms on the Cy groups), 30.7–24.1 (40 C, CH_2 carbon atoms on the Cy groups), 17.6–14.0 (4 C, C^1 and $\text{C}^{1'}$), 13.2 (1 C, C^5) ppm.

^{19}F NMR [376.54 MHz, *o*D F_2B , 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.9 (m, PhF), -139.5 (m, $\text{oC}_6\text{F}_2\text{H}_4$) ppm.

^{27}Al NMR [104.27 MHz, *o*D F_2B , 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [161.99 MHz, *o*D F_2B , 298 K]: $\delta = 21.0$ (m, 2 P, P^{I}), 5.7 (m, 2 P, P^{II}) ppm.

^{71}Ga NMR [122.03 MHz, *o*D F_2B , 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

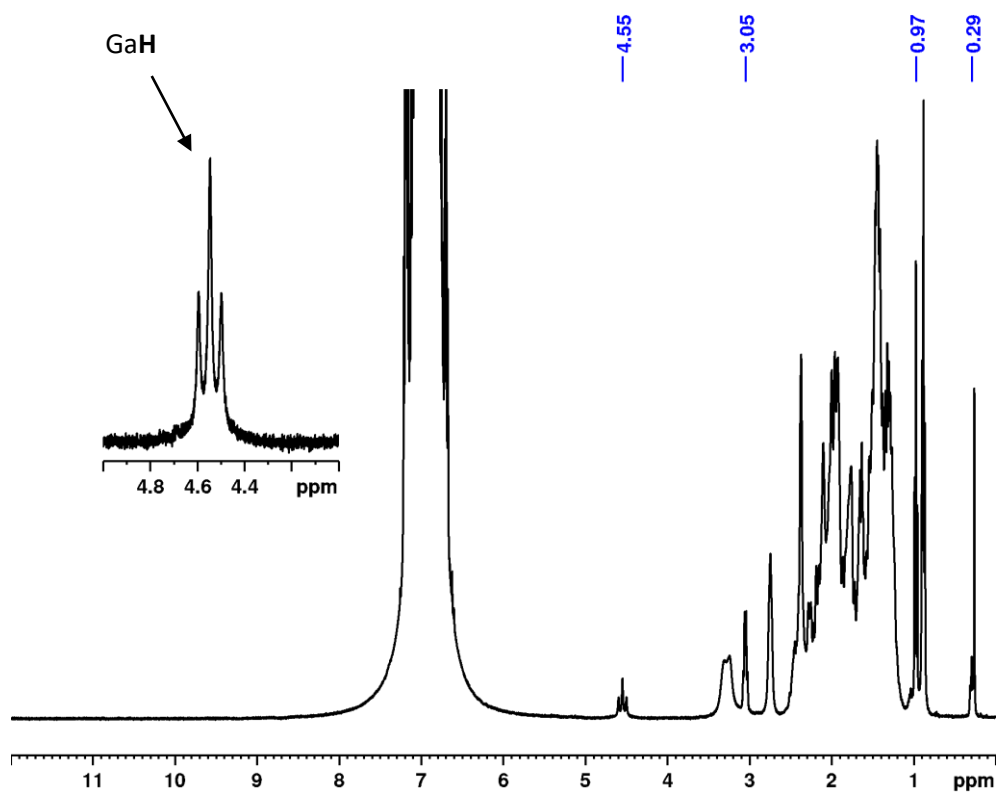


Figure S 69: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in oDFB at room temperature, 0.5 h after mixing the components.

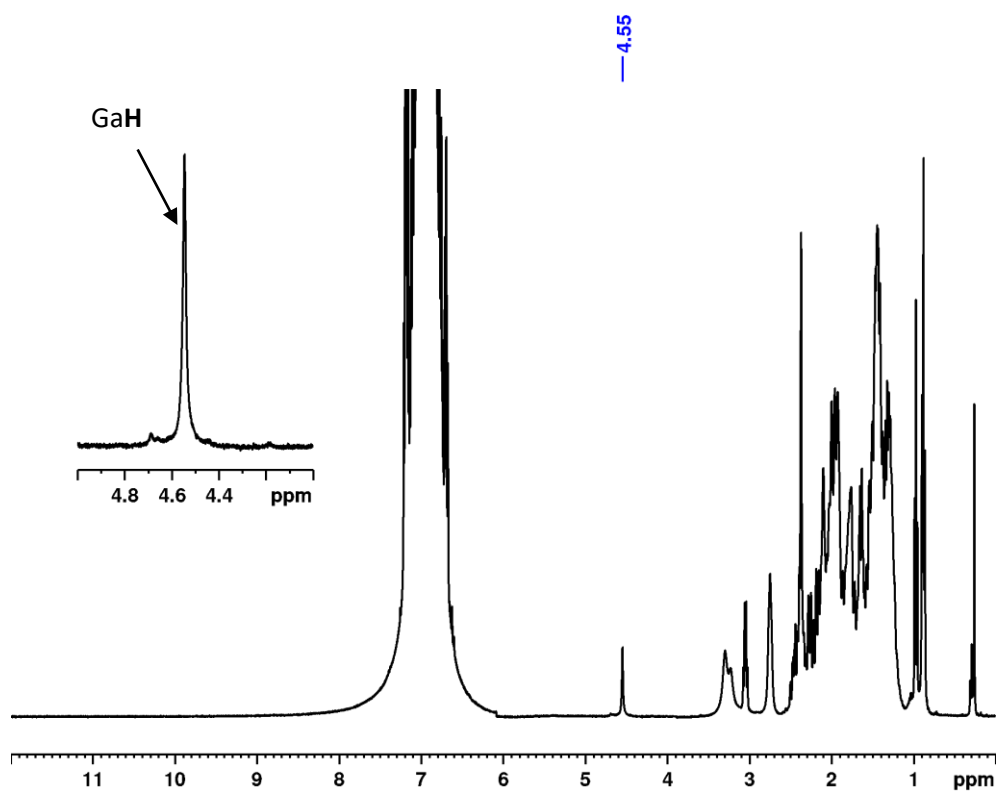


Figure S 70: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in oDFB at room temperature, 0.5 h after mixing the components.

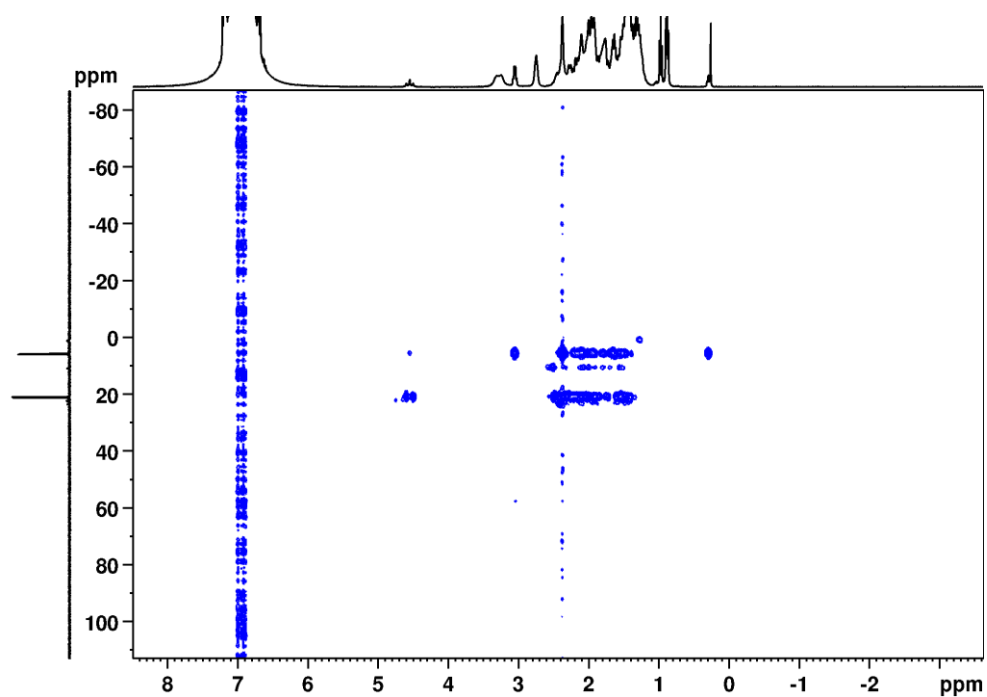


Figure S 71: $^1\text{H},^{31}\text{P}$ -HMBC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in *o*DFB at room temperature, 0.5 h after mixing the components.

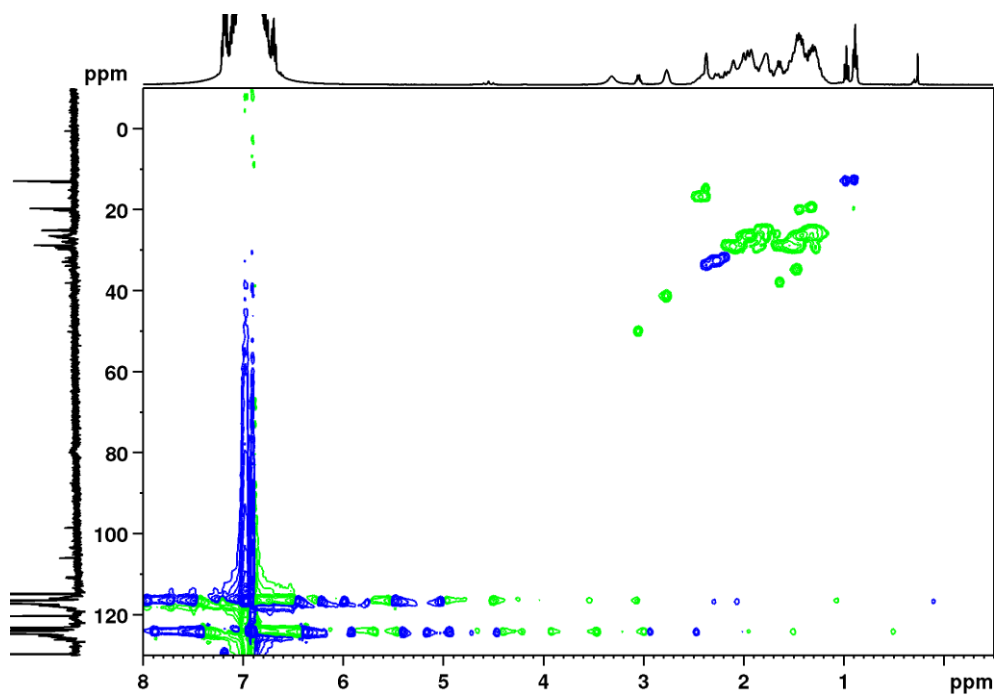


Figure S 72: Edited $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in *o*DFB at room temperature, 0.5 h after mixing the components.

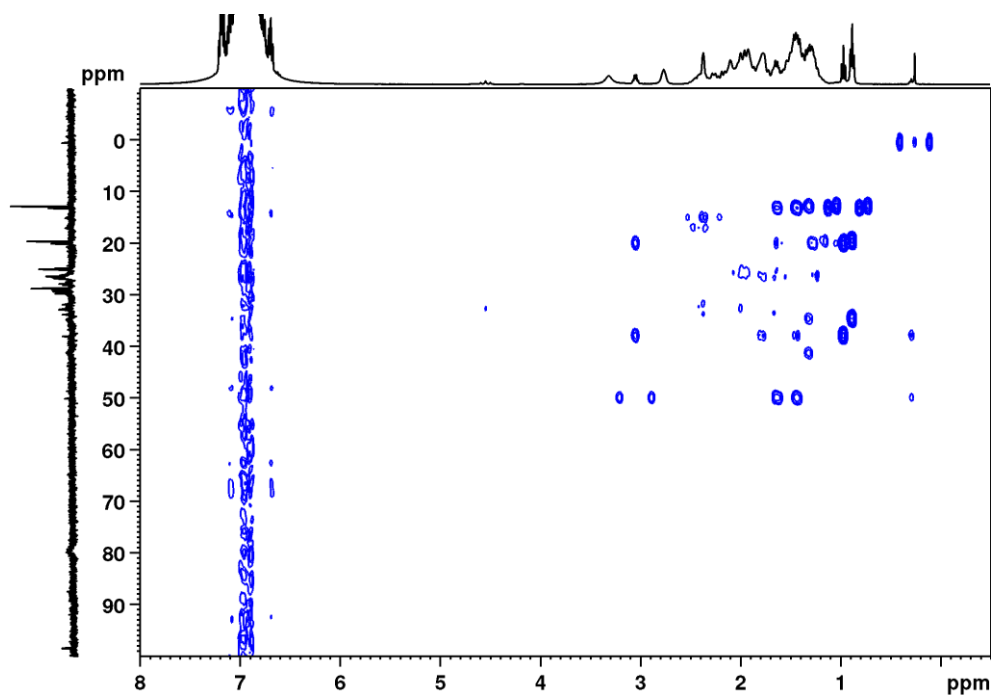


Figure S 73: ^1H , ^{13}C -HMBC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in *o*DFB at room temperature, 0.5 h after mixing the components.

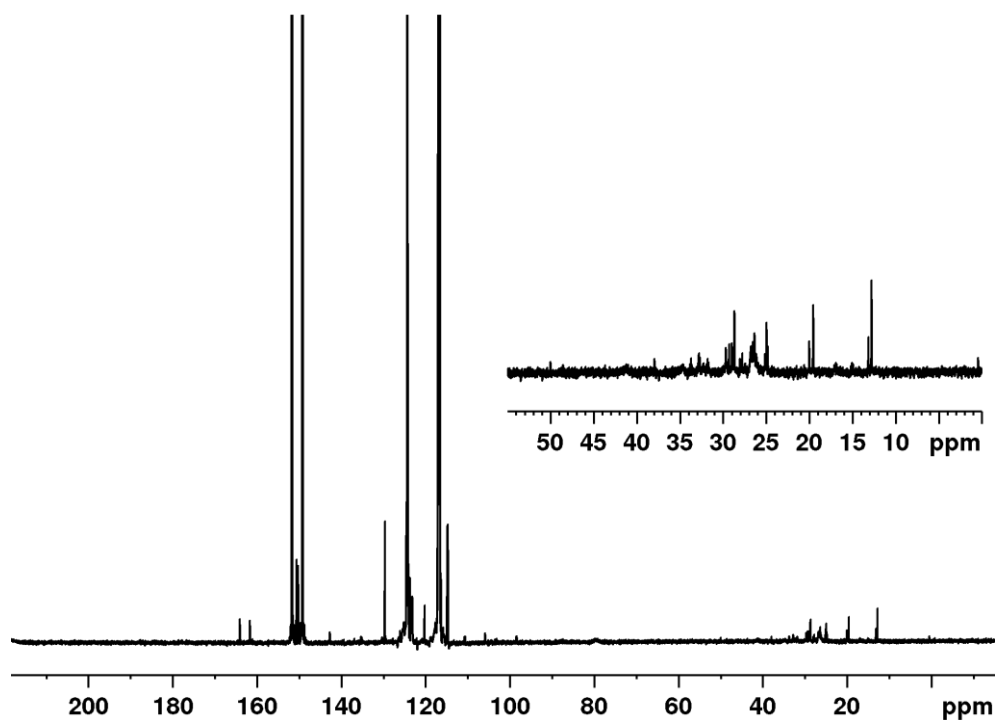


Figure S 74: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in *o*DFB at room temperature, 0.5 h after mixing the components.

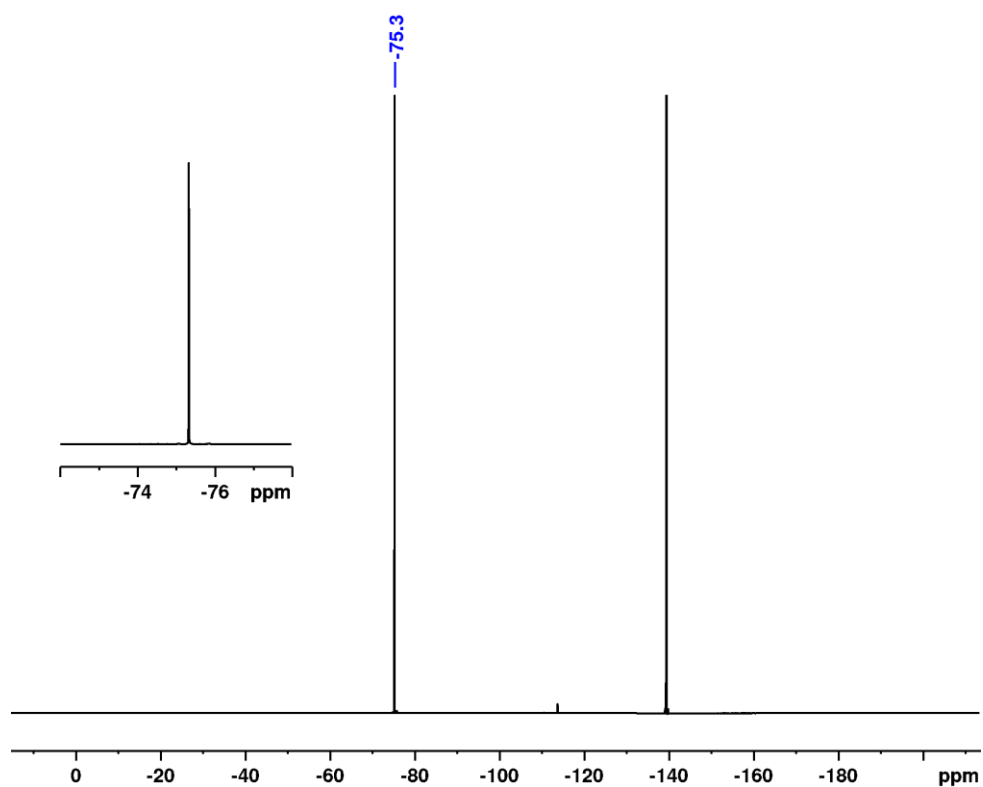


Figure S 75: ^{19}F NMR spectrum (376.53 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in oDFB at room temperature, 0.5 h after mixing the components.

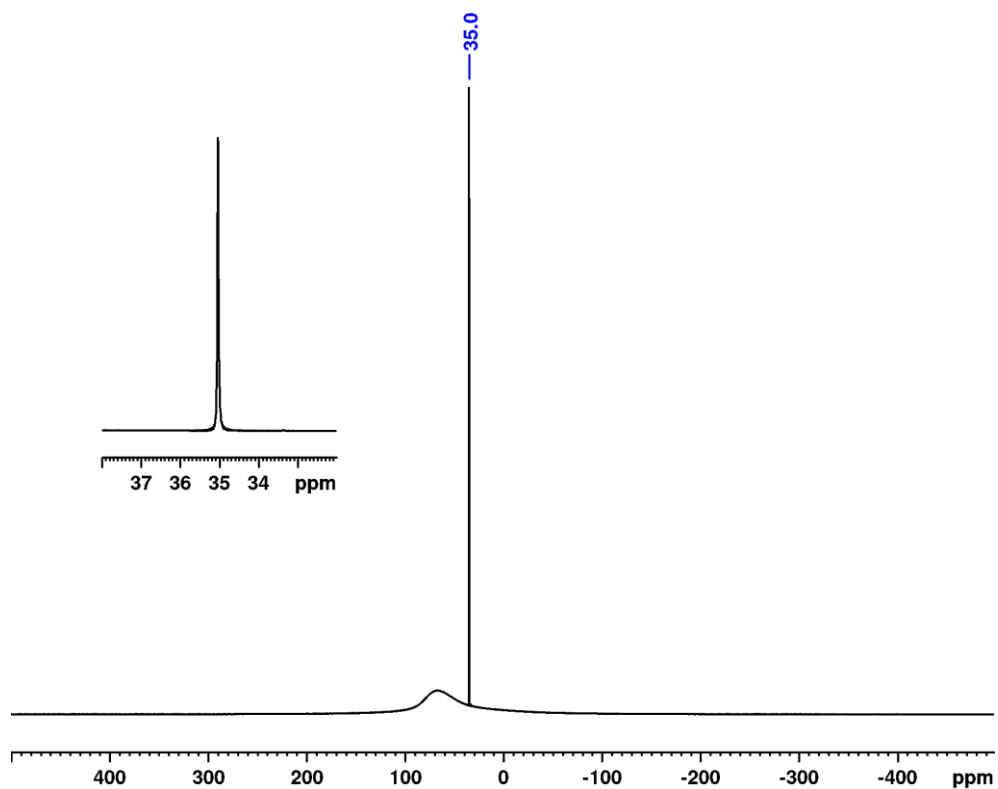


Figure S 76: ^{27}Al NMR spectrum (104.27 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in oDFB at room temperature, 0.5 h after mixing the components.

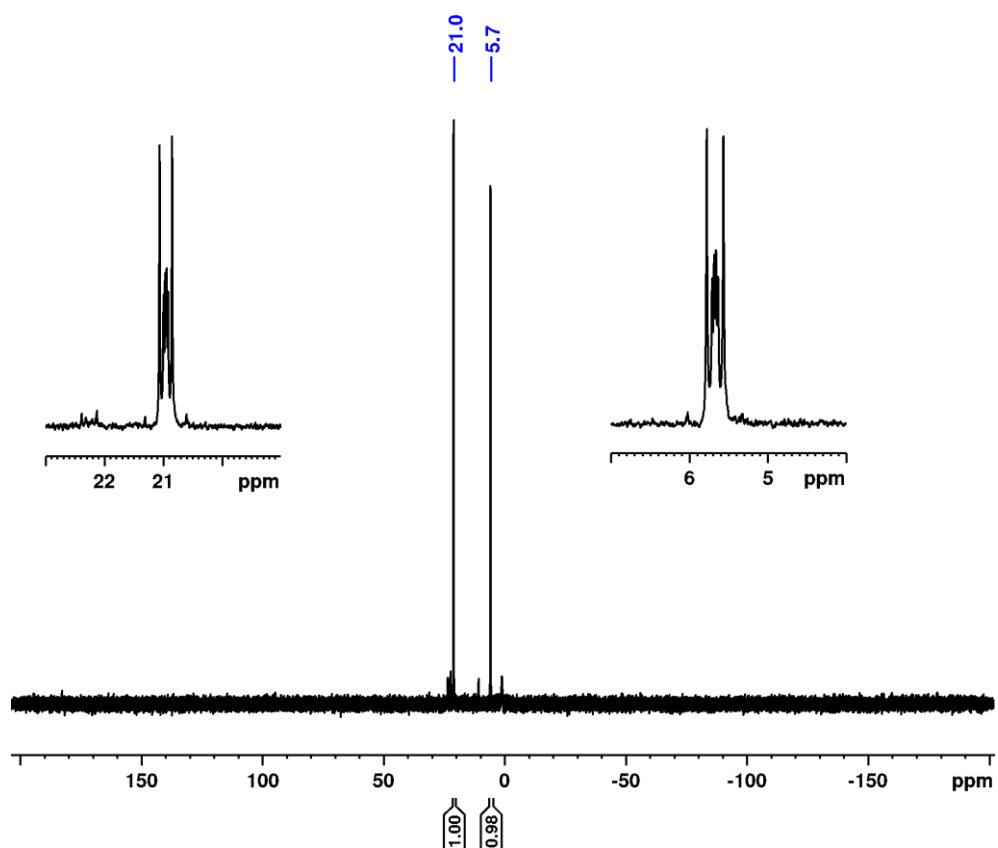
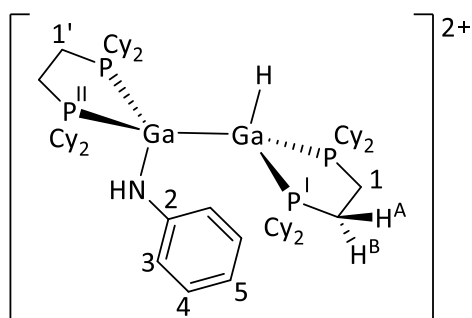


Figure S 77: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2nBu in oDFB at room temperature, 0.5 h after mixing the components.

4.6 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPh})][\text{pf}]_2$



^1H NMR [300.18 MHz, *o*DFB, calibrated at $\text{oC}_6\text{F}_2\text{H}_4 = 6.96$ ppm, 298 K]: $\delta = 7.20$ (m, 2 H, C^4H), 6.73 (m, 1 H, C^5H), 6.62 (m, 2 H, C^3H), 4.73 (t, 1 H, GaH , $^2J_{\text{H,P}} = 20.4$ Hz), 3.30 (m, 1 H, N-H), 2.50–2.33 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{A}}$, $\text{C}^{1'}\text{H}^{\text{B}}$), 2.42–2.24 (m, 8 H, CH protons of the Cy groups), 2.05–1.27 (m, 80 H, CH_2 protons of the Cy groups) ppm.

^{13}C NMR [75.48 MHz, *o*DFB, 298 K]: $\delta = 150.9$ (1 C, C^2), 129.6 (2 C, C^4), 117.9 (1 C, C^5), 115.3 (2 C, C^3), 33.4–31.7 (8 C, CH carbon atoms of the Cy groups), 29.1–25.3 (40 C, CH_2 carbon atoms on the Cy groups), 17.0–15.4 (4 C, C^1 and $\text{C}^{1'}$) ppm.

^{19}F NMR [282.45 MHz, *o*DFB, 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.8 (m, PhF), -139.5 (m, $\text{oC}_6\text{F}_2\text{H}_4$) ppm.

^{27}Al NMR [78.22 MHz, *o*DFB, 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [121.52 MHz, *o*DFB, 298 K]: $\delta = 20.1$ (m, 2 P, P^{I}), 8.5 (m, 2 P, P^{II}) ppm.

^{71}Ga NMR [91.54 MHz, *o*DFB, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

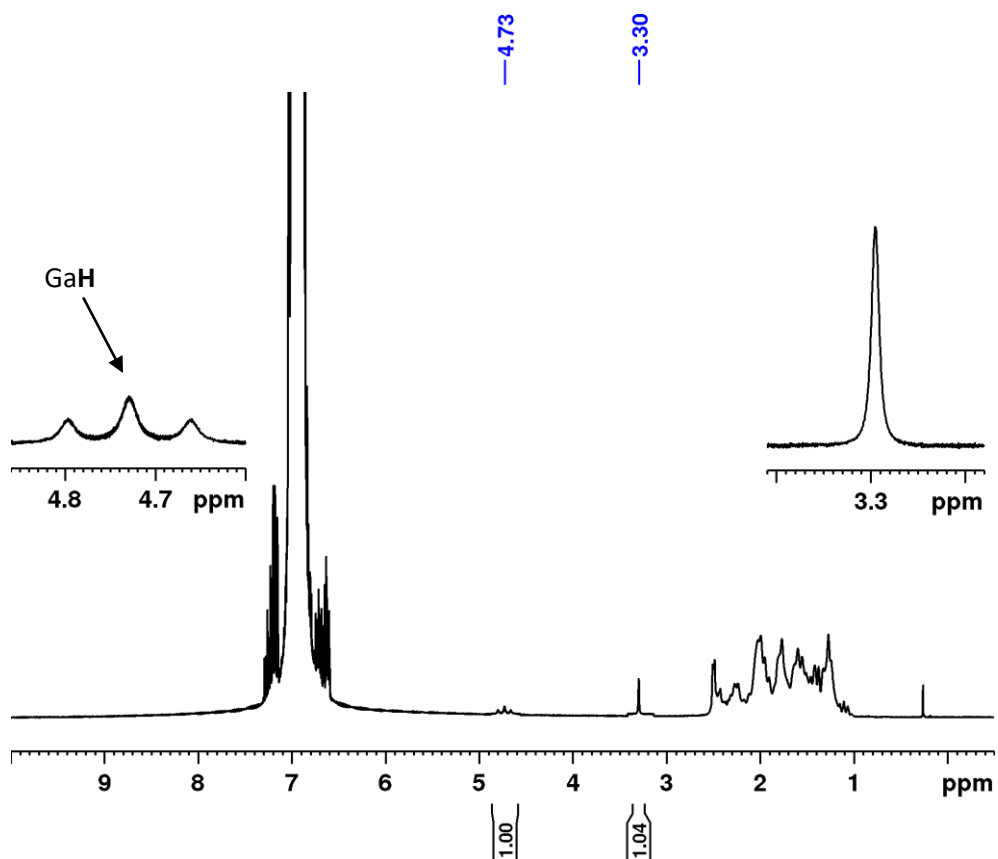


Figure S 78: ^1H NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in oDFB.

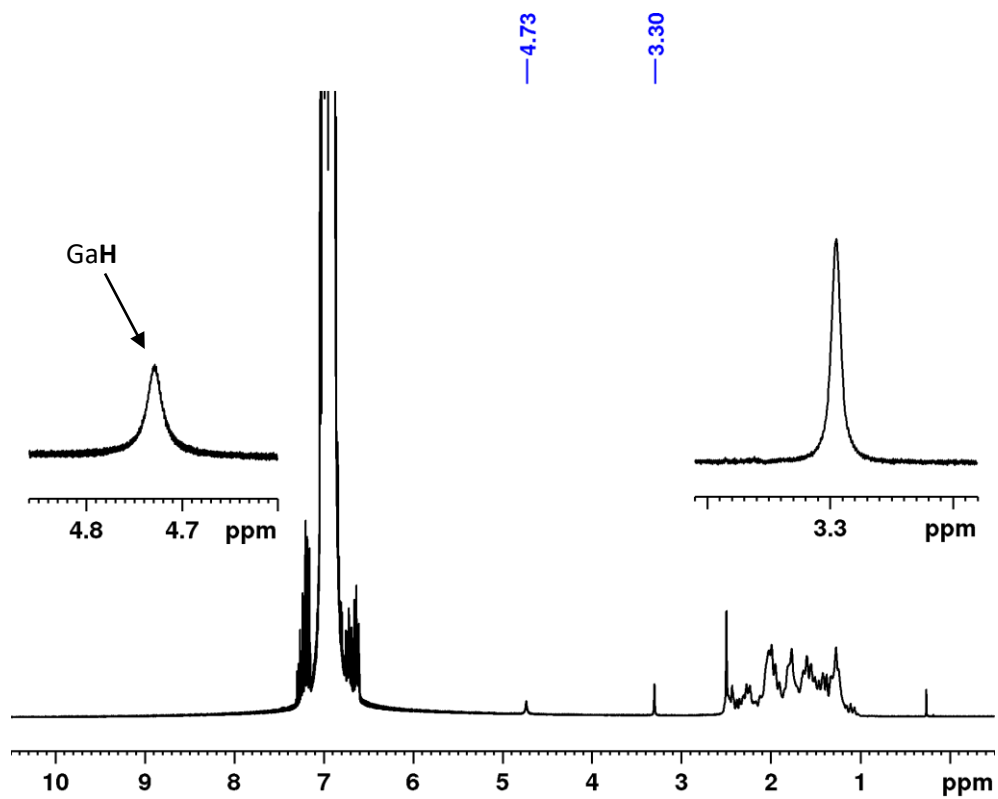


Figure S 79: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in oDFB.

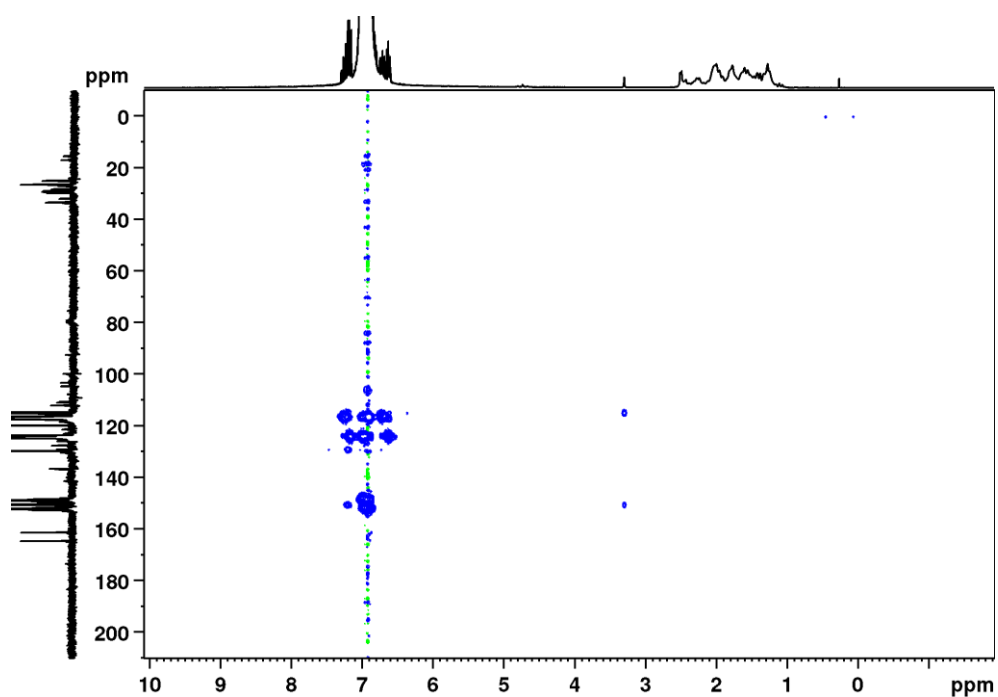


Figure S 80: ^1H , ^{13}C -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 8.0$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in oDFB.

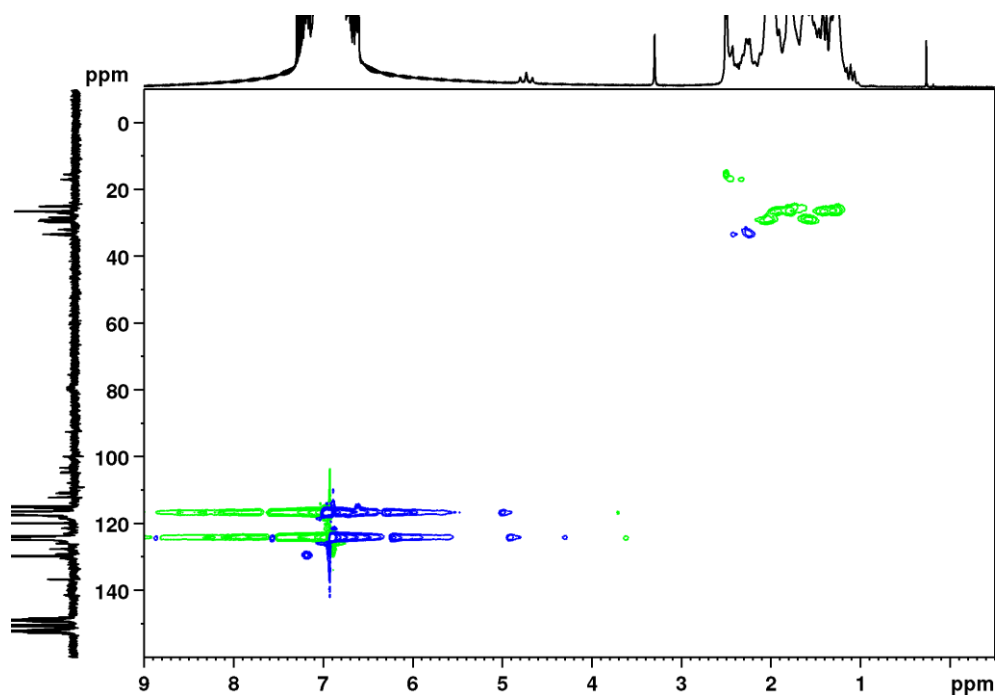


Figure S 81: Edited ^1H , ^{13}C -HSQC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in oDFB.

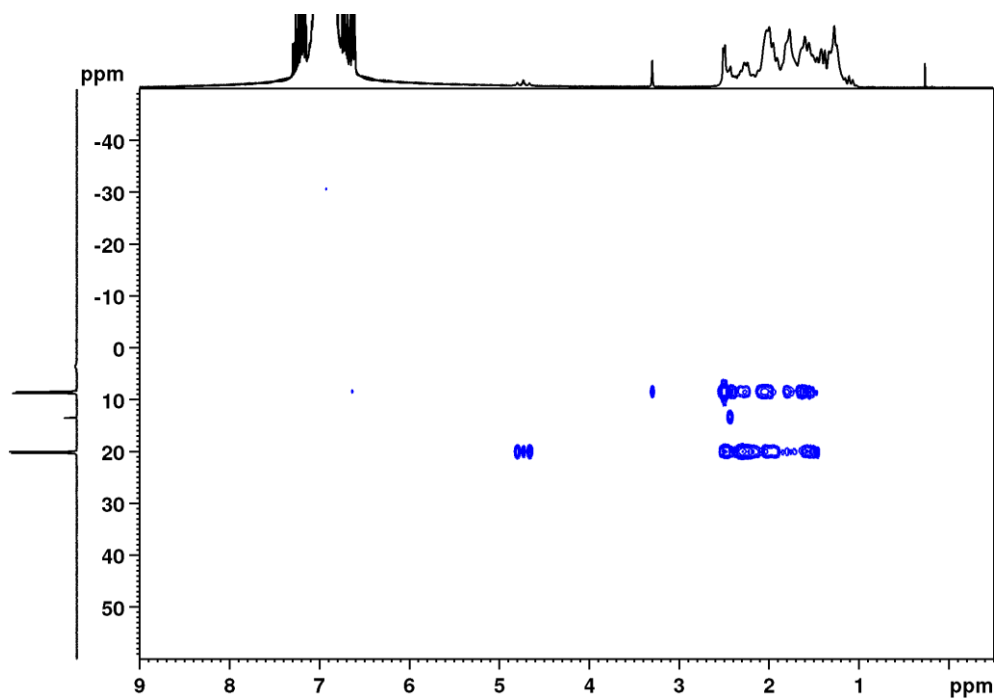


Figure S 82: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[(\text{Ga}(\text{dcpe}))_2][\text{pf}]_2$ and NH_2Ph in oDFB.

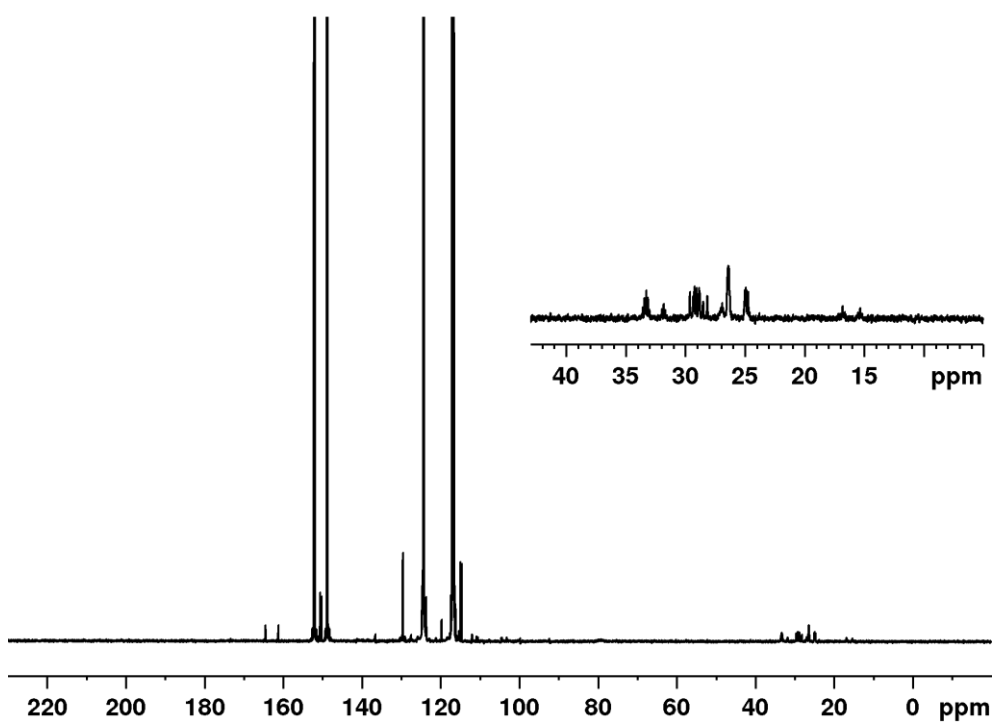


Figure S 83: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (75.48 MHz, oDFB, 298 K) of a mixture $[(\text{Ga}(\text{dcpe}))_2][\text{pf}]_2$ and NH_2Ph in oDFB.

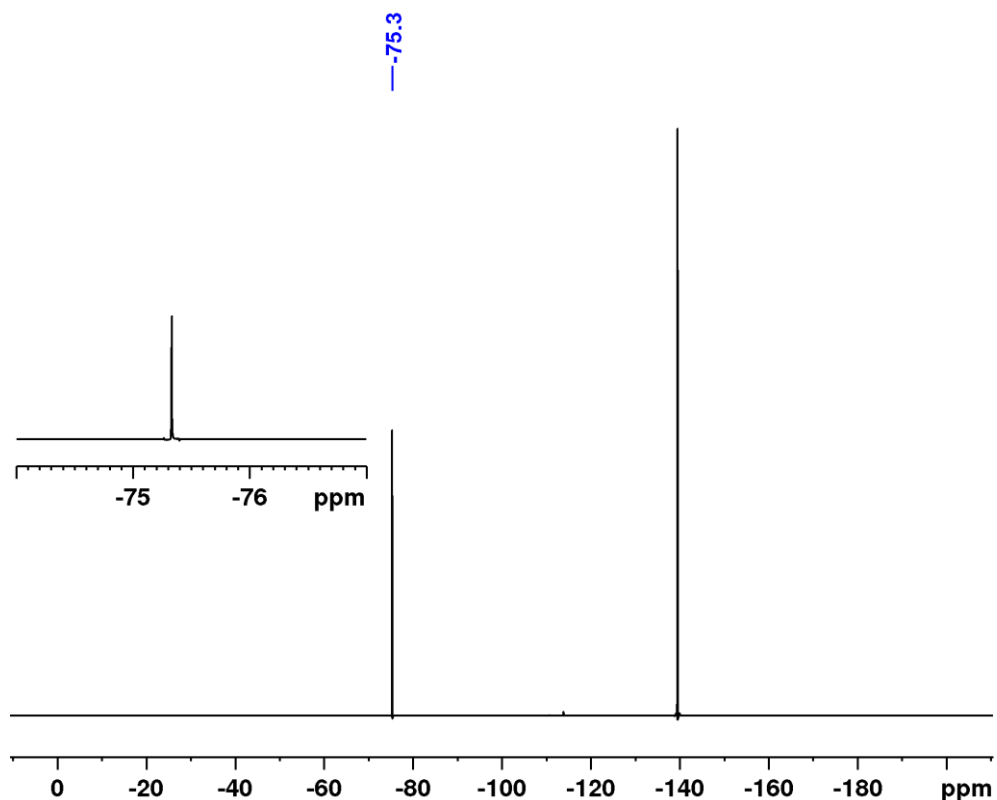


Figure S 84: ^{19}F NMR spectrum (188.31 MHz, oDFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})\}_2][\text{PF}]_2$ and NH_2Ph in oDFB

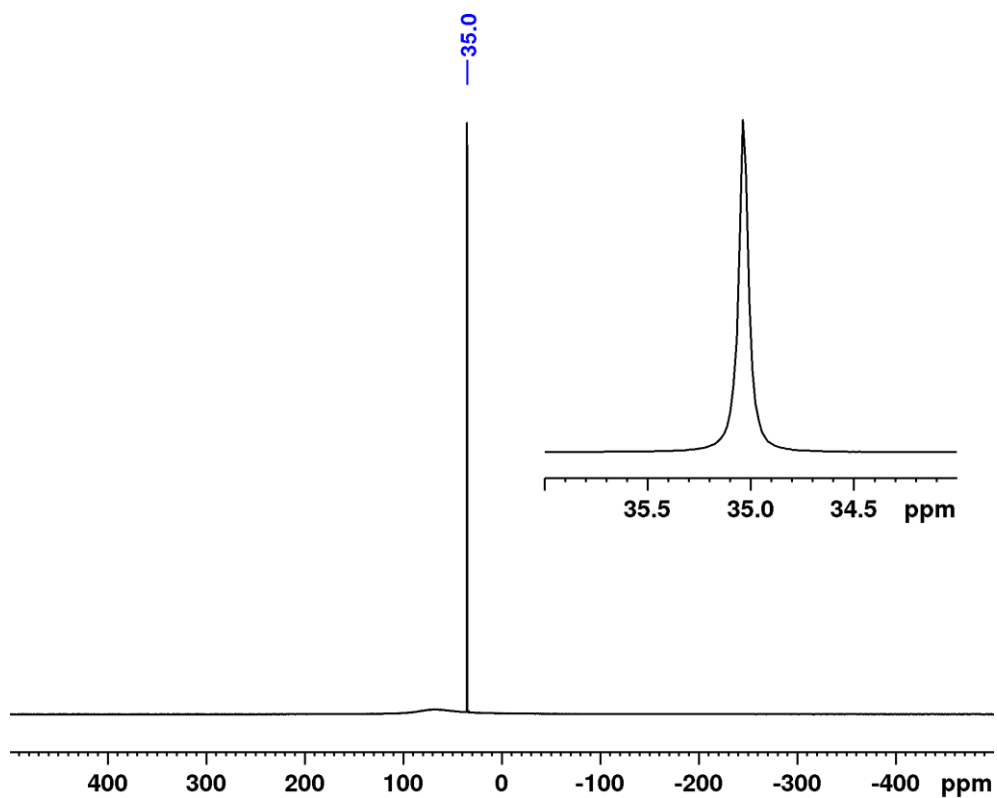


Figure S 85: ^{27}Al NMR spectrum (78.22 MHz, oDFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})\}_2][\text{PF}]_2$ and NH_2Ph in oDFB.

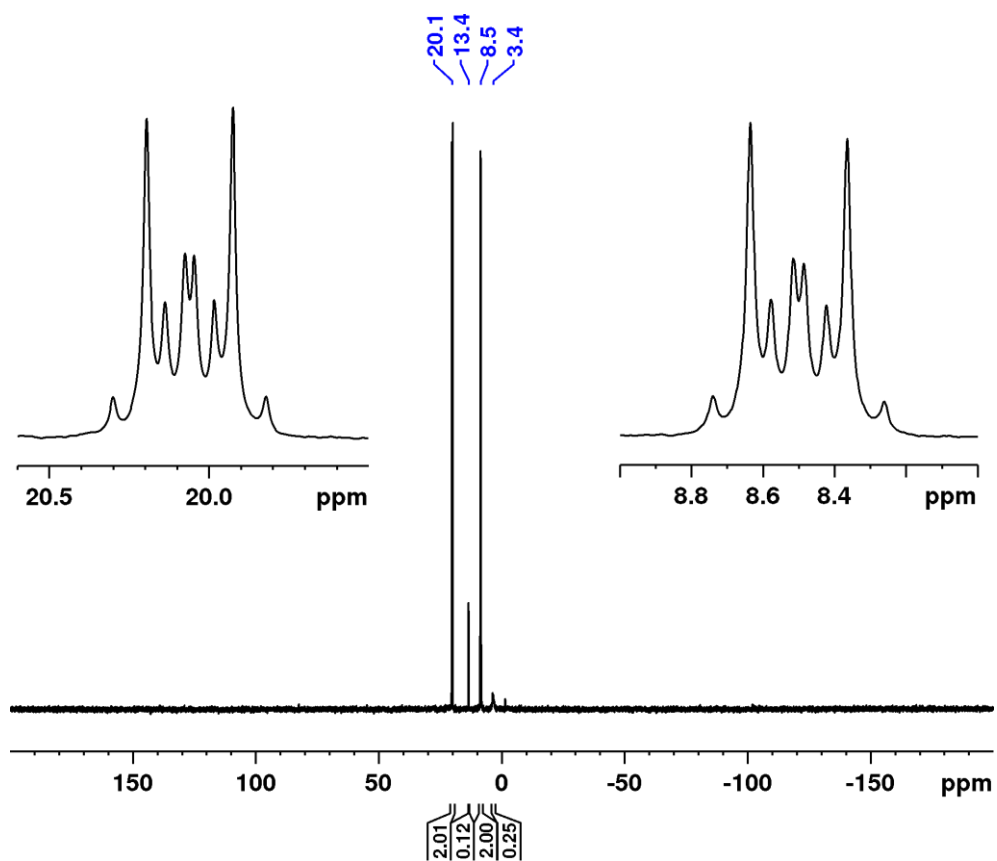


Figure S 86: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in oDFB.

4.6.1 Observed Intermediates during the Formation of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2\text{NPh}]^{2+}$

During the H–N bond activation with H_2NPh , one intermediate is observed in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum. The NMR findings for this species are similar to those for the intermediate with PhOH (section 4.4.1): It is characterized by a singlet in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum ($\delta(^{31}\text{P}) = 13.4$ ppm) and $J_{\text{H,P}}$ coupling constants of ca. 27 Hz. The ^1H signal of the corresponding GaH proton at ca. 5.25 ppm is remarkably broad, so that it cannot be determined whether the ^1H signal has a triplet or quintet splitting pattern in the non-decoupled ^1H NMR spectrum. Apparently, the intermediate is more stable for H_2NPh than for HOPh , since it is still present in the reaction mixture after several hours (see **Figure S 87** and **Figure S 89**). However, the signal intensities indicate that the concentration of this species decreases while the dimeric addition product is formed. A plausible structure is presented in **Figure S 87**.

Nevertheless, taking into account that the ^{31}P NMR and ^1H NMR shift of the P-Ga-H units in the intermediates observed during the reactions with HOPh , H_2NPh and HNPh_2 (sections 4.4.1, 4.6.1 and 4.7.1) is very similar, it cannot be ruled out that the NPh group acts as a bridging ligand with its aromatic π -system or that the NPh group is only weakly associated.

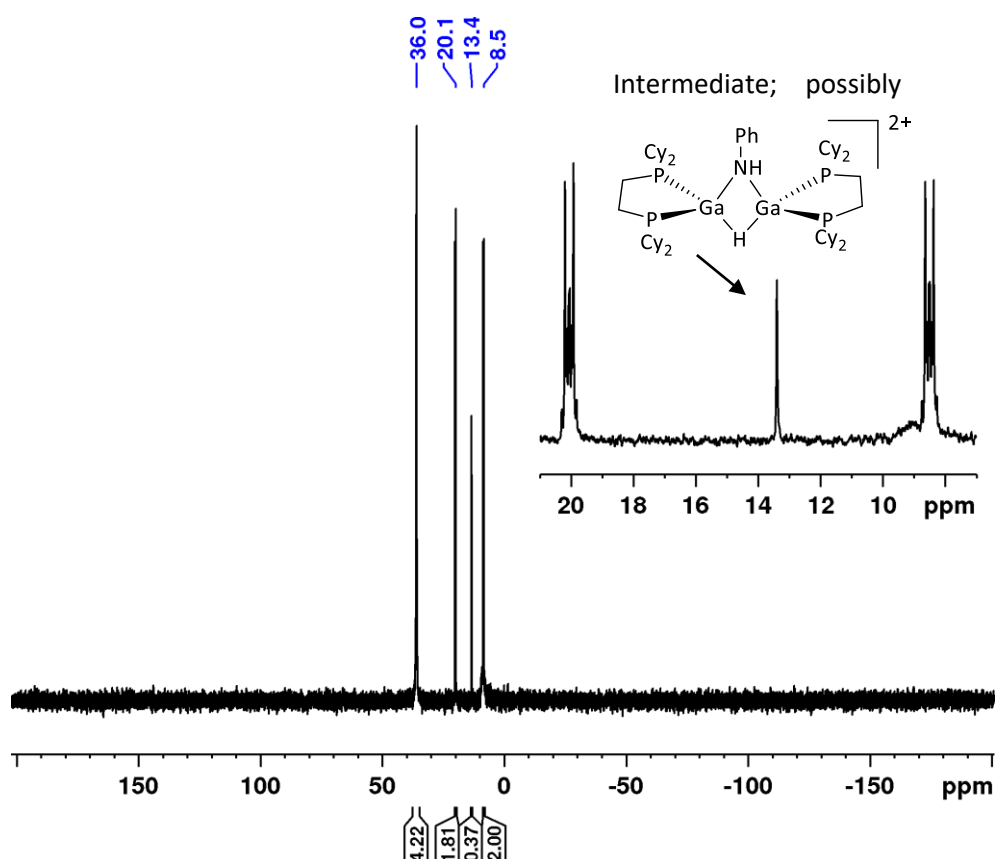


Figure S 87: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, *o*DFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NH_2Ph in *o*DFB, directly after mixing the components.

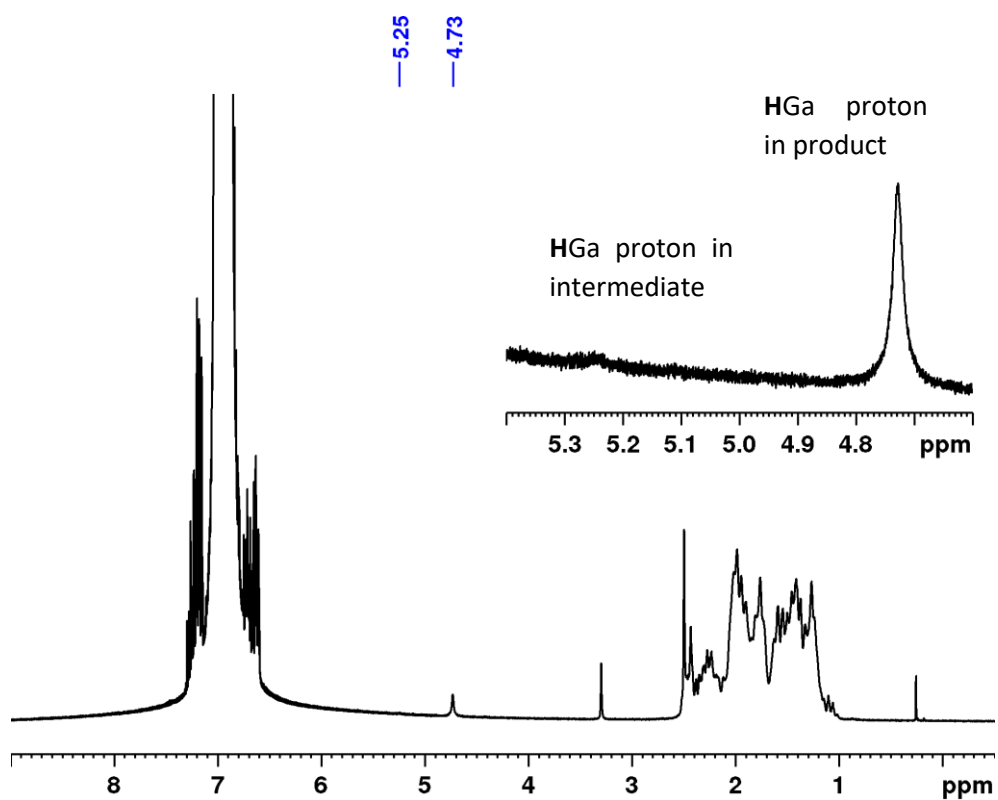


Figure S 88: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ and NH_2Ph in oDFB, 3 h after mixing the components.

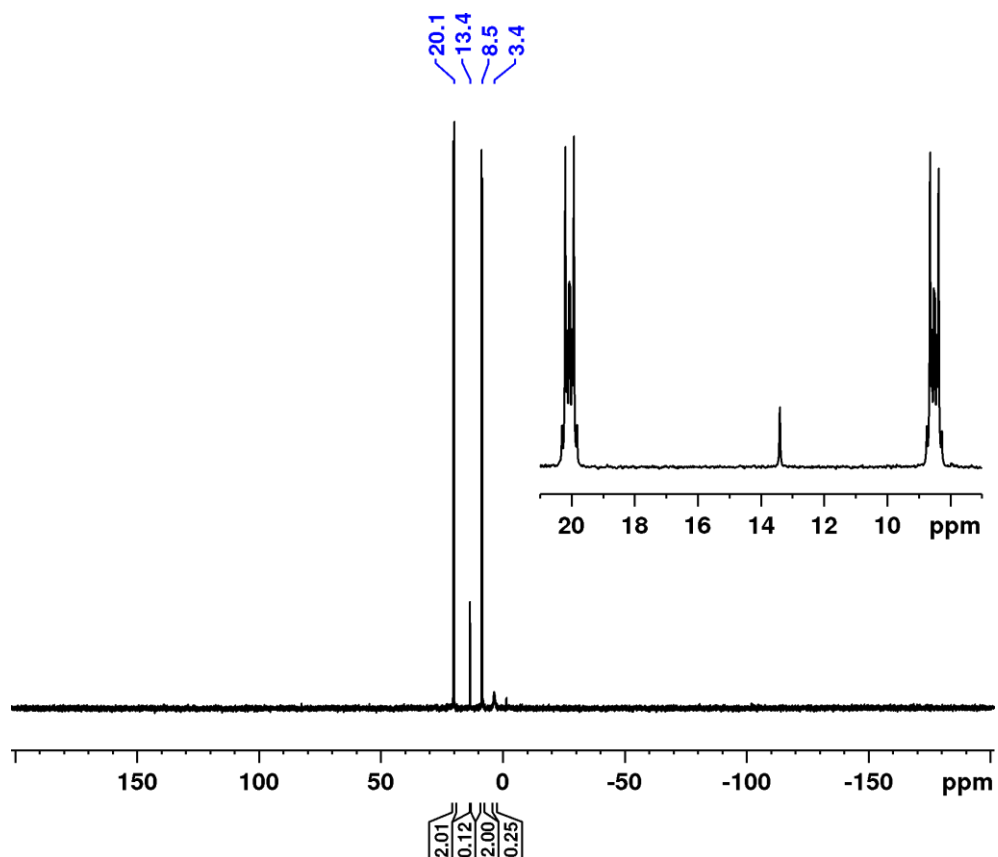
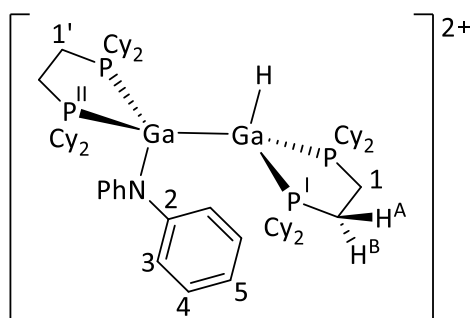


Figure S 89: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture $[\{\text{Ga}(\text{dcpe})_2\}][\text{pf}]_2$ and NH_2Ph in oDFB, 8 h after mixing the components.

4.7 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$



^1H NMR [300.18 MHz, *o*D F_2H_4 , calibrated at $\text{oC}_6\text{F}_2\text{H}_4 = 6.96$ ppm, 298 K]: $\delta = 7.39$ (m, 2 H, C^4H), 7.13 (1 H, C^5H), 6.85 (2 H, C^3H) 5.85 (br, HNPh_2 , starting material), 5.00 (t, 1 H, GaH , $^2J_{\text{H,P}} = 19.5$ Hz), 2.44–2.36 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{A}}$ and $\text{C}^{1'}\text{H}^{\text{B}}$), 2.34–1.52 (m, 8 H, CH protons of the Cy groups), 2.06–0.83 (m, 80 H, CH_2 protons of the Cy groups) ppm.

^{13}C NMR [100.62 MHz, *o*D F_2H_4 , 298 K]: $\delta = 150.7$ (1 C, C^2), 130.6 (2 C, C^4), 122.5 (1 C, C^5), 121.5 (2 C, C^3), 33.7–32.4 (8 C, CH carbon atoms of the Cy groups), 30.4–25.4 (40 C, CH_2 carbon atoms on the Cy groups), 16.5–14.6 (4 C, C^1 and $\text{C}^{1'}$) ppm.

^{19}F NMR [376.54 MHz, *o*D F_2H_4 , 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$, -113.8 (m, PhF), -139.5 (m, $\text{oC}_6\text{F}_2\text{H}_4$) ppm.

^{27}Al NMR [78.22 MHz, *o*D F_2H_4 , 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [161.99 MHz, *o*D F_2H_4 , 298 K]: $\delta = 30.7$ ($[\text{HdcpeH}]^+$), 21.6 (m, 2 P, P^{I}), 17.8 (unknown impurity), 5.5 (m, 2 P, P^{II}), -1.5 (m, $[\text{H}(\text{dcpe})\text{GaNPh}_2]^+$) ppm

^{71}Ga NMR [91.54 MHz, *o*D F_2H_4 , 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

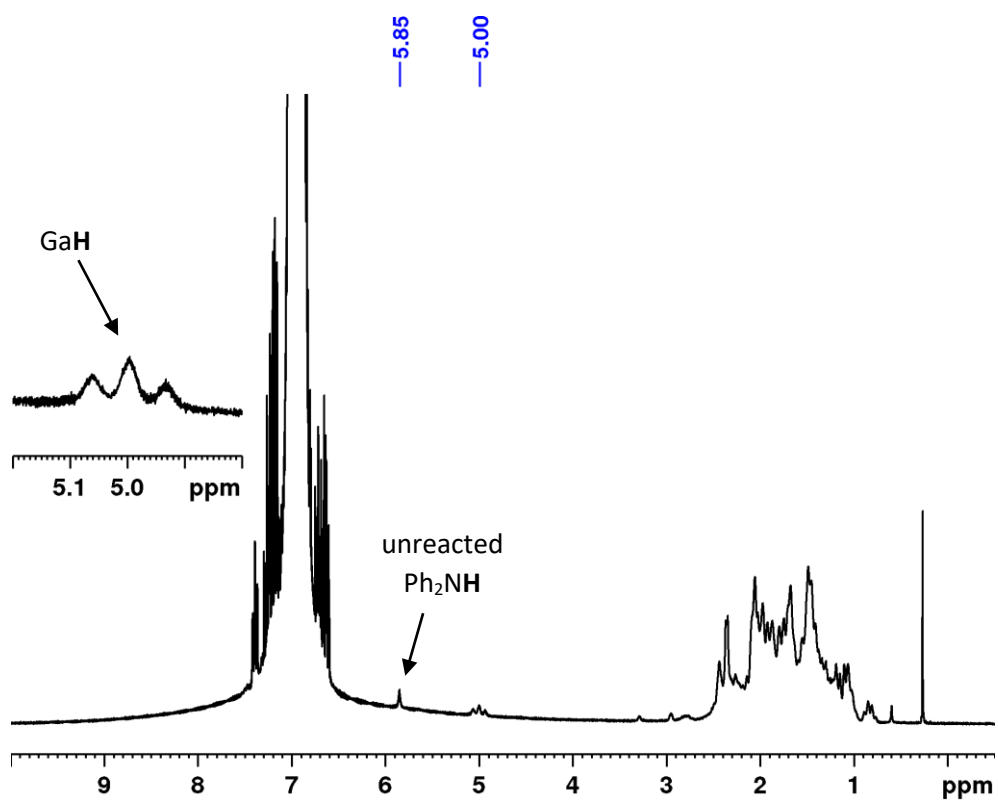


Figure S 90: ^1H NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NHPH_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

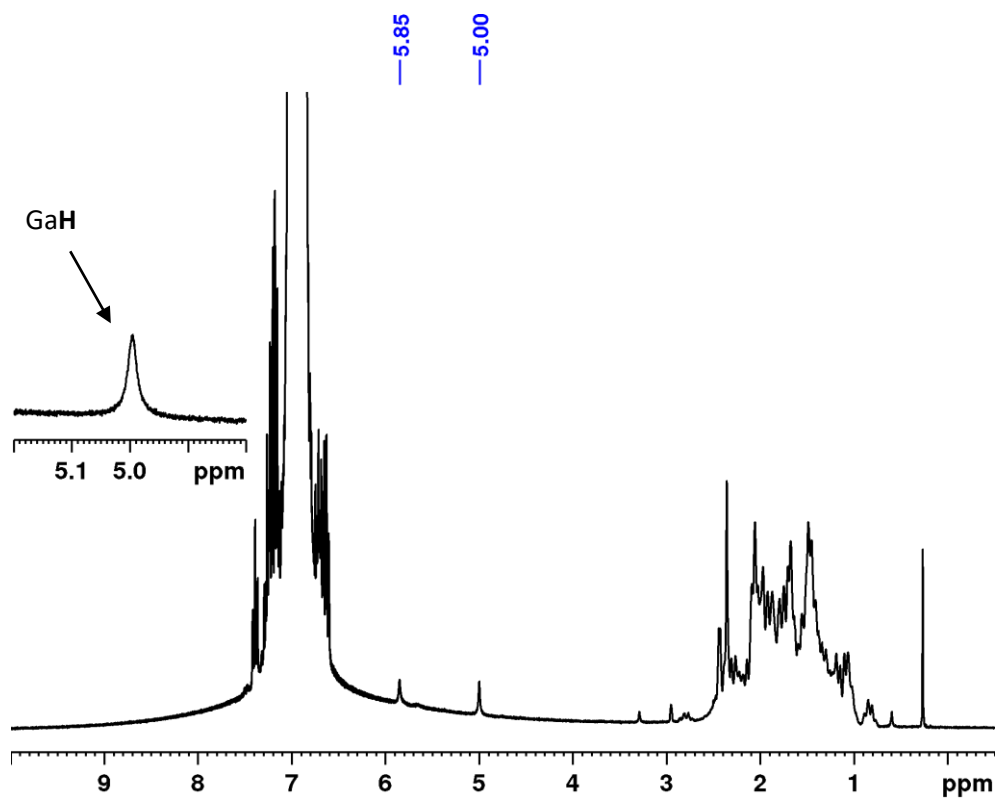


Figure S 91: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NHPH_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

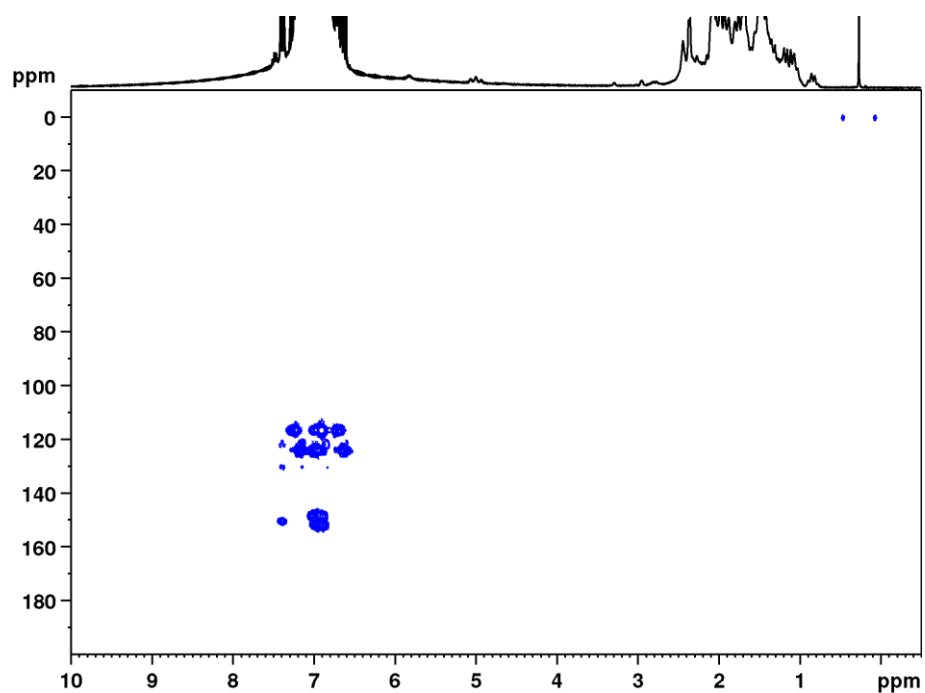


Figure S 92: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 8.0$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

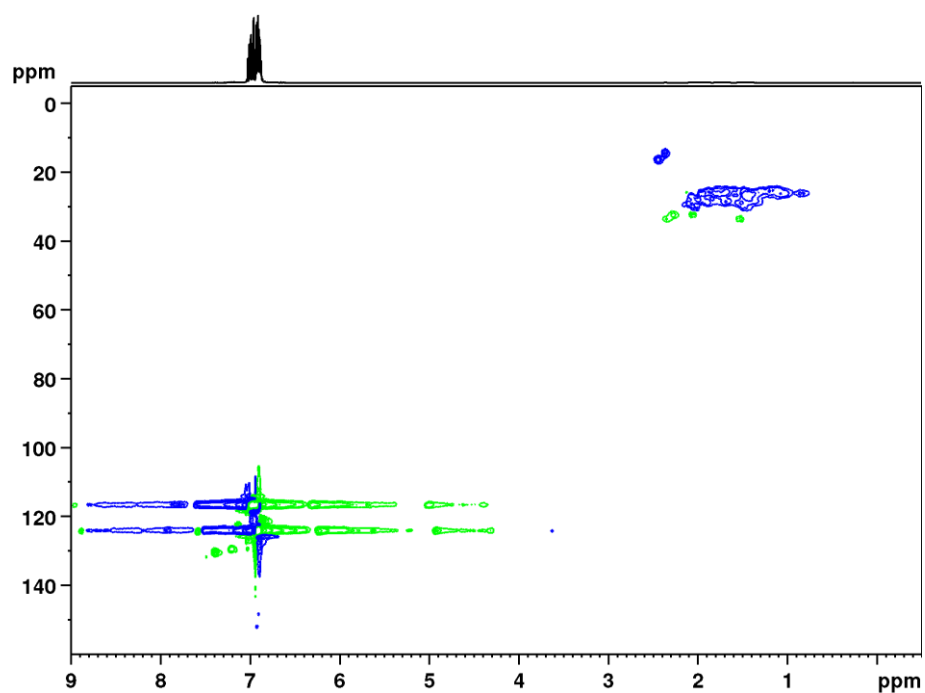


Figure S 93: Edited $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

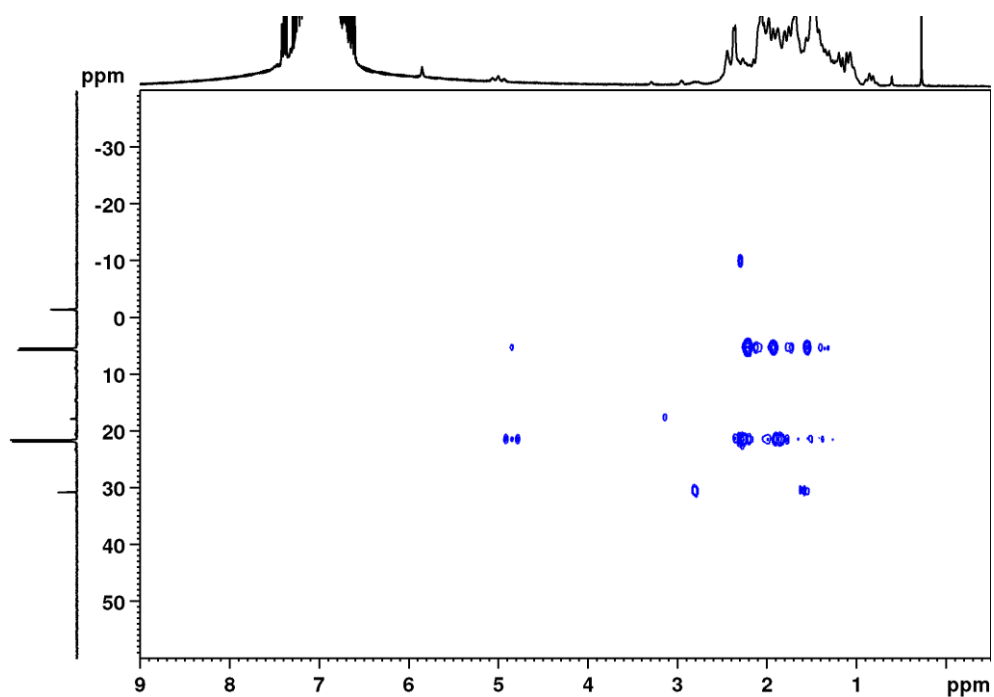


Figure S 94: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

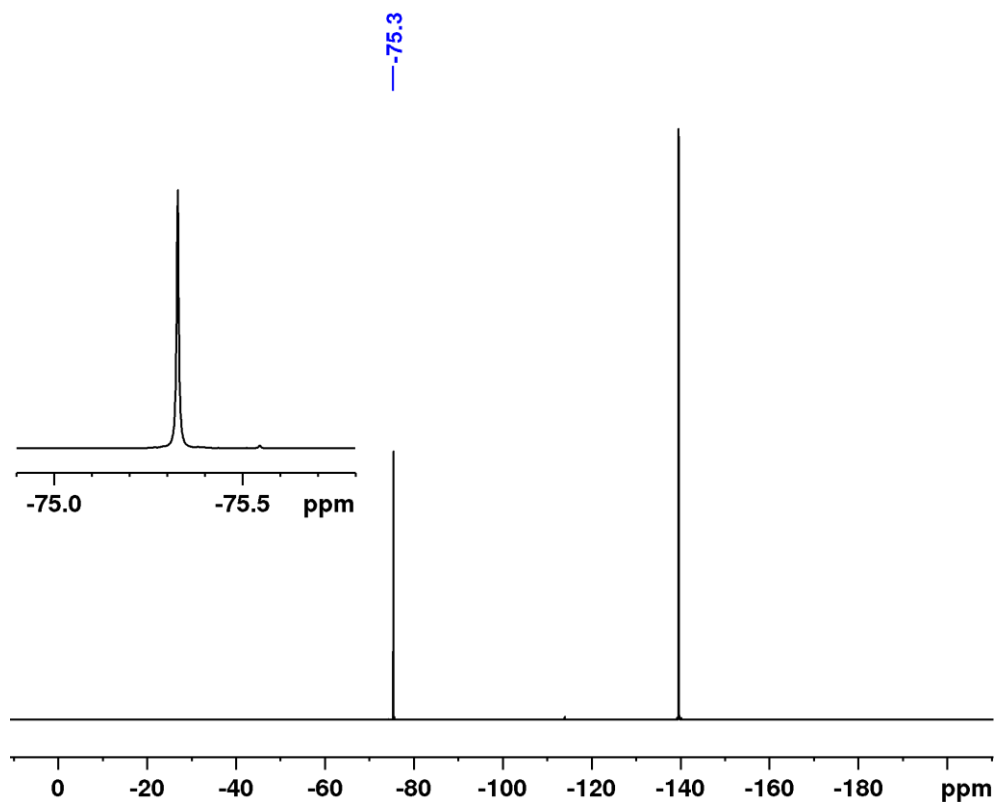


Figure S 95: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

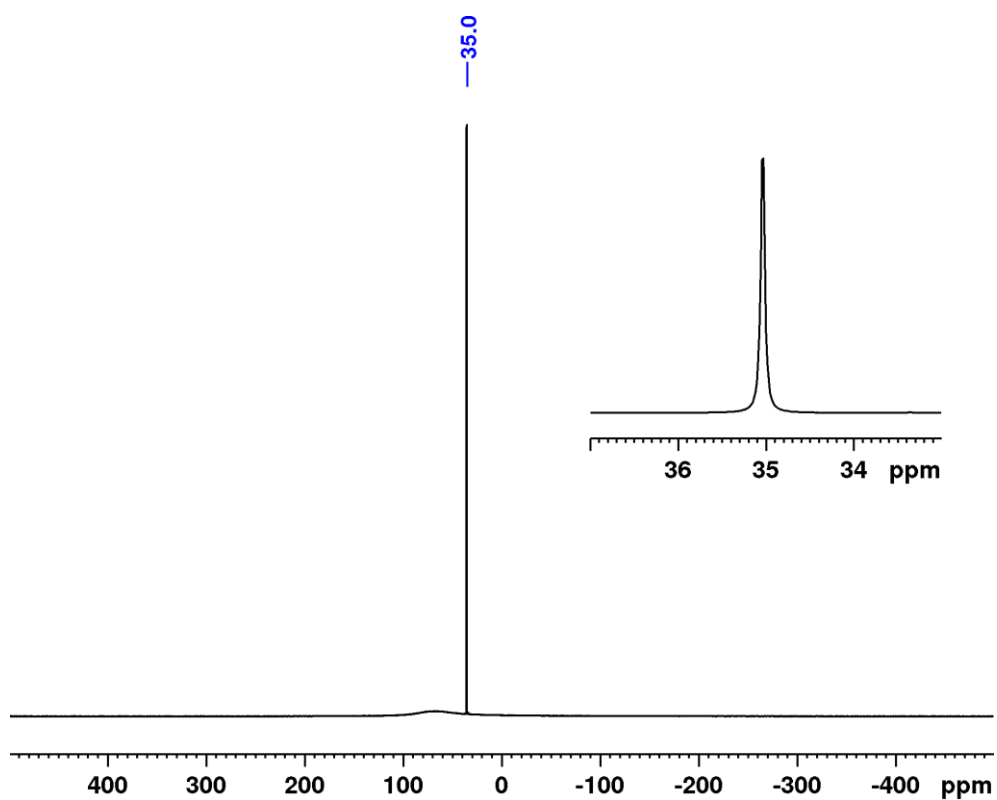


Figure S 96: ^{27}Al NMR spectrum (78.22 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

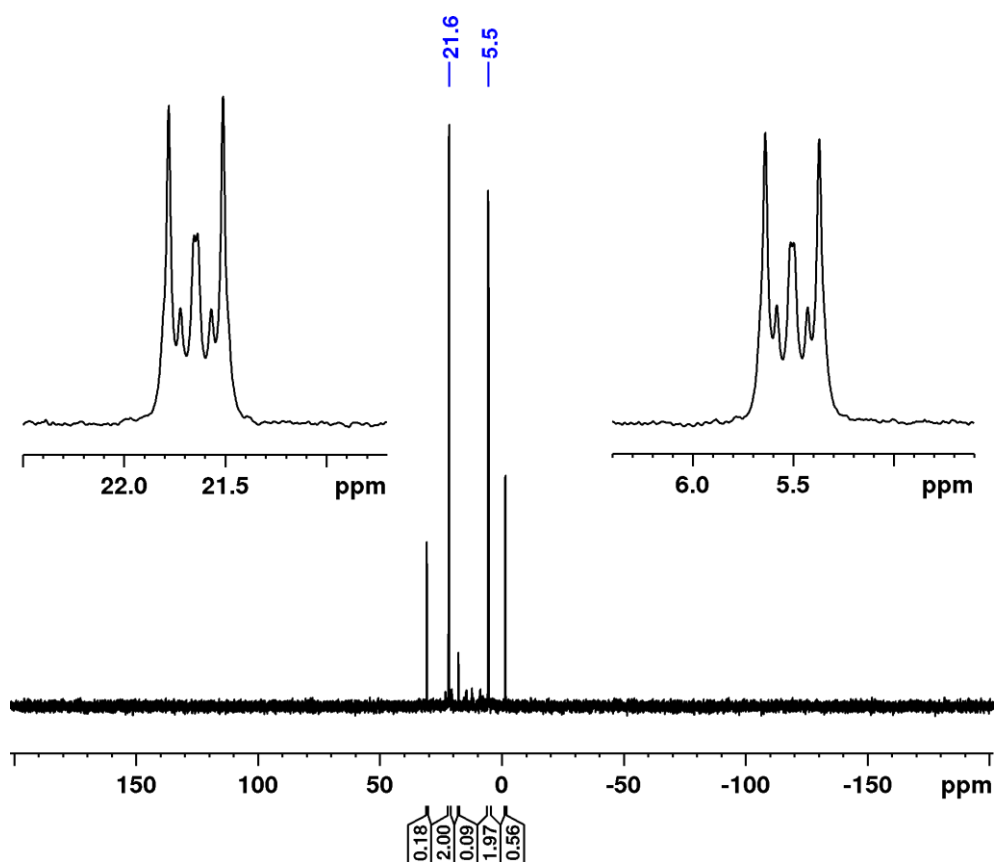


Figure S 97: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NHPh_2 in oDFB after heating the reaction mixture to 60 °C for 24 h.

4.7.1 Observed Intermediates during the Formation of $[H\{Ga(dcpe)\}_2NPh_2]^{2+}$

With $HNPh_2$, the reaction process is more complex than with $HOPh$ and H_2NPh (section 4.4.1 and 4.6.1) and seems to depend on the stoichiometry. When using sub-stoichiometric amounts of $HNPh_2$, the main intermediate is similar to those observed with $PhOH$ and H_2NPh (**Figure S 98** and **Figure S 100**). A plausible structure is presented in **Figure S 100**.

Nevertheless, taking into account that the ^{31}P NMR and ^1H NMR shift of the $P-Ga-H$ units in the intermediates observed during the reactions with $HOPh$, H_2NPh and $HNPh_2$ (sections 4.4.1, 4.6.1 and 4.7.1) is very similar, it cannot be ruled out that the NPh_2 group acts as a bridging ligand with its aromatic π -system or that the NPh_2 group is only weakly associated.

When using a surplus of $HNPh_2$, the reaction proceeds considerably faster at room temperature (*cf.* **Figure S 100** and **Figure S 105**). Besides this, and more importantly, another main intermediate is formed. It is characterized by a singlet in the $^{31}P\{^1H\}$ NMR spectrum, a doublet in the ^{31}P NMR spectrum ($\delta(^{31}P) = -1.5$ ppm) and by a $J_{H,P}$ coupling constant of 50 Hz, which is indicative of a $Ga^{III}-H$ species. The GaH proton shows a signal at 5.65 ppm. On the basis of these findings (**Figure S 101–Figure S 104**), we suggest that this species is a monomeric $[HGa(dcpe)NPh_2]^+$ complex, since, in the dimeric Ga^{II} addition products, the $^2J_{H,P}$ coupling constants are significantly smaller (ca. 20 Hz) and all phosphorous atoms in the molecule are chemically and magnetically equivalent. The putative monomer is quickly formed in solution and at room temperature slowly reacts further as the concentration of $\mathbf{1}^{2+}$ decreases (**Figure S 105**), indicating that the monomeric addition product reacts with the digallene under the formation of the final, dimeric Ga^{II} addition product.

It should be noted that both intermediates are present in reaction solutions of $\mathbf{1}^{2+}$ and $HNPh_2$, and that the applied stoichiometry merely influences their relative concentrations, underlining that, with $HNPh_2$, different reaction mechanisms are likely operative. In this context, it is unsurprising that a higher starting concentration of $HNPh_2$ leads to an increased formation of the monomeric intermediate. The somewhat more complex reaction mechanism compared to other substrates could be attributed to the high steric demand of $HNPh_2$, and a different coordination mode compared to other alcohols and amines: due to the electron delocalization over the $Ph-N-Ph$ system, the π systems are electron rich, while the nitrogen atom is comparatively electron poor.

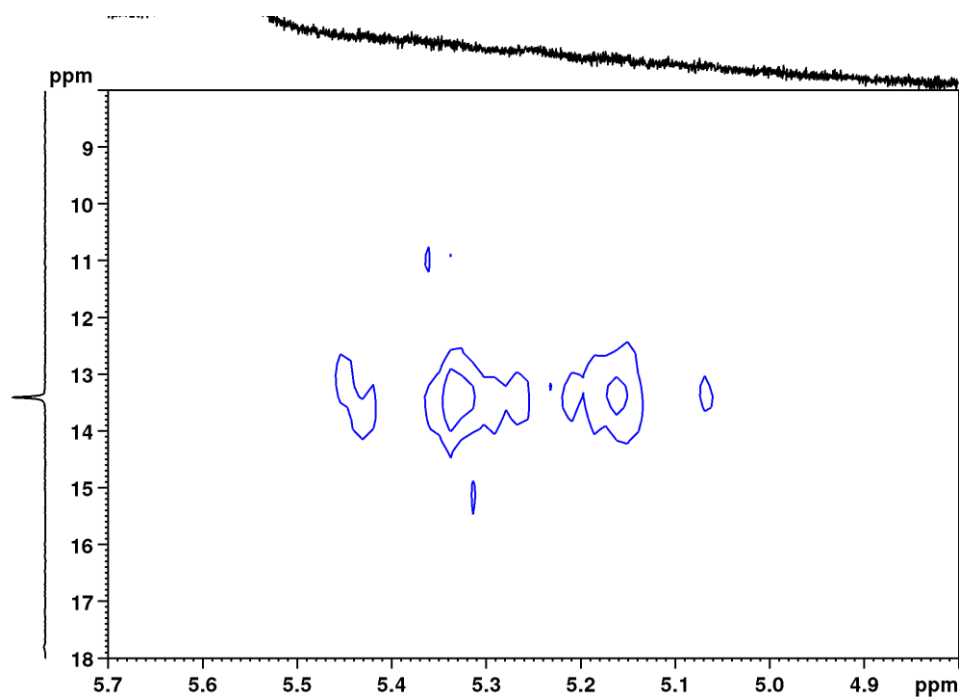


Figure S 98: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HNPh_2 (1 : 0.6) in oDFB, two days after mixing the components.

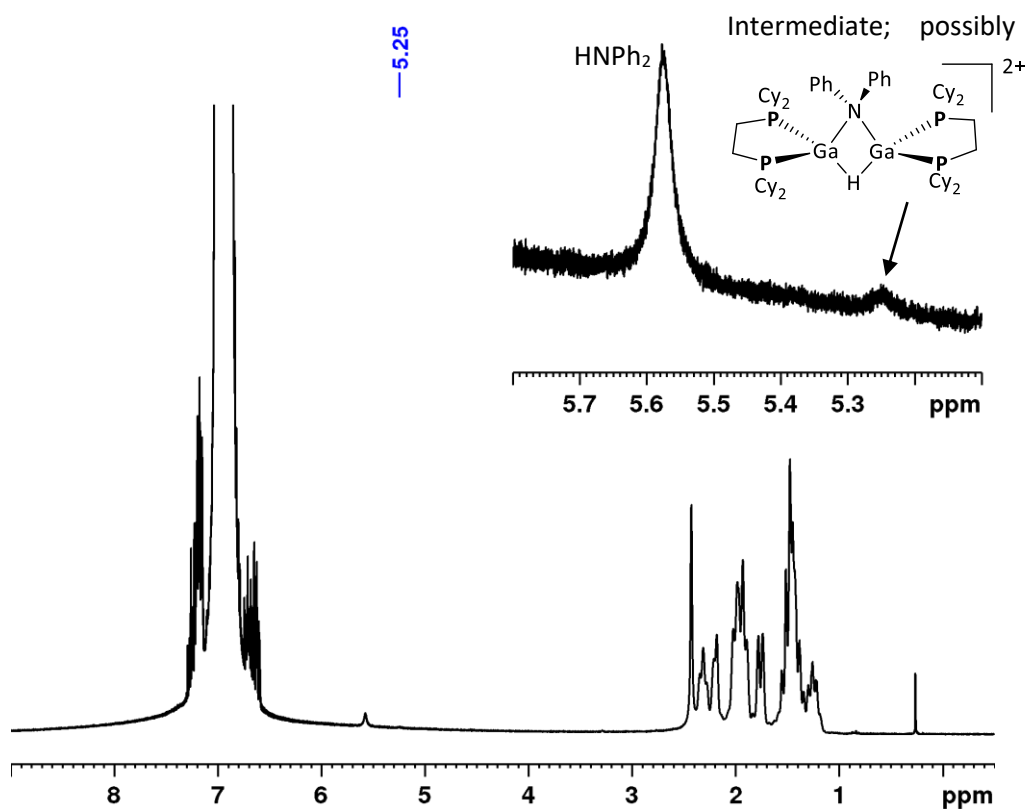


Figure S 99: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HNPh_2 (1 : 0.6) in oDFB, one day after mixing the components.

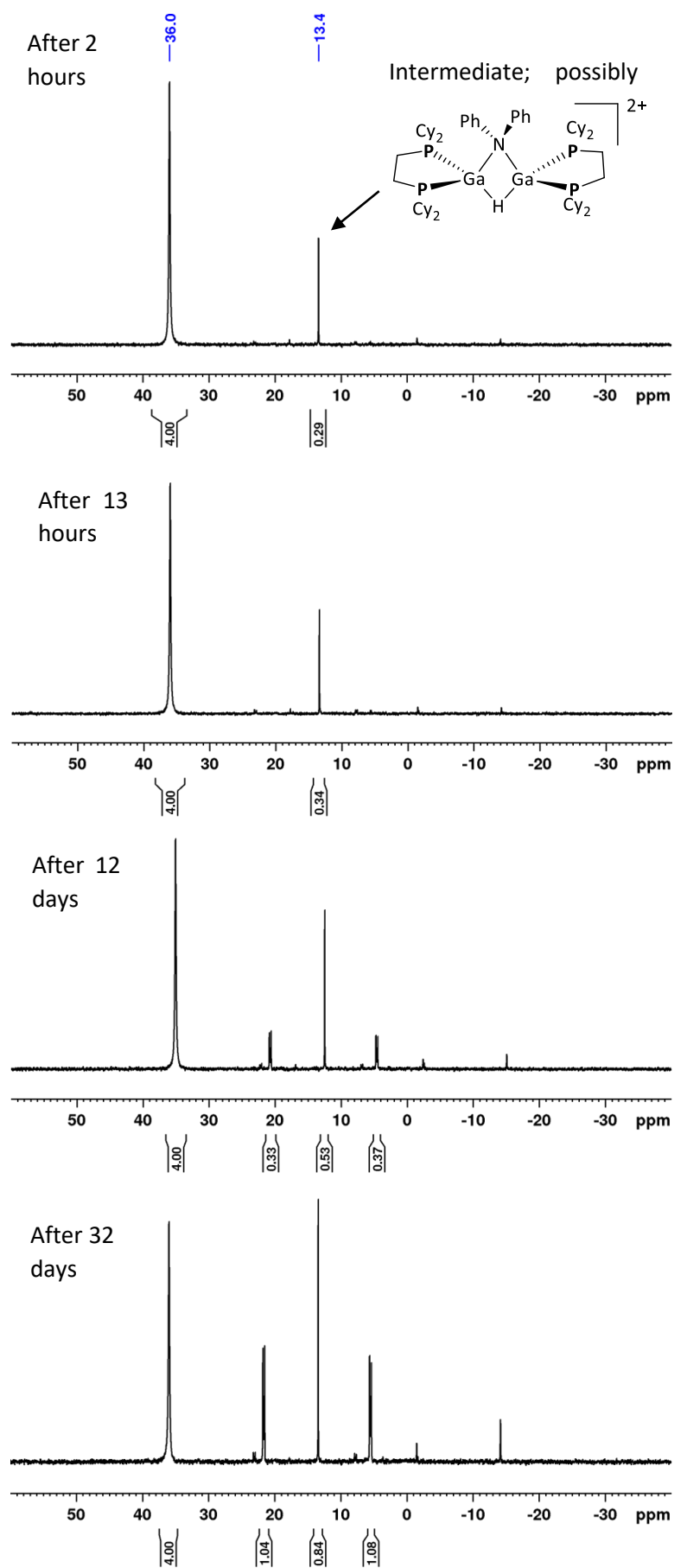


Figure S 100: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, *o*DfB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NHPh_2 (1 : 0.6) in *o*DfB at different times after mixing the components.

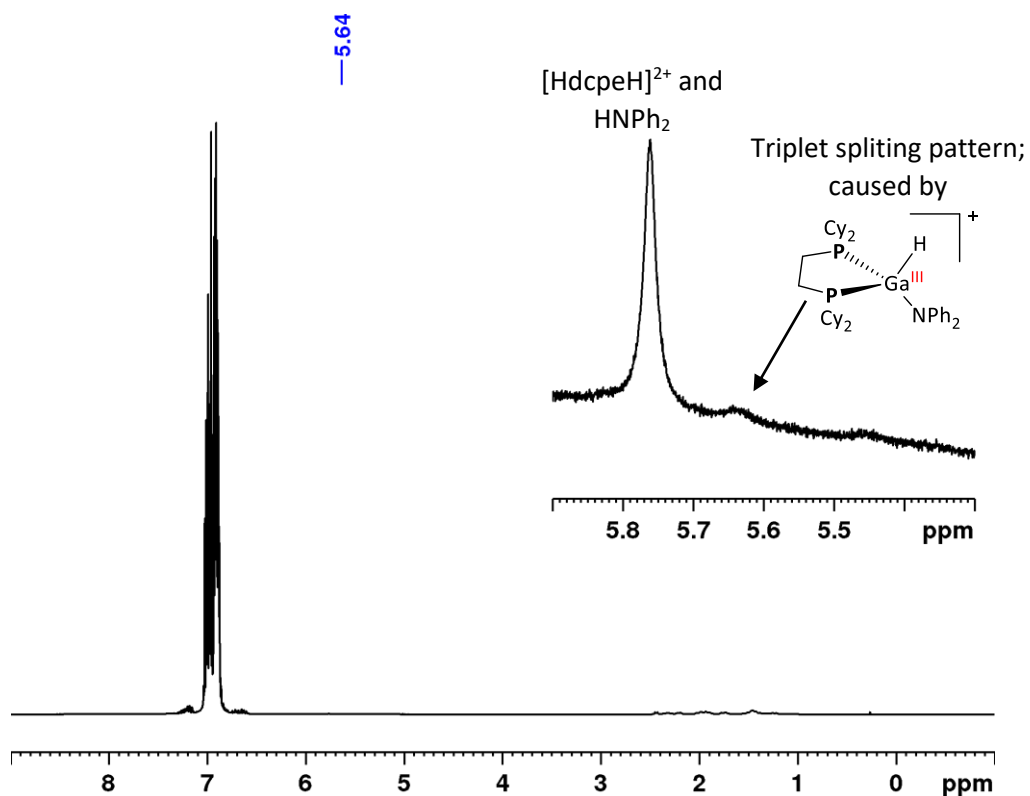


Figure S 101: ^1H NMR spectrum (300.18 MHz, *o*DFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HNPh_2 (1 : 1.2) in *o*DFB, 6 h after mixing the components.

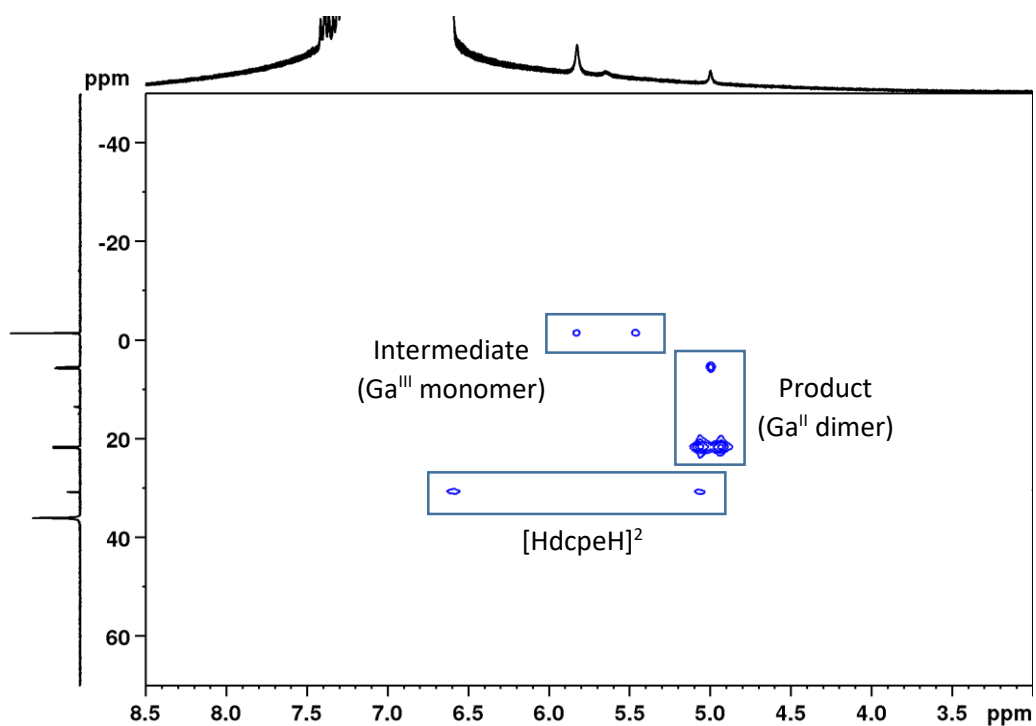


Figure S 102: $^1\text{H},^{31}\text{P}$ -HMBC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and HNPh_2 (1 : 1.2) in *o*DFB, one day after mixing the components.

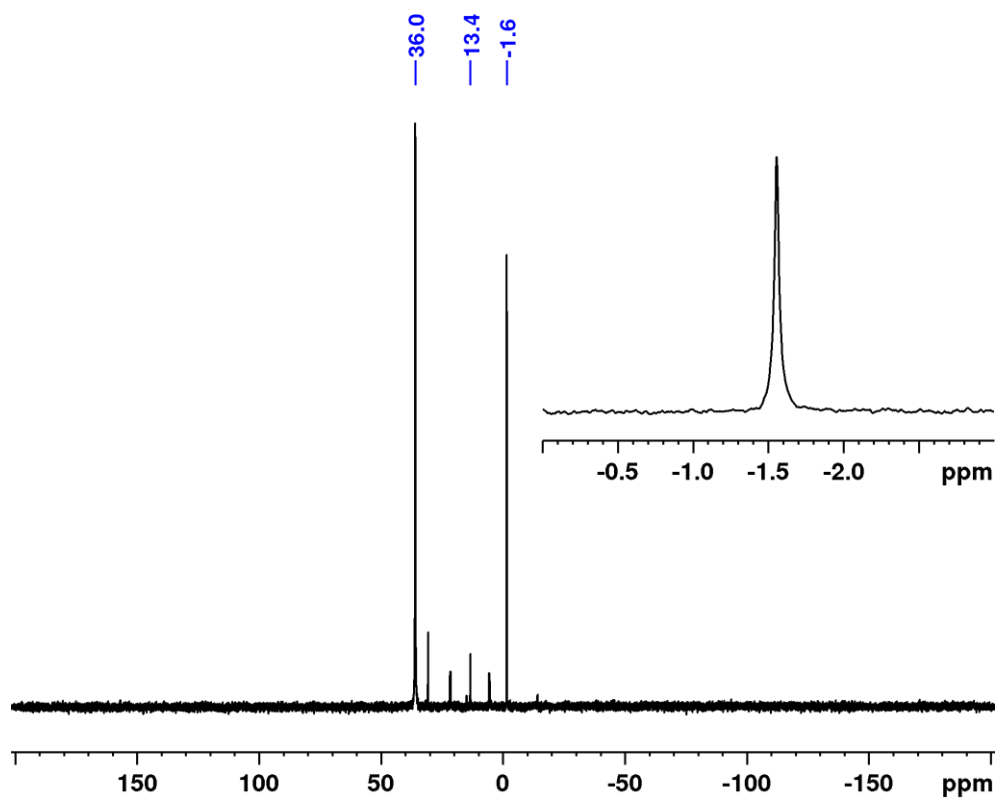


Figure S 103: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NPh_2 (1 : 1.2) in oDFB, 7 h after mixing the components.

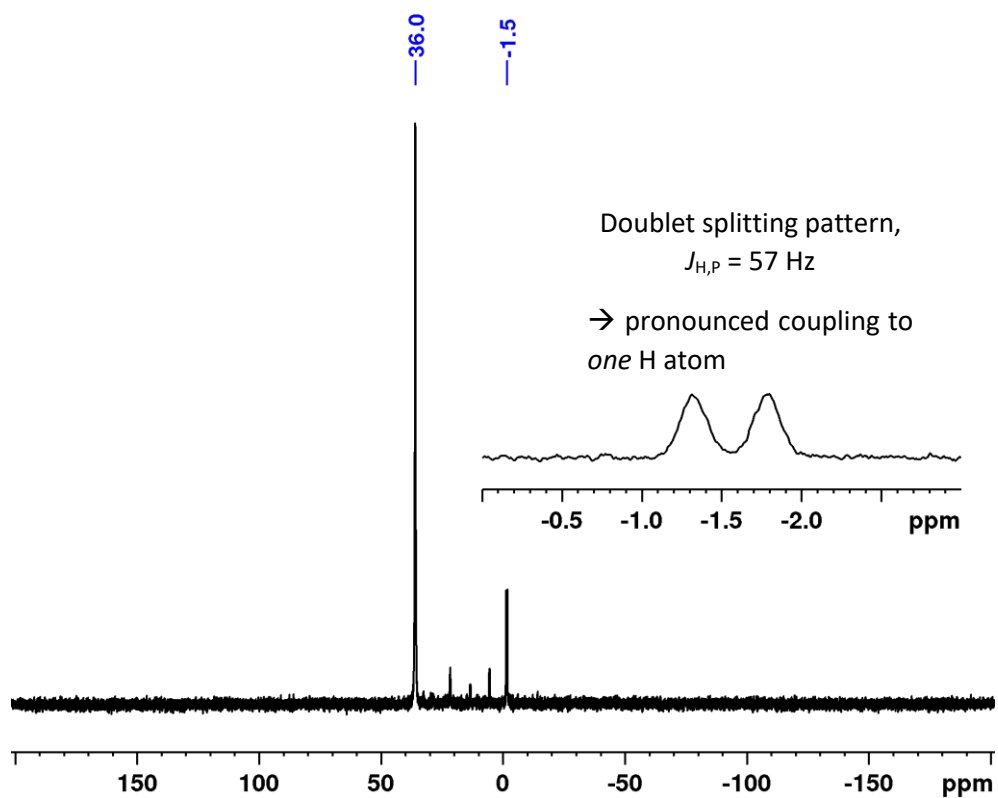


Figure S 104: ^{31}P NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NPh_2 (1 : 1.2) in oDFB, 7 h after mixing the components.

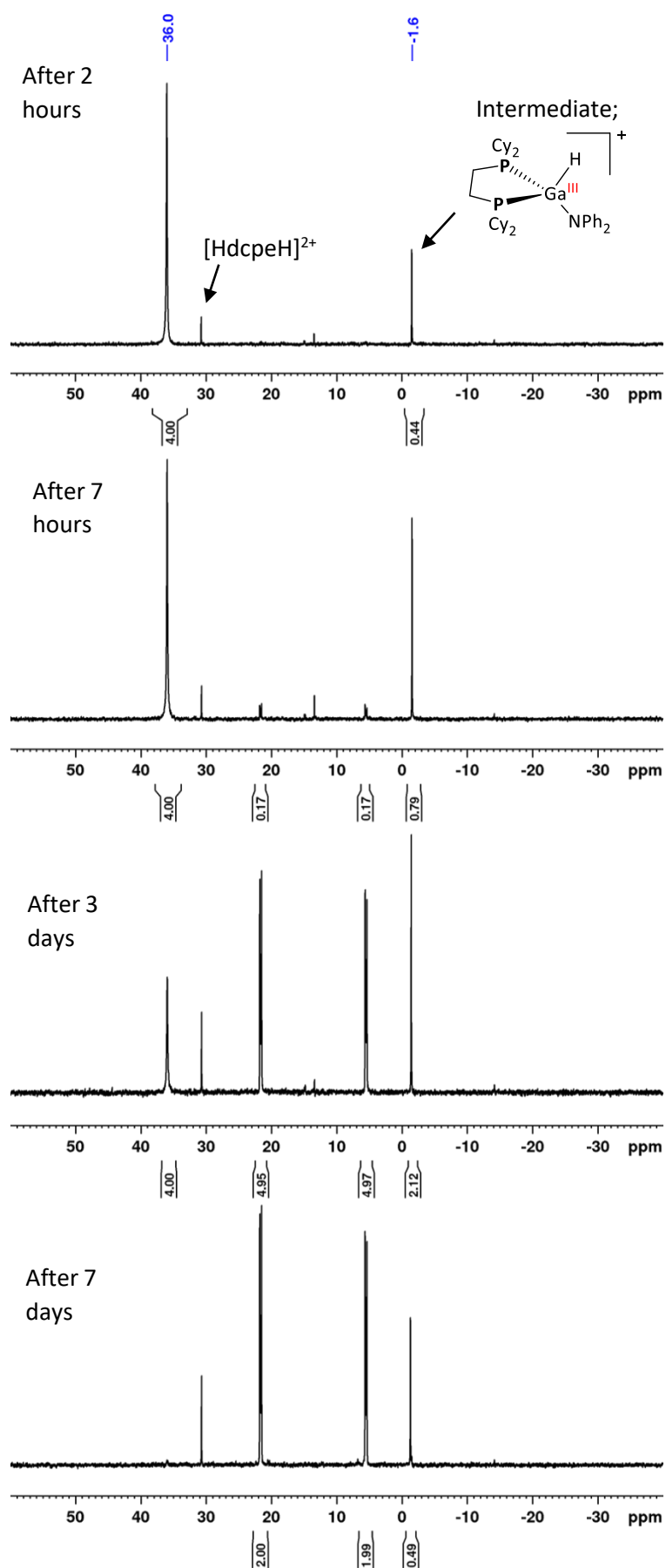
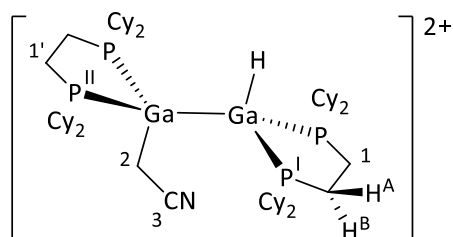


Figure S 105: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, *o*DfB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NPh_2 (1 : 1.2) in *o*DfB at different times after mixing the components.

4.8 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$



^1H NMR [300.18 MHz, *o*D₂F₆, calibrated at *o*C₆F₂H₄ = 6.96 ppm, 298 K]: δ = 4.68 (t, 1 H, GaH, $^2J_{\text{H,P}}$ = 20.8 Hz), 2.54–2.29 (m, 8 H, CH protons of the Cy groups), 2.50–2.44 (m, 8 H, C¹H^A, C¹H^B, C^{1'}H^A and C^{1'}H^B), 2.15–1.29 (m, 8 H, CH₂ protons of the Cy groups), 1.80 (t, 2 H, C²H₂, $^3J_{\text{H,P}}$ = 4.3 Hz) ppm.

^{13}C NMR [100.62 MHz, *o*D₂F₆, 298 K]: δ = 122.7 (1 C, C³N), 33.8–32.7 (8 C, CH carbon atoms of the Cy groups), 29.3–24.9 (40 C, CH₂ carbon atoms of the Cy groups), 16.6 and 15.6 (4 C, C¹ and C^{1'}), –2.5 (1 C, C²) ppm.

^{19}F NMR [376.54 MHz, *o*D₂F₆, 298 K]: δ = –75.3 (s, 36 F, [Al(OC(CF₃)₃)₄][–]), –113.9 (m, PhF), –139.5 (m, *o*C₆F₂H₄) ppm.

^{27}Al NMR [78.22 MHz, *o*D₂F₆, 298 K]: δ = 35.0 (s, 1 Al, [Al(OC(CF₃)₃)₄][–]) ppm.

^{31}P NMR [161.99 MHz, *o*D₂F₆, 298 K]: δ = 35.9 (digallene starting material), 23.1 (unknown impurity), 20.8 (m, 2 P, P^I), 14.9 (m, 2 P, P^{II}), 10.4 (unknown impurity) ppm.

^{71}Ga NMR [91.54 MHz, *o*D₂F₆, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

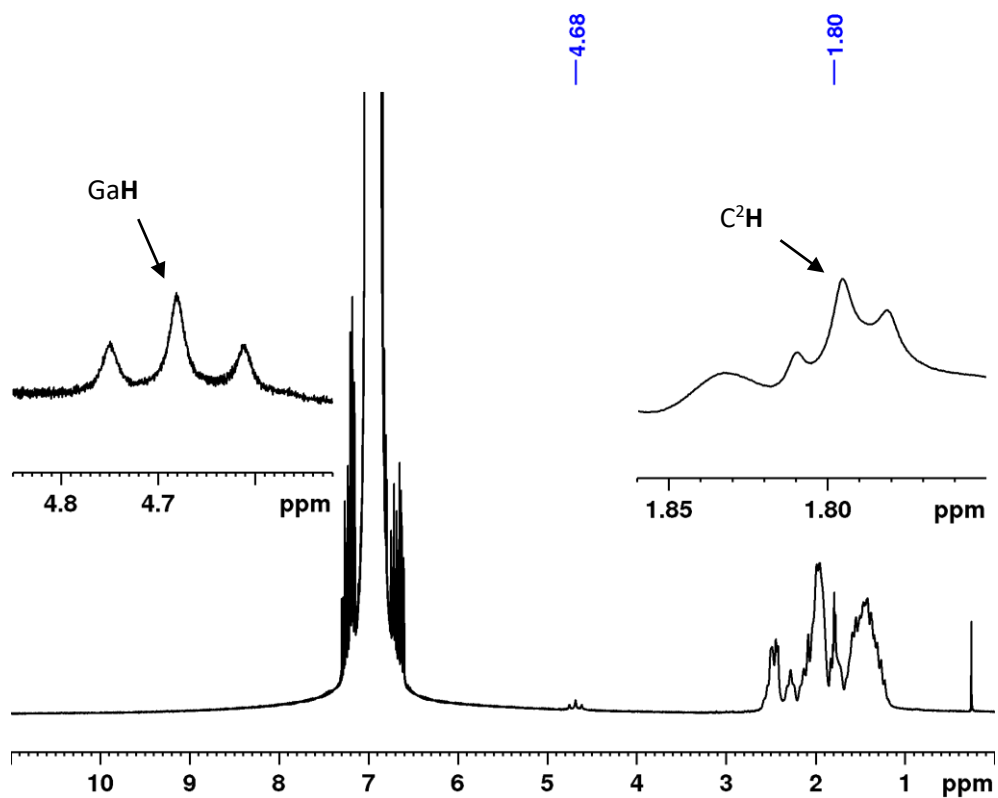


Figure S 106: ^1H NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_3$ in oDFB after heating the reaction mixture to $60\text{ }^\circ\text{C}$ for 4 days.

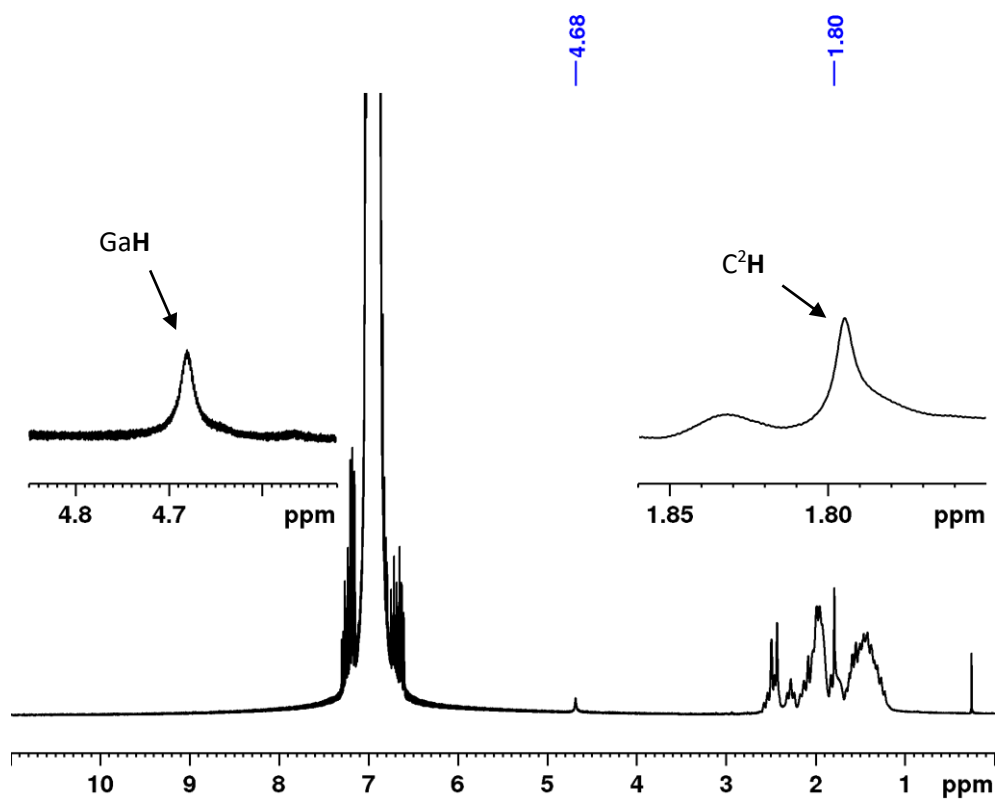


Figure S 107: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_3$ in oDFB after heating the reaction mixture to $60\text{ }^\circ\text{C}$ for 4 days.

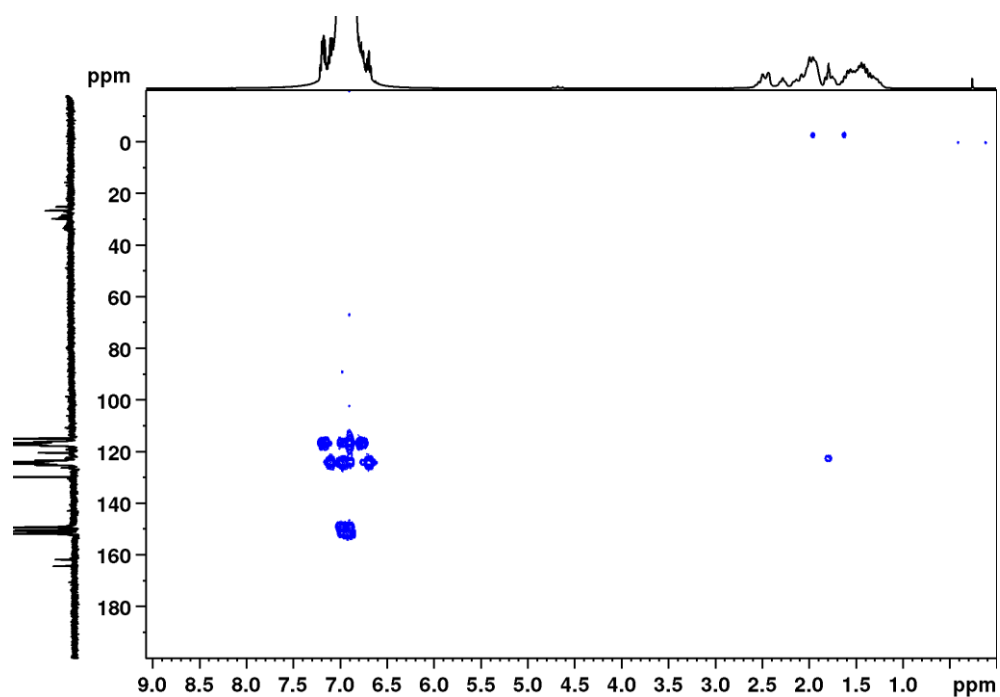


Figure S 108: ^1H , ^{13}C -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60 °C for 4 days.

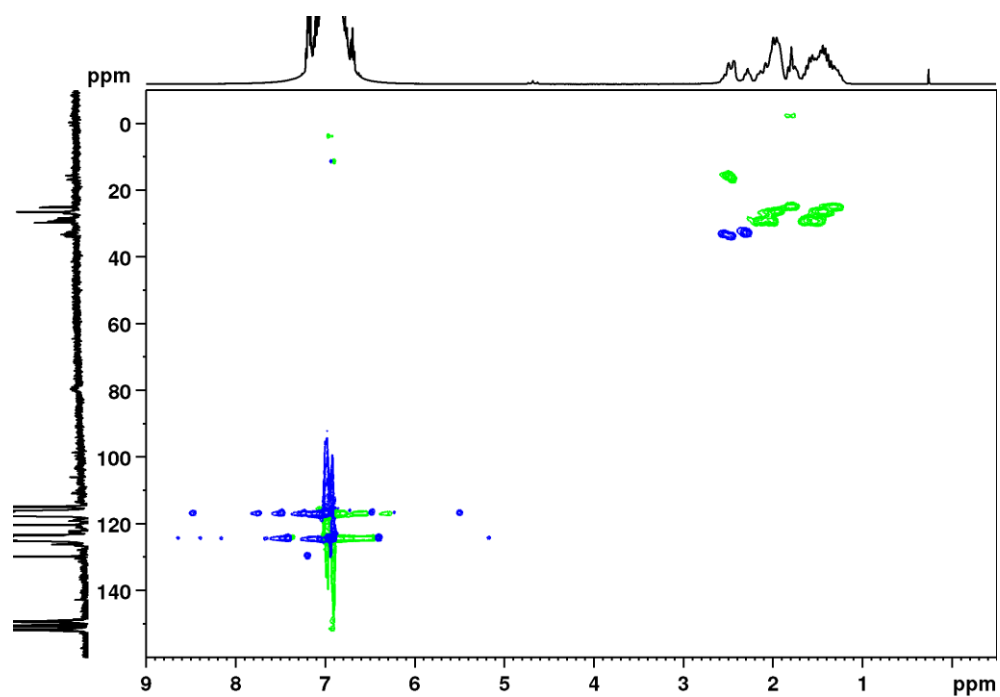


Figure S 109: Edited ^1H , ^{13}C -HSQC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60 °C for 4 days.

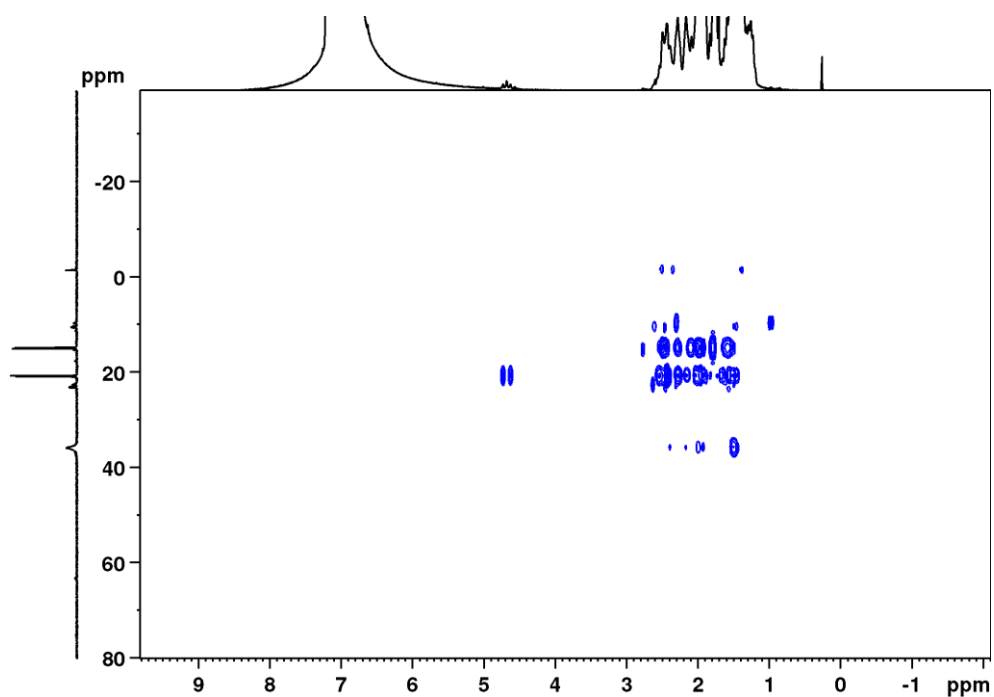


Figure S 110: $^1\text{H},^{31}\text{P}$ -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60°C for 4 days.

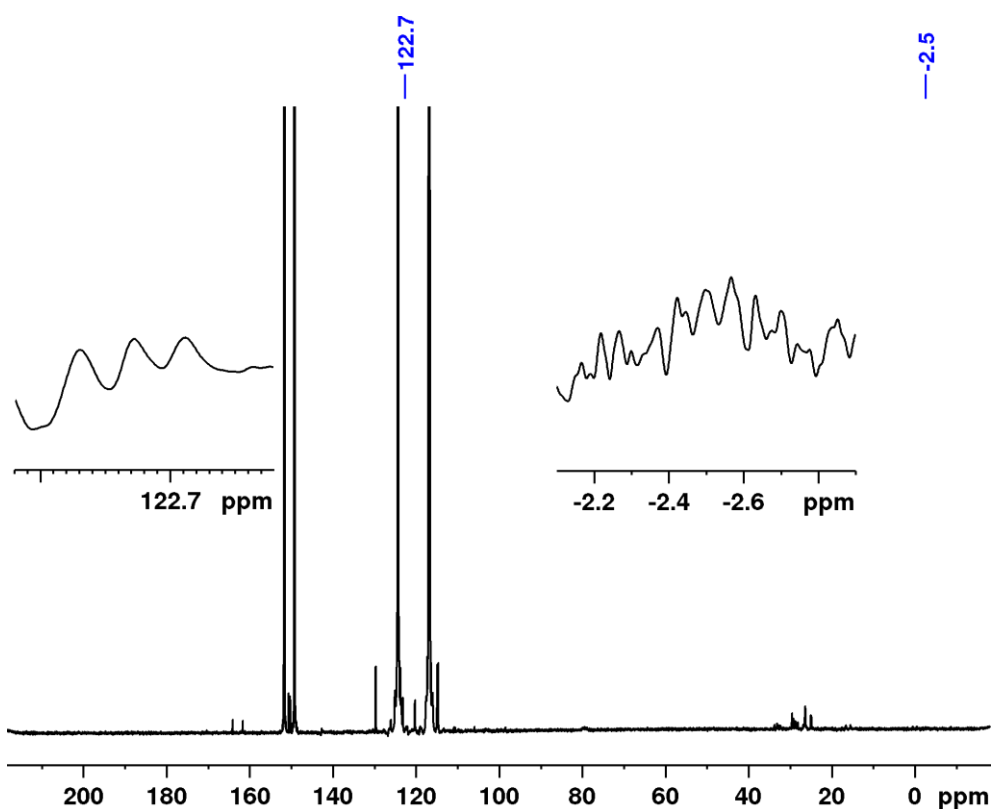


Figure S 111: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60°C for 4 days.

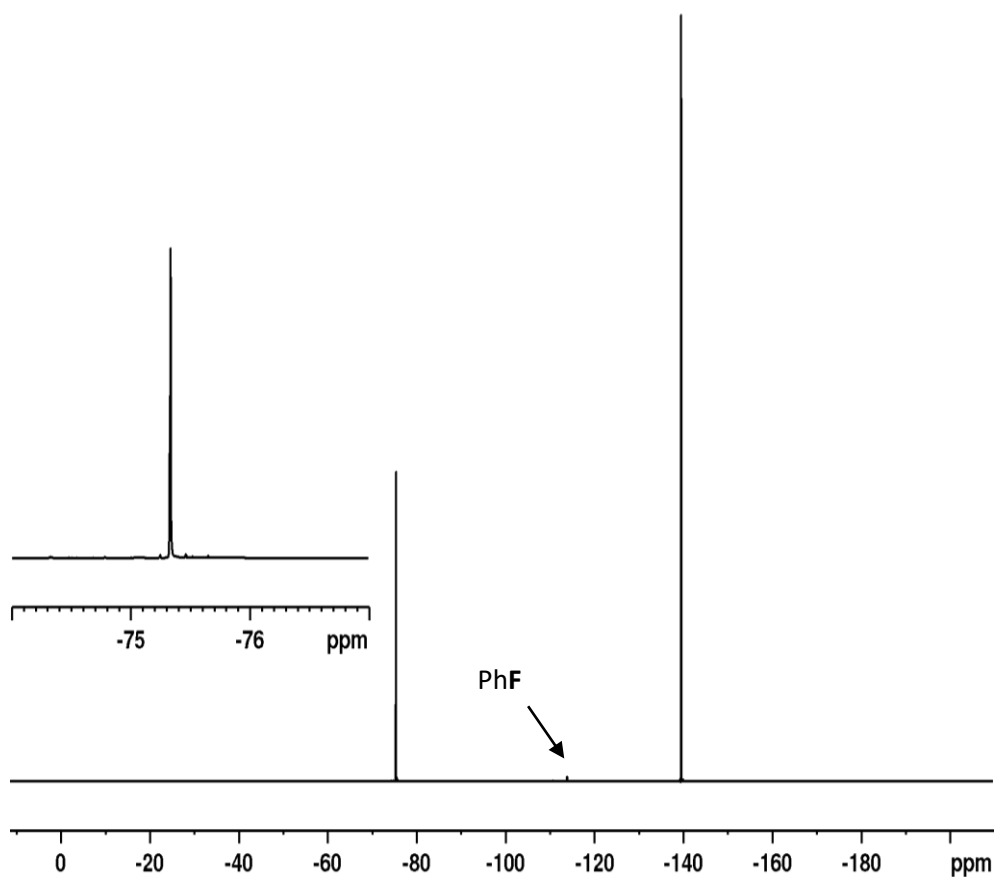


Figure S 112: ^{19}F NMR spectrum (376.54 MHz, oDFB , 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60°C for 4 days.

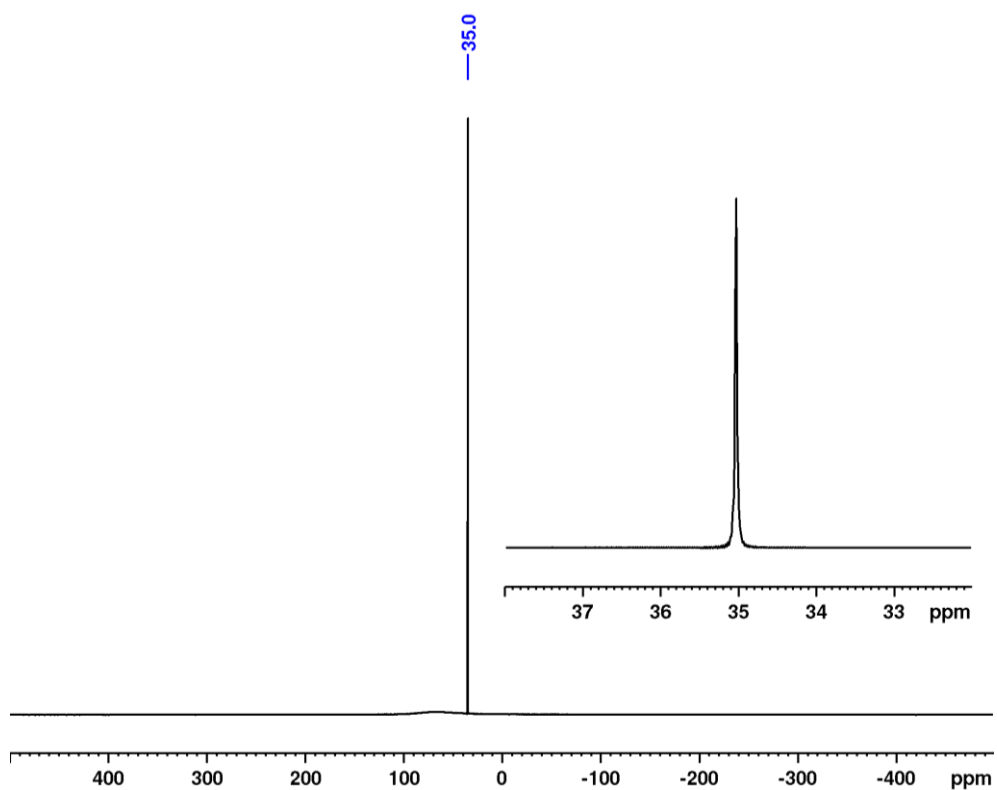


Figure S 113: ^{27}Al NMR spectrum (78.22 MHz, oDFB , 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and NC-CH_3 in oDFB after heating the reaction mixture to 60°C for 4 days.

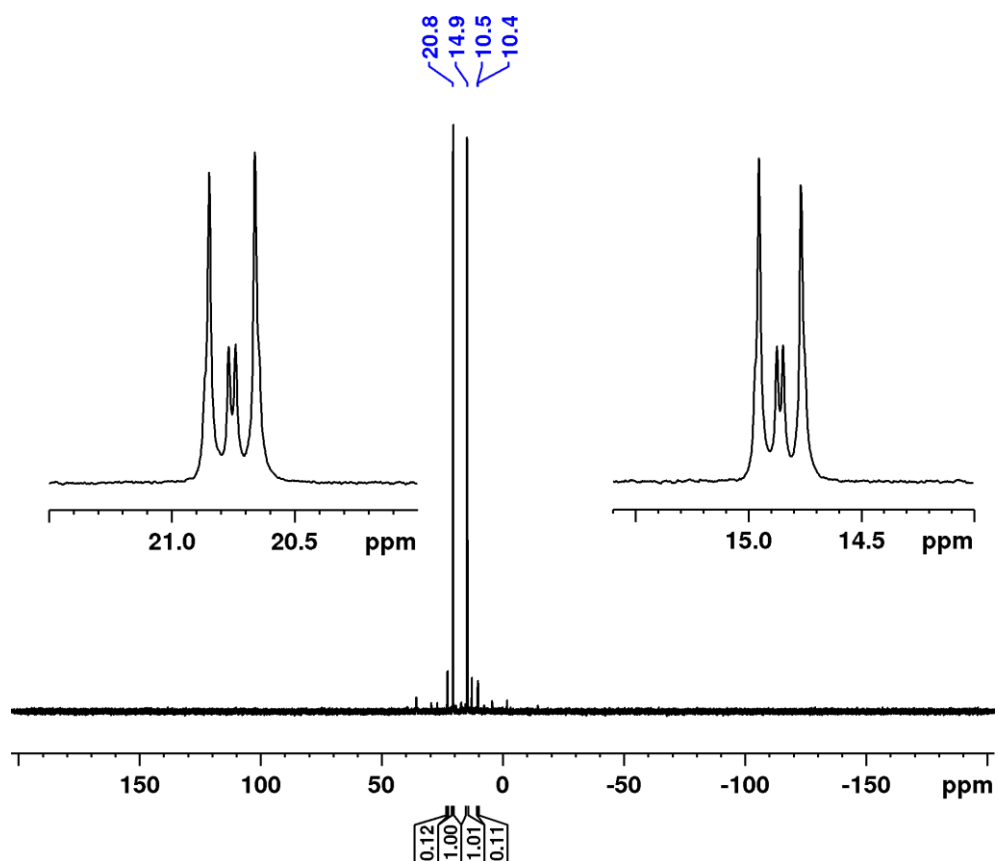


Figure S 114: $^{31}P\{^1H\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{Ga(dcpe)\}_2][pf]_2$ and NC-CH₃ in oDFB after heating the reaction mixture to 60 °C for 4 days.

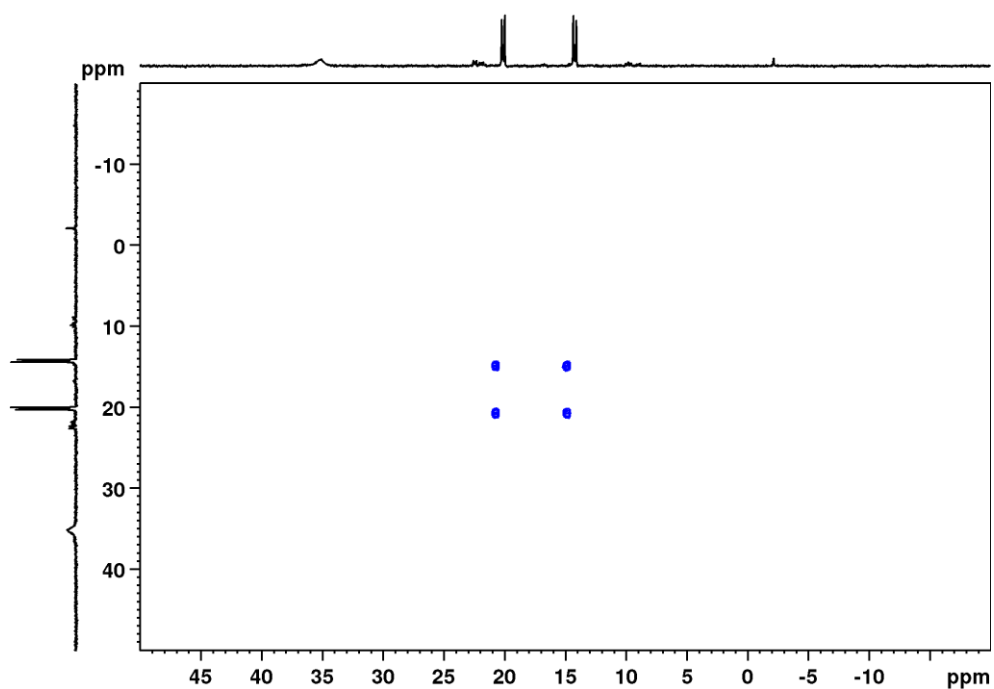
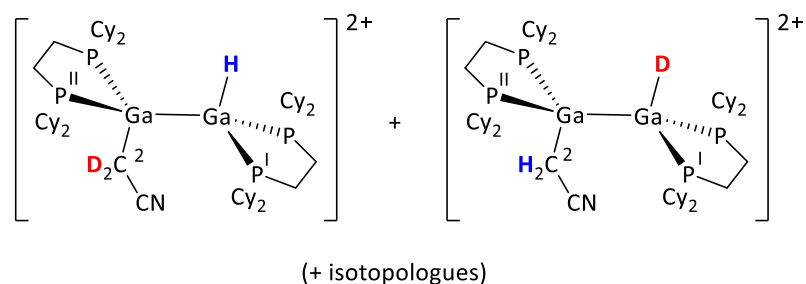


Figure S 115: $^{31}P\{^1H\}$ -COSY NMR spectrum (121.52 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{Ga(dcpe)\}_2][pf]_2$ and NC-CH₃ in oDFB after heating the reaction mixture to 60 °C for 4 days.

4.9 Reaction between H₃C–CN and D₃C–CN with [{Ga(dcpe)}₂][pf]₂



When heating a 2:1:1 mixture of **[1]**[pf]₂, acetonitrile and acetonitrile-*d*₃, the ¹H and ³¹P{¹H} spectra are similar to the spectra obtained for a 1:1 mixture of **[1]**[pf]₂ and acetonitrile (see section 4.4). Note that the more complex signals in the ³¹P{¹H} spectrum are caused by ³¹P/²D couplings and the isotope shifts on the ³¹P NMR resonances (**Figure S 114** vs. **Figure S 117**). Obviously, the H/D exchange in the Ga–CH₂CN and/or the Ga–H group leads only to small isotope shifts of the resonances of the phosphorous atoms and has no significant effect on the chemical shift of the GaH proton.

However, a noticeable isotope shift is observed for the carbon atom C²H₂/D₂ (ca. –3.1 vs –2.5 ppm). The fact that the GaH proton, which resonates at 4.67 ppm, shows a cross peak in the ¹H,¹³C NMR spectrum to *both* ¹³C signals (*cf.* **Figure S 118** and **Figure S 119**) clearly indicates that two different products were formed: one product with GaH/GaCH₂ and the other product with GaH/GaCD₂ moieties.

Strictly speaking, the analogous isotopologues with GaD/GaCH₂ and with GaD/GaCD₂ moieties are not detected with this NMR experiment. However, since our results prove that the X and CX₂CN parts of one CX₃CN substrate molecule (X = H or D) are not transferred to the same digallene molecule, it is reasonable to assume that these isotopologues were also formed.

It is important to note that, when heating a 1:1 mixture of [H{Ga(dcpe)}₂(CH₂CN)][pf]₂ and [D{Ga(dcpe)}₂(CD₂CN)][pf]₂ to 60 °C for 4 days, no formation of [H{Ga(dcpe)}₂(CD₂CN)][pf]₂ was observed. Thus, for the reaction of H₃C–CN and D₃C–CN with [{Ga(dcpe)}₂][pf]₂, scrambling of Ga–H and Ga–D can be ruled out.

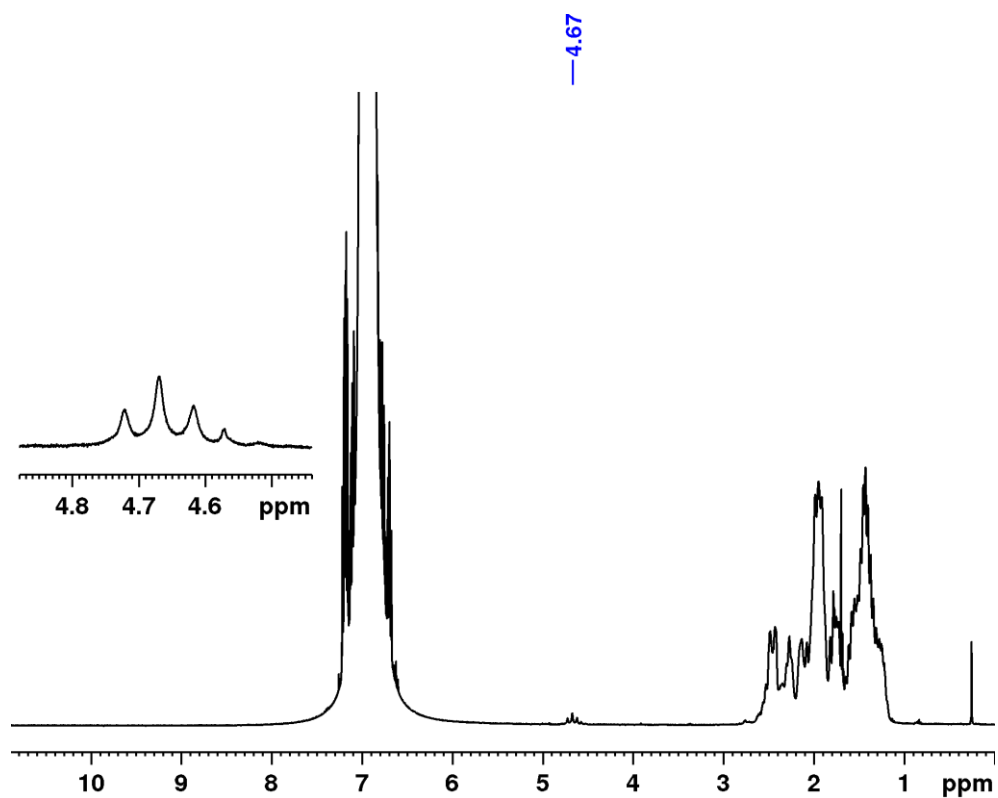


Figure S 116: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$, $\text{H}_3\text{C-CN}$ and $\text{D}_3\text{C-CN}$ (2 : 1 : 1) in oDFB after heating the reaction mixture to 60 °C for 2 days.

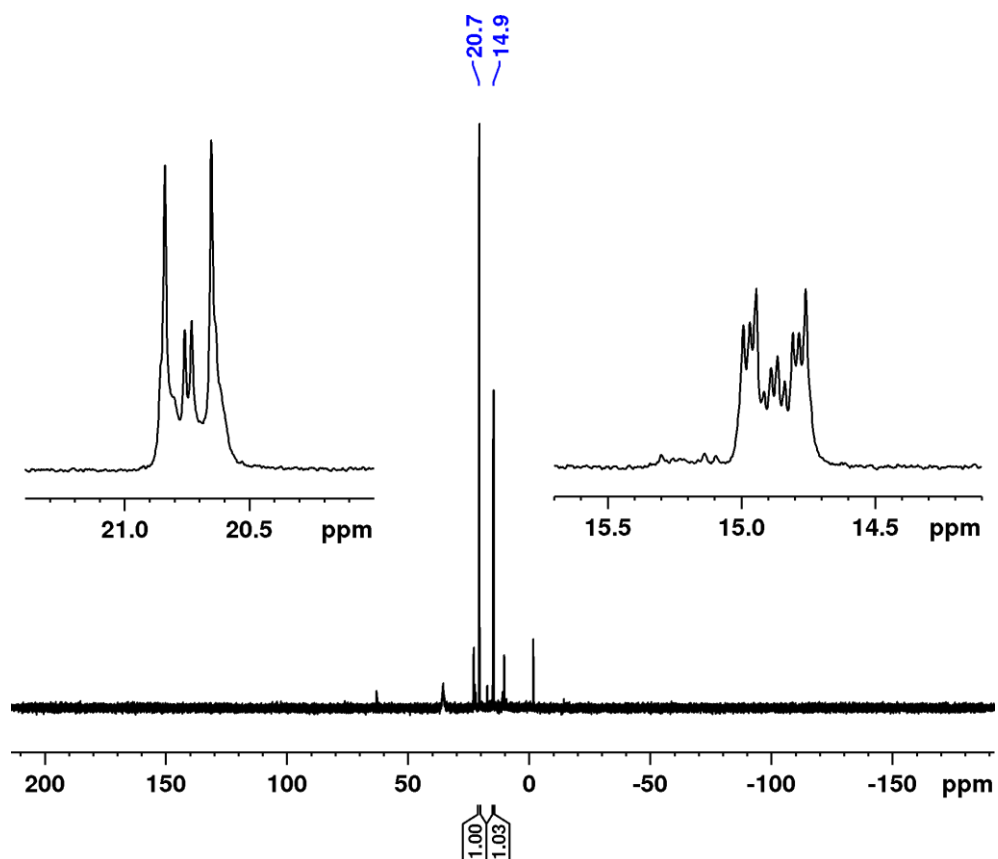


Figure S 117: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$, $\text{H}_3\text{C-CN}$ and $\text{D}_3\text{C-CN}$ (2 : 1 : 1) in oDFB after heating the reaction mixture to 60 °C for 2 days.

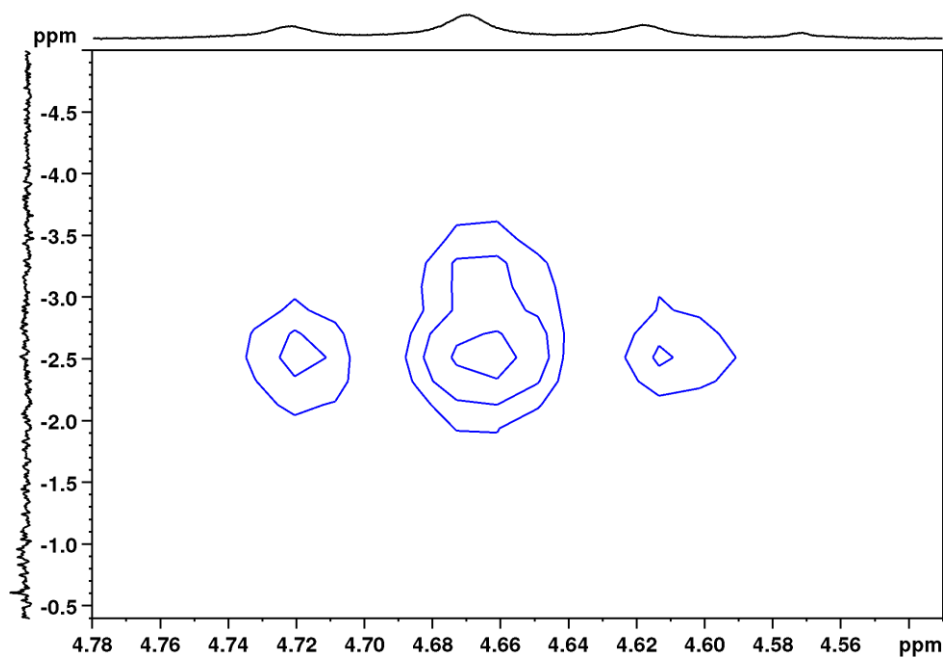


Figure S 118: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$, $\text{H}_3\text{C-CN}$ and $\text{D}_3\text{C-CN}$ (2 : 1 : 1) in oDFB after heating the reaction mixture to 60 °C for 2 days.

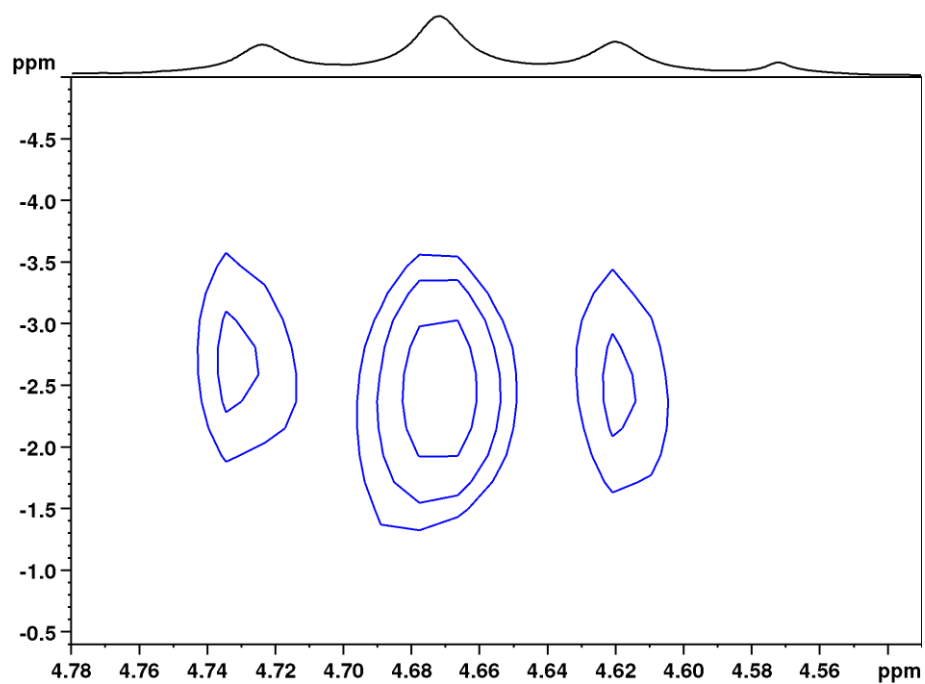
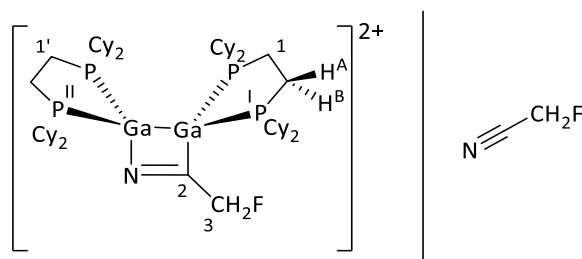


Figure S 119: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 16$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{H}_3\text{C-CN}$ in oDFB after heating the reaction mixture to 60 °C for 4 days (for comparison with Figure S 118).

4.10 [$\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_2\text{F})][\text{pf}]_2$ and its Decomposition in Solution

4.10.1 [$\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_2\text{F})][\text{pf}]_2$



^1H NMR [400.17 MHz, *o*DFOB, calibrated at $\text{oC}_6\text{F}_2\text{H}_4 = 6.96$ ppm, 298 K]: $\delta = 4.90$ (d, 2 H, C^3H_2 , $^2J_{\text{H,F}} = 51.0$ Hz), 4.76 (d, CH_2F in starting material, $^2J_{\text{H,F}} = 46.0$ Hz), 2.72–2.40 (m, 8 H, $\text{C}^1\text{H}^{\text{A}}$, $\text{C}^1\text{H}^{\text{B}}$, $\text{C}^{1'}\text{H}^{\text{A}}$ and $\text{C}^{1'}\text{H}^{\text{B}}$), 2.50–2.29 (m, 8 H, CH protons of the Cy groups), 2.10–1.26 (m, 80 H, CH_2 protons of the Cy groups) ppm.

^{13}C NMR [100.62 MHz, *o*DFOB, 298 K]: $\delta = 215.2$ (1 C, C^2), 87.4 (1 C, C^3), 113.6 and 66.0 (NC and CH_2F in starting material), 33.8–31.6 (8 C, CH carbon atoms of the Cy groups), 30.1–25.0 (40 C, CH_2 carbon atoms of the Cy groups), 15.8 and 15.5 (4 C, C^1 and $\text{C}^{1'}$) ppm.

^{19}F NMR [376.54 MHz, *o*DFOB, 298 K]: $\delta = -75.3$ (s, 36 F, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$), -113.9 (m, PhF), -139.5 (m, $\text{oC}_6\text{F}_2\text{H}_4$), -202.3 (t, 1 F, C^3F , $^2J_{\text{F,H}} = 51.0$ Hz), -232.5 (CH_2F in starting material) ppm.

^{27}Al NMR [104.27 MHz, *o*DFOB, 298 K]: $\delta = 35.0$ (s, 1 Al, $[\text{Al}(\text{OC}(\text{CF}_3)_3)_4]^-$) ppm.

^{31}P NMR [161.99 MHz, *o*DFOB, 298 K]: $\delta = 13.9$ (m, 2 P, P^{I}), 12.9 (m, 2 P, P^{II}) ppm.

^{71}Ga NMR [122.04 MHz, *o*DFOB, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

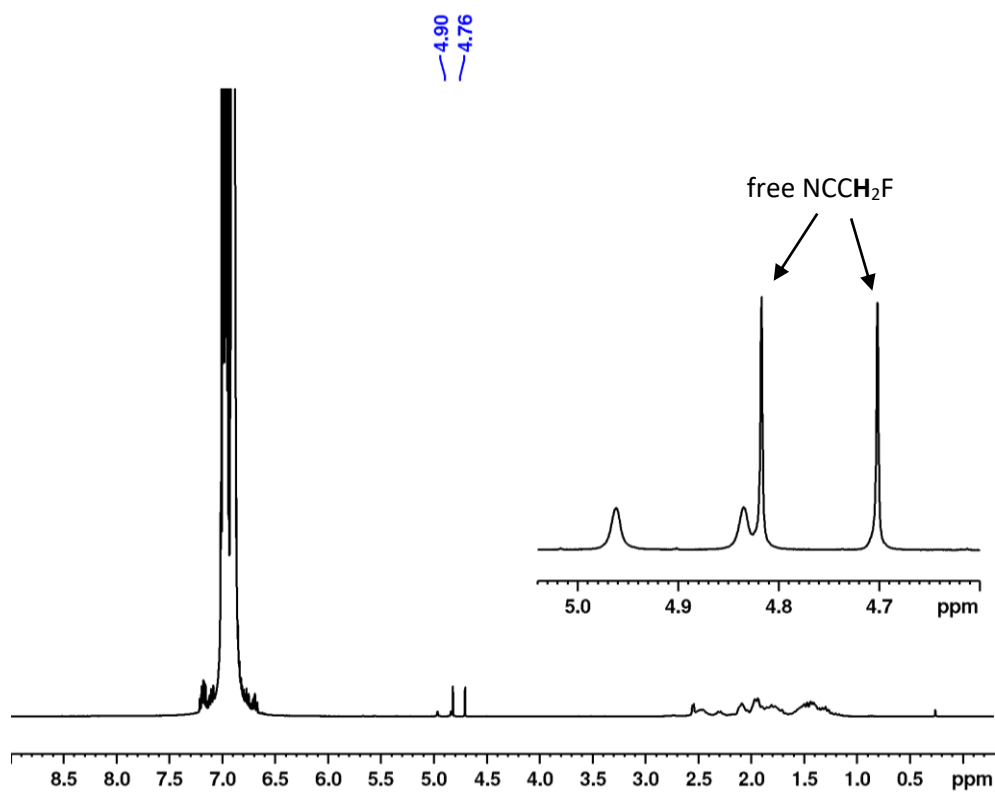


Figure S 120: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$, 3 h after mixing the components in oDFB.

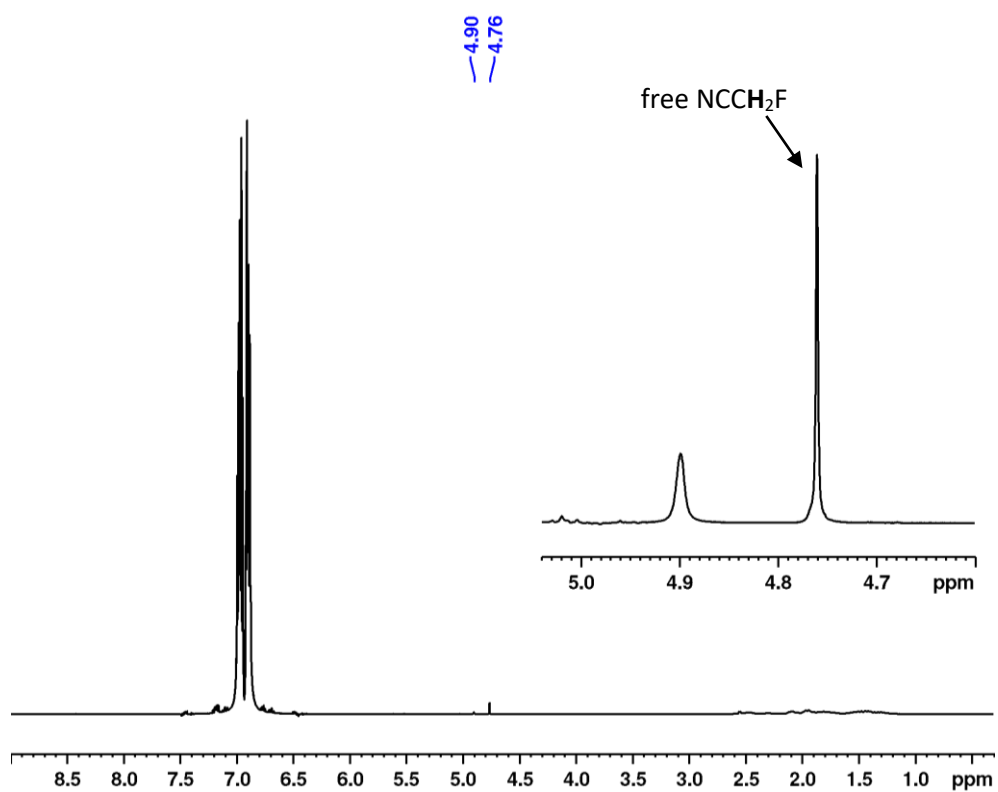


Figure S 121: $^1\text{H}\{^{19}\text{F}\}$ NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$, 3 h after mixing the components in oDFB.

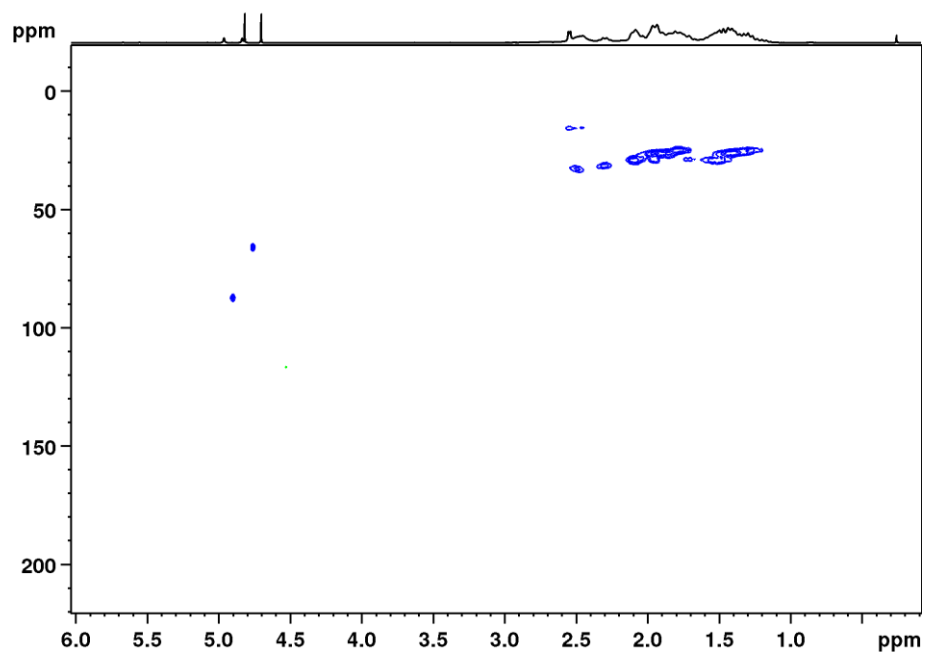


Figure S 122: $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$, 3 d after mixing the components in *o*DFB.

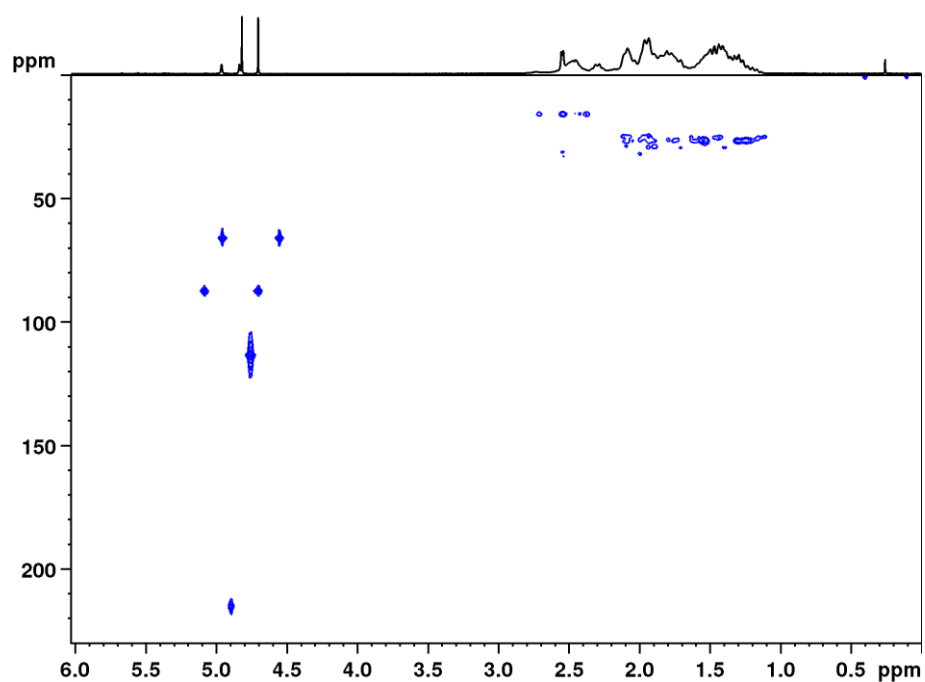


Figure S 123: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$, 3 d after mixing the components in *o*DFB.

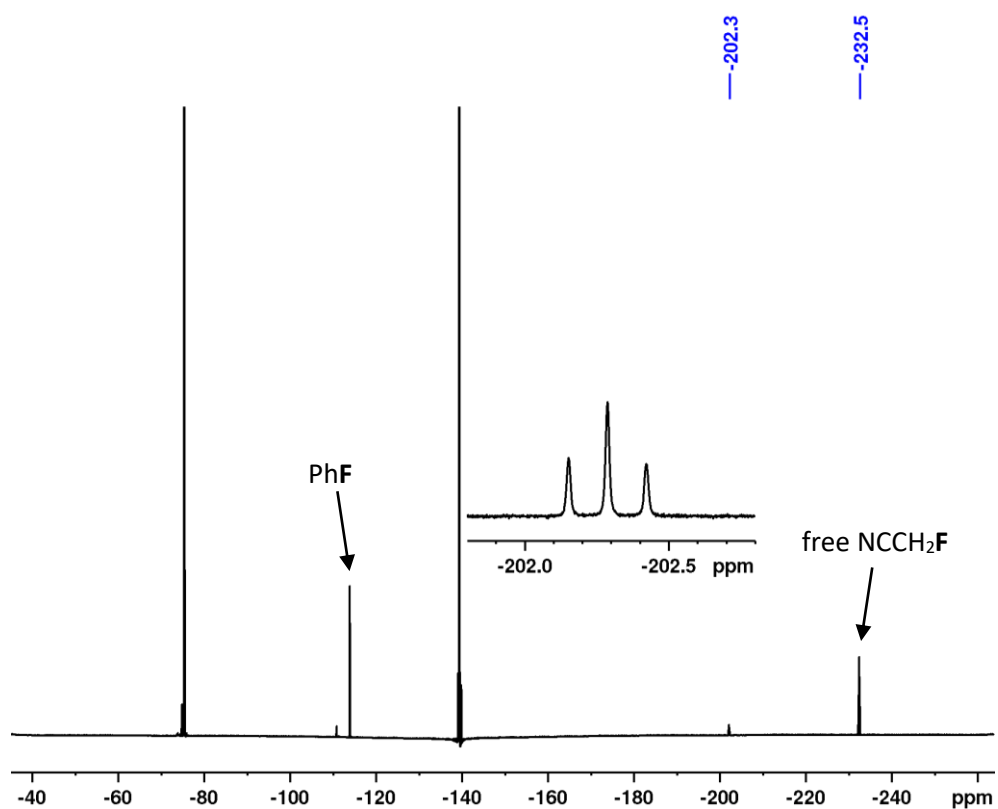


Figure S 124: ^{19}F NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$, 3 h after mixing the components in oDFB.

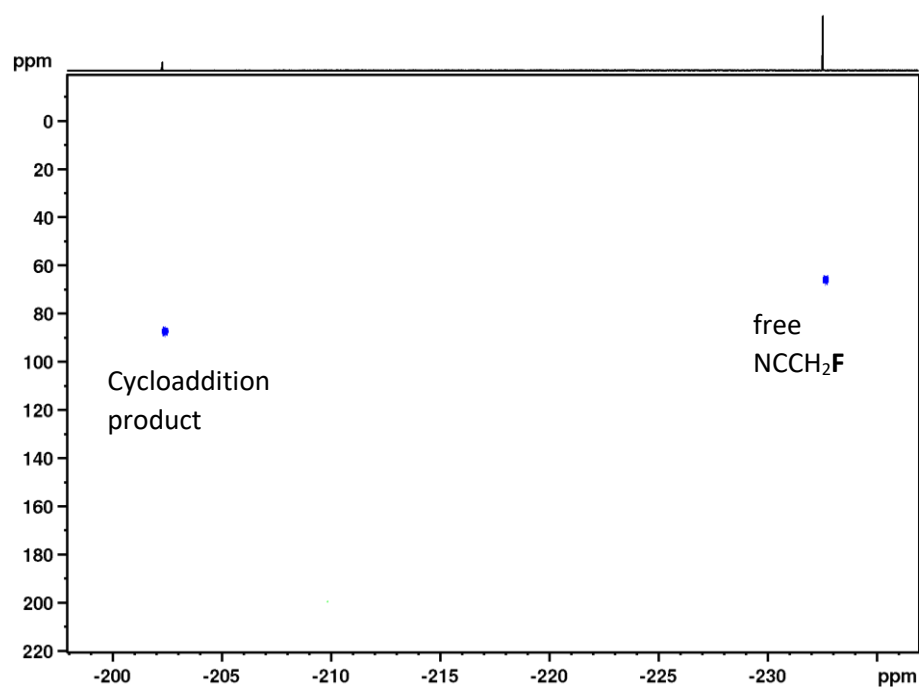


Figure S 125: ^{19}F , $^{13}\text{C}\{^1\text{H}\}$ -HSQC NMR spectrum (376.54 MHz, oDFB, 298 K, optimized for $J = 250$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$ in oDFB.

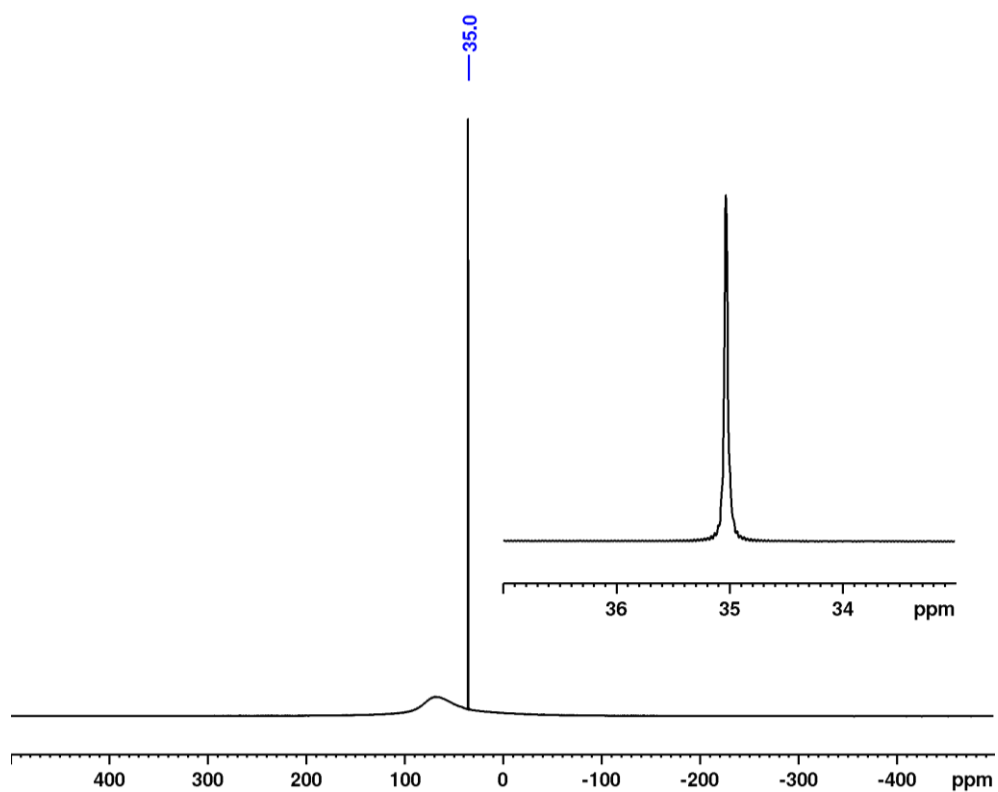


Figure S 126: ^{27}Al NMR spectrum (104.27 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$, 3 h after mixing the components in oDFB.

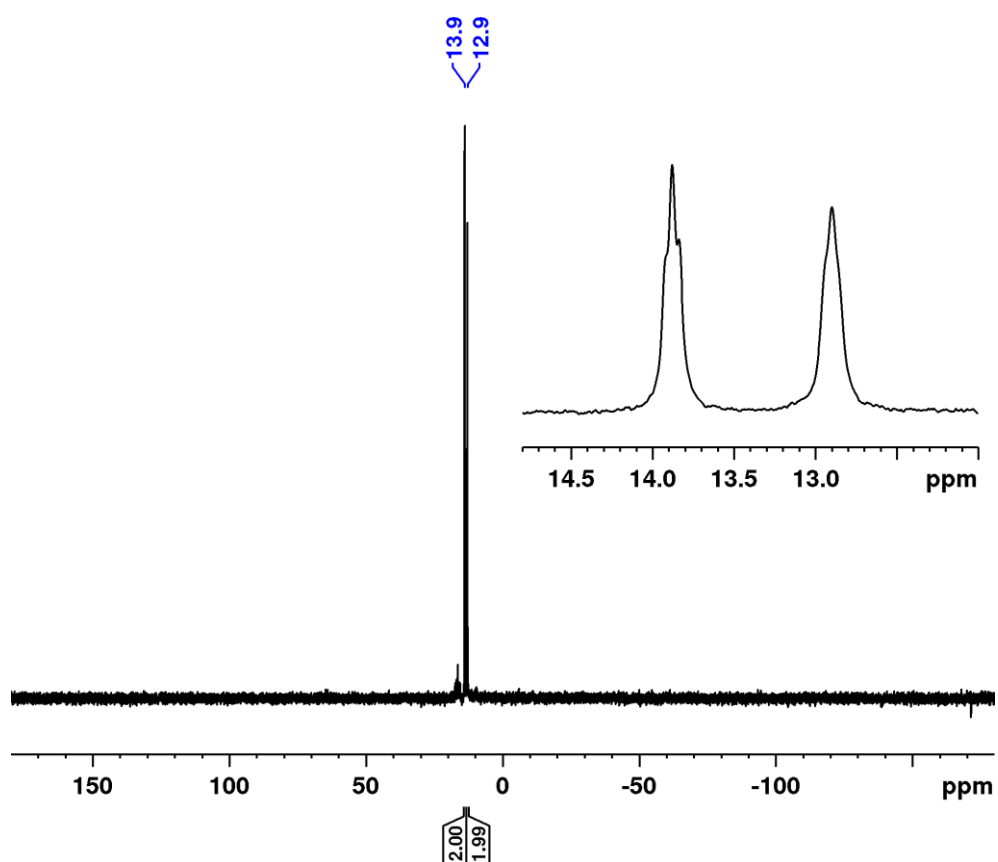


Figure S 127: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (81.01 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$, 3 h after mixing the components in oDFB.

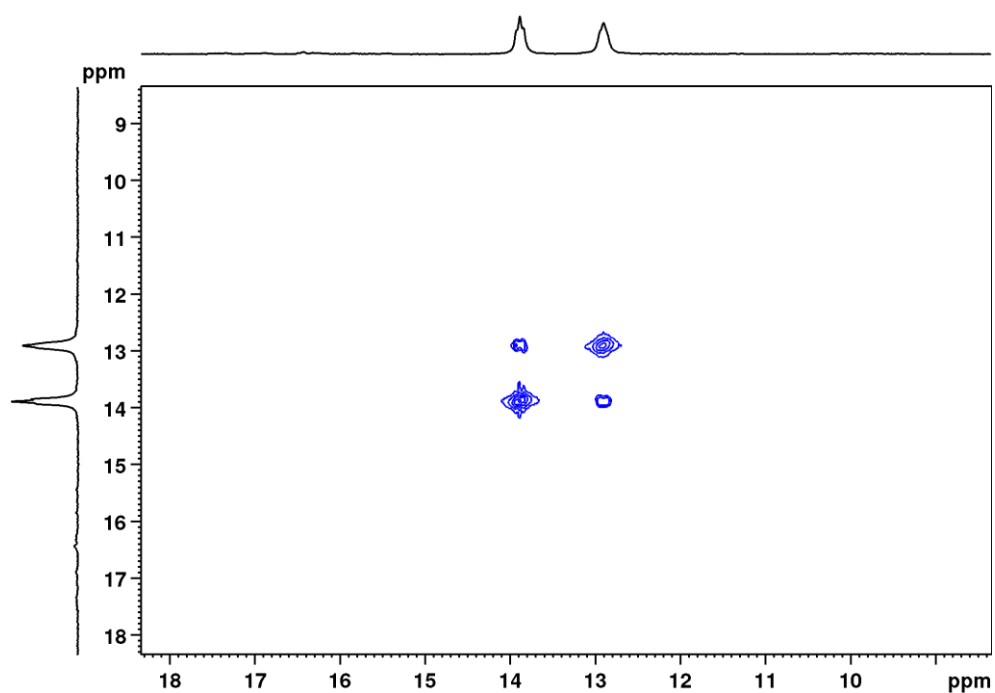


Figure S 128: $^{31}\text{P}\{^1\text{H}\}$ -COSY NMR spectrum (81.01 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$, 4 h after mixing the components in oDFB.

4.10.2 Decomposition of $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_2\text{F})]^{2+}$ in Solution

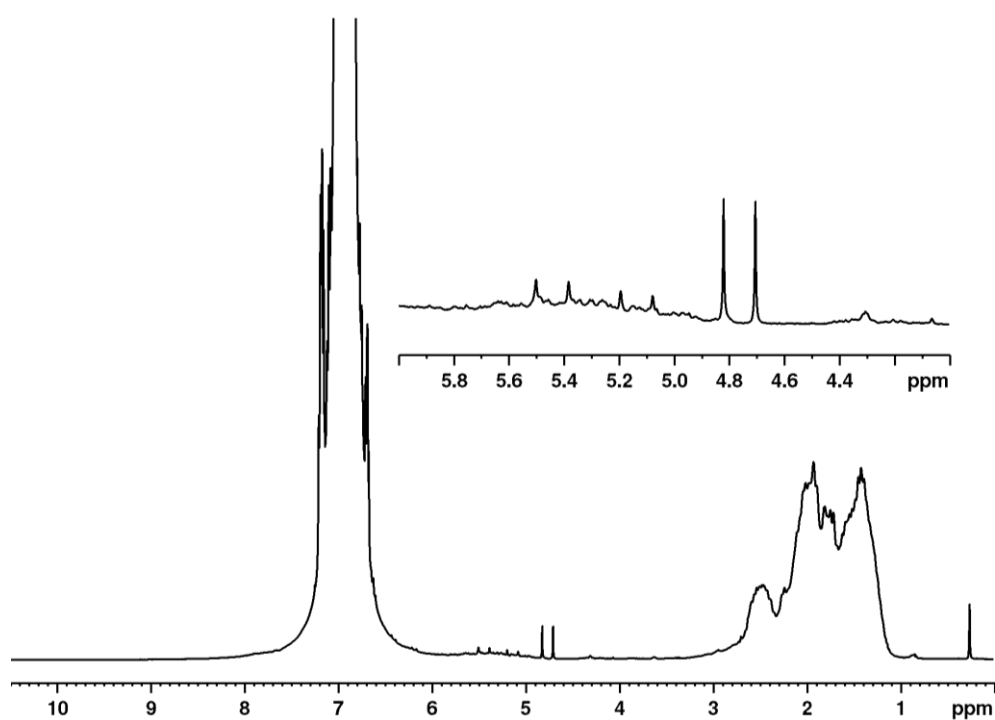


Figure S 129: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$ in oDFB, 4 weeks after mixing the components.

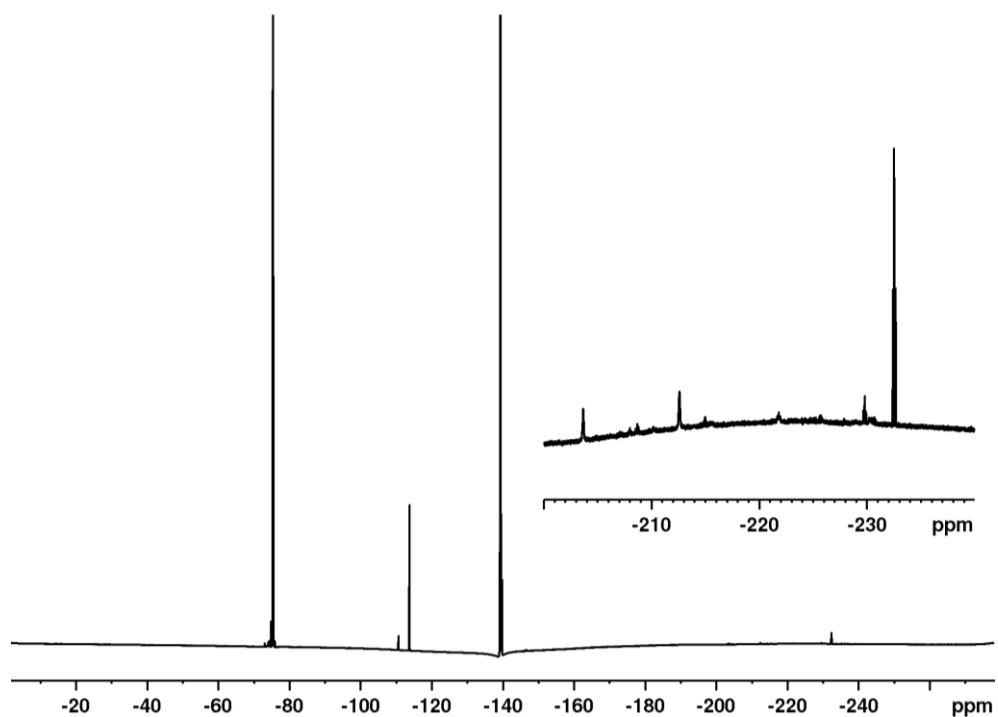


Figure S 130: ^{19}F NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB, 4 weeks after mixing the components.

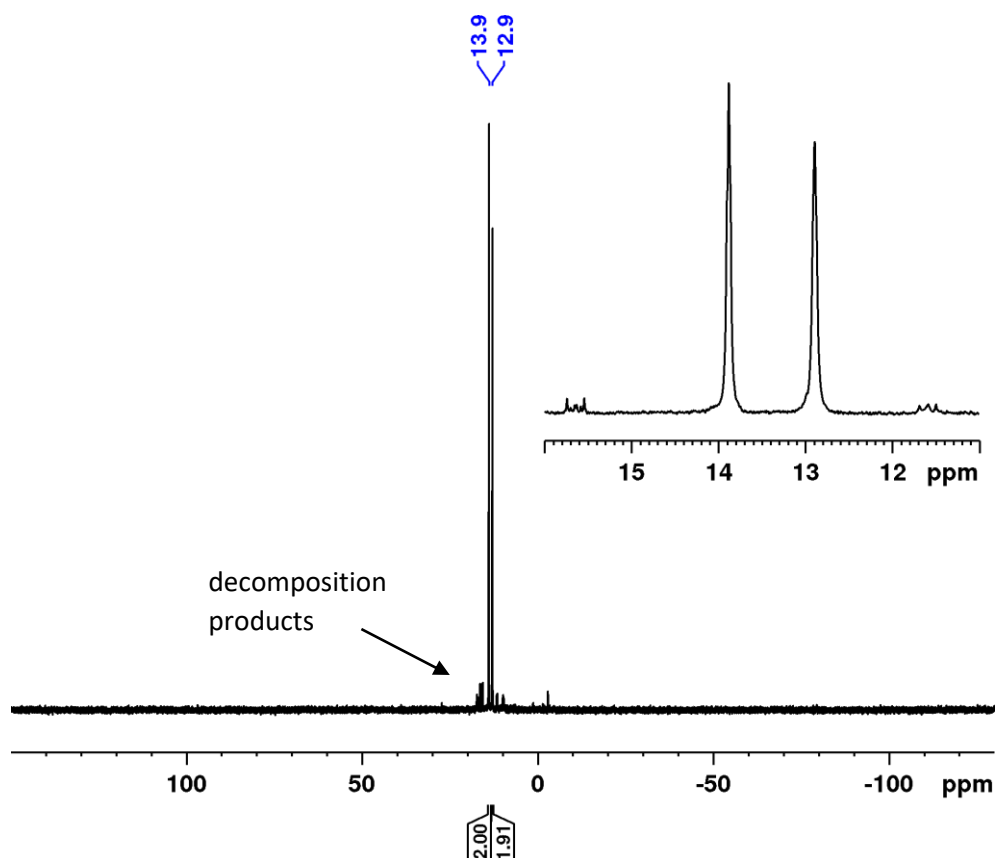


Figure S 131: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB, 2 days after mixing the components.

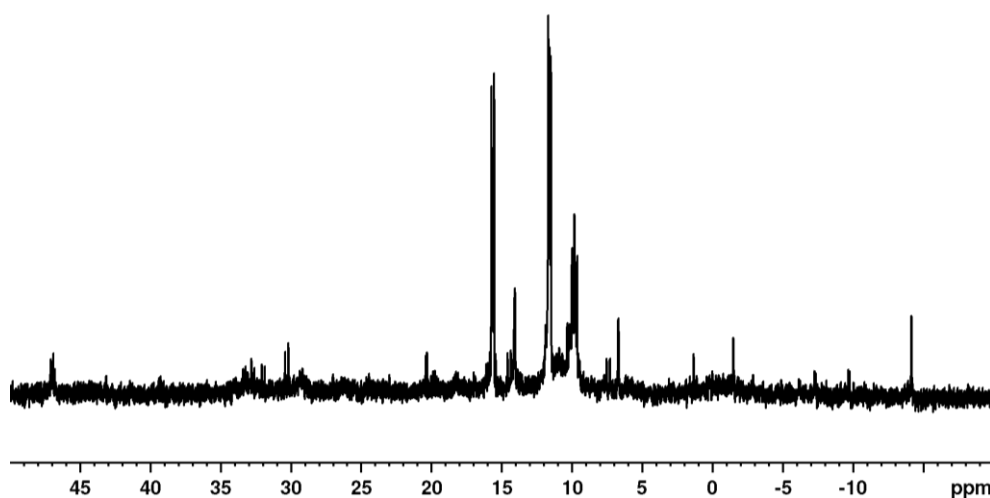


Figure S 132: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC}-\text{CH}_2\text{F}$ in oDFB, 4 weeks after mixing the components.

4.11 $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCPH})][\text{pf}]_2$ and its Decomposition in Solution

4.11.1 $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCPH})][\text{pf}]_2$

Due to the rapid decomposition of the putative $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCPH})]^{2+}$, which is already noticeable after 2 h (see broad signal at 32.8 ppm in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum in **Figure S 134**) and thus faster than for the cycloaddition product with NCCH_2F , the NMR signals could not be assigned in detail. However, the ^1H , ^{31}P crosspeak in the aromatic region and the AA'BB' spin system in the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum strongly indicate the formation of the cycloaddition product.

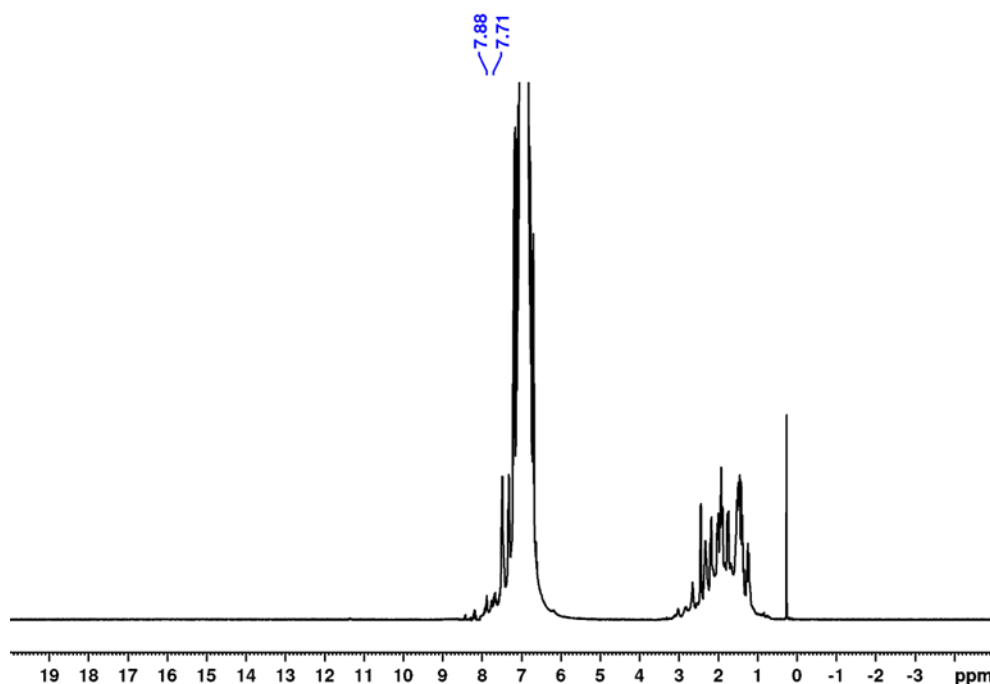


Figure S 133: ^1H NMR spectrum [400.17 MHz, 2FB, 298 K] of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and benzonitrile, 2 h after mixing the components in oDFB.

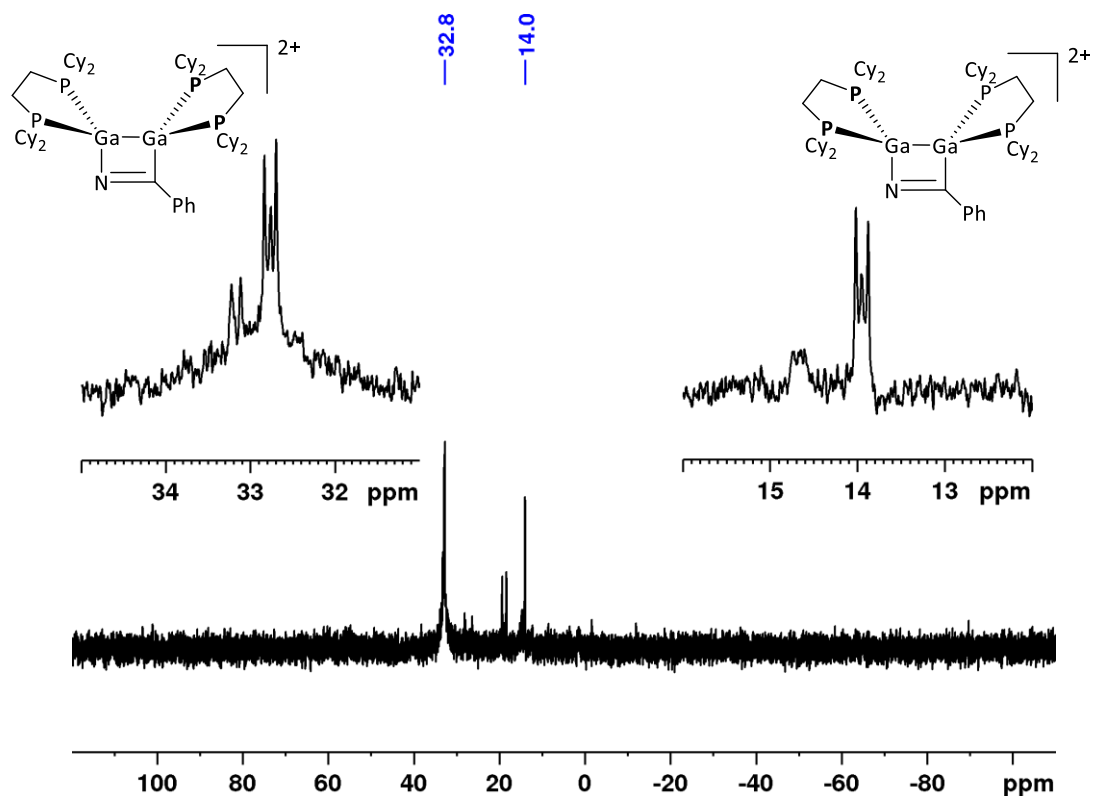


Figure S 134: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum [81.01 MHz, 2FB, 298 K] of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and benzonitrile, 2 h after mixing the components in oDFB.

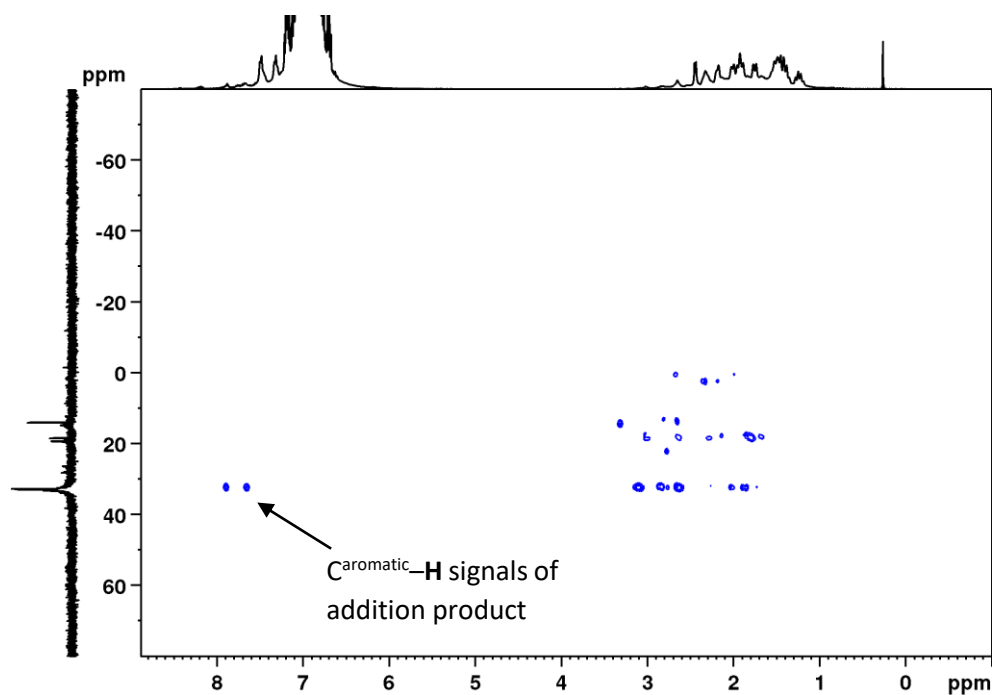


Figure S 135: $^1\text{H},^{31}\text{P}$ -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 15$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and benzonitrile, 5 h after mixing the components in oDFB.

4.11.2 Decomposition of $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCPH})]^{2+}$ in Solution

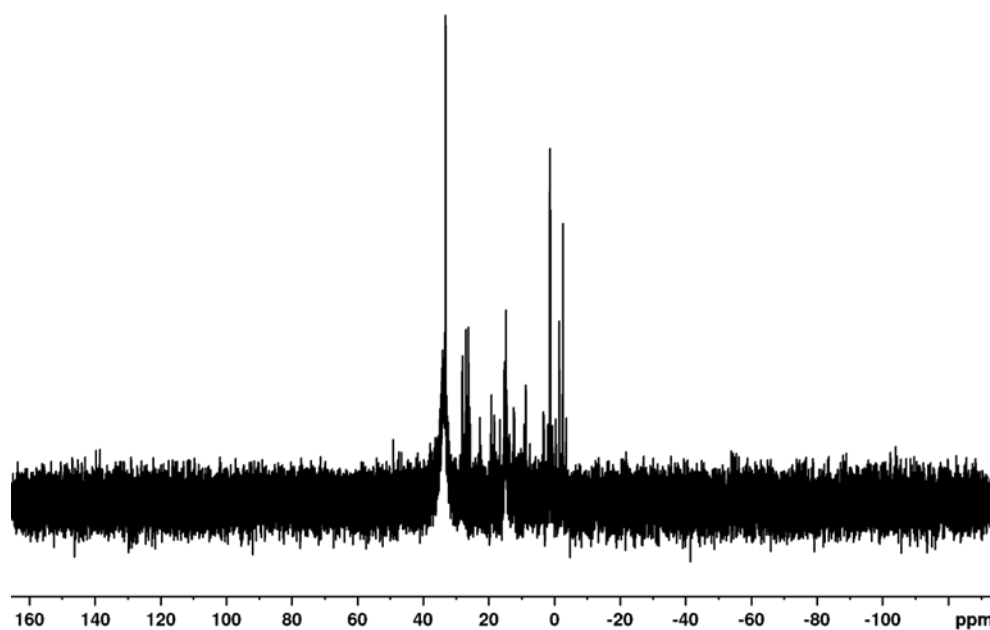
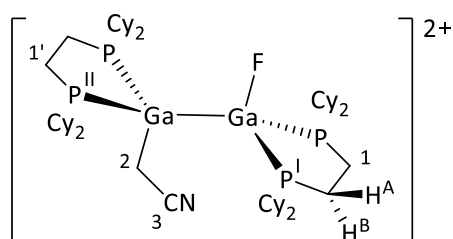


Figure S 136: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum [161.99 MHz, *o*DFB, 298 K] of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and benzonitrile, 1 d after mixing the components in *o*DFB.

4.12 $[F\{Ga(dcpe)\}_2(CH_2CN)][pf]_2$



^1H NMR [300.18 MHz, *o*DFB, calibrated at $oC_6F_2H_4$ = 6.96 ppm, 298 K]: δ = 2.65–2.34 (m, 8 H, C^1H^A , C^1H^B , $C^{1'}H^A$ and $C^{1'}H^B$), 2.48–2.33 (m, 8 H, CH protons of the Cy groups), 2.0–1.25 (m, 80 H, CH_2 protons of the Cy groups), 1.83 (t, 2 H, C^2H_2 , $^3J_{H,P}$ = 3.8 Hz) ppm.

^{13}C NMR [75.48 MHz, *o*DFB, 298 K]: δ = 123.1 (1 C, C^3N), 33.3–32.3 (8 C, CH carbon atoms of the Cy groups), 29.4–25.2 (40 C, CH_2 carbon atoms of the Cy groups), 15.5 and 14.8 (4 C, C^1 and $C^{1'}$), –3.5 (1 C, C^2) ppm.

^{19}F NMR [282.45 MHz, *o*DFB, 298 K]: δ = –75.3 (s, 36 F, $[Al(OC(CF_3)_3)_4]^-$), –113.9 (m, PhF), –139.5 (m, $oC_6F_2H_4$), –203.7 (t, 1 F, F–Ga, $^2J_{F,P}$ = 27.3 Hz) ppm.

^{27}Al NMR [78.22 MHz, *o*DFB, 298 K]: δ = 35.0 (s, 1 Al, $[Al(OC(CF_3)_3)_4]^-$) ppm.

^{31}P NMR [121.52 MHz, *o*DFB, 298 K]: δ = 30.3 (unknown impurity), 15.6 (m, 2 P, P^{II}), 11.6 (unknown impurity), 9.8 (m, 2 P, P^I) ppm.

^{71}Ga NMR [91.54 MHz, *o*DFB, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

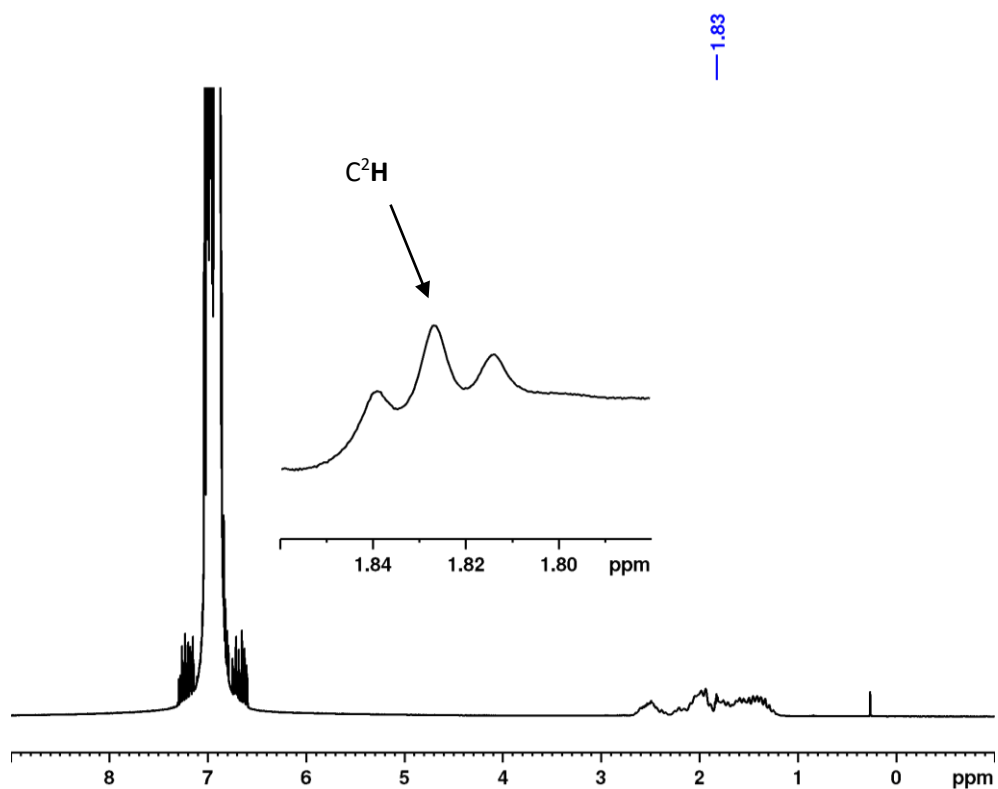


Figure S 137: ^1H NMR spectrum (300.18 MHz, oDFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\text{Ga}(\text{dcpe})]_2[\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB with *n*-pentane.

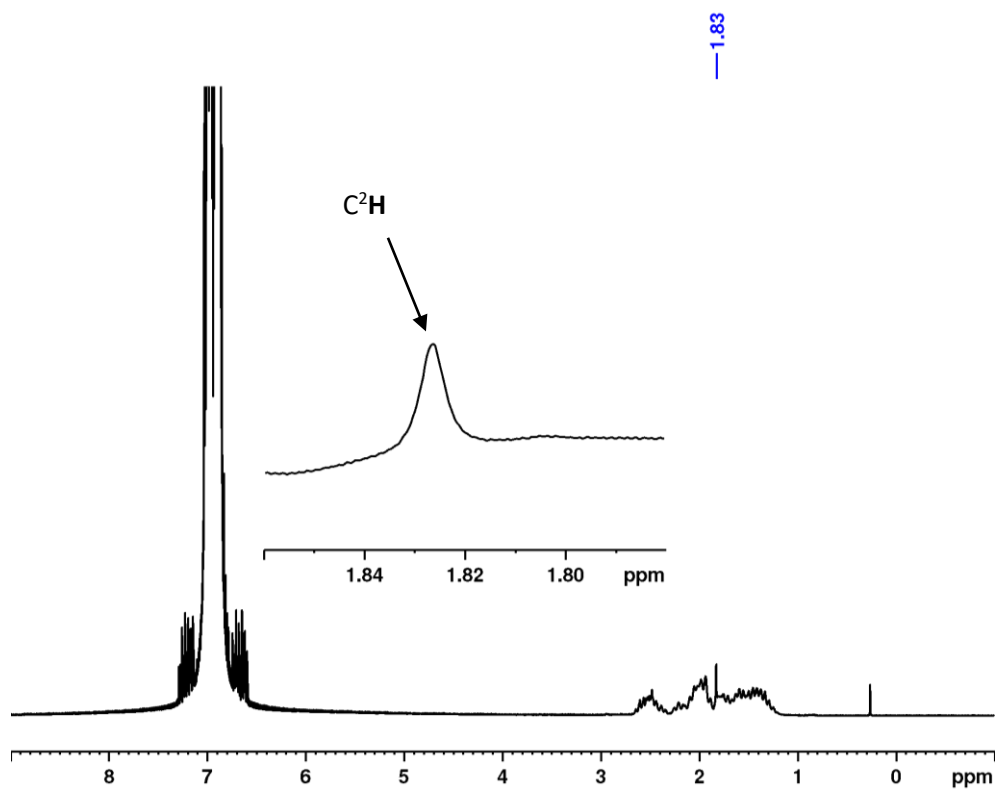


Figure S 138: $^1\text{H}\{^{31}\text{P}\}$ NMR spectrum (300.18 MHz, oDFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\text{Ga}(\text{dcpe})]_2[\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB with *n*-pentane.

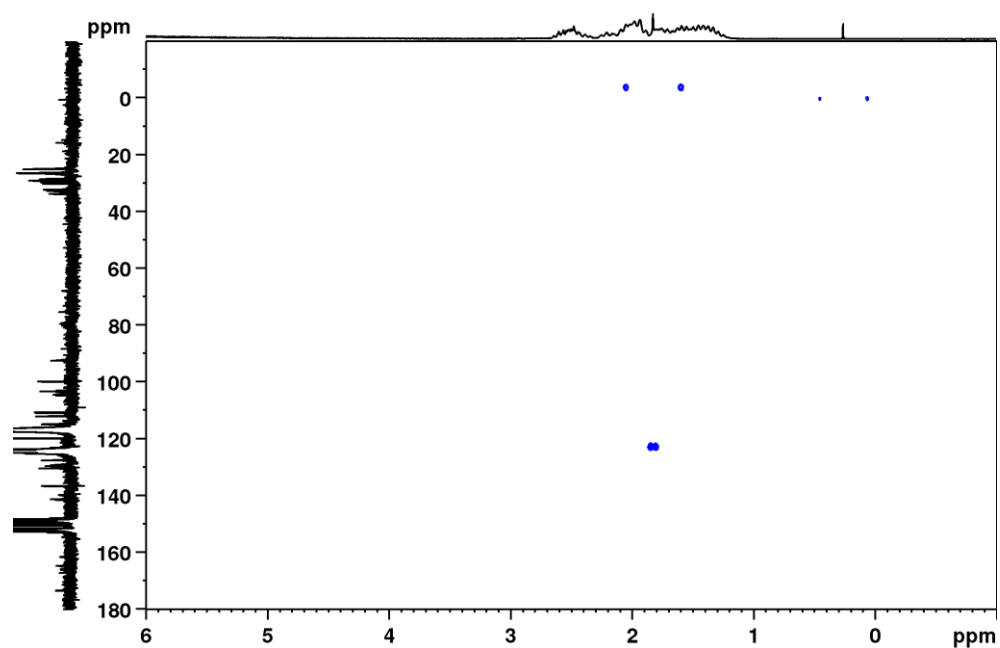


Figure S 139: ^1H , ^{13}C -HMBC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for $J = 8$ Hz) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

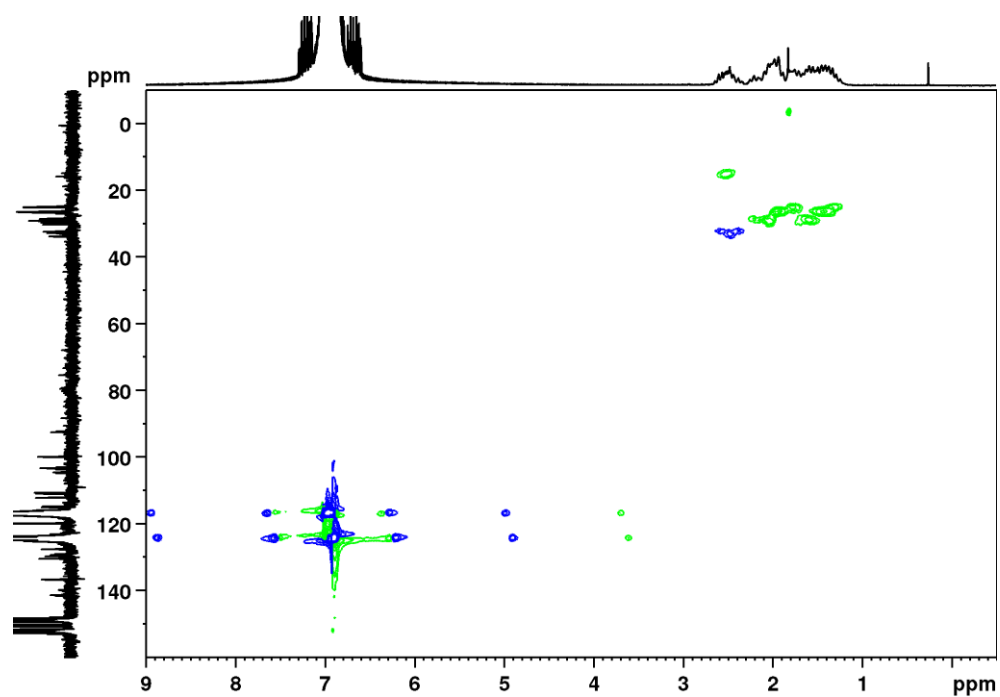


Figure S 140: Edited ^1H , ^{13}C -HSQC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for $J = 145$ Hz) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

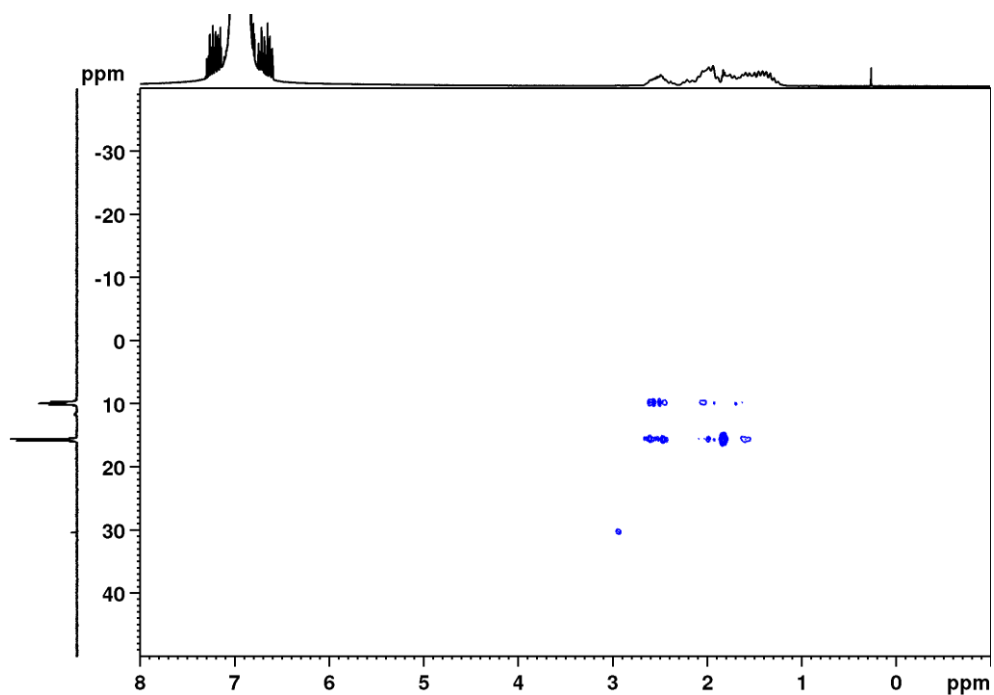


Figure S 141: ^1H , ^{31}P -HMBC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for $J = 15$ Hz) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

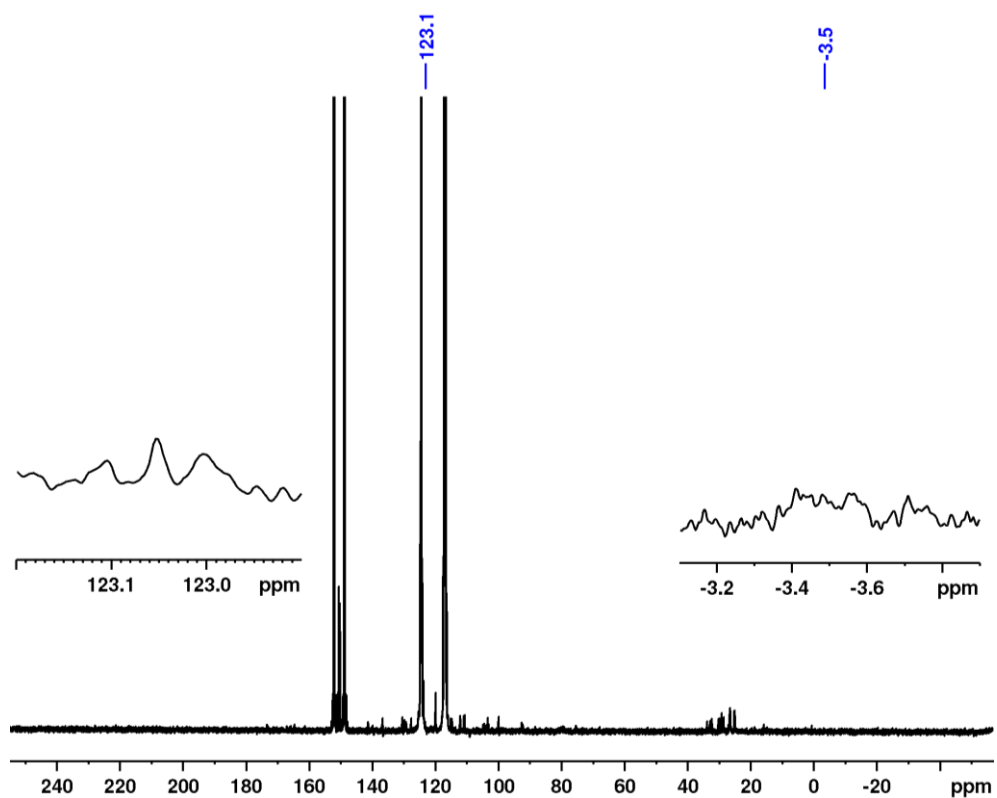


Figure S 142: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (75.48 MHz, *o*DFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

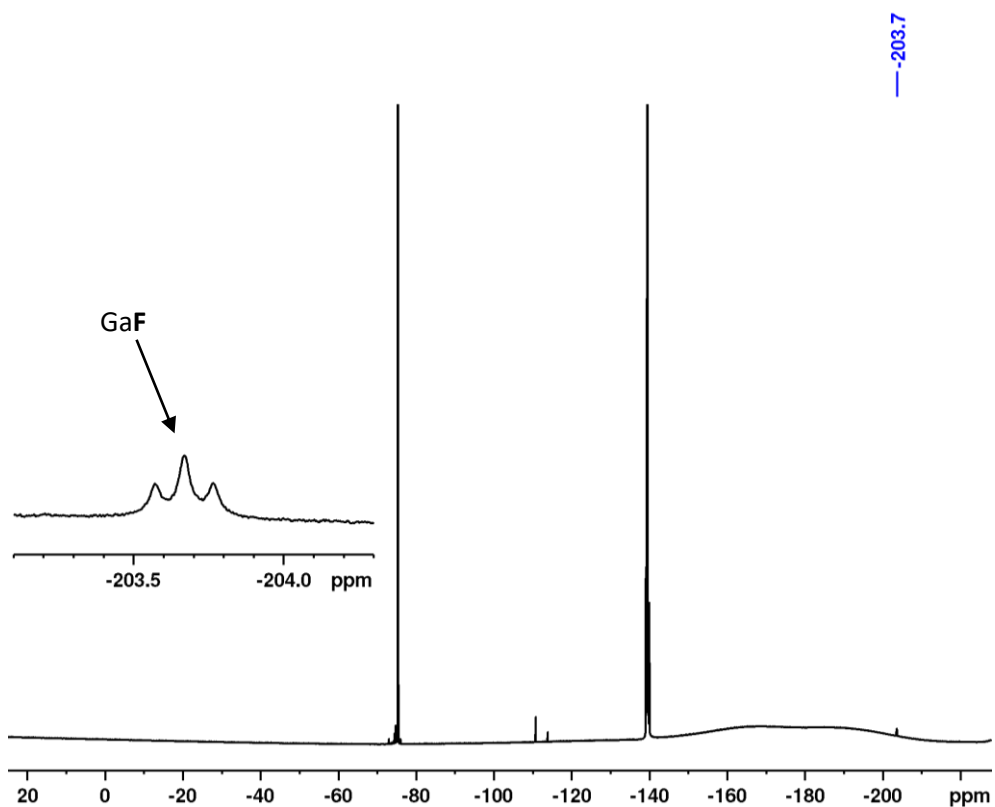


Figure S 143: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB with *n*-pentane.

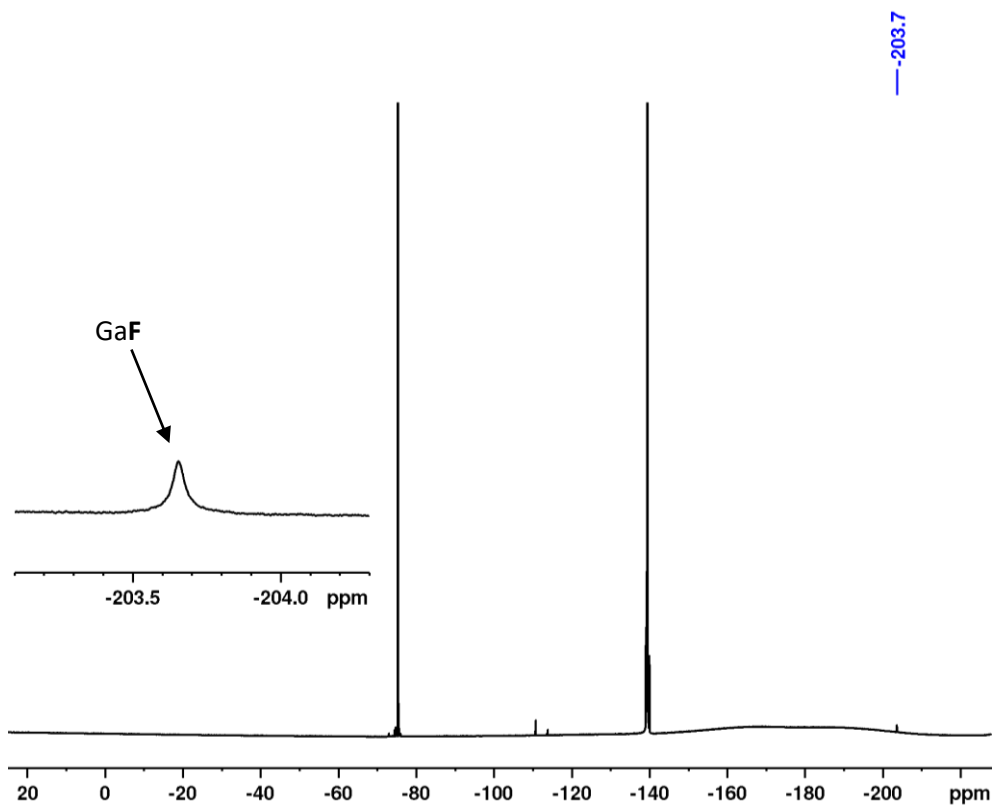


Figure S 144: $^{19}\text{F}\{^{31}\text{P}\}$ NMR spectrum (282.45 MHz, oDFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in oDFB with *n*-pentane.

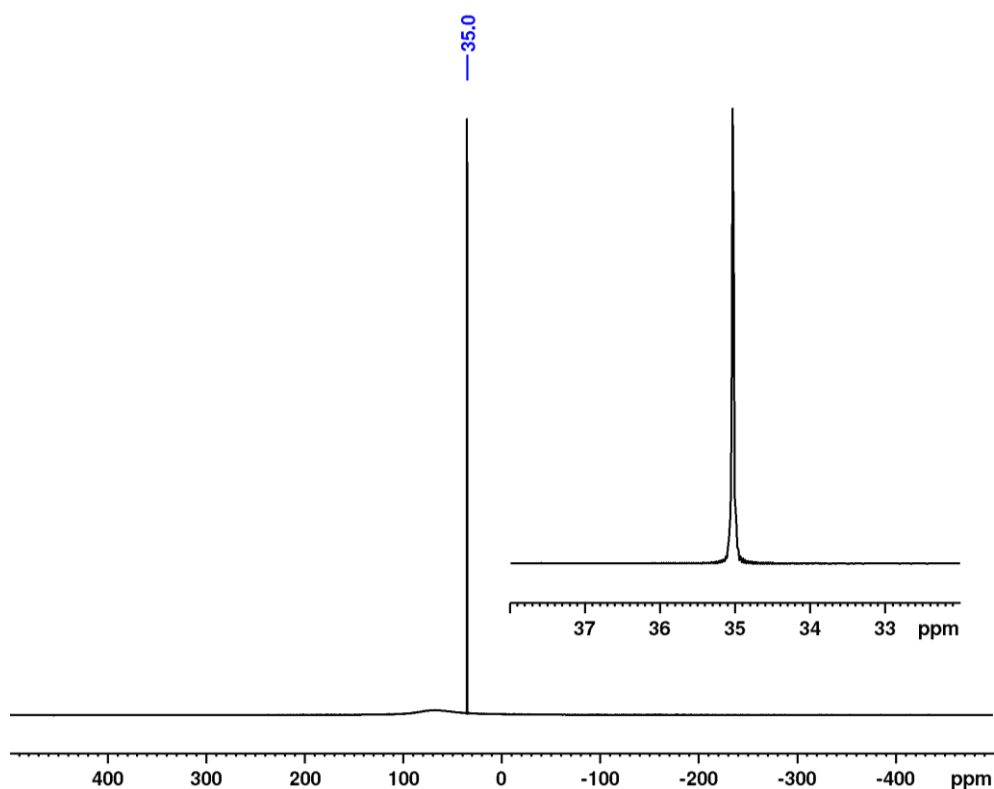


Figure S 145: ^{27}Al NMR spectrum (78.22 MHz, *o*DFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

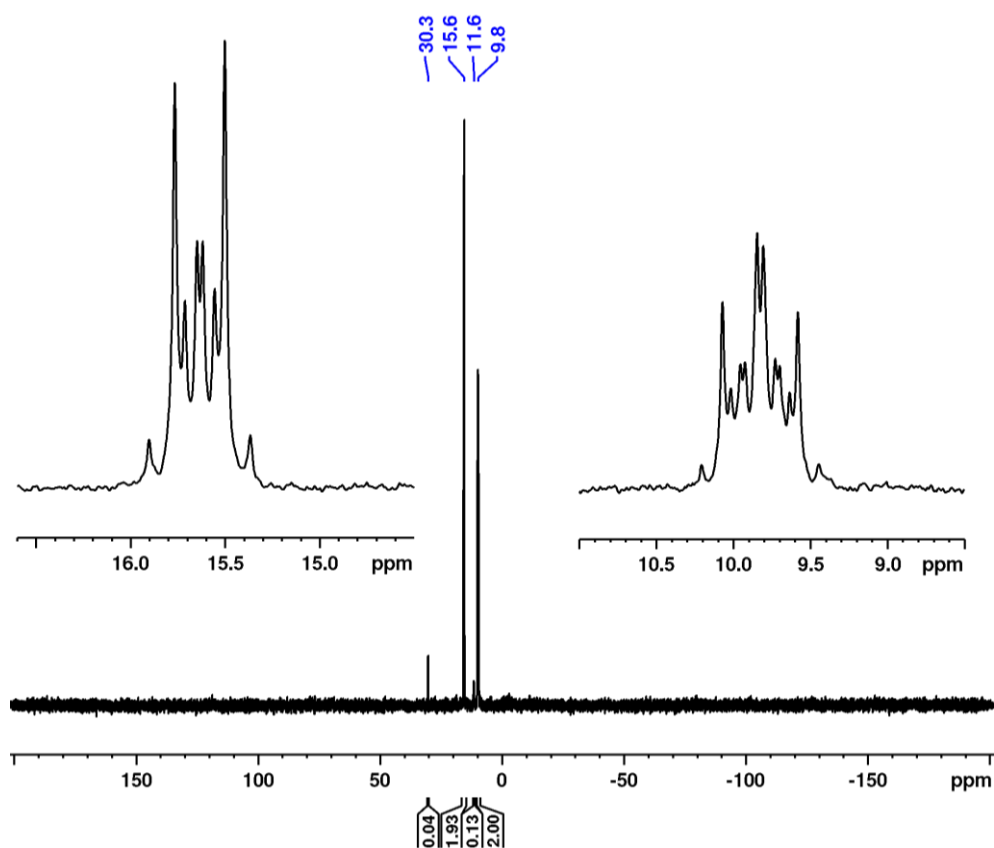


Figure S 146: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (78.22 MHz, *o*DFB, 298 K) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

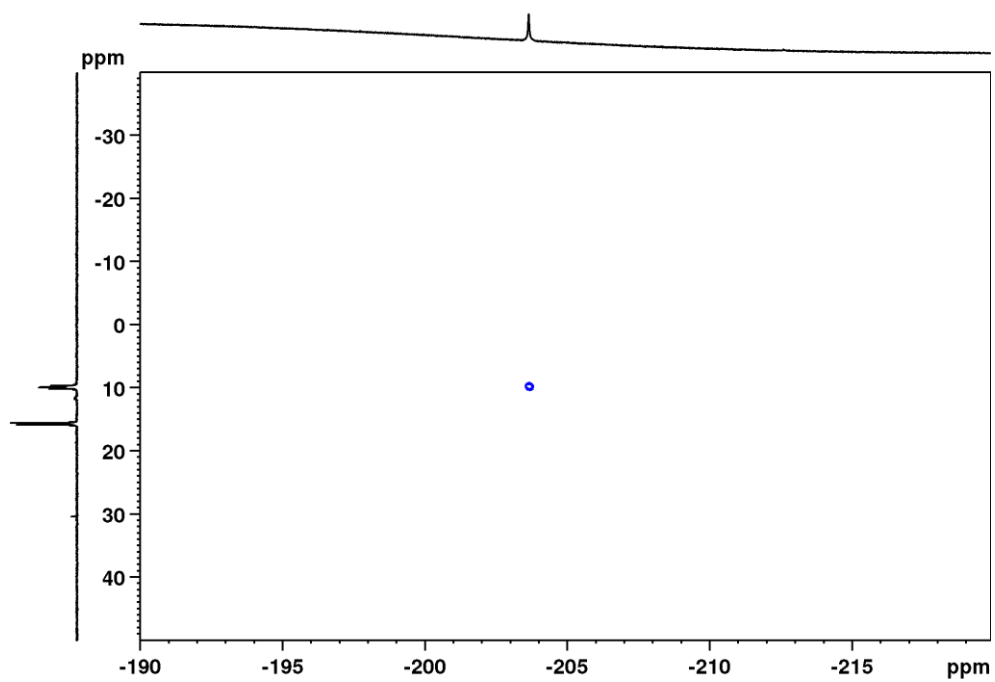
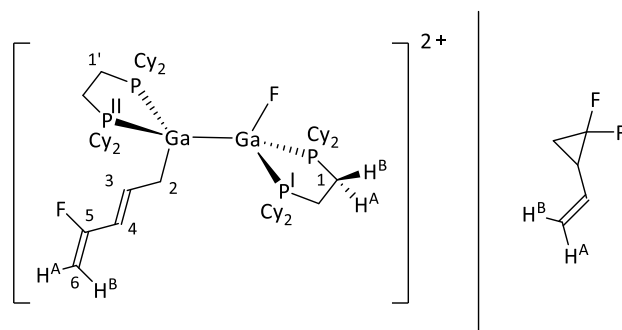


Figure S 147: ^{19}F , ^{31}P -HMBC NMR spectrum (282.45 MHz, *o*DFB, 298 K, optimized for $J = 30$ Hz) of the crystals obtained upon layering an equimolar solution of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and $\text{NC-CH}_2\text{F}$ in *o*DFB with *n*-pentane.

4.13 $[F\{Ga(dcpe)\}_2(C_5H_6F)][pf]_2$



^1H NMR [400.17 MHz, *o*D₂O, calibrated at *o*C₆F₂H₄ = 6.96 ppm, 298 K]: δ = 6.16 (m, 1 H, C³H), 5.95 (m, 1 H, C⁴H), 5.44, 5.15 and 5.06 (m, olefinic protons in the starting material), 4.65 (m, 1 H, C⁶H^A), 4.41 (m, 1 H, C⁶H^B), 2.63–2.41 (m, 8 H, C¹H^A, C¹H^B, C^{1'}H^A and C^{1'}H^B), 2.47–2.34 (m, 8 H, CH protons of the Cy groups), 2.21–1.28 (m, 80 H, CH₂ protons of the Cy groups), 2.21 (m, 2 H, C²H₂) ppm.

^{13}C NMR [100.62 MHz, *o*D₂O, 298 K]: δ = 160.9 (1 C, C⁵), 130.9 (1 C, C³), 121.1 (1 C, C⁴), 91.9 (1 C, C⁶), 32.8–32.6 (8 C, CH carbon atoms of the Cy groups), 30.0–24.9 (40 C, CH₂ carbon atoms of the Cy groups), 20.0 (1 C, C²), 15.8 and 14.8 (4 C, C¹ and C^{1'}) ppm.

^{19}F NMR [376.54 MHz, *o*D₂O, 298 K]: δ = –75.3 (s, 36 F, [Al(OC(CF₃)₃)₄][–]), –111.7 (ddd, 1 F, C⁵F, $^3J_{F,C6HB}$ = 50.3 Hz, $^3J_{F,C4H}$ = 24.9 Hz, $^3J_{F,C6HA}$ = 17.1 Hz), –113.9 (m, PhF), –128.7 and –142.0 (m, 2 F, CF₂-group in the starting material), –139.5 (m, *o*C₆F₂H₄), –204.0 (t, 1 F, GaF, $^2J_{F,P1}$ = 27.0 Hz) ppm.

^{27}Al NMR [78.22 MHz, *o*D₂O, 298 K]: δ = 35.0 (s, 1 Al, [Al(OC(CF₃)₃)₄][–]) ppm.

^{31}P NMR [161.99 MHz, *o*D₂O, 298 K]: δ = 15.5 (m, 2 P, P^{II}), 15.1 (unknown impurity), 13.4 (unknown impurity), 9.2 (m, 2 P, P^I), –1.5 (unknown impurity) ppm.

^{71}Ga NMR [122.04 MHz, *o*D₂O, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ^{71}Ga .

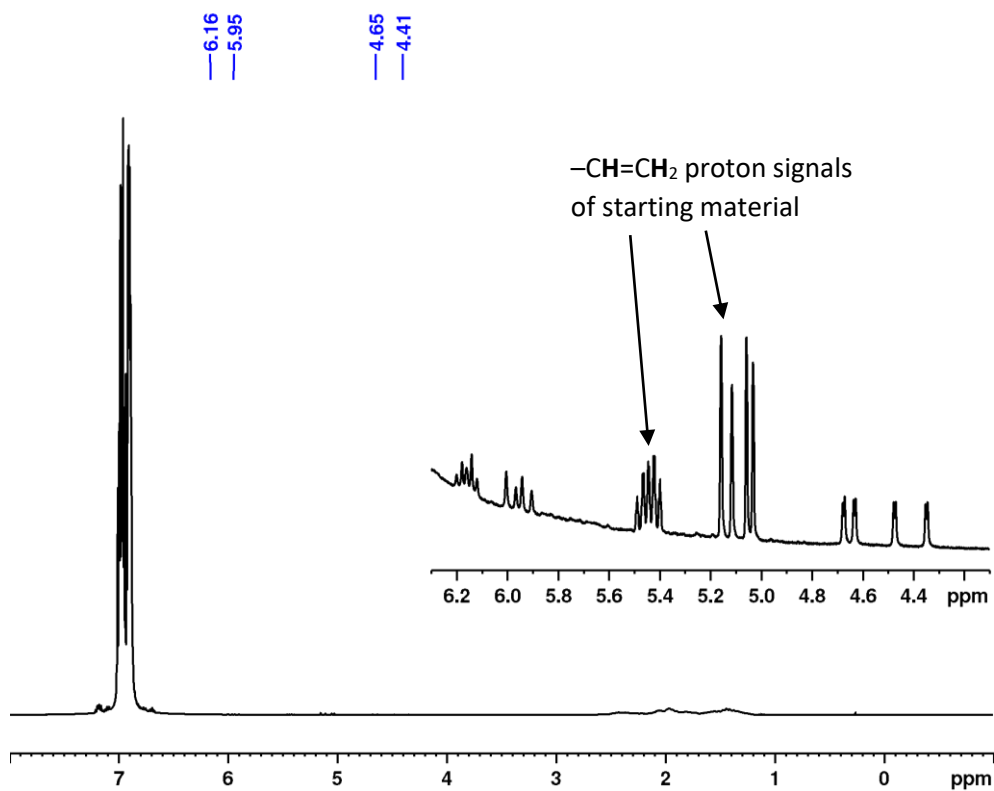


Figure S 148: ^1H NMR spectrum (400.17 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in oDFB.

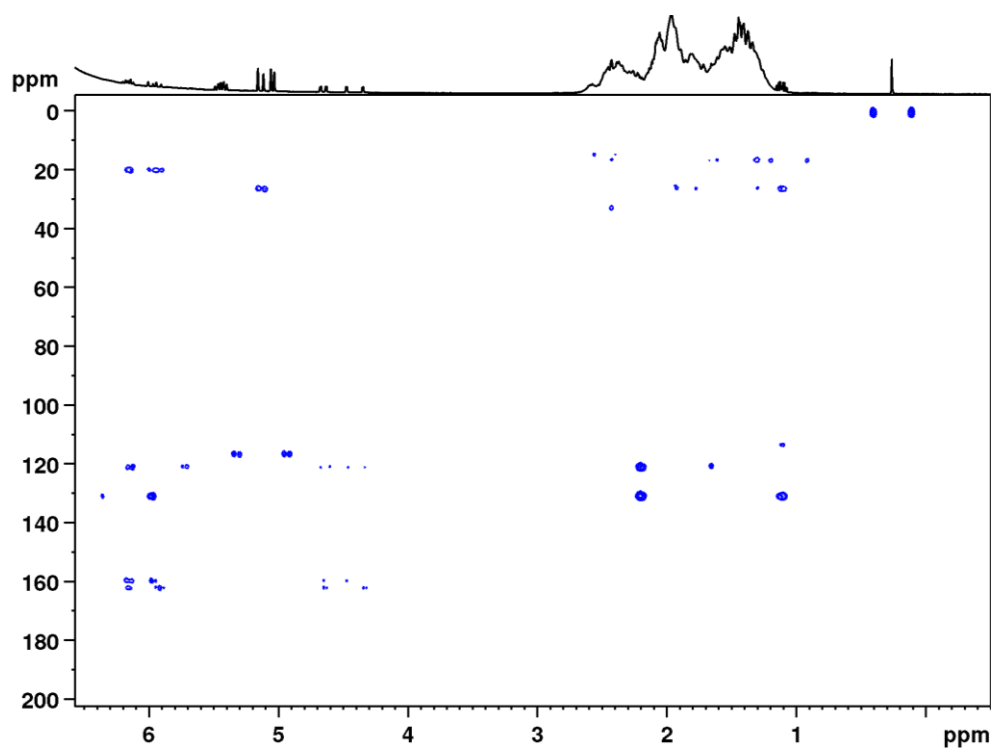


Figure S 149: ^1H , ^{13}C -HMBC NMR spectrum (400.17 MHz, oDFB, 298 K, optimized for $J = 8$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in oDFB.

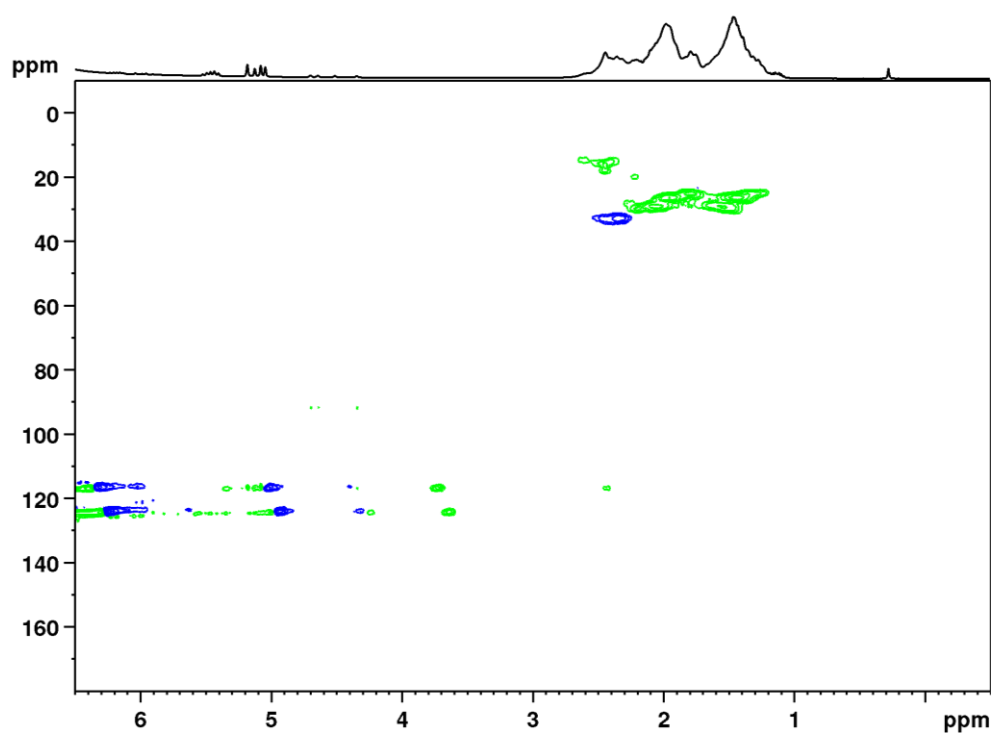


Figure S 150: Edited ^1H , ^{13}C -HSQC NMR spectrum (300.18 MHz, *o*DfB, 298 K, optimized for $J = 145$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in *o*DfB.

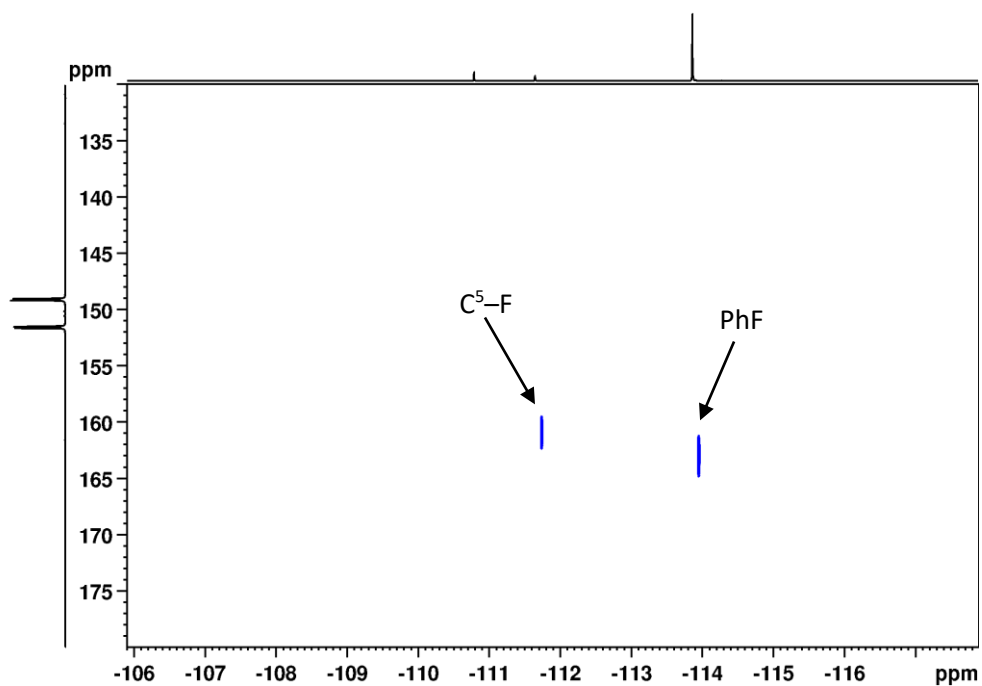


Figure S 151: ^{19}F , ^{13}C -HSQC NMR spectrum (376.54 MHz, *o*DfB, 298 K, optimized for $J = 280$ Hz) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in *o*DfB.

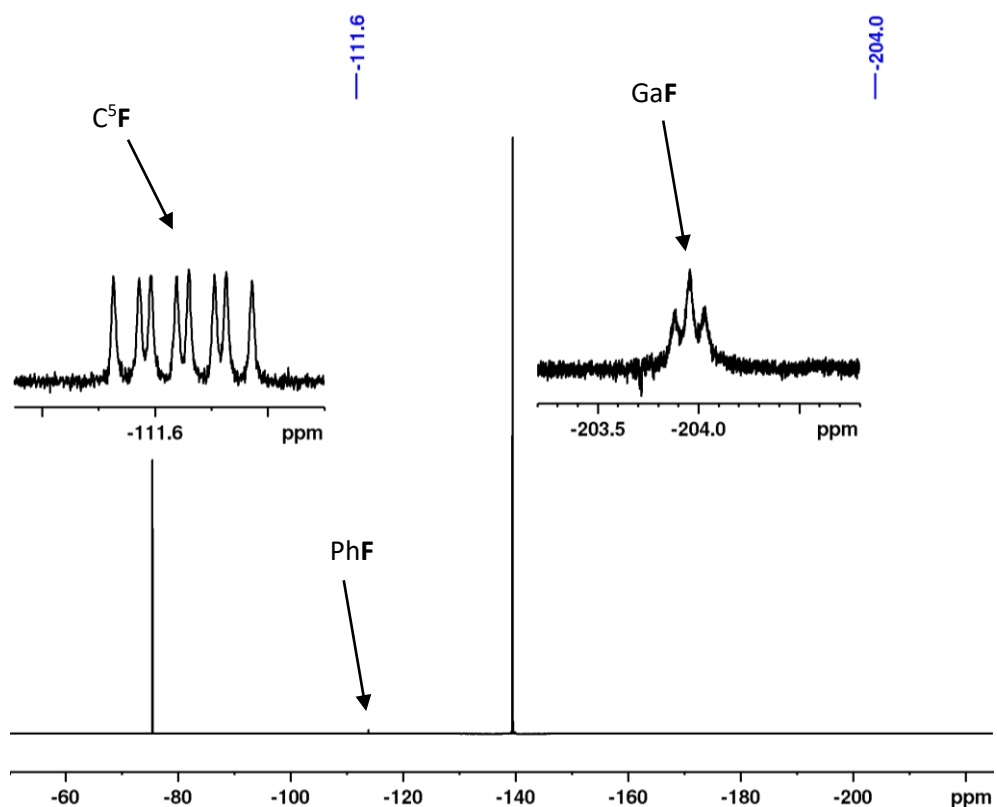


Figure S 152: ^{19}F NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in oDFB.

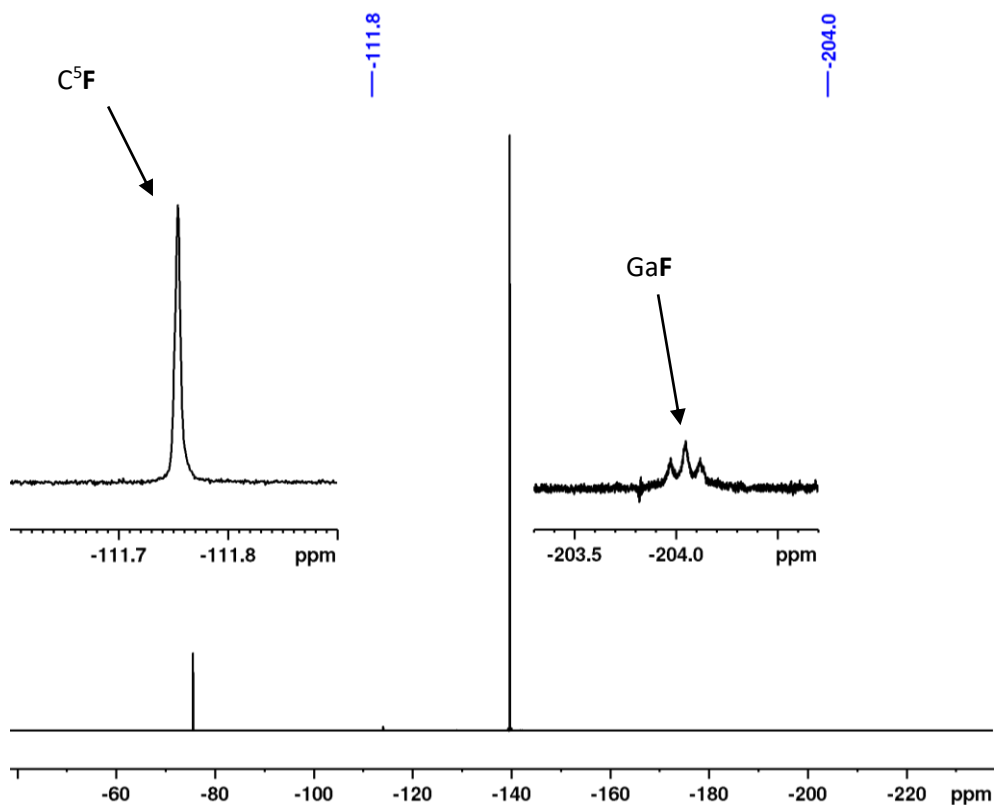


Figure S 153: $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (376.54 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in oDFB.

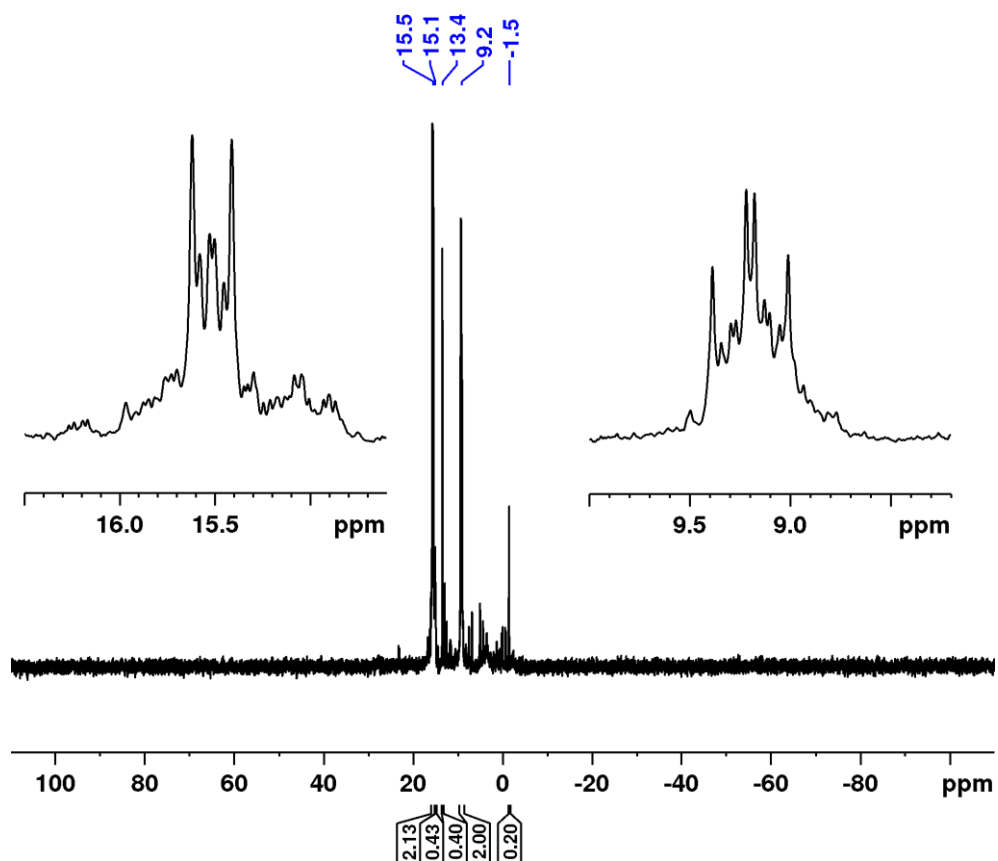
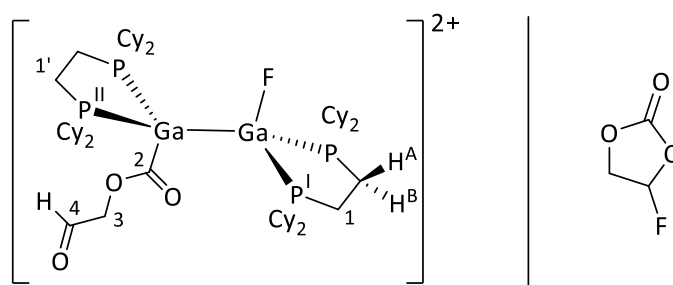


Figure S 154: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.99 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ and 1,1-difluorovinylcyclopropane in oDFB.

4.14 [F{Ga(dcpe)}₂(COOCH₂CHO)][pf]₂



¹H NMR [300.18 MHz, *o*D₂F₆, calibrated at *o*C₆F₂H₄ = 6.96 ppm, 298 K]: δ = 9.53 (s, 1 H, C⁴H), 6.09, 4.38 and 4.29 (m, 3 H, FEC starting material), 4.94 (s, 2 H, C³H₂), 2.61–2.35 (m, 8 H, CH protons of the Cy groups), 2.25–1.32 (m, 80 H, CH₂ protons of the Cy groups), 2.57–2.54 (m, 8 H, C¹H^A, C¹H^B, C^{1'}H^A and C^{1'}H^B) ppm.

¹³C NMR [100.62 MHz, *o*D₂F₆, 298 K]: δ = 193.3 (1 C, C⁴), 189.7 (1 C, C²), 67.2 (1 C, C³), 33.9–31.9 (8 C, CH carbon atoms of the Cy groups), 28.9–24.9 (40 C, CH₂ carbon atoms of the Cy groups), 16.1 and 14.8 (4 C, C¹ and C^{1'}) ppm.

¹⁹F NMR [282.45 MHz, *o*D₂F₆, 298 K]: δ = –75.3 (s, 36 F, [Al(OC(CF₃)₃)₄][–]), –113.9 (m, PhF), –121.8 (m, 1 F, FEC starting material), –139.5 (m, *o*C₆F₂H₄), –203.6 (t, 1 F, GaF, ²*J*_{F,P^I} = 26.8 Hz) ppm.

²⁷Al NMR [78.22 MHz, *o*D₂F₆, 298 K]: δ = 35.0 (s, 1 Al, [Al(OC(CF₃)₃)₄][–]) ppm.

³¹P NMR [121.51 MHz, *o*D₂F₆, 298 K]: δ = 30.6 (unknown impurity), 18.1 (m, 2 P, P^{II}), 9.9 (m, 2 P, P^I) ppm.

⁷¹Ga NMR [91.54 MHz, *o*D₂F₆, 298 K]: signal probably too broad to be detected, due to the quadrupolar relaxation of ⁷¹Ga.

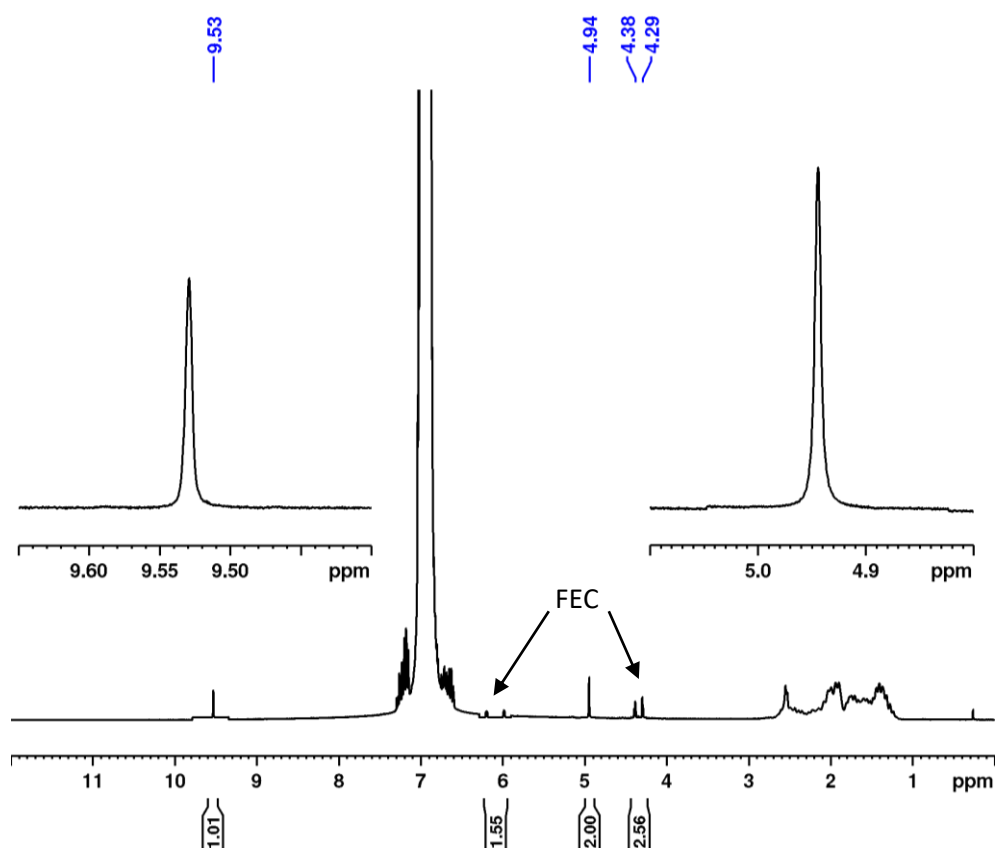


Figure S 155: ^1H NMR spectrum (300.18 MHz, *o*D₂O, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

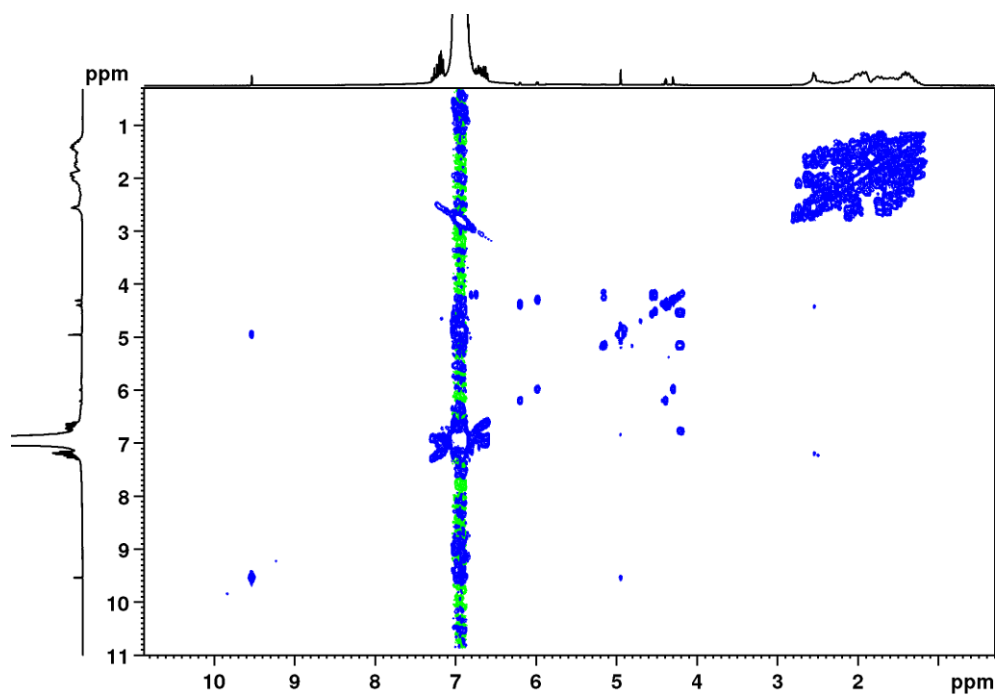


Figure S 156: ^1H -COSY NMR spectrum (300.18 MHz, *o*D₂O, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

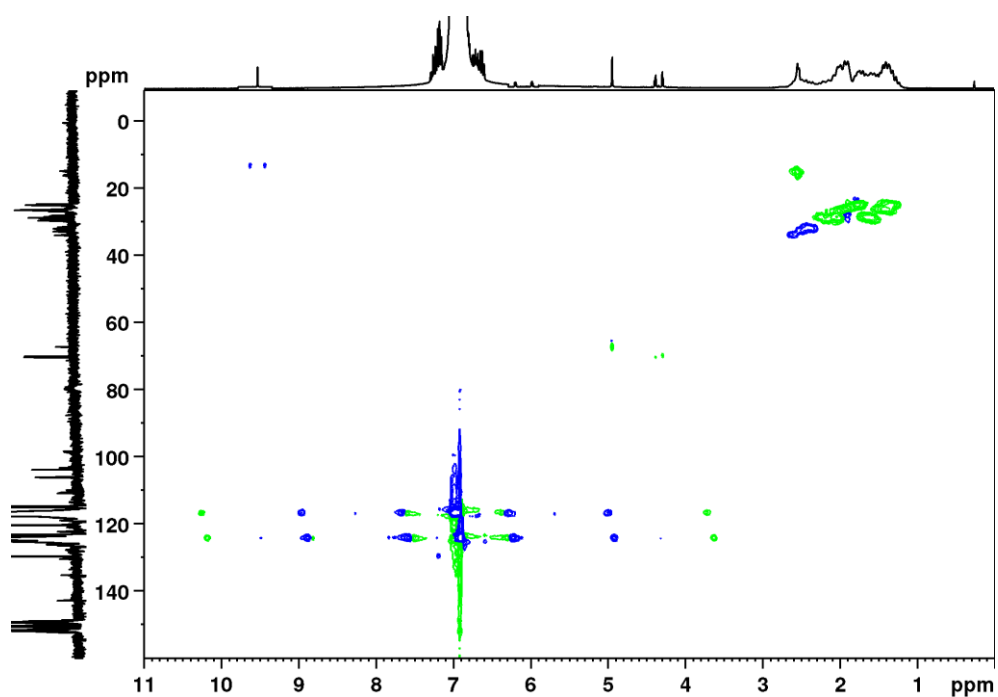


Figure S 157: Edited $^1\text{H},^{13}\text{C}$ -HSQC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 145$ Hz) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

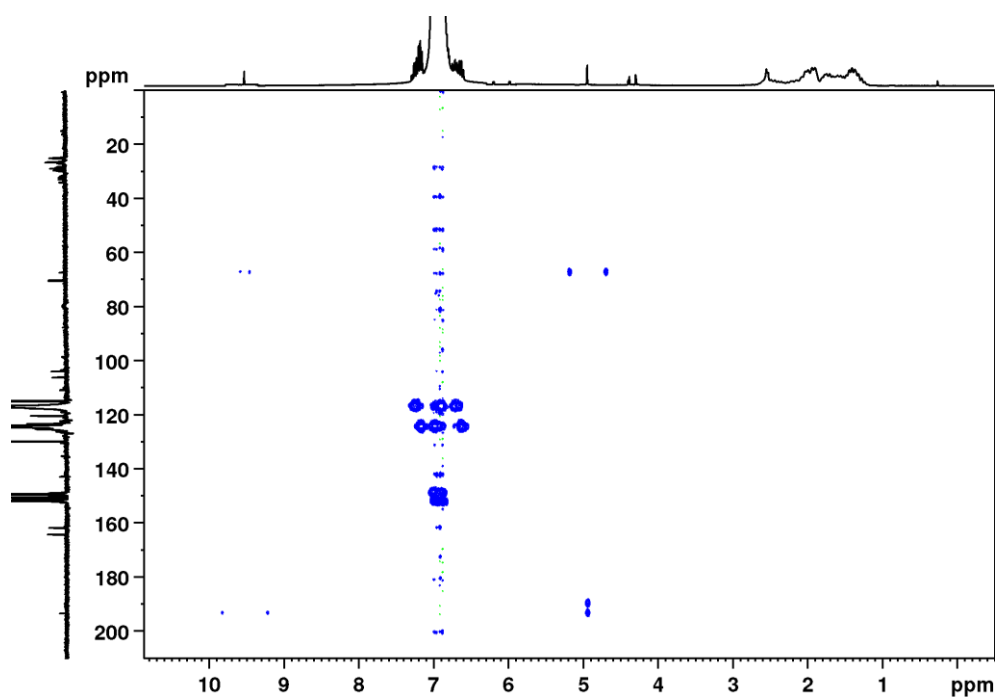


Figure S 158: $^1\text{H},^{13}\text{C}$ -HMBC NMR spectrum (300.18 MHz, oDFB, 298 K, optimized for $J = 10$ Hz) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

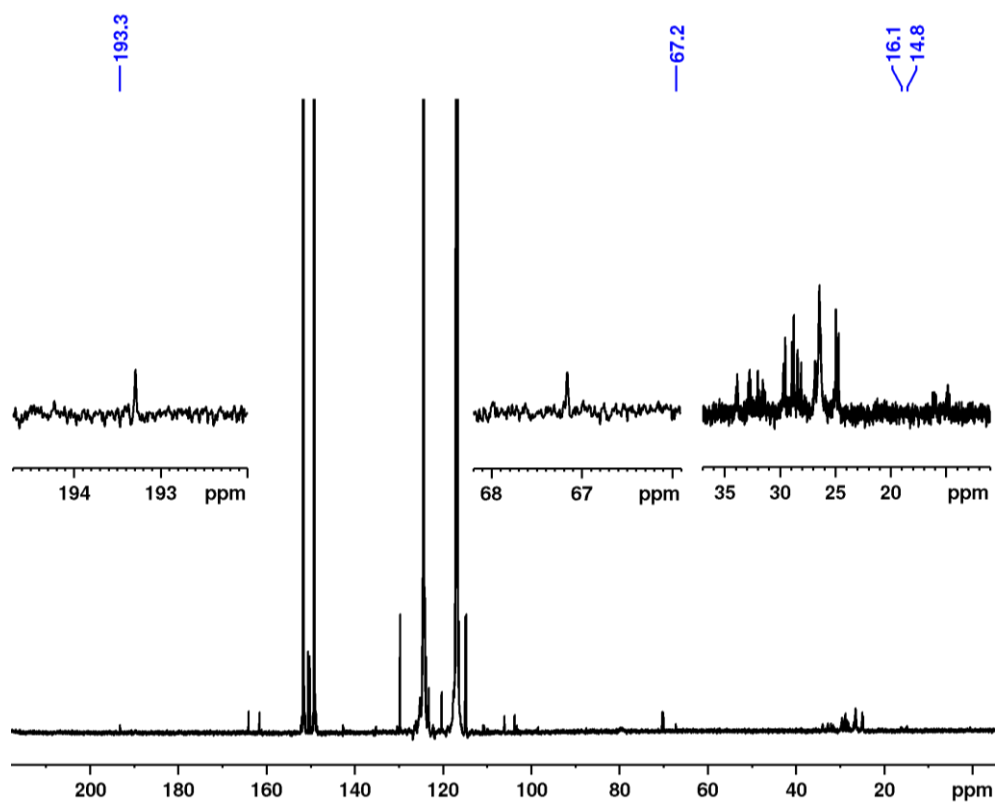


Figure S 159: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100.62 MHz, oDFB, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

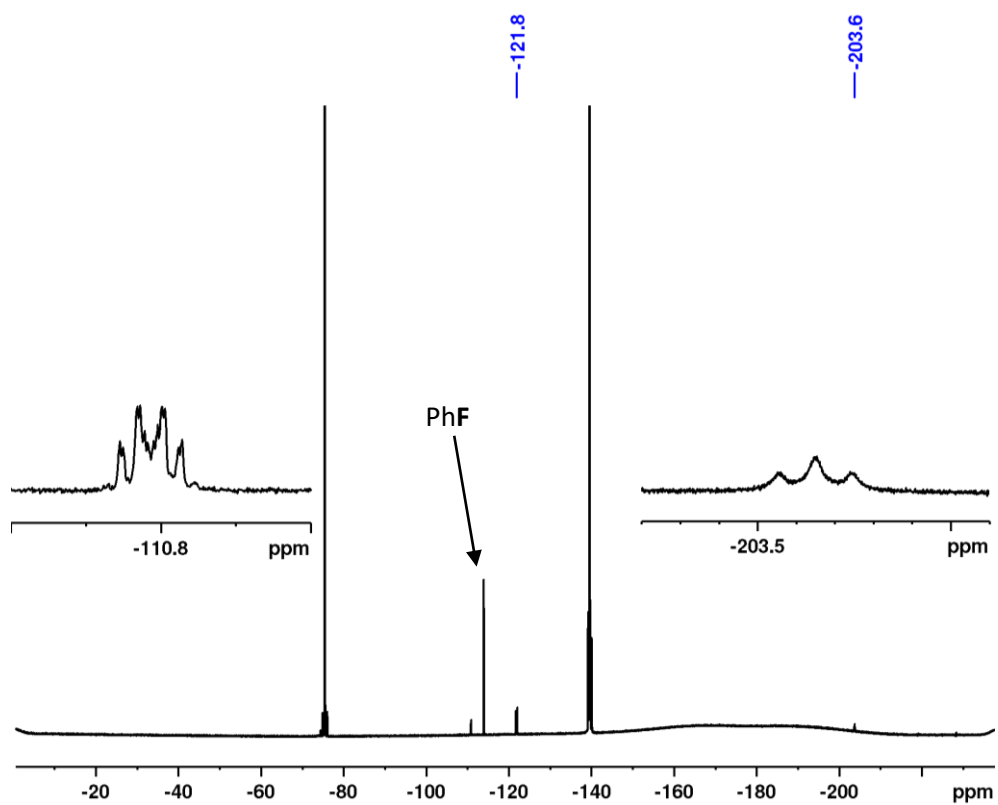


Figure S 160: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

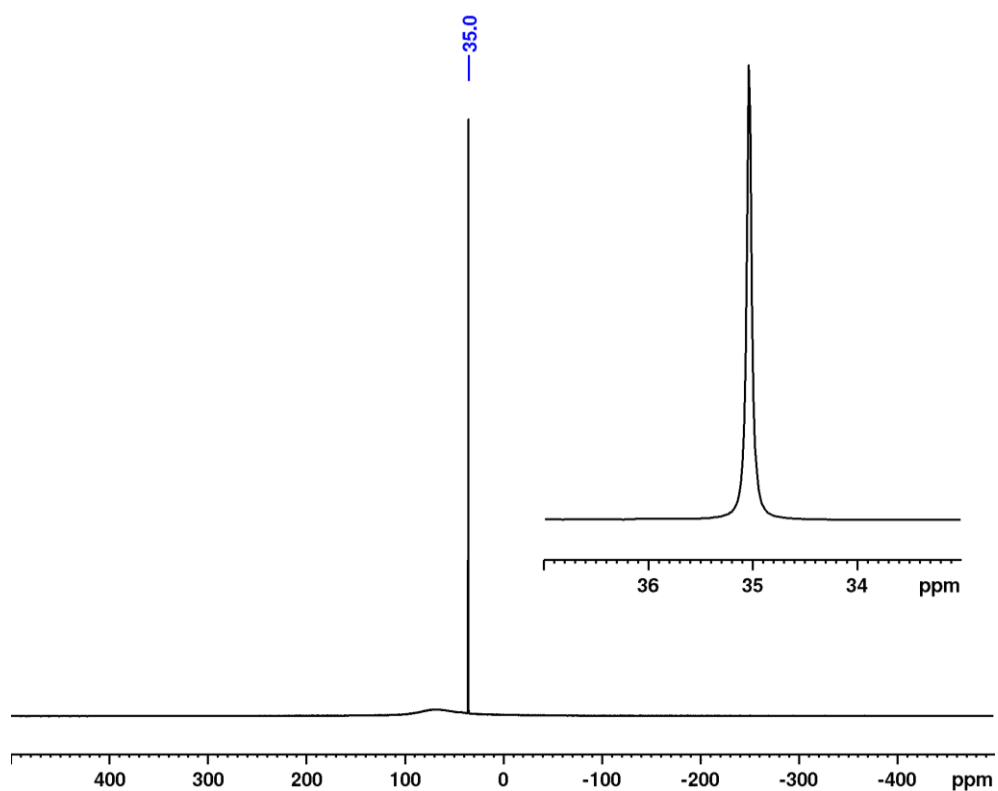


Figure S 161: ^{27}Al NMR spectrum (78.22 MHz, oDFB, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

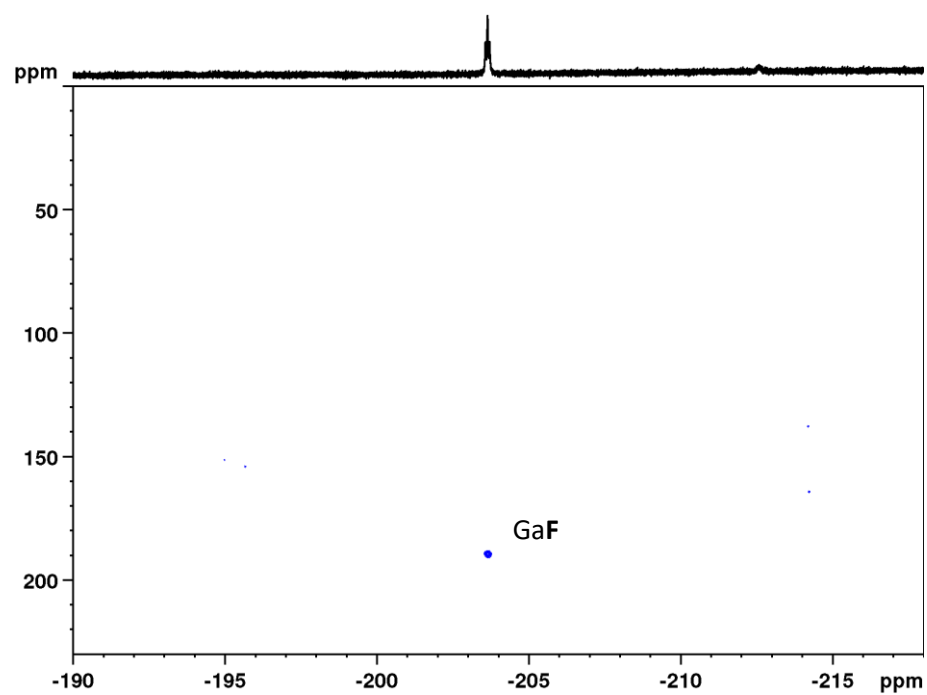


Figure S 162: ^{19}F , ^{13}C -HMBC NMR spectrum (376.54 MHz, oDFB, 298 K, optimized for $J = 20$ Hz) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

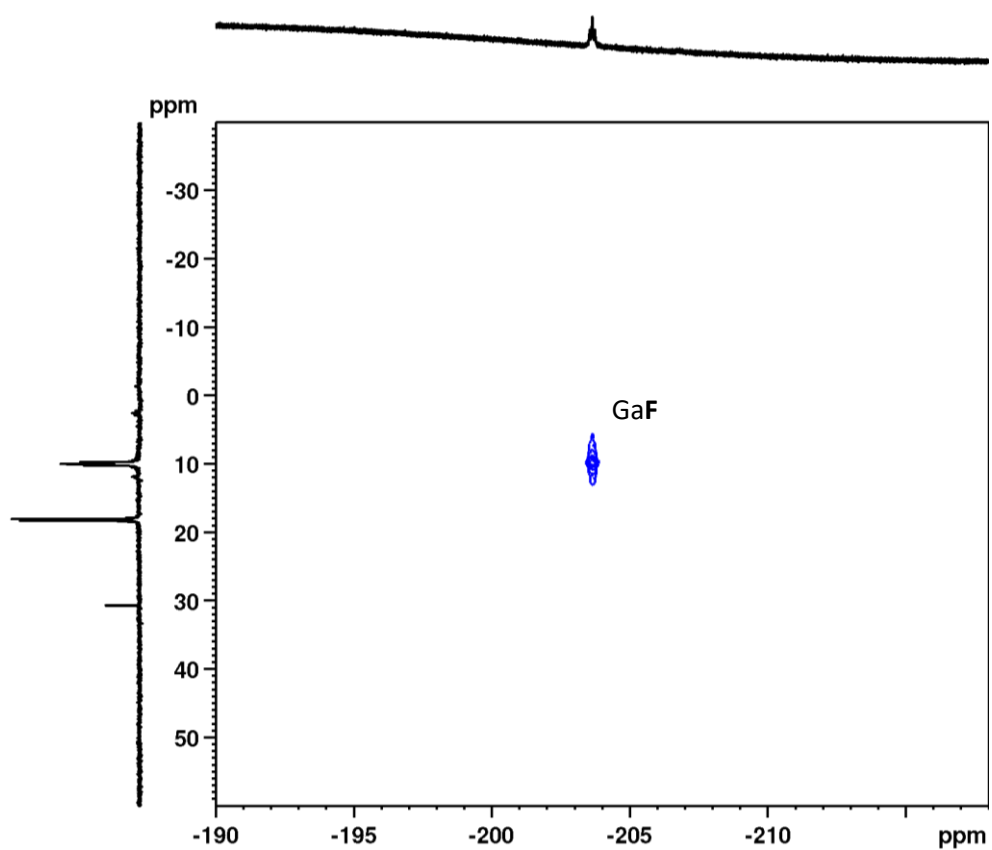


Figure S 163: $^{19}\text{F},^{31}\text{P}$ -HMBC NMR spectrum (282.45 MHz, oDFB, 298 K, optimized for $J = 30$ Hz) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

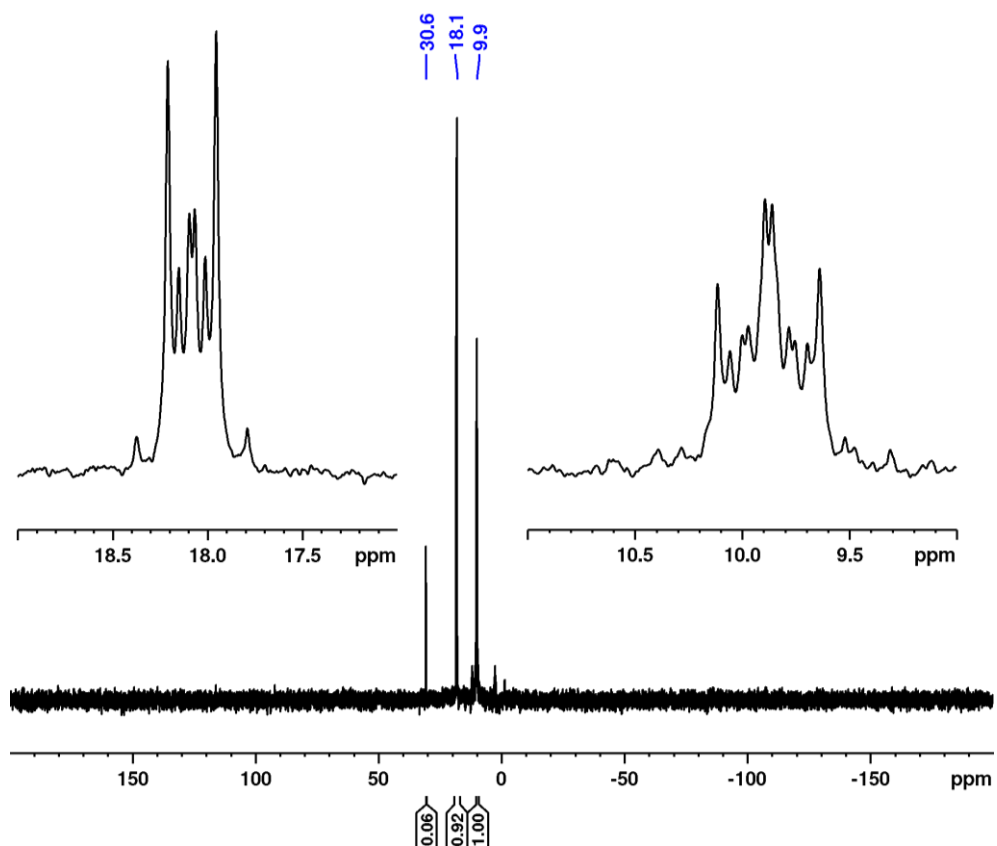
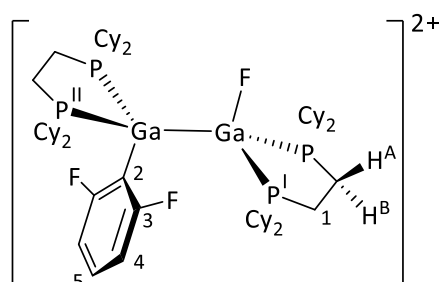


Figure S 164: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.51 MHz, oDFB, 298 K) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$.

4.15 $[\{Ga(dcpe)\}_2(C_6F_2H_3)][pf]_{5/3}[alfal]_{1/3}$



^1H NMR [400.17 MHz, 3FB, calibrated at 1,2,3- $C_6F_3H_3$ = 6.86 ppm, 298 K]: δ = 7.66 (m, 1 H, C^5H), 7.27 (m, 2 H, C^4H), 2.74–2.60 (m, 8 H, C^1H^A , C^1H^B , $C^{1'}H^A$ and $C^{1'}H^B$), 2.61–2.49 (m, 8 H, CH protons of the Cy groups), 2.40–1.22 (m, 80 H, CH_2 protons of the Cy groups) ppm.

^{13}C NMR [100.62 MHz, 3FB, 298 K]: δ = 166.4 (2 C, C^3), 134.4 (1 C, C^5), 114.0 (1 C, C^2), 111.9 (2 C, C^4), 34.9–32.6 (8 C, CH carbon atoms of the Cy groups), 29.4–24.9 (40 C, CH_2 carbon atoms of the Cy groups), 15.3 and 14.5 (4 C, C^1 and $C^{1'}$) ppm.

^{19}F NMR [282.45 MHz, 3FB, 298 K]: δ = –75.7 (s, 36 F, $[Al(OC(CF_3)_3)_4]^-$), –75.9 (s, 54 F, $[{(F_3C)_3C}Al-F-Al(OC(CF_3)_3)_3]^-$), –88.2 (m, 2 F, C^3F), –112.9 (m, PhF), –136.8 and –163.5 (m, 3FB solvent), –184.6 (s, 72 F, $[{(F_3C)_3C}Al-F-Al(OC(CF_3)_3)_3]^-$), –194.8 (t, 1 F, F–Ga, $^2J_{F,P1}$ = 27.3 Hz) ppm.

^{27}Al NMR [78.22 MHz, 3FB, 298 K]: δ = 34.8 (s, 1 Al, $[Al(OC(CF_3)_3)_4]^-$) ppm.

^{31}P NMR [121.52 MHz, 3FB, 298 K]: δ = 15.8 (m, 2 P, P^{II}), 12.0 (unknown impurity), 8.9 (m, 2 P, P^I) ppm.

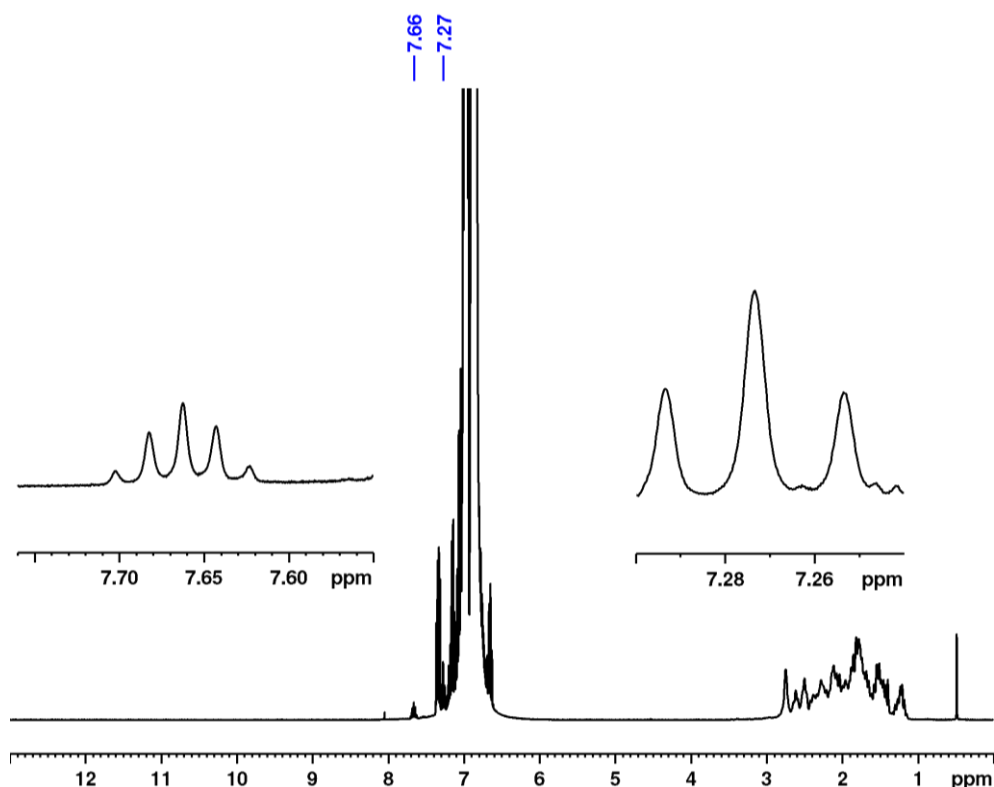


Figure S 165: ^1H NMR spectrum (400.17 MHz, 3FB, 298 K) of $[\{Ga(dcpe)\}_2][pf]_2$ in 3FB.

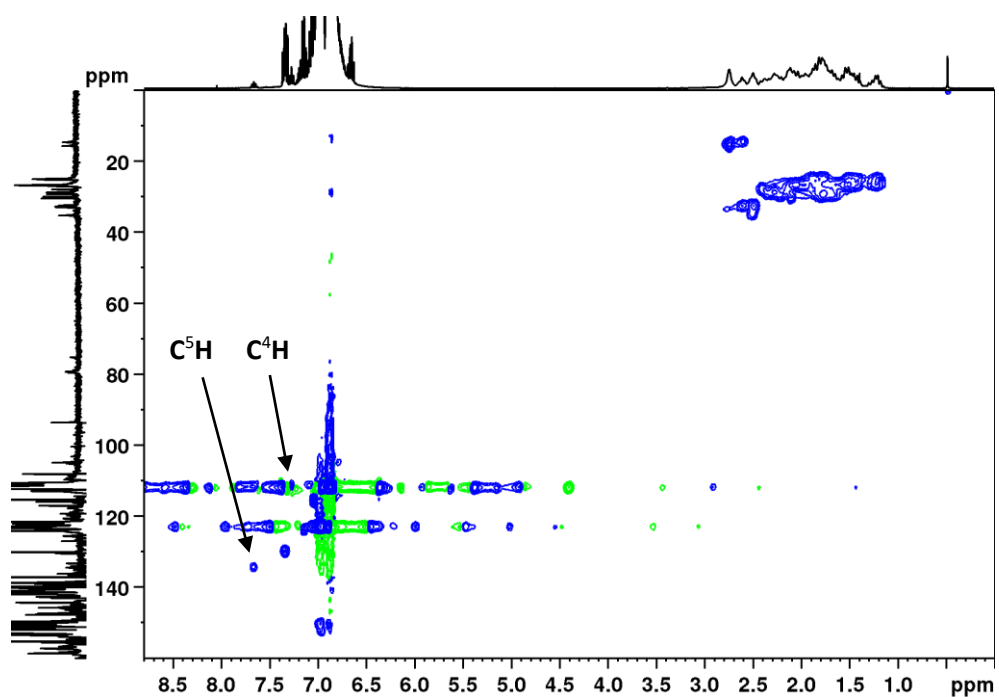


Figure S 166: ^1H , ^{13}C -HSQC NMR spectrum (400.17 MHz, 3FB, 298 K, optimized for $J = 145$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

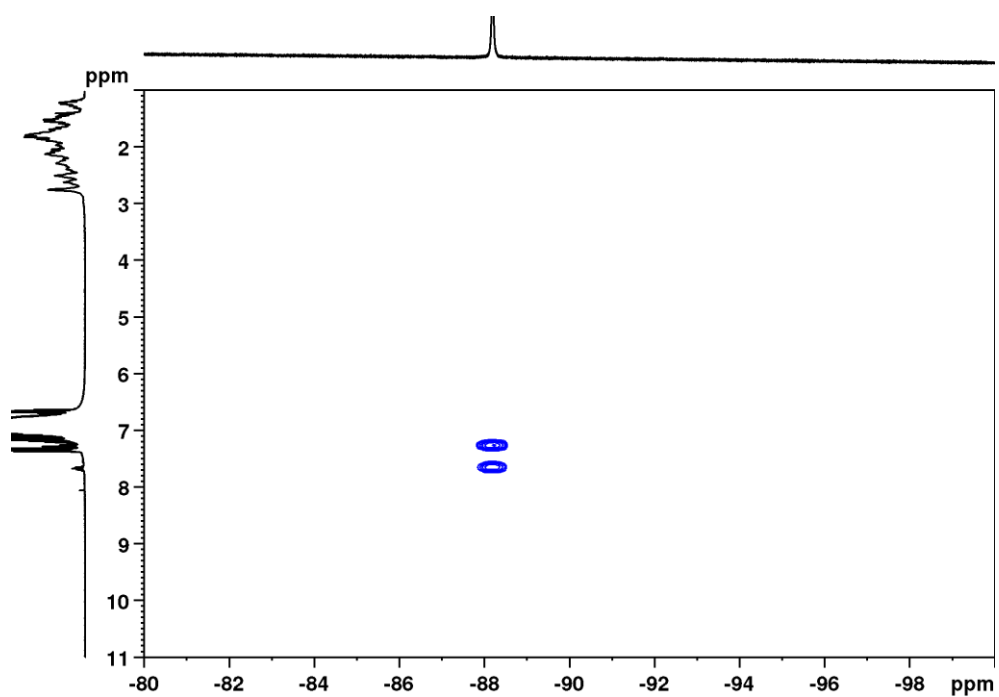


Figure S 167: ^1H , ^{19}F -COSY NMR spectrum (376.54 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

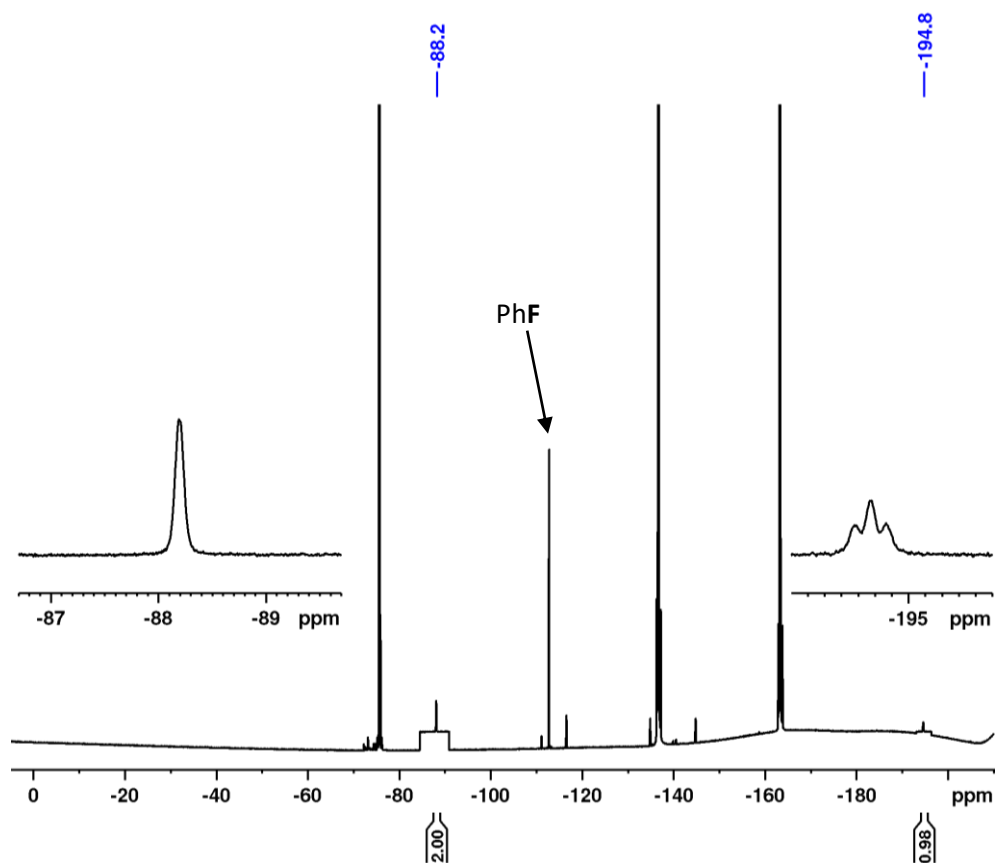


Figure S 168: ^{19}F NMR spectrum (282.45 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

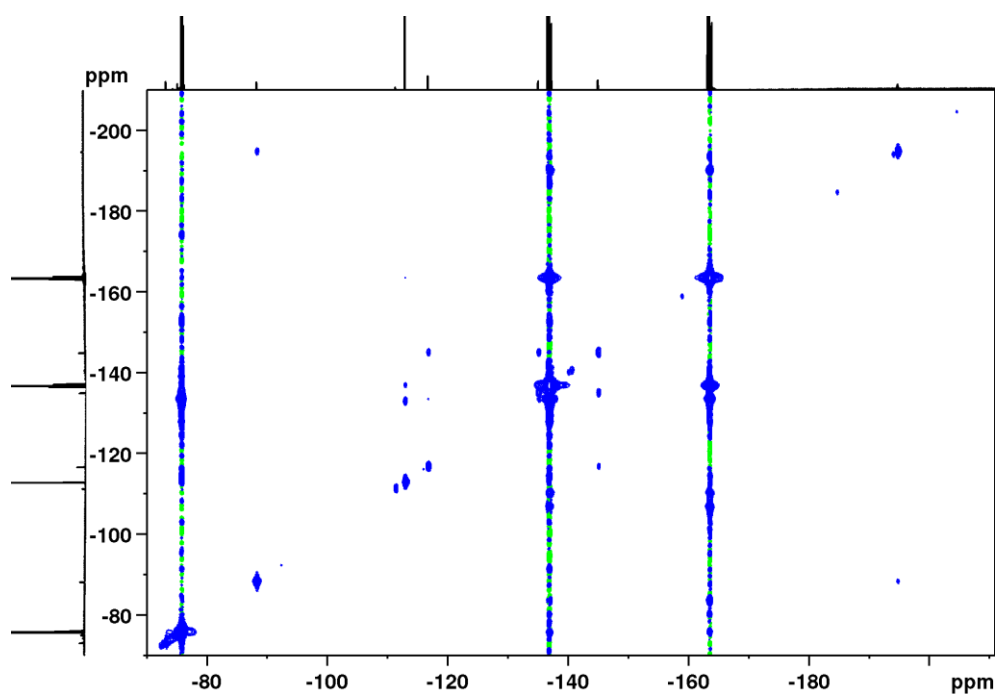


Figure S 169: ^{19}F -COSY NMR spectrum (376.54 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

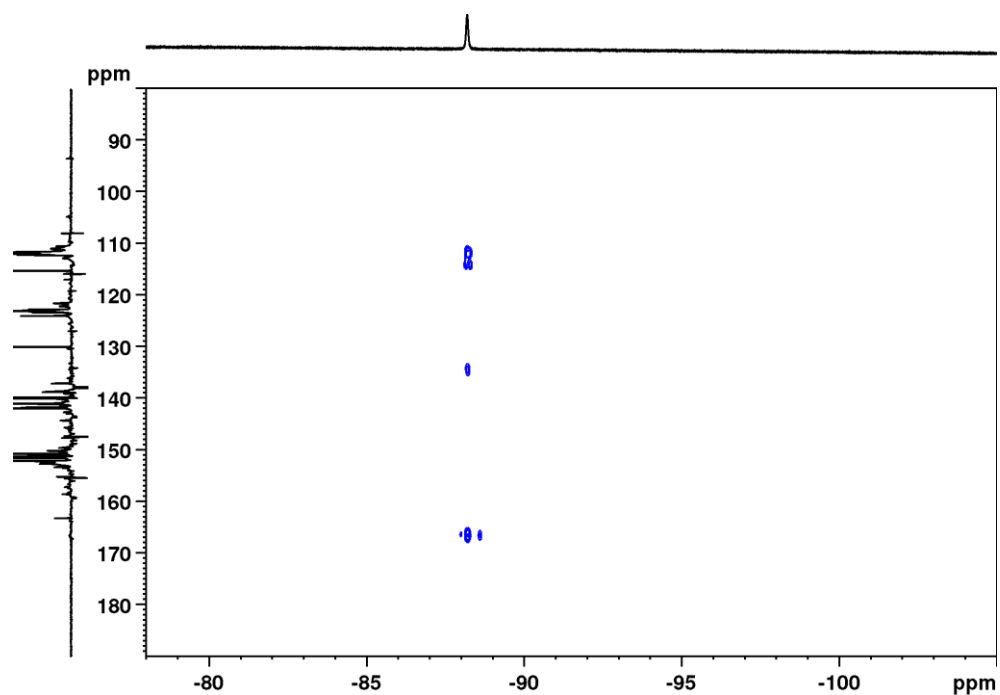


Figure S 170: ^{19}F , ^{13}C -HMBC NMR spectrum (376.54 MHz, 3FB, 298 K, optimized for $J = 30$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

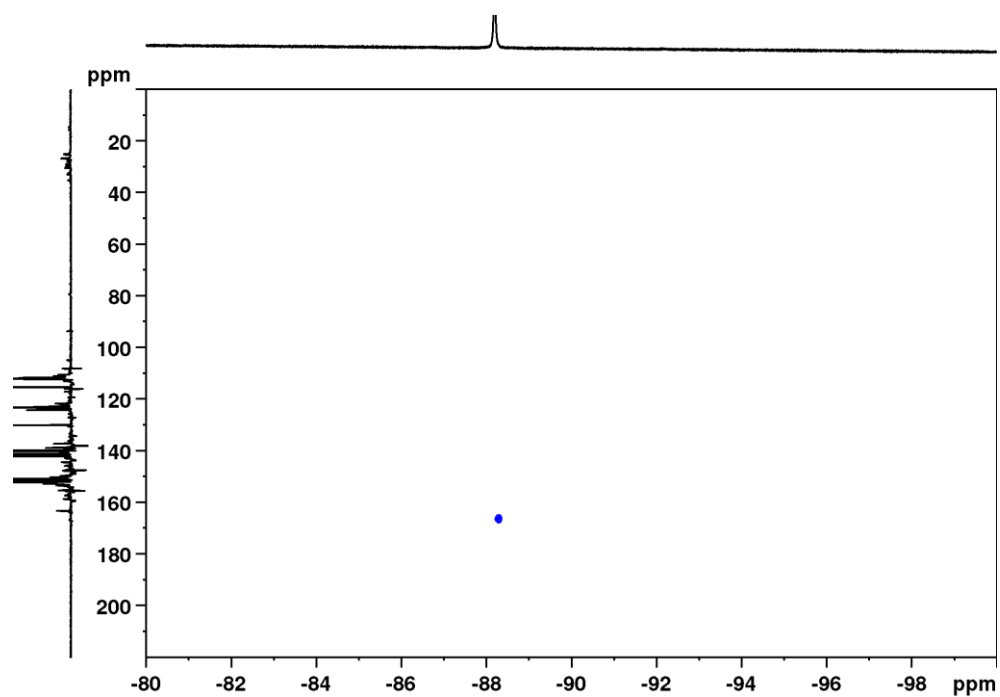


Figure S 171: ^{19}F , ^{13}C -HSQC NMR spectrum (376.54 MHz, 3FB, 298 K, optimized for $J = 250$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

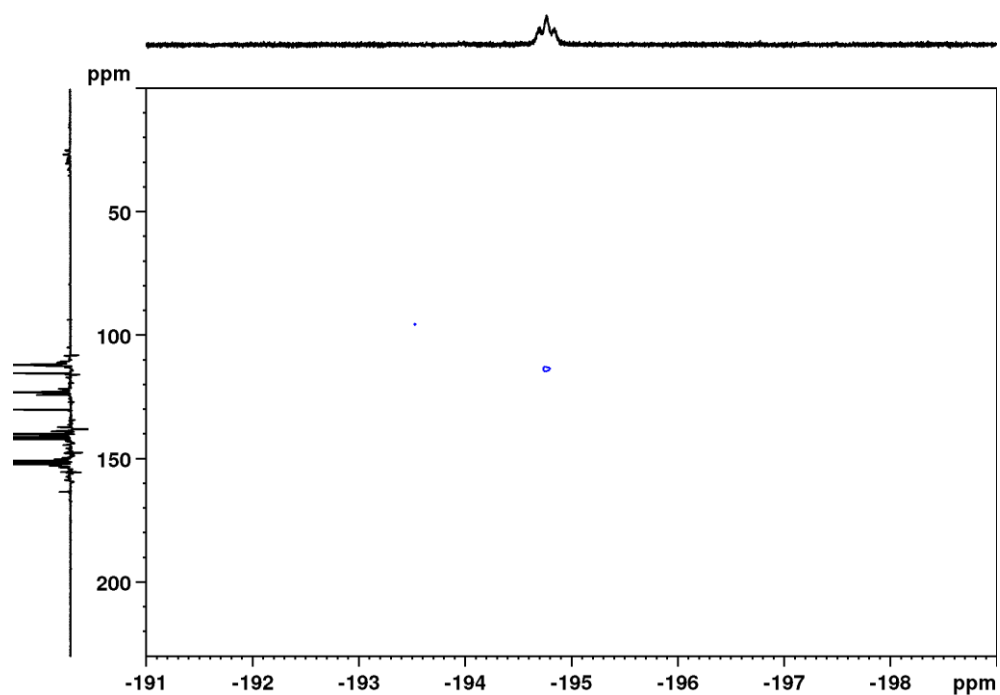


Figure S 172: ^{19}F , ^{13}C -HMBC NMR spectrum (376.54 MHz, 3FB, 298 K, optimized for $J = 20$ Hz) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

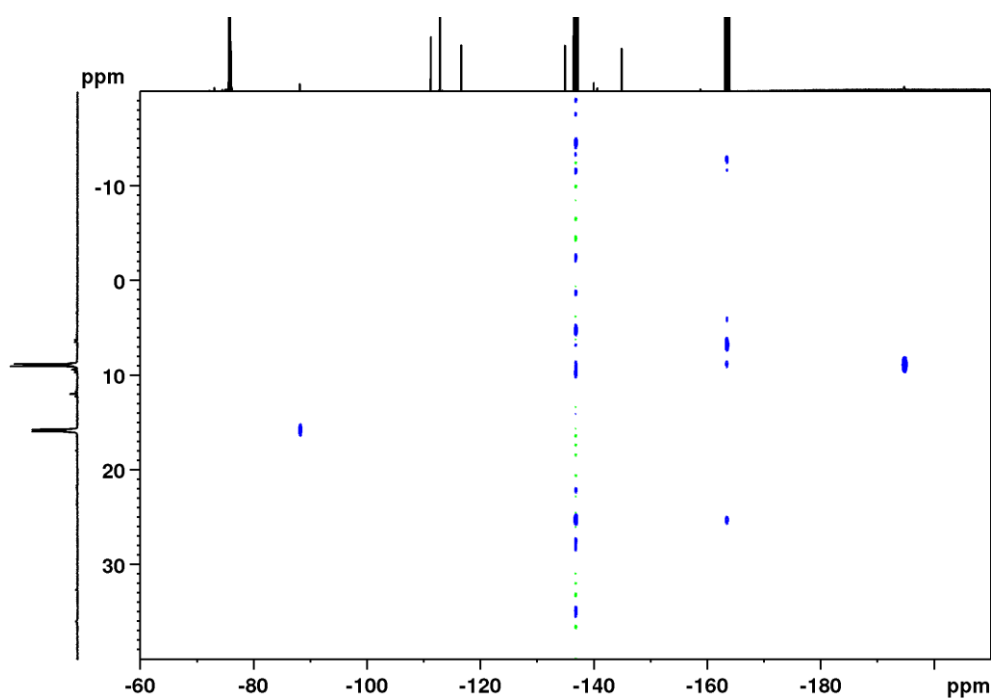


Figure S 173: ^{19}F , ^{31}P -COSY NMR spectrum (376.54 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

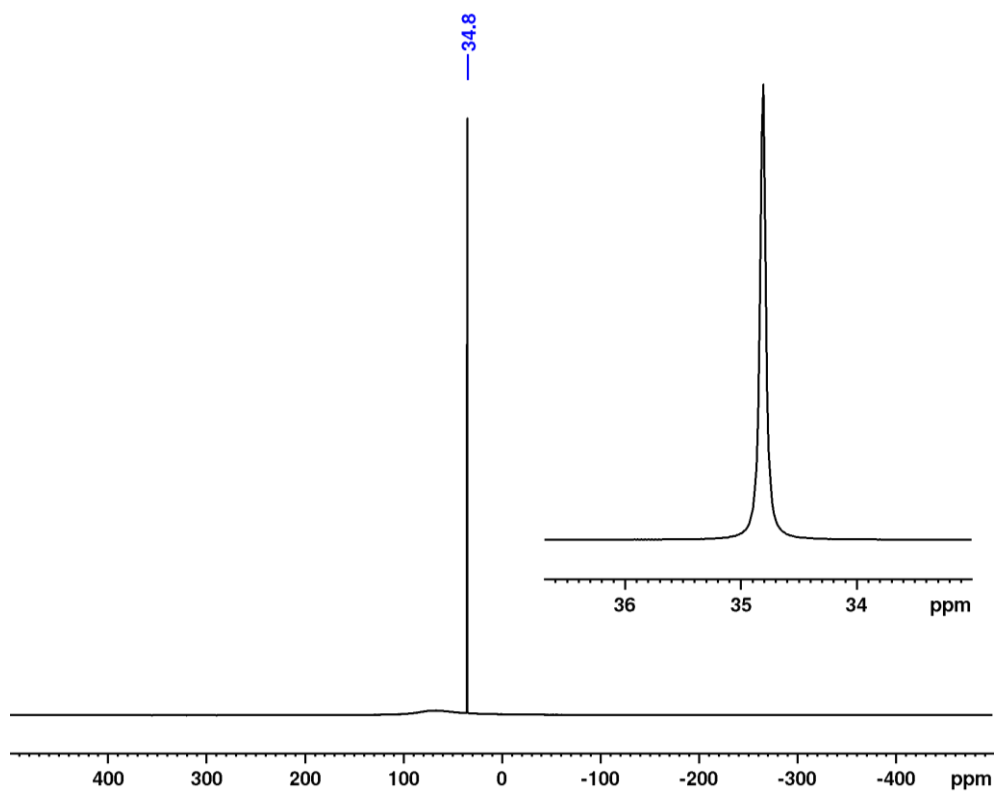


Figure S 174: ^{27}Al NMR spectrum (78.22 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

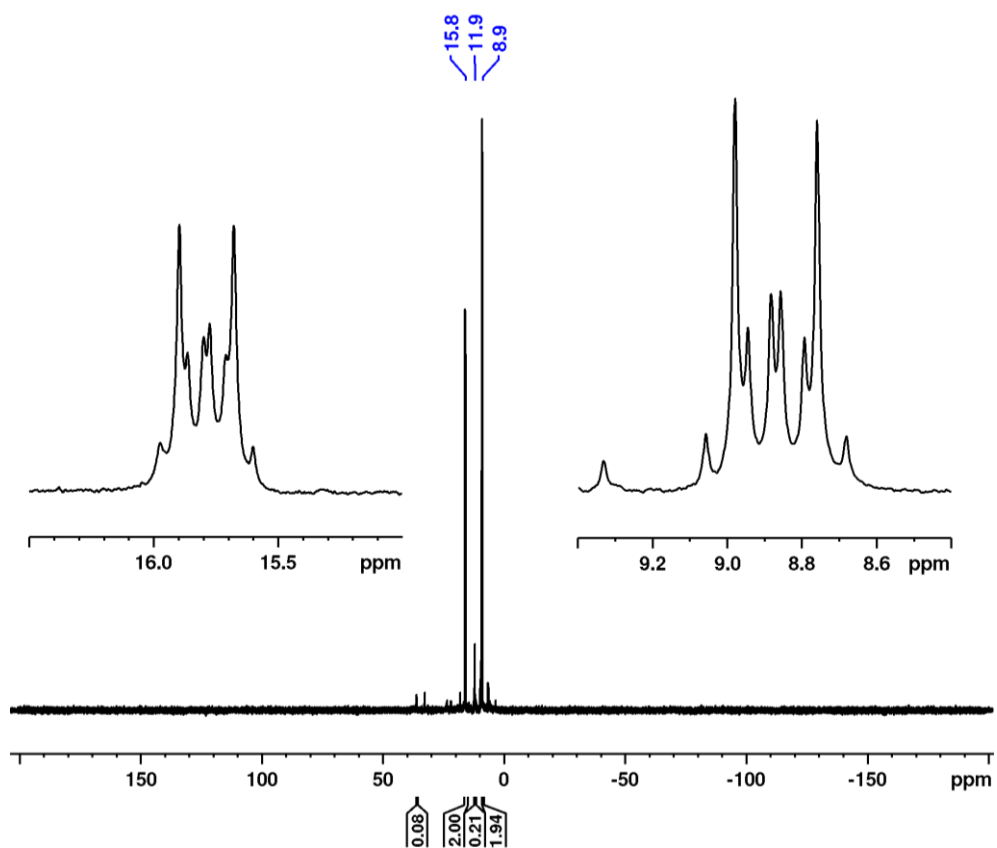


Figure S 175: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, 3FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 3FB.

4.16 Unselective Bond Activation Reactions

4.16.1 Reaction Between $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$ and PhCF_3

The NMR signals at ca. -200 ppm in the ^{19}F NMR spectrum (**Figure S 176**) of a mixture of $\mathbf{1}^{2+}$ and PhCF_3 probably indicate the presence of species with a P-Ga-F moiety and thus suggest that $\mathbf{1}^{2+}$ does cleave C-F bonds in this substrate, however in a somewhat unselective reaction and under the formation of a multitude of different reaction products as shown by the ^{19}F and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra.

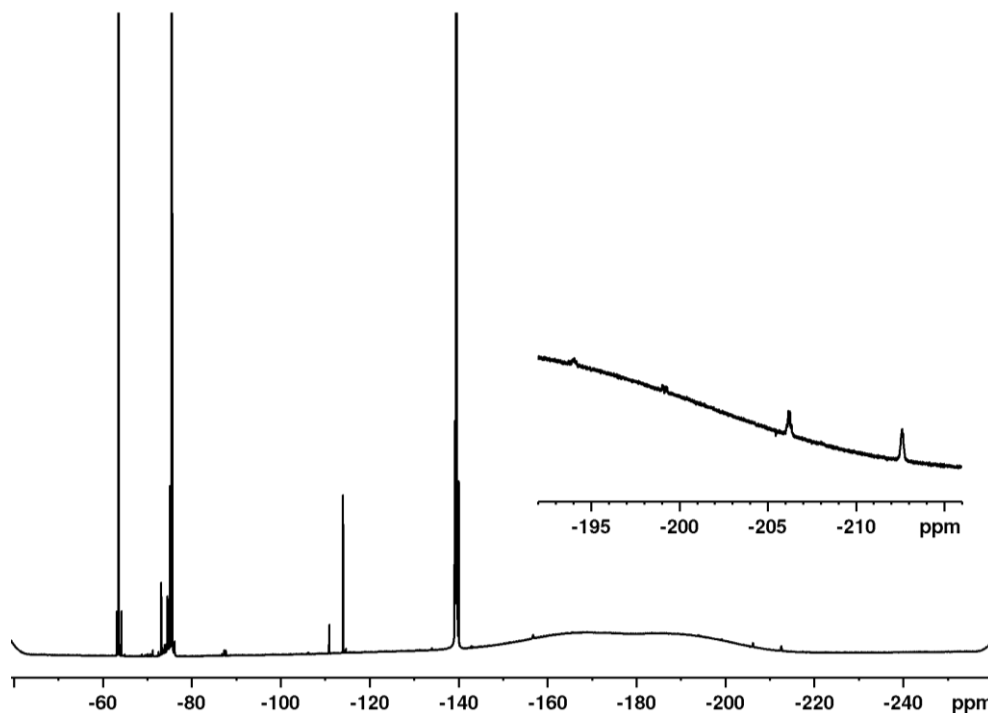


Figure S 176: ^{19}F NMR spectrum (282.45 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and a excess PhCF_3 in oDFB.

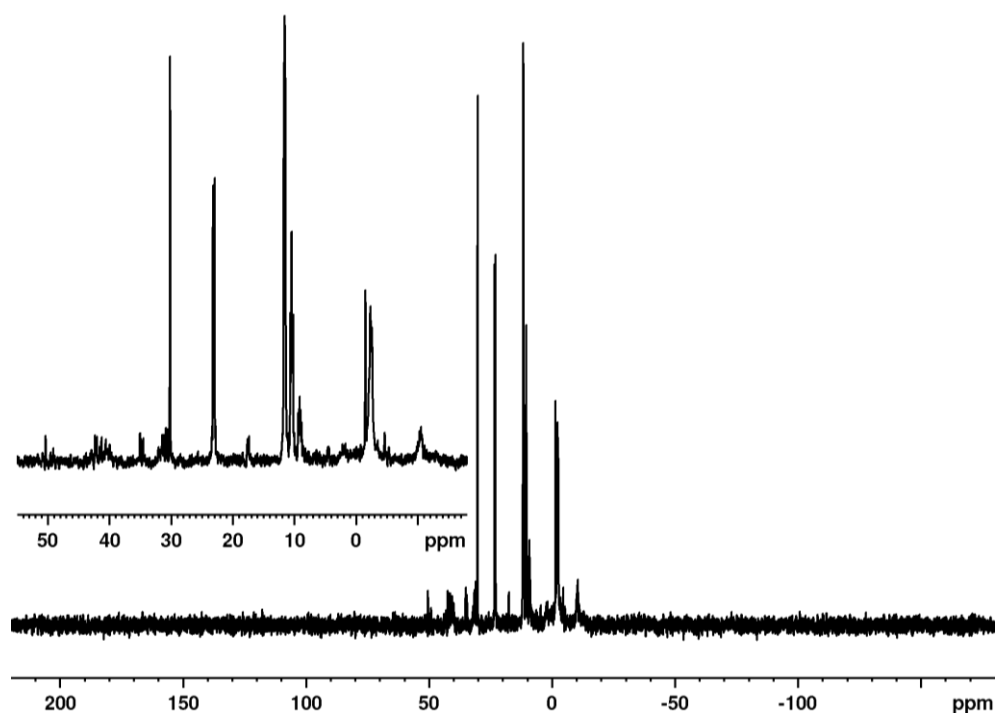


Figure S 177: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.52 MHz, oDFB, 298 K) of a mixture of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ and a excess PhCF_3 in oDFB.

4.16.2 Reaction Between $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$ and 4FB

When heating a solution of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ in 4FB for 3 days at 40 °C, the ^{19}F and ^{31}P NMR spectra indicate the formation of at least four different species with FGaP_2 moieties, which is confirmed by the ^{19}F , ^{31}P -COSY NMR spectrum (Figure S 178–Figure S 180). If 1^{2+} merely activated the C–F bonds in 4FB, only two isomeric products would have been expected. Thus, the results suggest that the products undergo consecutive reactions.

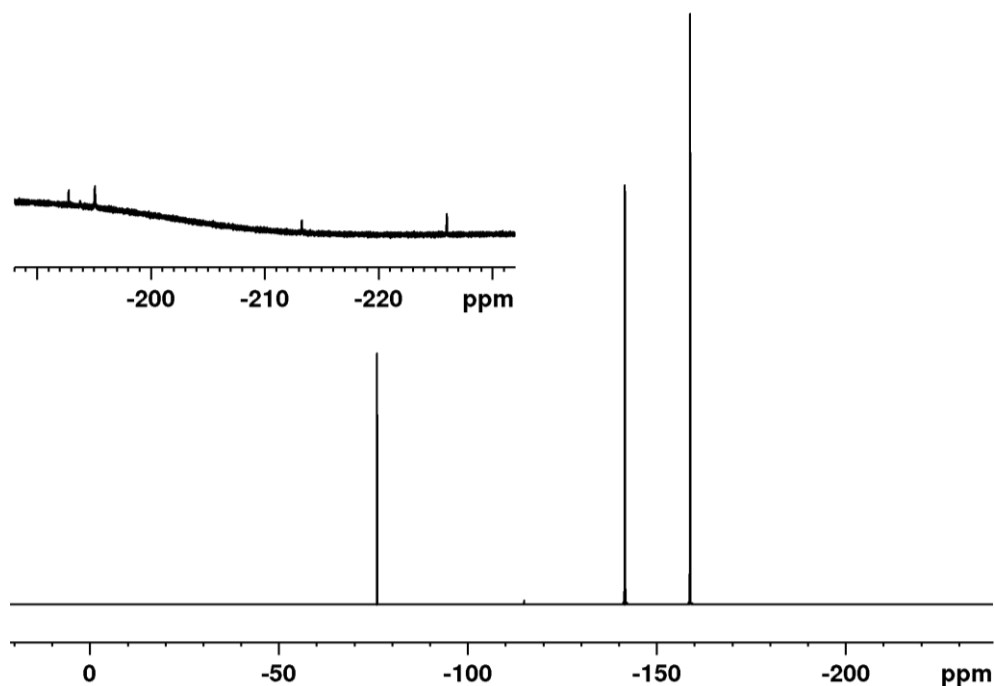


Figure S 178: $^{19}\text{F}\{^{31}\text{P}\}$ NMR spectrum (282.45 MHz, 4FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ in 4FB, after 3 d at 40 °C.

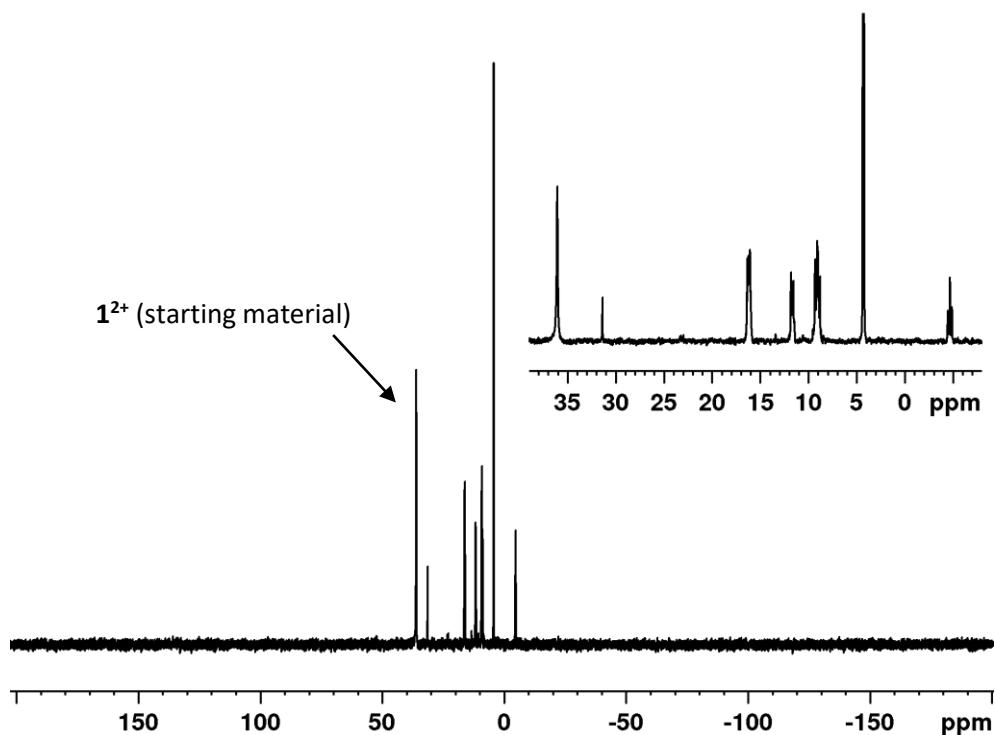


Figure S 179: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (121.51 MHz, 4FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][pf]_2$ in 4FB, after 3 d at 40 °C.

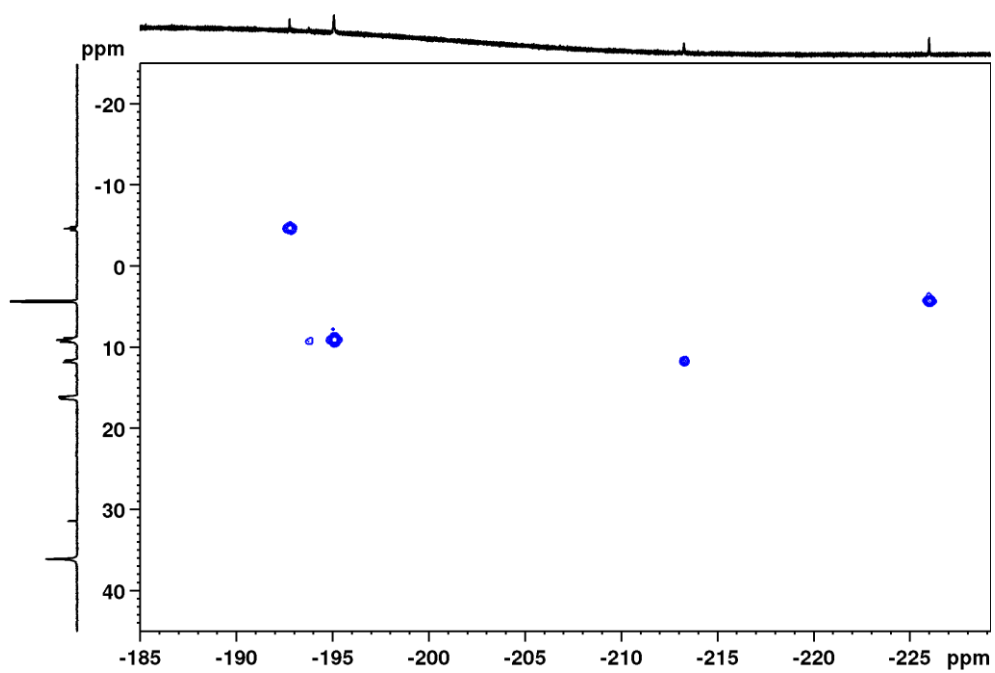


Figure S 180: ^{19}F , ^{31}P -COSY NMR spectrum (282.45 MHz, 4FB, 298 K) of $[\{\text{Ga}(\text{dcpe})\}_2][\text{pf}]_2$ in 4FB, after 3 d at 40 °C.

5 Vibrational Spectroscopy

5.1 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2934 (vw), 2859 (vw), 1637 (vw), 1508 (vw), 1451 (vw), 1414 (vw), 1351 (vw), 1297 (w), 1274 (m), 1238 (s), 1213 (vs), 1168 (m), 1049 (vw), 971 (vs), 890 (vw), 852 (vw), 830 (vw), 755 (vw), 726 (vs), 680 (vw), 644 (vw), 571 (vw), 559 (vw).

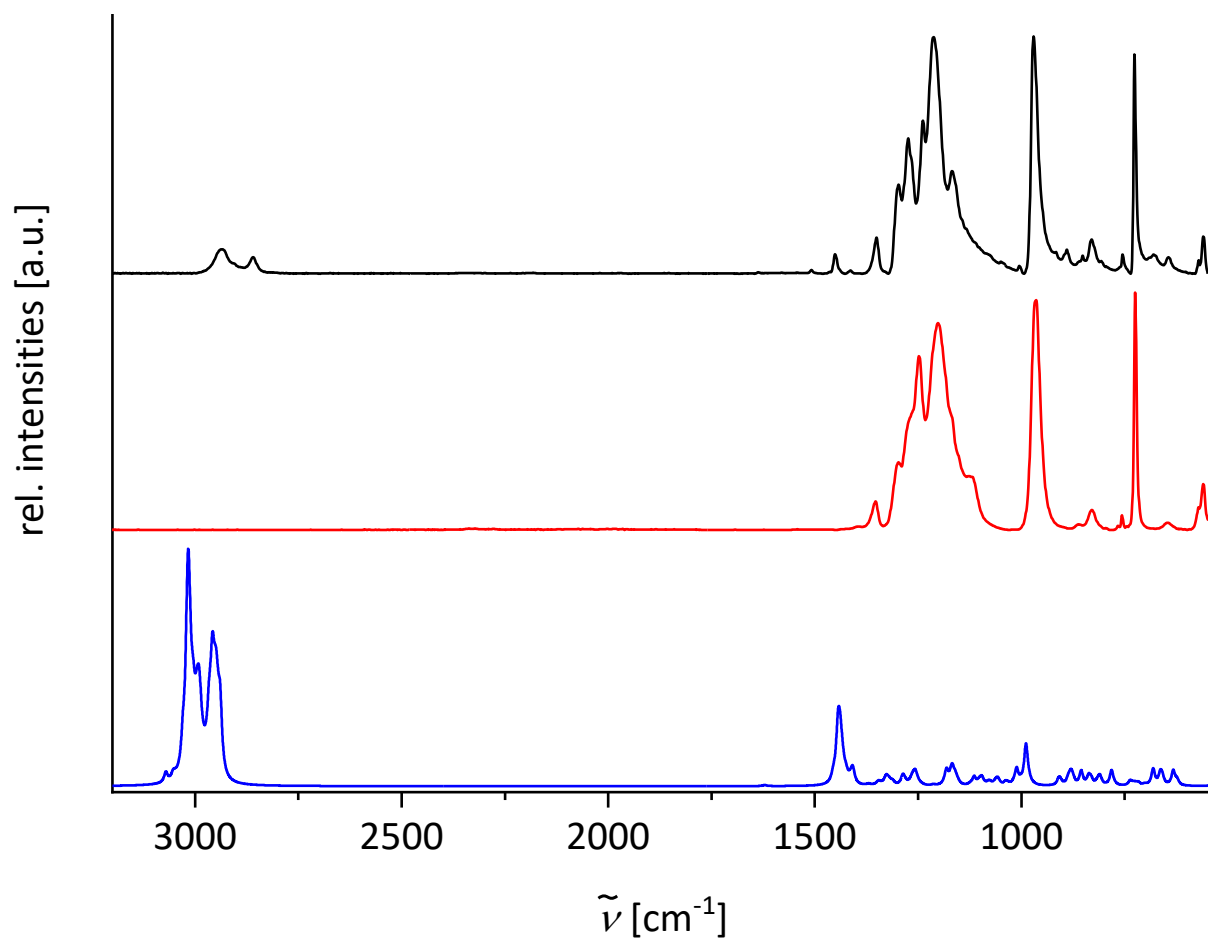


Figure S 181: Comparison of the experimental IR spectra of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$ (black) and NO[pf] (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})]^{2+}$ (blue).

Table S 11: IR bands and the assigned vibration modes in $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})][\text{pf}]_2$.

IR	Assignment
2934 (vw)	C–H (dcpe) ^a
2859 (vw)	C–H (dcpe) ^a
1637 (vw)	C=C ($\text{H}_5\text{C}_3=\text{C}_3\text{H}_5$ fragment) ^a
1508 (vw)	-
1451 (vw)	C–C, C–H (dcpe) ^a
1414 (vw)	C–H (dcpe) ^a
1351 (vw)	C–C, C–F ($[\text{pf}]^-$) ^b
1297 (w)	C–C, C–F, C–O, Al–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
1274 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1238 (s)	C–C, C–F ($[\text{pf}]^-$) ^b
1213 (vs)	C–C, C–O, C–F ($[\text{pf}]^-$) ^a
1168 (m)	C–C, C–F ($[\text{pf}]^-$) ^a
1049 (vw)	C–C, C–H (dcpe) ^a , C–H ($\text{H}_5\text{C}_3=\text{C}_3\text{H}_5$ fragment) ^a
971 (vs)	C–C, C–F ($[\text{pf}]^-$) ^b
890 (vw)	C–C, C–H (dcpe) ^a
852 (vw)	C–C, C–H (dcpe) ^a
830 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b , C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a
680 (vw)	C–C, CH_2 ($\text{H}_5\text{C}_3=\text{C}_3\text{H}_5$ fragment) ^a
644 (vw)	C–C, C–P (dcpe) ^a
571 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b
559 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.2 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2942 (vw), 2859 (vw), 1863 (vw), 1451 (vw), 1415 (vw), 1352 (vw), 1298 (w), 1274 (m), 1240 (m), 1213 (vs), 1164 (w), 1099 (vw), 1064 (vw), 1003 (vw), 971 (vs), 914 (vw), 888 (vw), 851 (vw), 833 (vw), 755 (vw), 726 (vs), 658 (vw), 643 (vw), 587 (vw), 571 (vw), 560 (vw).

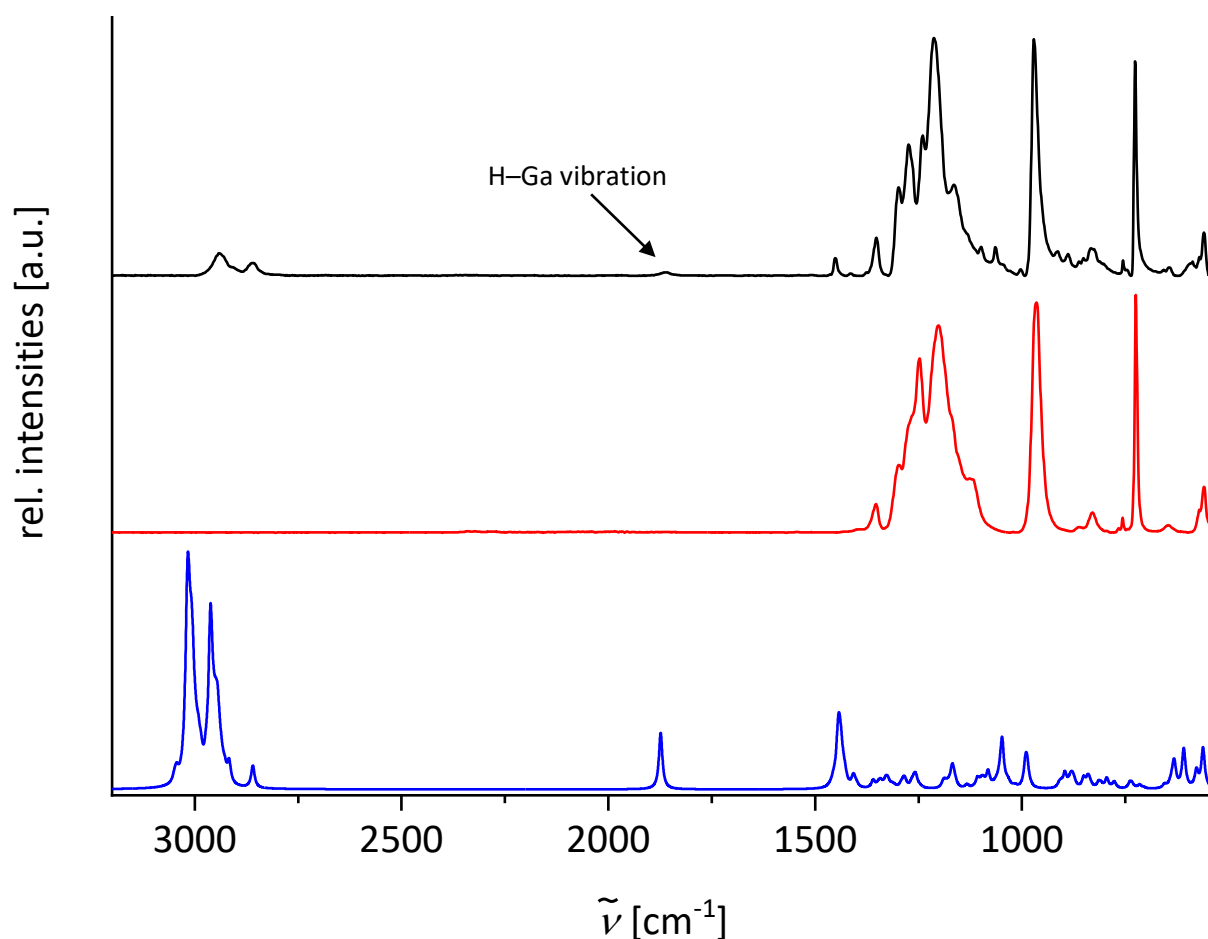


Figure S 182: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})]^{2+}$ (blue).

Table S 12: IR bands and the assigned vibration modes in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OEt})][\text{pf}]_2$.

IR	Assignment
2942 (vw)	C–H (dcpe) ^a
2859 (vw)	C–H (dcpe) ^a
1863 (vw)	Ga–H ^a
1451 (vw)	C–C, C–H (dcpe) ^a
1415 (vw)	C–H (dcpe) ^a
1352 (vw)	C–C, C–F ($[\text{pf}]^-$) ^b
1298 (w)	C–C, C–F, C–O, Al–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
1274 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1240 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1213 (vs)	C–C, C–O, C–F ($[\text{pf}]^-$) ^a
1164 (w)	C–C, C–F ($[\text{pf}]^-$) ^a
1099 (vw)	C–C, C–H (dcpe) ^a
1064 (vw)	C–O, C–C ($-\text{OCH}_2\text{CH}_3$) ^a
1003 (vw)	C–C, C–H (dcpe) ^a
971 (vs)	C–C, C–F ($[\text{pf}]^-$) ^b
914 (vw)	C–C, C–F, C–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
888 (vw)	C–C, C–H (dcpe) ^a
851 (vw)	C–C, C–H (dcpe) ^a
833 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b , C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a
658 (vw)	C–C, C–P (dcpe) ^a
643 (vw)	C–C, C–P (dcpe) ^a
587 (vw)	O–Ga, C–O, C–C ($-\text{OCH}_2\text{CH}_3$) ^a
571 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b
560 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.3 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2940 (vw), 2861 (vw), 1842 (vw), 1592 (vw), 1509 (vw), 1483 (vw), 1452 (vw), 1413 (vw), 1351 (vw), 1297 (w), 1274 (m), 1239 (s), 1210 (vs), 1166 (m), 1074 (vw), 1049 (vw), 1004 (vw), 970 (vs), 920 (vw), 889 (vw), 850 (vw), 831 (vw), 800 (vw), 756 (vw), 726 (vs), 695 (vw), 659 (vw), 645 (vw), 597 (vw), 571 (vw), 559 (vw).

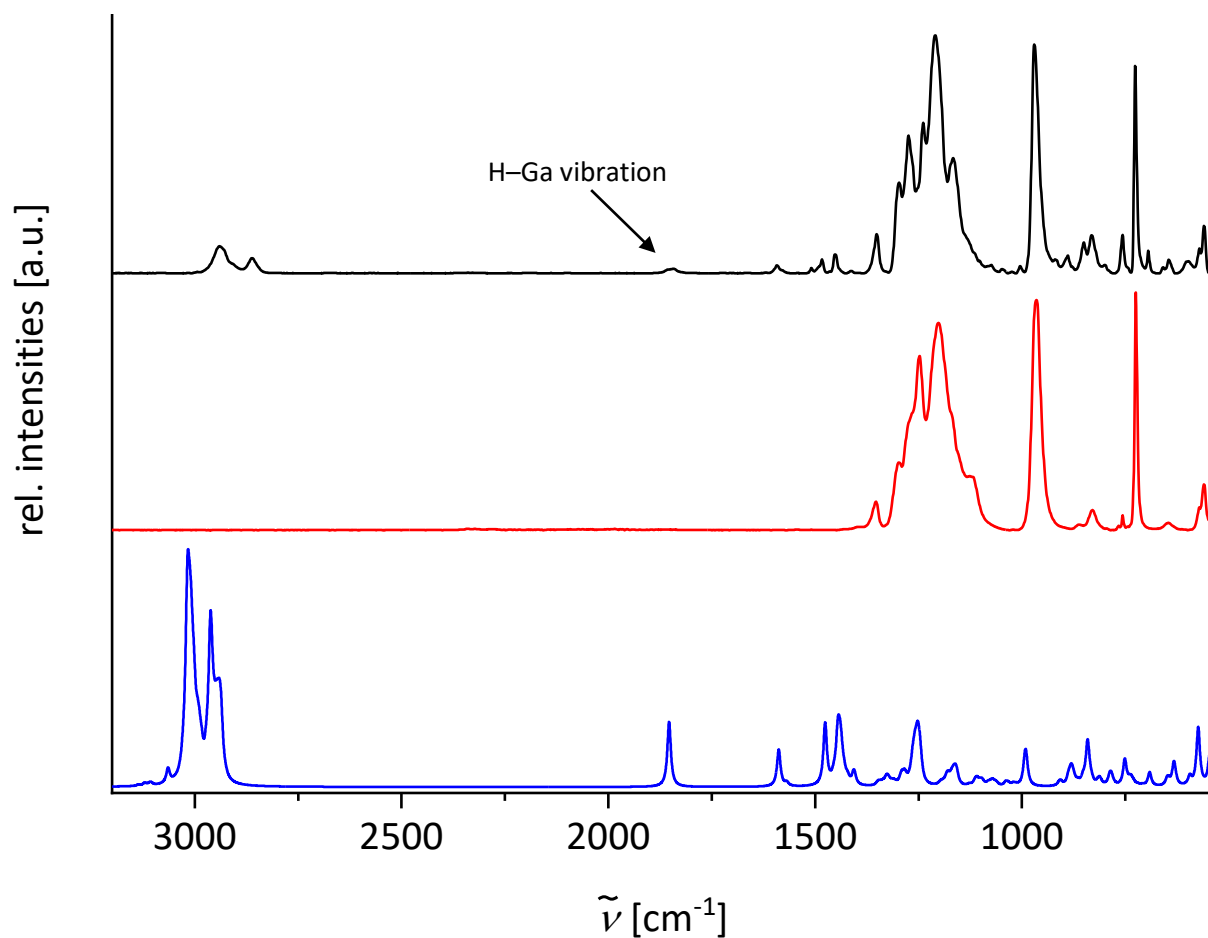


Figure S 183: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})]^{2+}$ (blue).

Table S 13: IR bands and the assigned vibration modes in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{OPh})][\text{pf}]_2$.

IR	Assignment
2940 (vw)	C–H (dcpe) ^a
2861 (vw)	C–H (dcpe) ^a
1842 (vw)	Ga–H ^a
1592 (vw)	C–C, C–O ($-\text{C}_6\text{H}_5$) ^a
1509 (vw)	-
1483 (vw)	C–H, C–C, C–O ($-\text{C}_6\text{H}_5$) ^a
1452 (vw)	C–C, C–H (dcpe) ^a
1413 (vw)	C–H (dcpe) ^a
1351 (vw)	C–C, C–F ($[\text{pf}]^-$) ^b
1297 (w)	C–C, C–F, C–O, Al–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
1274 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1239 (s)	C–C, C–F ($[\text{pf}]^-$) ^b
1210 (vs)	C–C, C–O, C–F ($[\text{pf}]^-$) ^a
1166 (m)	C–C, C–F ($[\text{pf}]^-$) ^a
1074 (vw)	C–C, C–H (dcpe) ^a
1049 (vw)	C–C, C–H (dcpe) ^a
1003 (vw)	C–C, C–H (dcpe) ^a
970 (vs)	C–C, C–F ($[\text{pf}]^-$) ^b
920 (vw)	C–C, C–F, C–O ($[\text{pf}]^-$) ^a
889 (vw)	C–C, C–H (dcpe) ^a
850 (vw)	C–C, C–H (dcpe) ^a
831 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b , C–C, C–H (dcpe) ^a
800 (vw)	C–H ($-\text{C}_6\text{H}_5$) ^a
756 (vw)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a
695 (vw)	C–H ($-\text{C}_6\text{H}_5$) ^a
659 (vw)	Ga–O, C–C ($-\text{C}_6\text{H}_5$) ^a , C–C, C–P (dcpe) ^a
645 (vw)	C–C, C–P (dcpe) ^a
597 (vw)	Ga–O, Ga–H, C–C ($-\text{C}_6\text{H}_5$) ^a
571 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b
559 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.4 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHnBu})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2942 (vw), 2863 (vw), 1862 (vw), 1453 (vw), 1417 (vw), 1351 (w), 1297 (m), 1273 (s), 1240 (s), 1211 (vs), 1164 (m), 1002 (vw), 970 (vs), 918 (vw), 889 (vw), 853 (vw), 832 (vw), 755 (vw), 726 (vs), 645 (vw), 612 (vw), 595 (vw), 571 (vw), 559 (vw).

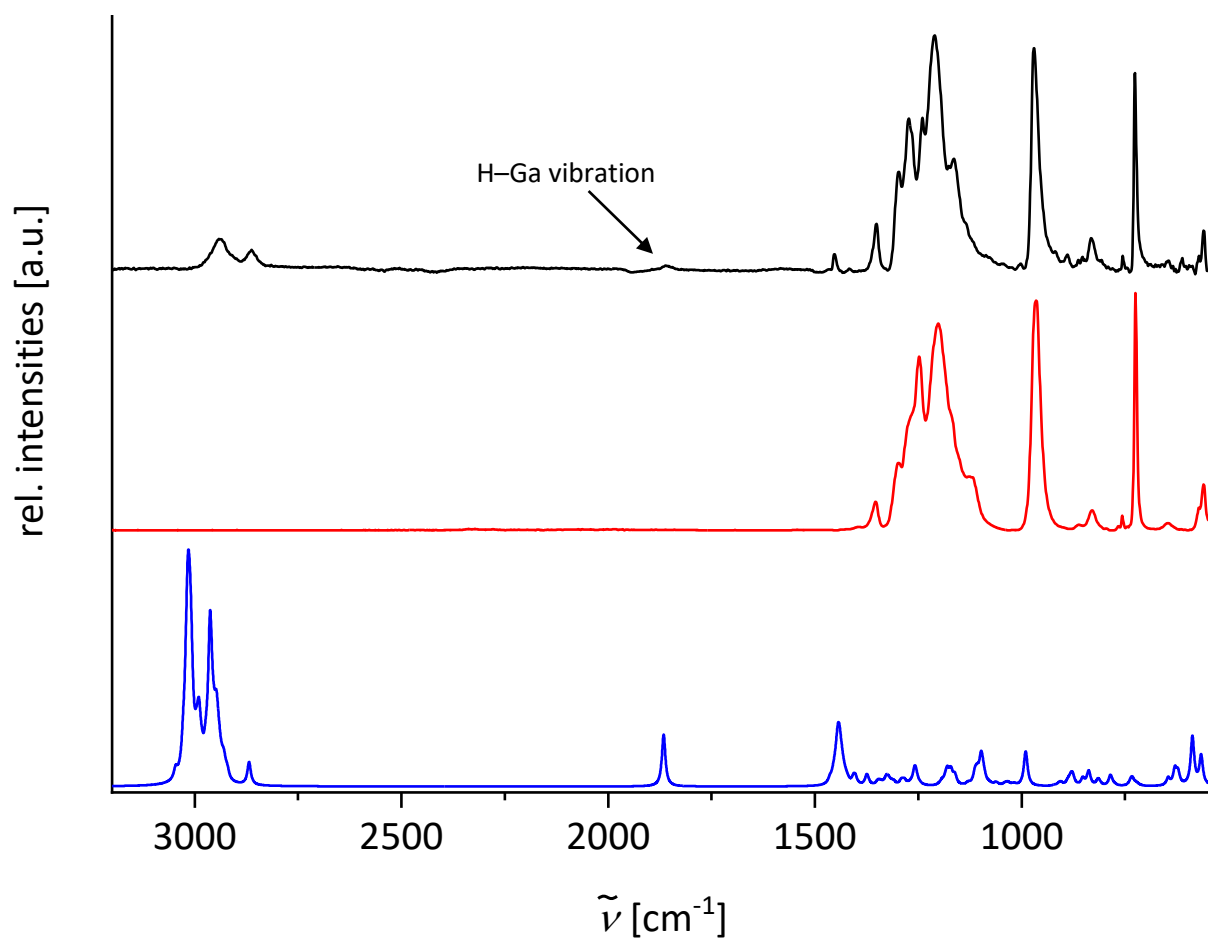


Figure S 184: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHnBu})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHnBu})]^{2+}$ (blue).

Table S 14: IR bands and the assigned vibration modes in $[H\{Ga(dcpe)\}_2(NHnBu)][pf]_2$.

IR	Assignment
2942 (vw)	C–H (dcpe) ^a
2863 (vw),	C–H (dcpe) ^a
1862 (vw)	Ga–H ^a
1453 (vw)	C–C, C–H (dcpe) ^a , C–C, C–H (–NHnBu) ^a
1417 (vw)	C–H (dcpe) ^a
1351 (w)	C–C, C–F ([<i>pf</i>] [–]) ^b
1297 (m)	C–C, C–F, C–O, Al–O ([<i>pf</i>] [–]) ^a , C–H (dcpe) ^a
1273 (s)	C–C, C–F ([<i>pf</i>] [–]) ^b
1240 (s)	C–C, C–F ([<i>pf</i>] [–]) ^b
1211 (vs)	C–C, C–O, C–F ([<i>pf</i>] [–]) ^a
1164 (m)	C–C, C–F ([<i>pf</i>] [–]) ^a
1002 (vw)	C–C, C–H (dcpe) ^a
970 (vs)	C–C, C–F ([<i>pf</i>] [–]) ^b
918 (vw)	C–C, C–F, C–O ([<i>pf</i>] [–]) ^a , C–H (dcpe) ^a
889 (vw)	C–C, C–H (dcpe) ^a
853 (vw)	C–C, C–H (dcpe) ^a
832 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b , C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ([<i>pf</i>] [–]) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ([<i>pf</i>] [–]) ^a , C–H, C–C (–NHnBu) ^a
645 (vw)	C–C, C–P (dcpe) ^a
612 (vw)	Ga–N, N–H, N–C (–NHnBu) ^a
595 (vw)	Ga–H, C–C, C–P (dcpe) ^a
571 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b
559 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.5 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPH})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2940 (vw), 2864 (vw), 1854 (vw), 1597 (vw), 1493 (vw), 1452 (vw), 1419 (vw), 1351 (vw), 1298 (w), 1275 (m), 1240 (s), 1212 (vs), 1168 (m), 1074 (vw), 1045 (vw), 1003 (vw), 971 (vs), 918 (vw), 888 (vw), 864 (vw), 849 (vw), 831 (vw), 749 (vw), 727 (vs), 690 (vw), 659 (vw), 648 (vw), 607 (vw), 571 (vw), 560 (vw).

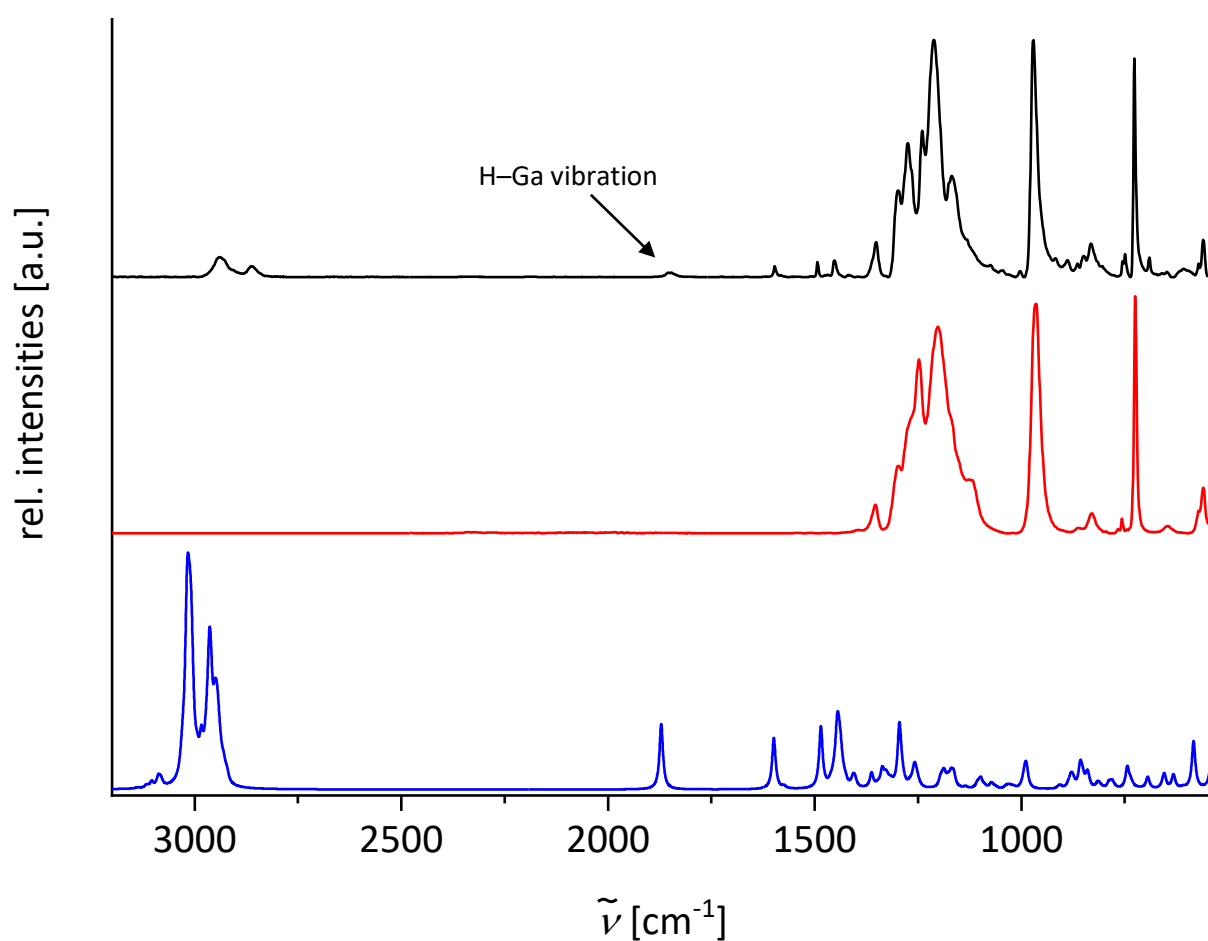


Figure S 185: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPH})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NHPH})]^{2+}$ (blue).

Table S 15: IR bands and the assigned vibration modes in $[H\{Ga(dcpe)\}_2(NHPh)][pf]_2$.

IR	Assignment
2940 (vw)	C–H (dcpe) ^a
2864 (vw),	C–H (dcpe) ^a
1854 (vw)	Ga–H ^a
1597 (vw)	C–C, C–N (–C ₆ H ₅) ^a
1493 (vw)	C–H, C–C, C–N (–C ₆ H ₅) ^a
1452 (vw)	C–C, C–H (dcpe) ^a
1419 (vw)	C–H (dcpe) ^a
1351 (vw)	C–C, C–F ([<i>pf</i>] [–]) ^b
1298 (w)	C–C, C–F, C–O, Al–O ([<i>pf</i>] [–]) ^a , C–H (dcpe) ^a
1275 (m)	C–C, C–F ([<i>pf</i>] [–]) ^b
1240 (s)	C–C, C–F ([<i>pf</i>] [–]) ^b
1212 (vs)	C–C, C–O, C–F ([<i>pf</i>] [–]) ^a
1168 (m)	C–C, C–F ([<i>pf</i>] [–]) ^a
1074 (vw)	C–C, C–H (dcpe) ^a
1045 (vw)	C–C, C–H (dcpe) ^a
1003 (vw)	C–C, C–H (dcpe) ^a
971 (vs)	C–C, C–F ([<i>pf</i>] [–]) ^b
918 (vw)	C–C, C–F, C–O ([<i>pf</i>] [–]) ^a
888 (vw)	C–C, C–H (dcpe) ^a
864 (vw)	C–C, C–H (dcpe) ^a
849 (vw)	C–C, C–H (dcpe) ^a
831 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b , C–C, C–H (dcpe) ^a
749 (vw)	C–C, C–F, Al–O ([<i>pf</i>] [–]) ^a , C–C, C–H (dcpe) ^a
727 (vs)	C–C, C–F, Al–O ([<i>pf</i>] [–]) ^a
690 (vw)	C–H (–C ₆ H ₅) ^a
659 (vw)	Ga–N, N–H, C–C (–C ₆ H ₅) ^a , C–C, C–P (dcpe) ^a
648 (vw)	C–C, C–P (dcpe) ^a
607 (vw)	Ga–N, Ga–H, N–H, C–C (–C ₆ H ₅) ^a
571 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b
560 (vw)	Al–O, C–C ([<i>pf</i>] [–]) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.6 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2937 (vw), 2861 (vw), 1834 (vw), 1585 (vw), 1483 (vw), 1451 (vw), 1351 (vw), 1298 (w), 1274 (m), 1239 (s), 1211 (vs), 1166 (w), 1134 (w), 1002 (vw), 971 (vs), 927 (vw), 915 (vw), 890 (vw), 869 (vw), 830 (vw), 752 (vw), 726 (vs), 703 (vw), 694 (vw), 605 (vw), 571 (vw), 559 (vw).

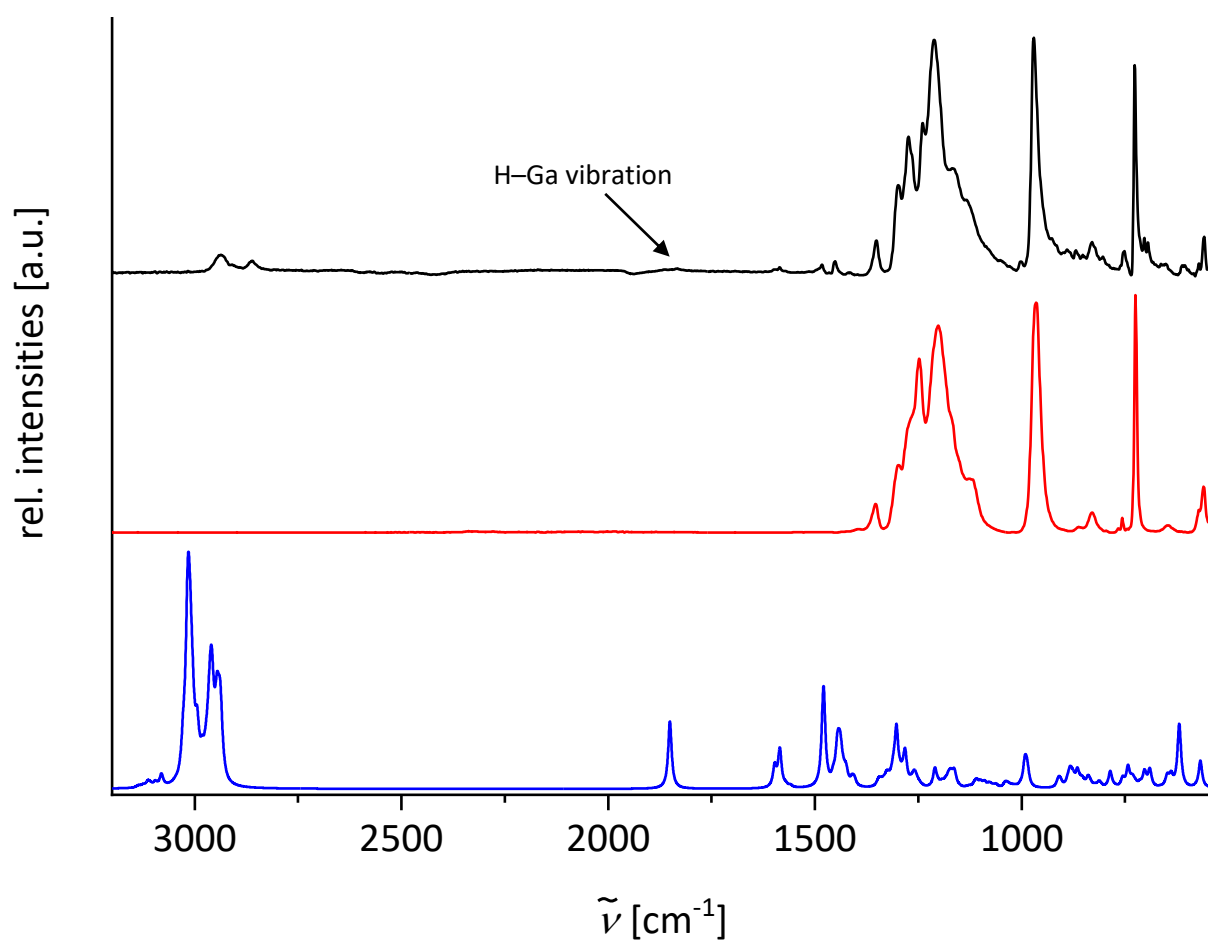


Figure S 186: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)]^{2+}$ (blue).

Table S 16: IR bands and the assigned vibration modes in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NPh}_2)][\text{pf}]_2$.

IR	Assignment
2937 (vw)	C–H (dcpe) ^a
2861 (vw)	C–H (dcpe) ^a
1834 (vw)	Ga–H ^a
1585 (vw)	C–C, C–N ($-\text{C}_6\text{H}_5$) ^a
1483 (vw)	C–H, C–C, C–N ($-\text{C}_6\text{H}_5$) ^a
1451 (vw)	C–C, C–H (dcpe) ^a , C–C, C–H ($-\text{C}_6\text{H}_5$) ^a
1351 (vw)	C–C, C–F ($[\text{pf}]^-$) ^b
1298 (w)	C–C, C–F, C–O, Al–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a , C–H ($-\text{C}_6\text{H}_5$) ^a
1274 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1239 (s)	C–C, C–F ($[\text{pf}]^-$) ^b
1211 (vs)	C–C, C–O, C–F ($[\text{pf}]^-$) ^a
1166 (w)	C–C, C–F ($[\text{pf}]^-$) ^a
1134 (w)	C–C, C–H (dcpe) ^a
1002 (vw)	C–C, C–H (dcpe) ^a
971 (vs)	C–C, C–F ($[\text{pf}]^-$) ^b
927 (vw)	-
915 (vw)	C–C, C–F, C–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a , C–H ($-\text{C}_6\text{H}_5$) ^a
890 (vw)	C–C, C–H (dcpe) ^a
869 (vw)	C–C, C–H (dcpe) ^a
830 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b , C–C, C–H (dcpe) ^a
752 (vw)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a
703 (vw)	C–C, C–P (dcpe) ^a , C–H ($-\text{C}_6\text{H}_5$) ^a
694 (vw)	C–H ($-\text{C}_6\text{H}_5$) ^a
605 (vw)	Ga–H, Ga–N, C–C ($-\text{C}_6\text{H}_5$) ^a
571 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b
559 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.7 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2940 (vw), 2862 (vw), 2223 (vw), 1851 (vw), 1509 (vw), 1453 (vw), 1351 (vw), 1296 (w), 1272 (m), 1238 (s), 1208 (vs), 1177 (m), 1164 (m), 1134 (w), 1102 (vw), 1085 (vw), 1000 (vw), 969 (vs), 918 (vw), 890 (vw), 853 (vw), 832 (vw), 755 (vw), 725 (s), 650 (vw), 571 (vw), 560 (vw).

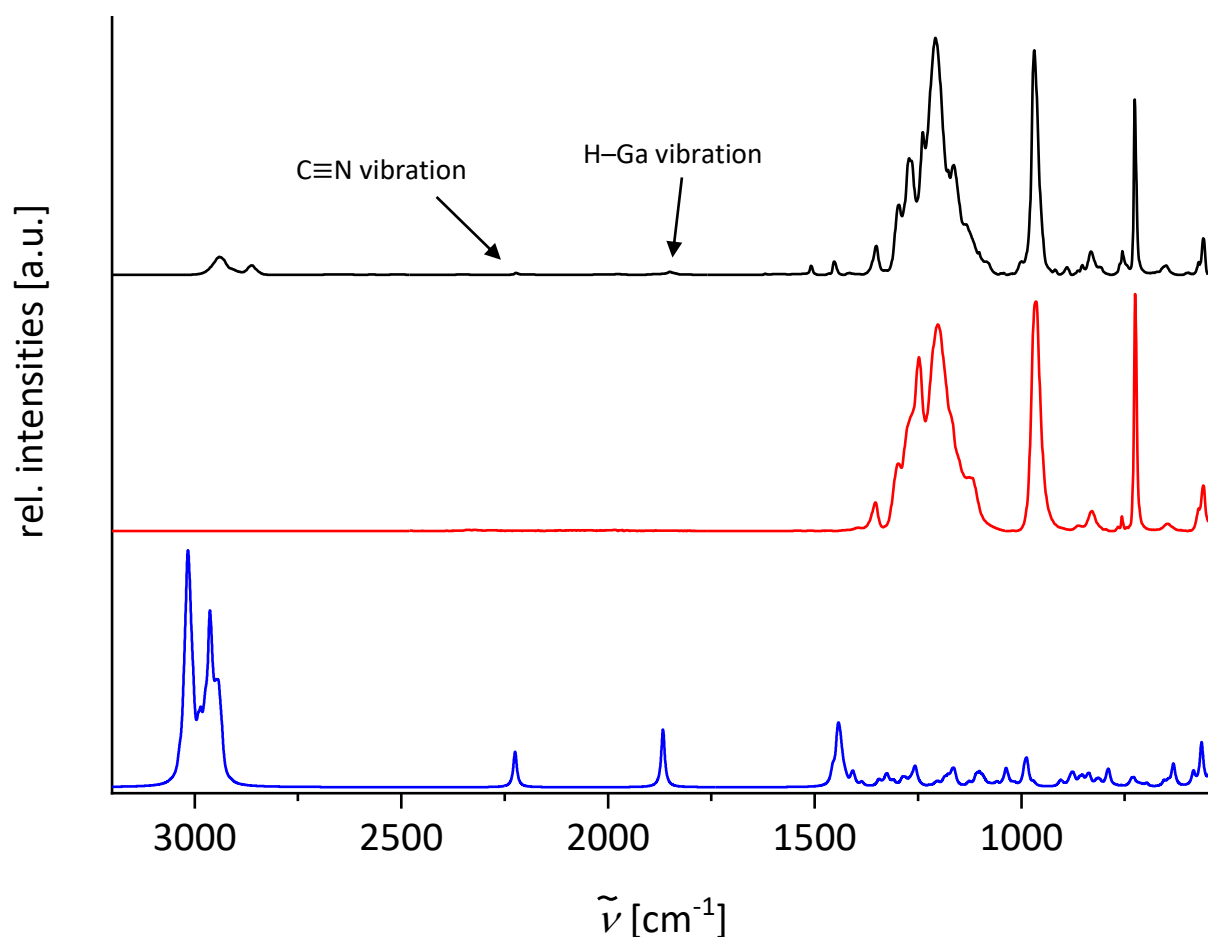


Figure S 187: Comparison of the experimental IR spectra of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$ (black) and NO[*pf*] (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})]^{2+}$ (blue).

Table S 17: IR bands and the assigned vibration modes in $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$.

IR	Assignment
2940 (vw)	C–H (dcpe) ^a
2862 (vw)	C–H (dcpe) ^a
2223 (vw)	$\text{C}\equiv\text{N}$ (CH_2CN fragment) ^a
1851 (vw)	Ga–H ^a
1509 (vw)	-
1453 (vw)	C–C, C–H (dcpe) ^a
1351 (vw)	C–C, C–F ($[\text{pf}]^-$) ^b
1296 (w)	C–C, C–F, C–O, Al–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
1272 (m)	C–C, C–F ($[\text{pf}]^-$) ^b
1238 (s)	C–C, C–F ($[\text{pf}]^-$) ^b
1208 (vs)	C–C, C–O, C–F ($[\text{pf}]^-$) ^a
1177 (m)	C–C, C–F ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
1164 (m)	C–C, C–F ($[\text{pf}]^-$) ^a
1134 (w)	-
1102 (vw)	C–C, C–H (dcpe) ^a , CH_2 (CH_2CN fragment) ^a
1085 (vw)	C–C, C–H (dcpe) ^a , CH_2 (CH_2CN fragment) ^a
1000 (vw)	C–C, C–H (dcpe) ^a
969 (s)	C–C, C–F ($[\text{pf}]^-$) ^b
918 (vw)	C–C, C–F, C–O ($[\text{pf}]^-$) ^a , C–H (dcpe) ^a
890 (vw)	C–C, C–H (dcpe) ^a
853 (vw)	C–C, C–H (dcpe) ^a
832 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b , C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a , C–C, C–H (dcpe) ^a
725 (s)	C–C, C–F, Al–O ($[\text{pf}]^-$) ^a
650 (vw)	C–C, C–P (dcpe) ^a
571 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b
560 (vw)	Al–O, C–C ($[\text{pf}]^-$) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.8 $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2940 (vw), 2864 (vw), 2221 (vw), 1508 (vw), 1453 (vw), 1418 (vw), 1351 (vw), 1298 (w), 1273 (s), 1240 (s), 1210 (vs), 1177 (m), 1164 (m), 1079 (vw), 1003 (vw), 970 (vs), 919 (vw), 890 (vw), 863 (vw), 852 (vw), 831 (vw), 755 (vw), 726 (vs), 657 (vw), 649 (vw), 583 (vw), 571 (vw), 560 (w).

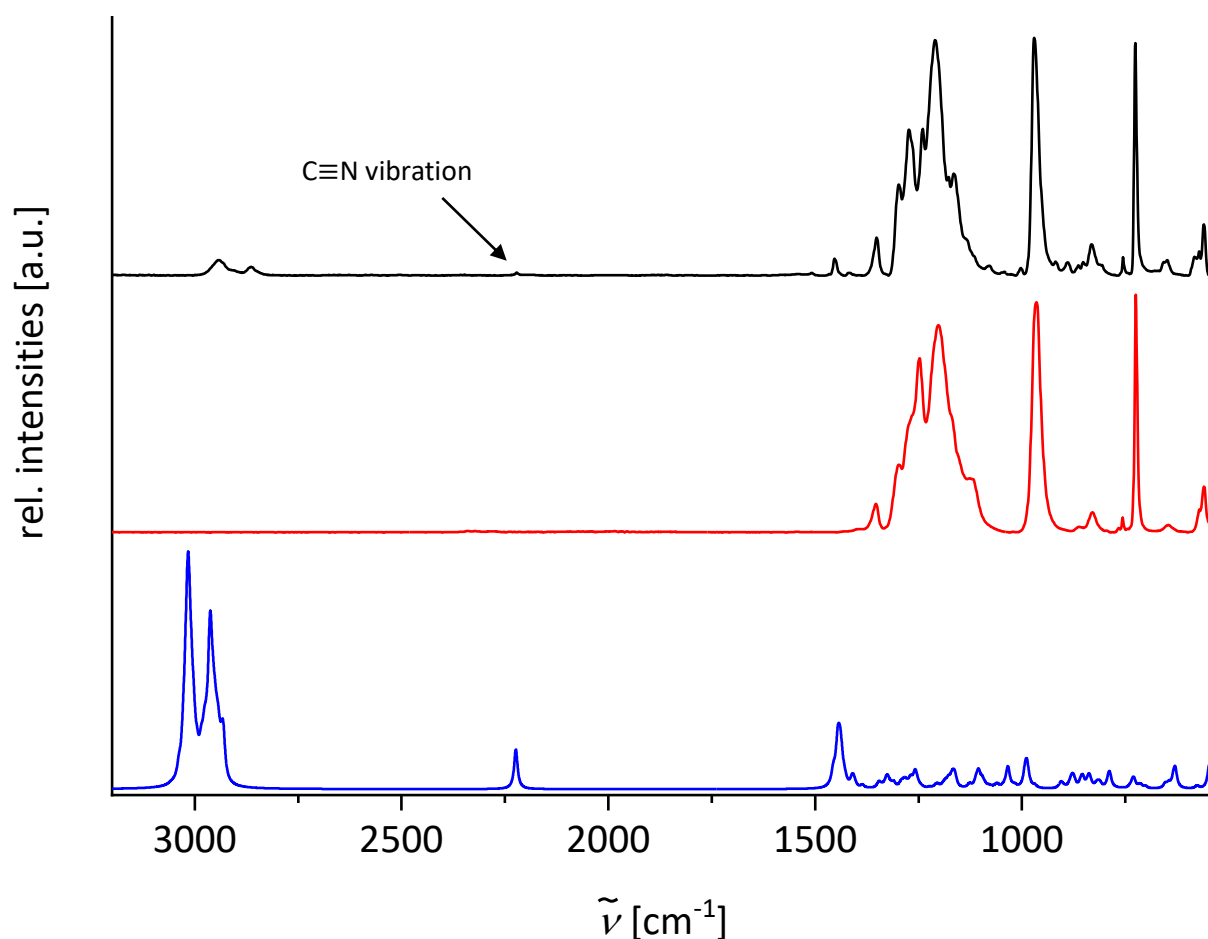


Figure S 188: Comparison of the experimental IR spectra of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})]^{2+}$ (blue).

Table S 18: IR bands and the assigned vibration modes in $[F\{Ga(dcpe)\}_2(CH_2CN)][pf]_2$.

IR	Assignment
2940 (vw)	C–H (dcpe) ^a
2864 (vw)	C–H (dcpe) ^a
2221 (vw)	C≡N (CH ₂ CN fragment) ^a
1508 (vw)	-
1453 (vw)	C–C, C–H (dcpe) ^a
1418 (vw)	C–H (dcpe) ^a
1351 (vw)	C–C, C–F ([<i>pf</i>] [−]) ^b
1298 (w)	C–C, C–F, C–O, Al–O ([<i>pf</i>] [−]) ^a , C–H (dcpe) ^a
1273 (s)	C–C, C–F ([<i>pf</i>] [−]) ^b
1240 (s)	C–C, C–F ([<i>pf</i>] [−]) ^b
1210 (vs)	C–C, C–O, C–F ([<i>pf</i>] [−]) ^a
1177 (m)	C–C, C–F ([<i>pf</i>] [−]) ^a , C–H (dcpe) ^a
1164 (m)	C–C, C–F ([<i>pf</i>] [−]) ^a
1079 (vw)	C–C, C–H (dcpe) ^a , CH ₂ (CH ₂ CN fragment) ^a
1003 (vw)	C–C, C–H (dcpe) ^a
970 (vs)	C–C, C–F ([<i>pf</i>] [−]) ^b
919 (vw)	C–C, C–F, C–O ([<i>pf</i>] [−]) ^a , C–H (dcpe) ^a
890 (vw)	C–C, C–H (dcpe) ^a
863 (vw)	C–C, C–H (dcpe) ^a
852 (vw)	C–C, C–H (dcpe) ^a
831 (vw)	Al–O, C–C ([<i>pf</i>] [−]) ^b , C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ([<i>pf</i>] [−]) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ([<i>pf</i>] [−]) ^a
657 (vw)	C–C, C–P (dcpe) ^a
649 (vw)	C–C, C–P (dcpe) ^a
583 (vw)	Ga–C, C–C, C–N (CH ₂ CN fragment) ^a
571 (vw)	Al–O, C–C ([<i>pf</i>] [−]) ^b
560 (w)	Al–O, C–C ([<i>pf</i>] [−]) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.9 $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2943 (vw), 2862 (vw), 1835 (vw), 1751 (vw), 1674 (vw), 1452 (vw), 1414 (vw), 1352 (w), 1297 (m), 1274 (s), 1240 (s), 1213 (vs), 1164 (m), 1077 (vw), 1043 (vw), 1003 (vw), 971 (vs), 918 (vw), 889 (vw), 834 (vw), 756 (vw), 726 (vs), 641 (vw), 586 (vw), 572 (vw), 560 (w).

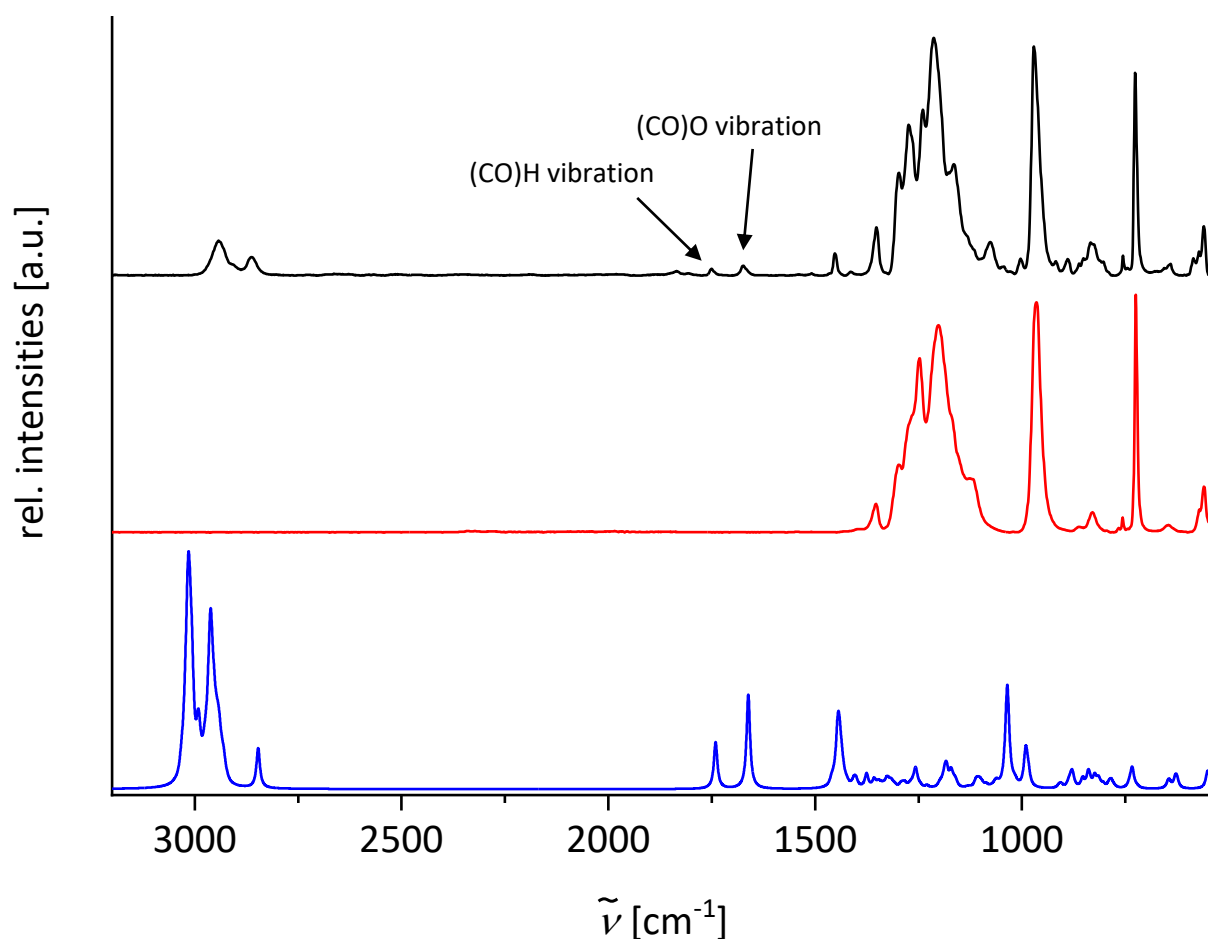


Figure S 189: Comparison of the experimental IR spectra of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})][\text{pf}]_2$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{COOCH}_2\text{CHO})]^{2+}$ (blue).

Table S 19: IR bands and the assigned vibration modes in $[F\{Ga(dcpe)\}_2(COOCH_2CHO)][pf]_2$.

IR	Assignment
2943 (vw)	C–H (dcpe) ^a
2862 (vw)	C–H (dcpe) ^a
1835 (vw)	-
1751 (vw)	(C=O)H (COOCH ₂ CHO fragment) ^a
1674 (vw)	(C=O)O (COOCH ₂ CHO fragment) ^a
1452 (vw)	C–C, C–H (dcpe) ^a
1414 (vw)	C–H (dcpe) ^a
1352 (w)	C–C, C–F ([<i>pf</i>] ⁻) ^b
1297 (m)	C–C, C–F, C–O, Al–O ([<i>pf</i>] ⁻) ^a , C–H (dcpe) ^a
1274 (s)	C–C, C–F ([<i>pf</i>] ⁻) ^b
1240 (s)	C–C, C–F ([<i>pf</i>] ⁻) ^b , CH ₂ (COOCH ₂ CHO fragment) ^a
1213 (vs)	C–C, C–O, C–F ([<i>pf</i>] ⁻) ^a
1164 (m)	C–C, C–F ([<i>pf</i>] ⁻) ^a
1077 (vw)	C–C, C–H (dcpe) ^a
1043 (vw)	C–C, C–H (dcpe) ^a , C–O, C–C (COOCH ₂ CHO fragment) ^a
1003 (vw)	C–C, C–H (dcpe) ^a
971 (vs)	C–C, C–F ([<i>pf</i>] ⁻) ^b
918 (vw)	C–C, C–F, C–O ([<i>pf</i>] ⁻) ^a , C–H (dcpe) ^a
889 (vw)	C–C, C–H (dcpe) ^a
834 (vw)	Al–O, C–C ([<i>pf</i>] ⁻) ^b , C–C, C–H (dcpe) ^a
756 (vw)	C–C, C–F, Al–O ([<i>pf</i>] ⁻) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ([<i>pf</i>] ⁻) ^a
641 (vw)	C–C, C–P (dcpe) ^a
586 (vw)	Ga–C, C–C, C–N (CH ₂ CN fragment) ^a
572 (vw)	Al–O, C–C ([<i>pf</i>] ⁻) ^b
560 (w)	Al–O, C–C ([<i>pf</i>] ⁻) ^b

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

5.10 $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfal}]_{1/3}$

FT-IR: $\tilde{\nu}$ [cm^{-1}] = 2938 (vw), 2865 (vw), 1608 (vw), 1453 (vw), 1418 (vw), 1351 (vw), 1298 (w), 1274 (m), 1240 (s), 1210 (vs), 1167 (m), 1087 (vw), 1004 (vw), 970 (vs), 918 (vw), 890 (vw), 866 (vw), 852 (vw), 824 (vw), 803 (vw), 787 (vw), 755 (vw), 726 (vs), 649 (vw), 571 (vw), 560 (vw).

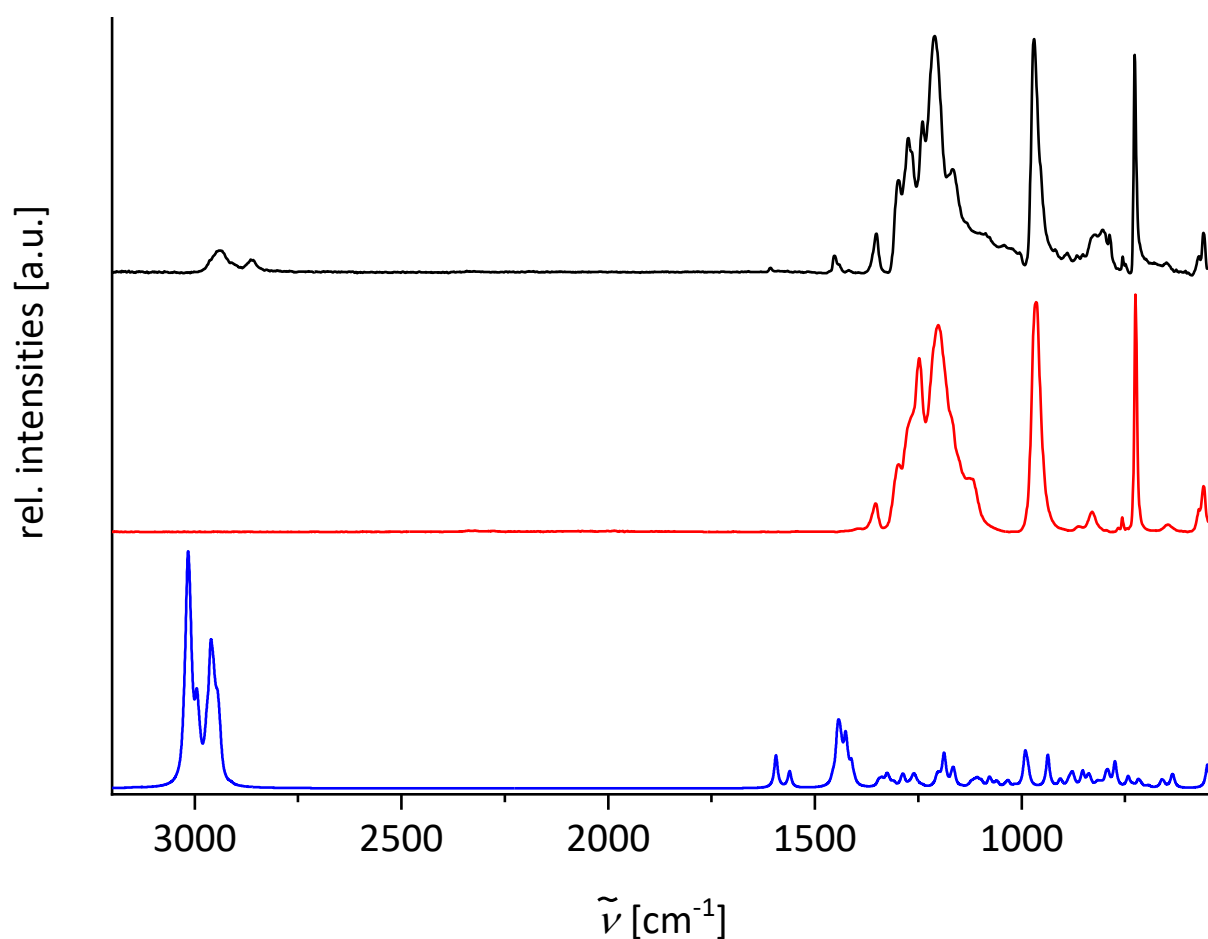


Figure S 190: Comparison of the experimental IR spectra of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)][\text{pf}]_{5/3}[\text{alfal}]_{1/3}$ (black) and $\text{NO}[\text{pf}]$ (red) with the calculated IR spectrum (RI-BP86(D3BJ)/def2-TZVPP) of $[\text{F}\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_2\text{H}_3)]^{2+}$ (blue).

Table S 20: IR bands and the assigned vibration modes in $[F\{Ga(dcpe)\}_2(C_6F_2H_3)][pf]_{5/3}[alfa]_{1/3}$.

IR	Assignment
2938 (vw)	C–H (dcpe) ^a
2865 (vw)	C–H (dcpe) ^a
1608 (vw)	C–C ($-C_6F_2H_3$) ^a
1453 (vw)	C–C, C–H (dcpe) ^a
1418 (vw)	C–H (dcpe) ^a
1351 (vw)	C–C, C–F ($[pf]^-$) ^b
1298 (w)	C–C, C–F, C–O, Al–O ($[pf]^-$) ^a , C–H (dcpe) ^a
1274 (m)	C–C, C–F ($[pf]^-$) ^b
1240 (s)	C–C, C–F ($[pf]^-$) ^b
1210 (vs)	C–C, C–O, C–F ($[pf]^-$) ^a
1167 (m)	C–C, C–F ($[pf]^-$) ^a
1087 (vw)	C–C, C–H (dcpe) ^a
1004 (vw)	C–C, C–H (dcpe) ^a
970 (vs)	C–C, C–F ($[pf]^-$) ^b
918 (vw)	C–C, C–F, C–O ($[pf]^-$) ^a , C–H (dcpe) ^a
890 (vw)	C–C, C–H (dcpe) ^a
866 (vw)	C–H ($-C_6F_2H_3$) ^a
852 (vw)	C–C, C–H (dcpe) ^a
824 (vw)	Al–O, C–C ($[pf]^-$) ^b , C–C, C–H (dcpe) ^a
803 (vw)	C–C, C–H (dcpe) ^a
787 (vw)	C–C, C–H (dcpe) ^a
755 (vw)	C–C, C–F, Al–O ($[pf]^-$) ^a , C–C, C–H (dcpe) ^a
726 (vs)	C–C, C–F, Al–O ($[pf]^-$) ^a
649 (vw)	C–C, C–P (dcpe) ^a
571 (vw)	Al–O, C–C ($[pf]^-$) ^b
560 (vw)	Al–O, C–C ($[pf]^-$) ^b , Ga–F ^a

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 6). b) Assignments based on literature values.^[34–36]

6 Quantum Chemical Calculations

6.1 EDA-NOCV Analysis

6.1.1 $[\{\text{Ga}(\text{dcpe})\}_2]^{2+} + \text{HOMe}$

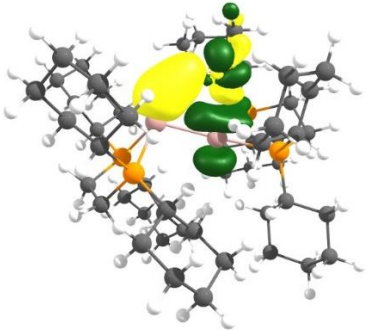
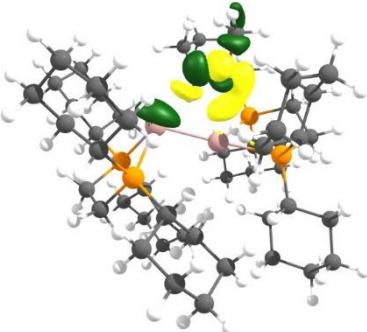
Energies	Orbital Interaction	Interacting Fragments: $[\{\text{Ga}(\text{dcpe})\}_2]^{2+} + \text{HOMe}$
ΔE_{int}		-16.8
ΔE_{Pauli}		38.7
$\Delta E_{\text{disp}}^{\text{I}}$		-11.1 (20.0 %)
$\Delta E_{\text{elstat}}^{\text{I}}$		-25.9 (46.6 %)
$\Delta E_{\text{orb}}^{\text{I}}$		-18.6 (33.5 %)
$\Delta E_{\text{orb}(1)}^{\text{II}}$	 $p(\text{HOMO and HOMO-1}) \rightarrow \sigma^*(\text{LUMO})$ and $s(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO})$	-9.41 (50.7 %) $ \nu_1=0.33 $
$\Delta E_{\text{orb}(2)}^{\text{II}}$	 $s(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO})$	-3.07 (16.5 %) $ \nu_2=0.16 $
$\Delta E_{\text{orb}(\text{rest})}^{\text{II}}$		-6.07 (32.7 %)

Figure S 191: Results of the EDA-NOCV analysis of the $1^{2+}/\text{HOMe}$ adduct. The shape of the deformation densities $\Delta\rho_{(1)}$ and $\Delta\rho_{(2)}$, corresponding to $\Delta E_{\text{orb}(1)}$ and $\Delta E_{\text{orb}(2)}$, are shown exemplarily (isosurface values: 0.0008 au). The eigenvalues ν_1 and ν_2 give the size of the charge migration in e. The direction of the charge flow of the deformation densities is green→yellow. All calculations were performed at the BP86(D3BJ)/def2-TZVPP level of theory; energy values are given in kcal mol⁻¹ instead of the typically recommended kJ mol⁻¹ for better comparability with other EDA-NOCV analyses in the literature. I) Values in parentheses show the contribution to the total attractive interaction. II) Values in parentheses show the contribution to the total orbital interaction ΔE_{orb} .

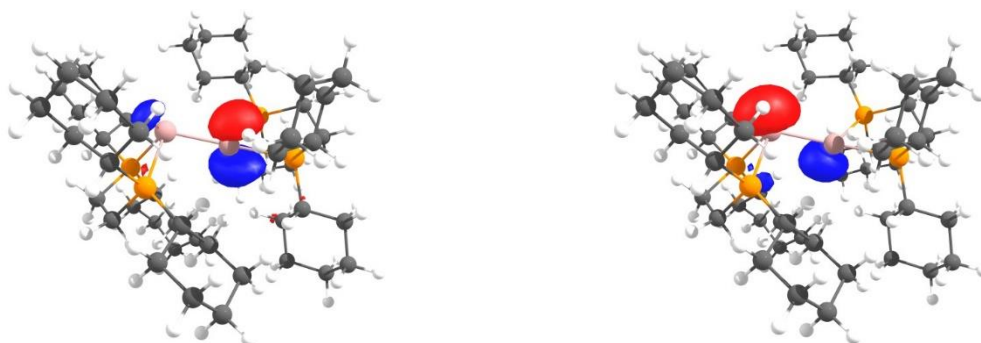


Figure S 192: LUMO (left) and HOMO (right) of the conformer of 1^{2+} interacting with H₂O (contour value: 0.06 au).



Figure S 193: HOMO (left), HOMO-1 (middle) and LUMO (right) of H₂O interacting with 1^{2+} (contour value: 0.08 au).

6.1.2 $[\{\text{Ga}(\text{dcpe})\}_2]^{2+} + \text{HNMe}_2$

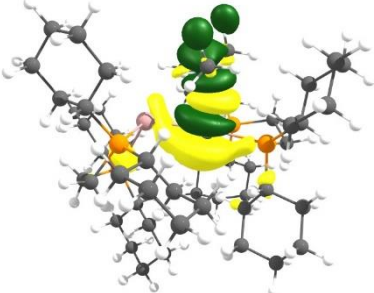
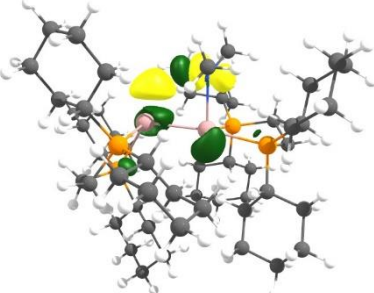
Energies	Orbital Interaction	Interacting Fragments: $[\{\text{Ga}(\text{dcpe})\}_2]^{2+} + \text{HNMe}_2$
ΔE_{int}		-37.1
ΔE_{Pauli}		97.3
$\Delta E_{\text{disp}}^{\text{I}}$		-19.4 (14.4 %)
$\Delta E_{\text{elstat}}^{\text{I}}$		-68.1 (50.6 %)
$\Delta E_{\text{orb}}^{\text{I}}$		-47.0 (34.9 %)
$\Delta E_{\text{orb}(1)}^{\text{II}}$	 $p(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO})$	-31.6 (67.3 %) $ \nu_1=0.55 $
$\Delta E_{\text{orb}(2)}^{\text{II}}$	 $s(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO and LUMO}+1)$	-2.79 (5.9 %) $ \nu_2=0.20 $
$\Delta E_{\text{orb}(\text{rest})}^{\text{II}}$		-12.6 (26.8 %)

Figure S 194: Results of the EDA-NOCV analysis of the $1^{2+}/\text{HNMe}_2$ adduct. The shape of the deformation densities $\Delta\rho_{(1)}$ and $\Delta\rho_{(2)}$, corresponding to $\Delta E_{\text{orb}(1)}$ and $\Delta E_{\text{orb}(2)}$, are shown exemplarily (isosurface values: 0.0008 au). The eigenvalue ν_1 and ν_2 give the size of the charge migration in e. The direction of the charge flow of the deformation densities is green→yellow. All calculations were performed at the BP86(D3BJ)/def2-TZVPP level of theory; energy values are given in kcal mol⁻¹ instead of the typically recommended kJ mol⁻¹ for better comparability with other EDA-NOCV analyses in the literature. I) Values in parentheses show the contribution to the total attractive interaction. II) Values in parentheses show the contribution to the total orbital interaction ΔE_{orb} .

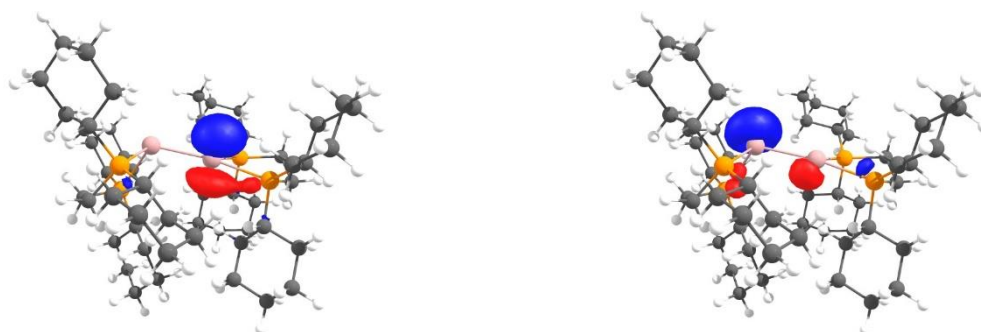


Figure S 195: LUMO (left) and HOMO (right) of $\mathbf{1}^{2+}$ interacting with HNMe_2 (contour value: 0.06 au).

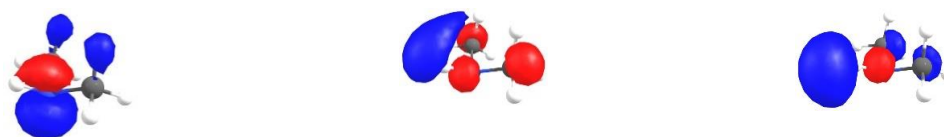


Figure S 196: HOMO (left), LUMO (middle) and LUMO+1 (right) of HNMe_2 interacting with $\mathbf{1}^{2+}$ (contour value: 0.08 au for the HOMO and 0.05 for the LUMO and LUMO+1).

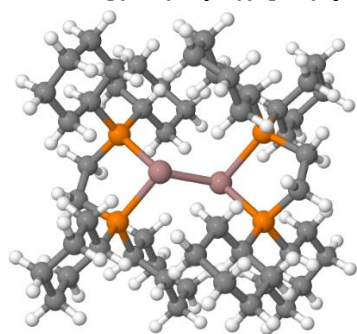
6.1.3 Summary of the EDA-NOCV Analysis

Deformation Density	Donor Fragment	Acceptor Fragment	Energies	Orbital Interaction (for E = N)	E = N, n = 2	E = O, n = 1
$\Delta\rho_{(1)}$	HOMO	LUMO	ΔE_{int}		-37.1	-16.8
			ΔE_{Pauli}		97.3	38.7
			$\Delta E_{\text{disp}}^{\text{i}}$		-19.4	-11.1
					(14.4 %)	(20.0 %)
			$\Delta E_{\text{elstat}}^{\text{i}}$		-68.1	-25.9
					(50.6 %)	(46.6 %)
			$\Delta E_{\text{orb}}^{\text{i}}$		-47.0	-18.6
					(34.9 %)	(33.5 %)
					-31.6	-9.41
$\Delta\rho_{(2)}$	HOMO	LUMO	$\Delta E_{\text{orb}(1)}^{\text{ii}}$	$p(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO})$	(67.3 %)	(50.7 %)
					$ v_1 =0.55 $	$ v_1 =0.33 $
		LUMO+1	$\Delta E_{\text{orb}(2)}^{\text{ii}}$	$s(\text{HOMO}) \rightarrow \sigma^*(\text{LUMO and LUMO}+1)$	-2.79	-3.07
					(5.9 %)	(16.5 %)
					$ v_2 =0.20 $	$ v_2 =0.16 $
			$\Delta E_{\text{orb}(\text{rest})}^{\text{ii}}$		-12.6	-6.07
					(26.8 %)	(32.7 %)

Figure S 197: EDA-NOCV results for $1^{2+}/\text{HOMe}$ and $1^{2+}/\text{HNMe}_2$ using the digallene and HOMe or HNMe₂ as interacting fragments. The shape of the deformation densities $\Delta\rho_{(1)-(2)}$, corresponding to $\Delta E_{\text{orb}(1)-(2)}$, and the fragment orbitals of 1^{2+} and HNMe₂ are shown exemplarily (isosurface values: 0.0008 au for $\Delta\rho_{(1)-(2)}$, 0.06 au for the molecular orbitals of 1^{2+} , 0.08 au for the HOMO of HNMe₂ and 0.05 au for the LUMO(+1) of HNMe₂). The eigenvalues $|v_1|$ and $|v_2|$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is green $\rightarrow$ yellow. All calculations were performed at the RI-BP86(D3BJ)/def2-TZVPP level of theory; energy values are given in kcal mol⁻¹ instead of kJ mol⁻¹ for better comparability with other EDA-NOCV analyses in the literature. ⁱ Values in parentheses show the contribution to the total attractive interaction. ⁱⁱ Values in parentheses show the contribution to the total orbital interaction ΔE_{orb} .

6.2 Optimized Geometries

6.2.1 $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$ (symmetric)



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: ci

Cartesian coordinates in Ångström:

Ga	0.1584484	0.1534239	-1.1905059
P	-1.3652058	-1.2914867	-2.4666176
P	-1.1570485	1.9737759	-2.1938223
C	-0.4055903	-2.5017094	-3.4750943
H	0.0137175	-3.1910370	-2.7201302
C	0.7774284	-1.8139854	-4.1772143
H	0.3983797	-1.0681914	-4.8945718
H	1.3853137	-1.2638291	-3.4389707
C	1.6369421	-2.8384969	-4.9271827
H	2.4573215	-2.3237125	-5.4458349
H	2.1033284	-3.5184107	-4.1955495
C	0.7964228	-3.6508002	-5.9177769
H	1.4224353	-4.4011099	-6.4187605
H	0.4178687	-2.9827826	-6.7090721
C	-0.3847753	-4.3297025	-5.2182058
H	-0.0074669	-5.0787867	-4.5024945
H	-1.0026757	-4.8750705	-5.9441454
C	-1.2559371	-3.3139886	-4.4651322
H	-2.0724400	-3.8332543	-3.9439414
H	-1.7239068	-2.6284249	-5.1903522
C	-2.6657171	-2.2562157	-1.5764739
H	-3.2235232	-2.7836203	-2.3699495
C	-2.0268698	-3.2921656	-0.6413073
H	-1.3664001	-3.9690668	-1.2015310
H	-1.3954349	-2.7542711	0.0885046
C	-3.0975920	-4.1009116	0.1012702
H	-3.6605394	-4.7053368	-0.6277519
H	-2.6147581	-4.8138831	0.7833757
C	-4.0650254	-3.1897617	0.8612423
H	-4.8399171	-3.7880660	1.3587033
H	-3.5200136	-2.6566134	1.6591413
C	-4.7045200	-2.1628740	-0.0761652
H	-5.3644830	-1.4861432	0.4837940
H	-5.3400993	-2.6824384	-0.8111666
C	-3.6402011	-1.3425909	-0.8155913
H	-4.1313574	-0.6447126	-1.5082629
H	-3.0682788	-0.7371619	-0.0919635
C	-2.2768733	-0.1987435	-3.6519421
H	-1.6511970	-0.1231405	-4.5501529
H	-3.2082265	-0.6974642	-3.9543526
C	-2.5822252	1.1998735	-3.0871682
H	-3.3999249	1.1447597	-2.3567889
H	-2.9131415	1.8716254	-3.8919112
C	-0.2024027	2.9069757	-3.4711712

H	-0.9307959	3.5464945	-3.9982197
C	0.8620315	3.7893758	-2.8036160
H	1.5165659	3.1414189	-2.1990898
H	0.3952760	4.5062417	-2.1138338
C	1.7135001	4.5328172	-3.8385279
H	1.0797234	5.2510921	-4.3830650
H	2.4813043	5.1250992	-3.3213488
C	2.3584435	3.5618131	-4.8301376
H	3.0726883	2.9133793	-4.2950171
H	2.9391186	4.1130444	-5.5813525
C	1.2972885	2.6950072	-5.5117519
H	1.7648615	1.9723505	-6.1946067
H	0.6438438	3.3317551	-6.1297452
C	0.4404669	1.9442961	-4.4853007
H	1.0727291	1.2227947	-3.9378114
H	-0.3318476	1.3627282	-5.0068547
C	-1.8515357	3.2195422	-1.0190245
H	-0.9492830	3.6574844	-0.5561574
C	-2.6815558	2.5745549	0.1015426
H	-2.1064295	1.7726876	0.5903233
H	-3.5795471	2.1006479	-0.3278081
C	-3.1125700	3.6326256	1.1234161
H	-3.7177061	3.1615350	1.9106383
H	-2.2125436	4.0385890	1.6175169
C	-3.8870729	4.7735577	0.4560522
H	-4.8394234	4.3816513	0.0629060
H	-4.1497221	5.5412483	1.1962304
C	-3.0832667	5.3970526	-0.6888454
H	-2.1883685	5.8966208	-0.2818060
H	-3.6713709	6.1749670	-1.1940597
C	-2.6396492	4.3436065	-1.7147138
H	-3.5270173	3.9139782	-2.2071143
H	-2.0360973	4.8186529	-2.5001920
Ga	-0.1584484	-0.1534239	1.1905059
P	1.3652058	1.2914867	2.4666176
P	1.1570485	-1.9737759	2.1938223
C	0.4055903	2.5017094	3.4750943
H	-0.0137175	3.1910370	2.7201302
C	-0.7774284	1.8139854	4.1772143
H	-0.3983797	1.0681914	4.8945718
H	-1.3853137	1.2638291	3.4389707
C	-1.6369421	2.8384969	4.9271827
H	-2.4573215	2.3237125	5.4458349
H	-2.1033284	3.5184107	4.1955495
C	-0.7964228	3.6508002	5.9177769
H	-1.4224353	4.4011099	6.4187605
H	-0.4178687	2.9827826	6.7090721
C	0.3847753	4.3297025	5.2182058
H	0.0074669	5.0787867	4.5024945
H	1.0026757	4.8750705	5.9441454
C	1.2559371	3.3139886	4.4651322
H	2.0724400	3.8332543	3.9439414
H	1.7239068	2.6284249	5.1903522
C	2.6657171	2.2562157	1.5764739
H	3.2235232	2.7836203	2.3699495
C	2.0268698	3.2921656	0.6413073
H	1.3664001	3.9690668	1.2015310
H	1.3954349	2.7542711	-0.0885046
C	3.0975920	4.1009116	-0.1012702
H	3.6605394	4.7053368	0.6277519
H	2.6147581	4.8138831	-0.7833757
C	4.0650254	3.1897617	-0.8612423

H	4.8399171	3.7880660	-1.3587033
H	3.5200136	2.6566134	-1.6591413
C	4.7045200	2.1628740	0.0761652
H	5.3644830	1.4861432	-0.4837940
H	5.3400993	2.6824384	0.8111666
C	3.6402011	1.3425909	0.8155913
H	4.1313574	0.6447126	1.5082629
H	3.0682788	0.7371619	0.0919635
C	2.2768733	0.1987435	3.6519421
H	1.6511970	0.1231405	4.5501529
H	3.2082265	0.6974642	3.9543526
C	2.5822252	-1.1998735	3.0871682
H	3.3999249	-1.1447597	2.3567889
H	2.9131415	-1.8716254	3.8919112
C	0.2024027	-2.9069757	3.4711712
H	0.9307959	-3.5464945	3.9982197
C	-0.8620315	-3.7893758	2.8036160
H	-1.5165659	-3.1414189	2.1990898
H	-0.3952760	-4.5062417	2.1138338
C	-1.7135001	-4.5328172	3.8385279
H	-1.0797234	-5.2510921	4.3830650
H	-2.4813043	-5.1250992	3.3213488
C	-2.3584435	-3.5618131	4.8301376
H	-3.0726883	-2.9133793	4.2950171
H	-2.9391186	-4.1130444	5.5813525
C	-1.2972885	-2.6950072	5.5117519
H	-1.7648615	-1.9723505	6.1946067
H	-0.6438438	-3.3317551	6.1297452
C	-0.4404669	-1.9442961	4.4853007
H	-1.0727291	-1.2227947	3.9378114
H	0.3318476	-1.3627282	5.0068547
C	1.8515357	-3.2195422	1.0190245
H	0.9492830	-3.6574844	0.5561574
C	2.6815558	-2.5745549	-0.1015426
H	2.1064295	-1.7726876	-0.5903233
H	3.5795471	-2.1006479	0.3278081
C	3.1125700	-3.6326256	-1.1234161
H	3.7177061	-3.1615350	-1.9106383
H	2.2125436	-4.0385890	-1.6175169
C	3.8870729	-4.7735577	-0.4560522
H	4.8394234	-4.3816513	-0.0629060
H	4.1497221	-5.5412483	-1.1962304
C	3.0832667	-5.3970526	0.6888454
H	2.1883685	-5.8966208	0.2818060
H	3.6713709	-6.1749670	1.1940597
C	2.6396492	-4.3436065	1.7147138
H	3.5270173	-3.9139782	2.2071143
H	2.0360973	-4.8186529	2.5001920

SCF energy GEOOPT = -7256.171633101 H
 ZPE = 3596. kJ/mol
 FREEH energy = 3772.42 kJ/mol
 FREEH entropy = 1.53132 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		-0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	au	10.92	0.02834	YES	NO
8	au	19.05	0.11990	YES	NO
9	ag	23.26	0.00000	NO	YES
10	au	27.23	0.30003	YES	NO
11	ag	29.95	0.00000	NO	YES
12	au	31.16	0.00344	YES	NO
13	ag	32.42	0.00000	NO	YES
14	au	35.04	0.11615	YES	NO
15	ag	38.82	0.00000	NO	YES
16	au	39.84	0.59894	YES	NO
17	ag	43.19	0.00000	NO	YES
18	au	45.36	0.03676	YES	NO
19	ag	46.46	0.00000	NO	YES
20	ag	52.19	0.00000	NO	YES
21	au	52.20	0.19501	YES	NO
22	ag	54.53	0.00000	NO	YES
23	au	56.54	0.55763	YES	NO
24	ag	62.69	0.00000	NO	YES
25	au	63.88	0.34385	YES	NO
26	ag	65.74	0.00000	NO	YES
27	au	70.23	0.76885	YES	NO
28	ag	71.99	0.00000	NO	YES
29	au	72.25	0.32231	YES	NO
30	au	74.90	0.57779	YES	NO
31	au	80.79	3.14781	YES	NO
32	ag	81.29	0.00000	NO	YES
33	ag	87.50	0.00000	NO	YES
34	au	87.57	0.23786	YES	NO
35	ag	89.44	0.00000	NO	YES
36	ag	122.40	0.00000	NO	YES
37	ag	123.60	0.00000	NO	YES
38	au	124.91	0.84170	YES	NO
39	au	132.09	0.45545	YES	NO
40	ag	141.86	0.00000	NO	YES
41	ag	143.22	0.00000	NO	YES
42	au	144.12	4.33625	YES	NO
43	ag	146.32	0.00000	NO	YES
44	au	147.91	6.62281	YES	NO
45	au	148.81	0.65115	YES	NO
46	ag	166.04	0.00000	NO	YES
47	au	179.11	0.78762	YES	NO
48	ag	179.57	0.00000	NO	YES
49	au	183.48	1.41280	YES	NO
50	ag	191.57	0.00000	NO	YES
51	au	195.42	5.29589	YES	NO
52	ag	200.26	0.00000	NO	YES
53	au	207.44	4.94899	YES	NO
54	ag	215.88	0.00000	NO	YES
55	au	216.74	0.22183	YES	NO
56	ag	217.07	0.00000	NO	YES
57	au	224.30	4.17799	YES	NO
58	ag	226.65	0.00000	NO	YES
59	au	228.02	0.46864	YES	NO
60	ag	235.18	0.00000	NO	YES
61	au	236.39	0.55059	YES	NO
62	au	238.71	0.88127	YES	NO
63	ag	238.87	0.00000	NO	YES
64	ag	244.15	0.00000	NO	YES
65	au	245.14	1.03950	YES	NO
66	ag	256.15	0.00000	NO	YES
67	au	273.65	1.91869	YES	NO

68	ag	276.04	0.00000	NO	YES
69	au	284.53	1.33108	YES	NO
70	ag	290.38	0.00000	NO	YES
71	au	306.25	0.96603	YES	NO
72	ag	307.29	0.00000	NO	YES
73	ag	314.10	0.00000	NO	YES
74	au	315.57	0.32591	YES	NO
75	au	329.88	1.75673	YES	NO
76	ag	330.40	0.00000	NO	YES
77	ag	333.67	0.00000	NO	YES
78	au	335.00	0.05537	YES	NO
79	au	341.51	5.85328	YES	NO
80	ag	343.01	0.00000	NO	YES
81	au	367.31	14.62782	YES	NO
82	ag	369.83	0.00000	NO	YES
83	ag	374.37	0.00000	NO	YES
84	au	375.80	1.16583	YES	NO
85	au	393.92	5.18499	YES	NO
86	ag	396.84	0.00000	NO	YES
87	ag	414.68	0.00000	NO	YES
88	au	415.23	3.60602	YES	NO
89	ag	423.10	0.00000	NO	YES
90	au	423.31	5.46848	YES	NO
91	au	425.89	4.09585	YES	NO
92	ag	426.38	0.00000	NO	YES
93	au	430.08	0.45619	YES	NO
94	ag	430.13	0.00000	NO	YES
95	au	431.18	0.03908	YES	NO
96	ag	431.49	0.00000	NO	YES
97	ag	432.06	0.00000	NO	YES
98	au	432.72	1.74943	YES	NO
99	au	434.81	0.95999	YES	NO
100	ag	434.82	0.00000	NO	YES
101	au	444.37	13.81677	YES	NO
102	ag	446.52	0.00000	NO	YES
103	ag	465.70	0.00000	NO	YES
104	au	466.28	7.59054	YES	NO
105	au	490.95	6.25621	YES	NO
106	ag	491.56	0.00000	NO	YES
107	au	493.95	10.03835	YES	NO
108	ag	494.12	0.00000	NO	YES
109	au	502.40	3.70124	YES	NO
110	ag	503.34	0.00000	NO	YES
111	au	516.65	27.94310	YES	NO
112	ag	516.84	0.00000	NO	YES
113	au	623.10	42.73833	YES	NO
114	ag	623.88	0.00000	NO	YES
115	au	639.50	24.26470	YES	NO
116	ag	639.97	0.00000	NO	YES
117	au	713.20	1.68828	YES	NO
118	ag	713.57	0.00000	NO	YES
119	au	721.58	5.54511	YES	NO
120	ag	722.01	0.00000	NO	YES
121	ag	732.56	0.00000	NO	YES
122	au	732.90	16.20991	YES	NO
123	ag	734.74	0.00000	NO	YES
124	au	735.00	8.60167	YES	NO
125	au	773.38	7.95127	YES	NO
126	ag	773.53	0.00000	NO	YES
127	ag	773.86	0.00000	NO	YES
128	au	774.01	3.17722	YES	NO
129	ag	774.86	0.00000	NO	YES

130	au	774.89	1.40374	YES	NO
131	au	775.47	2.43028	YES	NO
132	ag	775.62	0.00000	NO	YES
133	au	776.60	28.46908	YES	NO
134	ag	776.95	0.00000	NO	YES
135	au	809.92	0.17957	YES	NO
136	ag	810.27	0.00000	NO	YES
137	ag	811.30	0.00000	NO	YES
138	au	811.40	4.20853	YES	NO
139	au	812.26	4.75511	YES	NO
140	ag	812.51	0.00000	NO	YES
141	ag	814.14	0.00000	NO	YES
142	au	814.48	15.99134	YES	NO
143	ag	832.51	0.00000	NO	YES
144	au	833.13	3.84603	YES	NO
145	ag	836.07	0.00000	NO	YES
146	au	836.43	10.18262	YES	NO
147	au	836.96	5.30188	YES	NO
148	ag	837.01	0.00000	NO	YES
149	au	839.42	19.73473	YES	NO
150	ag	840.08	0.00000	NO	YES
151	au	850.21	36.73168	YES	NO
152	ag	852.64	0.00000	NO	YES
153	au	876.19	5.13054	YES	NO
154	ag	876.37	0.00000	NO	YES
155	au	876.74	3.12768	YES	NO
156	ag	876.76	0.00000	NO	YES
157	ag	876.93	0.00000	NO	YES
158	au	877.24	11.18007	YES	NO
159	au	877.97	8.07199	YES	NO
160	ag	878.32	0.00000	NO	YES
161	au	878.94	5.78210	YES	NO
162	ag	878.95	0.00000	NO	YES
163	au	879.90	8.96516	YES	NO
164	ag	880.35	0.00000	NO	YES
165	ag	882.20	0.00000	NO	YES
166	au	883.60	1.09277	YES	NO
167	au	885.11	4.89421	YES	NO
168	ag	886.60	0.00000	NO	YES
169	ag	903.16	0.00000	NO	YES
170	au	903.70	8.47169	YES	NO
171	au	904.02	5.11335	YES	NO
172	ag	904.74	0.00000	NO	YES
173	ag	909.39	0.00000	NO	YES
174	au	909.90	6.07043	YES	NO
175	au	910.90	1.41352	YES	NO
176	ag	911.08	0.00000	NO	YES
177	au	982.84	0.86840	YES	NO
178	ag	982.93	0.00000	NO	YES
179	ag	987.57	0.00000	NO	YES
180	au	987.72	15.41783	YES	NO
181	ag	989.22	0.00000	NO	YES
182	au	989.29	17.30737	YES	NO
183	ag	989.77	0.00000	NO	YES
184	au	990.28	19.90490	YES	NO
185	au	991.57	15.27192	YES	NO
186	ag	992.41	0.00000	NO	YES
187	ag	1015.67	0.00000	NO	YES
188	au	1015.85	5.89493	YES	NO
189	au	1016.31	1.04427	YES	NO
190	ag	1016.59	0.00000	NO	YES
191	au	1020.35	1.42697	YES	NO

192	ag	1020.35	0.00000	NO	YES
193	ag	1022.43	0.00000	NO	YES
194	au	1022.45	0.97360	YES	NO
195	au	1031.60	1.32464	YES	NO
196	ag	1031.80	0.00000	NO	YES
197	ag	1032.53	0.00000	NO	YES
198	au	1032.84	5.56758	YES	NO
199	ag	1039.07	0.00000	NO	YES
200	au	1039.10	6.77623	YES	NO
201	ag	1039.84	0.00000	NO	YES
202	au	1039.99	0.93500	YES	NO
203	au	1059.05	7.48427	YES	NO
204	ag	1059.16	0.00000	NO	YES
205	ag	1059.33	0.00000	NO	YES
206	au	1059.39	2.76014	YES	NO
207	au	1064.34	4.56036	YES	NO
208	ag	1066.25	0.00000	NO	YES
209	ag	1068.98	0.00000	NO	YES
210	au	1070.18	0.28314	YES	NO
211	ag	1071.70	0.00000	NO	YES
212	au	1071.75	0.11032	YES	NO
213	au	1071.84	0.05899	YES	NO
214	ag	1071.85	0.00000	NO	YES
215	au	1074.64	1.49684	YES	NO
216	ag	1074.70	0.00000	NO	YES
217	ag	1075.43	0.00000	NO	YES
218	au	1076.36	0.38739	YES	NO
219	au	1078.90	7.78022	YES	NO
220	ag	1079.64	0.00000	NO	YES
221	ag	1091.79	0.00000	NO	YES
222	au	1091.82	23.95138	YES	NO
223	au	1094.46	14.53236	YES	NO
224	ag	1094.60	0.00000	NO	YES
225	au	1100.84	0.56918	YES	NO
226	ag	1101.07	0.00000	NO	YES
227	ag	1105.68	0.00000	NO	YES
228	au	1106.58	20.88214	YES	NO
229	au	1126.37	16.46788	YES	NO
230	ag	1129.00	0.00000	NO	YES
231	au	1160.24	13.52143	YES	NO
232	ag	1160.58	0.00000	NO	YES
233	ag	1161.08	0.00000	NO	YES
234	au	1161.42	6.73747	YES	NO
235	ag	1169.02	0.00000	NO	YES
236	au	1169.64	18.15012	YES	NO
237	au	1171.57	19.69385	YES	NO
238	ag	1171.64	0.00000	NO	YES
239	au	1174.89	18.44753	YES	NO
240	ag	1175.06	0.00000	NO	YES
241	au	1177.91	20.65658	YES	NO
242	ag	1178.63	0.00000	NO	YES
243	au	1188.58	3.18668	YES	NO
244	ag	1189.07	0.00000	NO	YES
245	ag	1194.84	0.00000	NO	YES
246	au	1195.39	4.27526	YES	NO
247	au	1237.41	0.77382	YES	NO
248	ag	1237.64	0.00000	NO	YES
249	au	1244.37	0.63581	YES	NO
250	ag	1245.01	0.00000	NO	YES
251	ag	1245.28	0.00000	NO	YES
252	au	1245.63	1.39429	YES	NO
253	au	1245.93	0.29623	YES	NO

254	ag	1246.29	0.00000	NO	YES
255	au	1249.06	0.66203	YES	NO
256	ag	1249.10	0.00000	NO	YES
257	ag	1253.52	0.00000	NO	YES
258	au	1254.15	2.01793	YES	NO
259	ag	1255.06	0.00000	NO	YES
260	au	1255.79	13.01262	YES	NO
261	au	1257.13	12.93416	YES	NO
262	ag	1257.36	0.00000	NO	YES
263	au	1257.48	5.22470	YES	NO
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266	ag	1258.39	0.00000	NO	YES
267	au	1259.46	8.47516	YES	NO
268	ag	1259.73	0.00000	NO	YES
269	ag	1262.09	0.00000	NO	YES
270	au	1263.18	1.34468	YES	NO
271	au	1264.65	5.95954	YES	NO
272	ag	1265.47	0.00000	NO	YES
273	au	1266.21	5.34130	YES	NO
274	ag	1267.18	0.00000	NO	YES
275	ag	1280.78	0.00000	NO	YES
276	au	1280.82	2.51856	YES	NO
277	ag	1283.77	0.00000	NO	YES
278	au	1283.84	5.02350	YES	NO
279	au	1288.61	3.27386	YES	NO
280	ag	1289.23	0.00000	NO	YES
281	ag	1290.32	0.00000	NO	YES
282	au	1290.82	8.98306	YES	NO
283	ag	1309.11	0.00000	NO	YES
284	au	1309.17	1.57998	YES	NO
285	au	1309.98	4.48452	YES	NO
286	ag	1310.23	0.00000	NO	YES
287	au	1314.09	2.10566	YES	NO
288	ag	1314.40	0.00000	NO	YES
289	ag	1315.02	0.00000	NO	YES
290	au	1315.35	6.06773	YES	NO
291	ag	1321.62	0.00000	NO	YES
292	au	1322.07	0.53272	YES	NO
293	ag	1323.10	0.00000	NO	YES
294	au	1323.13	0.57774	YES	NO
295	ag	1323.33	0.00000	NO	YES
296	au	1323.77	10.72592	YES	NO
297	au	1324.41	8.28567	YES	NO
298	ag	1324.44	0.00000	NO	YES
299	au	1324.81	1.36301	YES	NO
300	ag	1325.57	0.00000	NO	YES
301	au	1325.72	2.14091	YES	NO
302	ag	1326.22	0.00000	NO	YES
303	ag	1326.97	0.00000	NO	YES
304	au	1327.11	11.45636	YES	NO
305	au	1327.71	2.69993	YES	NO
306	ag	1328.00	0.00000	NO	YES
307	au	1336.06	0.39128	YES	NO
308	ag	1336.18	0.00000	NO	YES
309	au	1337.08	1.04546	YES	NO
310	ag	1337.09	0.00000	NO	YES
311	au	1338.13	2.05205	YES	NO
312	ag	1338.19	0.00000	NO	YES
313	ag	1339.15	0.00000	NO	YES
314	au	1339.16	1.44737	YES	NO
315	au	1345.57	4.31126	YES	NO

316	ag	1345.59	0.00000	NO	YES
317	ag	1346.12	0.00000	NO	YES
318	au	1346.17	2.88933	YES	NO
319	ag	1348.73	0.00000	NO	YES
320	au	1348.89	2.34969	YES	NO
321	au	1350.18	0.97879	YES	NO
322	ag	1350.40	0.00000	NO	YES
323	au	1400.47	15.36926	YES	NO
324	ag	1400.52	0.00000	NO	YES
325	au	1405.73	14.25230	YES	NO
326	ag	1405.83	0.00000	NO	YES
327	au	1423.24	10.53652	YES	NO
328	ag	1423.42	0.00000	NO	YES
329	ag	1428.22	0.00000	NO	YES
330	au	1428.76	12.54397	YES	NO
331	ag	1430.80	0.00000	NO	YES
332	au	1431.17	3.73989	YES	NO
333	au	1433.32	1.58401	YES	NO
334	ag	1433.44	0.00000	NO	YES
335	ag	1434.55	0.00000	NO	YES
336	au	1435.02	12.40472	YES	NO
337	au	1435.08	7.17288	YES	NO
338	ag	1435.40	0.00000	NO	YES
339	au	1436.26	2.04622	YES	NO
340	ag	1437.29	0.00000	NO	YES
341	ag	1437.76	0.00000	NO	YES
342	au	1437.81	15.76739	YES	NO
343	au	1438.40	4.37829	YES	NO
344	ag	1438.47	0.00000	NO	YES
345	au	1438.59	3.80738	YES	NO
346	ag	1438.67	0.00000	NO	YES
347	ag	1439.19	0.00000	NO	YES
348	au	1439.36	11.93457	YES	NO
349	au	1440.13	3.51942	YES	NO
350	ag	1440.13	0.00000	NO	YES
351	au	1442.03	70.47082	YES	NO
352	ag	1442.46	0.00000	NO	YES
353	ag	1442.93	0.00000	NO	YES
354	au	1443.36	11.79264	YES	NO
355	ag	1444.42	0.00000	NO	YES
356	au	1444.64	15.16248	YES	NO
357	au	1446.72	38.19992	YES	NO
358	ag	1446.78	0.00000	NO	YES
359	ag	1452.54	0.00000	NO	YES
360	au	1452.86	3.38830	YES	NO
361	au	1453.24	7.52717	YES	NO
362	ag	1454.27	0.00000	NO	YES
363	ag	1454.59	0.00000	NO	YES
364	au	1454.74	1.48202	YES	NO
365	ag	1455.77	0.00000	NO	YES
366	au	1456.07	1.73107	YES	NO
367	ag	2919.84	0.00000	NO	YES
368	au	2919.86	26.35208	YES	NO
369	ag	2921.46	0.00000	NO	YES
370	au	2921.51	74.21241	YES	NO
371	au	2925.79	75.48958	YES	NO
372	ag	2926.39	0.00000	NO	YES
373	au	2927.35	9.09713	YES	NO
374	ag	2927.39	0.00000	NO	YES
375	ag	2930.28	0.00000	NO	YES
376	au	2930.29	30.14789	YES	NO
377	ag	2931.85	0.00000	NO	YES

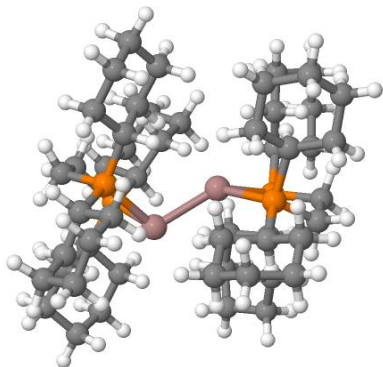
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379	ag	2933.08	0.00000	NO	YES
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382	au	2936.56	24.71459	YES	NO
383	ag	2937.30	0.00000	NO	YES
384	au	2937.31	25.21273	YES	NO
385	ag	2942.21	0.00000	NO	YES
386	au	2942.22	18.08738	YES	NO
387	au	2945.02	14.94226	YES	NO
388	ag	2945.04	0.00000	NO	YES
389	ag	2945.33	0.00000	NO	YES
390	au	2945.39	23.75846	YES	NO
391	au	2945.61	5.14390	YES	NO
392	ag	2945.67	0.00000	NO	YES
393	au	2946.21	2.94310	YES	NO
394	ag	2946.24	0.00000	NO	YES
395	au	2948.69	22.30099	YES	NO
396	ag	2948.70	0.00000	NO	YES
397	au	2955.88	3.73836	YES	NO
398	ag	2955.90	0.00000	NO	YES
399	au	2956.11	7.28972	YES	NO
400	ag	2956.11	0.00000	NO	YES
401	au	2956.97	21.45592	YES	NO
402	ag	2956.98	0.00000	NO	YES
403	au	2959.26	21.26361	YES	NO
404	ag	2959.26	0.00000	NO	YES
405	ag	2959.70	0.00000	NO	YES
406	au	2959.74	10.13724	YES	NO
407	au	2959.84	69.00169	YES	NO
408	ag	2959.87	0.00000	NO	YES
409	ag	2960.80	0.00000	NO	YES
410	au	2960.83	36.03664	YES	NO
411	au	2962.98	99.88988	YES	NO
412	ag	2963.08	0.00000	NO	YES
413	ag	2963.30	0.00000	NO	YES
414	au	2963.31	85.60392	YES	NO
415	ag	2977.08	0.00000	NO	YES
416	au	2977.16	106.69336	YES	NO
417	ag	2978.21	0.00000	NO	YES
418	au	2978.32	29.29696	YES	NO
419	au	2982.42	13.86777	YES	NO
420	ag	2982.43	0.00000	NO	YES
421	au	2988.48	9.64088	YES	NO
422	ag	2988.48	0.00000	NO	YES
423	ag	2998.26	0.00000	NO	YES
424	au	2998.29	43.23556	YES	NO
425	ag	3002.08	0.00000	NO	YES
426	au	3002.16	47.67971	YES	NO
427	au	3003.92	28.02357	YES	NO
428	ag	3003.93	0.00000	NO	YES
429	ag	3004.82	0.00000	NO	YES
430	au	3004.90	54.64863	YES	NO
431	ag	3005.78	0.00000	NO	YES
432	au	3005.81	96.75875	YES	NO
433	au	3006.38	10.01856	YES	NO
434	ag	3006.43	0.00000	NO	YES
435	ag	3009.93	0.00000	NO	YES
436	au	3009.95	43.64844	YES	NO
437	au	3010.06	8.90268	YES	NO
438	ag	3010.08	0.00000	NO	YES
439	ag	3010.90	0.00000	NO	YES

440	au	3010.91	15.39461	YES	NO
441	ag	3011.52	0.00000	NO	YES
442	au	3011.56	44.16445	YES	NO
443	au	3011.98	85.84790	YES	NO
444	ag	3012.00	0.00000	NO	YES
445	ag	3012.32	0.00000	NO	YES
446	au	3012.35	43.77723	YES	NO
447	au	3015.21	50.55656	YES	NO
448	ag	3015.23	0.00000	NO	YES
449	au	3015.59	61.33338	YES	NO
450	ag	3015.64	0.00000	NO	YES
451	au	3016.03	67.42986	YES	NO
452	ag	3016.06	0.00000	NO	YES
453	ag	3017.04	0.00000	NO	YES
454	au	3017.06	36.72299	YES	NO
455	ag	3018.37	0.00000	NO	YES
456	au	3018.38	42.26232	YES	NO
457	au	3019.44	67.69109	YES	NO
458	ag	3019.49	0.00000	NO	YES
459	au	3029.42	0.67149	YES	NO
460	ag	3029.43	0.00000	NO	YES
461	au	3044.33	2.35926	YES	NO
462	ag	3044.34	0.00000	NO	YES

\$end

Double hybrid single point energy = -7249.051030759942 H
 COSMO energy + OC correction = -7256.3196247836 H (in oDFB)
 COSMO energy + OC correction = -7256.326891604 H (in 3FB)

6.2.2 $[\{\text{Ga}(\text{dcpe})\}_2]^{2+}$ (asymmetric)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.1400311	17.4157585	-2.1819865
Ga	-4.5460621	17.2346598	-1.9146004
P	-1.6632199	18.9426330	-4.0809401
P	-6.0110963	19.0210663	-1.0697684
P	-1.6140671	15.6725487	-3.8598852
P	-5.6234988	15.9465445	-0.1330542
C	-5.1965751	20.7684785	-5.4294914
H	-5.3764832	21.4337763	-4.5668411
H	-6.1681912	20.3301913	-5.6972823
C	-0.3916335	14.4182724	-3.2756488
H	-0.0557914	13.8667918	-4.1707010
C	-4.5907092	14.8986651	0.9777028

H	-4.1660664	15.6514304	1.6679367
C	-4.0089464	15.6744279	-5.3422317
H	-3.4969453	16.0635864	-6.2376481
H	-4.2795328	16.5368188	-4.7148302
C	-7.1233732	19.5967900	-2.4198998
H	-6.4522031	20.1110999	-3.1268611
C	-7.1248073	18.2939274	0.2223841
H	-7.4507682	19.0865096	0.9097815
H	-8.0232661	17.9358787	-0.2987108
C	-3.2664390	22.1716644	-6.2498909
H	-2.8585507	22.7315324	-7.1021727
H	-3.3610124	22.8903097	-5.4191166
C	-2.2824049	21.0650539	-5.8464520
H	-1.3132297	21.5074148	-5.5796826
H	-2.1074264	20.4046353	-6.7106081
C	-4.2250528	19.6574012	-5.0141282
H	-4.1330709	18.9361558	-5.8422565
H	-4.6149555	19.0887350	-4.1542362
C	1.8311912	14.0575184	-2.1127721
H	2.2519512	13.5118704	-2.9728276
H	2.6723555	14.5702784	-1.6266851
C	-8.1576587	14.5547093	-0.1931210
H	-8.5953271	15.3906443	0.3713985
H	-7.8310659	13.8093784	0.5453320
C	-5.1658278	20.4798264	-0.3288040
H	-5.9543750	21.2014050	-0.0549506
C	-0.4188468	20.7996692	-2.4538526
H	-1.1713188	21.5425712	-2.7532516
H	-0.8590420	20.2151593	-1.6257994
C	0.8452317	21.5089904	-1.9559834
H	1.2204274	22.1782025	-2.7470105
H	0.5905929	22.1494009	-1.1001168
C	-7.7311198	18.3829296	-3.1477303
H	-6.9264300	17.7171623	-3.5061168
H	-8.3387022	17.7939098	-2.4398235
C	-4.6439829	21.5990958	-6.5913954
H	-4.5648276	20.9621474	-7.4876627
H	-5.3416991	22.4083270	-6.8450063
C	-8.2039444	20.5884335	-1.9596638
H	-7.7439412	21.4684974	-1.4884716
H	-8.8404086	20.1126962	-1.1959635
C	-4.2329740	21.1132941	-1.3735998
H	-4.8013122	21.4224105	-2.2627284
H	-3.5110926	20.3438956	-1.7011842
C	-2.6560209	13.5482807	-5.4597232
H	-1.9734203	12.8715113	-4.9301123
H	-2.1186626	13.9105876	-6.3512891
C	2.2562850	19.5768782	-2.7500699
H	2.6872497	20.1648867	-3.5765987
H	3.0159487	18.8362460	-2.4647185
C	-3.6200649	21.2783280	1.5127516
H	-4.3406199	22.0335184	1.8655240
H	-3.0485033	20.9566868	2.3938774
C	-9.6998104	19.8110695	-3.8520693
H	-10.3016302	20.1402608	-4.7094709
H	-10.3932646	19.3016655	-3.1624948
C	-5.3656494	13.8644368	1.8133298
H	-6.1889021	14.3417514	2.3631008

H	-5.8168142	13.1208006	1.1386271
C	1.1751165	13.0650604	-1.1486260
H	1.9031356	12.3074018	-0.8299335
H	0.8580871	13.5990070	-0.2367557
C	-8.6244231	18.8224168	-4.3138629
H	-7.9982495	19.2965747	-5.0864541
H	-9.0828364	17.9394403	-4.7799424
C	1.9360184	20.5048607	-1.5756098
H	1.5964334	19.9033012	-0.7156242
H	2.8423670	21.0323433	-1.2503889
C	-2.6925043	21.9054780	0.4682023
H	-2.1783577	22.7780182	0.8923478
H	-1.9089851	21.1785786	0.1963142
C	-6.3549659	13.8844282	-1.8636954
H	-5.9520761	13.1113129	-1.1914092
H	-5.5087380	14.2590248	-2.4628106
C	-4.3871817	20.0807020	0.9372437
H	-3.6748399	19.2768776	0.6794076
H	-5.0712589	19.6789026	1.6982539
C	-6.9552791	15.0274457	-1.0245302
H	-7.3252054	15.7883322	-1.7394502
C	-3.4695963	22.3063617	-0.7884630
C	-8.6369475	12.7954972	-1.9581457
H	-9.4065718	12.3896954	-2.6280147
H	-8.3333083	11.9685872	-1.2954832
C	-9.2185982	13.9343642	-1.1140847
H	-10.0626024	13.5744840	-0.5105740
H	-9.6203403	14.7164914	-1.7800985
C	-1.0492210	13.4381985	-2.2919280
H	-1.9161868	12.9408688	-2.7483733
H	-1.4276175	14.0159508	-1.4352853
C	-4.4177737	13.1500474	2.7867202
H	-4.0397098	13.8776446	3.5233576
H	-4.9787064	12.3945685	3.3532548
C	-5.2660924	14.9147786	-5.7785587
H	-5.9316979	15.5883049	-6.3367869
H	-5.8199277	14.5983752	-4.8787311
C	-3.2394944	12.5061833	2.0498102
H	-3.6140581	11.7029922	1.3935709
H	-2.5590478	12.0293805	2.7677258
C	-3.4140588	14.2566676	0.2270626
H	-3.7936597	13.5396397	-0.5174389
H	-2.8676637	15.0366854	-0.3269356
C	-9.0782433	21.0195237	-3.1456844
H	-9.8604037	21.7053769	-2.7938777
H	-8.4608502	21.5873361	-3.8608553
C	-3.9125368	12.7803022	-5.8991068
H	-3.6217983	11.9377685	-6.5408906
H	-4.3899962	12.3432266	-5.0060112
C	-7.4247483	13.2649977	-2.7695793
H	-6.9917792	12.4293317	-3.3369752
H	-7.7468637	14.0162338	-3.5102714
C	-4.9121461	13.6868383	-6.6231110
H	-5.8198407	13.1233644	-6.8781822
H	-4.4745877	14.0197078	-7.5785319
C	-0.0422863	12.3959458	-1.7920151
H	-0.5358706	11.7198855	-1.0793822
H	0.2829493	11.7699352	-2.6387057

C	-2.4810579	13.5371166	1.2076273
H	-2.0146935	14.2840904	1.8708815
H	-1.6620324	13.0547242	0.6564453
C	-0.1167236	19.8424688	-3.6198206
H	0.2022710	20.4261396	-4.4990009
C	1.0012244	18.8525143	-3.2506245
H	1.2551666	18.2235328	-4.1154483
H	0.6323137	18.1764832	-2.4573726
C	0.8249104	15.0976860	-2.6217495
H	1.3209659	15.7808495	-3.3251397
H	0.4720543	15.7139145	-1.7758713
C	-0.7622388	16.5134592	-5.2720334
H	0.3005441	16.5467460	-5.0027341
H	-0.8424538	15.8734469	-6.1620186
C	-1.2802671	17.9248138	-5.5801269
H	-2.2217611	17.8682858	-6.1420251
H	-0.5610084	18.4649697	-6.2116665
C	-3.0514304	14.7453703	-4.5793520
H	-3.5821631	14.3692372	-3.6860414
C	-2.8454304	20.2393408	-4.6745010
H	-2.9663055	20.9082800	-3.8074152
C	-6.4598837	17.1463493	0.9919752
H	-7.1932291	16.6265419	1.6242413
H	-5.6723263	17.5279323	1.6559347
H	-4.1835599	23.1084638	-0.5425269
H	-2.7916944	22.7191057	-1.5490877

SCF energy GEOOPT = -7256.165972908 H

ZPE = 3596. kJ/mol

FREEH energy = 3772.30 kJ/mol

FREEH entropy = 1.54579 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	5.60	0.02921	YES	YES
	8	a	14.49	0.09237	YES	YES
	9	a	18.34	0.04973	YES	YES
	10	a	21.38	0.00934	YES	YES
	11	a	24.72	0.18559	YES	YES
	12	a	31.02	0.02820	YES	YES
	13	a	32.99	0.01686	YES	YES
	14	a	37.52	0.54758	YES	YES
	15	a	38.20	0.15959	YES	YES
	16	a	40.60	0.01272	YES	YES
	17	a	44.19	0.05895	YES	YES
	18	a	45.66	0.07682	YES	YES
	19	a	48.35	0.36329	YES	YES
	20	a	50.21	0.40208	YES	YES
	21	a	54.17	0.12647	YES	YES
	22	a	55.24	0.02185	YES	YES
	23	a	56.88	0.23762	YES	YES

24	a	59.30	0.25587	YES	YES
25	a	62.06	0.70547	YES	YES
26	a	66.43	0.01693	YES	YES
27	a	68.31	0.53916	YES	YES
28	a	70.30	0.18098	YES	YES
29	a	70.82	0.21743	YES	YES
30	a	74.78	0.56183	YES	YES
31	a	75.26	1.11375	YES	YES
32	a	79.80	0.11096	YES	YES
33	a	83.53	0.02828	YES	YES
34	a	90.88	0.72598	YES	YES
35	a	93.76	0.24452	YES	YES
36	a	115.11	0.25430	YES	YES
37	a	118.54	0.14634	YES	YES
38	a	126.71	0.64539	YES	YES
39	a	129.74	0.63618	YES	YES
40	a	134.60	0.70480	YES	YES
41	a	138.19	0.38911	YES	YES
42	a	140.39	1.71561	YES	YES
43	a	143.44	4.06558	YES	YES
44	a	150.66	0.47706	YES	YES
45	a	155.70	2.19328	YES	YES
46	a	166.59	0.28568	YES	YES
47	a	176.91	1.16162	YES	YES
48	a	179.03	3.79459	YES	YES
49	a	184.19	1.58206	YES	YES
50	a	193.58	2.16127	YES	YES
51	a	196.46	4.36579	YES	YES
52	a	209.26	0.93483	YES	YES
53	a	210.63	0.09032	YES	YES
54	a	215.98	0.19627	YES	YES
55	a	220.80	0.23868	YES	YES
56	a	223.90	0.03107	YES	YES
57	a	227.56	0.60939	YES	YES
58	a	228.75	1.06302	YES	YES
59	a	229.14	0.28396	YES	YES
60	a	233.69	0.43944	YES	YES
61	a	235.62	0.43678	YES	YES
62	a	238.03	0.47443	YES	YES
63	a	240.15	0.49777	YES	YES
64	a	246.43	0.29210	YES	YES
65	a	251.03	0.75064	YES	YES
66	a	258.23	0.91817	YES	YES
67	a	267.43	0.44555	YES	YES
68	a	278.76	0.08445	YES	YES
69	a	281.44	0.75155	YES	YES
70	a	288.00	1.83350	YES	YES
71	a	296.79	0.93188	YES	YES
72	a	305.22	0.49218	YES	YES
73	a	310.22	0.07571	YES	YES
74	a	313.49	1.44016	YES	YES
75	a	328.62	0.91241	YES	YES
76	a	329.81	0.12971	YES	YES
77	a	331.70	1.32254	YES	YES
78	a	337.31	1.69886	YES	YES
79	a	337.95	0.55834	YES	YES
80	a	340.05	1.90703	YES	YES
81	a	363.40	9.12894	YES	YES

82	a	376.74	3.22200	YES	YES
83	a	379.32	0.76792	YES	YES
84	a	379.90	0.77747	YES	YES
85	a	389.82	2.36932	YES	YES
86	a	393.68	2.82144	YES	YES
87	a	407.96	0.38918	YES	YES
88	a	416.71	2.44917	YES	YES
89	a	420.58	1.01770	YES	YES
90	a	422.53	4.32763	YES	YES
91	a	427.58	2.16925	YES	YES
92	a	429.00	0.65612	YES	YES
93	a	429.95	0.19550	YES	YES
94	a	430.66	0.01708	YES	YES
95	a	431.02	0.30943	YES	YES
96	a	432.67	0.67428	YES	YES
97	a	432.81	0.60428	YES	YES
98	a	433.82	0.15674	YES	YES
99	a	436.12	3.72126	YES	YES
100	a	436.66	0.11765	YES	YES
101	a	444.56	3.04352	YES	YES
102	a	455.79	7.20500	YES	YES
103	a	461.94	4.84136	YES	YES
104	a	467.55	5.59207	YES	YES
105	a	491.98	7.41526	YES	YES
106	a	492.20	0.10203	YES	YES
107	a	494.40	5.33297	YES	YES
108	a	495.79	2.38117	YES	YES
109	a	501.32	2.86295	YES	YES
110	a	502.25	1.06203	YES	YES
111	a	510.42	11.50638	YES	YES
112	a	512.90	11.64469	YES	YES
113	a	630.74	10.57444	YES	YES
114	a	631.24	31.47386	YES	YES
115	a	640.53	9.45194	YES	YES
116	a	659.99	13.02658	YES	YES
117	a	698.16	3.22720	YES	YES
118	a	713.97	1.86963	YES	YES
119	a	722.12	2.26615	YES	YES
120	a	726.16	6.80034	YES	YES
121	a	731.76	3.41117	YES	YES
122	a	734.13	6.27124	YES	YES
123	a	734.64	10.98773	YES	YES
124	a	737.72	4.82574	YES	YES
125	a	770.86	17.96929	YES	YES
126	a	772.45	0.19428	YES	YES
127	a	772.61	1.62363	YES	YES
128	a	773.40	0.46258	YES	YES
129	a	773.77	2.81775	YES	YES
130	a	774.07	0.23767	YES	YES
131	a	775.53	0.31499	YES	YES
132	a	775.81	0.35677	YES	YES
133	a	777.98	2.70472	YES	YES
134	a	778.93	20.97526	YES	YES
135	a	806.30	0.79658	YES	YES
136	a	808.02	0.79539	YES	YES
137	a	809.13	4.07129	YES	YES
138	a	810.40	8.67380	YES	YES
139	a	811.33	3.63027	YES	YES

140	a	811.62	4.71022	YES	YES
141	a	812.52	5.24530	YES	YES
142	a	817.55	2.69117	YES	YES
143	a	832.22	7.85337	YES	YES
144	a	832.46	2.72644	YES	YES
145	a	836.42	1.46023	YES	YES
146	a	837.14	3.03395	YES	YES
147	a	837.34	0.94584	YES	YES
148	a	838.18	5.21479	YES	YES
149	a	839.17	6.95602	YES	YES
150	a	839.48	2.78899	YES	YES
151	a	847.05	26.03745	YES	YES
152	a	853.14	16.74959	YES	YES
153	a	873.95	6.11511	YES	YES
154	a	874.46	0.48082	YES	YES
155	a	874.83	1.81762	YES	YES
156	a	875.21	3.82529	YES	YES
157	a	875.78	1.36512	YES	YES
158	a	876.35	3.37225	YES	YES
159	a	877.55	4.60848	YES	YES
160	a	878.41	1.47950	YES	YES
161	a	878.87	2.74180	YES	YES
162	a	879.09	0.88281	YES	YES
163	a	879.79	0.71525	YES	YES
164	a	881.11	9.04059	YES	YES
165	a	881.34	6.24871	YES	YES
166	a	883.05	0.92634	YES	YES
167	a	884.58	3.84416	YES	YES
168	a	884.90	0.53337	YES	YES
169	a	902.88	3.48941	YES	YES
170	a	903.32	2.69034	YES	YES
171	a	904.05	3.71855	YES	YES
172	a	905.61	0.28919	YES	YES
173	a	906.74	4.24244	YES	YES
174	a	909.35	2.12428	YES	YES
175	a	909.98	0.47250	YES	YES
176	a	911.31	1.56442	YES	YES
177	a	986.04	4.32259	YES	YES
178	a	986.16	2.45655	YES	YES
179	a	987.42	3.67968	YES	YES
180	a	987.69	15.11743	YES	YES
181	a	988.33	17.20171	YES	YES
182	a	989.15	6.68161	YES	YES
183	a	989.68	6.00834	YES	YES
184	a	990.43	21.00824	YES	YES
185	a	991.52	5.89036	YES	YES
186	a	996.64	0.56748	YES	YES
187	a	1012.85	0.63239	YES	YES
188	a	1014.55	3.07582	YES	YES
189	a	1015.26	2.25135	YES	YES
190	a	1016.17	1.74140	YES	YES
191	a	1016.63	0.47621	YES	YES
192	a	1019.00	1.08577	YES	YES
193	a	1019.62	0.23971	YES	YES
194	a	1021.81	0.54438	YES	YES
195	a	1028.77	0.73605	YES	YES
196	a	1030.11	1.22312	YES	YES
197	a	1032.03	1.86296	YES	YES

198	a	1036.06	2.10696	YES	YES
199	a	1036.67	1.40700	YES	YES
200	a	1038.52	1.13307	YES	YES
201	a	1038.61	2.89361	YES	YES
202	a	1040.00	2.26759	YES	YES
203	a	1055.59	2.77414	YES	YES
204	a	1057.41	0.30216	YES	YES
205	a	1058.55	4.84573	YES	YES
206	a	1059.15	1.95294	YES	YES
207	a	1060.35	1.79098	YES	YES
208	a	1063.53	0.60971	YES	YES
209	a	1066.19	4.35659	YES	YES
210	a	1067.41	0.30958	YES	YES
211	a	1069.87	0.02893	YES	YES
212	a	1069.93	0.37413	YES	YES
213	a	1071.15	0.19897	YES	YES
214	a	1071.67	0.03775	YES	YES
215	a	1072.36	0.12016	YES	YES
216	a	1072.43	0.04906	YES	YES
217	a	1072.89	0.26693	YES	YES
218	a	1075.09	0.09984	YES	YES
219	a	1078.01	4.34237	YES	YES
220	a	1081.79	4.52295	YES	YES
221	a	1089.43	3.86274	YES	YES
222	a	1090.54	7.07676	YES	YES
223	a	1093.24	9.49564	YES	YES
224	a	1094.23	1.96142	YES	YES
225	a	1101.30	2.22160	YES	YES
226	a	1101.58	2.91683	YES	YES
227	a	1107.94	7.84187	YES	YES
228	a	1113.84	15.63624	YES	YES
229	a	1122.90	7.30113	YES	YES
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232	a	1159.10	3.10454	YES	YES
233	a	1160.75	13.21422	YES	YES
234	a	1165.25	7.77947	YES	YES
235	a	1167.53	17.44087	YES	YES
236	a	1168.08	7.28312	YES	YES
237	a	1168.39	5.37125	YES	YES
238	a	1170.60	2.99027	YES	YES
239	a	1173.24	12.73883	YES	YES
240	a	1175.38	5.68750	YES	YES
241	a	1179.25	9.18478	YES	YES
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243	a	1188.37	0.34325	YES	YES
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246	a	1210.40	1.93410	YES	YES
247	a	1234.79	1.16516	YES	YES
248	a	1236.88	0.90999	YES	YES
249	a	1243.95	0.50754	YES	YES
250	a	1244.63	1.01203	YES	YES
251	a	1245.27	0.27179	YES	YES
252	a	1245.75	0.90102	YES	YES
253	a	1246.84	0.20829	YES	YES
254	a	1247.95	0.43148	YES	YES
255	a	1249.45	0.57365	YES	YES

256	a	1250.21	0.11833	YES	YES
257	a	1252.32	1.44104	YES	YES
258	a	1252.91	3.55024	YES	YES
259	a	1253.36	1.00007	YES	YES
260	a	1253.69	1.25921	YES	YES
261	a	1255.91	1.42298	YES	YES
262	a	1256.13	0.31522	YES	YES
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265	a	1257.97	6.70051	YES	YES
266	a	1258.76	1.19905	YES	YES
267	a	1260.01	6.13873	YES	YES
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271	a	1263.91	1.88849	YES	YES
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274	a	1270.16	2.92880	YES	YES
275	a	1281.34	3.42211	YES	YES
276	a	1281.71	0.31525	YES	YES
277	a	1282.67	2.91932	YES	YES
278	a	1284.20	2.80575	YES	YES
279	a	1285.87	3.64522	YES	YES
280	a	1288.07	1.72686	YES	YES
281	a	1288.24	3.67588	YES	YES
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284	a	1306.93	0.19187	YES	YES
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292	a	1320.13	5.59232	YES	YES
293	a	1321.78	1.87052	YES	YES
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297	a	1323.36	0.23910	YES	YES
298	a	1323.75	2.27828	YES	YES
299	a	1324.32	2.24276	YES	YES
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309	a	1336.75	0.41510	YES	YES
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311	a	1337.70	0.09367	YES	YES
312	a	1337.99	0.64814	YES	YES
313	a	1338.29	0.08050	YES	YES

314	a	1338.74	0.48646	YES	YES
315	a	1343.19	2.01883	YES	YES
316	a	1343.88	1.13015	YES	YES
317	a	1345.28	2.63813	YES	YES
318	a	1345.79	1.08132	YES	YES
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345	a	1438.88	4.76994	YES	YES
346	a	1439.22	2.97146	YES	YES
347	a	1439.31	1.73109	YES	YES
348	a	1439.49	5.39297	YES	YES
349	a	1439.79	4.67700	YES	YES
350	a	1441.13	0.37875	YES	YES
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352	a	1442.62	19.25412	YES	YES
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358	a	1448.10	9.42241	YES	YES
359	a	1452.22	2.69947	YES	YES
360	a	1452.96	0.18968	YES	YES
361	a	1453.60	5.19679	YES	YES
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365	a	1456.11	0.11915	YES	YES
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367	a	2897.57	3.84486	YES	YES
368	a	2907.50	37.12499	YES	YES
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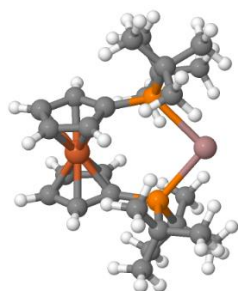
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384	a	2943.34	8.69451	YES	YES
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388	a	2945.68	14.48020	YES	YES
389	a	2946.05	8.37251	YES	YES
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391	a	2947.32	10.53313	YES	YES
392	a	2948.67	5.47790	YES	YES
393	a	2950.47	3.42387	YES	YES
394	a	2951.11	13.95218	YES	YES
395	a	2951.71	9.63144	YES	YES
396	a	2955.45	4.56821	YES	YES
397	a	2955.72	4.75074	YES	YES
398	a	2956.28	6.09112	YES	YES
399	a	2956.77	4.61390	YES	YES
400	a	2957.49	5.42021	YES	YES
401	a	2959.02	9.68538	YES	YES
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410	a	2964.08	26.64028	YES	YES
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413	a	2972.31	14.41920	YES	YES
414	a	2973.53	9.63789	YES	YES
415	a	2974.49	24.55338	YES	YES
416	a	2980.93	21.24916	YES	YES
417	a	2982.47	16.98522	YES	YES
418	a	2982.80	3.91048	YES	YES
419	a	2984.85	4.51076	YES	YES
420	a	2985.84	10.79564	YES	YES
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422	a	2988.16	4.13223	YES	YES
423	a	2990.21	29.55315	YES	YES
424	a	2995.41	20.82539	YES	YES
425	a	2997.24	33.82276	YES	YES
426	a	2998.93	21.21414	YES	YES
427	a	3000.29	21.76372	YES	YES
428	a	3001.84	29.07383	YES	YES
429	a	3003.21	7.02976	YES	YES

430	a	3003.33	31.06212	YES	YES
431	a	3003.65	40.65606	YES	YES
432	a	3004.73	30.81451	YES	YES
433	a	3005.72	14.93254	YES	YES
434	a	3007.20	17.92703	YES	YES
435	a	3008.70	16.49923	YES	YES
436	a	3009.01	17.70426	YES	YES
437	a	3010.88	23.03653	YES	YES
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447	a	3016.13	25.17473	YES	YES
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449	a	3017.76	29.13775	YES	YES
450	a	3018.24	18.20136	YES	YES
451	a	3018.44	26.37214	YES	YES
452	a	3018.52	30.26508	YES	YES
453	a	3018.70	38.31006	YES	YES
454	a	3018.78	20.55836	YES	YES
455	a	3019.00	37.35209	YES	YES
456	a	3019.44	20.92608	YES	YES
457	a	3020.41	19.57105	YES	YES
458	a	3022.54	30.77771	YES	YES
459	a	3026.79	2.26441	YES	YES
460	a	3028.45	0.47743	YES	YES
461	a	3037.58	1.65825	YES	YES
462	a	3045.01	1.01003	YES	YES

\$end

Double hybrid single point energy = -7249.045868529255 H
COSMO energy + OC correction = -7256.3135866390 H (in oDFB)

6.2.3 [Ga(dtbpf)]⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

Ga	1.3340101	0.7103251	-1.6910945
Fe	-1.4416557	-0.7680499	1.8240354
P	1.4515160	-1.3293270	-0.0156445
P	-0.9233779	1.6106840	-0.6535103

C	2.9173717	-0.9557545	1.1196518
C	4.0636630	-0.3455371	0.2886896
H	4.8444071	0.0013958	0.9807442
H	3.7327066	0.5284629	-0.2924488
H	4.5246076	-1.0543225	-0.4024500
C	2.4584702	0.1432028	2.0950183
H	3.3092300	0.4250096	2.7316312
H	1.6341756	-0.1661113	2.7422596
H	2.1464461	1.0445321	1.5485967
C	3.4302609	-2.1838793	1.8836448
H	4.2044614	-1.8660524	2.5977025
H	3.8891666	-2.9157699	1.2090067
H	2.6410950	-2.6925149	2.4481413
C	1.7810402	-2.8286782	-1.1414207
C	3.1854799	-2.7510500	-1.7577681
H	3.2700432	-3.5339974	-2.5251485
H	3.9744832	-2.9329088	-1.0201034
H	3.3741531	-1.7872250	-2.2496438
C	0.7614803	-2.7257826	-2.2927097
H	0.9589202	-3.5265380	-3.0198778
H	0.8518902	-1.7704069	-2.8358008
H	-0.2724764	-2.8433380	-1.9535066
C	1.5986087	-4.1616458	-0.4045854
H	1.7577205	-4.9868709	-1.1143836
H	0.5896331	-4.2652478	0.0108381
H	2.3188613	-4.2825891	0.4121714
C	-0.5884974	3.4624734	-0.3660202
C	0.7727246	3.5396479	0.3527260
H	1.0555657	4.5952300	0.4741431
H	1.5733367	3.0588489	-0.2335302
H	0.7491529	3.0932857	1.3518268
C	-1.6698529	4.1227565	0.4986562
H	-1.3995880	5.1758674	0.6661545
H	-1.7627377	3.6396077	1.4780634
H	-2.6522692	4.1050725	0.0139263
C	-0.4499524	4.2066556	-1.7021590
H	-0.0901200	5.2248325	-1.4951590
H	-1.4065684	4.3008569	-2.2272933
H	0.2782719	3.7308566	-2.3728276
C	-2.2322232	1.3224847	-1.9881350
C	-1.6307880	1.6438789	-3.3708171
H	-2.3501012	1.3303655	-4.1409708
H	-0.6970428	1.0909244	-3.5536704
H	-1.4275681	2.7064084	-3.5202142
C	-2.5419273	-0.1854654	-1.9921017
H	-3.2586578	-0.3943383	-2.7990347
H	-2.9695624	-0.5444003	-1.0527971
H	-1.6345948	-0.7696246	-2.2015403
C	-3.5125190	2.1422571	-1.7785684
H	-4.2599361	1.8401707	-2.5271535
H	-3.3309539	3.2148138	-1.9130204
H	-3.9527357	1.9955748	-0.7861827
C	0.0665994	-1.8859521	1.0180100
C	-0.0268175	-2.1149682	2.4415982
H	0.7461528	-1.9329534	3.1775001
C	-1.3313847	-2.6141425	2.7403954
H	-1.7051119	-2.8452409	3.7325837
C	-2.0651820	-2.7066996	1.5208739

H	-3.0964412	-3.0267461	1.4150410
C	-1.2197451	-2.2527289	0.4644991
H	-1.5069921	-2.1822197	-0.5749297
C	-1.6107927	1.0638279	0.9355171
C	-0.8661686	1.1418669	2.1745331
H	0.1596528	1.4652310	2.2795184
C	-1.7009437	0.6998239	3.2443192
H	-1.4099275	0.6251507	4.2868354
C	-2.9615251	0.3264594	2.6913918
H	-3.8024867	-0.0900873	3.2361817
C	-2.9153492	0.5475124	1.2809657
H	-3.7307844	0.3428104	0.5988296

SCF energy GEOOPT = -4889.656646528 H

ZPE = 1642. kJ/mol

FREEH energy = 1740.85 kJ/mol

FREEH entropy = 0.91153 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
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	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
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	9	a	51.22	0.01467	YES	YES
	10	a	63.92	0.00047	YES	YES
	11	a	68.40	0.01244	YES	YES
	12	a	81.20	0.02355	YES	YES
	13	a	86.41	0.05064	YES	YES
	14	a	98.40	0.01733	YES	YES
	15	a	100.81	1.61369	YES	YES
	16	a	105.48	0.57629	YES	YES
	17	a	112.36	3.66740	YES	YES
	18	a	118.02	2.48191	YES	YES
	19	a	123.00	0.03746	YES	YES
	20	a	140.70	1.56419	YES	YES
	21	a	144.73	0.17300	YES	YES
	22	a	162.54	4.99398	YES	YES
	23	a	164.93	5.50181	YES	YES
	24	a	176.86	0.23128	YES	YES
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	27	a	202.01	0.70757	YES	YES
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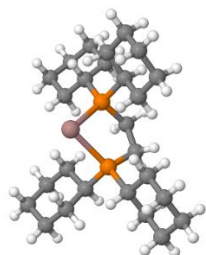
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43	a	274.91	0.17628	YES	YES
44	a	275.52	0.18438	YES	YES
45	a	299.82	0.58622	YES	YES
46	a	303.14	0.98451	YES	YES
47	a	327.83	0.17024	YES	YES
48	a	329.51	0.25125	YES	YES
49	a	353.00	0.75363	YES	YES
50	a	357.24	1.78391	YES	YES
51	a	360.17	1.70800	YES	YES
52	a	366.88	0.80772	YES	YES
53	a	369.35	0.26028	YES	YES
54	a	374.60	2.54529	YES	YES
55	a	377.97	0.25407	YES	YES
56	a	397.70	2.14447	YES	YES
57	a	399.09	1.55236	YES	YES
58	a	406.74	0.53627	YES	YES
59	a	418.01	3.79568	YES	YES
60	a	424.27	11.97697	YES	YES
61	a	426.15	1.04674	YES	YES
62	a	454.44	26.14071	YES	YES
63	a	455.17	33.41743	YES	YES
64	a	470.70	28.34704	YES	YES
65	a	472.99	5.45387	YES	YES
66	a	493.07	10.82827	YES	YES
67	a	511.09	8.93660	YES	YES
68	a	520.04	1.88306	YES	YES
69	a	554.04	9.22505	YES	YES
70	a	557.94	0.49833	YES	YES
71	a	572.21	0.03280	YES	YES
72	a	576.39	0.61146	YES	YES
73	a	588.92	0.68833	YES	YES
74	a	589.80	5.93916	YES	YES
75	a	612.88	4.14284	YES	YES
76	a	617.67	2.09488	YES	YES
77	a	792.01	1.31164	YES	YES
78	a	792.74	11.44072	YES	YES
79	a	794.05	0.56729	YES	YES
80	a	797.72	9.63041	YES	YES
81	a	799.02	1.52764	YES	YES
82	a	806.92	33.00966	YES	YES
83	a	813.33	0.27220	YES	YES
84	a	818.99	2.35948	YES	YES
85	a	820.82	5.49590	YES	YES
86	a	823.35	2.66079	YES	YES
87	a	840.92	1.68043	YES	YES
88	a	849.98	0.56699	YES	YES
89	a	871.71	1.08083	YES	YES
90	a	875.62	3.12171	YES	YES
91	a	878.54	1.29784	YES	YES
92	a	879.86	1.02529	YES	YES
93	a	912.60	1.00705	YES	YES
94	a	913.17	0.98053	YES	YES
95	a	914.81	0.87345	YES	YES

96	a	915.30	2.91219	YES	YES
97	a	918.08	1.14623	YES	YES
98	a	918.99	1.23487	YES	YES
99	a	920.48	1.24629	YES	YES
100	a	921.34	0.62893	YES	YES
101	a	932.71	0.02879	YES	YES
102	a	933.28	0.05146	YES	YES
103	a	940.17	0.20481	YES	YES
104	a	940.47	0.35373	YES	YES
105	a	987.51	0.34096	YES	YES
106	a	988.01	1.11524	YES	YES
107	a	998.55	1.57478	YES	YES
108	a	999.56	0.85163	YES	YES
109	a	1002.52	0.16138	YES	YES
110	a	1002.77	1.77485	YES	YES
111	a	1006.75	4.88165	YES	YES
112	a	1007.19	5.75941	YES	YES
113	a	1026.50	0.91952	YES	YES
114	a	1030.18	2.88953	YES	YES
115	a	1032.77	13.84986	YES	YES
116	a	1035.61	7.96022	YES	YES
117	a	1052.33	1.31973	YES	YES
118	a	1052.99	1.03629	YES	YES
119	a	1149.12	0.38458	YES	YES
120	a	1149.70	13.65429	YES	YES
121	a	1153.89	74.61034	YES	YES
122	a	1154.44	10.62833	YES	YES
123	a	1158.58	31.19319	YES	YES
124	a	1160.14	1.21805	YES	YES
125	a	1167.88	1.25735	YES	YES
126	a	1171.11	2.81632	YES	YES
127	a	1179.48	1.57039	YES	YES
128	a	1182.18	3.09711	YES	YES
129	a	1189.26	0.58648	YES	YES
130	a	1189.67	0.64676	YES	YES
131	a	1192.52	0.13359	YES	YES
132	a	1192.97	0.09317	YES	YES
133	a	1197.52	0.68292	YES	YES
134	a	1199.92	1.07967	YES	YES
135	a	1291.58	3.30019	YES	YES
136	a	1293.77	0.97520	YES	YES
137	a	1345.62	4.68351	YES	YES
138	a	1347.71	4.78599	YES	YES
139	a	1353.52	0.46528	YES	YES
140	a	1354.05	2.01193	YES	YES
141	a	1356.79	3.96416	YES	YES
142	a	1357.18	9.00760	YES	YES
143	a	1357.25	10.61419	YES	YES
144	a	1358.29	25.15581	YES	YES
145	a	1360.95	0.51661	YES	YES
146	a	1361.40	0.11603	YES	YES
147	a	1378.24	9.63993	YES	YES
148	a	1379.58	0.12004	YES	YES
149	a	1383.48	22.39773	YES	YES
150	a	1384.08	3.82420	YES	YES
151	a	1389.61	8.58764	YES	YES
152	a	1390.17	19.20312	YES	YES
153	a	1403.26	0.99047	YES	YES

154	a	1405.12	0.38824	YES	YES
155	a	1419.90	1.23855	YES	YES
156	a	1421.24	0.16435	YES	YES
157	a	1422.63	0.44963	YES	YES
158	a	1423.35	0.84758	YES	YES
159	a	1429.93	1.63478	YES	YES
160	a	1430.54	1.45825	YES	YES
161	a	1431.03	0.52053	YES	YES
162	a	1431.72	0.68037	YES	YES
163	a	1438.06	2.45102	YES	YES
164	a	1438.56	1.56689	YES	YES
165	a	1440.96	3.46917	YES	YES
166	a	1442.53	0.47142	YES	YES
167	a	1449.16	11.77392	YES	YES
168	a	1449.56	13.00698	YES	YES
169	a	1452.43	0.64157	YES	YES
170	a	1454.21	2.73101	YES	YES
171	a	1454.52	0.13004	YES	YES
172	a	1455.24	5.65510	YES	YES
173	a	1461.31	7.43010	YES	YES
174	a	1461.62	1.60086	YES	YES
175	a	1469.04	0.54332	YES	YES
176	a	1469.66	39.60082	YES	YES
177	a	1473.10	8.52824	YES	YES
178	a	1473.58	10.58823	YES	YES
179	a	2934.53	29.61942	YES	YES
180	a	2935.24	7.93811	YES	YES
181	a	2954.48	10.27662	YES	YES
182	a	2954.99	11.77017	YES	YES
183	a	2964.82	12.22909	YES	YES
184	a	2965.02	9.42190	YES	YES
185	a	2965.23	17.02532	YES	YES
186	a	2965.25	15.24119	YES	YES
187	a	2970.53	23.41089	YES	YES
188	a	2970.56	10.30363	YES	YES
189	a	2971.37	40.15295	YES	YES
190	a	2971.56	14.02125	YES	YES
191	a	3008.10	40.83059	YES	YES
192	a	3008.37	3.13370	YES	YES
193	a	3014.84	43.69602	YES	YES
194	a	3015.29	0.87705	YES	YES
195	a	3024.07	52.64528	YES	YES
196	a	3024.21	3.08250	YES	YES
197	a	3027.29	27.38493	YES	YES
198	a	3027.44	8.75558	YES	YES
199	a	3039.25	13.41654	YES	YES
200	a	3039.47	21.65080	YES	YES
201	a	3041.93	4.12218	YES	YES
202	a	3042.18	5.44432	YES	YES
203	a	3059.84	11.34124	YES	YES
204	a	3060.95	10.99189	YES	YES
205	a	3066.44	5.74832	YES	YES
206	a	3066.63	6.00897	YES	YES
207	a	3068.30	0.70470	YES	YES
208	a	3068.69	1.58205	YES	YES
209	a	3069.41	23.07829	YES	YES
210	a	3069.88	20.57266	YES	YES
211	a	3087.75	5.84663	YES	YES

212	a	3089.73	5.54856	YES	YES
213	a	3096.85	8.43750	YES	YES
214	a	3097.71	8.11361	YES	YES
215	a	3164.17	0.08086	YES	YES
216	a	3164.24	0.04353	YES	YES
217	a	3175.76	0.52228	YES	YES
218	a	3175.97	0.55337	YES	YES
219	a	3190.73	1.72736	YES	YES
220	a	3190.96	0.88210	YES	YES
221	a	3211.58	1.56128	YES	YES
222	a	3212.15	0.55721	YES	YES
§end					

6.2.4 [Ga(dcpe)]⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c2

Cartesian coordinates in Ångström:

```

Ga  -0.0000000  0.0000000  2.1405337
P   -0.8248189 -1.3619484  0.0539142
P    0.8248189  1.3619484  0.0539142
C   -0.6357848 -3.1979283 -0.0094537
H   -1.1360682 -3.5434903  0.9114336
C    0.8443289 -3.6071087  0.0903907
H    1.3951521 -3.2215623 -0.7837176
H    1.3041363 -3.1544345  0.9815559
C    0.9859215 -5.1342066  0.1317948
H    2.0501133 -5.4057855  0.1672848
H    0.5339179 -5.5106019  1.0640086
C    0.3013669 -5.7929551 -1.0702716
H    0.3855310 -6.8860300 -1.0016948
H    0.8241859 -5.4968287 -1.9952410
C   -1.1708431 -5.3804236 -1.1673308
H   -1.7192636 -5.7675003 -0.2928228
H   -1.6400715 -5.8276164 -2.0545850
C   -1.3230729 -3.8538575 -1.2184240
H   -2.3871924 -3.5794911 -1.2544409
H   -0.8645465 -3.4763636 -2.1468307
C   -2.6423860 -1.0104920  0.0739993
H   -3.0692707 -1.3201210 -0.8949880
C   -3.3311397 -1.7989335  1.2028181
H   -3.2323513 -2.8790424  1.0296238
H   -2.8207352 -1.5842816  2.1582862
C   -4.8133698 -1.4247313  1.3254850
H   -5.3425501 -1.7428587  0.4122133
H   -5.2626818 -1.9833320  2.1579177
C   -5.0006725  0.0818038  1.5237919
H   -6.0690650  0.3294338  1.5821941

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H	-4.5558601	0.3821582	2.4873921
C	-4.3360965	0.8683862	0.3914939
H	-4.4363324	1.9505390	0.5551098
H	-4.8457052	0.6457362	-0.5605252
C	-2.8550467	0.5047090	0.2534973
H	-2.4075561	1.0602304	-0.5804686
H	-2.3247758	0.8343915	1.1714412
C	-0.1921759	-0.7444434	-1.5816450
H	0.6858801	-1.3633783	-1.8084444
H	-0.9337067	-0.9517217	-2.3657344
C	0.1921759	0.7444434	-1.5816450
H	-0.6858801	1.3633783	-1.8084444
H	0.9337067	0.9517217	-2.3657344
C	2.6423860	1.0104920	0.0739993
H	3.0692707	1.3201210	-0.8949880
C	3.3311397	1.7989335	1.2028181
H	2.8207352	1.5842816	2.1582862
H	3.2323513	2.8790424	1.0296238
C	4.8133698	1.4247313	1.3254850
H	5.3425501	1.7428587	0.4122133
H	5.2626818	1.9833320	2.1579177
C	5.0006725	-0.0818038	1.5237919
H	4.5558601	-0.3821582	2.4873921
H	6.0690650	-0.3294338	1.5821941
C	4.3360965	-0.8683862	0.3914939
H	4.4363324	-1.9505390	0.5551098
H	4.8457052	-0.6457362	-0.5605252
C	2.8550467	-0.5047090	0.2534973
H	2.3247758	-0.8343915	1.1714412
H	2.4075561	-1.0602304	-0.5804686
C	0.6357848	3.1979283	-0.0094537
H	1.1360682	3.5434903	0.9114336
C	-0.8443289	3.6071087	0.0903907
H	-1.3041363	3.1544345	0.9815559
H	-1.3951521	3.2215623	-0.7837176
C	-0.9859215	5.1342066	0.1317948
H	-2.0501133	5.4057855	0.1672848
H	-0.5339179	5.5106019	1.0640086
C	-0.3013669	5.7929551	-1.0702716
H	-0.8241859	5.4968287	-1.9952410
H	-0.3855310	6.8860300	-1.0016948
C	1.1708431	5.3804236	-1.1673308
H	1.7192636	5.7675003	-0.2928228
H	1.6400715	5.8276164	-2.0545850
C	1.3230729	3.8538575	-1.2184240
H	0.8645465	3.4763636	-2.1468307
H	2.3871924	3.5794911	-1.2544409

SCF energy GEOOPT = -3628.083122169 H

ZPE = 1793. kJ/mol

FREEH energy = 1880.12 kJ/mol

FREEH entropy = 0.87088 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.11	0.00661	YES	YES
8	b	33.06	0.06666	YES	YES
9	a	37.74	0.01490	YES	YES
10	b	41.10	0.19935	YES	YES
11	a	43.43	0.14321	YES	YES
12	a	44.73	0.12202	YES	YES
13	b	48.82	0.30806	YES	YES
14	b	53.51	0.02964	YES	YES
15	b	66.89	0.41674	YES	YES
16	a	68.14	0.02005	YES	YES
17	a	69.51	0.09832	YES	YES
18	b	70.78	0.00378	YES	YES
19	a	117.66	0.49772	YES	YES
20	b	122.06	0.92535	YES	YES
21	b	127.83	1.56923	YES	YES
22	a	133.13	1.90038	YES	YES
23	a	138.51	1.66315	YES	YES
24	a	171.47	1.95694	YES	YES
25	b	174.93	0.69242	YES	YES
26	a	194.48	2.09142	YES	YES
27	b	197.60	1.49132	YES	YES
28	b	217.60	0.07493	YES	YES
29	a	220.19	0.73480	YES	YES
30	b	225.13	0.32084	YES	YES
31	a	225.31	0.31537	YES	YES
32	b	238.42	0.08895	YES	YES
33	a	240.87	0.11064	YES	YES
34	b	260.42	1.43153	YES	YES
35	a	266.72	1.63134	YES	YES
36	b	299.72	0.59961	YES	YES
37	a	306.46	0.03497	YES	YES
38	a	329.34	0.21523	YES	YES
39	b	329.47	0.57446	YES	YES
40	b	347.20	0.50944	YES	YES
41	b	357.21	5.24551	YES	YES
42	a	359.48	0.04198	YES	YES
43	a	394.93	0.16971	YES	YES
44	b	415.85	3.19822	YES	YES
45	a	422.43	0.04872	YES	YES
46	b	424.06	2.18169	YES	YES
47	a	430.34	0.04491	YES	YES
48	b	430.84	0.00417	YES	YES
49	a	431.88	0.00051	YES	YES
50	b	432.93	0.52317	YES	YES
51	a	442.26	0.31041	YES	YES
52	b	465.65	5.92144	YES	YES
53	a	491.13	0.34154	YES	YES
54	b	491.95	4.77065	YES	YES
55	a	504.50	0.06260	YES	YES
56	b	515.21	19.49590	YES	YES
57	b	629.17	17.07453	YES	YES
58	a	631.36	4.21466	YES	YES
59	b	715.06	4.99029	YES	YES
60	a	723.69	0.04839	YES	YES

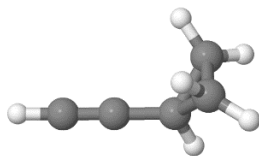
61	a	733.94	1.56253	YES	YES
62	b	735.58	7.43648	YES	YES
63	b	761.61	19.02670	YES	YES
64	a	769.81	0.00017	YES	YES
65	b	770.16	0.36372	YES	YES
66	a	773.92	0.02165	YES	YES
67	b	774.07	0.59070	YES	YES
68	a	808.40	1.21964	YES	YES
69	b	810.68	2.87258	YES	YES
70	a	811.29	0.01120	YES	YES
71	b	811.61	7.48938	YES	YES
72	a	830.62	2.12633	YES	YES
73	b	837.33	6.32493	YES	YES
74	a	837.73	0.20426	YES	YES
75	b	839.04	10.97779	YES	YES
76	a	847.88	0.87667	YES	YES
77	b	872.23	3.30381	YES	YES
78	a	873.53	3.20144	YES	YES
79	b	875.89	10.86205	YES	YES
80	a	876.79	0.11450	YES	YES
81	a	877.41	0.48725	YES	YES
82	b	877.65	4.67778	YES	YES
83	b	880.22	0.64513	YES	YES
84	a	882.39	1.65081	YES	YES
85	b	900.81	1.65889	YES	YES
86	a	902.72	0.39748	YES	YES
87	b	907.78	3.46702	YES	YES
88	a	908.21	0.00566	YES	YES
89	b	987.01	1.36911	YES	YES
90	a	987.21	3.49851	YES	YES
91	b	988.85	19.54758	YES	YES
92	a	990.41	7.08185	YES	YES
93	a	992.95	3.11147	YES	YES
94	b	1015.80	0.06209	YES	YES
95	a	1016.05	0.96177	YES	YES
96	b	1021.20	0.48647	YES	YES
97	a	1021.45	0.39336	YES	YES
98	b	1029.04	0.00374	YES	YES
99	a	1030.01	1.36771	YES	YES
100	b	1038.38	5.23720	YES	YES
101	a	1038.75	0.32159	YES	YES
102	b	1058.62	0.89348	YES	YES
103	a	1058.63	0.04103	YES	YES
104	b	1059.28	5.26938	YES	YES
105	a	1066.02	0.04466	YES	YES
106	b	1070.38	1.63959	YES	YES
107	a	1071.68	0.05294	YES	YES
108	b	1072.79	2.57365	YES	YES
109	a	1075.48	0.06778	YES	YES
110	b	1076.21	1.59387	YES	YES
111	a	1087.26	1.35924	YES	YES
112	b	1090.77	6.91920	YES	YES
113	a	1098.70	0.04139	YES	YES
114	b	1105.40	9.11553	YES	YES
115	a	1128.82	0.46273	YES	YES
116	a	1158.22	3.35191	YES	YES
117	b	1159.01	0.54633	YES	YES
118	b	1168.36	27.28763	YES	YES

119	a	1169.24	0.55143	YES	YES
120	b	1173.07	3.54121	YES	YES
121	a	1174.03	1.24330	YES	YES
122	b	1187.91	3.76277	YES	YES
123	a	1189.86	0.48539	YES	YES
124	b	1225.63	2.24782	YES	YES
125	a	1243.51	0.21010	YES	YES
126	b	1246.39	2.55224	YES	YES
127	a	1247.52	0.47355	YES	YES
128	b	1251.09	0.25653	YES	YES
129	a	1252.55	0.00025	YES	YES
130	a	1253.99	0.03421	YES	YES
131	b	1254.02	5.35525	YES	YES
132	b	1257.31	5.33201	YES	YES
133	a	1257.99	2.25084	YES	YES
134	b	1258.97	8.68072	YES	YES
135	a	1259.09	1.53097	YES	YES
136	b	1262.47	4.40384	YES	YES
137	a	1263.08	0.00747	YES	YES
138	a	1282.75	0.68572	YES	YES
139	b	1282.80	3.92766	YES	YES
140	b	1288.61	5.81457	YES	YES
141	a	1288.88	0.76799	YES	YES
142	b	1310.96	3.12029	YES	YES
143	a	1311.56	0.01058	YES	YES
144	b	1314.47	1.20909	YES	YES
145	a	1314.48	0.13065	YES	YES
146	b	1322.26	1.92844	YES	YES
147	a	1322.75	1.00005	YES	YES
148	a	1323.66	1.50123	YES	YES
149	b	1323.67	1.22809	YES	YES
150	b	1324.93	1.99484	YES	YES
151	a	1324.95	0.87471	YES	YES
152	b	1327.28	3.63970	YES	YES
153	a	1327.74	7.93669	YES	YES
154	b	1335.90	0.10096	YES	YES
155	a	1335.96	1.04938	YES	YES
156	a	1337.14	0.00707	YES	YES
157	b	1337.32	0.23492	YES	YES
158	b	1344.78	5.33673	YES	YES
159	a	1344.98	0.97021	YES	YES
160	b	1347.83	2.27450	YES	YES
161	a	1347.87	0.04968	YES	YES
162	b	1406.11	6.73795	YES	YES
163	a	1410.39	1.42430	YES	YES
164	b	1411.48	8.90924	YES	YES
165	a	1413.34	8.15444	YES	YES
166	b	1430.05	2.29886	YES	YES
167	a	1431.54	1.51490	YES	YES
168	a	1434.41	0.00176	YES	YES
169	b	1435.49	6.50186	YES	YES
170	a	1436.11	1.55432	YES	YES
171	b	1436.30	17.67660	YES	YES
172	b	1438.22	6.02175	YES	YES
173	a	1438.32	2.25378	YES	YES
174	b	1439.83	0.49641	YES	YES
175	a	1439.87	0.00024	YES	YES
176	a	1442.89	30.48399	YES	YES

177	b	1443.05	1.79744	YES	YES
178	b	1444.69	16.79287	YES	YES
179	a	1444.83	4.49806	YES	YES
180	a	1452.37	1.22471	YES	YES
181	b	1452.54	4.72776	YES	YES
182	b	1454.87	0.28154	YES	YES
183	a	1455.38	0.00687	YES	YES
184	b	2851.40	142.52655	YES	YES
185	a	2853.79	9.61907	YES	YES
186	b	2928.67	10.21872	YES	YES
187	a	2928.72	1.79025	YES	YES
188	a	2938.10	0.04259	YES	YES
189	b	2938.17	29.02088	YES	YES
190	b	2942.53	14.97135	YES	YES
191	a	2942.57	9.39953	YES	YES
192	b	2942.71	18.36806	YES	YES
193	a	2942.79	1.76327	YES	YES
194	a	2944.69	1.57410	YES	YES
195	b	2944.77	25.66260	YES	YES
196	b	2947.71	17.82401	YES	YES
197	a	2947.81	6.30882	YES	YES
198	a	2952.06	4.69832	YES	YES
199	b	2952.30	12.76826	YES	YES
200	b	2952.57	7.40247	YES	YES
201	a	2952.79	1.85790	YES	YES
202	b	2955.88	0.22918	YES	YES
203	a	2955.93	8.74273	YES	YES
204	b	2958.18	76.46042	YES	YES
205	a	2958.29	1.12222	YES	YES
206	b	2958.89	11.64694	YES	YES
207	a	2958.89	89.91379	YES	YES
208	b	2978.99	6.41121	YES	YES
209	a	2984.72	3.62729	YES	YES
210	b	2991.33	9.04792	YES	YES
211	a	2991.43	44.06557	YES	YES
212	a	3000.85	1.03700	YES	YES
213	b	3000.89	55.97565	YES	YES
214	a	3005.54	4.50975	YES	YES
215	b	3005.57	37.30448	YES	YES
216	a	3007.94	0.07594	YES	YES
217	b	3007.97	66.03052	YES	YES
218	b	3008.22	37.83825	YES	YES
219	a	3008.27	8.56363	YES	YES
220	b	3009.76	37.55844	YES	YES
221	a	3009.80	31.68979	YES	YES
222	b	3011.57	21.96275	YES	YES
223	a	3011.62	33.03292	YES	YES
224	a	3013.08	18.27614	YES	YES
225	b	3013.09	52.21455	YES	YES
226	b	3014.15	43.37986	YES	YES
227	a	3014.18	3.95885	YES	YES
228	b	3014.94	21.83648	YES	YES
229	a	3015.09	37.24130	YES	YES
230	a	3021.88	0.21182	YES	YES
231	b	3038.54	4.65595	YES	YES

\$end

6.2.5 HCCC₃H₅



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: cs

Cartesian coordinates in Ångström:

```
C   -2.4798527   -0.4282591   0.0000000
C   -1.2697989   -0.5097138   0.0000000
H   -3.5462910   -0.3590792   0.0000000
C    0.1603871   -0.5971183   0.0000000
C    0.9853149    0.4419296    0.7504470
C    0.9853149    0.4419296   -0.7504470
H    0.5589582   -1.6127203    0.0000000
H    1.8709108    0.0851723    1.2728924
H    0.4320339    1.2263757    1.2618571
H    0.4320339    1.2263757   -1.2618571
H    1.8709108    0.0851723   -1.2728924
```

SCF energy GEOOPT = -194.1292951041 H

ZPE = 231.1 kJ/mol

FREEH energy = 244.93 kJ/mol

FREEH entropy = 0.29943 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a'	194.01	1.39950	YES	YES
8		a''	200.39	1.62749	YES	YES
9		a'	491.03	7.84414	YES	YES
10		a''	502.40	0.96116	YES	YES
11		a''	576.24	55.38173	YES	YES
12		a'	638.17	46.98139	YES	YES
13		a'	740.33	2.18504	YES	YES
14		a'	793.18	0.95453	YES	YES
15		a''	799.29	7.92883	YES	YES
16		a''	861.42	1.72724	YES	YES
17		a'	948.04	20.44498	YES	YES
18		a'	1016.07	7.08727	YES	YES
19		a''	1036.74	5.81888	YES	YES
20		a''	1072.95	1.43513	YES	YES
21		a'	1104.93	0.35992	YES	YES
22		a''	1163.97	0.77694	YES	YES
23		a'	1185.58	0.52862	YES	YES
24		a'	1337.13	3.12190	YES	YES
25		a''	1420.77	2.90184	YES	YES
26		a'	1450.17	0.99458	YES	YES
27		a'	2150.14	32.54722	YES	YES

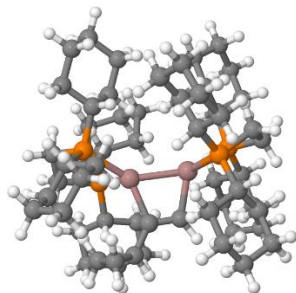
28	a''	3071.44	16.74176	YES	YES
29	a'	3073.40	4.98742	YES	YES
30	a'	3077.10	6.83209	YES	YES
31	a''	3154.61	0.11165	YES	YES
32	a'	3169.51	9.21200	YES	YES
33	a'	3405.87	74.89504	YES	YES

\$end

Double hybrid single point energy = -193.765731385910 H

COSMO energy + OC correction = -194.1351446828 H (in oDFB)

6.2.6 $[\{\text{Ga}(\text{dcpe})\}_2(\text{HCCC}_3\text{H}_5)]^{2+}$



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

```

Ga  -2.4757386   17.2482330  -2.7111462
Ga  -4.0653228   17.8416555  -0.9742568
P   -1.6232113   18.8844879  -4.2518510
P   -6.0520188   19.1902998  -0.8125894
P   -2.0361340   15.6067784  -4.3885897
P   -5.3065183   16.1961036   0.2639921
C   -5.0922555   20.9731535  -5.3049401
H   -5.2669110   21.4920130  -4.3461119
H   -6.0700144   20.6021877  -5.6432941
C   -1.0588376   14.1822544  -3.7494945
H   -0.8162823   13.5291975  -4.6042466
C   -4.2193203   15.3651721   1.4918713
H   -3.6043160   16.2112457   1.8473038
C   -4.3991076   16.0644342  -5.8031462
H   -3.8347658   16.5996254  -6.5840451
H   -4.6327305   16.7978575  -5.0157469
C   -6.8967885   19.2809399  -2.4522027
H   -6.2150025   19.8918346  -3.0663763
C   -7.2134220   18.2601783   0.2995513
H   -7.7877635   18.9757308   0.9024827
H   -7.9355784   17.7532581  -0.3542856
C   -3.1321013   22.4579217  -5.8815286
H   -2.7111224   23.1403930  -6.6318354
H   -3.2222225   23.0367016  -4.9473219
C   -2.1672018   21.2869028  -5.6523852
H   -1.1957185   21.6647786  -5.3060637
H   -1.9869014   20.7709108  -6.6096668
C   -4.1415757   19.7927071  -5.0724276
H   -4.0578035   19.2185035  -6.0089693

```

H	-4.5418554	19.1022127	-4.3140093
C	0.9985302	13.4929134	-2.4373836
H	1.3226914	12.7831577	-3.2154399
H	1.9120994	13.8712657	-1.9589193
C	-7.0201526	13.9064543	0.0414317
H	-7.5781934	14.3040177	0.9009391
H	-6.2526164	13.2286385	0.4447032
C	-5.8670952	20.9176675	-0.2084687
H	-6.8222947	21.4299271	-0.4124198
C	-0.2548179	20.4461517	-2.4343129
H	-0.9398402	21.2794415	-2.6481431
H	-0.7422504	19.8110068	-1.6769212
C	1.0647579	20.9871210	-1.8712660
H	1.4971019	21.7113671	-2.5807494
H	0.8637743	21.5398010	-0.9431748
C	-2.2389525	17.8886439	-0.0706494
C	-6.9972448	17.8884351	-3.0960998
H	-6.0005052	17.4218278	-3.1441380
H	-7.6230011	17.2382390	-2.4626023
C	-4.5166655	21.9695616	-6.3155129
H	-4.4414621	21.4827629	-7.3017719
H	-5.1994408	22.8206013	-6.4401971
C	-8.2673544	19.9766587	-2.4022768
H	-8.1761213	20.9878232	-1.9832106
H	-8.9417101	19.4144656	-1.7356498
C	-4.7490013	21.6024079	-1.0184965
H	-4.9844790	21.5806091	-2.0934459
H	-3.8143133	21.0289118	-0.8877821
C	-3.2136059	13.8655468	-6.2889988
H	-2.6300868	13.0447572	-5.8497926
H	-2.5933764	14.3075395	-7.0858770
C	2.3266508	19.0673515	-2.9072472
H	2.8011390	19.7253083	-3.6531850
H	3.0310184	18.2443841	-2.7235526
C	-5.3745855	22.4301142	1.7545758
H	-6.3151605	22.9906024	1.6297543
H	-5.1414943	22.4456194	2.8277055
C	-8.9947299	18.6627820	-4.4460057
H	-9.4116879	18.7435449	-5.4587903
H	-9.7018535	18.0457867	-3.8670476
C	-4.9074261	14.7357317	2.7139943
H	-5.5632922	15.4648525	3.2103371
H	-5.5426847	13.8962103	2.3981907
C	0.1151008	12.7686133	-1.4186788
H	0.6616117	11.9302090	-0.9668426
H	-0.1352136	13.4625416	-0.5984084
C	-7.6329922	17.9634905	-4.4880976
H	-6.9561223	18.5108807	-5.1639539
H	-7.7329929	16.9500126	-4.8991072
C	2.0683639	19.8583191	-1.6222479
H	1.6710467	19.1807587	-0.8477588
H	3.0105232	20.2653970	-1.2319231
C	-4.2626424	23.1145662	0.9532219
H	-4.1572607	24.1600639	1.2717671
H	-3.2994429	22.6246779	1.1713638
C	-5.5594608	14.4902085	-1.9524800
H	-4.7445698	13.8395560	-1.6014058
H	-5.0838966	15.3206159	-2.4966779

C	-5.5897907	20.9796880	1.3010831
H	-4.6904362	20.3894032	1.5323807
H	-6.4213479	20.5321886	1.8642725
C	-6.3326672	15.0371883	-0.7402185
H	-7.1224890	15.7024519	-1.1350630
C	-4.5379413	23.0477848	-0.5521284
C	-7.2086851	12.5724269	-2.1048651
H	-7.9032677	12.0423780	-2.7701584
H	-6.4648142	11.8291506	-1.7734699
C	-7.9565996	13.1171899	-0.8837365
H	-8.4240640	12.2970367	-0.3225489
H	-8.7760022	13.7757897	-1.2164801
C	-1.9414311	13.4119288	-2.7479316
H	-2.8379784	13.0191763	-3.2482377
H	-2.2896088	14.1201209	-1.9768315
C	-3.8449406	14.2289932	3.7002559
H	-3.2807442	15.0901075	4.0948752
H	-4.3382011	13.7567498	4.5605277
C	-5.6842139	15.5029719	-6.4222940
H	-6.2718382	16.3221993	-6.8586279
H	-6.3011300	15.0601441	-5.6233669
C	-2.8767400	13.2480944	3.0304697
H	-3.4270218	12.3404235	2.7316266
H	-2.1103180	12.9242828	3.7472693
C	-3.2627789	14.3798756	0.7978115
H	-3.8358322	13.5273053	0.4001665
H	-2.7699658	14.8755548	-0.0517162
C	-8.8892993	20.0486866	-3.8040438
H	-9.8787335	20.5210124	-3.7413118
H	-8.2693804	20.7034603	-4.4376985
C	-4.5087145	13.3172304	-6.9043399
H	-4.2627451	12.5808119	-7.6809763
H	-5.0735265	12.7755068	-6.1275375
C	-6.4943336	13.6931677	-2.8676859
H	-5.9264557	13.2766004	-3.7129472
H	-7.2417242	14.3788621	-3.3020006
C	-5.3779455	14.4383959	-7.4800488
H	-6.3122586	14.0256134	-7.8832724
H	-4.8535791	14.9080123	-8.3286765
C	-1.1747242	12.2690397	-2.0735534
H	-1.8257935	11.7836164	-1.3326473
H	-0.9313827	11.5011578	-2.8253078
C	-2.2168137	13.8689961	1.7948330
H	-1.5768442	14.7130961	2.1001020
H	-1.5606801	13.1387492	1.3008478
C	-1.7898612	18.2930885	1.2726022
C	-1.4385970	17.3064827	-1.0008804
C	-0.0208047	19.6101876	-3.7086577
H	0.3310614	20.2702980	-4.5195219
C	1.0241267	18.5016556	-3.4856812
H	1.2329273	17.9828261	-4.4328019
H	0.6112291	17.7545621	-2.7894995
C	0.2481436	14.6595417	-3.0907840
H	0.8961545	15.1530360	-3.8283524
H	0.0050968	15.4098768	-2.3218966
C	-1.0059567	16.4794448	-5.6536666
H	0.0312598	16.3680804	-5.3130862
H	-1.0830733	15.9506558	-6.6137717

C	-1.3422998	17.9725393	-5.8389890
H	-2.2648361	18.0844946	-6.4232153
H	-0.5434111	18.4674329	-6.4080616
C	-3.5293080	14.9335453	-5.2299584
H	-4.0963797	14.4586929	-4.4117992
C	-2.7533484	20.2891341	-4.6395973
H	-2.8698679	20.7984074	-3.6665693
C	-6.5068302	17.2374763	1.2067845
H	-7.2469711	16.6071431	1.7185427
H	-5.9271141	17.7492938	1.9881686
H	-5.4380731	23.6377036	-0.7888131
H	-3.7108091	23.4995331	-1.1173558
H	-0.8364743	17.8621433	1.5898470
C	-2.7779695	18.6115201	2.3781833
C	-2.0268294	19.7294793	1.7222464
H	-2.5640943	20.3719405	1.0270293
H	-1.2317448	20.2224196	2.2771666
H	-2.5204271	18.3363215	3.3988858
H	-3.8351840	18.5062549	2.1317631
H	-0.3964590	17.0495839	-0.7619430

SCF energy GEOOPT = -7450.377337511 H

ZPE = 3838. kJ/mol

FREEH energy = 4027.98 kJ/mol

FREEH entropy = 1.60876 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	13.83	0.00960	YES	YES
	8	a	19.27	0.00019	YES	YES
	9	a	24.07	0.01285	YES	YES
	10	a	25.42	0.02064	YES	YES
	11	a	30.02	0.01028	YES	YES
	12	a	32.00	0.03532	YES	YES
	13	a	34.71	0.03614	YES	YES
	14	a	39.86	0.01175	YES	YES
	15	a	41.13	0.13570	YES	YES
	16	a	43.96	0.03518	YES	YES
	17	a	45.90	0.01412	YES	YES
	18	a	46.41	0.08010	YES	YES
	19	a	48.86	0.11645	YES	YES
	20	a	50.23	0.09911	YES	YES
	21	a	52.60	0.02668	YES	YES
	22	a	57.21	0.42082	YES	YES
	23	a	58.70	0.07567	YES	YES
	24	a	60.58	0.02312	YES	YES
	25	a	63.41	0.05150	YES	YES
	26	a	65.65	0.27149	YES	YES
	27	a	67.20	0.10318	YES	YES
	28	a	68.20	0.13599	YES	YES
	29	a	70.30	0.01824	YES	YES

30	a	72.75	0.05123	YES	YES
31	a	77.25	0.09314	YES	YES
32	a	80.41	0.09975	YES	YES
33	a	85.53	0.48363	YES	YES
34	a	90.30	0.29856	YES	YES
35	a	91.83	0.25467	YES	YES
36	a	97.97	0.15407	YES	YES
37	a	107.45	0.11449	YES	YES
38	a	117.35	1.59591	YES	YES
39	a	122.43	0.18172	YES	YES
40	a	130.29	0.59461	YES	YES
41	a	132.70	1.04868	YES	YES
42	a	135.72	0.71459	YES	YES
43	a	136.56	0.22997	YES	YES
44	a	140.18	0.09158	YES	YES
45	a	142.05	0.85446	YES	YES
46	a	147.03	1.57991	YES	YES
47	a	155.24	0.43138	YES	YES
48	a	159.81	0.86509	YES	YES
49	a	166.21	4.22422	YES	YES
50	a	173.96	0.62185	YES	YES
51	a	176.54	2.95004	YES	YES
52	a	179.82	0.60623	YES	YES
53	a	187.71	2.38952	YES	YES
54	a	194.37	1.59001	YES	YES
55	a	199.79	0.07052	YES	YES
56	a	212.08	0.24064	YES	YES
57	a	213.86	0.15057	YES	YES
58	a	219.50	0.28151	YES	YES
59	a	220.25	0.30793	YES	YES
60	a	223.24	0.37716	YES	YES
61	a	224.65	0.72179	YES	YES
62	a	226.87	0.24842	YES	YES
63	a	229.52	0.08512	YES	YES
64	a	230.83	0.17932	YES	YES
65	a	235.23	0.32792	YES	YES
66	a	238.75	4.70354	YES	YES
67	a	241.34	3.00309	YES	YES
68	a	243.52	6.70382	YES	YES
69	a	245.21	0.78892	YES	YES
70	a	249.64	1.63739	YES	YES
71	a	254.92	0.84787	YES	YES
72	a	263.34	2.83746	YES	YES
73	a	278.05	1.63375	YES	YES
74	a	280.66	0.10844	YES	YES
75	a	285.13	3.88628	YES	YES
76	a	294.81	0.20678	YES	YES
77	a	297.78	0.08692	YES	YES
78	a	305.27	0.33725	YES	YES
79	a	309.59	0.07004	YES	YES
80	a	313.51	0.12300	YES	YES
81	a	330.14	0.06657	YES	YES
82	a	330.64	0.89917	YES	YES
83	a	334.94	0.31849	YES	YES
84	a	336.33	0.28070	YES	YES
85	a	340.07	0.18560	YES	YES
86	a	344.30	0.76580	YES	YES
87	a	370.05	0.03528	YES	YES

88	a	374.95	1.62513	YES	YES
89	a	380.36	0.79713	YES	YES
90	a	382.61	2.67074	YES	YES
91	a	393.04	1.16050	YES	YES
92	a	394.68	0.06588	YES	YES
93	a	406.47	6.54967	YES	YES
94	a	410.94	0.79943	YES	YES
95	a	411.74	1.57526	YES	YES
96	a	414.03	2.16432	YES	YES
97	a	420.90	4.42824	YES	YES
98	a	424.70	2.63789	YES	YES
99	a	428.09	0.47782	YES	YES
100	a	430.12	0.01398	YES	YES
101	a	430.35	0.12212	YES	YES
102	a	430.81	0.24992	YES	YES
103	a	431.41	0.15837	YES	YES
104	a	431.70	0.47551	YES	YES
105	a	433.18	0.41847	YES	YES
106	a	435.66	1.81684	YES	YES
107	a	437.98	0.17807	YES	YES
108	a	445.35	0.61122	YES	YES
109	a	453.84	21.86624	YES	YES
110	a	456.89	10.72690	YES	YES
111	a	462.15	6.28153	YES	YES
112	a	472.11	3.96954	YES	YES
113	a	492.40	4.53112	YES	YES
114	a	494.08	1.92704	YES	YES
115	a	496.17	4.84756	YES	YES
116	a	497.36	0.91533	YES	YES
117	a	501.31	2.07755	YES	YES
118	a	503.53	0.52494	YES	YES
119	a	511.24	22.40132	YES	YES
120	a	514.86	9.79425	YES	YES
121	a	516.68	9.36567	YES	YES
122	a	622.72	26.86636	YES	YES
123	a	626.25	12.94094	YES	YES
124	a	630.01	18.96446	YES	YES
125	a	642.27	11.41750	YES	YES
126	a	656.37	12.72589	YES	YES
127	a	700.90	1.65354	YES	YES
128	a	718.65	1.02599	YES	YES
129	a	723.10	2.06286	YES	YES
130	a	727.66	2.62101	YES	YES
131	a	733.12	9.24385	YES	YES
132	a	736.64	3.93601	YES	YES
133	a	737.81	2.29119	YES	YES
134	a	738.45	2.54109	YES	YES
135	a	765.27	5.99367	YES	YES
136	a	770.45	0.36450	YES	YES
137	a	771.87	0.93471	YES	YES
138	a	773.60	1.37246	YES	YES
139	a	774.18	0.75442	YES	YES
140	a	775.08	0.13148	YES	YES
141	a	776.60	0.34429	YES	YES
142	a	776.73	3.39679	YES	YES
143	a	777.39	0.64708	YES	YES
144	a	777.62	11.03896	YES	YES
145	a	779.20	13.62549	YES	YES

146	a	793.53	12.94623	YES	YES
147	a	803.21	22.01088	YES	YES
148	a	807.61	0.13053	YES	YES
149	a	809.41	2.32168	YES	YES
150	a	809.64	10.08681	YES	YES
151	a	811.38	6.26455	YES	YES
152	a	811.95	0.65018	YES	YES
153	a	813.64	3.15742	YES	YES
154	a	815.39	1.82603	YES	YES
155	a	816.94	2.88968	YES	YES
156	a	830.22	4.36376	YES	YES
157	a	831.65	5.81222	YES	YES
158	a	835.71	7.88385	YES	YES
159	a	837.49	0.16594	YES	YES
160	a	838.25	1.61321	YES	YES
161	a	838.43	2.72638	YES	YES
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163	a	839.45	1.43828	YES	YES
164	a	848.33	17.64114	YES	YES
165	a	850.68	24.46209	YES	YES
166	a	852.67	8.03190	YES	YES
167	a	872.06	0.39868	YES	YES
168	a	872.15	3.64385	YES	YES
169	a	872.61	3.31246	YES	YES
170	a	876.69	0.41723	YES	YES
171	a	877.26	3.69474	YES	YES
172	a	877.59	1.22448	YES	YES
173	a	878.27	1.92314	YES	YES
174	a	878.47	4.85870	YES	YES
175	a	879.48	2.42680	YES	YES
176	a	880.07	4.54643	YES	YES
177	a	880.53	2.72546	YES	YES
178	a	881.30	1.92002	YES	YES
179	a	881.77	1.97747	YES	YES
180	a	883.58	5.70047	YES	YES
181	a	883.75	10.05065	YES	YES
182	a	885.89	4.69474	YES	YES
183	a	886.64	1.43387	YES	YES
184	a	902.96	1.31666	YES	YES
185	a	904.10	1.57417	YES	YES
186	a	904.64	2.62674	YES	YES
187	a	905.29	0.60639	YES	YES
188	a	907.87	1.28549	YES	YES
189	a	908.22	2.93096	YES	YES
190	a	910.27	1.39891	YES	YES
191	a	910.93	0.64703	YES	YES
192	a	961.04	16.93418	YES	YES
193	a	977.72	0.30154	YES	YES
194	a	979.45	0.06382	YES	YES
195	a	986.97	10.18269	YES	YES
196	a	987.93	5.69113	YES	YES
197	a	988.97	3.83580	YES	YES
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206	a	1016.42	0.59758	YES	YES
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208	a	1018.04	0.64410	YES	YES
209	a	1019.18	0.28792	YES	YES
210	a	1020.91	0.56549	YES	YES
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212	a	1026.52	3.76132	YES	YES
213	a	1030.32	0.96424	YES	YES
214	a	1031.39	0.61372	YES	YES
215	a	1032.05	2.19363	YES	YES
216	a	1037.29	0.26161	YES	YES
217	a	1038.87	2.68617	YES	YES
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219	a	1040.17	0.74148	YES	YES
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227	a	1065.66	0.23331	YES	YES
228	a	1068.11	1.53045	YES	YES
229	a	1071.18	0.21366	YES	YES
230	a	1071.86	0.13419	YES	YES
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232	a	1072.80	0.36140	YES	YES
233	a	1073.09	0.28645	YES	YES
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235	a	1074.21	0.04187	YES	YES
236	a	1074.71	0.00184	YES	YES
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239	a	1081.18	0.29164	YES	YES
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243	a	1093.05	6.97128	YES	YES
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254	a	1161.43	10.07024	YES	YES
255	a	1166.70	8.80013	YES	YES
256	a	1167.41	3.23246	YES	YES
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259	a	1170.72	5.22947	YES	YES
260	a	1173.13	1.17621	YES	YES
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262	a	1176.80	11.51142	YES	YES
263	a	1179.14	4.45605	YES	YES
264	a	1183.27	5.90328	YES	YES
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266	a	1189.65	1.71991	YES	YES
267	a	1192.19	0.78102	YES	YES
268	a	1195.78	3.42147	YES	YES
269	a	1215.50	2.32908	YES	YES
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271	a	1240.95	0.33053	YES	YES
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273	a	1245.96	0.18865	YES	YES
274	a	1246.45	0.29518	YES	YES
275	a	1246.81	0.15743	YES	YES
276	a	1248.60	1.31763	YES	YES
277	a	1250.13	0.31260	YES	YES
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294	a	1266.08	2.42149	YES	YES
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296	a	1270.62	2.76837	YES	YES
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301	a	1285.82	2.60914	YES	YES
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306	a	1307.36	0.63914	YES	YES
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312	a	1313.33	1.85154	YES	YES
313	a	1316.53	1.76102	YES	YES
314	a	1318.53	0.26749	YES	YES
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352	a	1425.78	3.42864	YES	YES
353	a	1428.88	6.49164	YES	YES
354	a	1429.65	0.89834	YES	YES
355	a	1430.34	6.02826	YES	YES
356	a	1430.79	1.87469	YES	YES
357	a	1431.60	1.29854	YES	YES
358	a	1432.18	3.56750	YES	YES
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361	a	1436.14	6.02185	YES	YES
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363	a	1437.20	8.21757	YES	YES
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370	a	1439.20	1.07756	YES	YES
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372	a	1439.51	9.61186	YES	YES
373	a	1440.29	0.33405	YES	YES
374	a	1440.96	2.93794	YES	YES
375	a	1441.18	4.55381	YES	YES
376	a	1442.88	14.48813	YES	YES
377	a	1443.37	9.79893	YES	YES

378	a	1443.46	9.30311	YES	YES
379	a	1443.72	14.02779	YES	YES
380	a	1444.61	11.25344	YES	YES
381	a	1445.27	12.20184	YES	YES
382	a	1446.08	1.57378	YES	YES
383	a	1446.47	8.75985	YES	YES
384	a	1447.03	9.45148	YES	YES
385	a	1452.96	2.01768	YES	YES
386	a	1454.02	1.10412	YES	YES
387	a	1454.04	2.24916	YES	YES
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390	a	1456.25	0.59531	YES	YES
391	a	1456.98	1.66852	YES	YES
392	a	1457.43	4.22030	YES	YES
393	a	1496.35	27.45574	YES	YES
394	a	2921.12	4.34691	YES	YES
395	a	2926.60	9.26967	YES	YES
396	a	2929.14	29.51824	YES	YES
397	a	2934.55	2.37943	YES	YES
398	a	2935.42	23.25792	YES	YES
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400	a	2937.44	7.31816	YES	YES
401	a	2939.14	11.90830	YES	YES
402	a	2942.15	4.08589	YES	YES
403	a	2942.35	30.73751	YES	YES
404	a	2942.72	4.51313	YES	YES
405	a	2942.83	16.58556	YES	YES
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411	a	2947.96	9.34052	YES	YES
412	a	2948.80	14.23071	YES	YES
413	a	2949.07	3.06583	YES	YES
414	a	2949.24	16.22504	YES	YES
415	a	2950.30	1.21053	YES	YES
416	a	2950.83	12.04129	YES	YES
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419	a	2953.62	5.11691	YES	YES
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430	a	2959.83	41.87217	YES	YES
431	a	2959.96	39.88728	YES	YES
432	a	2960.55	21.94560	YES	YES
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434	a	2962.29	28.45909	YES	YES
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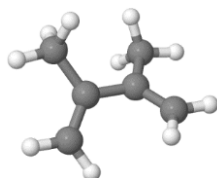
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448	a	2989.16	7.33568	YES	YES
449	a	2989.61	3.02786	YES	YES
450	a	2990.34	4.81962	YES	YES
451	a	2990.64	48.70715	YES	YES
452	a	2997.78	17.10712	YES	YES
453	a	2999.20	34.32927	YES	YES
454	a	3000.30	33.14459	YES	YES
455	a	3001.43	12.99461	YES	YES
456	a	3002.33	25.39084	YES	YES
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459	a	3007.90	14.75811	YES	YES
460	a	3008.05	20.41656	YES	YES
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462	a	3009.05	15.27233	YES	YES
463	a	3009.20	25.18603	YES	YES
464	a	3009.97	14.56281	YES	YES
465	a	3010.82	11.69681	YES	YES
466	a	3011.21	29.47897	YES	YES
467	a	3011.34	17.58817	YES	YES
468	a	3011.92	34.04993	YES	YES
469	a	3012.54	12.36376	YES	YES
470	a	3013.06	20.20372	YES	YES
471	a	3014.09	17.14155	YES	YES
472	a	3014.69	19.70028	YES	YES
473	a	3015.74	35.12652	YES	YES
474	a	3015.84	26.31170	YES	YES
475	a	3015.94	13.02755	YES	YES
476	a	3016.39	30.20828	YES	YES
477	a	3016.48	26.72726	YES	YES
478	a	3017.40	30.31877	YES	YES
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486	a	3021.87	33.24974	YES	YES
487	a	3026.87	2.54915	YES	YES
488	a	3030.55	0.46655	YES	YES
489	a	3038.73	1.33430	YES	YES
490	a	3044.59	0.50792	YES	YES
491	a	3049.24	7.49962	YES	YES
492	a	3051.06	15.45352	YES	YES
493	a	3071.00	5.66412	YES	YES

494	a	3142.77	2.52553	YES	YES
495	a	3161.36	4.77742	YES	YES

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Double hybrid single point energy = -7442.885925002109 H
 COSMO energy + OC correction = -7450.5235382757 H (in oDFB)

6.2.7 C₆H₁₀



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c2

Cartesian coordinates in Ångström:

C	-0.7326713	-0.1241313	0.2400331
C	0.7326713	0.1241313	0.2400331
C	-1.3477486	-0.6658435	1.3045998
C	-1.4941578	0.2353353	-1.0114284
H	-0.7870871	-0.9724776	2.1868274
H	-2.4259748	-0.8287519	1.3120231
C	1.3477486	0.6658435	1.3045998
C	1.4941578	-0.2353353	-1.0114284
H	0.7870871	0.9724776	2.1868274
H	2.4259748	0.8287519	1.3120231
H	-1.1680258	-0.3741357	-1.8674761
H	-1.3264762	1.2869564	-1.2892828
H	-2.5706840	0.0785652	-0.8752504
H	1.3264762	-1.2869564	-1.2892828
H	2.5706840	-0.0785652	-0.8752504
H	1.1680258	0.3741357	-1.8674761

SCF energy GEOOPT = -234.7340258129 H
 ZPE = 359.9 kJ/mol
 FREEH energy = 379.48 kJ/mol
 FREEH entropy = 0.33996 kJ/mol/K

\$vibrational spectrum

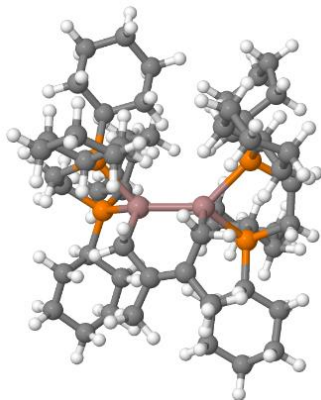
#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	78.62	0.00018	YES	YES
8		b	176.14	0.12493	YES	YES
9		a	206.75	0.24604	YES	YES
10		a	257.48	0.00303	YES	YES
11		b	276.17	5.84921	YES	YES
12		a	358.38	0.63935	YES	YES

13	b	444.07	0.58020	YES	YES
14	b	514.18	8.76247	YES	YES
15	a	550.22	3.68092	YES	YES
16	b	685.14	0.68633	YES	YES
17	a	712.13	0.09922	YES	YES
18	a	757.18	1.94561	YES	YES
19	b	884.56	71.81242	YES	YES
20	a	885.07	9.05260	YES	YES
21	b	910.07	0.20203	YES	YES
22	a	952.51	2.37956	YES	YES
23	a	977.23	4.25876	YES	YES
24	b	1001.35	2.32254	YES	YES
25	b	1027.74	0.02229	YES	YES
26	a	1036.47	0.02025	YES	YES
27	b	1182.34	6.44214	YES	YES
28	a	1285.51	3.15694	YES	YES
29	b	1353.23	5.55225	YES	YES
30	a	1360.76	6.56987	YES	YES
31	b	1387.38	1.21752	YES	YES
32	a	1401.40	1.59209	YES	YES
33	b	1427.48	16.70381	YES	YES
34	a	1431.50	3.87081	YES	YES
35	b	1445.66	16.48187	YES	YES
36	a	1452.24	4.83373	YES	YES
37	a	1622.51	17.91000	YES	YES
38	b	1648.53	11.46982	YES	YES
39	b	2955.73	7.57400	YES	YES
40	a	2957.36	36.69059	YES	YES
41	b	3005.02	25.51495	YES	YES
42	a	3007.77	2.91476	YES	YES
43	b	3049.44	37.60871	YES	YES
44	a	3050.71	1.24401	YES	YES
45	b	3067.55	13.08597	YES	YES
46	a	3069.05	5.46481	YES	YES
47	b	3155.29	19.86228	YES	YES
48	a	3156.44	3.88690	YES	YES

\$end

Double hybrid single point energy = -234.285983195144 H
COSMO energy + OC correction = -234.7372988397 H (in oDFB)

6.2.8 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{H}_{10})]^{2+}$



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	12.6601144	9.8744342	5.2774439
Ga	10.8479666	8.2781817	5.4641419
P	15.0005722	9.8753690	5.8721927
P	12.6433176	12.1215292	6.1802405
P	11.0977186	5.8950774	5.2754690
P	9.2188250	7.7696855	7.1872097
C	6.8140916	8.1563306	5.7495857
H	6.5659380	7.0913600	5.8622400
H	7.4273168	8.2510253	4.8420640
C	11.0462054	3.8759374	3.2261026
H	11.5707852	3.1435024	3.8544833
H	9.9711772	3.7510040	3.4172739
C	11.9245232	9.2764073	2.3931455
C	13.2754858	5.2232039	1.7882246
H	12.7446289	5.9446296	1.1480906
H	14.3479704	5.3603588	1.5902029
C	12.3475495	3.5831456	6.4137761
H	12.9256003	3.3806306	5.4999988
H	11.3806360	3.0732302	6.2994528
C	14.5349992	9.3122023	8.5645502
H	14.6659384	10.3836942	8.7865740
H	13.4797533	9.1754410	8.2799229
C	11.7747477	14.7357069	5.2863243
H	11.5439580	15.0945758	6.2981588
H	12.8283549	14.9796258	5.0912848
C	10.8703472	15.4560524	4.2748696
H	11.1723365	15.1725589	3.2531612
C	16.9367047	9.0492336	7.7732108
H	17.5771782	8.7071443	6.9495350
H	17.1845757	10.1083800	7.9517882
C	10.7397152	8.6274944	2.5583625
C	15.4079727	11.6430525	6.2807316
H	16.3973935	11.8795072	5.8673520
H	15.5043634	11.7034046	7.3725963
C	8.8975460	5.9468552	7.0118265
H	9.4079950	5.4525451	7.8487759
C	12.1523875	5.1006477	6.5658181
H	11.5708258	5.2686240	7.4887809
C	14.3640802	12.6542295	5.7836369
H	14.5682269	13.6494499	6.2015352
H	14.4040633	12.7482633	4.6887325
C	7.6143031	8.6542191	6.9636517
H	7.0220537	8.4527994	7.8717248
C	9.6943217	8.0182742	8.9574276
H	9.7892392	9.1123797	9.0563335
C	16.1720537	9.3386518	4.5562850
H	17.1753377	9.3735403	5.0139169
C	12.8342383	3.8014109	1.4289200
H	13.4401667	3.0748490	1.9955760
H	13.0249903	3.6030546	0.3658096
C	13.1069666	3.0197660	7.6218200
H	13.2586918	1.9400094	7.4907796
H	12.4911183	3.1421046	8.5283969
C	12.3377001	10.3831981	3.3173159
H	13.1802927	10.9494303	2.9035557

H	11.5008379	11.0915171	3.4259768
C	9.3937064	15.1047850	4.4882517
H	8.7723548	15.6099525	3.7369099
H	9.0670088	15.4856715	5.4701533
C	14.2578856	5.2458182	7.9461183
H	13.6979128	5.4634940	8.8713654
H	15.2325151	5.7450409	8.0470522
C	16.8813908	8.3250922	1.8703356
H	15.9129679	8.2770489	1.3462282
H	17.6381138	7.9812887	1.1527275
C	11.3516679	3.5855505	1.7492915
H	10.7389129	4.2471312	1.1154394
H	11.0510793	2.5564902	1.5105220
C	12.8464090	9.0539960	1.2255860
H	13.8772598	8.8921681	1.5769178
H	12.5722602	8.1972664	0.6030456
H	12.8792228	9.9408973	0.5731022
C	16.1661218	10.2709054	3.3351334
H	16.4133457	11.3013908	3.6292232
H	15.1554612	10.2929603	2.9018031
C	12.4465673	12.3137884	8.0037285
H	13.3892272	11.8845637	8.3880166
C	12.3412225	13.7538363	8.5291909
H	11.4025683	14.2012728	8.1698649
H	13.1608089	14.3757992	8.1426570
C	11.0650865	7.3908054	9.2525565
H	11.0063066	6.3022498	9.0894019
C	9.3769824	5.3573404	5.6741575
H	9.3100043	4.2612219	5.6982908
H	8.7440263	5.7041582	4.8449503
C	12.9794807	5.5486752	3.2561014
H	13.2348886	6.5958406	3.4750007
H	13.6102573	4.9151295	3.8988634
C	8.6295191	7.5257194	9.9532792
H	8.4708747	6.4435113	9.8168984
H	7.6642839	8.0146384	9.7666696
C	7.8993992	10.1636996	6.8773701
H	8.5741422	10.3405057	6.0242080
H	8.4305486	10.5072369	7.7772667
C	10.0642577	12.8548105	5.4294536
H	9.7770213	13.1307626	6.4566276
H	9.9269276	11.7658348	5.3445230
C	5.8319250	10.4737974	5.4579963
H	4.8988667	11.0416971	5.3463286
H	6.4241214	10.6578887	4.5456818
C	17.2478573	8.2409277	9.0402541
H	18.3062306	8.3688635	9.3039226
H	17.1065466	7.1684084	8.8274415
C	16.8449979	7.3932882	3.0851613
H	17.8501247	7.3295261	3.5324094
H	16.5742510	6.3723637	2.7810928
C	14.8681394	8.5214202	9.8340748
H	14.6233660	7.4604108	9.6739708
H	14.2310325	8.8709407	10.6576600
C	16.3470975	8.6545245	10.2060255
H	16.5629516	9.7005103	10.4806149
H	16.5702093	8.0484760	11.0941993
C	11.2887332	11.4584062	10.0747048

H	12.2068472	10.9729570	10.4468787
H	10.4454998	10.8605331	10.4507246
C	5.5290358	8.9764677	5.5724581
H	4.8636736	8.8012835	6.4333785
H	4.9900688	8.6217518	4.6836366
C	11.3041155	11.4366320	8.5427192
H	11.4132685	10.4094281	8.1609481
H	10.3437636	11.8134599	8.1579616
C	11.4951294	5.3042791	3.5806986
H	10.9154040	6.0013427	2.9577577
C	12.3416296	13.7585372	10.0636527
H	12.2483827	14.7897911	10.4295303
H	13.3123044	13.3831629	10.4282092
C	13.4928520	5.8292658	6.7534115
H	13.3076820	6.9060063	6.8886232
H	14.0990716	5.7286166	5.8407445
C	6.6121266	10.9705071	6.6781878
H	6.8608911	12.0362911	6.5742636
H	5.9835925	10.8826545	7.5789698
C	14.4489004	3.7318046	7.8137790
H	15.0998108	3.5209533	6.9492211
H	14.9673404	3.3367389	8.6976012
C	11.2114968	12.8877490	10.6211733
H	11.2456149	12.8759143	11.7187417
H	10.2408894	13.3307738	10.3435024
C	10.4320924	7.1507739	11.6932252
H	10.7437227	7.3739336	12.7223265
H	10.3411380	6.0538280	11.6264577
C	15.8570794	7.8909851	4.1468952
H	14.8313421	7.8600117	3.7427995
H	15.8740312	7.2245744	5.0217890
C	11.4957526	7.6329581	10.7033993
H	11.6752247	8.7091959	10.8511175
H	12.4518989	7.1257609	10.8896272
C	9.0732174	7.7897243	11.3986679
H	8.3089912	7.4110584	12.0905051
H	9.1331329	8.8781431	11.5640580
C	17.1653406	9.7742040	2.2805806
H	17.1310571	10.4348508	1.4038025
H	18.1864384	9.8479703	2.6885006
C	9.8667664	8.8675360	3.7544884
H	9.6578767	9.9361988	3.9260300
H	8.9006891	8.3674025	3.6353180
C	15.4510184	8.9234639	7.3933205
H	15.2431450	7.8744994	7.1293173
C	11.5398280	13.2182937	5.1961173
H	11.7935029	12.9137629	4.1643503
C	9.1641084	13.5905649	4.4312812
H	9.3812709	13.2215294	3.4152476
H	8.1107561	13.3503312	4.6335878
H	11.8180020	7.7764976	8.5475243
H	7.8245387	5.7595663	7.1489767
C	10.1336568	7.7264304	1.5080558
H	10.8669713	7.2431289	0.8536952
H	9.4593628	8.3108773	0.8610262
H	9.5085214	6.9396359	1.9551324
H	11.0226184	16.5407134	4.3562086

SCF energy GEOOPT = -7490.973352785 H
 ZPE = 3967. kJ/mol
 FREEH energy = 4162.64 kJ/mol
 FREEH entropy = 1.64570 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	16.49	0.09374	YES	YES
8		a	21.66	0.01143	YES	YES
9		a	24.04	0.02387	YES	YES
10		a	25.92	0.01705	YES	YES
11		a	29.59	0.01135	YES	YES
12		a	31.67	0.07051	YES	YES
13		a	34.92	0.04518	YES	YES
14		a	36.34	0.03290	YES	YES
15		a	39.02	0.00360	YES	YES
16		a	40.96	0.02259	YES	YES
17		a	42.44	0.15281	YES	YES
18		a	44.50	0.05784	YES	YES
19		a	45.26	0.02585	YES	YES
20		a	49.41	0.20735	YES	YES
21		a	51.77	0.04295	YES	YES
22		a	54.40	0.01055	YES	YES
23		a	58.01	0.05446	YES	YES
24		a	58.84	0.00701	YES	YES
25		a	62.25	0.22735	YES	YES
26		a	66.60	0.33690	YES	YES
27		a	70.79	0.04763	YES	YES
28		a	72.48	0.05365	YES	YES
29		a	76.90	0.00052	YES	YES
30		a	78.62	0.06519	YES	YES
31		a	80.13	0.04335	YES	YES
32		a	86.62	0.03243	YES	YES
33		a	87.49	0.05855	YES	YES
34		a	91.90	0.38483	YES	YES
35		a	93.31	0.25461	YES	YES
36		a	103.59	0.30471	YES	YES
37		a	108.45	1.47250	YES	YES
38		a	110.24	0.53474	YES	YES
39		a	113.14	0.32487	YES	YES
40		a	123.07	0.38844	YES	YES
41		a	123.22	0.11254	YES	YES
42		a	131.46	1.64917	YES	YES
43		a	134.97	1.77575	YES	YES
44		a	136.93	0.25516	YES	YES
45		a	141.06	0.42402	YES	YES
46		a	144.28	1.12166	YES	YES
47		a	148.14	1.68958	YES	YES
48		a	150.70	1.24861	YES	YES
49		a	156.45	3.06318	YES	YES
50		a	159.65	0.79027	YES	YES

51	a	166.07	3.36006	YES	YES
52	a	173.58	1.17828	YES	YES
53	a	176.99	1.54698	YES	YES
54	a	179.48	0.71956	YES	YES
55	a	188.61	5.73690	YES	YES
56	a	191.88	1.62359	YES	YES
57	a	195.70	0.99107	YES	YES
58	a	212.32	0.47633	YES	YES
59	a	213.33	0.14964	YES	YES
60	a	214.17	0.33292	YES	YES
61	a	217.04	0.27417	YES	YES
62	a	222.16	1.36390	YES	YES
63	a	222.82	0.39081	YES	YES
64	a	227.00	0.18364	YES	YES
65	a	228.55	0.03574	YES	YES
66	a	230.73	0.03191	YES	YES
67	a	234.94	0.56258	YES	YES
68	a	235.91	0.05115	YES	YES
69	a	240.19	0.56828	YES	YES
70	a	241.76	1.27969	YES	YES
71	a	243.37	0.42524	YES	YES
72	a	248.71	0.52500	YES	YES
73	a	271.11	0.19203	YES	YES
74	a	281.65	0.23630	YES	YES
75	a	283.61	0.33930	YES	YES
76	a	285.01	0.81799	YES	YES
77	a	289.92	0.63383	YES	YES
78	a	295.28	0.11709	YES	YES
79	a	300.62	0.27111	YES	YES
80	a	303.70	1.68162	YES	YES
81	a	311.67	0.22499	YES	YES
82	a	312.74	0.46585	YES	YES
83	a	318.87	5.86196	YES	YES
84	a	331.63	0.62128	YES	YES
85	a	333.59	0.10094	YES	YES
86	a	335.38	0.56167	YES	YES
87	a	339.15	0.06041	YES	YES
88	a	344.25	0.24878	YES	YES
89	a	345.71	0.61578	YES	YES
90	a	365.30	2.65412	YES	YES
91	a	371.53	0.26364	YES	YES
92	a	373.38	0.56479	YES	YES
93	a	377.84	1.12042	YES	YES
94	a	381.32	2.82627	YES	YES
95	a	384.87	0.17145	YES	YES
96	a	395.18	1.61241	YES	YES
97	a	397.02	0.41912	YES	YES
98	a	409.18	0.12341	YES	YES
99	a	409.78	0.69686	YES	YES
100	a	416.36	1.98028	YES	YES
101	a	418.36	1.05075	YES	YES
102	a	424.03	6.05493	YES	YES
103	a	425.17	0.05411	YES	YES
104	a	429.17	0.05034	YES	YES
105	a	430.03	0.03315	YES	YES
106	a	430.24	0.07392	YES	YES
107	a	431.09	0.02063	YES	YES
108	a	433.10	0.08789	YES	YES

109	a	434.95	0.75053	YES	YES
110	a	438.34	0.47030	YES	YES
111	a	439.23	0.44949	YES	YES
112	a	454.92	5.45367	YES	YES
113	a	457.98	4.48553	YES	YES
114	a	469.20	2.93496	YES	YES
115	a	470.96	3.55929	YES	YES
116	a	480.47	0.46177	YES	YES
117	a	493.10	3.76144	YES	YES
118	a	494.74	3.65226	YES	YES
119	a	495.56	1.24302	YES	YES
120	a	497.27	2.39963	YES	YES
121	a	502.62	1.05520	YES	YES
122	a	504.62	2.61864	YES	YES
123	a	512.81	10.52460	YES	YES
124	a	513.74	8.25779	YES	YES
125	a	516.88	0.59686	YES	YES
126	a	532.16	4.47593	YES	YES
127	a	623.25	10.77864	YES	YES
128	a	632.17	20.59625	YES	YES
129	a	633.20	9.75284	YES	YES
130	a	658.54	7.43428	YES	YES
131	a	659.68	8.50201	YES	YES
132	a	663.93	22.21521	YES	YES
133	a	681.18	33.94316	YES	YES
134	a	700.91	2.07137	YES	YES
135	a	703.35	1.03841	YES	YES
136	a	716.07	4.20802	YES	YES
137	a	720.44	2.51727	YES	YES
138	a	723.33	2.29505	YES	YES
139	a	728.17	2.30734	YES	YES
140	a	729.32	2.69660	YES	YES
141	a	736.00	3.66957	YES	YES
142	a	737.22	5.82319	YES	YES
143	a	769.17	0.10314	YES	YES
144	a	771.06	0.14885	YES	YES
145	a	773.92	0.40040	YES	YES
146	a	774.20	0.09924	YES	YES
147	a	774.25	0.07130	YES	YES
148	a	774.48	0.73095	YES	YES
149	a	775.23	0.13010	YES	YES
150	a	777.39	0.01490	YES	YES
151	a	781.68	25.57763	YES	YES
152	a	782.20	5.93954	YES	YES
153	a	806.63	1.65394	YES	YES
154	a	807.79	1.87141	YES	YES
155	a	809.73	5.05624	YES	YES
156	a	810.17	2.39380	YES	YES
157	a	811.03	5.98412	YES	YES
158	a	812.08	3.88418	YES	YES
159	a	815.39	3.59286	YES	YES
160	a	817.30	2.58944	YES	YES
161	a	830.36	4.49551	YES	YES
162	a	831.71	6.29328	YES	YES
163	a	836.60	5.64274	YES	YES
164	a	837.01	10.41758	YES	YES
165	a	837.79	0.72918	YES	YES
166	a	838.36	0.51575	YES	YES

167	a	839.07	0.59615	YES	YES
168	a	839.32	0.68814	YES	YES
169	a	854.93	19.73811	YES	YES
170	a	856.07	9.22351	YES	YES
171	a	873.75	1.00990	YES	YES
172	a	874.64	4.26720	YES	YES
173	a	875.59	0.18762	YES	YES
174	a	876.58	0.82395	YES	YES
175	a	876.77	0.61646	YES	YES
176	a	877.40	3.93083	YES	YES
177	a	877.86	2.33912	YES	YES
178	a	877.94	2.97581	YES	YES
179	a	879.58	7.74743	YES	YES
180	a	879.99	0.62392	YES	YES
181	a	881.44	4.61192	YES	YES
182	a	882.29	2.16019	YES	YES
183	a	882.94	3.91896	YES	YES
184	a	884.13	1.97275	YES	YES
185	a	886.89	6.29510	YES	YES
186	a	887.16	3.56774	YES	YES
187	a	903.41	0.55577	YES	YES
188	a	904.23	0.57097	YES	YES
189	a	904.57	3.52165	YES	YES
190	a	905.31	1.24064	YES	YES
191	a	908.44	3.66251	YES	YES
192	a	909.24	5.61807	YES	YES
193	a	909.37	1.59976	YES	YES
194	a	909.96	1.35123	YES	YES
195	a	910.37	2.05440	YES	YES
196	a	970.72	1.21381	YES	YES
197	a	979.75	0.52171	YES	YES
198	a	981.02	5.37688	YES	YES
199	a	985.01	2.16231	YES	YES
200	a	987.27	9.48155	YES	YES
201	a	987.78	4.04935	YES	YES
202	a	988.26	7.37263	YES	YES
203	a	988.53	11.07148	YES	YES
204	a	989.34	38.05776	YES	YES
205	a	989.70	11.74312	YES	YES
206	a	990.50	1.11015	YES	YES
207	a	991.15	2.37618	YES	YES
208	a	1001.24	5.70401	YES	YES
209	a	1011.59	31.62966	YES	YES
210	a	1012.65	0.50378	YES	YES
211	a	1014.03	0.16444	YES	YES
212	a	1016.06	0.07327	YES	YES
213	a	1016.70	0.15509	YES	YES
214	a	1017.68	0.82640	YES	YES
215	a	1018.58	0.75064	YES	YES
216	a	1019.22	1.18483	YES	YES
217	a	1019.80	0.08600	YES	YES
218	a	1032.29	2.92118	YES	YES
219	a	1032.59	0.28180	YES	YES
220	a	1036.45	0.41773	YES	YES
221	a	1037.13	0.76184	YES	YES
222	a	1038.46	0.74432	YES	YES
223	a	1038.64	3.94980	YES	YES
224	a	1039.88	0.66286	YES	YES

225	a	1040.66	0.25868	YES	YES
226	a	1055.23	4.54768	YES	YES
227	a	1055.60	1.34447	YES	YES
228	a	1058.04	5.83314	YES	YES
229	a	1059.54	0.96587	YES	YES
230	a	1060.10	1.84784	YES	YES
231	a	1060.49	0.23251	YES	YES
232	a	1060.90	2.72514	YES	YES
233	a	1064.35	3.84015	YES	YES
234	a	1064.77	0.02165	YES	YES
235	a	1069.76	0.02489	YES	YES
236	a	1070.54	0.09987	YES	YES
237	a	1072.12	0.19204	YES	YES
238	a	1072.40	0.16727	YES	YES
239	a	1072.60	0.03640	YES	YES
240	a	1073.09	0.34782	YES	YES
241	a	1074.20	0.95049	YES	YES
242	a	1074.95	0.30684	YES	YES
243	a	1077.61	2.88534	YES	YES
244	a	1078.63	0.50528	YES	YES
245	a	1079.40	4.26020	YES	YES
246	a	1085.26	1.07815	YES	YES
247	a	1093.41	2.97799	YES	YES
248	a	1094.06	2.10815	YES	YES
249	a	1095.89	4.98235	YES	YES
250	a	1098.13	8.81324	YES	YES
251	a	1102.58	3.28271	YES	YES
252	a	1103.66	2.61434	YES	YES
253	a	1114.05	12.51638	YES	YES
254	a	1115.50	4.83374	YES	YES
255	a	1122.97	1.65746	YES	YES
256	a	1125.78	1.10577	YES	YES
257	a	1153.88	5.97511	YES	YES
258	a	1159.97	13.28936	YES	YES
259	a	1160.50	2.63715	YES	YES
260	a	1166.32	14.47463	YES	YES
261	a	1166.86	1.51657	YES	YES
262	a	1167.48	7.45985	YES	YES
263	a	1168.16	2.26902	YES	YES
264	a	1169.65	6.66549	YES	YES
265	a	1170.02	7.40207	YES	YES
266	a	1173.78	2.98636	YES	YES
267	a	1180.64	15.51001	YES	YES
268	a	1181.34	3.44870	YES	YES
269	a	1182.06	8.43088	YES	YES
270	a	1182.26	1.83560	YES	YES
271	a	1184.59	2.20214	YES	YES
272	a	1188.38	1.14164	YES	YES
273	a	1212.58	0.65242	YES	YES
274	a	1213.04	1.49405	YES	YES
275	a	1239.10	0.36053	YES	YES
276	a	1239.83	0.21509	YES	YES
277	a	1241.90	0.46657	YES	YES
278	a	1242.33	0.72391	YES	YES
279	a	1246.05	0.34143	YES	YES
280	a	1247.03	0.31993	YES	YES
281	a	1248.62	0.94211	YES	YES
282	a	1249.14	0.12800	YES	YES

283	a	1249.93	0.73217	YES	YES
284	a	1251.06	0.55215	YES	YES
285	a	1251.85	2.12769	YES	YES
286	a	1252.45	2.59710	YES	YES
287	a	1254.09	0.13669	YES	YES
288	a	1255.16	1.50496	YES	YES
289	a	1256.51	3.19205	YES	YES
290	a	1256.68	9.80796	YES	YES
291	a	1257.60	2.26777	YES	YES
292	a	1258.01	5.00716	YES	YES
293	a	1259.05	0.44042	YES	YES
294	a	1259.82	0.95898	YES	YES
295	a	1260.72	1.74496	YES	YES
296	a	1261.69	2.11076	YES	YES
297	a	1261.81	3.40430	YES	YES
298	a	1263.70	4.04530	YES	YES
299	a	1264.43	3.70870	YES	YES
300	a	1266.16	1.65483	YES	YES
301	a	1268.15	1.81073	YES	YES
302	a	1268.62	1.09197	YES	YES
303	a	1270.50	1.21676	YES	YES
304	a	1280.20	4.11518	YES	YES
305	a	1281.60	0.12257	YES	YES
306	a	1283.90	1.54715	YES	YES
307	a	1284.50	2.17130	YES	YES
308	a	1286.41	9.29247	YES	YES
309	a	1287.02	5.53122	YES	YES
310	a	1288.88	1.45374	YES	YES
311	a	1289.27	2.46815	YES	YES
312	a	1305.10	0.20816	YES	YES
313	a	1306.29	0.26338	YES	YES
314	a	1310.44	1.29066	YES	YES
315	a	1311.01	0.50243	YES	YES
316	a	1311.28	0.78648	YES	YES
317	a	1312.17	3.76831	YES	YES
318	a	1313.63	0.94604	YES	YES
319	a	1314.75	0.82332	YES	YES
320	a	1318.40	1.54824	YES	YES
321	a	1319.33	2.82743	YES	YES
322	a	1321.23	1.03170	YES	YES
323	a	1321.58	1.87922	YES	YES
324	a	1322.48	1.06732	YES	YES
325	a	1323.28	1.09475	YES	YES
326	a	1324.00	1.30999	YES	YES
327	a	1324.07	1.08329	YES	YES
328	a	1324.22	0.22426	YES	YES
329	a	1324.51	0.48385	YES	YES
330	a	1324.82	0.57439	YES	YES
331	a	1325.16	0.33281	YES	YES
332	a	1326.80	2.75167	YES	YES
333	a	1327.55	9.36543	YES	YES
334	a	1330.23	0.34203	YES	YES
335	a	1330.55	3.19777	YES	YES
336	a	1336.50	0.13928	YES	YES
337	a	1336.73	0.17128	YES	YES
338	a	1336.87	0.81135	YES	YES
339	a	1337.12	0.49281	YES	YES
340	a	1337.77	0.12572	YES	YES

341	a	1337.89	0.10678	YES	YES
342	a	1338.60	0.05921	YES	YES
343	a	1339.10	0.10639	YES	YES
344	a	1343.44	0.06260	YES	YES
345	a	1343.61	0.20033	YES	YES
346	a	1344.53	2.33615	YES	YES
347	a	1344.75	2.34536	YES	YES
348	a	1345.25	0.24757	YES	YES
349	a	1347.11	1.59981	YES	YES
350	a	1347.31	1.68038	YES	YES
351	a	1347.97	0.68896	YES	YES
352	a	1355.06	0.78943	YES	YES
353	a	1369.65	2.92879	YES	YES
354	a	1402.99	0.95090	YES	YES
355	a	1406.84	3.40229	YES	YES
356	a	1407.25	11.59440	YES	YES
357	a	1409.36	8.46103	YES	YES
358	a	1409.64	10.66404	YES	YES
359	a	1415.29	7.77603	YES	YES
360	a	1422.47	0.08692	YES	YES
361	a	1423.76	10.16142	YES	YES
362	a	1425.39	5.51916	YES	YES
363	a	1427.15	2.12668	YES	YES
364	a	1429.83	3.82391	YES	YES
365	a	1431.25	8.17101	YES	YES
366	a	1432.42	0.36359	YES	YES
367	a	1432.66	0.72911	YES	YES
368	a	1433.50	9.33397	YES	YES
369	a	1433.95	3.54271	YES	YES
370	a	1435.33	1.81190	YES	YES
371	a	1435.43	7.85943	YES	YES
372	a	1435.98	4.56263	YES	YES
373	a	1436.44	2.17668	YES	YES
374	a	1437.11	7.07509	YES	YES
375	a	1437.61	7.54787	YES	YES
376	a	1437.95	9.60613	YES	YES
377	a	1438.34	9.20473	YES	YES
378	a	1438.56	3.89930	YES	YES
379	a	1438.89	0.59795	YES	YES
380	a	1439.13	8.69295	YES	YES
381	a	1439.76	4.64563	YES	YES
382	a	1439.89	10.18077	YES	YES
383	a	1440.03	0.45043	YES	YES
384	a	1440.58	6.01985	YES	YES
385	a	1441.63	13.49025	YES	YES
386	a	1442.15	11.84162	YES	YES
387	a	1442.69	3.47492	YES	YES
388	a	1443.16	23.61681	YES	YES
389	a	1443.63	17.38177	YES	YES
390	a	1444.49	17.78732	YES	YES
391	a	1444.96	13.64962	YES	YES
392	a	1445.52	3.12766	YES	YES
393	a	1445.98	12.14269	YES	YES
394	a	1447.26	1.37556	YES	YES
395	a	1451.61	2.21192	YES	YES
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398	a	1454.38	1.52842	YES	YES

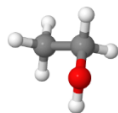
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403	a	1457.67	1.67649	YES	YES
404	a	1621.38	2.39499	YES	YES
405	a	2926.21	0.52903	YES	YES
406	a	2933.09	3.68719	YES	YES
407	a	2938.16	15.77901	YES	YES
408	a	2938.50	18.43248	YES	YES
409	a	2938.87	38.08872	YES	YES
410	a	2939.19	18.05833	YES	YES
411	a	2939.88	6.02832	YES	YES
412	a	2940.62	35.90173	YES	YES
413	a	2942.25	2.27852	YES	YES
414	a	2942.79	8.12098	YES	YES
415	a	2944.16	4.18949	YES	YES
416	a	2944.58	5.83371	YES	YES
417	a	2944.58	4.22436	YES	YES
418	a	2945.50	11.42107	YES	YES
419	a	2946.03	12.52108	YES	YES
420	a	2946.15	11.07793	YES	YES
421	a	2946.78	19.89235	YES	YES
422	a	2948.03	15.41885	YES	YES
423	a	2948.59	14.57699	YES	YES
424	a	2949.14	15.65197	YES	YES
425	a	2949.87	13.16501	YES	YES
426	a	2950.05	11.64002	YES	YES
427	a	2950.09	10.55898	YES	YES
428	a	2950.54	19.83777	YES	YES
429	a	2951.46	8.85069	YES	YES
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431	a	2952.99	20.33472	YES	YES
432	a	2954.01	12.19250	YES	YES
433	a	2954.92	6.67086	YES	YES
434	a	2955.41	16.13624	YES	YES
435	a	2956.26	6.76586	YES	YES
436	a	2957.08	20.07831	YES	YES
437	a	2957.19	14.05127	YES	YES
438	a	2957.37	12.86969	YES	YES
439	a	2957.53	25.54882	YES	YES
440	a	2957.67	15.56948	YES	YES
441	a	2958.36	30.52073	YES	YES
442	a	2958.64	20.85563	YES	YES
443	a	2960.22	36.82764	YES	YES
444	a	2962.65	28.82036	YES	YES
445	a	2965.08	16.14306	YES	YES
446	a	2965.49	20.92146	YES	YES
447	a	2966.33	19.12933	YES	YES
448	a	2966.78	8.14881	YES	YES
449	a	2967.61	8.22019	YES	YES
450	a	2967.74	11.86231	YES	YES
451	a	2968.75	14.57127	YES	YES
452	a	2973.80	11.85309	YES	YES
453	a	2973.82	7.12100	YES	YES
454	a	2978.50	11.63512	YES	YES
455	a	2979.09	4.31296	YES	YES
456	a	2981.44	9.64805	YES	YES

457	a	2982.18	6.01551	YES	YES
458	a	2986.58	48.05383	YES	YES
459	a	2987.12	5.09901	YES	YES
460	a	2988.00	2.03421	YES	YES
461	a	2989.63	49.49689	YES	YES
462	a	2991.45	10.60437	YES	YES
463	a	2991.51	20.02657	YES	YES
464	a	2991.56	12.90993	YES	YES
465	a	2991.98	7.50388	YES	YES
466	a	2992.08	10.81959	YES	YES
467	a	2993.13	12.54649	YES	YES
468	a	2994.95	39.04498	YES	YES
469	a	2997.00	32.91840	YES	YES
470	a	2998.77	23.08348	YES	YES
471	a	3002.40	30.54927	YES	YES
472	a	3003.54	6.74468	YES	YES
473	a	3004.74	17.55315	YES	YES
474	a	3005.29	38.21074	YES	YES
475	a	3006.11	25.64183	YES	YES
476	a	3010.16	14.46579	YES	YES
477	a	3010.55	9.79084	YES	YES
478	a	3010.65	15.75189	YES	YES
479	a	3011.35	24.10546	YES	YES
480	a	3012.90	13.63644	YES	YES
481	a	3014.03	39.08969	YES	YES
482	a	3014.24	17.94758	YES	YES
483	a	3014.43	23.47118	YES	YES
484	a	3014.85	22.11121	YES	YES
485	a	3014.88	1.90674	YES	YES
486	a	3015.54	16.62094	YES	YES
487	a	3016.02	26.65750	YES	YES
488	a	3016.30	11.40235	YES	YES
489	a	3016.36	26.39929	YES	YES
490	a	3016.46	47.51240	YES	YES
491	a	3016.71	13.19962	YES	YES
492	a	3017.14	21.32211	YES	YES
493	a	3017.66	15.45451	YES	YES
494	a	3017.88	33.43171	YES	YES
495	a	3018.18	28.15309	YES	YES
496	a	3018.25	19.53407	YES	YES
497	a	3019.34	18.47844	YES	YES
498	a	3019.84	34.60449	YES	YES
499	a	3019.95	34.35528	YES	YES
500	a	3021.75	22.17190	YES	YES
501	a	3026.44	4.83403	YES	YES
502	a	3028.13	11.08196	YES	YES
503	a	3029.19	16.38171	YES	YES
504	a	3029.42	25.58440	YES	YES
505	a	3031.60	7.57417	YES	YES
506	a	3039.37	1.78179	YES	YES
507	a	3039.55	1.82791	YES	YES
508	a	3047.85	6.06601	YES	YES
509	a	3053.39	12.51112	YES	YES
510	a	3070.73	20.59903	YES	YES

\$end

Double hybrid single point energy = -7483.398135452510 H
COSMO energy + OC correction = -7491.1196653206 (in oDFB)

6.2.9 EtOH



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

O	-2.0682522	1.3205384	0.4754789
C	-3.4961656	1.4394881	0.5199099
H	-3.8091119	2.4733390	0.2843073
H	-3.7650506	1.2502773	1.5681229
C	-4.2034914	0.4504537	-0.3980239
H	-3.9510116	0.6394265	-1.4524210
H	-5.2952508	0.5370450	-0.2983930
H	-3.9127273	-0.5800273	-0.1551024
H	-1.7874988	1.4837693	-0.4390388

SCF energy GEOOPT = -155.1205854950 H

ZPE = 203.6 kJ/mol

FREEH energy = 215.02 kJ/mol

FREEH entropy = 0.27115 kJ/mol/K

\$vibrational spectrum

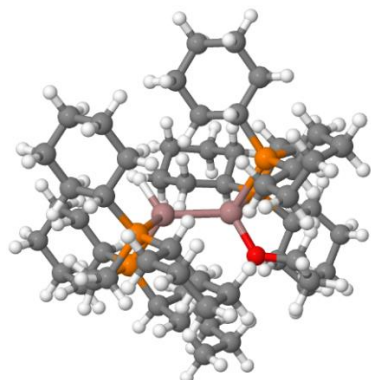
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#			cm** (-1)	km/mol	IR	RAMAN
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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	256.65	3.13145	YES	YES
8		a	273.67	103.63565	YES	YES
9		a	408.33	12.33647	YES	YES
10		a	781.75	3.21810	YES	YES
11		a	859.25	11.51120	YES	YES
12		a	1030.97	73.36766	YES	YES
13		a	1034.89	47.66579	YES	YES
14		a	1099.51	3.49889	YES	YES
15		a	1241.53	10.04921	YES	YES
16		a	1329.30	1.02629	YES	YES
17		a	1355.35	3.37722	YES	YES
18		a	1372.17	41.69523	YES	YES
19		a	1441.30	7.08622	YES	YES
20		a	1445.50	2.02265	YES	YES
21		a	1467.72	1.11946	YES	YES
22		a	2909.98	67.74161	YES	YES
23		a	2956.17	17.41557	YES	YES
24		a	3000.06	7.75822	YES	YES
25		a	3025.22	48.95406	YES	YES
26		a	3042.05	30.41449	YES	YES
27		a	3703.24	13.26086	YES	YES

\$end

Double hybrid single point energy = -154.860751543774 H

COSMO energy + OC correction = -155.1276140019 H (in oDFB)

6.2.10 [H{Ga(dcpe)}₂(OEt)]²⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

Ga	0.0323728	1.3341080	-0.0701687
Ga	-0.1559380	-1.0792664	0.0054747
O	-1.8724623	-1.7197872	0.2040362
C	-2.2175130	-3.0876618	0.3837749
H	-1.3297686	-3.7032286	0.6346682
H	-2.6155682	-3.4949400	-0.5634810
C	-3.2614498	-3.2320431	1.4778943
H	-4.1539462	-2.6439376	1.2293481
H	-2.8738190	-2.8699265	2.4394616
H	-3.5639304	-4.2814022	1.5968842
P	-1.2884495	2.5736011	-1.6331869
P	-1.0654664	2.5667392	1.6762742
C	-2.7125358	1.6480951	-2.3395502
H	-3.2845208	2.3661529	-2.9509961
C	-3.6217002	1.0991734	-1.2283520
H	-3.0298130	0.4477135	-0.5658073
H	-4.0187244	1.9229703	-0.6194247
C	-4.7823240	0.2851909	-1.8111874
H	-5.3939137	-0.1138733	-0.9904078
H	-5.4375958	0.9476906	-2.3995154
C	-4.2660733	-0.8503725	-2.6971290
H	-3.6980083	-1.5553523	-2.0686786
H	-5.1056962	-1.4108793	-3.1293700
C	-3.3622737	-0.3103562	-3.8089048
H	-3.9540456	0.3242758	-4.4879217
H	-2.9657260	-1.1311029	-4.4223919
C	-2.1988719	0.5127912	-3.2423820
H	-1.5857322	0.9138122	-4.0621196
H	-1.5454616	-0.1432538	-2.6408164
C	-0.3567176	3.3277187	-3.0393034
H	0.0015577	2.4598637	-3.6200302
C	-1.2518644	4.1909526	-3.9471377
H	-2.1018769	3.6063069	-4.3253615
H	-1.6712037	5.0239103	-3.3597916
C	-0.4452211	4.7605571	-5.1222529

H	-0.1147916	3.9299868	-5.7677277
H	-1.0971299	5.3948178	-5.7379613
C	0.7747001	5.5476880	-4.6368568
H	0.4382940	6.4356931	-4.0764768
H	1.3510223	5.9212244	-5.4936791
C	1.6631990	4.6843038	-3.7373691
H	2.5171716	5.2644542	-3.3616143
H	2.0828873	3.8551566	-4.3303263
C	0.8778774	4.1075644	-2.5519147
H	1.5179167	3.4583240	-1.9382472
H	0.5575015	4.9399430	-1.9042901
C	-1.9432833	3.9945035	-0.6432179
H	-1.1576254	4.7602772	-0.6904965
H	-2.8251825	4.4104846	-1.1496354
C	-2.2787808	3.6760117	0.8240761
H	-3.2469994	3.1649473	0.8911961
H	-2.3723116	4.6084174	1.3975320
C	-2.0275592	1.6512102	2.9593266
H	-1.2751321	1.0112107	3.4510395
C	-3.0878420	0.7385984	2.3191755
H	-3.7973157	1.3521896	1.7419680
H	-2.6241937	0.0351733	1.6115265
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H	-4.6566763	-0.6293692	2.8939166
H	-3.2048662	-0.7490456	3.8827805
C	-4.4858902	0.9004110	4.4330251
H	-5.2469507	1.5408159	3.9572577
H	-5.0082776	0.3174905	5.2034425
C	-3.4109623	1.7820982	5.0727859
H	-2.6992845	1.1506417	5.6307014
H	-3.8559952	2.4707820	5.8034898
C	-2.6422325	2.5866679	4.0161011
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C	0.1627483	3.6223681	2.5544214
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C	1.1998470	2.7126278	3.2399724
H	1.6668403	2.0718361	2.4726296
H	0.7062481	2.0444060	3.9610560
C	2.2900741	3.5334343	3.9386704
H	1.8436566	4.0931447	4.7762401
H	3.0340795	2.8548922	4.3796889
C	2.9570983	4.5107386	2.9672589
H	3.4833957	3.9425930	2.1817058
H	3.7188642	5.1047207	3.4893059
C	1.9198258	5.4322642	2.3189775
H	2.4007350	6.1148456	1.6051130
H	1.4562228	6.0643178	3.0934622
C	0.8293328	4.6282234	1.5993269
H	1.2773741	4.0818323	0.7540653
H	0.0749854	5.3122077	1.1834565
P	0.9999592	-2.4398657	-1.6913398
P	1.2366262	-2.3049586	1.6182709
C	-0.0811166	-3.7485714	-2.4095418
H	-0.4368169	-4.3199643	-1.5341717
C	0.6274380	-4.7129874	-3.3743205
H	1.4882898	-5.1970138	-2.8913484
H	1.0167556	-4.1456810	-4.2345831

C	-0.3578341	-5.7778620	-3.8792257
H	0.1561319	-6.4458714	-4.5834031
H	-0.6783054	-6.4034663	-3.0300789
C	-1.5845820	-5.1403830	-4.5392019
H	-2.2888202	-5.9191899	-4.8603610
H	-1.2713644	-4.6074878	-5.4523199
C	-2.2779277	-4.1570119	-3.5916752
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H	-3.1258725	-3.6682736	-4.0912005
C	-1.3021254	-3.0937354	-3.0758086
H	-0.9624816	-2.4747893	-3.9230430
H	-1.7998981	-2.4190607	-2.3658031
C	1.8122111	-1.5387049	-3.0910497
H	1.0998369	-1.6610489	-3.9255459
C	3.1673862	-2.1304362	-3.5194595
H	3.8802729	-2.0504044	-2.6832855
H	3.0705335	-3.1982029	-3.7559757
C	3.7315471	-1.3653394	-4.7240557
H	3.0653185	-1.5101241	-5.5901605
H	4.7043562	-1.7912891	-5.0041198
C	3.8659678	0.1297111	-4.4215672
H	4.6130407	0.2746328	-3.6235770
H	4.2442256	0.6643996	-5.3029478
C	2.5275212	0.7258937	-3.9752246
H	2.6477645	1.7846775	-3.7066720
H	1.8135579	0.6910529	-4.8154660
C	1.9344335	-0.0362945	-2.7871092
H	0.9447910	0.3714240	-2.5307987
H	2.5686492	0.1108237	-1.8972008
C	2.3078442	-3.3300952	-0.7351056
H	2.6587253	-4.1952240	-1.3129374
H	3.1653999	-2.6523128	-0.6287536
C	1.7944928	-3.7685291	0.6459834
H	2.5734337	-4.3197405	1.1882164
H	0.9289320	-4.4405143	0.5515858
C	0.3226758	-2.9102176	3.0972104
H	-0.4702276	-3.5549207	2.6803590
C	-0.3550803	-1.7133487	3.7906262
H	0.4163775	-0.9966052	4.1203836
H	-0.9981038	-1.1887305	3.0680652
C	-1.1718163	-2.1676773	5.0066631
H	-1.5927356	-1.2890286	5.5157544
H	-2.0283963	-2.7676834	4.6578570
C	-0.3332217	-3.0014037	5.9795917
H	-0.9573047	-3.3453478	6.8149197
H	0.4565184	-2.3694534	6.4188567
C	0.3099583	-4.1958162	5.2697739
H	-0.4752990	-4.8805858	4.9103435
H	0.9323056	-4.7712485	5.9680858
C	1.1660440	-3.7366651	4.0820343
H	1.9936991	-3.1171406	4.4613184
H	1.6157445	-4.6029679	3.5764312
C	2.7640083	-1.4269702	2.2019378
H	2.4501446	-0.9932713	3.1684238
C	3.1579432	-0.2643071	1.2766838
H	2.3008272	0.3980004	1.1020792
H	3.4463742	-0.6603092	0.2877582
C	4.3280937	0.5311864	1.8628576

H	4.6041434	1.3427602	1.1751371
H	3.9951141	1.0121600	2.7980040
C	5.5319981	-0.3697281	2.1536383
H	5.9361023	-0.7553726	1.2027845
H	6.3387536	0.2105807	2.6207381
C	5.1384679	-1.5474891	3.0502645
H	4.8458425	-1.1739772	4.0452565
H	5.9958451	-2.2155563	3.2079500
C	3.9721160	-2.3473928	2.4524320
H	3.7074796	-3.1828836	3.1125085
H	4.2971487	-2.7869486	1.4952145
H	1.4544991	2.0030036	-0.1693886

SCF energy GEOOPT = -7411.352212692 H

ZPE = 3797. kJ/mol

FREEH energy = 3985.92 kJ/mol

FREEH entropy = 1.61294 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	9.83	0.03113	YES	YES
	8	a	13.87	0.13365	YES	YES
	9	a	23.41	0.01402	YES	YES
	10	a	24.96	0.01587	YES	YES
	11	a	31.05	0.07830	YES	YES
	12	a	33.76	0.03696	YES	YES
	13	a	34.78	0.00637	YES	YES
	14	a	38.25	0.03727	YES	YES
	15	a	40.59	0.08942	YES	YES
	16	a	41.05	0.09038	YES	YES
	17	a	44.26	0.03041	YES	YES
	18	a	49.01	0.31025	YES	YES
	19	a	50.45	0.25772	YES	YES
	20	a	51.90	0.06587	YES	YES
	21	a	53.59	0.06690	YES	YES
	22	a	56.72	0.16422	YES	YES
	23	a	58.62	0.10483	YES	YES
	24	a	61.53	0.10374	YES	YES
	25	a	63.05	0.41311	YES	YES
	26	a	65.20	0.34347	YES	YES
	27	a	66.56	0.73003	YES	YES
	28	a	68.93	0.35784	YES	YES
	29	a	70.40	0.70672	YES	YES
	30	a	74.99	0.92608	YES	YES
	31	a	76.71	0.02888	YES	YES
	32	a	78.53	0.67139	YES	YES
	33	a	84.40	0.16392	YES	YES
	34	a	88.24	0.05423	YES	YES
	35	a	89.62	0.25283	YES	YES
	36	a	97.84	0.31199	YES	YES
	37	a	99.90	2.23602	YES	YES

38	a	116.90	1.94676	YES	YES
39	a	120.00	1.76699	YES	YES
40	a	122.40	1.28925	YES	YES
41	a	123.81	6.49059	YES	YES
42	a	129.59	0.61747	YES	YES
43	a	132.83	0.21378	YES	YES
44	a	143.24	1.81364	YES	YES
45	a	143.70	0.40296	YES	YES
46	a	146.27	0.35769	YES	YES
47	a	154.04	1.50628	YES	YES
48	a	161.03	2.89493	YES	YES
49	a	169.91	13.28954	YES	YES
50	a	171.97	1.78199	YES	YES
51	a	174.80	0.20188	YES	YES
52	a	179.57	0.23622	YES	YES
53	a	184.64	2.64478	YES	YES
54	a	188.48	1.88397	YES	YES
55	a	193.13	1.20642	YES	YES
56	a	204.26	3.59864	YES	YES
57	a	206.51	9.10843	YES	YES
58	a	212.42	0.57451	YES	YES
59	a	217.19	0.68591	YES	YES
60	a	220.28	0.04639	YES	YES
61	a	223.19	2.73981	YES	YES
62	a	227.78	2.15820	YES	YES
63	a	231.39	0.10120	YES	YES
64	a	232.86	0.60050	YES	YES
65	a	234.90	0.25510	YES	YES
66	a	237.06	0.24909	YES	YES
67	a	237.72	0.20429	YES	YES
68	a	240.08	0.32756	YES	YES
69	a	241.27	0.71827	YES	YES
70	a	253.14	0.12241	YES	YES
71	a	256.37	0.25645	YES	YES
72	a	272.08	0.72963	YES	YES
73	a	275.34	3.06281	YES	YES
74	a	282.33	6.70057	YES	YES
75	a	291.93	0.07468	YES	YES
76	a	298.97	4.57063	YES	YES
77	a	306.18	0.15647	YES	YES
78	a	308.73	0.15202	YES	YES
79	a	309.82	0.04215	YES	YES
80	a	312.59	0.06036	YES	YES
81	a	330.45	0.44899	YES	YES
82	a	330.94	0.70168	YES	YES
83	a	333.12	0.16757	YES	YES
84	a	335.06	2.17408	YES	YES
85	a	337.26	2.69220	YES	YES
86	a	346.21	3.90936	YES	YES
87	a	349.27	1.30482	YES	YES
88	a	370.03	3.76274	YES	YES
89	a	373.29	0.51788	YES	YES
90	a	374.12	2.01670	YES	YES
91	a	382.97	1.29714	YES	YES
92	a	393.74	0.19970	YES	YES
93	a	402.96	0.04731	YES	YES
94	a	411.59	0.35701	YES	YES
95	a	412.41	1.05553	YES	YES

96	a	421.00	2.77876	YES	YES
97	a	422.88	0.19435	YES	YES
98	a	427.87	0.61447	YES	YES
99	a	428.73	0.12095	YES	YES
100	a	429.89	0.05366	YES	YES
101	a	430.28	0.17555	YES	YES
102	a	430.93	0.33954	YES	YES
103	a	431.22	0.27281	YES	YES
104	a	434.23	0.67609	YES	YES
105	a	434.76	0.81655	YES	YES
106	a	435.68	0.00451	YES	YES
107	a	440.51	3.20291	YES	YES
108	a	446.85	4.11163	YES	YES
109	a	457.34	1.59580	YES	YES
110	a	463.90	3.58077	YES	YES
111	a	466.05	4.52987	YES	YES
112	a	489.60	4.73988	YES	YES
113	a	493.38	2.98461	YES	YES
114	a	493.56	1.34699	YES	YES
115	a	497.98	0.05856	YES	YES
116	a	501.70	0.58460	YES	YES
117	a	503.16	3.16800	YES	YES
118	a	514.91	3.40142	YES	YES
119	a	516.76	18.52331	YES	YES
120	a	562.05	81.91880	YES	YES
121	a	577.87	34.84836	YES	YES
122	a	608.61	80.51144	YES	YES
123	a	631.49	47.66552	YES	YES
124	a	635.84	16.96188	YES	YES
125	a	641.90	5.70406	YES	YES
126	a	655.04	7.48193	YES	YES
127	a	705.80	2.80675	YES	YES
128	a	715.69	6.21369	YES	YES
129	a	716.62	1.67335	YES	YES
130	a	726.90	1.17001	YES	YES
131	a	734.16	8.40476	YES	YES
132	a	736.31	0.73463	YES	YES
133	a	739.06	9.68957	YES	YES
134	a	741.22	0.70151	YES	YES
135	a	770.25	0.52730	YES	YES
136	a	771.28	0.52931	YES	YES
137	a	773.29	0.26489	YES	YES
138	a	773.46	0.65267	YES	YES
139	a	773.84	0.31724	YES	YES
140	a	776.51	0.06923	YES	YES
141	a	777.17	0.20655	YES	YES
142	a	777.38	12.09491	YES	YES
143	a	778.32	0.06245	YES	YES
144	a	785.13	0.57913	YES	YES
145	a	794.83	20.58850	YES	YES
146	a	807.78	1.13301	YES	YES
147	a	808.29	3.39034	YES	YES
148	a	809.01	0.27726	YES	YES
149	a	809.71	3.08494	YES	YES
150	a	812.76	1.25149	YES	YES
151	a	813.25	0.77268	YES	YES
152	a	814.66	2.51363	YES	YES
153	a	814.83	6.87381	YES	YES

154	a	832.93	3.55528	YES	YES
155	a	833.63	0.29133	YES	YES
156	a	837.02	3.35219	YES	YES
157	a	837.41	1.39193	YES	YES
158	a	838.47	5.67875	YES	YES
159	a	839.99	4.59503	YES	YES
160	a	840.28	5.11410	YES	YES
161	a	841.60	6.87229	YES	YES
162	a	850.48	18.57119	YES	YES
163	a	852.07	1.83245	YES	YES
164	a	872.00	1.82885	YES	YES
165	a	873.70	6.22828	YES	YES
166	a	875.18	2.17166	YES	YES
167	a	875.78	0.76768	YES	YES
168	a	876.03	1.74289	YES	YES
169	a	877.22	4.84461	YES	YES
170	a	877.95	0.98370	YES	YES
171	a	878.96	1.11840	YES	YES
172	a	879.46	2.92183	YES	YES
173	a	879.67	5.35609	YES	YES
174	a	880.30	2.65765	YES	YES
175	a	880.81	2.94516	YES	YES
176	a	882.14	3.73990	YES	YES
177	a	882.64	1.72832	YES	YES
178	a	884.66	3.27697	YES	YES
179	a	885.92	4.59479	YES	YES
180	a	896.04	29.46404	YES	YES
181	a	903.00	0.88299	YES	YES
182	a	903.50	1.07668	YES	YES
183	a	903.87	2.14733	YES	YES
184	a	905.43	2.28385	YES	YES
185	a	908.27	4.38560	YES	YES
186	a	908.40	2.39339	YES	YES
187	a	909.84	1.67933	YES	YES
188	a	911.57	2.09098	YES	YES
189	a	978.54	2.04632	YES	YES
190	a	986.14	7.64088	YES	YES
191	a	986.69	3.25243	YES	YES
192	a	987.11	8.16808	YES	YES
193	a	987.51	8.60984	YES	YES
194	a	988.40	16.50649	YES	YES
195	a	991.24	18.91670	YES	YES
196	a	991.28	7.56347	YES	YES
197	a	991.84	15.83146	YES	YES
198	a	993.20	0.98754	YES	YES
199	a	1014.63	1.44909	YES	YES
200	a	1015.22	0.51167	YES	YES
201	a	1016.84	0.75272	YES	YES
202	a	1017.14	0.79972	YES	YES
203	a	1017.43	0.18114	YES	YES
204	a	1018.82	0.42363	YES	YES
205	a	1020.30	0.78255	YES	YES
206	a	1020.99	0.55171	YES	YES
207	a	1030.32	1.15668	YES	YES
208	a	1031.17	2.27162	YES	YES
209	a	1031.80	1.50661	YES	YES
210	a	1033.39	1.50920	YES	YES
211	a	1034.61	3.34470	YES	YES

212	a	1036.58	1.02579	YES	YES
213	a	1037.81	3.28785	YES	YES
214	a	1038.64	1.15443	YES	YES
215	a	1047.95	95.31731	YES	YES
216	a	1053.42	15.05579	YES	YES
217	a	1057.72	2.26636	YES	YES
218	a	1059.92	2.98580	YES	YES
219	a	1060.87	0.94822	YES	YES
220	a	1061.91	1.33074	YES	YES
221	a	1063.35	2.11010	YES	YES
222	a	1065.93	2.22420	YES	YES
223	a	1067.04	0.89053	YES	YES
224	a	1068.62	0.33987	YES	YES
225	a	1071.24	0.12596	YES	YES
226	a	1071.96	0.39626	YES	YES
227	a	1072.35	0.16698	YES	YES
228	a	1072.38	0.07230	YES	YES
229	a	1072.79	0.60819	YES	YES
230	a	1072.84	0.18611	YES	YES
231	a	1074.13	0.06919	YES	YES
232	a	1074.67	0.06605	YES	YES
233	a	1081.84	32.22897	YES	YES
234	a	1087.56	1.25522	YES	YES
235	a	1092.71	8.82700	YES	YES
236	a	1094.80	2.16162	YES	YES
237	a	1096.65	7.87853	YES	YES
238	a	1100.02	1.90960	YES	YES
239	a	1100.39	4.42061	YES	YES
240	a	1106.74	6.13195	YES	YES
241	a	1107.37	5.10904	YES	YES
242	a	1108.09	7.68433	YES	YES
243	a	1116.84	1.10848	YES	YES
244	a	1132.20	6.21579	YES	YES
245	a	1135.40	1.51449	YES	YES
246	a	1159.62	2.38291	YES	YES
247	a	1161.06	4.14697	YES	YES
248	a	1163.49	3.80773	YES	YES
249	a	1164.86	3.80838	YES	YES
250	a	1165.87	3.57725	YES	YES
251	a	1167.36	20.00488	YES	YES
252	a	1169.62	18.83925	YES	YES
253	a	1170.79	3.30170	YES	YES
254	a	1176.93	5.63608	YES	YES
255	a	1181.30	5.28150	YES	YES
256	a	1186.99	6.63437	YES	YES
257	a	1187.39	3.12809	YES	YES
258	a	1189.33	1.22879	YES	YES
259	a	1189.69	2.28087	YES	YES
260	a	1190.53	0.48960	YES	YES
261	a	1191.34	4.97111	YES	YES
262	a	1235.94	0.44199	YES	YES
263	a	1241.15	0.12873	YES	YES
264	a	1242.81	0.17141	YES	YES
265	a	1244.42	0.41637	YES	YES
266	a	1245.52	0.71750	YES	YES
267	a	1246.24	0.68430	YES	YES
268	a	1247.80	0.49561	YES	YES
269	a	1247.89	0.56541	YES	YES

270	a	1248.95	0.93833	YES	YES
271	a	1250.12	0.44709	YES	YES
272	a	1251.63	0.06995	YES	YES
273	a	1253.06	0.54106	YES	YES
274	a	1254.55	0.38407	YES	YES
275	a	1255.92	8.54554	YES	YES
276	a	1256.13	0.32841	YES	YES
277	a	1257.19	3.35991	YES	YES
278	a	1257.52	0.72275	YES	YES
279	a	1257.90	3.52165	YES	YES
280	a	1258.37	2.76273	YES	YES
281	a	1258.65	3.00457	YES	YES
282	a	1259.28	3.56478	YES	YES
283	a	1261.29	5.43867	YES	YES
284	a	1261.57	1.28848	YES	YES
285	a	1262.81	1.34891	YES	YES
286	a	1263.84	1.33536	YES	YES
287	a	1265.18	1.11141	YES	YES
288	a	1266.08	1.63115	YES	YES
289	a	1267.38	6.19833	YES	YES
290	a	1272.31	0.01449	YES	YES
291	a	1280.58	2.17621	YES	YES
292	a	1281.62	2.74599	YES	YES
293	a	1283.04	3.31872	YES	YES
294	a	1284.86	6.79348	YES	YES
295	a	1285.19	1.80745	YES	YES
296	a	1286.17	6.88592	YES	YES
297	a	1290.50	4.77003	YES	YES
298	a	1293.37	4.27057	YES	YES
299	a	1305.71	1.47721	YES	YES
300	a	1307.61	0.70098	YES	YES
301	a	1311.19	2.04087	YES	YES
302	a	1311.51	1.38059	YES	YES
303	a	1312.32	1.21518	YES	YES
304	a	1313.82	1.46353	YES	YES
305	a	1315.52	0.77223	YES	YES
306	a	1315.73	1.07605	YES	YES
307	a	1320.80	1.33202	YES	YES
308	a	1322.88	0.83389	YES	YES
309	a	1323.05	1.13128	YES	YES
310	a	1323.26	0.93384	YES	YES
311	a	1323.68	2.47407	YES	YES
312	a	1323.77	0.41317	YES	YES
313	a	1324.13	2.05302	YES	YES
314	a	1324.16	0.63681	YES	YES
315	a	1324.21	1.21072	YES	YES
316	a	1324.43	0.38340	YES	YES
317	a	1326.35	4.44736	YES	YES
318	a	1327.54	1.23372	YES	YES
319	a	1328.26	1.42056	YES	YES
320	a	1328.66	3.96205	YES	YES
321	a	1329.52	6.45570	YES	YES
322	a	1332.06	2.61448	YES	YES
323	a	1336.43	0.34611	YES	YES
324	a	1336.54	0.25162	YES	YES
325	a	1337.16	0.87047	YES	YES
326	a	1337.51	0.34351	YES	YES
327	a	1338.09	0.51737	YES	YES

328	a	1338.48	0.55926	YES	YES
329	a	1339.92	0.55800	YES	YES
330	a	1340.41	1.59692	YES	YES
331	a	1342.41	8.11193	YES	YES
332	a	1344.43	0.41088	YES	YES
333	a	1344.61	2.16798	YES	YES
334	a	1346.16	1.27972	YES	YES
335	a	1346.45	0.68244	YES	YES
336	a	1346.87	0.91503	YES	YES
337	a	1346.97	1.30371	YES	YES
338	a	1349.26	0.73924	YES	YES
339	a	1350.21	2.04753	YES	YES
340	a	1359.79	15.93628	YES	YES
341	a	1399.94	6.89819	YES	YES
342	a	1406.48	10.00549	YES	YES
343	a	1406.69	6.30828	YES	YES
344	a	1408.80	9.56179	YES	YES
345	a	1423.58	1.69076	YES	YES
346	a	1427.37	7.57959	YES	YES
347	a	1428.28	4.99521	YES	YES
348	a	1429.27	5.33592	YES	YES
349	a	1431.06	2.40379	YES	YES
350	a	1431.18	7.09911	YES	YES
351	a	1432.57	0.85323	YES	YES
352	a	1433.21	2.91213	YES	YES
353	a	1434.44	1.18844	YES	YES
354	a	1435.36	9.70092	YES	YES
355	a	1435.62	5.10993	YES	YES
356	a	1436.35	0.60983	YES	YES
357	a	1436.84	1.83664	YES	YES
358	a	1437.14	1.55001	YES	YES
359	a	1437.33	4.28065	YES	YES
360	a	1437.61	2.17804	YES	YES
361	a	1437.76	5.62090	YES	YES
362	a	1438.24	10.28535	YES	YES
363	a	1438.56	3.46726	YES	YES
364	a	1438.86	11.30964	YES	YES
365	a	1439.41	5.02899	YES	YES
366	a	1439.76	5.24448	YES	YES
367	a	1440.37	0.53216	YES	YES
368	a	1440.68	5.18798	YES	YES
369	a	1441.15	8.22643	YES	YES
370	a	1441.48	15.71927	YES	YES
371	a	1442.91	16.17863	YES	YES
372	a	1443.47	15.31451	YES	YES
373	a	1443.62	15.57944	YES	YES
374	a	1444.50	14.35823	YES	YES
375	a	1445.27	27.71620	YES	YES
376	a	1445.75	4.52912	YES	YES
377	a	1446.89	4.95459	YES	YES
378	a	1447.73	3.62458	YES	YES
379	a	1452.76	1.08680	YES	YES
380	a	1453.79	1.49932	YES	YES
381	a	1454.69	1.97690	YES	YES
382	a	1454.99	4.71093	YES	YES
383	a	1455.60	2.30708	YES	YES
384	a	1455.86	0.50451	YES	YES
385	a	1456.44	0.28255	YES	YES

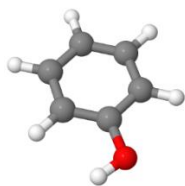
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389	a	2859.58	45.85833	YES	YES
390	a	2917.06	42.76606	YES	YES
391	a	2927.25	3.94727	YES	YES
392	a	2927.82	17.72685	YES	YES
393	a	2933.48	15.59732	YES	YES
394	a	2935.55	3.43637	YES	YES
395	a	2936.40	3.97593	YES	YES
396	a	2937.98	8.02690	YES	YES
397	a	2938.14	5.67695	YES	YES
398	a	2938.23	6.41780	YES	YES
399	a	2940.18	10.15621	YES	YES
400	a	2941.45	6.36579	YES	YES
401	a	2942.59	8.98376	YES	YES
402	a	2942.77	6.75261	YES	YES
403	a	2943.57	9.83091	YES	YES
404	a	2943.69	9.23029	YES	YES
405	a	2944.87	23.67822	YES	YES
406	a	2944.91	6.84541	YES	YES
407	a	2945.14	19.14164	YES	YES
408	a	2946.34	12.46320	YES	YES
409	a	2946.60	14.93082	YES	YES
410	a	2947.62	1.84909	YES	YES
411	a	2947.72	12.67336	YES	YES
412	a	2949.06	7.28434	YES	YES
413	a	2949.55	8.30536	YES	YES
414	a	2950.45	17.61445	YES	YES
415	a	2950.68	3.55373	YES	YES
416	a	2950.79	22.84283	YES	YES
417	a	2952.75	9.28789	YES	YES
418	a	2953.39	9.14339	YES	YES
419	a	2953.90	6.03801	YES	YES
420	a	2954.67	5.13798	YES	YES
421	a	2955.19	4.06635	YES	YES
422	a	2956.40	6.73530	YES	YES
423	a	2956.54	7.62067	YES	YES
424	a	2956.85	4.24835	YES	YES
425	a	2956.89	16.16846	YES	YES
426	a	2957.60	6.59099	YES	YES
427	a	2957.98	6.39375	YES	YES
428	a	2958.73	3.16965	YES	YES
429	a	2959.89	8.76335	YES	YES
430	a	2960.58	31.99795	YES	YES
431	a	2961.11	31.02000	YES	YES
432	a	2961.47	50.02324	YES	YES
433	a	2961.96	10.69781	YES	YES
434	a	2962.11	82.21763	YES	YES
435	a	2963.23	29.91025	YES	YES
436	a	2963.41	34.66156	YES	YES
437	a	2963.91	41.99386	YES	YES
438	a	2970.80	11.49466	YES	YES
439	a	2973.10	20.95409	YES	YES
440	a	2980.89	2.85658	YES	YES
441	a	2985.36	4.36743	YES	YES
442	a	2985.54	32.01239	YES	YES
443	a	2990.19	6.05714	YES	YES

444	a	2991.51	26.83125	YES	YES
445	a	2991.96	7.29953	YES	YES
446	a	2992.37	18.21689	YES	YES
447	a	2997.52	33.65051	YES	YES
448	a	2997.83	1.77262	YES	YES
449	a	2999.28	18.59780	YES	YES
450	a	3003.40	17.32267	YES	YES
451	a	3003.44	24.44318	YES	YES
452	a	3004.42	30.71837	YES	YES
453	a	3005.03	18.79301	YES	YES
454	a	3005.62	17.15359	YES	YES
455	a	3007.12	16.62391	YES	YES
456	a	3007.33	3.10658	YES	YES
457	a	3007.59	15.50157	YES	YES
458	a	3007.69	42.44592	YES	YES
459	a	3008.12	44.36907	YES	YES
460	a	3009.45	15.73188	YES	YES
461	a	3009.70	14.45610	YES	YES
462	a	3010.42	16.53969	YES	YES
463	a	3011.46	22.91429	YES	YES
464	a	3013.00	16.59921	YES	YES
465	a	3013.69	21.48135	YES	YES
466	a	3014.16	19.21156	YES	YES
467	a	3014.62	26.76086	YES	YES
468	a	3015.40	37.93841	YES	YES
469	a	3015.44	12.47552	YES	YES
470	a	3015.94	17.81329	YES	YES
471	a	3016.24	7.77740	YES	YES
472	a	3016.42	38.74599	YES	YES
473	a	3016.93	19.46057	YES	YES
474	a	3017.69	34.41203	YES	YES
475	a	3017.82	23.26810	YES	YES
476	a	3017.92	29.54159	YES	YES
477	a	3018.09	34.14230	YES	YES
478	a	3018.29	20.05418	YES	YES
479	a	3018.79	24.49297	YES	YES
480	a	3019.30	15.95602	YES	YES
481	a	3019.53	19.21951	YES	YES
482	a	3019.80	33.62877	YES	YES
483	a	3024.84	14.96994	YES	YES
484	a	3030.42	0.08546	YES	YES
485	a	3032.93	1.34937	YES	YES
486	a	3038.50	0.67206	YES	YES
487	a	3043.69	22.06002	YES	YES
488	a	3046.48	0.54871	YES	YES
489	a	3048.83	14.11245	YES	YES

\$end

Double hybrid single point energy = -7403.975779491784 H
 COSMO energy + OC correction = -7411.4994578365 H (in oDFB)

6.2.11 PhOH



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: cs

Cartesian coordinates in Ångström:

O	1.3319757	-2.1255567	0.0000000
C	0.6090030	-0.9583424	0.0000000
C	-0.7912461	-0.9410843	0.0000000
H	-1.3473176	-1.8813969	0.0000000
C	-1.4700835	0.2791366	0.0000000
H	-2.5601197	0.2838856	0.0000000
C	-0.7629095	1.4831124	0.0000000
H	-1.2950572	2.4332757	0.0000000
C	0.6353513	1.4556534	0.0000000
H	1.1985243	2.3890018	0.0000000
C	1.3254354	0.2443727	0.0000000
H	2.4141062	0.2112185	0.0000000
H	0.7123377	-2.8732763	0.0000000

SCF energy GEOOPT = -307.6259677609 H

ZPE = 267.0 kJ/mol

FREEH energy = 281.85 kJ/mol

FREEH entropy = 0.31440 kJ/mol/K

\$vibrational spectrum

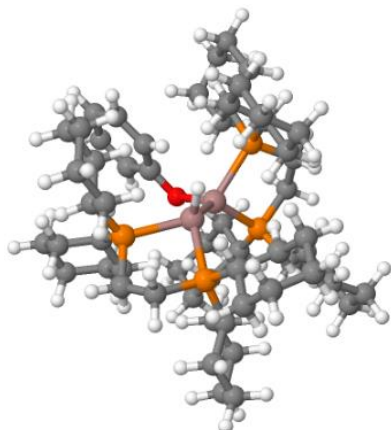
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#			cm** (-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	219.63	0.80421	YES	YES
8		a''	367.74	91.63266	YES	YES
9		a'	392.77	9.53439	YES	YES
10		a''	405.93	0.30821	YES	YES
11		a''	497.25	14.04645	YES	YES
12		a'	520.76	1.52776	YES	YES
13		a'	614.15	0.39648	YES	YES
14		a''	677.78	25.09697	YES	YES
15		a''	736.51	55.28477	YES	YES
16		a''	792.83	0.00047	YES	YES
17		a'	810.69	19.47492	YES	YES
18		a''	857.22	5.53024	YES	YES
19		a''	927.24	0.09408	YES	YES
20		a''	946.05	0.04918	YES	YES
21		a'	990.81	1.92608	YES	YES
22		a'	1020.19	4.54383	YES	YES
23		a'	1066.46	13.96494	YES	YES
24		a'	1146.20	7.56746	YES	YES

25	a'	1157.10	23.85152	YES	YES
26	a'	1162.36	126.32063	YES	YES
27	a'	1252.23	69.88939	YES	YES
28	a'	1324.93	12.75173	YES	YES
29	a'	1355.44	14.73199	YES	YES
30	a'	1461.74	26.28463	YES	YES
31	a'	1487.50	47.98834	YES	YES
32	a'	1592.84	46.65641	YES	YES
33	a'	1603.87	30.93651	YES	YES
34	a'	3080.24	14.87537	YES	YES
35	a'	3101.93	0.28134	YES	YES
36	a'	3110.00	16.05929	YES	YES
37	a'	3123.93	16.04588	YES	YES
38	a'	3130.49	5.92187	YES	YES
39	a'	3703.45	44.54951	YES	YES

§end

Double hybrid single point energy = -307.083414303859H
 COSMO energy + OC correction = -307.6350898506 H (in oDFB)

6.2.12 [H{Ga(dcpe)}₂(OPh)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	15.2549201	12.9883647	16.3768647
Ga	16.4757343	13.9973158	18.2399182
P	15.1147957	15.1942440	19.8698037
P	17.6601611	13.0440696	20.1162747
P	15.2102155	10.6831385	15.7134324
P	16.1978642	13.4788979	14.2244877
O	17.8443833	15.2119224	17.7839774
C	15.5590980	14.4075585	21.4827759
H	15.3121650	15.1020596	22.2980233
H	14.9074654	13.5329203	21.6025202
C	17.0388906	14.0006610	21.5691934
H	17.2294233	13.4303983	22.4882873
H	17.6687822	14.8967811	21.6150068
C	15.3991064	10.7945304	13.8803365
H	15.6296042	9.8040762	13.4677828
H	14.4054980	11.0740167	13.5054522

C	16.4528269	11.8225998	13.4379225
H	16.4437189	11.9333865	12.3446036
H	17.4594463	11.4836812	13.7164240
C	17.6075596	16.3999801	17.1842860
C	18.6805902	17.2990257	17.0362181
H	19.6622406	17.0085211	17.4094680
C	18.4815339	18.5410328	16.4371416
H	19.3231741	19.2257858	16.3355071
C	17.2148457	18.9198338	15.9763227
H	17.0647581	19.8946105	15.5159078
C	16.1474193	18.0328320	16.1180052
H	15.1543694	18.3116398	15.7651827
C	16.3402410	16.7826240	16.7115268
H	15.4990362	16.0922053	16.8087287
C	13.3040256	14.9578910	19.6402967
H	12.8034123	15.4164823	20.5096945
C	12.9444991	13.4629626	19.5877515
H	13.2136935	12.9627735	20.5284879
H	13.5368931	12.9848515	18.7897428
C	11.4527158	13.2572372	19.3010199
H	11.2385610	12.1814466	19.2369868
H	10.8652016	13.6422871	20.1499549
C	11.0259593	13.9719447	18.0163850
H	9.9501439	13.8335449	17.8446498
H	11.5487715	13.5186024	17.1573698
C	11.3652429	15.4639573	18.0821215
H	11.0894755	15.9660170	17.1446238
H	10.7726941	15.9418784	18.8788426
C	12.8571610	15.6863032	18.3575462
H	13.0754585	16.7606731	18.4295086
H	13.4390014	15.2940203	17.5072034
C	15.4564987	16.9986027	20.0032485
H	15.3206689	17.3608591	18.9707266
C	16.9197507	17.2727791	20.3942905
H	17.0823509	16.9479644	21.4356582
H	17.6077111	16.7033307	19.7565888
C	17.2096345	18.7744438	20.2923827
H	17.1058707	19.0815880	19.2391337
H	18.2532998	18.9687907	20.5751413
C	16.2525117	19.5802648	21.1764322
H	16.4503973	19.3438756	22.2351875
H	16.4400959	20.6559509	21.0592673
C	14.7879607	19.2662764	20.8531006
H	14.5522669	19.6224138	19.8369055
H	14.1177361	19.8038815	21.5374333
C	14.4909463	17.7595752	20.9256571
H	13.4449413	17.5749484	20.6448973
H	14.6127980	17.4077190	21.9634230
C	19.4952630	13.2372517	20.0605677
H	19.8914220	12.6071027	20.8757638
C	19.9632506	14.6869405	20.2795411
H	19.6575215	15.0493257	21.2703865
H	19.4837053	15.3286572	19.5258919
C	21.4899326	14.7867731	20.1559581
H	21.7937628	15.8345812	20.2849353
H	21.9596608	14.2223742	20.9780078
C	21.9891457	14.2417465	18.8152212
H	23.0844088	14.3019680	18.7648914

H	21.5989200	14.8688601	17.9967532
C	21.5256057	12.7979922	18.6069389
H	21.8514665	12.4216502	17.6266941
H	21.9930423	12.1460727	19.3627545
C	20.0005954	12.6916621	18.7118821
H	19.6842359	11.6483418	18.5760754
H	19.5396142	13.2849883	17.9073701
C	17.3134553	11.2575352	20.4082263
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C	15.8307559	10.9222764	20.1739268
H	15.5140405	11.2729042	19.1784919
H	15.2110531	11.4606640	20.9087741
C	15.5798341	9.4170211	20.3211515
H	14.5085772	9.2062976	20.1981536
H	16.1039023	8.8862146	19.5080316
C	16.0775356	8.8875615	21.6697270
H	15.4735818	9.3301159	22.4788802
H	15.9258110	7.8015484	21.7281211
C	17.5528162	9.2313449	21.8923566
H	18.1732679	8.7049844	21.1484692
H	17.8849614	8.8820866	22.8789801
C	17.7974126	10.7417336	21.7731579
H	17.2467873	11.2557205	22.5772638
H	18.8629735	10.9657865	21.9202706
C	16.4698942	9.5003704	16.3673411
H	15.9976228	9.1018509	17.2829975
C	17.7662278	10.2212756	16.7747131
H	18.2349308	10.6653298	15.8817896
H	17.5366666	11.0614109	17.4478642
C	18.7479170	9.2417630	17.4280595
H	19.6818465	9.7615050	17.6842184
H	18.3158426	8.8806424	18.3770176
C	19.0426501	8.0423131	16.5218286
H	19.7090172	7.3361429	17.0345989
H	19.5843200	8.3887325	15.6263327
C	17.7512416	7.3417360	16.0929619
H	17.2620797	6.8915386	16.9723090
H	17.9716800	6.5170502	15.4021084
C	16.7813480	8.3242622	15.4241985
H	15.8633453	7.8070890	15.1189226
H	17.2498212	8.7146670	14.5061260
C	15.0687885	14.4341455	13.1249663
H	15.6197934	14.5739409	12.1790416
C	14.7911407	15.8089538	13.7542686
H	15.7291048	16.3513849	13.9311573
H	14.3257604	15.6527345	14.7426453
C	13.8478780	16.6421735	12.8804512
H	13.6481242	17.6042206	13.3725930
H	14.3486915	16.8776254	11.9275146
C	12.5422936	15.8930108	12.6028940
H	11.9960178	15.7469784	13.5501343
H	11.8889058	16.4904090	11.9533858
C	12.8207820	14.5310157	11.9615225
H	13.2772039	14.6803967	10.9696689
H	11.8843318	13.9814093	11.7943211
C	13.7625047	13.6788129	12.8238169
H	13.9772528	12.7355335	12.3018593
H	13.2638853	13.4263915	13.7747421

C	17.8170476	14.3455977	14.2942927
H	17.5994936	15.2328752	14.9136417
C	18.3585462	14.8230671	12.9386085
H	18.5573732	13.9546449	12.2888533
H	17.6191221	15.4500812	12.4222934
C	19.6539828	15.6196576	13.1523049
H	19.4160432	16.5314296	13.7243168
H	20.0487593	15.9479088	12.1814771
C	20.7032519	14.8001302	13.9098066
H	21.6035768	15.4053259	14.0818550
H	21.0171166	13.9449416	13.2884141
C	20.1531663	14.2848830	15.2434071
H	20.8964137	13.6500263	15.7457530
H	19.9474434	15.1314939	15.9152453
C	18.8553532	13.4956200	15.0448062
H	18.4508294	13.1735381	16.0157582
H	19.0780491	12.5849691	14.4642513
C	13.5158742	10.0215003	15.9980235
H	12.8825458	10.7702383	15.4874226
C	13.1720084	10.0574344	17.4954384
H	13.3636989	11.0611476	17.9040245
H	13.8304192	9.3583065	18.0351778
C	11.7099713	9.6576158	17.7280170
H	11.4958316	9.6506217	18.8061824
H	11.0558553	10.4239051	17.2807011
C	11.3963033	8.2910756	17.1101338
H	11.9661604	7.5111024	17.6418684
H	10.3343610	8.0485552	17.2484181
C	11.7581795	8.2557541	15.6221028
H	11.1130738	8.9562527	15.0670070
H	11.5697589	7.2580819	15.2034581
C	13.2279318	8.6371871	15.3951014
H	13.4662740	8.6177455	14.3222544
H	13.8706822	7.8882548	15.8836904
H	13.7166213	13.3137332	16.2170787

SCF energy GEOOPT = -7563.875389214 H

ZPE = 3862. kJ/mol

FREEH energy = 4054.64 kJ/mol

FREEH entropy = 1.63198 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	14.37	0.12208	YES	YES
	8	a	17.48	0.00050	YES	YES
	9	a	20.97	0.05192	YES	YES
	10	a	25.46	0.09588	YES	YES
	11	a	32.99	0.11293	YES	YES
	12	a	34.84	0.02998	YES	YES
	13	a	38.03	0.01755	YES	YES
	14	a	40.46	0.02035	YES	YES

15	a	41.65	0.06482	YES	YES
16	a	42.17	0.06873	YES	YES
17	a	42.45	0.10838	YES	YES
18	a	44.32	0.02438	YES	YES
19	a	47.60	0.01750	YES	YES
20	a	48.84	0.00366	YES	YES
21	a	51.34	0.41177	YES	YES
22	a	53.96	0.16881	YES	YES
23	a	54.11	0.00690	YES	YES
24	a	58.97	0.09732	YES	YES
25	a	59.08	0.20270	YES	YES
26	a	63.48	0.02023	YES	YES
27	a	63.71	0.32885	YES	YES
28	a	66.08	0.07733	YES	YES
29	a	67.98	0.01477	YES	YES
30	a	71.40	0.01913	YES	YES
31	a	73.75	0.45551	YES	YES
32	a	79.13	0.08182	YES	YES
33	a	81.50	0.17087	YES	YES
34	a	84.82	0.05708	YES	YES
35	a	90.56	0.06441	YES	YES
36	a	95.11	0.61804	YES	YES
37	a	98.92	0.19252	YES	YES
38	a	103.06	0.66303	YES	YES
39	a	119.49	0.70717	YES	YES
40	a	127.89	0.82497	YES	YES
41	a	130.05	0.20481	YES	YES
42	a	131.46	4.25941	YES	YES
43	a	136.64	0.03807	YES	YES
44	a	139.59	2.58519	YES	YES
45	a	142.99	1.86986	YES	YES
46	a	149.30	0.18461	YES	YES
47	a	151.10	6.60128	YES	YES
48	a	155.71	3.36143	YES	YES
49	a	160.16	1.18870	YES	YES
50	a	163.63	7.15696	YES	YES
51	a	172.09	0.11639	YES	YES
52	a	185.24	2.18259	YES	YES
53	a	188.62	6.12267	YES	YES
54	a	190.50	2.94194	YES	YES
55	a	202.83	1.14813	YES	YES
56	a	209.99	1.77112	YES	YES
57	a	212.73	0.74000	YES	YES
58	a	217.01	0.69324	YES	YES
59	a	218.19	0.16176	YES	YES
60	a	221.75	0.15334	YES	YES
61	a	223.84	0.25419	YES	YES
62	a	225.39	0.98682	YES	YES
63	a	226.83	1.25676	YES	YES
64	a	232.66	0.12796	YES	YES
65	a	238.68	0.29912	YES	YES
66	a	239.17	0.11322	YES	YES
67	a	242.12	1.14715	YES	YES
68	a	243.37	3.09789	YES	YES
69	a	245.66	0.41197	YES	YES
70	a	252.72	1.59766	YES	YES
71	a	256.10	0.73484	YES	YES
72	a	257.38	0.73192	YES	YES

73	a	269.65	2.14814	YES	YES
74	a	275.34	0.27150	YES	YES
75	a	279.68	5.07936	YES	YES
76	a	285.25	0.95394	YES	YES
77	a	296.78	4.79977	YES	YES
78	a	306.88	0.04605	YES	YES
79	a	308.92	1.07389	YES	YES
80	a	311.28	0.29714	YES	YES
81	a	311.64	0.53823	YES	YES
82	a	326.90	0.99346	YES	YES
83	a	329.31	0.74084	YES	YES
84	a	333.41	0.27267	YES	YES
85	a	334.28	0.13865	YES	YES
86	a	336.52	1.27827	YES	YES
87	a	339.95	0.63714	YES	YES
88	a	373.48	2.11865	YES	YES
89	a	377.16	2.71033	YES	YES
90	a	378.16	2.21521	YES	YES
91	a	382.39	0.02619	YES	YES
92	a	392.59	0.96445	YES	YES
93	a	401.64	0.20826	YES	YES
94	a	413.40	2.18294	YES	YES
95	a	414.54	1.96006	YES	YES
96	a	415.63	0.90649	YES	YES
97	a	424.50	1.94804	YES	YES
98	a	426.32	0.42489	YES	YES
99	a	428.52	0.22219	YES	YES
100	a	428.87	0.15894	YES	YES
101	a	429.97	0.90279	YES	YES
102	a	431.59	0.51498	YES	YES
103	a	431.89	0.28993	YES	YES
104	a	432.86	0.48976	YES	YES
105	a	433.74	0.20120	YES	YES
106	a	434.25	0.30092	YES	YES
107	a	436.55	0.21021	YES	YES
108	a	440.14	1.68906	YES	YES
109	a	449.60	4.09486	YES	YES
110	a	450.45	1.21797	YES	YES
111	a	457.19	5.26421	YES	YES
112	a	465.44	6.88462	YES	YES
113	a	493.21	2.29356	YES	YES
114	a	494.78	2.85258	YES	YES
115	a	495.13	3.19741	YES	YES
116	a	497.23	2.94347	YES	YES
117	a	502.81	1.00444	YES	YES
118	a	506.53	8.40648	YES	YES
119	a	507.18	5.48359	YES	YES
120	a	509.19	12.50000	YES	YES
121	a	517.94	18.67793	YES	YES
122	a	519.52	10.90098	YES	YES
123	a	546.03	57.47772	YES	YES
124	a	573.77	113.99102	YES	YES
125	a	594.17	17.22989	YES	YES
126	a	629.76	8.52627	YES	YES
127	a	632.00	14.04521	YES	YES
128	a	632.95	26.86790	YES	YES
129	a	645.72	7.04388	YES	YES
130	a	648.79	11.15250	YES	YES

131	a	691.21	27.00282	YES	YES
132	a	708.79	2.61208	YES	YES
133	a	719.65	2.43784	YES	YES
134	a	725.96	0.50672	YES	YES
135	a	730.71	5.70017	YES	YES
136	a	735.67	1.55428	YES	YES
137	a	736.35	8.07450	YES	YES
138	a	738.18	4.43564	YES	YES
139	a	742.56	4.29300	YES	YES
140	a	751.23	51.21416	YES	YES
141	a	768.93	0.08130	YES	YES
142	a	773.78	0.09821	YES	YES
143	a	774.39	0.33472	YES	YES
144	a	775.59	0.07268	YES	YES
145	a	777.09	0.10095	YES	YES
146	a	778.00	0.14462	YES	YES
147	a	778.59	0.66439	YES	YES
148	a	780.48	0.38201	YES	YES
149	a	783.46	15.59284	YES	YES
150	a	787.70	17.40270	YES	YES
151	a	799.48	0.17907	YES	YES
152	a	808.75	1.63222	YES	YES
153	a	810.58	0.46350	YES	YES
154	a	811.06	4.42785	YES	YES
155	a	812.21	1.39783	YES	YES
156	a	812.68	1.91405	YES	YES
157	a	812.90	2.44495	YES	YES
158	a	815.33	1.76295	YES	YES
159	a	816.04	4.36658	YES	YES
160	a	831.45	4.92843	YES	YES
161	a	833.75	3.79553	YES	YES
162	a	837.62	0.50953	YES	YES
163	a	838.14	0.65853	YES	YES
164	a	838.85	9.07150	YES	YES
165	a	839.15	1.53229	YES	YES
166	a	839.57	7.41459	YES	YES
167	a	840.95	3.42159	YES	YES
168	a	841.52	65.97412	YES	YES
169	a	846.88	3.38326	YES	YES
170	a	852.60	11.61394	YES	YES
171	a	864.94	6.30374	YES	YES
172	a	873.84	1.89206	YES	YES
173	a	874.16	2.29598	YES	YES
174	a	874.51	2.59243	YES	YES
175	a	875.95	1.75780	YES	YES
176	a	876.83	2.02479	YES	YES
177	a	878.06	6.41311	YES	YES
178	a	879.23	5.01709	YES	YES
179	a	880.31	0.50365	YES	YES
180	a	880.45	7.09578	YES	YES
181	a	880.70	1.17649	YES	YES
182	a	880.98	2.63982	YES	YES
183	a	881.83	9.12841	YES	YES
184	a	882.54	1.58700	YES	YES
185	a	885.43	6.02367	YES	YES
186	a	887.71	10.56051	YES	YES
187	a	889.10	0.91011	YES	YES
188	a	903.74	0.45379	YES	YES

189	a	904.97	2.48300	YES	YES
190	a	905.90	0.74600	YES	YES
191	a	906.08	1.39444	YES	YES
192	a	907.83	3.73151	YES	YES
193	a	910.22	1.18966	YES	YES
194	a	910.64	2.44890	YES	YES
195	a	911.37	0.19477	YES	YES
196	a	945.26	0.20218	YES	YES
197	a	971.80	0.10457	YES	YES
198	a	981.38	0.68250	YES	YES
199	a	983.94	0.09092	YES	YES
200	a	988.05	2.75681	YES	YES
201	a	988.96	8.13382	YES	YES
202	a	989.42	9.86602	YES	YES
203	a	990.01	6.73740	YES	YES
204	a	990.95	17.82739	YES	YES
205	a	991.44	8.66617	YES	YES
206	a	992.88	8.55059	YES	YES
207	a	993.49	10.83658	YES	YES
208	a	993.75	8.16740	YES	YES
209	a	1014.01	1.46828	YES	YES
210	a	1014.54	0.38227	YES	YES
211	a	1015.86	0.02547	YES	YES
212	a	1016.28	0.76856	YES	YES
213	a	1017.51	0.31597	YES	YES
214	a	1020.36	0.34918	YES	YES
215	a	1020.61	1.39353	YES	YES
216	a	1021.18	0.10967	YES	YES
217	a	1021.71	2.37523	YES	YES
218	a	1029.98	1.43052	YES	YES
219	a	1030.35	0.09072	YES	YES
220	a	1032.23	0.98958	YES	YES
221	a	1034.91	2.50542	YES	YES
222	a	1035.79	1.36481	YES	YES
223	a	1037.66	2.50222	YES	YES
224	a	1039.23	1.13961	YES	YES
225	a	1040.57	3.00839	YES	YES
226	a	1057.71	0.19134	YES	YES
227	a	1059.38	1.63852	YES	YES
228	a	1060.65	0.08090	YES	YES
229	a	1061.71	1.43796	YES	YES
230	a	1061.85	1.46077	YES	YES
231	a	1065.21	3.68459	YES	YES
232	a	1065.94	0.32303	YES	YES
233	a	1068.59	1.01278	YES	YES
234	a	1069.99	0.49856	YES	YES
235	a	1070.89	0.11520	YES	YES
236	a	1071.15	1.88035	YES	YES
237	a	1072.02	0.29406	YES	YES
238	a	1072.30	6.47567	YES	YES
239	a	1072.72	0.26802	YES	YES
240	a	1073.30	0.18108	YES	YES
241	a	1073.49	0.19096	YES	YES
242	a	1074.02	0.04101	YES	YES
243	a	1076.88	2.26470	YES	YES
244	a	1081.89	5.98152	YES	YES
245	a	1094.45	3.81946	YES	YES
246	a	1095.49	2.37376	YES	YES

247	a	1098.37	5.13140	YES	YES
248	a	1101.06	4.28655	YES	YES
249	a	1107.18	4.58716	YES	YES
250	a	1107.86	4.36045	YES	YES
251	a	1110.54	4.56536	YES	YES
252	a	1113.67	7.23815	YES	YES
253	a	1125.66	1.74707	YES	YES
254	a	1128.79	1.83687	YES	YES
255	a	1149.77	0.22048	YES	YES
256	a	1157.20	15.53964	YES	YES
257	a	1160.32	2.17383	YES	YES
258	a	1160.60	13.28223	YES	YES
259	a	1162.47	5.60471	YES	YES
260	a	1164.26	1.46266	YES	YES
261	a	1165.53	13.66032	YES	YES
262	a	1169.00	6.39340	YES	YES
263	a	1170.90	2.07754	YES	YES
264	a	1171.39	6.74027	YES	YES
265	a	1178.17	11.37222	YES	YES
266	a	1180.85	8.79007	YES	YES
267	a	1183.94	5.85775	YES	YES
268	a	1189.54	2.64173	YES	YES
269	a	1194.65	2.23837	YES	YES
270	a	1195.13	3.40185	YES	YES
271	a	1199.20	1.17734	YES	YES
272	a	1201.76	1.12797	YES	YES
273	a	1240.50	0.91407	YES	YES
274	a	1242.03	1.24770	YES	YES
275	a	1245.29	19.74770	YES	YES
276	a	1245.84	6.93045	YES	YES
277	a	1246.40	7.55115	YES	YES
278	a	1247.25	0.49115	YES	YES
279	a	1248.13	6.51768	YES	YES
280	a	1248.58	5.03075	YES	YES
281	a	1249.16	21.38940	YES	YES
282	a	1251.11	1.16190	YES	YES
283	a	1252.01	41.32421	YES	YES
284	a	1253.19	12.95704	YES	YES
285	a	1254.57	10.79304	YES	YES
286	a	1254.89	0.56423	YES	YES
287	a	1256.23	2.92797	YES	YES
288	a	1257.12	4.42639	YES	YES
289	a	1257.76	7.60571	YES	YES
290	a	1258.18	15.92880	YES	YES
291	a	1258.39	8.79545	YES	YES
292	a	1260.81	16.18501	YES	YES
293	a	1261.05	1.02223	YES	YES
294	a	1261.76	6.19704	YES	YES
295	a	1263.72	2.63683	YES	YES
296	a	1264.44	2.93713	YES	YES
297	a	1264.70	13.17240	YES	YES
298	a	1265.14	9.40695	YES	YES
299	a	1269.03	3.07506	YES	YES
300	a	1270.08	1.64963	YES	YES
301	a	1274.56	1.85672	YES	YES
302	a	1279.91	0.40067	YES	YES
303	a	1281.91	7.93124	YES	YES
304	a	1284.05	6.76892	YES	YES

305	a	1285.27	3.48631	YES	YES
306	a	1286.14	2.29432	YES	YES
307	a	1288.66	4.85353	YES	YES
308	a	1291.13	7.24316	YES	YES
309	a	1291.61	4.80365	YES	YES
310	a	1294.26	3.76066	YES	YES
311	a	1305.11	2.71734	YES	YES
312	a	1308.36	1.35844	YES	YES
313	a	1310.38	1.20792	YES	YES
314	a	1311.42	2.89328	YES	YES
315	a	1311.48	0.84555	YES	YES
316	a	1314.84	1.46825	YES	YES
317	a	1316.57	1.45076	YES	YES
318	a	1318.23	0.60925	YES	YES
319	a	1321.62	2.91062	YES	YES
320	a	1321.99	1.92351	YES	YES
321	a	1322.46	0.47433	YES	YES
322	a	1323.02	0.34280	YES	YES
323	a	1323.56	0.37437	YES	YES
324	a	1324.32	2.92488	YES	YES
325	a	1324.46	1.41180	YES	YES
326	a	1324.80	0.56213	YES	YES
327	a	1325.20	0.49959	YES	YES
328	a	1325.60	1.58676	YES	YES
329	a	1325.79	0.15611	YES	YES
330	a	1326.57	2.81818	YES	YES
331	a	1327.95	0.54680	YES	YES
332	a	1328.39	2.22231	YES	YES
333	a	1329.30	6.16966	YES	YES
334	a	1332.56	0.53707	YES	YES
335	a	1336.97	0.44299	YES	YES
336	a	1337.26	4.01899	YES	YES
337	a	1337.41	0.18883	YES	YES
338	a	1337.81	0.33030	YES	YES
339	a	1338.06	0.08250	YES	YES
340	a	1338.20	0.05920	YES	YES
341	a	1338.81	0.32037	YES	YES
342	a	1339.17	0.13151	YES	YES
343	a	1339.60	0.28135	YES	YES
344	a	1344.31	2.35613	YES	YES
345	a	1344.96	0.56582	YES	YES
346	a	1345.09	0.32415	YES	YES
347	a	1346.72	1.68327	YES	YES
348	a	1346.78	2.23283	YES	YES
349	a	1349.50	1.52044	YES	YES
350	a	1350.01	0.47277	YES	YES
351	a	1350.76	0.97957	YES	YES
352	a	1404.79	8.83531	YES	YES
353	a	1404.85	5.43816	YES	YES
354	a	1407.14	8.50251	YES	YES
355	a	1407.84	6.97610	YES	YES
356	a	1419.90	2.02817	YES	YES
357	a	1421.82	8.72899	YES	YES
358	a	1427.30	1.92869	YES	YES
359	a	1428.33	0.85561	YES	YES
360	a	1429.62	3.61514	YES	YES
361	a	1430.34	8.17764	YES	YES
362	a	1432.68	2.24527	YES	YES

363	a	1433.86	1.97238	YES	YES
364	a	1434.46	2.35075	YES	YES
365	a	1436.12	7.34078	YES	YES
366	a	1436.38	2.68026	YES	YES
367	a	1436.87	8.44497	YES	YES
368	a	1437.15	5.42842	YES	YES
369	a	1437.47	5.27098	YES	YES
370	a	1437.81	0.93595	YES	YES
371	a	1438.14	6.71046	YES	YES
372	a	1438.38	4.97397	YES	YES
373	a	1438.73	2.28899	YES	YES
374	a	1439.33	3.66598	YES	YES
375	a	1439.40	5.00650	YES	YES
376	a	1439.59	3.70361	YES	YES
377	a	1440.06	4.44484	YES	YES
378	a	1440.20	10.29502	YES	YES
379	a	1441.08	2.85738	YES	YES
380	a	1441.93	9.75656	YES	YES
381	a	1442.36	2.05498	YES	YES
382	a	1443.00	15.69547	YES	YES
383	a	1443.88	7.22510	YES	YES
384	a	1444.61	14.18938	YES	YES
385	a	1445.04	6.91133	YES	YES
386	a	1445.58	40.87799	YES	YES
387	a	1446.19	1.85346	YES	YES
388	a	1447.31	7.21682	YES	YES
389	a	1451.79	1.75711	YES	YES
390	a	1453.23	2.56015	YES	YES
391	a	1453.81	5.36453	YES	YES
392	a	1454.79	0.76649	YES	YES
393	a	1455.06	0.31950	YES	YES
394	a	1455.48	2.04158	YES	YES
395	a	1456.48	0.36127	YES	YES
396	a	1458.60	2.86447	YES	YES
397	a	1475.84	121.19521	YES	YES
398	a	1568.43	6.91131	YES	YES
399	a	1588.02	72.51622	YES	YES
400	a	1853.18	127.44482	YES	YES
401	a	2924.43	2.81687	YES	YES
402	a	2931.94	3.20659	YES	YES
403	a	2933.65	12.94933	YES	YES
404	a	2935.85	23.96962	YES	YES
405	a	2936.67	26.26373	YES	YES
406	a	2937.07	22.87281	YES	YES
407	a	2937.09	3.61856	YES	YES
408	a	2939.00	11.31471	YES	YES
409	a	2939.57	0.43054	YES	YES
410	a	2939.70	25.35663	YES	YES
411	a	2940.86	12.19668	YES	YES
412	a	2941.46	18.90799	YES	YES
413	a	2941.77	8.42300	YES	YES
414	a	2942.72	17.44220	YES	YES
415	a	2943.99	8.80472	YES	YES
416	a	2944.23	9.41815	YES	YES
417	a	2945.61	6.88700	YES	YES
418	a	2946.67	9.95194	YES	YES
419	a	2946.99	13.60839	YES	YES
420	a	2947.10	9.61891	YES	YES

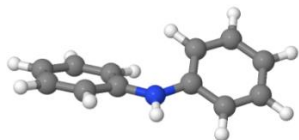
421	a	2947.15	16.28841	YES	YES
422	a	2947.36	3.78492	YES	YES
423	a	2949.94	24.84121	YES	YES
424	a	2950.51	0.35508	YES	YES
425	a	2951.44	8.37137	YES	YES
426	a	2952.69	12.19059	YES	YES
427	a	2952.94	12.61469	YES	YES
428	a	2953.99	7.20606	YES	YES
429	a	2955.45	2.65718	YES	YES
430	a	2955.77	12.38134	YES	YES
431	a	2956.33	2.77701	YES	YES
432	a	2957.65	8.91904	YES	YES
433	a	2957.86	5.99005	YES	YES
434	a	2958.07	2.82519	YES	YES
435	a	2958.69	11.55284	YES	YES
436	a	2959.12	6.07934	YES	YES
437	a	2960.07	34.96864	YES	YES
438	a	2960.50	16.85739	YES	YES
439	a	2961.36	33.87820	YES	YES
440	a	2961.47	32.38227	YES	YES
441	a	2962.20	22.58178	YES	YES
442	a	2962.42	50.72060	YES	YES
443	a	2962.78	33.58646	YES	YES
444	a	2963.21	28.12372	YES	YES
445	a	2965.13	30.81235	YES	YES
446	a	2968.58	8.77525	YES	YES
447	a	2972.02	9.88181	YES	YES
448	a	2972.50	14.16191	YES	YES
449	a	2983.74	33.46931	YES	YES
450	a	2985.34	0.54146	YES	YES
451	a	2988.00	3.88567	YES	YES
452	a	2989.43	45.22784	YES	YES
453	a	2992.89	21.84662	YES	YES
454	a	2994.57	19.33624	YES	YES
455	a	2994.98	14.57507	YES	YES
456	a	2997.36	2.12854	YES	YES
457	a	3000.84	27.22731	YES	YES
458	a	3001.23	26.01276	YES	YES
459	a	3001.87	34.85838	YES	YES
460	a	3004.08	25.97433	YES	YES
461	a	3005.10	20.81462	YES	YES
462	a	3007.29	5.52585	YES	YES
463	a	3007.37	31.89315	YES	YES
464	a	3007.69	19.04130	YES	YES
465	a	3007.80	24.26779	YES	YES
466	a	3008.80	27.28612	YES	YES
467	a	3009.66	23.12102	YES	YES
468	a	3010.57	7.62176	YES	YES
469	a	3010.66	30.51999	YES	YES
470	a	3011.55	12.85168	YES	YES
471	a	3012.09	34.88854	YES	YES
472	a	3012.11	11.91676	YES	YES
473	a	3012.33	14.64274	YES	YES
474	a	3012.67	20.68037	YES	YES
475	a	3014.48	31.75015	YES	YES
476	a	3015.81	43.73472	YES	YES
477	a	3016.45	22.38832	YES	YES
478	a	3016.62	17.37536	YES	YES

479	a	3016.92	17.21726	YES	YES
480	a	3017.26	19.30054	YES	YES
481	a	3017.37	23.87894	YES	YES
482	a	3017.48	4.99925	YES	YES
483	a	3017.51	44.80340	YES	YES
484	a	3018.19	28.88480	YES	YES
485	a	3018.25	16.05277	YES	YES
486	a	3019.15	31.26831	YES	YES
487	a	3019.33	16.90469	YES	YES
488	a	3019.60	18.74422	YES	YES
489	a	3019.83	21.50981	YES	YES
490	a	3022.24	16.86284	YES	YES
491	a	3027.76	7.03048	YES	YES
492	a	3028.30	12.72725	YES	YES
493	a	3032.32	1.59768	YES	YES
494	a	3035.15	1.21029	YES	YES
495	a	3045.25	0.88040	YES	YES
496	a	3052.77	0.26821	YES	YES
497	a	3064.70	28.66553	YES	YES
498	a	3105.38	3.64997	YES	YES
499	a	3109.11	3.41923	YES	YES
500	a	3121.17	5.02853	YES	YES
501	a	3136.35	2.41675	YES	YES

\$end

Double hybrid single point energy = -7556.212272619291 H
COSMO enery + OC correction = -7564.0224598681 H (in oDFB)

6.2.13 HNPh₂



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
Symmetry: c2

Cartesian coordinates in Ångström:

H	-2.0277022	2.2948717	2.3545109
C	-2.0994247	1.8853110	1.3466016
C	-3.2673503	2.0661356	0.6014583
H	-4.1158509	2.6023540	1.0239277
C	-3.3267870	1.5538320	-0.6978155
H	-4.2264014	1.6882635	-1.2986907
C	-2.2474930	0.8561895	-1.2332830
H	-2.3082603	0.4434822	-2.2420668
C	-1.0709239	0.6661732	-0.4831060
C	-1.0061567	1.2013719	0.8167076
H	-0.0912977	1.1062499	1.3973107
H	4.1158509	-2.6023540	1.0239277
C	3.2673503	-2.0661356	0.6014583
C	2.0994247	-1.8853110	1.3466016
H	2.0277022	-2.2948717	2.3545109
C	1.0061567	-1.2013719	0.8167076
H	0.0912977	-1.1062499	1.3973107
C	1.0709239	-0.6661732	-0.4831060
C	2.2474930	-0.8561895	-1.2332830

H	2.3082603	-0.4434822	-2.2420668
C	3.3267870	-1.5538320	-0.6978155
H	4.2264014	-1.6882635	-1.2986907
N	0.0000000	0.0000000	-1.0809386
H	-0.0000000	0.0000000	-2.0944000

SCF energy GEOOPT = -518.9110712150 H

ZPE = 505.3 kJ/mol

FREEH energy = 533.10 kJ/mol

FREEH entropy = 0.42326 kJ/mol/K

\$vibrational spectrum

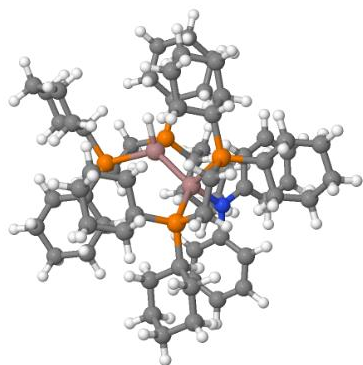
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#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b	34.70	0.96053	YES	YES
8		a	51.79	0.01339	YES	YES
9		a	105.00	0.01997	YES	YES
10		b	211.01	4.32617	YES	YES
11		a	219.71	0.39138	YES	YES
12		a	304.04	0.21503	YES	YES
13		b	327.79	3.12441	YES	YES
14		b	378.67	111.24827	YES	YES
15		b	401.47	1.80539	YES	YES
16		a	408.32	0.55764	YES	YES
17		a	484.76	2.78715	YES	YES
18		b	494.33	30.92078	YES	YES
19		b	564.85	3.59097	YES	YES
20		a	609.55	0.41690	YES	YES
21		b	614.78	1.48263	YES	YES
22		a	637.41	1.20126	YES	YES
23		b	682.06	61.48215	YES	YES
24		a	690.22	8.03696	YES	YES
25		b	733.02	80.96426	YES	YES
26		a	736.27	6.15904	YES	YES
27		b	798.51	1.72736	YES	YES
28		a	800.54	0.02004	YES	YES
29		a	816.78	0.08278	YES	YES
30		b	859.44	5.43365	YES	YES
31		a	877.07	1.11833	YES	YES
32		b	877.24	2.81236	YES	YES
33		b	932.15	0.08290	YES	YES
34		a	936.45	0.00015	YES	YES
35		b	948.79	0.80605	YES	YES
36		a	957.86	0.18082	YES	YES
37		b	988.17	6.56880	YES	YES
38		a	989.33	0.50624	YES	YES
39		b	1025.11	8.56469	YES	YES
40		a	1026.52	0.30624	YES	YES
41		b	1074.64	3.03414	YES	YES
42		a	1087.08	9.98489	YES	YES
43		b	1148.31	0.36807	YES	YES
44		a	1148.73	1.46048	YES	YES
45		b	1166.17	16.91784	YES	YES
46		a	1171.82	2.20247	YES	YES
47		a	1225.69	3.69980	YES	YES
48		b	1246.25	21.72136	YES	YES

49	b	1311.88	117.71877	YES	YES
50	a	1319.09	0.13223	YES	YES
51	a	1347.16	3.36461	YES	YES
52	b	1350.50	89.27851	YES	YES
53	b	1411.06	28.97426	YES	YES
54	a	1455.11	3.14714	YES	YES
55	b	1483.07	103.61249	YES	YES
56	a	1488.09	4.61259	YES	YES
57	b	1510.22	314.38206	YES	YES
58	a	1578.55	8.49564	YES	YES
59	b	1584.83	15.88874	YES	YES
60	b	1594.72	306.55038	YES	YES
61	a	1607.51	6.75258	YES	YES
62	b	3086.10	12.76804	YES	YES
63	a	3086.41	10.85731	YES	YES
64	b	3100.24	1.90992	YES	YES
65	a	3100.81	1.26232	YES	YES
66	b	3109.08	6.13028	YES	YES
67	a	3109.33	35.45085	YES	YES
68	b	3125.59	41.38305	YES	YES
69	a	3126.91	0.70672	YES	YES
70	b	3131.90	2.19791	YES	YES
71	a	3138.72	3.22969	YES	YES
72	a	3534.65	18.05234	YES	YES

\$end

Double hybrid single point energy = -517.948290328414 H
 COSMO energy + OC correction = -518.9204541244 H (in oDFB)

6.2.14 [H{Ga(dcpe)}₂(NPh₂)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	15.8345254	15.7008335	15.7583697
H	16.4129480	17.0787599	15.2417361
Ga	14.1966392	15.7607551	17.5814181
P	17.8143307	14.3320836	16.0266561
P	15.5826409	14.5650722	13.6604906
P	14.1680710	18.0013843	18.6431219
P	11.7891351	16.0762750	17.2400814
N	14.3980450	14.5273292	19.0583049
C	12.4588702	18.6328611	18.3527256
H	12.2142605	19.3632120	19.1370553
H	12.4658475	19.1799942	17.4028188
C	11.4085437	17.5181676	18.3306587
H	10.4257814	17.9211621	18.0533248

H	11.2993219	17.0847562	19.3332583
C	17.9148771	13.2884503	14.4966218
H	18.5661248	13.8196095	13.7904689
H	18.4204071	12.3460432	14.7486401
C	16.5491794	13.0106557	13.8525869
H	15.9532150	12.3378756	14.4824728
H	16.6748876	12.5230014	12.8765371
C	15.3120176	19.2959712	17.9892472
H	15.1050914	20.2025380	18.5833576
C	15.0739640	19.6186751	16.5050313
H	14.0553682	20.0008679	16.3507166
H	15.1721915	18.6961108	15.9137889
C	16.0868456	20.6527882	15.9945391
H	15.9152455	20.8301952	14.9237362
H	15.9130433	21.6151019	16.5026068
C	17.5293612	20.2016478	16.2423760
H	17.7295012	19.2869950	15.6580920
H	18.2332885	20.9662156	15.8873441
C	17.7600735	19.9096601	17.7267052
H	17.6473292	20.8374897	18.3101897
H	18.7860937	19.5558988	17.9007669
C	16.7674818	18.8618582	18.2370358
H	16.9373809	18.6545522	19.3027121
H	16.9425104	17.9190512	17.6931245
C	14.4072000	17.9404515	20.4726231
H	15.3637259	17.4062093	20.5859989
C	13.3244866	17.0824468	21.1482755
H	12.3578836	17.6110723	21.1000365
H	13.2095871	16.1269134	20.6198422
C	13.6877039	16.8520558	22.6193605
H	12.9137613	16.2398219	23.1037411
H	14.6260470	16.2755742	22.6655960
C	13.8503617	18.1871416	23.3538373
H	14.1575286	18.0150263	24.3940607
H	12.8734942	18.6966973	23.3979910
C	14.8650075	19.0960469	22.6520473
H	15.8689512	18.6466123	22.7233092
H	14.9204928	20.0708009	23.1553632
C	14.5287565	19.3056593	21.1658473
H	13.5808289	19.8612316	21.0729690
H	15.3096945	19.9211260	20.6991122
C	11.4597961	16.5839740	15.4888961
H	11.5049749	15.6270966	14.9397184
C	10.0682669	17.2026629	15.2720660
H	9.9940078	18.1411559	15.8447465
H	9.2828310	16.5370500	15.6508767
C	9.8290811	17.5016268	13.7862835
H	9.8094341	16.5512833	13.2270397
H	8.8385779	17.9584969	13.6592890
C	10.9195548	18.4103502	13.2147844
H	10.7496652	18.5862067	12.1441616
H	10.8678850	19.3965956	13.7047997
C	12.3081846	17.8063279	13.4384408
H	13.0910555	18.4816705	13.0665098
H	12.3941526	16.8744844	12.8541340
C	12.5579416	17.4963793	14.9183776
H	12.5804545	18.4437438	15.4757222
H	13.5486302	17.0333980	15.0507562
C	10.5308587	14.7875519	17.7240607
H	11.0379769	14.2092654	18.5117369
C	10.2506199	13.8452643	16.5423637
H	9.8474831	14.4201338	15.6952779

H	11.1924112	13.3920441	16.2055056
C	9.2399808	12.7513919	16.9062377
H	9.0241603	12.1498357	16.0116996
H	9.6918432	12.0753911	17.6453149
C	7.9542029	13.3413332	17.4879751
H	7.2641871	12.5362639	17.7737266
H	7.4354882	13.9401484	16.7207089
C	8.2709151	14.2243820	18.6964359
H	8.7299317	13.6117120	19.4893491
H	7.3522199	14.6536374	19.1187525
C	9.2317823	15.3614060	18.3232736
H	8.7354903	16.0287017	17.6026288
H	9.4492265	15.9599422	19.2170347
C	13.4199517	13.5205602	19.2475783
C	12.6942322	13.3982678	20.4470373
H	12.8865816	14.0929301	21.2630944
C	11.7475259	12.3854494	20.6036509
H	11.2024197	12.3006288	21.5433081
C	11.5013447	11.4788525	19.5685274
H	10.7748183	10.6786641	19.7013951
C	12.1968924	11.6083150	18.3645157
H	12.0122828	10.9089103	17.5494598
C	13.1407385	12.6224803	18.2042015
H	13.6944148	12.7121815	17.2694099
C	15.5066135	14.6056138	19.9014059
C	16.5232143	15.5488639	19.6305683
H	16.4384949	16.1868018	18.7500101
C	17.6451089	15.6783285	20.4474988
H	18.3928082	16.4346966	20.2089434
C	17.8146298	14.8484983	21.5564196
H	18.6866329	14.9476376	22.1998056
C	16.8384759	13.8811878	21.8168339
H	16.9555533	13.2081241	22.6660537
C	15.7069869	13.7553268	21.0136279
H	14.9757270	12.9860255	21.2479094
C	16.5054395	15.6200357	12.4601000
H	17.3197225	16.0248229	13.0877199
C	15.6369205	16.8173836	12.0385245
H	15.2185630	17.3096475	12.9296182
H	14.7865108	16.4613995	11.4353151
C	16.4640011	17.8146251	11.2183117
H	15.8229057	18.6431025	10.8868495
H	17.2380489	18.2543362	11.8687865
C	17.1292735	17.1349607	10.0170142
H	16.3515863	16.7928547	9.3143147
H	17.7469831	17.8576979	9.4674852
C	17.9797392	15.9370105	10.4520815
H	18.4235790	15.4407093	9.5786383
H	18.8196659	16.2895746	11.0739994
C	17.1529782	14.9216889	11.2546477
H	17.7947141	14.0905075	11.5811387
H	16.3809087	14.4862115	10.6049325
C	19.3889776	15.2888991	16.0814460
H	20.1993191	14.5396116	16.0621752
C	19.4665773	16.0780987	17.3983153
H	18.6040927	16.7636852	17.4444086
H	19.3776703	15.4037115	18.2599832
C	20.7637680	16.8898134	17.4848200
H	20.7712813	17.4702764	18.4182706
H	21.6191348	16.1975948	17.5429098
C	20.9323910	17.8113070	16.2738162
H	20.1376532	18.5757196	16.2819883

H	21.8865210	18.3512251	16.3358340
C	20.8537150	17.0223018	14.9639288
H	21.7081339	16.3295826	14.8983255
H	20.9316659	17.6979129	14.1010742
C	19.5468401	16.2241546	14.8705048
H	19.5289624	15.6549666	13.9293747
H	18.6919315	16.9197662	14.8441524
C	13.9159245	14.1122878	13.0259928
H	13.3859882	15.0784253	12.9598977
C	13.1775256	13.2358134	14.0548529
H	13.7336281	12.2971133	14.2075770
H	13.1470932	13.7464952	15.0315576
C	11.7620208	12.8967665	13.5710548
H	11.2717710	12.2362313	14.2986805
H	11.1621055	13.8219769	13.5322914
C	11.7769328	12.2469580	12.1853269
H	12.2844893	11.2701577	12.2453885
H	10.7501098	12.0439343	11.8531962
C	12.4991771	13.1351336	11.1711824
H	11.9368104	14.0742623	11.0374036
H	12.5352410	12.6502615	10.1865106
C	13.9248735	13.4662115	11.6294779
H	14.4017221	14.1372132	10.9045993
H	14.5246885	12.5424568	11.6545566
C	17.7734918	13.1720857	17.4510861
H	17.5313262	13.8142768	18.3139436
C	19.0993730	12.4512275	17.7326199
H	19.3828330	11.8302176	16.8661446
H	19.9118521	13.1735786	17.8896289
C	18.9474969	11.5598005	18.9744557
H	19.8936184	11.0367424	19.1683241
H	18.7532097	12.2041411	19.8475125
C	17.8005993	10.5568307	18.8131144
H	17.6940238	9.9551483	19.7257535
H	18.0440285	9.8509217	18.0014259
C	16.4811844	11.2672373	18.4956879
H	16.1806647	11.8849270	19.3543119
H	15.6742179	10.5401458	18.3300043
C	16.6220052	12.1699315	17.2663261
H	15.6836637	12.7124108	17.0786705
H	16.8223452	11.5400041	16.3835508

SCF energy GEOOPT = -7775.157050149 H

ZPE = 4103. kJ/mol

FREEH energy = 4307.76 kJ/mol

FREEH entropy = 1.69830 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	16.54	0.05790	YES	YES
	8	a	20.21	0.01515	YES	YES
	9	a	23.70	0.04546	YES	YES
	10	a	28.01	0.00140	YES	YES
	11	a	30.05	0.09282	YES	YES
	12	a	33.82	0.04400	YES	YES

13	a	36.43	0.03616	YES	YES
14	a	38.30	0.16492	YES	YES
15	a	42.32	0.01818	YES	YES
16	a	42.73	0.03859	YES	YES
17	a	44.57	0.15007	YES	YES
18	a	46.31	0.22601	YES	YES
19	a	50.64	0.08237	YES	YES
20	a	52.39	0.04584	YES	YES
21	a	54.13	0.09599	YES	YES
22	a	56.17	0.03978	YES	YES
23	a	56.60	0.05212	YES	YES
24	a	58.45	0.11317	YES	YES
25	a	60.78	0.03550	YES	YES
26	a	63.32	0.21647	YES	YES
27	a	68.15	0.10036	YES	YES
28	a	69.32	0.08881	YES	YES
29	a	72.66	0.08128	YES	YES
30	a	74.84	0.20032	YES	YES
31	a	76.81	0.10243	YES	YES
32	a	79.28	0.13917	YES	YES
33	a	80.40	0.08558	YES	YES
34	a	84.35	0.21168	YES	YES
35	a	86.62	0.24487	YES	YES
36	a	90.56	0.05214	YES	YES
37	a	94.81	0.04953	YES	YES
38	a	99.49	1.04265	YES	YES
39	a	105.77	0.14915	YES	YES
40	a	113.17	0.40540	YES	YES
41	a	117.42	0.71260	YES	YES
42	a	123.02	2.58232	YES	YES
43	a	124.35	0.12862	YES	YES
44	a	131.40	1.55619	YES	YES
45	a	136.06	2.43822	YES	YES
46	a	139.04	0.10195	YES	YES
47	a	141.54	4.92556	YES	YES
48	a	147.40	1.64473	YES	YES
49	a	151.59	1.23959	YES	YES
50	a	153.60	1.80427	YES	YES
51	a	154.24	3.11864	YES	YES
52	a	158.85	0.23118	YES	YES
53	a	168.13	1.70193	YES	YES
54	a	168.64	2.16593	YES	YES
55	a	186.03	4.28931	YES	YES
56	a	187.56	5.54166	YES	YES
57	a	191.92	1.89312	YES	YES
58	a	206.70	2.30570	YES	YES
59	a	209.94	0.47234	YES	YES
60	a	211.18	1.18237	YES	YES
61	a	216.97	0.44644	YES	YES
62	a	219.39	0.32143	YES	YES
63	a	220.76	0.42007	YES	YES
64	a	221.99	0.78989	YES	YES
65	a	226.50	2.14264	YES	YES
66	a	229.63	0.25479	YES	YES
67	a	233.80	1.33842	YES	YES
68	a	235.18	0.20633	YES	YES
69	a	237.34	0.15662	YES	YES
70	a	239.35	0.83400	YES	YES
71	a	241.09	1.91189	YES	YES
72	a	245.68	0.54849	YES	YES
73	a	246.56	0.94903	YES	YES
74	a	247.70	1.67635	YES	YES

75	a	254.37	0.48157	YES	YES
76	a	264.39	0.73231	YES	YES
77	a	265.43	2.06273	YES	YES
78	a	273.31	0.29244	YES	YES
79	a	277.68	1.13903	YES	YES
80	a	285.32	0.39141	YES	YES
81	a	291.60	2.90717	YES	YES
82	a	309.90	0.15892	YES	YES
83	a	310.26	0.46942	YES	YES
84	a	311.34	0.10359	YES	YES
85	a	312.79	0.15210	YES	YES
86	a	321.65	6.50432	YES	YES
87	a	329.67	1.02892	YES	YES
88	a	330.54	0.07750	YES	YES
89	a	334.26	0.21032	YES	YES
90	a	334.96	0.06499	YES	YES
91	a	339.09	0.33129	YES	YES
92	a	340.67	1.22070	YES	YES
93	a	363.86	0.47549	YES	YES
94	a	377.40	0.74933	YES	YES
95	a	380.29	1.00266	YES	YES
96	a	387.52	1.36200	YES	YES
97	a	389.67	0.37018	YES	YES
98	a	394.01	8.44521	YES	YES
99	a	399.18	0.63660	YES	YES
100	a	411.34	0.48319	YES	YES
101	a	412.28	0.98786	YES	YES
102	a	416.85	0.71902	YES	YES
103	a	420.03	1.10523	YES	YES
104	a	425.50	0.15888	YES	YES
105	a	426.42	2.59356	YES	YES
106	a	427.44	0.15256	YES	YES
107	a	429.26	0.51917	YES	YES
108	a	430.26	0.27194	YES	YES
109	a	430.48	0.12554	YES	YES
110	a	432.25	0.18105	YES	YES
111	a	432.92	0.13254	YES	YES
112	a	434.11	0.53872	YES	YES
113	a	437.40	0.36346	YES	YES
114	a	441.26	2.46175	YES	YES
115	a	445.26	1.57592	YES	YES
116	a	449.23	2.67741	YES	YES
117	a	451.91	4.04898	YES	YES
118	a	463.81	7.69032	YES	YES
119	a	464.61	0.90238	YES	YES
120	a	492.28	1.07048	YES	YES
121	a	494.14	2.51020	YES	YES
122	a	497.53	1.10048	YES	YES
123	a	497.95	3.83030	YES	YES
124	a	499.47	5.04015	YES	YES
125	a	501.04	10.83095	YES	YES
126	a	503.86	0.87137	YES	YES
127	a	510.39	11.00929	YES	YES
128	a	512.01	12.18936	YES	YES
129	a	514.78	8.32454	YES	YES
130	a	567.63	57.22360	YES	YES
131	a	579.76	0.87807	YES	YES
132	a	614.85	1.49377	YES	YES
133	a	616.51	8.70519	YES	YES
134	a	618.84	125.62923	YES	YES
135	a	638.13	13.38952	YES	YES
136	a	638.33	9.00420	YES	YES

137	a	646.08	12.48219	YES	YES
138	a	649.03	12.53964	YES	YES
139	a	664.74	1.03881	YES	YES
140	a	689.91	36.92177	YES	YES
141	a	700.39	5.39459	YES	YES
142	a	703.01	27.72527	YES	YES
143	a	714.01	7.86276	YES	YES
144	a	724.98	7.08516	YES	YES
145	a	729.96	2.77073	YES	YES
146	a	731.38	7.51011	YES	YES
147	a	731.84	4.99596	YES	YES
148	a	734.69	3.58692	YES	YES
149	a	742.33	29.81982	YES	YES
150	a	743.41	12.37670	YES	YES
151	a	755.53	18.31608	YES	YES
152	a	771.82	0.60138	YES	YES
153	a	772.15	0.18835	YES	YES
154	a	772.84	0.29454	YES	YES
155	a	774.83	0.24220	YES	YES
156	a	775.44	0.07817	YES	YES
157	a	776.28	0.55565	YES	YES
158	a	776.67	0.29962	YES	YES
159	a	781.15	0.25458	YES	YES
160	a	785.41	23.49967	YES	YES
161	a	786.02	10.60684	YES	YES
162	a	797.09	0.42585	YES	YES
163	a	806.79	1.73526	YES	YES
164	a	810.22	2.42059	YES	YES
165	a	811.36	2.06726	YES	YES
166	a	812.15	0.88953	YES	YES
167	a	812.76	2.51553	YES	YES
168	a	813.50	1.88993	YES	YES
169	a	813.63	2.25494	YES	YES
170	a	817.83	1.29924	YES	YES
171	a	823.43	3.69561	YES	YES
172	a	832.54	3.73161	YES	YES
173	a	834.41	1.94774	YES	YES
174	a	836.81	5.32290	YES	YES
175	a	838.41	2.50297	YES	YES
176	a	838.68	1.34390	YES	YES
177	a	839.46	5.43504	YES	YES
178	a	840.37	5.73916	YES	YES
179	a	840.95	1.65252	YES	YES
180	a	849.13	3.65923	YES	YES
181	a	853.43	11.36124	YES	YES
182	a	858.88	6.83855	YES	YES
183	a	865.13	31.41418	YES	YES
184	a	873.88	5.66361	YES	YES
185	a	874.86	2.86405	YES	YES
186	a	875.69	3.02179	YES	YES
187	a	876.88	3.56247	YES	YES
188	a	877.38	1.37457	YES	YES
189	a	878.61	2.66484	YES	YES
190	a	879.56	1.88663	YES	YES
191	a	879.92	4.84511	YES	YES
192	a	880.34	1.11112	YES	YES
193	a	880.91	1.24879	YES	YES
194	a	882.01	2.35475	YES	YES
195	a	882.54	3.69035	YES	YES
196	a	882.91	3.74534	YES	YES
197	a	883.51	6.33401	YES	YES
198	a	884.06	9.81285	YES	YES

199	a	886.59	1.19740	YES	YES
200	a	889.00	8.78367	YES	YES
201	a	904.17	2.19195	YES	YES
202	a	905.28	1.17357	YES	YES
203	a	905.61	2.34507	YES	YES
204	a	906.02	1.77881	YES	YES
205	a	907.25	2.38570	YES	YES
206	a	908.80	6.07999	YES	YES
207	a	909.41	1.92581	YES	YES
208	a	911.84	9.43840	YES	YES
209	a	912.50	1.58492	YES	YES
210	a	943.30	0.56546	YES	YES
211	a	957.28	0.31625	YES	YES
212	a	970.56	0.17517	YES	YES
213	a	980.11	0.17930	YES	YES
214	a	984.61	3.54380	YES	YES
215	a	985.70	6.42650	YES	YES
216	a	985.82	15.57351	YES	YES
217	a	987.80	7.35869	YES	YES
218	a	989.83	6.40578	YES	YES
219	a	990.02	12.99679	YES	YES
220	a	990.68	1.94279	YES	YES
221	a	991.94	9.31683	YES	YES
222	a	992.85	20.77695	YES	YES
223	a	993.20	7.12713	YES	YES
224	a	997.00	0.45783	YES	YES
225	a	1003.54	3.82396	YES	YES
226	a	1013.92	1.51974	YES	YES
227	a	1014.56	0.49628	YES	YES
228	a	1015.65	0.26901	YES	YES
229	a	1017.15	0.25142	YES	YES
230	a	1017.95	0.62188	YES	YES
231	a	1020.37	0.49181	YES	YES
232	a	1021.29	1.24287	YES	YES
233	a	1022.38	0.03065	YES	YES
234	a	1025.55	3.22008	YES	YES
235	a	1031.55	1.07334	YES	YES
236	a	1032.02	3.75871	YES	YES
237	a	1033.17	0.65472	YES	YES
238	a	1036.25	1.00807	YES	YES
239	a	1036.94	2.66989	YES	YES
240	a	1039.20	3.90206	YES	YES
241	a	1040.26	1.97132	YES	YES
242	a	1040.55	0.92423	YES	YES
243	a	1041.03	2.68009	YES	YES
244	a	1057.93	0.08951	YES	YES
245	a	1058.91	0.14320	YES	YES
246	a	1060.56	2.72770	YES	YES
247	a	1061.94	1.88031	YES	YES
248	a	1062.31	0.99530	YES	YES
249	a	1065.98	1.58039	YES	YES
250	a	1067.06	1.06840	YES	YES
251	a	1068.38	0.87421	YES	YES
252	a	1070.41	0.63163	YES	YES
253	a	1071.01	0.11061	YES	YES
254	a	1071.75	0.06106	YES	YES
255	a	1073.20	0.63757	YES	YES
256	a	1073.63	0.06002	YES	YES
257	a	1073.86	0.03613	YES	YES
258	a	1073.88	0.72571	YES	YES
259	a	1074.59	0.04226	YES	YES
260	a	1075.42	2.27087	YES	YES

261	a	1079.10	6.22385	YES	YES
262	a	1079.46	0.75190	YES	YES
263	a	1089.18	9.38482	YES	YES
264	a	1092.66	3.04448	YES	YES
265	a	1097.90	1.12980	YES	YES
266	a	1099.37	6.82218	YES	YES
267	a	1100.38	2.61568	YES	YES
268	a	1107.12	2.84949	YES	YES
269	a	1108.93	8.15849	YES	YES
270	a	1109.19	3.32547	YES	YES
271	a	1114.35	7.01507	YES	YES
272	a	1126.90	3.14806	YES	YES
273	a	1133.80	1.19387	YES	YES
274	a	1150.11	1.19260	YES	YES
275	a	1153.01	0.48724	YES	YES
276	a	1159.92	4.31291	YES	YES
277	a	1160.43	2.43911	YES	YES
278	a	1162.53	10.56694	YES	YES
279	a	1162.97	6.51686	YES	YES
280	a	1164.19	9.76598	YES	YES
281	a	1167.69	3.07932	YES	YES
282	a	1170.31	3.37079	YES	YES
283	a	1171.18	7.25787	YES	YES
284	a	1171.66	10.46504	YES	YES
285	a	1176.58	14.24670	YES	YES
286	a	1178.48	4.74227	YES	YES
287	a	1184.34	9.17017	YES	YES
288	a	1191.37	4.32917	YES	YES
289	a	1192.13	2.48848	YES	YES
290	a	1195.57	3.29714	YES	YES
291	a	1201.94	3.32066	YES	YES
292	a	1202.79	2.51440	YES	YES
293	a	1207.58	2.11912	YES	YES
294	a	1209.84	37.41837	YES	YES
295	a	1239.34	0.95555	YES	YES
296	a	1243.99	0.55303	YES	YES
297	a	1244.51	1.38582	YES	YES
298	a	1246.30	0.08666	YES	YES
299	a	1247.64	1.04935	YES	YES
300	a	1248.18	1.87396	YES	YES
301	a	1248.90	0.44627	YES	YES
302	a	1250.60	0.76833	YES	YES
303	a	1250.94	0.73658	YES	YES
304	a	1253.24	3.75362	YES	YES
305	a	1254.17	1.75052	YES	YES
306	a	1255.07	0.11625	YES	YES
307	a	1255.83	4.29209	YES	YES
308	a	1256.41	1.95883	YES	YES
309	a	1257.59	0.13769	YES	YES
310	a	1258.37	5.27064	YES	YES
311	a	1258.64	3.31423	YES	YES
312	a	1259.68	1.80209	YES	YES
313	a	1259.86	5.96601	YES	YES
314	a	1260.59	2.43288	YES	YES
315	a	1262.12	5.08380	YES	YES
316	a	1264.38	1.84173	YES	YES
317	a	1265.00	0.19545	YES	YES
318	a	1266.20	0.56598	YES	YES
319	a	1266.64	4.79522	YES	YES
320	a	1268.54	0.46349	YES	YES
321	a	1269.37	1.20968	YES	YES
322	a	1274.58	1.85309	YES	YES

323	a	1281.33	5.91174	YES	YES
324	a	1281.75	56.44966	YES	YES
325	a	1283.35	3.42999	YES	YES
326	a	1285.64	0.91997	YES	YES
327	a	1286.26	3.86735	YES	YES
328	a	1287.30	6.22202	YES	YES
329	a	1289.84	3.69848	YES	YES
330	a	1293.80	9.85486	YES	YES
331	a	1295.22	4.60937	YES	YES
332	a	1302.69	113.84761	YES	YES
333	a	1308.19	6.46309	YES	YES
334	a	1309.62	7.55478	YES	YES
335	a	1309.91	3.63870	YES	YES
336	a	1310.39	1.51507	YES	YES
337	a	1310.81	6.53749	YES	YES
338	a	1312.40	3.68327	YES	YES
339	a	1314.08	0.82730	YES	YES
340	a	1315.10	5.41611	YES	YES
341	a	1318.11	2.30606	YES	YES
342	a	1322.26	3.54317	YES	YES
343	a	1322.94	1.35047	YES	YES
344	a	1322.99	1.68009	YES	YES
345	a	1323.34	0.45595	YES	YES
346	a	1323.51	0.73426	YES	YES
347	a	1323.62	1.49030	YES	YES
348	a	1324.15	0.40008	YES	YES
349	a	1324.58	2.23100	YES	YES
350	a	1324.93	0.31194	YES	YES
351	a	1325.81	0.44718	YES	YES
352	a	1326.38	2.94860	YES	YES
353	a	1326.43	2.40137	YES	YES
354	a	1327.36	4.05385	YES	YES
355	a	1328.03	4.93612	YES	YES
356	a	1331.17	0.91601	YES	YES
357	a	1331.98	1.17267	YES	YES
358	a	1334.21	5.81572	YES	YES
359	a	1335.93	0.47450	YES	YES
360	a	1336.46	0.42702	YES	YES
361	a	1337.04	0.35963	YES	YES
362	a	1337.65	0.15104	YES	YES
363	a	1337.77	0.07692	YES	YES
364	a	1337.91	0.66348	YES	YES
365	a	1338.62	0.89621	YES	YES
366	a	1339.04	0.80442	YES	YES
367	a	1342.01	5.99690	YES	YES
368	a	1344.75	4.00328	YES	YES
369	a	1345.12	2.56132	YES	YES
370	a	1345.87	1.95035	YES	YES
371	a	1346.47	1.11228	YES	YES
372	a	1348.06	2.61869	YES	YES
373	a	1349.36	0.60113	YES	YES
374	a	1349.94	0.27561	YES	YES
375	a	1349.98	0.61111	YES	YES
376	a	1404.34	5.23255	YES	YES
377	a	1404.40	8.65664	YES	YES
378	a	1409.81	8.37946	YES	YES
379	a	1409.95	6.35378	YES	YES
380	a	1420.50	2.00391	YES	YES
381	a	1423.78	10.67542	YES	YES
382	a	1425.10	12.96768	YES	YES
383	a	1426.28	4.00902	YES	YES
384	a	1427.70	2.36717	YES	YES

385	a	1431.00	12.97254	YES	YES
386	a	1432.94	1.31013	YES	YES
387	a	1435.24	2.59409	YES	YES
388	a	1435.38	0.76094	YES	YES
389	a	1435.81	6.55177	YES	YES
390	a	1436.10	4.44686	YES	YES
391	a	1436.71	0.47175	YES	YES
392	a	1436.92	2.87415	YES	YES
393	a	1437.31	4.31503	YES	YES
394	a	1437.64	5.37653	YES	YES
395	a	1438.18	2.16975	YES	YES
396	a	1438.31	7.21541	YES	YES
397	a	1438.68	8.85155	YES	YES
398	a	1438.93	1.14098	YES	YES
399	a	1439.20	1.88027	YES	YES
400	a	1439.38	3.22454	YES	YES
401	a	1439.89	5.17657	YES	YES
402	a	1440.04	9.45738	YES	YES
403	a	1440.05	1.33184	YES	YES
404	a	1440.48	12.05818	YES	YES
405	a	1441.86	1.80982	YES	YES
406	a	1442.73	9.33267	YES	YES
407	a	1443.64	12.76936	YES	YES
408	a	1444.27	7.55801	YES	YES
409	a	1444.38	2.13652	YES	YES
410	a	1445.67	15.37502	YES	YES
411	a	1445.88	4.34070	YES	YES
412	a	1446.34	26.09205	YES	YES
413	a	1447.86	5.72846	YES	YES
414	a	1451.91	0.42222	YES	YES
415	a	1453.08	0.06975	YES	YES
416	a	1453.61	2.42404	YES	YES
417	a	1454.10	3.36847	YES	YES
418	a	1455.66	6.60104	YES	YES
419	a	1456.35	0.69311	YES	YES
420	a	1456.78	2.36145	YES	YES
421	a	1457.16	2.15632	YES	YES
422	a	1478.82	185.98085	YES	YES
423	a	1481.43	31.79222	YES	YES
424	a	1559.15	4.26580	YES	YES
425	a	1570.52	4.73107	YES	YES
426	a	1584.86	79.86673	YES	YES
427	a	1597.27	43.45019	YES	YES
428	a	1850.75	141.75479	YES	YES
429	a	2929.69	4.84606	YES	YES
430	a	2934.03	13.77454	YES	YES
431	a	2935.61	4.32757	YES	YES
432	a	2936.62	1.90965	YES	YES
433	a	2937.04	55.22016	YES	YES
434	a	2938.01	7.29435	YES	YES
435	a	2939.10	41.92789	YES	YES
436	a	2939.23	5.66887	YES	YES
437	a	2940.01	18.19973	YES	YES
438	a	2940.12	16.40863	YES	YES
439	a	2940.54	1.81536	YES	YES
440	a	2942.43	3.85946	YES	YES
441	a	2942.98	8.58667	YES	YES
442	a	2944.04	13.18943	YES	YES
443	a	2944.16	12.47078	YES	YES
444	a	2944.85	15.86369	YES	YES
445	a	2945.39	15.57322	YES	YES
446	a	2945.57	16.77727	YES	YES

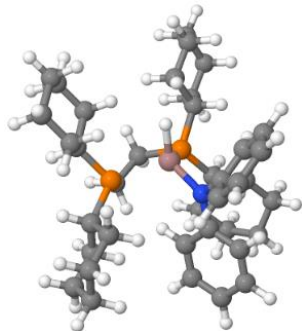
447	a	2945.98	3.03449	YES	YES
448	a	2946.60	10.85436	YES	YES
449	a	2947.05	4.29063	YES	YES
450	a	2947.35	38.27637	YES	YES
451	a	2948.21	5.73999	YES	YES
452	a	2950.38	17.35534	YES	YES
453	a	2952.86	11.48470	YES	YES
454	a	2953.97	11.32050	YES	YES
455	a	2955.96	2.62553	YES	YES
456	a	2956.85	12.10648	YES	YES
457	a	2956.97	13.09841	YES	YES
458	a	2957.47	14.12160	YES	YES
459	a	2957.50	21.76256	YES	YES
460	a	2958.24	12.89851	YES	YES
461	a	2958.69	30.88269	YES	YES
462	a	2958.88	3.99888	YES	YES
463	a	2960.01	32.87376	YES	YES
464	a	2960.79	31.49216	YES	YES
465	a	2961.13	8.02140	YES	YES
466	a	2962.47	31.21799	YES	YES
467	a	2962.61	38.44517	YES	YES
468	a	2964.45	12.93454	YES	YES
469	a	2966.00	26.73634	YES	YES
470	a	2966.21	22.92360	YES	YES
471	a	2969.47	17.69395	YES	YES
472	a	2969.92	3.85840	YES	YES
473	a	2972.11	17.14425	YES	YES
474	a	2974.19	7.72154	YES	YES
475	a	2976.24	13.94704	YES	YES
476	a	2982.08	37.09502	YES	YES
477	a	2987.15	3.27728	YES	YES
478	a	2987.90	5.62591	YES	YES
479	a	2988.16	1.26924	YES	YES
480	a	2991.84	8.89294	YES	YES
481	a	2993.95	2.16439	YES	YES
482	a	2994.01	4.02503	YES	YES
483	a	2994.25	24.64261	YES	YES
484	a	2994.53	54.55326	YES	YES
485	a	3000.64	18.66530	YES	YES
486	a	3004.88	28.45634	YES	YES
487	a	3005.12	9.91812	YES	YES
488	a	3005.19	32.50134	YES	YES
489	a	3006.76	7.57041	YES	YES
490	a	3008.20	25.22859	YES	YES
491	a	3009.16	19.11384	YES	YES
492	a	3009.35	23.71512	YES	YES
493	a	3010.06	31.73251	YES	YES
494	a	3010.39	26.10916	YES	YES
495	a	3010.99	10.41388	YES	YES
496	a	3011.94	7.86630	YES	YES
497	a	3011.96	23.17570	YES	YES
498	a	3012.90	22.84511	YES	YES
499	a	3013.16	21.39481	YES	YES
500	a	3013.52	23.43276	YES	YES
501	a	3014.39	29.86588	YES	YES
502	a	3014.62	29.01656	YES	YES
503	a	3015.56	24.13635	YES	YES
504	a	3015.74	39.42287	YES	YES
505	a	3016.15	25.51639	YES	YES
506	a	3016.70	28.61573	YES	YES
507	a	3016.76	9.93661	YES	YES
508	a	3016.93	23.35626	YES	YES

509	a	3017.35	32.94431	YES	YES
510	a	3017.55	18.92042	YES	YES
511	a	3017.74	1.17341	YES	YES
512	a	3017.95	7.51506	YES	YES
513	a	3017.97	28.01447	YES	YES
514	a	3019.00	36.48330	YES	YES
515	a	3019.23	22.59793	YES	YES
516	a	3021.26	16.52274	YES	YES
517	a	3021.85	4.44321	YES	YES
518	a	3025.86	23.52711	YES	YES
519	a	3028.38	20.89357	YES	YES
520	a	3028.67	27.53393	YES	YES
521	a	3032.78	1.06262	YES	YES
522	a	3035.71	0.42635	YES	YES
523	a	3045.43	0.73404	YES	YES
524	a	3049.07	1.49088	YES	YES
525	a	3080.64	25.11114	YES	YES
526	a	3095.56	9.49720	YES	YES
527	a	3106.73	4.62486	YES	YES
528	a	3109.54	0.97156	YES	YES
529	a	3112.00	5.13029	YES	YES
530	a	3114.78	6.89120	YES	YES
531	a	3124.80	4.62221	YES	YES
532	a	3133.24	1.27232	YES	YES
533	a	3136.01	2.86186	YES	YES
534	a	3140.54	1.17225	YES	YES

§end

Double hybrid single point energy = -7767.058128041005 H
 COSMO energy + OC correction = -7775.3012445274 H (in oDFB)

6.2.15 [H{Ga(dcpe)}(NPh₂)]⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.0386955	0.3040672	-0.2318020
P	-3.9287312	-0.7225160	-1.3542358
P	-2.2989890	2.2031226	-1.7299851
C	-3.8757635	-2.5011513	-1.9007240
H	-4.8730374	-2.8822165	-1.6178971
C	-2.8155247	-3.2774499	-1.0931042
H	-1.8212109	-2.8649219	-1.3149448
H	-2.9806459	-3.1405650	-0.0149302
C	-2.8357887	-4.7658206	-1.4559400
H	-2.0486447	-5.2873877	-0.8943187
H	-3.7947870	-5.2106675	-1.1413936
C	-2.6477896	-4.9665880	-2.9625143
H	-2.6800133	-6.0357221	-3.2124330

H	-1.6498424	-4.6014164	-3.2554669
C	-3.7189875	-4.2091236	-3.7527256
H	-4.7117489	-4.6298061	-3.5222767
H	-3.5680238	-4.3364376	-4.8337327
C	-3.7165785	-2.7110636	-3.4158713
H	-4.5252473	-2.2041696	-3.9612920
H	-2.7675156	-2.2753174	-3.7593630
C	-5.4397886	-0.6360091	-0.2894434
H	-6.2555639	-1.0550048	-0.9061847
C	-5.2366071	-1.5329154	0.9482937
H	-5.0324453	-2.5685305	0.6447015
H	-4.3502941	-1.1800263	1.5010791
C	-6.4601009	-1.4952258	1.8721632
H	-7.3225666	-1.9434636	1.3520040
H	-6.2663384	-2.1202387	2.7545838
C	-6.8021963	-0.0626461	2.2876579
H	-7.6946858	-0.0530779	2.9277769
H	-5.9766723	0.3499134	2.8910536
C	-7.0237583	0.8198193	1.0572064
H	-7.2340535	1.8568679	1.3542093
H	-7.9101572	0.4652368	0.5060164
C	-5.8082889	0.7972831	0.1211160
H	-6.0241500	1.4057928	-0.7678604
H	-4.9474339	1.2549134	0.6335003
C	-4.1938516	0.3649057	-2.8312607
H	-3.5230111	-0.0193470	-3.6117228
H	-5.2198315	0.2368053	-3.2045796
C	-3.9049849	1.8591109	-2.5837666
H	-4.6807922	2.3012139	-1.9465791
H	-3.9305221	2.4029260	-3.5375787
C	-0.9869850	2.5502940	-2.9844101
H	-1.1325723	3.6095698	-3.2576356
C	0.3928371	2.4035271	-2.3132192
H	0.5091810	1.3742237	-1.9470926
H	0.4624836	3.0652133	-1.4361174
C	1.5200497	2.7133350	-3.3036583
H	1.4761405	3.7761774	-3.5946836
H	2.4883626	2.5603737	-2.8079063
C	1.4073746	1.8321312	-4.5505076
H	1.5346775	0.7762744	-4.2623144
H	2.2142829	2.0685618	-5.2575037
C	0.0457164	2.0154351	-5.2284538
H	-0.0389664	1.3630992	-6.1088480
H	-0.0466089	3.0517338	-5.5940809
C	-1.1094176	1.7117428	-4.2642978
H	-1.0768803	0.6458806	-4.0056401
H	-2.0719034	1.9084401	-4.7595326
C	-2.5288193	3.8134065	-0.8451637
H	-1.5013188	4.0760891	-0.5353322
C	-3.3921590	3.6841891	0.4194924
H	-3.0007866	2.8938539	1.0738523
H	-4.4132502	3.3859892	0.1302399
C	-3.4598093	5.0197270	1.1715085
H	-4.1004798	4.9096430	2.0573943
H	-2.4531218	5.2729056	1.5424453
C	-3.9728515	6.1466797	0.2705924
H	-5.0218195	5.9447247	-0.0042393
H	-3.9718605	7.1005773	0.8152918
C	-3.1307405	6.2637486	-1.0031780
H	-2.1069748	6.5773065	-0.7413048
H	-3.5365605	7.0404037	-1.6660641
C	-3.0665040	4.9292881	-1.7598542

H	-4.0796740	4.6602206	-2.1005705
H	-2.4461173	5.0403605	-2.6598188
N	-0.3448486	-0.5413770	-0.3385837
H	2.1564171	-0.7968461	4.3522880
C	1.6537959	-0.7441819	3.3874702
C	1.3206804	0.4940777	2.8361823
H	1.5672207	1.4132596	3.3670533
C	0.6838223	0.5599606	1.5947014
H	0.4429499	1.5251960	1.1465390
C	0.3569023	-0.6126113	0.9015738
C	0.6893686	-1.8554168	1.4625941
H	0.4322325	-2.7664035	0.9221902
C	1.3400042	-1.9178861	2.6936190
H	1.5938317	-2.8879088	3.1205616
H	-2.4625404	0.6628826	1.2253118
H	2.2506615	-1.2104200	-0.6743726
C	1.6263655	-1.3684482	-1.5513969
C	0.2480018	-1.0593251	-1.4870606
C	-0.5107297	-1.2568690	-2.6561122
H	-1.5723013	-1.0112680	-2.6342938
C	0.0564493	-1.7585350	-3.8255570
H	-0.5680385	-1.9019800	-4.7085291
C	1.4148470	-2.0730106	-3.8718030
H	1.8634294	-2.4676715	-4.7814942
C	2.1888935	-1.8653702	-2.7240456
H	3.2552304	-2.0905455	-2.7421403

SCF energy GEOOPT = -4147.035923940 H

ZPE = 2297. kJ/mol

FREEH energy = 2413.54 kJ/mol

FREEH entropy = 1.10070 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	8.47	0.03686	YES	YES
	8	a	16.66	0.01783	YES	YES
	9	a	27.07	0.52404	YES	YES
	10	a	28.33	0.03075	YES	YES
	11	a	33.97	0.04953	YES	YES
	12	a	41.17	0.02811	YES	YES
	13	a	43.41	0.05671	YES	YES
	14	a	46.07	0.03959	YES	YES
	15	a	47.72	0.18347	YES	YES
	16	a	49.23	0.08881	YES	YES
	17	a	53.19	0.07482	YES	YES
	18	a	65.69	0.48457	YES	YES
	19	a	68.63	0.08934	YES	YES
	20	a	77.96	0.54508	YES	YES
	21	a	79.30	0.75044	YES	YES
	22	a	84.45	0.12926	YES	YES
	23	a	91.90	0.12313	YES	YES
	24	a	99.36	0.24876	YES	YES
	25	a	120.96	2.70227	YES	YES
	26	a	124.99	1.66750	YES	YES
	27	a	137.60	1.05970	YES	YES

28	a	141.32	2.21633	YES	YES
29	a	143.29	0.37779	YES	YES
30	a	160.88	0.06179	YES	YES
31	a	166.97	1.02356	YES	YES
32	a	174.75	3.62899	YES	YES
33	a	181.62	1.63936	YES	YES
34	a	200.55	0.91465	YES	YES
35	a	211.07	0.00670	YES	YES
36	a	214.25	0.08731	YES	YES
37	a	223.04	0.27073	YES	YES
38	a	227.92	0.04379	YES	YES
39	a	232.88	0.07506	YES	YES
40	a	235.45	1.14007	YES	YES
41	a	239.23	0.40246	YES	YES
42	a	242.22	0.24653	YES	YES
43	a	247.68	3.85012	YES	YES
44	a	278.62	8.77044	YES	YES
45	a	288.80	1.02179	YES	YES
46	a	294.21	1.11905	YES	YES
47	a	301.48	1.75720	YES	YES
48	a	308.37	0.24093	YES	YES
49	a	324.95	5.80699	YES	YES
50	a	329.67	5.50246	YES	YES
51	a	333.42	2.91632	YES	YES
52	a	343.18	0.94415	YES	YES
53	a	359.41	0.76184	YES	YES
54	a	378.44	6.85410	YES	YES
55	a	386.67	0.45525	YES	YES
56	a	405.55	6.33301	YES	YES
57	a	405.91	0.83007	YES	YES
58	a	410.75	0.76391	YES	YES
59	a	414.24	2.30792	YES	YES
60	a	422.63	2.26787	YES	YES
61	a	428.34	3.85987	YES	YES
62	a	428.67	1.51777	YES	YES
63	a	429.05	1.33140	YES	YES
64	a	430.67	2.10717	YES	YES
65	a	437.49	0.70813	YES	YES
66	a	439.42	2.42348	YES	YES
67	a	461.81	6.88193	YES	YES
68	a	488.70	1.03109	YES	YES
69	a	492.53	4.91458	YES	YES
70	a	497.68	27.12255	YES	YES
71	a	499.10	4.13363	YES	YES
72	a	507.73	11.22555	YES	YES
73	a	510.68	16.83546	YES	YES
74	a	547.87	80.47246	YES	YES
75	a	569.72	23.46812	YES	YES
76	a	607.39	67.59195	YES	YES
77	a	614.83	0.03805	YES	YES
78	a	618.50	4.31164	YES	YES
79	a	626.99	15.29901	YES	YES
80	a	650.11	5.62053	YES	YES
81	a	668.55	1.03782	YES	YES
82	a	691.97	42.74104	YES	YES
83	a	694.65	23.00549	YES	YES
84	a	712.90	0.88099	YES	YES
85	a	713.29	0.50554	YES	YES
86	a	732.45	0.98324	YES	YES
87	a	736.82	3.93426	YES	YES
88	a	739.61	46.83566	YES	YES
89	a	751.94	11.66010	YES	YES

90	a	768.78	0.30614	YES	YES
91	a	771.07	0.24944	YES	YES
92	a	774.53	0.20515	YES	YES
93	a	777.33	0.11969	YES	YES
94	a	785.03	10.16167	YES	YES
95	a	799.04	1.89675	YES	YES
96	a	807.83	1.37949	YES	YES
97	a	809.76	2.33183	YES	YES
98	a	811.04	0.33828	YES	YES
99	a	813.88	5.69412	YES	YES
100	a	816.39	0.81247	YES	YES
101	a	834.84	0.39240	YES	YES
102	a	836.53	1.52393	YES	YES
103	a	837.02	4.37006	YES	YES
104	a	838.78	10.38829	YES	YES
105	a	849.24	7.79070	YES	YES
106	a	857.16	2.95561	YES	YES
107	a	871.78	11.55998	YES	YES
108	a	872.93	10.10646	YES	YES
109	a	874.83	0.91420	YES	YES
110	a	876.91	3.02549	YES	YES
111	a	878.73	4.05154	YES	YES
112	a	880.00	4.34236	YES	YES
113	a	880.62	1.96333	YES	YES
114	a	882.20	3.48837	YES	YES
115	a	883.04	5.83982	YES	YES
116	a	887.01	3.52750	YES	YES
117	a	905.25	1.60957	YES	YES
118	a	905.89	1.84922	YES	YES
119	a	908.50	0.20599	YES	YES
120	a	910.37	0.32425	YES	YES
121	a	916.82	21.86346	YES	YES
122	a	935.95	0.14691	YES	YES
123	a	947.73	0.00964	YES	YES
124	a	965.00	0.36453	YES	YES
125	a	971.76	0.04061	YES	YES
126	a	979.98	0.88908	YES	YES
127	a	987.39	2.13653	YES	YES
128	a	988.92	8.68647	YES	YES
129	a	989.34	17.09849	YES	YES
130	a	990.42	3.91198	YES	YES
131	a	994.62	3.14191	YES	YES
132	a	996.42	0.27486	YES	YES
133	a	1017.52	0.76662	YES	YES
134	a	1018.93	0.19186	YES	YES
135	a	1019.32	0.59686	YES	YES
136	a	1021.46	0.21862	YES	YES
137	a	1023.59	4.28036	YES	YES
138	a	1028.75	5.11142	YES	YES
139	a	1031.62	1.56921	YES	YES
140	a	1032.74	0.76184	YES	YES
141	a	1035.03	1.05702	YES	YES
142	a	1038.63	0.48631	YES	YES
143	a	1061.95	1.18303	YES	YES
144	a	1063.34	0.34389	YES	YES
145	a	1064.92	0.06681	YES	YES
146	a	1067.40	0.39977	YES	YES
147	a	1070.95	0.41619	YES	YES
148	a	1071.20	0.00731	YES	YES
149	a	1071.98	7.15160	YES	YES
150	a	1073.27	0.12551	YES	YES
151	a	1073.91	0.07500	YES	YES

152	a	1081.34	8.75272	YES	YES
153	a	1085.57	3.63613	YES	YES
154	a	1092.85	1.22788	YES	YES
155	a	1097.99	7.95054	YES	YES
156	a	1106.07	2.01665	YES	YES
157	a	1107.91	3.94634	YES	YES
158	a	1127.29	2.30044	YES	YES
159	a	1146.91	1.71826	YES	YES
160	a	1151.72	0.08446	YES	YES
161	a	1158.96	4.08726	YES	YES
162	a	1162.27	5.16237	YES	YES
163	a	1165.19	2.13914	YES	YES
164	a	1167.95	7.81724	YES	YES
165	a	1168.33	7.21252	YES	YES
166	a	1169.23	5.22173	YES	YES
167	a	1178.74	10.21795	YES	YES
168	a	1186.42	11.55140	YES	YES
169	a	1192.65	3.97687	YES	YES
170	a	1194.87	11.16162	YES	YES
171	a	1207.32	45.15775	YES	YES
172	a	1244.30	1.93097	YES	YES
173	a	1246.58	0.34239	YES	YES
174	a	1248.87	0.49019	YES	YES
175	a	1250.45	2.68488	YES	YES
176	a	1251.27	1.62489	YES	YES
177	a	1254.66	3.38331	YES	YES
178	a	1257.27	2.83753	YES	YES
179	a	1258.17	9.39902	YES	YES
180	a	1259.83	1.56996	YES	YES
181	a	1260.26	6.22012	YES	YES
182	a	1263.27	2.16734	YES	YES
183	a	1265.83	2.95733	YES	YES
184	a	1270.69	2.06966	YES	YES
185	a	1272.03	0.09714	YES	YES
186	a	1284.78	57.17092	YES	YES
187	a	1286.17	2.99301	YES	YES
188	a	1287.94	1.85112	YES	YES
189	a	1289.22	3.16593	YES	YES
190	a	1290.90	1.15858	YES	YES
191	a	1302.79	70.48134	YES	YES
192	a	1304.04	68.54780	YES	YES
193	a	1311.65	1.69433	YES	YES
194	a	1316.43	0.65913	YES	YES
195	a	1318.10	2.18516	YES	YES
196	a	1318.34	1.25582	YES	YES
197	a	1323.42	0.60428	YES	YES
198	a	1323.87	0.33164	YES	YES
199	a	1324.13	1.15653	YES	YES
200	a	1325.00	0.16565	YES	YES
201	a	1327.23	6.14073	YES	YES
202	a	1329.77	4.24311	YES	YES
203	a	1330.56	2.98972	YES	YES
204	a	1333.70	1.53451	YES	YES
205	a	1334.57	1.78461	YES	YES
206	a	1337.75	0.02159	YES	YES
207	a	1338.79	0.09869	YES	YES
208	a	1339.75	0.26408	YES	YES
209	a	1340.59	0.67809	YES	YES
210	a	1344.94	1.26412	YES	YES
211	a	1345.43	5.27586	YES	YES
212	a	1346.68	1.52673	YES	YES
213	a	1348.03	1.04929	YES	YES

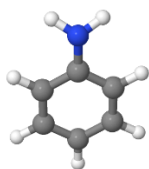
214	a	1350.27	0.36689	YES	YES
215	a	1402.25	10.64019	YES	YES
216	a	1405.06	7.82134	YES	YES
217	a	1429.94	3.10376	YES	YES
218	a	1431.38	1.11258	YES	YES
219	a	1432.88	2.64635	YES	YES
220	a	1435.94	3.67515	YES	YES
221	a	1436.13	3.95857	YES	YES
222	a	1436.74	5.15367	YES	YES
223	a	1437.59	1.04811	YES	YES
224	a	1438.15	7.22300	YES	YES
225	a	1438.49	7.30288	YES	YES
226	a	1438.87	3.21257	YES	YES
227	a	1440.17	3.52690	YES	YES
228	a	1440.52	3.67395	YES	YES
229	a	1441.02	8.71665	YES	YES
230	a	1443.16	12.25194	YES	YES
231	a	1444.27	28.81546	YES	YES
232	a	1445.29	6.15605	YES	YES
233	a	1446.49	5.87304	YES	YES
234	a	1447.88	1.61688	YES	YES
235	a	1453.96	1.29087	YES	YES
236	a	1454.88	3.62062	YES	YES
237	a	1455.83	3.83879	YES	YES
238	a	1457.38	0.87483	YES	YES
239	a	1478.53	120.75911	YES	YES
240	a	1481.14	76.31145	YES	YES
241	a	1562.05	6.33230	YES	YES
242	a	1576.78	6.19735	YES	YES
243	a	1586.81	67.89705	YES	YES
244	a	1598.84	54.40354	YES	YES
245	a	1945.97	85.30339	YES	YES
246	a	2924.52	4.91929	YES	YES
247	a	2930.06	9.30618	YES	YES
248	a	2931.74	1.95246	YES	YES
249	a	2940.18	9.96719	YES	YES
250	a	2942.63	11.27738	YES	YES
251	a	2943.50	23.66285	YES	YES
252	a	2944.76	48.75525	YES	YES
253	a	2944.88	3.73426	YES	YES
254	a	2945.81	9.60808	YES	YES
255	a	2946.55	17.70666	YES	YES
256	a	2947.97	12.60091	YES	YES
257	a	2948.24	11.71112	YES	YES
258	a	2953.51	1.24335	YES	YES
259	a	2954.88	4.78266	YES	YES
260	a	2956.28	1.30665	YES	YES
261	a	2958.59	3.93398	YES	YES
262	a	2959.00	19.43977	YES	YES
263	a	2960.08	91.64648	YES	YES
264	a	2961.41	15.77413	YES	YES
265	a	2962.23	24.17542	YES	YES
266	a	2964.11	16.41615	YES	YES
267	a	2967.61	30.79144	YES	YES
268	a	2971.21	18.55152	YES	YES
269	a	2975.97	10.76359	YES	YES
270	a	2980.78	2.53633	YES	YES
271	a	2992.65	4.98245	YES	YES
272	a	3003.96	24.02910	YES	YES
273	a	3004.89	36.35496	YES	YES
274	a	3005.87	31.72155	YES	YES
275	a	3006.32	28.18822	YES	YES

276	a	3008.59	14.55472	YES	YES
277	a	3008.67	7.80635	YES	YES
278	a	3009.25	16.48764	YES	YES
279	a	3010.25	41.76204	YES	YES
280	a	3010.57	22.13824	YES	YES
281	a	3011.39	26.66006	YES	YES
282	a	3012.27	35.17953	YES	YES
283	a	3012.86	17.62738	YES	YES
284	a	3013.12	24.81900	YES	YES
285	a	3013.90	27.91701	YES	YES
286	a	3015.13	50.98714	YES	YES
287	a	3015.71	1.48280	YES	YES
288	a	3017.66	11.24042	YES	YES
289	a	3021.59	25.49408	YES	YES
290	a	3024.62	2.67542	YES	YES
291	a	3027.60	1.18437	YES	YES
292	a	3033.19	5.09482	YES	YES
293	a	3044.53	0.80465	YES	YES
294	a	3085.39	20.12450	YES	YES
295	a	3090.78	16.46139	YES	YES
296	a	3100.13	27.06604	YES	YES
297	a	3103.75	2.04303	YES	YES
298	a	3108.63	7.23877	YES	YES
299	a	3112.93	4.93438	YES	YES
300	a	3119.44	13.18970	YES	YES
301	a	3131.02	1.56081	YES	YES
302	a	3131.34	11.66769	YES	YES
303	a	3135.87	3.67807	YES	YES

\$end

Double hybrid single point energy = -4142.522672211521 H
 COSMO energy + OC correction = -4147.0879874357 H (in oDFB)

6.2.16 H₂NPh



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

H	1.3133090	-0.0242037	2.0620512
C	0.7657024	0.0113832	1.1184513
C	-0.6357611	0.1335595	1.1366725
N	-1.3342593	0.1509879	2.3460866
C	-1.3231472	0.1721490	-0.0902798
H	-2.4109544	0.2624532	-0.0929077
C	-0.6261103	0.0909604	-1.2943070
H	-1.1798836	0.1248201	-2.2329902
C	0.7662424	-0.0304241	-1.3080256
H	1.3071670	-0.0924302	-2.2511231
C	1.4529476	-0.0690118	-0.0912804
H	2.5393659	-0.1613606	-0.0808145
H	-0.8006918	0.4680206	3.1490065
H	-2.2533766	0.5795064	2.3084402

SCF energy GEOPT = -287.7508036819 H

ZPE = 298.9 kJ/mol
 FREEH energy = 314.54 kJ/mol
 FREEH entropy = 0.31853 kJ/mol/K

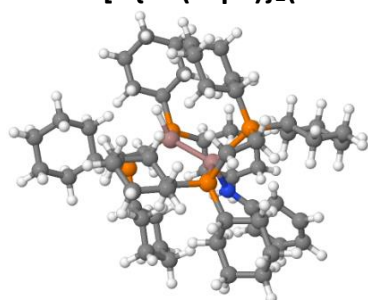
\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	211.51	4.96821	YES	YES
8		a	306.11	17.15264	YES	YES
9		a	371.34	0.00787	YES	YES
10		a	402.40	0.19282	YES	YES
11		a	487.72	74.28704	YES	YES
12		a	521.57	9.07873	YES	YES
13		a	568.60	237.47743	YES	YES
14		a	617.35	0.32415	YES	YES
15		a	682.82	31.08616	YES	YES
16		a	737.71	54.80911	YES	YES
17		a	795.91	0.06249	YES	YES
18		a	815.35	2.44832	YES	YES
19		a	852.69	7.90059	YES	YES
20		a	926.13	0.00049	YES	YES
21		a	941.52	0.04377	YES	YES
22		a	988.27	1.38143	YES	YES
23		a	1024.43	3.42000	YES	YES
24		a	1036.98	3.65303	YES	YES
25		a	1106.00	3.59680	YES	YES
26		a	1146.73	1.28524	YES	YES
27		a	1166.39	8.92545	YES	YES
28		a	1278.28	53.50489	YES	YES
29		a	1324.18	0.01238	YES	YES
30		a	1351.06	7.18185	YES	YES
31		a	1460.65	1.19007	YES	YES
32		a	1490.58	57.15474	YES	YES
33		a	1582.05	4.23351	YES	YES
34		a	1597.43	5.02515	YES	YES
35		a	1612.36	146.50477	YES	YES
36		a	3085.38	18.81532	YES	YES
37		a	3086.32	5.11989	YES	YES
38		a	3103.39	2.44230	YES	YES
39		a	3108.63	33.67040	YES	YES
40		a	3127.10	13.04485	YES	YES
41		a	3479.48	12.26652	YES	YES
42		a	3578.56	11.70990	YES	YES

\$end

Double hybrid single point energy = -287.221982147440 H
 COSMO energy + OC correction = -287.7602991828 H (in oDFB)

6.2.17 [H{Ga(dcpe)}₂(HNPh)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-0.3577689	0.2200689	-1.7938063
P	-2.2846772	-0.8764139	-2.8843464
P	-1.4422902	2.3512686	-2.4680828
C	-2.1382314	-2.2197539	-4.1750213
H	-2.9501106	-2.9155689	-3.8974830
C	-0.8013214	-2.9681117	-4.0446411
H	0.0278603	-2.2691839	-4.2263625
H	-0.6851664	-3.3374578	-3.0175710
C	-0.7168948	-4.1279273	-5.0430651
H	0.2654966	-4.6129214	-4.9576215
H	-1.4688744	-4.8924026	-4.7859644
C	-0.9485268	-3.6438731	-6.4761932
H	-0.9024127	-4.4886739	-7.1760230
H	-0.1404178	-2.9506298	-6.7610463
C	-2.2988998	-2.9342166	-6.5946026
H	-3.1106034	-3.6506963	-6.3877299
H	-2.4596597	-2.5677726	-7.6176863
C	-2.4068302	-1.7549059	-5.6173141
H	-3.4047180	-1.3029630	-5.6970167
H	-1.6760540	-0.9867963	-5.9102559
C	-3.4121638	-1.6162947	-1.6170186
H	-4.2835931	-1.9763084	-2.1934003
C	-2.7263204	-2.8249262	-0.9574203
H	-2.4369711	-3.5660659	-1.7149102
H	-1.7929691	-2.4821330	-0.4780837
C	-3.6323534	-3.4748140	0.0935245
H	-4.5205725	-3.8954723	-0.4045600
H	-3.1087506	-4.3225151	0.5558876
C	-4.0708684	-2.4598945	1.1508996
H	-4.7311740	-2.9359786	1.8879925
H	-3.1859843	-2.0981077	1.7017178
C	-4.7768772	-1.2696067	0.4977781
H	-5.0594215	-0.5232476	1.2530532
H	-5.7142719	-1.6124556	0.0310023
C	-3.8982957	-0.6022250	-0.5693763
H	-4.4716791	0.1982820	-1.0554315
H	-3.0262965	-0.1370166	-0.0815991
C	-3.2265467	0.5073565	-3.6673321
H	-2.8055150	0.6315014	-4.6728735
H	-4.2729371	0.1958062	-3.7983148
C	-3.1575651	1.8386311	-2.9103100
H	-3.7145960	1.7847077	-1.9670707

H	-3.6227804	2.6322560	-3.5102079
C	-0.7562479	3.3364339	-3.8801721
H	-1.1660383	4.3488331	-3.7195190
C	0.7732563	3.4078965	-3.7553324
H	1.1889798	2.3944666	-3.8421632
H	1.0481621	3.7856385	-2.7611196
C	1.3754510	4.2983235	-4.8465131
H	1.0457850	5.3397693	-4.6966245
H	2.4703183	4.2969856	-4.7541104
C	0.9517613	3.8180644	-6.2372929
H	1.3699532	2.8147600	-6.4165698
H	1.3670194	4.4781427	-7.0103725
C	-0.5749018	3.7659867	-6.3582742
H	-0.8722481	3.3934838	-7.3481459
H	-0.9863699	4.7849839	-6.2710371
C	-1.2014476	2.8747070	-5.2750504
H	-0.8775464	1.8389769	-5.4414044
H	-2.2973777	2.9025195	-5.3602130
C	-1.6868852	3.5965925	-1.1163811
H	-0.7057292	4.0926750	-1.0249009
C	-2.0218375	2.9309087	0.2259404
H	-1.2348135	2.2101332	0.4970825
H	-2.9525309	2.3482727	0.1308914
C	-2.1948926	3.9739919	1.3359241
H	-2.4706530	3.4701943	2.2724794
H	-1.2260404	4.4716695	1.5149905
C	-3.2318979	5.0375440	0.9681103
H	-4.2264553	4.5682329	0.8907097
H	-3.3028276	5.7887217	1.7659796
C	-2.8771385	5.7027972	-0.3631789
H	-1.9288394	6.2554451	-0.2611694
H	-3.6407623	6.4405386	-0.6435704
C	-2.7407577	4.6611017	-1.4809608
H	-3.7169143	4.1732534	-1.6281785
H	-2.4866844	5.1581446	-2.4267569
Ga	-0.0812018	-0.2558546	0.6094572
P	1.3575473	1.2063474	1.9175657
P	1.4119326	-2.0564789	1.2988553
C	0.5094694	2.3083497	3.1349859
H	-0.0209226	3.0468571	2.5128334
C	-0.5419713	1.5328304	3.9502244
H	-0.0466174	0.7292081	4.5195143
H	-1.2582050	1.0434756	3.2757568
C	-1.2690887	2.4562220	4.9369194
H	-1.9778355	1.8651655	5.5329843
H	-1.8691120	3.1884124	4.3725620
C	-0.2875808	3.2023093	5.8440180
H	-0.8311191	3.8820809	6.5135127
H	0.2365552	2.4799149	6.4914973
C	0.7388765	3.9808545	5.0176558
H	0.2271860	4.7688005	4.4407326
H	1.4594937	4.4897821	5.6719262
C	1.4945112	3.0597122	4.0494948
H	2.2075620	3.6486094	3.4560622
H	2.0833881	2.3332366	4.6321292
C	2.5371414	2.2569364	0.9655522
H	3.1042412	2.8313197	1.7171511
C	1.7727320	3.2382718	0.0645539

H	1.0910927	3.8597285	0.6633716
H	1.1490372	2.6545739	-0.6359715
C	2.7423342	4.1181482	-0.7317641
H	3.3232120	4.7416091	-0.0332188
H	2.1791974	4.8167881	-1.3665488
C	3.6933644	3.2622509	-1.5725259
H	4.3895459	3.9007595	-2.1318969
H	3.1135697	2.6942810	-2.3186575
C	4.4691768	2.2857247	-0.6861250
H	5.1201591	1.6422638	-1.2940787
H	5.1320532	2.8490119	-0.0100409
C	3.5308152	1.4110630	0.1537057
H	4.1262362	0.7738704	0.8204276
H	2.9623755	0.7385710	-0.5101660
C	2.3881530	0.0697827	2.9449752
H	1.7968948	-0.1303356	3.8468712
H	3.2916219	0.6057779	3.2679387
C	2.7768147	-1.2404209	2.2476857
H	3.5782209	-1.0510869	1.5267608
H	3.1716633	-1.9601453	2.9791373
C	0.6361473	-3.2193542	2.5186646
H	1.4462142	-3.9185020	2.7944718
C	-0.5229099	-4.0126932	1.8963366
H	-1.2621274	-3.2970085	1.5037748
H	-0.1675233	-4.6108636	1.0476654
C	-1.2019128	-4.9296438	2.9209872
H	-0.4927405	-5.7128288	3.2338748
H	-2.0436365	-5.4484721	2.4411301
C	-1.6743366	-4.1482844	4.1476898
H	-2.4544473	-3.4288743	3.8475287
H	-2.1357844	-4.8258758	4.8780627
C	-0.5052453	-3.3963949	4.7858339
H	-0.8436709	-2.8095718	5.6508564
H	0.2316460	-4.1211495	5.1680230
C	0.1797665	-2.4622255	3.7798870
H	-0.5215121	-1.6647827	3.4841413
H	1.0390329	-1.9799347	4.2651786
C	2.2249335	-3.0987431	-0.0067798
H	2.5109301	-4.0333574	0.5072300
C	1.2223624	-3.4306037	-1.1277840
H	0.3084539	-3.8796096	-0.7191497
H	0.9281096	-2.4877133	-1.6177414
C	1.8608871	-4.3576267	-2.1663503
H	1.1237150	-4.6159192	-2.9364129
H	2.1491273	-5.3056308	-1.6833743
C	3.0900275	-3.6983752	-2.7922187
H	2.7808552	-2.7913700	-3.3379177
H	3.5542240	-4.3665923	-3.5296388
C	4.1053681	-3.3300575	-1.7085969
H	4.5011261	-4.2515052	-1.2519664
H	4.9671387	-2.8043568	-2.1426045
C	3.4918979	-2.4581035	-0.6036135
H	3.2323492	-1.4707621	-1.0203921
H	4.2492720	-2.2878293	0.1724656
N	1.2975045	-0.0508660	-2.6576718
H	2.0826975	-0.1134294	-2.0159124
C	1.6951012	-0.0516111	-3.9827400
C	0.7475999	-0.0339118	-5.0194856

C	3.0602548	-0.0771181	-4.3395501
C	3.4446713	-0.0886995	-5.6781671
C	2.4883507	-0.0753187	-6.7001834
C	1.1352811	-0.0476533	-6.3575385
H	-0.3090093	-0.0132006	-4.7534280
H	3.8172485	-0.0843958	-3.5525892
H	4.5051075	-0.1077600	-5.9284573
H	2.7952073	-0.0853717	-7.7441192
H	0.3752207	-0.0340838	-7.1396044
H	-1.3268391	-0.4590205	1.5540712

SCF energy GEOOPT = -7543.978421672 H

ZPE = 3896. kJ/mol

FREEH energy = 4089.00 kJ/mol

FREEH entropy = 1.62556 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	6.99	0.03919	YES	YES
	8	a	19.21	0.25651	YES	YES
	9	a	22.49	0.17209	YES	YES
	10	a	23.37	0.22137	YES	YES
	11	a	28.05	0.17723	YES	YES
	12	a	32.91	0.02007	YES	YES
	13	a	36.59	0.02516	YES	YES
	14	a	40.08	0.19591	YES	YES
	15	a	41.95	0.08727	YES	YES
	16	a	44.13	0.09592	YES	YES
	17	a	47.77	0.03305	YES	YES
	18	a	49.43	0.01026	YES	YES
	19	a	51.62	0.06249	YES	YES
	20	a	52.21	0.27895	YES	YES
	21	a	59.47	0.06207	YES	YES
	22	a	61.51	0.13039	YES	YES
	23	a	62.98	0.06066	YES	YES
	24	a	65.28	0.25711	YES	YES
	25	a	68.29	0.13794	YES	YES
	26	a	70.64	0.20848	YES	YES
	27	a	71.85	0.34657	YES	YES
	28	a	73.69	0.15649	YES	YES
	29	a	76.55	0.03894	YES	YES
	30	a	79.03	0.31724	YES	YES
	31	a	83.99	0.05082	YES	YES
	32	a	86.10	0.13586	YES	YES
	33	a	89.71	0.54068	YES	YES
	34	a	91.55	0.11609	YES	YES
	35	a	97.41	0.26707	YES	YES
	36	a	99.44	0.20004	YES	YES
	37	a	101.25	0.02267	YES	YES
	38	a	110.16	0.17984	YES	YES
	39	a	125.70	1.13262	YES	YES

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129	a	653.49	11.73197	YES	YES
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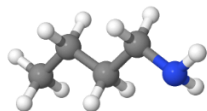
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438	a	2961.65	36.03176	YES	YES
439	a	2961.94	17.46237	YES	YES
440	a	2963.48	56.29388	YES	YES
441	a	2964.51	48.61855	YES	YES
442	a	2965.06	40.47399	YES	YES
443	a	2965.97	10.24961	YES	YES
444	a	2966.16	18.46880	YES	YES
445	a	2968.63	39.22507	YES	YES

446	a	2972.27	24.24426	YES	YES
447	a	2973.46	12.29547	YES	YES
448	a	2973.80	0.91762	YES	YES
449	a	2980.00	9.20098	YES	YES
450	a	2982.36	2.11569	YES	YES
451	a	2983.56	32.84738	YES	YES
452	a	2984.49	23.97838	YES	YES
453	a	2986.28	5.53465	YES	YES
454	a	2990.67	3.50537	YES	YES
455	a	2993.16	4.92859	YES	YES
456	a	2994.34	23.41609	YES	YES
457	a	3003.29	28.00268	YES	YES
458	a	3006.19	37.51877	YES	YES
459	a	3006.29	3.61712	YES	YES
460	a	3006.33	23.32577	YES	YES
461	a	3007.84	19.49740	YES	YES
462	a	3008.13	24.73956	YES	YES
463	a	3008.69	27.07875	YES	YES
464	a	3008.78	10.11682	YES	YES
465	a	3008.98	6.47253	YES	YES
466	a	3009.07	27.12135	YES	YES
467	a	3009.76	24.27477	YES	YES
468	a	3010.07	9.74635	YES	YES
469	a	3010.30	19.64373	YES	YES
470	a	3011.92	9.25471	YES	YES
471	a	3011.94	19.76634	YES	YES
472	a	3012.42	16.44853	YES	YES
473	a	3012.69	17.10797	YES	YES
474	a	3013.13	35.31934	YES	YES
475	a	3013.34	14.76329	YES	YES
476	a	3014.04	17.33042	YES	YES
477	a	3015.69	34.88127	YES	YES
478	a	3015.94	34.14006	YES	YES
479	a	3016.61	35.88679	YES	YES
480	a	3016.91	25.48875	YES	YES
481	a	3017.69	30.19720	YES	YES
482	a	3018.41	22.70458	YES	YES
483	a	3018.60	44.97284	YES	YES
484	a	3018.78	28.47614	YES	YES
485	a	3019.22	19.45754	YES	YES
486	a	3019.44	21.86784	YES	YES
487	a	3019.98	5.13293	YES	YES
488	a	3020.95	54.27220	YES	YES
489	a	3021.06	8.52143	YES	YES
490	a	3026.61	17.26543	YES	YES
491	a	3028.19	8.86876	YES	YES
492	a	3028.63	6.29084	YES	YES
493	a	3031.18	13.95385	YES	YES
494	a	3032.30	9.64803	YES	YES
495	a	3034.82	0.32561	YES	YES
496	a	3038.37	0.22130	YES	YES
497	a	3048.27	0.57137	YES	YES
498	a	3063.19	0.39000	YES	YES
499	a	3081.42	13.65875	YES	YES
500	a	3087.99	20.25649	YES	YES
501	a	3104.28	11.46131	YES	YES
502	a	3116.82	5.54143	YES	YES
503	a	3138.33	2.12619	YES	YES

504 a 3491.34 15.62770 YES YES
\$end

Double hybrid single point energy = -7536.336316713699 H
COSMO energy + OC correction = -7544.1277460103 H (in oDFB)

6.2.18 H₂NnBu



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

N	-1.2439487	-1.9609154	-0.0850574
C	0.2091963	-1.7514658	0.0058493
H	-1.7320070	-1.0641260	-0.0902246
H	-1.5734254	-2.4581697	0.7449915
C	0.9489535	-3.0866512	-0.0104457
H	0.5245099	-1.1771113	0.9011477
H	0.5160770	-1.1575826	-0.8696770
C	2.4709193	-2.9339773	0.0341031
H	0.6494581	-3.6447751	-0.9114307
H	0.6190101	-3.6934686	0.8512992
C	3.2048810	-4.2760478	0.0284190
H	2.7550881	-2.3609787	0.9319221
H	2.7991429	-2.3299016	-0.8275767
H	2.9195667	-4.8865335	0.8975024
H	4.2947238	-4.1423259	0.0578309
H	2.9629745	-4.8550895	-0.8744430

SCF energy GEOOPT = -213.9066145926 H
ZPE = 381.6 kJ/mol
FREEH energy = 400.35 kJ/mol
FREEH entropy = 0.33937 kJ/mol/K

\$vibrational spectrum

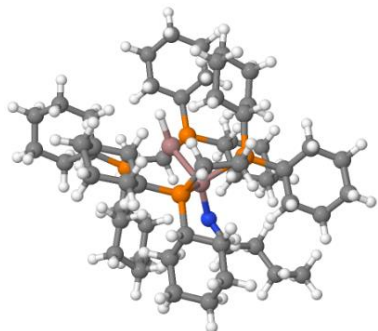
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	102.56	2.39019	YES	YES
8		a	110.25	1.48207	YES	YES
9		a	172.97	0.99504	YES	YES
10		a	238.76	6.19505	YES	YES
11		a	243.23	29.60202	YES	YES
12		a	385.53	0.04480	YES	YES
13		a	421.65	8.91091	YES	YES
14		a	722.19	3.56525	YES	YES
15		a	777.61	16.61253	YES	YES

16	a	822.99	111.37202	YES	YES
17	a	880.43	1.30093	YES	YES
18	a	925.72	5.42881	YES	YES
19	a	956.72	3.28780	YES	YES
20	a	1033.10	0.13483	YES	YES
21	a	1047.56	3.24407	YES	YES
22	a	1071.53	8.23842	YES	YES
23	a	1125.95	5.72198	YES	YES
24	a	1187.49	0.19968	YES	YES
25	a	1227.12	1.51849	YES	YES
26	a	1270.77	1.04424	YES	YES
27	a	1285.65	0.69096	YES	YES
28	a	1293.31	1.39709	YES	YES
29	a	1341.18	0.76899	YES	YES
30	a	1363.82	3.34678	YES	YES
31	a	1377.87	11.58551	YES	YES
32	a	1439.30	0.20509	YES	YES
33	a	1446.29	0.41544	YES	YES
34	a	1452.38	7.48408	YES	YES
35	a	1459.91	4.93648	YES	YES
36	a	1470.78	2.77310	YES	YES
37	a	1604.96	24.12132	YES	YES
38	a	2859.16	81.16524	YES	YES
39	a	2928.61	9.52036	YES	YES
40	a	2943.11	33.69859	YES	YES
41	a	2958.58	30.52485	YES	YES
42	a	2963.40	41.08585	YES	YES
43	a	2966.81	10.24408	YES	YES
44	a	2991.76	50.11259	YES	YES
45	a	3023.37	55.95006	YES	YES
46	a	3030.03	37.88536	YES	YES
47	a	3396.74	2.22330	YES	YES
48	a	3477.05	0.13320	YES	YES

\$end

Double hybrid single point energy = -213.511849899828 H
COSMO energy + OC correction = -213.9128469055 H (in oDFB)

6.2.19 [H{Ga(dcpe)}₂(HN*n*Bu)]²⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
Ga -0.3504018 0.5347406 -1.8842889

P	-2.1571665	-0.7530468	-2.9618482
P	-1.7289064	2.5081166	-2.3988973
C	-1.6754000	-1.8717089	-4.3582907
H	-0.8181624	-2.4367936	-3.9491927
C	-1.1687409	-1.0688390	-5.5681739
H	-1.9987365	-0.4803652	-5.9901046
H	-0.3934011	-0.3565410	-5.2584388
C	-0.6339525	-2.0072081	-6.6560027
H	-0.2866561	-1.4156081	-7.5139757
H	0.2468375	-2.5437918	-6.2672616
C	-1.7010451	-3.0152104	-7.0901876
H	-1.2907347	-3.7046550	-7.8399183
H	-2.5306757	-2.4795185	-7.5801108
C	-2.2394640	-3.7989536	-5.8904173
H	-1.4356283	-4.4276525	-5.4724771
H	-3.0403060	-4.4829855	-6.2022341
C	-2.7650917	-2.8700508	-4.7857382
H	-3.1038083	-3.4740791	-3.9336671
H	-3.6428537	-2.3151479	-5.1559638
C	-3.1621406	-1.7743768	-1.7992771
H	-3.9257855	-2.2534424	-2.4359107
C	-2.3098557	-2.8765719	-1.1521375
H	-1.7975875	-3.4761277	-1.9190570
H	-1.5210639	-2.4017577	-0.5416740
C	-3.1811333	-3.7743390	-0.2653843
H	-3.9119140	-4.3016898	-0.8994317
H	-2.5626879	-4.5526349	0.2015717
C	-3.9240292	-2.9574970	0.7964237
H	-4.5655372	-3.6130395	1.4003438
H	-3.1958172	-2.5039258	1.4896762
C	-4.7545497	-1.8413070	0.1593004
H	-5.2407109	-1.2329005	0.9341684
H	-5.5630466	-2.2835001	-0.4449608
C	-3.8959906	-0.9395417	-0.7373766
H	-4.5425694	-0.1932998	-1.2179846
H	-3.1608972	-0.3958305	-0.1216639
C	-3.3388057	0.5023042	-3.6268001
H	-3.0200198	0.7188179	-4.6527630
H	-4.3426461	0.0588324	-3.6897406
C	-3.3869137	1.8036921	-2.8049998
H	-3.8874023	1.6346544	-1.8425402
H	-3.9746151	2.5624773	-3.3397060
C	-1.2263720	3.5796989	-3.8177079
H	-1.9088778	4.4465011	-3.7873042
C	0.2122159	4.0737414	-3.5855436
H	0.8729790	3.2058763	-3.4441890
H	0.2567191	4.6553551	-2.6543965
C	0.7168789	4.9266147	-4.7542144
H	0.1421731	5.8659405	-4.7980957
H	1.7632781	5.2079618	-4.5717636
C	0.5793308	4.1849866	-6.0861477
H	1.2287698	3.2941515	-6.0805623
H	0.9264011	4.8195366	-6.9122268
C	-0.8725526	3.7611427	-6.3234309
H	-0.9697223	3.2144152	-7.2714317
H	-1.5042962	4.6595090	-6.4147374
C	-1.4048135	2.8886175	-5.1791978
H	-0.8723928	1.9247135	-5.1801859

H	-2.4676181	2.6669728	-5.3515084
C	-2.0198126	3.6763192	-0.9930777
H	-1.0878046	4.2654202	-0.9466799
C	-2.1774515	2.9383933	0.3432208
H	-1.2998113	2.3001388	0.5218952
H	-3.0467126	2.2616170	0.3006551
C	-2.3540712	3.9228087	1.5039066
H	-2.5043317	3.3643039	2.4382265
H	-1.4218913	4.5013472	1.6257126
C	-3.5145605	4.8907661	1.2583426
H	-4.4624246	4.3278547	1.2461933
H	-3.5902492	5.6100593	2.0846916
C	-3.3424176	5.6261773	-0.0732460
H	-2.4489144	6.2701865	-0.0277638
H	-4.1969338	6.2898812	-0.2613371
C	-3.1949441	4.6403680	-1.2402938
H	-4.1273742	4.0621644	-1.3386803
H	-3.0588298	5.1911734	-2.1810658
Ga	-0.1797497	-0.0455239	0.5046913
P	1.4370681	1.3112729	1.7274523
P	1.1686041	-1.9637917	1.1614292
C	0.7535672	2.3550759	3.0940415
H	0.2291113	3.1677529	2.5616480
C	-0.2837057	1.5953425	3.9367392
H	0.2066490	0.7432625	4.4338299
H	-1.0659194	1.1752627	3.2893502
C	-0.8944716	2.5078712	5.0078241
H	-1.6096824	1.9339802	5.6130071
H	-1.4710124	3.3074897	4.5143334
C	0.1844542	3.1352608	5.8943333
H	-0.2719923	3.8130490	6.6278939
H	0.6890009	2.3436381	6.4728117
C	1.2190279	3.8858759	5.0521676
H	0.7376500	4.7442024	4.5551780
H	2.0130547	4.2983477	5.6892467
C	1.8449697	2.9765439	3.9848273
H	2.5654981	3.5505114	3.3864578
H	2.4099245	2.1720962	4.4831226
C	2.5098752	2.4403236	0.7371377
H	3.0866363	3.0105577	1.4853561
C	1.6603981	3.4280258	-0.0783096
H	0.9690367	3.9770973	0.5781318
H	1.0515507	2.8557926	-0.7982596
C	2.5611776	4.4033135	-0.8442451
H	3.1334699	5.0114059	-0.1249877
H	1.9462527	5.1070763	-1.4211716
C	3.5244369	3.6467177	-1.7624173
H	4.1712648	4.3507541	-2.3025034
H	2.9426330	3.0950053	-2.5184290
C	4.3755506	2.6562327	-0.9628954
H	5.0363511	2.0860989	-1.6303816
H	5.0319158	3.2112228	-0.2732874
C	3.5074336	1.6836866	-0.1530209
H	4.1543956	1.0383608	0.4571919
H	2.9466989	1.0380171	-0.8447071
C	2.5904257	0.0948187	2.5116638
H	2.1866167	-0.1221222	3.5079146
H	3.5653085	0.5780692	2.6647553

C	2.7635527	-1.2017417	1.7030462
H	3.3336870	-1.0043165	0.7846548
H	3.3348592	-1.9379911	2.2850031
C	0.5477978	-2.9564250	2.5999789
H	1.4137141	-3.5473113	2.9453766
C	-0.5647713	-3.9105259	2.1386244
H	-1.3626096	-3.3107530	1.6754208
H	-0.1904412	-4.5984752	1.3687894
C	-1.1529086	-4.7155298	3.3030418
H	-0.3836042	-5.4001290	3.6953633
H	-1.9701601	-5.3477873	2.9287684
C	-1.6444878	-3.8019152	4.4271661
H	-2.4841684	-3.1874632	4.0612315
H	-2.0336884	-4.3997424	5.2618176
C	-0.5165814	-2.8872843	4.9078520
H	-0.8741012	-2.2081477	5.6941505
H	0.2830675	-3.4964311	5.3596201
C	0.0642438	-2.0612713	3.7536694
H	-0.7041492	-1.3709724	3.3716927
H	0.8911226	-1.4452755	4.1305040
C	1.5907667	-3.1943847	-0.1481358
H	0.6315878	-3.7089464	-0.3296183
C	2.0045001	-2.5325365	-1.4684992
H	1.2338877	-1.8194724	-1.7947673
H	2.9334443	-1.9545320	-1.3229502
C	2.2338200	-3.5908528	-2.5543129
H	2.5557276	-3.1015569	-3.4831365
H	1.2720430	-4.0854784	-2.7744450
C	3.2568907	-4.6409855	-2.1121917
H	4.2427388	-4.1608787	-1.9966350
H	3.3746065	-5.4077800	-2.8894860
C	2.8490624	-5.2891795	-0.7861473
H	1.9191336	-5.8644138	-0.9275160
H	3.6122603	-6.0063064	-0.4553874
C	2.6245506	-4.2382386	0.3098535
H	3.5788347	-3.7327723	0.5290334
H	2.3014651	-4.7281392	1.2388041
H	-1.4463623	-0.1328703	1.4381754
N	1.2964759	0.6535832	-2.7608036
C	1.6908676	0.8026922	-4.1532467
H	2.0155203	0.1488032	-2.2481745
C	2.2820706	-0.4626011	-4.7729214
H	2.4313737	1.6209148	-4.2592303
H	0.8212198	1.1275785	-4.7417012
C	2.6643840	-0.2984161	-6.2443496
H	1.5597528	-1.2881302	-4.6596727
H	3.1735429	-0.7565557	-4.1917152
C	3.2982312	-1.5566215	-6.8375390
H	3.3587048	0.5504668	-6.3471307
H	1.7659371	-0.0253964	-6.8221033
H	4.2231037	-1.8216162	-6.3062355
H	3.5516199	-1.4201857	-7.8961213
H	2.6169083	-2.4167791	-6.7674876

SCF energy GEOOPT = -7470.128410288 H

ZPE = 3976. kJ/mol

FREEH energy = 4172.32 kJ/mol

FREEH entropy = 1.67823 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	2.19	0.07543	YES	YES
8		a	13.92	0.01323	YES	YES
9		a	18.50	0.03970	YES	YES
10		a	22.34	0.04428	YES	YES
11		a	23.19	0.09033	YES	YES
12		a	27.83	0.11344	YES	YES
13		a	31.07	0.02150	YES	YES
14		a	36.67	0.01145	YES	YES
15		a	38.84	0.16138	YES	YES
16		a	40.25	0.03127	YES	YES
17		a	43.17	0.02154	YES	YES
18		a	44.01	0.02768	YES	YES
19		a	46.77	0.17609	YES	YES
20		a	49.09	0.16373	YES	YES
21		a	52.63	0.06986	YES	YES
22		a	54.05	0.14223	YES	YES
23		a	56.57	0.04852	YES	YES
24		a	60.55	0.07518	YES	YES
25		a	62.98	0.06500	YES	YES
26		a	64.90	0.14052	YES	YES
27		a	69.43	0.22564	YES	YES
28		a	70.46	0.16222	YES	YES
29		a	70.80	0.04169	YES	YES
30		a	76.70	0.06604	YES	YES
31		a	79.23	0.17023	YES	YES
32		a	84.39	1.25185	YES	YES
33		a	84.85	0.03629	YES	YES
34		a	88.30	0.69645	YES	YES
35		a	93.04	0.16282	YES	YES
36		a	97.08	0.44843	YES	YES
37		a	100.26	1.01313	YES	YES
38		a	103.20	0.17958	YES	YES
39		a	112.82	3.59552	YES	YES
40		a	126.50	0.89926	YES	YES
41		a	130.75	0.29552	YES	YES
42		a	134.48	1.16383	YES	YES
43		a	138.39	4.40123	YES	YES
44		a	142.66	2.98650	YES	YES
45		a	145.46	2.38872	YES	YES
46		a	146.47	0.09310	YES	YES
47		a	148.51	0.50094	YES	YES
48		a	149.82	0.65943	YES	YES
49		a	155.05	1.26754	YES	YES
50		a	158.90	1.07139	YES	YES
51		a	162.29	1.06123	YES	YES
52		a	176.61	3.17161	YES	YES
53		a	176.92	4.28651	YES	YES
54		a	182.72	0.12558	YES	YES

55	a	184.00	0.47903	YES	YES
56	a	193.40	1.71034	YES	YES
57	a	201.66	2.03702	YES	YES
58	a	205.13	0.88681	YES	YES
59	a	206.46	1.91763	YES	YES
60	a	209.72	1.55855	YES	YES
61	a	215.66	1.69194	YES	YES
62	a	216.99	0.28809	YES	YES
63	a	218.83	0.15764	YES	YES
64	a	222.84	0.96547	YES	YES
65	a	225.18	1.77567	YES	YES
66	a	229.12	1.58724	YES	YES
67	a	233.85	0.05170	YES	YES
68	a	237.09	0.08482	YES	YES
69	a	238.12	1.25665	YES	YES
70	a	240.16	0.10683	YES	YES
71	a	243.43	0.82408	YES	YES
72	a	247.22	0.15926	YES	YES
73	a	248.36	0.35374	YES	YES
74	a	249.30	0.72130	YES	YES
75	a	268.05	3.13407	YES	YES
76	a	277.51	2.42452	YES	YES
77	a	279.15	1.33900	YES	YES
78	a	290.61	0.29522	YES	YES
79	a	293.46	0.03445	YES	YES
80	a	299.99	0.99635	YES	YES
81	a	306.49	0.67674	YES	YES
82	a	314.00	0.14916	YES	YES
83	a	315.71	0.26356	YES	YES
84	a	329.86	0.35995	YES	YES
85	a	330.85	0.55906	YES	YES
86	a	333.91	0.42558	YES	YES
87	a	336.30	0.45735	YES	YES
88	a	341.46	2.15113	YES	YES
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91	a	368.49	0.93491	YES	YES
92	a	371.97	3.28294	YES	YES
93	a	373.97	0.73496	YES	YES
94	a	377.48	1.73206	YES	YES
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96	a	394.28	0.94041	YES	YES
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98	a	410.57	1.34733	YES	YES
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137	a	731.56	6.04835	YES	YES
138	a	732.48	10.09255	YES	YES
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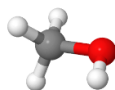
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498	a	3018.45	15.97433	YES	YES
499	a	3018.73	22.41265	YES	YES
500	a	3020.13	35.02180	YES	YES
501	a	3020.93	29.44446	YES	YES
502	a	3021.09	29.72766	YES	YES
503	a	3027.34	19.27462	YES	YES
504	a	3027.62	36.12253	YES	YES
505	a	3028.71	0.41250	YES	YES
506	a	3032.87	0.38376	YES	YES
507	a	3045.44	1.20848	YES	YES
508	a	3046.31	22.20679	YES	YES
509	a	3051.88	0.12270	YES	YES
510	a	3473.48	2.39057	YES	YES

\$end

Double hybrid single point energy = -7462.609810716432 H
 COSMO enery + OC correction = -7470.2746861071 H (in oDFB)

6.2.20 H₂O



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: cs

Cartesian coordinates in Ångström:

C	-0.3322226	0.1433998	0.0000000
O	1.0961566	0.1316259	0.0000000
H	-0.7564967	-0.3393027	0.8971508
H	-0.7564967	-0.3393027	-0.8971508
H	-0.6380192	1.1962799	0.0000000
H	1.3870785	-0.7927002	0.0000000

SCF energy GEOOPT = -115.7836368041 H

ZPE = 130.4 kJ/mol

FREEH energy = 139.26 kJ/mol

FREEH entropy = 0.23919 kJ/mol/K

\$vibrational spectrum

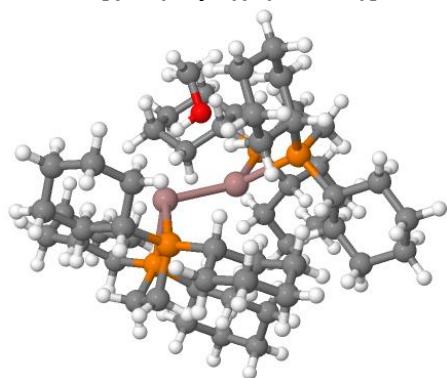
#	mode	symmetry	wave number cm ⁻¹	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	292.69	108.23880	YES	YES
8		a'	1008.65	114.53489	YES	YES
9		a'	1052.66	0.49233	YES	YES
10		a''	1130.93	0.15557	YES	YES
11		a'	1335.47	21.72847	YES	YES
12		a'	1429.72	4.03162	YES	YES
13		a''	1444.98	1.85912	YES	YES
14		a'	1461.40	3.88303	YES	YES
15		a'	2914.46	65.88322	YES	YES
16		a''	2960.91	64.43070	YES	YES
17		a'	3042.99	26.49602	YES	YES
18		a'	3724.49	19.80111	YES	YES

\$end

Double hybrid single point energy = -115.598907709007 H

COSMO energy + OC correction = -115.7907813795 H (in oDFB)

6.2.21 $[\{\text{Ga}(\text{dcpe})\}_2(\text{HOMe})]^{2+}$



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-1.8119855	17.4103192	-2.1630161
Ga	-4.2436345	17.3728123	-1.5945255
P	-1.5290345	18.9837592	-4.0637196
P	-5.9971214	19.0173815	-1.0124205
P	-1.7108377	15.7323112	-3.9584634
P	-5.4821849	15.9715273	-0.0045377
C	-5.0516407	20.9789514	-5.1882256
H	-5.1920936	21.6071693	-4.2911890
H	-6.0411899	20.5764885	-5.4479432
C	-0.6125365	14.3247353	-3.4883585
H	-0.4275565	13.7314807	-4.3997147
C	-4.4645193	14.9601372	1.1512123
H	-4.1058610	15.7201128	1.8659821
C	-4.2057120	16.0520236	-5.2145283
H	-3.7393128	16.4520898	-6.1294472
H	-4.3243075	16.8946394	-4.5163122
C	-7.0164667	19.3428217	-2.5128393
H	-6.3596414	19.9540568	-3.1525289
C	-7.1392749	18.2198505	0.2110051
H	-7.5942311	18.9861143	0.8524465
H	-7.9553884	17.7644772	-0.3672143
C	-3.1138803	22.3733920	-6.0021287
H	-2.7198029	22.9670441	-6.8378898
H	-3.1648051	23.0503713	-5.1333686
C	-2.1450924	21.2254401	-5.6876755
H	-1.1584854	21.6332634	-5.4316486
H	-2.0123450	20.6065467	-6.5895735
C	-4.0940745	19.8272099	-4.8583204
H	-4.0518985	19.1453129	-5.7225514
H	-4.4646876	19.2275874	-4.0111860
C	1.6183272	13.6748803	-2.4715615
H	1.8936070	13.0545339	-3.3398531
H	2.5567196	14.0738229	-2.0629261
C	-7.9658170	14.5144221	-0.1479962
H	-8.4526535	15.3611405	0.3568554
H	-7.6575937	13.8116643	0.6385467
C	-5.4275139	20.6539281	-0.3815072
H	-6.2554323	21.3604413	-0.5638130
C	-0.0816977	20.7295752	-2.4732603
H	-0.8384217	21.5033177	-2.6690066

H	-0.4560928	20.1223201	-1.6294426
C	1.2469979	21.3855821	-2.0783913
H	1.5618296	22.0752621	-2.8783060
H	1.0999592	21.9980780	-1.1780664
C	-7.3151629	18.0280756	-3.2530974
H	-6.3771317	17.4828862	-3.4587235
H	-7.9265428	17.3769185	-2.6055854
C	-4.5149512	21.8511480	-6.3268003
H	-4.4790416	21.2559575	-7.2540471
H	-5.2002680	22.6873916	-6.5192328
C	-8.3050523	20.1365911	-2.2431627
H	-8.0786084	21.0890036	-1.7439640
H	-8.9550077	19.5648628	-1.5610462
C	-4.2075443	21.0845541	-1.2173296
H	-4.4738424	21.1179067	-2.2834737
H	-3.4179881	20.3211887	-1.1057800
C	-3.0942226	13.8113674	-5.5666870
H	-2.4464404	13.0405702	-5.1289784
H	-2.5954674	14.1647546	-6.4838688
C	2.5175889	19.4517406	-3.0831903
H	2.8816210	20.0626865	-3.9252446
H	3.2807831	18.6823509	-2.9025408
C	-4.5633746	22.0125052	1.5629121
H	-5.3555722	22.7708148	1.4541221
H	-4.3120610	21.9763923	2.6316740
C	-9.3589923	19.0897695	-4.2987711
H	-9.8684089	19.3013188	-5.2482450
H	-10.0580723	18.4834445	-3.6991921
C	-5.2239968	13.8830115	1.9447084
H	-6.0815788	14.3204435	2.4749662
H	-5.6253648	13.1301798	1.2495156
C	0.9027479	12.8085806	-1.4313041
H	1.5415368	11.9670709	-1.1320304
H	0.7242296	13.4069657	-0.5214629
C	-8.0822781	18.2819977	-4.5550935
H	-7.4304020	18.8307394	-5.2538268
H	-8.3212723	17.3232779	-5.0356832
C	2.3405387	20.3390921	-1.8482417
H	2.0700851	19.7110272	-0.9827114
H	3.2893032	20.8302633	-1.5946368
C	-3.3418777	22.4288613	0.7367143
H	-2.9857934	23.4165828	1.0579553
H	-2.5169199	21.7203584	0.9211542
C	-6.0675874	13.8285859	-1.7029245
H	-5.6723770	13.0941585	-0.9850112
H	-5.2062061	14.2022321	-2.2793720
C	-5.1033024	20.6457913	1.1194992
H	-4.3435406	19.8750053	1.3085881
H	-5.9958551	20.3873728	1.7069134
C	-6.7348492	14.9868467	-0.9386040
H	-7.0874515	15.7071322	-1.6998894
C	-3.6682113	22.4430498	-0.7595005
C	-8.3118072	12.6680044	-1.8522175
H	-9.0366237	12.2094079	-2.5378273
H	-8.0159772	11.8809719	-1.1394067
C	-8.9639753	13.8252060	-1.0891361
H	-9.8269927	13.4685194	-0.5111511
H	-9.3528299	14.5656015	-1.8085131

C	-1.3248017	13.4503050	-2.4427483
H	-2.2727533	13.0594865	-2.8394292
H	-1.5780954	14.0881126	-1.5810051
C	-4.2786010	13.1927438	2.9383203
H	-3.9505818	13.9248792	3.6944371
H	-4.8266356	12.4097063	3.4794231
C	-5.5670948	15.4495711	-5.5731252
H	-6.2042381	16.2177546	-6.0336251
H	-6.0720536	15.1353038	-4.6437725
C	-3.0542920	12.6026199	2.2313846
H	-3.3789585	11.7993271	1.5491680
H	-2.3821726	12.1360141	2.9636679
C	-3.2326101	14.3798726	0.4376652
H	-3.5575455	13.6630596	-0.3317195
H	-2.6946420	15.1869593	-0.0844195
C	-9.0568983	20.3954238	-3.5567464
H	-9.9861061	20.9414018	-3.3460395
H	-8.4458633	21.0521108	-4.1971699
C	-4.4574984	13.2013324	-5.9277891
H	-4.3153337	12.3746194	-6.6366774
H	-4.8995843	12.7612632	-5.0182538
C	-7.0776686	13.1401813	-2.6273233
H	-6.5954125	12.2958992	-3.1395901
H	-7.3888066	13.8490952	-3.4129401
C	-5.4164456	14.2452171	-6.5079477
H	-6.3965810	13.7908237	-6.7067213
H	-5.0316616	14.5911452	-7.4812091
C	-0.4345173	12.2952969	-1.9711914
H	-0.9653694	11.7121852	-1.2050405
H	-0.2530730	11.6090696	-2.8140957
C	-2.3058712	13.6740862	1.4324446
H	-1.8849239	14.4211631	2.1259200
H	-1.4535369	13.2342036	0.8954139
H	-2.2208677	17.8683061	0.1342929
C	0.0822109	19.8152882	-3.7009254
H	0.3411709	20.4289684	-4.5792511
C	1.1987258	18.7793366	-3.4825395
H	1.3464588	18.1802807	-4.3927140
H	0.8895575	18.0818437	-2.6829230
C	0.7321576	14.8358361	-2.9401896
H	1.2650050	15.4280342	-3.6973462
H	0.5328669	15.5122896	-2.0903671
C	-0.8637590	16.5464892	-5.3879966
H	0.2093096	16.4897006	-5.1662194
H	-1.0316077	15.9478382	-6.2943474
C	-1.2814628	18.0059826	-5.6206571
H	-2.2420387	18.0448106	-6.1502350
H	-0.5444486	18.5154134	-6.2572134
C	-3.2837648	14.9896795	-4.5996958
H	-3.7703341	14.6151396	-3.6812440
C	-2.6867230	20.3519751	-4.5413410
H	-2.7521901	20.9729457	-3.6328034
C	-6.4200486	17.1582981	1.0535687
H	-7.1320782	16.6206344	1.6949690
H	-5.6749405	17.6272903	1.7101121
H	-4.4177150	23.2235102	-0.9675410
H	-2.7761150	22.7016091	-1.3483566
O	-3.0294685	18.0068265	0.6887852

C	-2.6784068	17.9531993	2.0845794
H	-2.2056620	16.9948012	2.3431264
H	-3.6029612	18.0619846	2.6633262
H	-2.0017904	18.7768018	2.3510021

SCF energy GEOOPT = -7371.970295588 H

ZPE = 3730. kJ/mol

FREEH energy = 3918.92 kJ/mol

FREEH entropy = 1.62593 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	6.25	1.53960	YES	YES
8		a	15.26	0.34833	YES	YES
9		a	19.52	0.64436	YES	YES
10		a	23.31	0.17285	YES	YES
11		a	31.79	0.06641	YES	YES
12		a	33.49	0.08692	YES	YES
13		a	34.55	0.18631	YES	YES
14		a	36.98	0.04047	YES	YES
15		a	39.94	0.03587	YES	YES
16		a	40.90	0.34395	YES	YES
17		a	43.20	0.34500	YES	YES
18		a	44.72	0.96493	YES	YES
19		a	46.95	0.34157	YES	YES
20		a	49.83	0.23032	YES	YES
21		a	50.64	0.17764	YES	YES
22		a	54.19	0.04556	YES	YES
23		a	56.37	0.07736	YES	YES
24		a	58.11	0.14972	YES	YES
25		a	60.20	0.22543	YES	YES
26		a	63.62	0.86252	YES	YES
27		a	66.48	0.21892	YES	YES
28		a	69.28	0.62718	YES	YES
29		a	71.09	0.35062	YES	YES
30		a	71.71	0.25229	YES	YES
31		a	74.22	2.90120	YES	YES
32		a	78.21	0.14690	YES	YES
33		a	79.77	0.92765	YES	YES
34		a	82.14	1.28135	YES	YES
35		a	87.84	0.27066	YES	YES
36		a	91.14	1.23426	YES	YES
37		a	97.01	0.31757	YES	YES
38		a	100.10	0.23767	YES	YES
39		a	110.97	3.06116	YES	YES
40		a	119.79	1.51391	YES	YES
41		a	120.44	2.24276	YES	YES
42		a	128.50	0.22078	YES	YES
43		a	130.35	0.87992	YES	YES
44		a	134.03	0.11439	YES	YES
45		a	139.51	0.19662	YES	YES

46	a	140.56	1.07432	YES	YES
47	a	144.19	0.68493	YES	YES
48	a	151.12	0.89169	YES	YES
49	a	151.69	4.97875	YES	YES
50	a	157.02	0.77162	YES	YES
51	a	167.93	0.91369	YES	YES
52	a	177.62	0.64599	YES	YES
53	a	180.38	3.58522	YES	YES
54	a	186.48	1.13986	YES	YES
55	a	193.02	2.85323	YES	YES
56	a	197.81	2.77559	YES	YES
57	a	200.68	5.13366	YES	YES
58	a	211.43	0.13561	YES	YES
59	a	215.01	0.64650	YES	YES
60	a	217.75	0.11293	YES	YES
61	a	221.99	0.16656	YES	YES
62	a	223.22	0.14393	YES	YES
63	a	226.11	0.59392	YES	YES
64	a	227.36	0.24359	YES	YES
65	a	230.63	0.08722	YES	YES
66	a	231.82	0.15805	YES	YES
67	a	232.60	1.05696	YES	YES
68	a	239.69	0.45491	YES	YES
69	a	243.14	0.01031	YES	YES
70	a	244.78	1.70453	YES	YES
71	a	250.40	0.80219	YES	YES
72	a	254.42	2.21962	YES	YES
73	a	266.50	0.90740	YES	YES
74	a	279.22	0.69533	YES	YES
75	a	281.85	0.92617	YES	YES
76	a	287.49	0.42560	YES	YES
77	a	297.89	3.42716	YES	YES
78	a	304.86	0.47606	YES	YES
79	a	308.65	0.11220	YES	YES
80	a	313.98	1.28411	YES	YES
81	a	329.12	1.21500	YES	YES
82	a	329.51	0.11422	YES	YES
83	a	331.69	0.58309	YES	YES
84	a	336.87	2.31680	YES	YES
85	a	337.35	0.46159	YES	YES
86	a	338.72	1.61801	YES	YES
87	a	363.08	7.85183	YES	YES
88	a	377.53	0.20875	YES	YES
89	a	379.36	5.14416	YES	YES
90	a	381.64	0.81915	YES	YES
91	a	389.32	0.31724	YES	YES
92	a	393.12	3.04411	YES	YES
93	a	405.74	0.10218	YES	YES
94	a	416.12	1.04414	YES	YES
95	a	420.66	2.68434	YES	YES
96	a	422.12	4.55116	YES	YES
97	a	425.82	3.97612	YES	YES
98	a	429.00	1.06993	YES	YES
99	a	429.76	0.24454	YES	YES
100	a	430.95	0.07283	YES	YES
101	a	432.03	0.63816	YES	YES
102	a	432.26	0.14316	YES	YES
103	a	432.52	0.96756	YES	YES

104	a	433.44	0.59618	YES	YES
105	a	436.33	2.16542	YES	YES
106	a	436.56	0.70427	YES	YES
107	a	447.87	2.73532	YES	YES
108	a	456.43	5.30822	YES	YES
109	a	462.80	4.21487	YES	YES
110	a	468.34	3.94310	YES	YES
111	a	490.76	5.67951	YES	YES
112	a	492.00	3.26298	YES	YES
113	a	494.42	4.44574	YES	YES
114	a	494.87	0.36001	YES	YES
115	a	501.74	0.76781	YES	YES
116	a	502.66	1.53895	YES	YES
117	a	509.11	8.92466	YES	YES
118	a	513.15	9.21575	YES	YES
119	a	532.36	16.25014	YES	YES
120	a	629.46	13.79927	YES	YES
121	a	630.30	24.33945	YES	YES
122	a	641.26	11.00818	YES	YES
123	a	660.58	12.56488	YES	YES
124	a	699.80	1.94537	YES	YES
125	a	714.32	1.21510	YES	YES
126	a	719.05	1.89873	YES	YES
127	a	728.59	8.78978	YES	YES
128	a	731.53	3.68670	YES	YES
129	a	733.62	4.00887	YES	YES
130	a	735.25	10.11832	YES	YES
131	a	740.07	4.57649	YES	YES
132	a	771.41	16.96430	YES	YES
133	a	773.05	0.10569	YES	YES
134	a	773.09	0.17235	YES	YES
135	a	773.78	5.00919	YES	YES
136	a	774.12	0.55089	YES	YES
137	a	774.84	0.18401	YES	YES
138	a	775.66	0.06032	YES	YES
139	a	775.83	0.65907	YES	YES
140	a	777.42	0.27469	YES	YES
141	a	779.49	20.47598	YES	YES
142	a	806.15	0.57435	YES	YES
143	a	808.05	1.52303	YES	YES
144	a	810.11	11.76834	YES	YES
145	a	810.50	5.55919	YES	YES
146	a	811.92	3.63403	YES	YES
147	a	812.94	3.78128	YES	YES
148	a	813.26	0.62075	YES	YES
149	a	817.05	2.91999	YES	YES
150	a	831.95	7.24674	YES	YES
151	a	832.10	1.67029	YES	YES
152	a	836.90	2.42083	YES	YES
153	a	837.50	3.12527	YES	YES
154	a	837.93	2.19095	YES	YES
155	a	838.27	0.42606	YES	YES
156	a	839.00	4.37873	YES	YES
157	a	840.02	10.52088	YES	YES
158	a	847.39	26.31287	YES	YES
159	a	849.56	15.15883	YES	YES
160	a	873.67	4.87200	YES	YES
161	a	874.26	2.10008	YES	YES

162	a	874.63	1.82371	YES	YES
163	a	876.50	1.83477	YES	YES
164	a	876.96	2.07686	YES	YES
165	a	877.18	3.04762	YES	YES
166	a	877.94	3.37976	YES	YES
167	a	878.40	1.45225	YES	YES
168	a	879.12	3.68947	YES	YES
169	a	879.89	0.27201	YES	YES
170	a	880.15	0.68783	YES	YES
171	a	881.41	2.22495	YES	YES
172	a	881.94	1.26698	YES	YES
173	a	882.79	11.72797	YES	YES
174	a	883.39	2.58232	YES	YES
175	a	885.60	2.56710	YES	YES
176	a	902.73	2.75182	YES	YES
177	a	903.57	3.72397	YES	YES
178	a	904.93	2.62198	YES	YES
179	a	905.45	1.70353	YES	YES
180	a	907.10	1.58161	YES	YES
181	a	909.46	0.96052	YES	YES
182	a	910.08	0.69549	YES	YES
183	a	911.01	0.98651	YES	YES
184	a	974.91	123.00962	YES	YES
185	a	983.75	2.04422	YES	YES
186	a	985.73	2.60443	YES	YES
187	a	987.61	5.86262	YES	YES
188	a	988.20	7.20959	YES	YES
189	a	988.54	14.04278	YES	YES
190	a	989.31	17.73301	YES	YES
191	a	989.69	2.67082	YES	YES
192	a	990.85	23.75586	YES	YES
193	a	991.20	0.20106	YES	YES
194	a	994.96	0.75530	YES	YES
195	a	1013.72	0.57176	YES	YES
196	a	1014.90	3.44640	YES	YES
197	a	1015.60	0.43645	YES	YES
198	a	1017.16	1.06557	YES	YES
199	a	1017.49	0.46765	YES	YES
200	a	1018.54	0.94107	YES	YES
201	a	1020.98	0.55531	YES	YES
202	a	1021.65	0.30296	YES	YES
203	a	1030.11	0.97709	YES	YES
204	a	1030.70	0.88204	YES	YES
205	a	1032.88	1.95863	YES	YES
206	a	1035.84	0.71612	YES	YES
207	a	1037.10	1.81050	YES	YES
208	a	1037.65	2.83849	YES	YES
209	a	1038.29	1.51314	YES	YES
210	a	1040.92	1.87601	YES	YES
211	a	1056.46	2.63148	YES	YES
212	a	1057.30	1.98825	YES	YES
213	a	1057.95	2.05723	YES	YES
214	a	1059.46	2.04123	YES	YES
215	a	1060.86	1.91363	YES	YES
216	a	1063.31	1.50190	YES	YES
217	a	1065.25	2.31445	YES	YES
218	a	1067.41	2.00445	YES	YES
219	a	1070.21	0.42902	YES	YES

220	a	1070.88	0.83484	YES	YES
221	a	1071.16	0.88178	YES	YES
222	a	1071.73	0.03344	YES	YES
223	a	1072.10	8.95161	YES	YES
224	a	1072.60	11.33716	YES	YES
225	a	1072.75	0.08600	YES	YES
226	a	1074.06	0.28187	YES	YES
227	a	1074.53	0.09466	YES	YES
228	a	1075.37	3.39942	YES	YES
229	a	1080.63	3.67218	YES	YES
230	a	1089.64	5.44004	YES	YES
231	a	1090.07	1.52970	YES	YES
232	a	1092.41	4.62920	YES	YES
233	a	1094.22	8.51879	YES	YES
234	a	1100.65	1.30785	YES	YES
235	a	1104.08	1.61069	YES	YES
236	a	1109.12	6.49690	YES	YES
237	a	1112.91	12.30384	YES	YES
238	a	1118.62	5.94842	YES	YES
239	a	1121.14	0.53504	YES	YES
240	a	1130.34	2.04150	YES	YES
241	a	1158.55	6.02212	YES	YES
242	a	1159.90	4.41960	YES	YES
243	a	1161.46	15.76034	YES	YES
244	a	1165.96	7.83686	YES	YES
245	a	1166.98	11.68896	YES	YES
246	a	1167.71	6.05372	YES	YES
247	a	1168.80	10.89216	YES	YES
248	a	1170.19	4.47206	YES	YES
249	a	1175.09	4.65140	YES	YES
250	a	1177.19	16.96248	YES	YES
251	a	1178.18	3.13603	YES	YES
252	a	1179.44	4.86324	YES	YES
253	a	1187.00	1.25522	YES	YES
254	a	1190.00	0.56995	YES	YES
255	a	1191.11	1.46681	YES	YES
256	a	1209.43	1.67681	YES	YES
257	a	1232.61	0.87608	YES	YES
258	a	1236.93	0.88393	YES	YES
259	a	1244.00	0.58210	YES	YES
260	a	1244.99	1.45321	YES	YES
261	a	1245.90	1.20322	YES	YES
262	a	1246.77	0.34208	YES	YES
263	a	1246.94	0.19512	YES	YES
264	a	1247.76	0.48470	YES	YES
265	a	1249.50	0.15019	YES	YES
266	a	1250.14	0.11053	YES	YES
267	a	1250.52	1.22232	YES	YES
268	a	1253.55	1.29892	YES	YES
269	a	1253.74	1.78534	YES	YES
270	a	1254.35	2.75629	YES	YES
271	a	1255.23	7.15428	YES	YES
272	a	1255.68	4.20947	YES	YES
273	a	1256.93	0.79435	YES	YES
274	a	1257.46	2.21013	YES	YES
275	a	1258.30	5.12989	YES	YES
276	a	1259.09	0.80612	YES	YES
277	a	1259.79	0.85738	YES	YES

278	a	1261.07	0.51991	YES	YES
279	a	1261.67	3.15998	YES	YES
280	a	1262.36	1.86073	YES	YES
281	a	1264.67	1.06996	YES	YES
282	a	1266.48	0.89826	YES	YES
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286	a	1282.01	0.56006	YES	YES
287	a	1283.01	0.77376	YES	YES
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289	a	1284.69	6.03769	YES	YES
290	a	1287.60	3.67320	YES	YES
291	a	1289.89	3.23359	YES	YES
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293	a	1306.11	0.72122	YES	YES
294	a	1306.81	0.96315	YES	YES
295	a	1308.99	1.20885	YES	YES
296	a	1310.36	0.58986	YES	YES
297	a	1311.77	2.60866	YES	YES
298	a	1314.20	1.09517	YES	YES
299	a	1315.13	1.78249	YES	YES
300	a	1315.87	0.31930	YES	YES
301	a	1319.18	5.10475	YES	YES
302	a	1319.81	2.94184	YES	YES
303	a	1321.29	1.64766	YES	YES
304	a	1321.88	11.95030	YES	YES
305	a	1322.08	19.01400	YES	YES
306	a	1322.35	2.80368	YES	YES
307	a	1322.87	17.97604	YES	YES
308	a	1323.58	1.52971	YES	YES
309	a	1324.51	0.42538	YES	YES
310	a	1324.53	4.08699	YES	YES
311	a	1324.82	2.33748	YES	YES
312	a	1325.17	0.36083	YES	YES
313	a	1326.19	17.51951	YES	YES
314	a	1327.39	4.08470	YES	YES
315	a	1328.13	1.35737	YES	YES
316	a	1328.72	17.60001	YES	YES
317	a	1330.04	8.62839	YES	YES
318	a	1335.90	0.38870	YES	YES
319	a	1336.12	0.42032	YES	YES
320	a	1336.55	0.69807	YES	YES
321	a	1337.05	0.24154	YES	YES
322	a	1337.34	0.35965	YES	YES
323	a	1337.84	0.21313	YES	YES
324	a	1338.30	0.00554	YES	YES
325	a	1338.79	0.58304	YES	YES
326	a	1343.54	0.83587	YES	YES
327	a	1343.82	0.91475	YES	YES
328	a	1344.34	2.95963	YES	YES
329	a	1345.68	0.41756	YES	YES
330	a	1346.26	0.86160	YES	YES
331	a	1347.24	0.80268	YES	YES
332	a	1348.28	2.95600	YES	YES
333	a	1349.59	1.31049	YES	YES
334	a	1400.99	5.78308	YES	YES
335	a	1404.01	9.16138	YES	YES

336	a	1405.38	6.08923	YES	YES
337	a	1407.30	8.05003	YES	YES
338	a	1419.75	0.77427	YES	YES
339	a	1423.67	5.90766	YES	YES
340	a	1425.49	4.52130	YES	YES
341	a	1427.47	6.80716	YES	YES
342	a	1428.36	1.78650	YES	YES
343	a	1429.34	0.95611	YES	YES
344	a	1430.84	1.08901	YES	YES
345	a	1432.64	1.26687	YES	YES
346	a	1433.48	0.82327	YES	YES
347	a	1434.14	3.00860	YES	YES
348	a	1434.73	2.11254	YES	YES
349	a	1435.47	3.64139	YES	YES
350	a	1435.94	1.67720	YES	YES
351	a	1436.54	8.73481	YES	YES
352	a	1436.62	7.21009	YES	YES
353	a	1437.92	5.20808	YES	YES
354	a	1437.96	0.83770	YES	YES
355	a	1438.22	5.84432	YES	YES
356	a	1438.61	3.07054	YES	YES
357	a	1438.84	15.11555	YES	YES
358	a	1439.17	0.56547	YES	YES
359	a	1439.24	2.84105	YES	YES
360	a	1439.60	10.27745	YES	YES
361	a	1439.83	2.05835	YES	YES
362	a	1441.02	2.88299	YES	YES
363	a	1441.68	0.50943	YES	YES
364	a	1442.05	6.17978	YES	YES
365	a	1443.00	34.28170	YES	YES
366	a	1443.20	3.88323	YES	YES
367	a	1443.73	17.81368	YES	YES
368	a	1444.35	4.11826	YES	YES
369	a	1444.91	19.64006	YES	YES
370	a	1446.04	3.90139	YES	YES
371	a	1447.09	8.29684	YES	YES
372	a	1452.50	0.07532	YES	YES
373	a	1453.43	3.57501	YES	YES
374	a	1453.62	4.03260	YES	YES
375	a	1454.35	0.34997	YES	YES
376	a	1454.56	2.14250	YES	YES
377	a	1455.07	2.27555	YES	YES
378	a	1455.99	1.84550	YES	YES
379	a	1457.78	0.63305	YES	YES
380	a	1462.65	5.67388	YES	YES
381	a	2911.80	27.96639	YES	YES
382	a	2914.27	57.25676	YES	YES
383	a	2919.56	18.47430	YES	YES
384	a	2920.64	0.68475	YES	YES
385	a	2925.16	12.25340	YES	YES
386	a	2926.41	5.34982	YES	YES
387	a	2929.58	5.60501	YES	YES
388	a	2931.22	21.99346	YES	YES
389	a	2938.43	14.32021	YES	YES
390	a	2938.69	26.48850	YES	YES
391	a	2939.76	22.22796	YES	YES
392	a	2941.57	18.17863	YES	YES
393	a	2941.77	5.14619	YES	YES

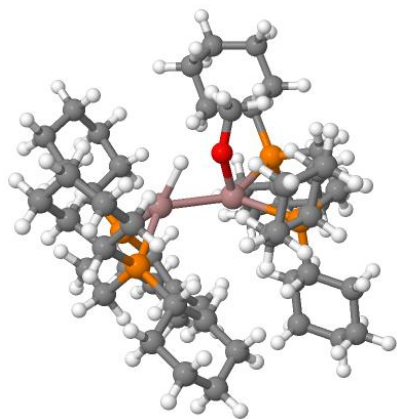
394	a	2942.66	10.45755	YES	YES
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396	a	2943.31	8.99932	YES	YES
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400	a	2945.64	11.20805	YES	YES
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409	a	2952.24	3.76174	YES	YES
410	a	2954.31	37.64141	YES	YES
411	a	2955.21	4.16885	YES	YES
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413	a	2955.83	10.12128	YES	YES
414	a	2956.39	6.96326	YES	YES
415	a	2957.47	5.90783	YES	YES
416	a	2958.46	23.39598	YES	YES
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418	a	2959.50	26.87666	YES	YES
419	a	2959.68	43.94515	YES	YES
420	a	2959.87	32.30996	YES	YES
421	a	2960.20	38.44115	YES	YES
422	a	2960.68	25.68580	YES	YES
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424	a	2962.73	31.16430	YES	YES
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426	a	2964.46	27.21234	YES	YES
427	a	2965.87	19.74209	YES	YES
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430	a	2977.91	12.18207	YES	YES
431	a	2981.68	13.50270	YES	YES
432	a	2983.00	25.08076	YES	YES
433	a	2985.12	6.12918	YES	YES
434	a	2985.56	16.38886	YES	YES
435	a	2985.81	3.98719	YES	YES
436	a	2987.97	6.69916	YES	YES
437	a	2991.15	34.40746	YES	YES
438	a	2992.37	9.97127	YES	YES
439	a	2993.49	23.79679	YES	YES
440	a	2994.92	28.78164	YES	YES
441	a	2998.38	22.05057	YES	YES
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443	a	2999.72	22.07762	YES	YES
444	a	3000.74	19.56322	YES	YES
445	a	3002.60	18.20167	YES	YES
446	a	3003.52	34.36819	YES	YES
447	a	3005.81	12.63885	YES	YES
448	a	3007.19	16.06485	YES	YES
449	a	3007.45	31.89802	YES	YES
450	a	3007.55	6.42729	YES	YES
451	a	3008.92	18.81915	YES	YES

452	a	3009.59	23.83447	YES	YES
453	a	3010.21	23.39358	YES	YES
454	a	3011.25	18.32836	YES	YES
455	a	3012.37	17.35961	YES	YES
456	a	3012.99	32.12803	YES	YES
457	a	3013.26	15.55026	YES	YES
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459	a	3015.49	26.37769	YES	YES
460	a	3015.79	28.75807	YES	YES
461	a	3016.33	17.65614	YES	YES
462	a	3016.67	13.05374	YES	YES
463	a	3016.97	56.04565	YES	YES
464	a	3017.06	14.64269	YES	YES
465	a	3017.47	38.10863	YES	YES
466	a	3017.63	21.56489	YES	YES
467	a	3018.16	34.63575	YES	YES
468	a	3018.34	22.02954	YES	YES
469	a	3018.61	18.12990	YES	YES
470	a	3018.75	25.18441	YES	YES
471	a	3019.43	22.38270	YES	YES
472	a	3022.78	31.73705	YES	YES
473	a	3023.33	14.40830	YES	YES
474	a	3028.11	0.78431	YES	YES
475	a	3029.92	1.90293	YES	YES
476	a	3030.78	7.96827	YES	YES
477	a	3039.33	0.79364	YES	YES
478	a	3044.02	1.01348	YES	YES
479	a	3052.34	12.76965	YES	YES
480	a	3288.70	487.20134	YES	YES

\$end

Double hybrid single point energy = -7364.660701520127 H
 COSMO energy + OC correction = -7372.1170406266 H (in oDFB)

6.2.22 [{Ga(dcpe)}₂(H-OMe)]²⁺ (Transition State)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-1.9641607	17.3490663	-2.4150484
Ga	-4.1368328	17.4807333	-1.2484970
P	-1.5266385	18.9597120	-4.1514037
P	-5.9796118	19.0243290	-0.8948943

P	-1.7395523	15.6889084	-4.1003547
P	-5.4158143	15.9939341	0.1729033
C	-5.0698684	20.9411338	-5.2145810
H	-5.2108249	21.5454305	-4.3015593
H	-6.0574655	20.5374195	-5.4789288
C	-0.7031874	14.2724543	-3.5428056
H	-0.5071504	13.6295474	-4.4168548
C	-4.4473090	14.9679248	1.3575942
H	-4.1163338	15.7145713	2.1007651
C	-4.2162174	16.1086780	-5.3339683
H	-3.7269013	16.5483399	-6.2180188
H	-4.3363767	16.9134849	-4.5941356
C	-6.9604940	19.2970814	-2.4317054
H	-6.2875432	19.8924989	-3.0699057
C	-7.1368568	18.2101896	0.3078029
H	-7.6149788	18.9742388	0.9349516
H	-7.9348414	17.7458800	-0.2881931
C	-3.1470835	22.3729293	-6.0011587
H	-2.7610778	22.9893487	-6.8240139
H	-3.2018445	23.0290913	-5.1168539
C	-2.1665482	21.2275020	-5.7155469
H	-1.1830246	21.6372255	-5.4498582
H	-2.0288148	20.6316990	-6.6324250
C	-4.1031459	19.7887026	-4.9152154
H	-4.0580825	19.1281405	-5.7957429
H	-4.4647565	19.1700365	-4.0789319
C	1.4519802	13.6149973	-2.3757850
H	1.7425136	12.9229698	-3.1826256
H	2.3850763	14.0094307	-1.9512497
C	-7.8519603	14.4983208	-0.1647643
H	-8.3846186	15.3221659	0.3315977
H	-7.5804752	13.7790037	0.6203391
C	-5.4739601	20.6827089	-0.2769962
H	-6.3456192	21.3482206	-0.3977114
C	-0.1408447	20.6395918	-2.4483671
H	-0.8934058	21.4197225	-2.6341721
H	-0.5372227	19.9953562	-1.6441069
C	1.1735562	21.2818177	-1.9877176
H	1.5087621	22.0073360	-2.7466152
H	0.9969397	21.8529399	-1.0658550
C	-7.2426337	17.9669776	-3.1494371
H	-6.3011425	17.4189642	-3.3203100
H	-7.8716883	17.3323042	-2.5025385
C	-4.5443020	21.8445187	-6.3336980
H	-4.5056989	21.2718099	-7.2749281
H	-5.2375887	22.6787939	-6.5048242
C	-8.2540778	20.0986455	-2.2101145
H	-8.0371808	21.0626583	-1.7297712
H	-8.9189979	19.5442060	-1.5279369
C	-4.3204260	21.1908870	-1.1654261
H	-4.6398430	21.2345599	-2.2171142
H	-3.4897761	20.4680699	-1.1035422
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H	-2.5242996	13.0497351	-5.3294884
H	-2.6102948	14.2193518	-6.6515825
C	2.4828801	19.3992547	-3.0389144
H	2.8679111	20.0484482	-3.8420591
H	3.2445192	18.6256447	-2.8701781

C	-4.5765380	22.0410483	1.6539323
H	-5.4120262	22.7581239	1.6059661
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C	-9.2648668	19.0060046	-4.2627699
H	-9.7539752	19.1958430	-5.2274386
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H	0.4496847	13.5280802	-0.4625959
C	-7.9830494	18.1937159	-4.4721995
H	-7.3161084	18.7265016	-5.1691318
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C	2.2644953	20.2297063	-1.7713619
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H	-5.4861240	13.1407971	-0.8945835
H	-4.9579070	14.2962824	-2.1233306
C	-5.0678623	20.6584112	1.2044478
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H	-5.9120676	20.3372839	1.8317079
C	-6.5838022	15.0133571	-0.8644680
H	-6.9002529	15.7482717	-1.6263352
C	-3.8304306	22.5669414	-0.7018535
C	-8.0561375	12.6956086	-1.9368838
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H	-7.7901465	11.8941328	-1.2284515
C	-8.7765675	13.8192792	-1.1850999
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H	-9.1336067	14.5729781	-1.9072372
C	-1.4989140	13.4810544	-2.4872925
H	-2.4267600	13.0816331	-2.9210347
H	-1.7950719	14.1784817	-1.6855774
C	-4.3356889	13.1807940	3.1305087
H	-4.0464001	13.9059515	3.9085901
H	-4.9040814	12.3892709	3.6371327
C	-5.5775642	15.5465584	-5.7536869
H	-6.1879256	16.3468134	-6.1946140
H	-6.1120555	15.2013922	-4.8528030
C	-3.0775239	12.6036509	2.4739362
H	-3.3668561	11.8031538	1.7726838
H	-2.4356738	12.1358205	3.2320757
C	-3.1864164	14.3917933	0.6862654
H	-3.4834657	13.6742737	-0.0931300
H	-2.6270208	15.1945368	0.1805537
C	-8.9784764	20.3277244	-3.5441326
H	-9.9115892	20.8782593	-3.3648167
H	-8.3540074	20.9702033	-4.1859956
C	-4.5096805	13.2902016	-6.1753829
H	-4.3700930	12.4880493	-6.9123268
H	-4.9865050	12.8281027	-5.2951205
C	-6.7853962	13.2110775	-2.6195857

H	-6.2569627	12.3901883	-3.1245976
H	-7.0609276	13.9376230	-3.4022007
C	-5.4248845	14.3822354	-6.7374497
H	-6.4087022	13.9615697	-6.9855211
H	-5.0021032	14.7607536	-7.6825480
C	-0.6688760	12.3417956	-1.8854608
H	-1.2583215	11.8325561	-1.1095243
H	-0.4654550	11.5900911	-2.6649738
C	-2.2996201	13.6842666	1.7159689
H	-1.9124002	14.4287238	2.4314356
H	-1.4239315	13.2512269	1.2122115
H	-1.8469573	17.7996677	-0.7192333
C	0.0660061	19.7807271	-3.7101931
H	0.3432033	20.4326191	-4.5550920
C	1.1798063	18.7386706	-3.5049016
H	1.3569046	18.1812637	-4.4364062
H	0.8497260	18.0082756	-2.7453683
C	0.6347975	14.7706184	-2.9661492
H	1.2223467	15.2875210	-3.7378901
H	0.4246289	15.5117093	-2.1751136
C	-0.8434909	16.5238324	-5.4852336
H	0.2208642	16.4584565	-5.2256049
H	-0.9812400	15.9448535	-6.4090619
C	-1.2451983	17.9940483	-5.7095282
H	-2.1882169	18.0482623	-6.2684436
H	-0.4841573	18.5014812	-6.3185134
C	-3.3216278	15.0012886	-4.7578128
H	-3.8194779	14.6092824	-3.8533338
C	-2.6993686	20.3203465	-4.5920843
H	-2.7687071	20.9129492	-3.6640770
C	-6.4397559	17.1544688	1.1815906
H	-7.1771577	16.6011609	1.7794564
H	-5.7454608	17.6346847	1.8858173
H	-4.6297083	23.3105504	-0.8517353
H	-2.9855085	22.8857157	-1.3293219
O	-2.8405888	18.2049840	0.1376718
C	-2.5867143	17.9413751	1.5162619
H	-2.1347596	16.9467709	1.6584626
H	-3.5141682	17.9913169	2.1066742
H	-1.8951251	18.6988019	1.9112447

SCF energy GEOOPT = -7371.954494974 H

ZPE = 3716. kJ/mol

FREEH energy = 3902.07 kJ/mol

FREEH entropy = 1.59765 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1		a	-1057.34	0.00000	YES	YES
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7			0.00	0.00000	-	-
8		a	7.20	0.05992	YES	YES
9		a	17.25	0.04854	YES	YES

10	a	18.39	0.01895	YES	YES
11	a	28.48	0.04829	YES	YES
12	a	28.83	0.07213	YES	YES
13	a	31.81	0.00032	YES	YES
14	a	32.88	0.01586	YES	YES
15	a	35.80	0.05993	YES	YES
16	a	38.27	0.00376	YES	YES
17	a	39.20	0.08458	YES	YES
18	a	41.54	0.50280	YES	YES
19	a	43.66	0.14789	YES	YES
20	a	48.25	0.00846	YES	YES
21	a	49.81	0.08091	YES	YES
22	a	52.55	0.03439	YES	YES
23	a	54.23	0.15399	YES	YES
24	a	56.92	0.18868	YES	YES
25	a	60.10	0.18651	YES	YES
26	a	62.13	0.30989	YES	YES
27	a	64.88	0.21432	YES	YES
28	a	66.30	0.25012	YES	YES
29	a	68.25	0.13176	YES	YES
30	a	71.76	0.08433	YES	YES
31	a	73.78	0.04257	YES	YES
32	a	77.45	0.10898	YES	YES
33	a	82.00	0.85072	YES	YES
34	a	85.08	0.15286	YES	YES
35	a	94.26	0.86105	YES	YES
36	a	101.49	0.25817	YES	YES
37	a	106.79	1.45812	YES	YES
38	a	116.80	7.97934	YES	YES
39	a	119.17	3.60925	YES	YES
40	a	125.46	0.42274	YES	YES
41	a	129.05	0.81485	YES	YES
42	a	134.82	0.09815	YES	YES
43	a	136.43	1.42465	YES	YES
44	a	138.69	0.55216	YES	YES
45	a	141.14	1.17132	YES	YES
46	a	145.11	4.03154	YES	YES
47	a	153.27	1.72132	YES	YES
48	a	156.12	1.77727	YES	YES
49	a	163.27	0.76515	YES	YES
50	a	165.61	1.80963	YES	YES
51	a	170.68	0.90730	YES	YES
52	a	181.98	2.95855	YES	YES
53	a	186.35	1.07813	YES	YES
54	a	188.50	0.88038	YES	YES
55	a	200.33	1.87779	YES	YES
56	a	207.64	0.20573	YES	YES
57	a	212.88	0.65752	YES	YES
58	a	213.72	3.98114	YES	YES
59	a	216.26	0.72366	YES	YES
60	a	220.43	0.57269	YES	YES
61	a	221.65	0.15720	YES	YES
62	a	223.25	0.42654	YES	YES
63	a	227.27	0.08705	YES	YES
64	a	228.09	0.23138	YES	YES
65	a	229.20	0.23272	YES	YES
66	a	233.59	0.09217	YES	YES
67	a	237.23	0.74996	YES	YES

68	a	240.08	0.00759	YES	YES
69	a	244.40	0.65370	YES	YES
70	a	246.70	0.95463	YES	YES
71	a	256.87	0.43956	YES	YES
72	a	270.52	21.11884	YES	YES
73	a	280.18	5.37174	YES	YES
74	a	282.08	1.12257	YES	YES
75	a	286.73	8.26621	YES	YES
76	a	290.01	17.13334	YES	YES
77	a	299.24	2.15802	YES	YES
78	a	307.02	0.02916	YES	YES
79	a	309.69	0.28166	YES	YES
80	a	313.84	0.08388	YES	YES
81	a	327.89	0.27271	YES	YES
82	a	329.70	1.51948	YES	YES
83	a	331.15	0.31005	YES	YES
84	a	336.81	5.27547	YES	YES
85	a	339.67	1.55253	YES	YES
86	a	342.99	0.74974	YES	YES
87	a	360.46	34.86679	YES	YES
88	a	370.50	14.04369	YES	YES
89	a	380.34	2.67966	YES	YES
90	a	382.19	5.58838	YES	YES
91	a	383.74	0.44909	YES	YES
92	a	393.23	0.40054	YES	YES
93	a	397.79	0.93906	YES	YES
94	a	406.09	0.16384	YES	YES
95	a	413.42	0.75242	YES	YES
96	a	419.84	1.89799	YES	YES
97	a	421.95	4.67648	YES	YES
98	a	425.97	3.64803	YES	YES
99	a	428.26	0.24275	YES	YES
100	a	429.13	0.54225	YES	YES
101	a	430.16	0.10672	YES	YES
102	a	430.82	0.08320	YES	YES
103	a	431.25	0.16310	YES	YES
104	a	432.12	0.88240	YES	YES
105	a	433.37	0.67282	YES	YES
106	a	436.78	2.11260	YES	YES
107	a	437.28	0.73057	YES	YES
108	a	445.29	3.57317	YES	YES
109	a	457.23	4.75126	YES	YES
110	a	462.74	5.62404	YES	YES
111	a	469.00	3.09015	YES	YES
112	a	491.94	5.19050	YES	YES
113	a	493.52	3.27750	YES	YES
114	a	494.35	1.94316	YES	YES
115	a	496.33	1.69952	YES	YES
116	a	502.43	2.27018	YES	YES
117	a	503.26	0.26890	YES	YES
118	a	510.05	8.82438	YES	YES
119	a	515.01	11.90509	YES	YES
120	a	629.22	7.28395	YES	YES
121	a	630.18	34.66088	YES	YES
122	a	641.41	9.97628	YES	YES
123	a	657.31	12.85658	YES	YES
124	a	700.30	1.51020	YES	YES
125	a	715.71	1.58414	YES	YES

126	a	720.27	1.82603	YES	YES
127	a	731.70	6.98011	YES	YES
128	a	731.88	3.47500	YES	YES
129	a	735.43	3.17566	YES	YES
130	a	738.06	5.36189	YES	YES
131	a	740.24	4.11928	YES	YES
132	a	767.93	30.94780	YES	YES
133	a	770.29	1.96973	YES	YES
134	a	772.94	0.38235	YES	YES
135	a	773.77	0.13565	YES	YES
136	a	774.50	0.18602	YES	YES
137	a	774.84	1.11287	YES	YES
138	a	775.13	0.18326	YES	YES
139	a	775.54	0.19607	YES	YES
140	a	775.91	0.51585	YES	YES
141	a	781.28	16.98602	YES	YES
142	a	792.03	12.71965	YES	YES
143	a	805.20	0.78691	YES	YES
144	a	808.57	2.24736	YES	YES
145	a	809.76	10.11781	YES	YES
146	a	810.23	8.47190	YES	YES
147	a	811.98	2.62825	YES	YES
148	a	813.04	2.61834	YES	YES
149	a	813.81	1.11511	YES	YES
150	a	816.49	3.26968	YES	YES
151	a	831.58	6.56804	YES	YES
152	a	832.58	2.94039	YES	YES
153	a	836.77	2.84838	YES	YES
154	a	837.60	0.40234	YES	YES
155	a	837.95	5.14731	YES	YES
156	a	838.55	1.16832	YES	YES
157	a	838.99	4.25794	YES	YES
158	a	839.30	7.13700	YES	YES
159	a	847.55	15.85901	YES	YES
160	a	850.91	16.57577	YES	YES
161	a	871.21	1.10944	YES	YES
162	a	873.00	4.68778	YES	YES
163	a	874.31	1.59924	YES	YES
164	a	876.23	2.00106	YES	YES
165	a	876.78	5.11338	YES	YES
166	a	877.28	0.33935	YES	YES
167	a	877.65	3.17873	YES	YES
168	a	878.11	1.37209	YES	YES
169	a	878.99	3.33482	YES	YES
170	a	879.88	3.01380	YES	YES
171	a	880.42	0.87239	YES	YES
172	a	880.71	3.65413	YES	YES
173	a	881.61	1.78135	YES	YES
174	a	883.22	3.72809	YES	YES
175	a	883.52	11.23844	YES	YES
176	a	885.97	0.47393	YES	YES
177	a	902.72	1.70895	YES	YES
178	a	903.90	3.07186	YES	YES
179	a	904.95	2.74607	YES	YES
180	a	905.33	1.79222	YES	YES
181	a	907.86	1.27622	YES	YES
182	a	909.79	1.47166	YES	YES
183	a	910.15	0.76125	YES	YES

184	a	910.53	0.77204	YES	YES
185	a	979.78	1.50594	YES	YES
186	a	981.67	0.21353	YES	YES
187	a	987.34	0.55318	YES	YES
188	a	987.74	16.66157	YES	YES
189	a	988.30	7.48471	YES	YES
190	a	988.77	18.43162	YES	YES
191	a	988.89	4.79610	YES	YES
192	a	989.66	0.08541	YES	YES
193	a	990.71	2.06883	YES	YES
194	a	991.01	27.12745	YES	YES
195	a	1010.42	101.15655	YES	YES
196	a	1012.92	8.22496	YES	YES
197	a	1015.01	3.76374	YES	YES
198	a	1015.98	0.11937	YES	YES
199	a	1016.60	3.75092	YES	YES
200	a	1017.65	1.04948	YES	YES
201	a	1018.31	1.98393	YES	YES
202	a	1020.93	0.60727	YES	YES
203	a	1021.65	0.15180	YES	YES
204	a	1029.00	0.96861	YES	YES
205	a	1029.73	1.09654	YES	YES
206	a	1031.94	1.96229	YES	YES
207	a	1034.02	2.36082	YES	YES
208	a	1036.91	2.06029	YES	YES
209	a	1038.15	1.83229	YES	YES
210	a	1038.69	1.79186	YES	YES
211	a	1040.21	1.09526	YES	YES
212	a	1057.19	2.58296	YES	YES
213	a	1058.10	1.91384	YES	YES
214	a	1058.79	1.00834	YES	YES
215	a	1060.05	0.92709	YES	YES
216	a	1060.89	2.18893	YES	YES
217	a	1064.59	1.49157	YES	YES
218	a	1064.86	0.33585	YES	YES
219	a	1067.66	1.67264	YES	YES
220	a	1069.63	0.12004	YES	YES
221	a	1070.42	0.18911	YES	YES
222	a	1071.01	1.02111	YES	YES
223	a	1072.13	0.20754	YES	YES
224	a	1072.58	0.04015	YES	YES
225	a	1072.64	0.24740	YES	YES
226	a	1073.79	0.05040	YES	YES
227	a	1074.05	0.01818	YES	YES
228	a	1075.74	5.13393	YES	YES
229	a	1080.86	3.58163	YES	YES
230	a	1091.13	1.12193	YES	YES
231	a	1091.75	4.89483	YES	YES
232	a	1091.92	4.80964	YES	YES
233	a	1094.89	8.77123	YES	YES
234	a	1101.47	0.77604	YES	YES
235	a	1104.72	1.72850	YES	YES
236	a	1109.66	7.74998	YES	YES
237	a	1113.49	10.36528	YES	YES
238	a	1120.71	5.16083	YES	YES
239	a	1120.99	2.07396	YES	YES
240	a	1128.73	1.62093	YES	YES
241	a	1129.92	1.07862	YES	YES

242	a	1159.15	6.75570	YES	YES
243	a	1160.02	0.56568	YES	YES
244	a	1161.51	12.07117	YES	YES
245	a	1165.36	11.16790	YES	YES
246	a	1166.60	2.22400	YES	YES
247	a	1167.24	9.10596	YES	YES
248	a	1169.12	15.96158	YES	YES
249	a	1170.33	3.37324	YES	YES
250	a	1175.82	7.34067	YES	YES
251	a	1177.91	16.30863	YES	YES
252	a	1178.86	3.10739	YES	YES
253	a	1180.95	6.13960	YES	YES
254	a	1186.87	0.51476	YES	YES
255	a	1188.86	0.97534	YES	YES
256	a	1190.88	1.93825	YES	YES
257	a	1211.10	1.89297	YES	YES
258	a	1235.63	0.51776	YES	YES
259	a	1238.77	0.91097	YES	YES
260	a	1244.24	0.94713	YES	YES
261	a	1245.03	0.97354	YES	YES
262	a	1246.34	1.00851	YES	YES
263	a	1246.74	0.39574	YES	YES
264	a	1247.11	0.62435	YES	YES
265	a	1248.43	0.35562	YES	YES
266	a	1249.99	0.07518	YES	YES
267	a	1250.45	0.88525	YES	YES
268	a	1250.66	0.20033	YES	YES
269	a	1253.27	2.08247	YES	YES
270	a	1254.31	0.49500	YES	YES
271	a	1255.28	9.32361	YES	YES
272	a	1255.52	1.47616	YES	YES
273	a	1256.27	3.62227	YES	YES
274	a	1257.31	1.26886	YES	YES
275	a	1257.74	3.84674	YES	YES
276	a	1258.48	4.90509	YES	YES
277	a	1259.91	0.31341	YES	YES
278	a	1260.17	1.94401	YES	YES
279	a	1260.56	2.74286	YES	YES
280	a	1261.91	0.30602	YES	YES
281	a	1262.50	0.83495	YES	YES
282	a	1266.11	0.01640	YES	YES
283	a	1266.82	0.67611	YES	YES
284	a	1268.19	1.75939	YES	YES
285	a	1268.99	2.30849	YES	YES
286	a	1280.61	2.36675	YES	YES
287	a	1281.37	4.46809	YES	YES
288	a	1282.45	0.28526	YES	YES
289	a	1284.94	3.57779	YES	YES
290	a	1285.10	3.37695	YES	YES
291	a	1287.33	3.42050	YES	YES
292	a	1290.44	2.04579	YES	YES
293	a	1291.64	6.61407	YES	YES
294	a	1306.56	0.74374	YES	YES
295	a	1308.10	0.68738	YES	YES
296	a	1309.94	1.17419	YES	YES
297	a	1310.68	1.05769	YES	YES
298	a	1313.04	1.66704	YES	YES
299	a	1313.26	0.46531	YES	YES

300	a	1314.48	1.25469	YES	YES
301	a	1317.39	0.32884	YES	YES
302	a	1320.02	2.15417	YES	YES
303	a	1321.26	0.53947	YES	YES
304	a	1321.91	1.82241	YES	YES
305	a	1322.07	1.48783	YES	YES
306	a	1322.63	0.45109	YES	YES
307	a	1323.22	9.70332	YES	YES
308	a	1324.20	2.94021	YES	YES
309	a	1324.24	1.23881	YES	YES
310	a	1324.64	0.80797	YES	YES
311	a	1324.94	3.86403	YES	YES
312	a	1325.14	5.10252	YES	YES
313	a	1326.84	7.66334	YES	YES
314	a	1327.70	7.81703	YES	YES
315	a	1328.88	12.80254	YES	YES
316	a	1328.99	3.83313	YES	YES
317	a	1330.50	2.95842	YES	YES
318	a	1333.65	92.29254	YES	YES
319	a	1336.22	0.09521	YES	YES
320	a	1336.49	0.20053	YES	YES
321	a	1336.64	2.52915	YES	YES
322	a	1337.43	3.22959	YES	YES
323	a	1337.56	0.48372	YES	YES
324	a	1338.20	0.46696	YES	YES
325	a	1338.52	1.54386	YES	YES
326	a	1339.27	3.42166	YES	YES
327	a	1343.32	0.99307	YES	YES
328	a	1344.00	2.77893	YES	YES
329	a	1344.55	0.26217	YES	YES
330	a	1345.67	0.98039	YES	YES
331	a	1346.53	1.78696	YES	YES
332	a	1346.78	1.28256	YES	YES
333	a	1348.91	1.74540	YES	YES
334	a	1349.50	1.00699	YES	YES
335	a	1398.69	6.41410	YES	YES
336	a	1404.73	9.01512	YES	YES
337	a	1405.19	9.93548	YES	YES
338	a	1406.01	3.79330	YES	YES
339	a	1416.64	8.46702	YES	YES
340	a	1424.89	3.78708	YES	YES
341	a	1426.74	4.78051	YES	YES
342	a	1430.26	6.79484	YES	YES
343	a	1430.96	0.91976	YES	YES
344	a	1431.57	0.34589	YES	YES
345	a	1431.89	1.33955	YES	YES
346	a	1432.60	0.09327	YES	YES
347	a	1433.27	4.21216	YES	YES
348	a	1433.92	2.08714	YES	YES
349	a	1434.49	0.06599	YES	YES
350	a	1434.91	9.64740	YES	YES
351	a	1435.45	1.96902	YES	YES
352	a	1436.00	10.98018	YES	YES
353	a	1436.50	10.94070	YES	YES
354	a	1437.51	1.96525	YES	YES
355	a	1438.16	8.33885	YES	YES
356	a	1438.20	3.93505	YES	YES
357	a	1438.46	4.61280	YES	YES

358	a	1438.63	4.35165	YES	YES
359	a	1438.97	3.66733	YES	YES
360	a	1439.12	4.97317	YES	YES
361	a	1439.32	4.94368	YES	YES
362	a	1439.61	3.55378	YES	YES
363	a	1439.65	2.30936	YES	YES
364	a	1441.08	7.25625	YES	YES
365	a	1441.83	3.93680	YES	YES
366	a	1442.62	6.77885	YES	YES
367	a	1443.15	35.80344	YES	YES
368	a	1444.14	7.55985	YES	YES
369	a	1444.61	2.07034	YES	YES
370	a	1444.86	25.58122	YES	YES
371	a	1445.13	7.19669	YES	YES
372	a	1446.53	9.60285	YES	YES
373	a	1450.79	1.66620	YES	YES
374	a	1452.36	0.64301	YES	YES
375	a	1453.53	3.62030	YES	YES
376	a	1454.39	1.26879	YES	YES
377	a	1454.69	4.38660	YES	YES
378	a	1455.29	1.25107	YES	YES
379	a	1455.41	5.68938	YES	YES
380	a	1456.44	0.58983	YES	YES
381	a	1458.07	4.15160	YES	YES
382	a	2924.38	21.41184	YES	YES
383	a	2926.87	37.17627	YES	YES
384	a	2928.32	5.95618	YES	YES
385	a	2928.80	59.60198	YES	YES
386	a	2930.66	7.01232	YES	YES
387	a	2931.75	7.70536	YES	YES
388	a	2931.90	19.08792	YES	YES
389	a	2932.61	1.20233	YES	YES
390	a	2938.77	10.51096	YES	YES
391	a	2939.45	0.69848	YES	YES
392	a	2939.75	7.74688	YES	YES
393	a	2941.21	21.08619	YES	YES
394	a	2941.94	4.13524	YES	YES
395	a	2942.62	7.32746	YES	YES
396	a	2943.11	8.59553	YES	YES
397	a	2943.19	18.84330	YES	YES
398	a	2943.91	14.13355	YES	YES
399	a	2944.46	11.59728	YES	YES
400	a	2945.34	9.76448	YES	YES
401	a	2945.72	6.46232	YES	YES
402	a	2945.92	13.54803	YES	YES
403	a	2946.14	6.11828	YES	YES
404	a	2947.20	11.43114	YES	YES
405	a	2949.73	0.86261	YES	YES
406	a	2949.92	9.38537	YES	YES
407	a	2950.05	22.77988	YES	YES
408	a	2950.15	4.06202	YES	YES
409	a	2951.47	28.57850	YES	YES
410	a	2952.05	8.70128	YES	YES
411	a	2953.53	0.62213	YES	YES
412	a	2955.24	4.45110	YES	YES
413	a	2955.41	7.57802	YES	YES
414	a	2955.42	8.99412	YES	YES
415	a	2956.20	7.70647	YES	YES

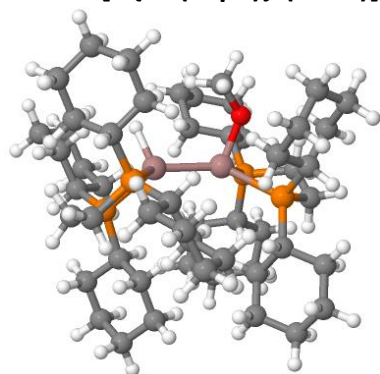
416	a	2957.32	5.42526	YES	YES
417	a	2958.07	12.31387	YES	YES
418	a	2958.68	14.72924	YES	YES
419	a	2959.37	11.47001	YES	YES
420	a	2959.79	34.38437	YES	YES
421	a	2959.98	32.86785	YES	YES
422	a	2960.30	41.57005	YES	YES
423	a	2960.98	16.72947	YES	YES
424	a	2961.72	18.32178	YES	YES
425	a	2961.83	58.14074	YES	YES
426	a	2962.66	22.97244	YES	YES
427	a	2965.01	25.22910	YES	YES
428	a	2966.19	19.04644	YES	YES
429	a	2971.49	15.39705	YES	YES
430	a	2974.78	11.44347	YES	YES
431	a	2978.40	22.86103	YES	YES
432	a	2979.35	6.09883	YES	YES
433	a	2984.74	3.73619	YES	YES
434	a	2985.90	28.70768	YES	YES
435	a	2985.96	4.03512	YES	YES
436	a	2988.97	6.07821	YES	YES
437	a	2991.16	14.27318	YES	YES
438	a	2991.74	37.61671	YES	YES
439	a	2992.37	17.41710	YES	YES
440	a	2994.48	23.36883	YES	YES
441	a	2995.49	18.71208	YES	YES
442	a	2997.13	23.65118	YES	YES
443	a	2997.56	21.11691	YES	YES
444	a	2999.20	43.57171	YES	YES
445	a	3000.31	5.83795	YES	YES
446	a	3001.28	18.83906	YES	YES
447	a	3002.09	34.46485	YES	YES
448	a	3004.05	32.78734	YES	YES
449	a	3005.85	15.71079	YES	YES
450	a	3007.38	27.81319	YES	YES
451	a	3007.49	10.15276	YES	YES
452	a	3009.18	15.06322	YES	YES
453	a	3009.44	23.06888	YES	YES
454	a	3009.68	22.16669	YES	YES
455	a	3010.88	25.65647	YES	YES
456	a	3010.96	18.59929	YES	YES
457	a	3011.68	23.43593	YES	YES
458	a	3011.96	17.77802	YES	YES
459	a	3012.64	22.47167	YES	YES
460	a	3014.10	17.87893	YES	YES
461	a	3014.48	26.95070	YES	YES
462	a	3014.68	11.03760	YES	YES
463	a	3014.81	23.06187	YES	YES
464	a	3016.36	25.39532	YES	YES
465	a	3017.06	30.45275	YES	YES
466	a	3017.10	9.87280	YES	YES
467	a	3017.34	23.55986	YES	YES
468	a	3017.48	43.26205	YES	YES
469	a	3017.89	24.60695	YES	YES
470	a	3018.02	37.90353	YES	YES
471	a	3018.08	18.81995	YES	YES
472	a	3018.23	24.38528	YES	YES
473	a	3019.02	25.20187	YES	YES

474	a	3019.12	21.34789	YES	YES
475	a	3022.59	32.33831	YES	YES
476	a	3024.71	12.25449	YES	YES
477	a	3026.35	5.42856	YES	YES
478	a	3029.25	0.82805	YES	YES
479	a	3036.12	1.37438	YES	YES
480	a	3044.05	0.61742	YES	YES

\$end

Double hybrid single point energy = -7364.642355164008 H
 COSMO energy + OC correction = -7372.1015196706 H (in oDFB)

6.2.23 [H{Ga(dcpe)}₂(OMe)]²⁺ (*syn*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.2158517	17.2831098	-2.4356251
Ga	-4.0345940	17.6984071	-0.8965123
P	-1.4944858	18.9056695	-4.0399729
P	-6.0683501	19.0357245	-0.9210266
P	-2.0147850	15.6292530	-4.1487876
P	-5.3277291	16.0474393	0.2517611
C	-4.9660946	21.0367638	-5.0213262
H	-5.0968088	21.6286673	-4.0995381
H	-5.9619635	20.6630962	-5.2992568
C	-1.0591847	14.1488840	-3.6004569
H	-0.9287955	13.5107523	-4.4905190
C	-4.3115518	15.1731415	1.5078591
H	-4.0455329	16.0065604	2.1826357
C	-4.3683780	16.1766537	-5.5465217
H	-3.7860433	16.6313511	-6.3640920
H	-4.5337670	16.9626217	-4.7938066
C	-7.0141523	19.2621958	-2.4848092
H	-6.3777616	19.9292476	-3.0884723
C	-7.2077398	18.1234456	0.2240937
H	-7.8001343	18.8475001	0.7985037
H	-7.9142130	17.5707440	-0.4109002
C	-3.0007145	22.4288738	-5.7692064
H	-2.5943732	23.0545979	-6.5748830
H	-3.0428527	23.0643331	-4.8694142
C	-2.0525181	21.2510682	-5.5095413
H	-1.0585149	21.6264595	-5.2323359
H	-1.9293881	20.6753508	-6.4413668

C	-4.0336882	19.8521488	-4.7374093
H	-4.0127320	19.2037621	-5.6275263
H	-4.4177356	19.2355986	-3.9092187
C	1.0488206	13.2705276	-2.5072911
H	1.2538306	12.5759749	-3.3379999
H	2.0246496	13.5662191	-2.0989786
C	-7.5726024	14.2900174	-0.1818520
H	-8.2077057	15.0291782	0.3271381
H	-7.2381617	13.5784723	0.5864461
C	-5.7191970	20.7168574	-0.2514299
H	-6.5912021	21.3417495	-0.5093444
C	0.0224999	20.3177934	-2.2203479
H	-0.7263347	21.1218979	-2.2740566
H	-0.3365079	19.5926386	-1.4709977
C	1.3735726	20.8852572	-1.7679845
H	1.6829412	21.6841532	-2.4611888
H	1.2598236	21.3537242	-0.7808492
C	-7.1673015	17.9307638	-3.2382713
H	-6.1806731	17.4657774	-3.3963020
H	-7.7532253	17.2287726	-2.6211595
C	-4.4090223	21.9446487	-6.1211276
H	-4.3794455	21.3891332	-7.0729916
H	-5.0788348	22.8000315	-6.2802885
C	-8.3763727	19.9490284	-2.2810785
H	-8.2530603	20.9128069	-1.7686642
H	-9.0113164	19.3223830	-1.6342856
C	-4.4802255	21.2708280	-0.9821458
H	-4.6509582	21.2808149	-2.0694666
H	-3.6311404	20.5921104	-0.7951255
C	-3.3414018	13.8892490	-5.9543690
H	-2.8083419	13.0481192	-5.4913682
H	-2.7060924	14.2565627	-6.7770295
C	2.5786300	19.1035398	-3.0892035
H	2.9356880	19.8288120	-3.8382224
H	3.3296257	18.3029383	-3.0466743
C	-5.1712181	22.1482835	1.7528349
H	-6.0221555	22.8250839	1.5708622
H	-5.0104032	22.1344064	2.8392366
C	-9.2416555	18.8334174	-4.3822240
H	-9.7190849	19.0048084	-5.3561558
H	-9.9185497	18.1721149	-3.8162687
C	-5.0415355	14.0857654	2.3127435
H	-5.9677003	14.4796448	2.7548059
H	-5.3311968	13.2662646	1.6360809
C	0.2109702	12.5592679	-1.4415965
H	0.7359750	11.6669040	-1.0761232
H	0.0824610	13.2277187	-0.5733818
C	-7.8941532	18.1309043	-4.5736961
H	-7.2558123	18.7319359	-5.2421675
H	-8.0357178	17.1594460	-5.0651279
C	2.4486286	19.7956879	-1.7294707
H	2.1849761	19.0489824	-0.9619879
H	3.4135419	20.2255136	-1.4299621
C	-3.9305224	22.6884474	1.0345445
H	-3.7057488	23.7066071	1.3789149
H	-3.0580353	22.0670201	1.2961347
C	-5.4721553	13.9584362	-1.5770769
H	-5.0612032	13.2296382	-0.8617900

H	-4.6102601	14.4757354	-2.0263442
C	-5.5309024	20.7350654	1.2751455
H	-4.7297296	20.0293498	1.5404332
H	-6.4499393	20.3979034	1.7758161
C	-6.3546262	14.9689361	-0.8262582
H	-6.7324084	15.6844837	-1.5806110
C	-4.1237386	22.6757767	-0.4849457
C	-7.5191597	12.5437282	-2.0247924
H	-8.1142372	12.0530906	-2.8065100
H	-7.1879514	11.7469460	-1.3391296
C	-8.3834776	13.5484196	-1.2544464
H	-9.2367656	13.0396999	-0.7865033
H	-8.8062368	14.2842570	-1.9595066
C	-1.9024142	13.3966930	-2.5538727
H	-2.8645480	13.0857365	-2.9855492
H	-2.1310440	14.0912390	-1.7282677
C	-4.1209511	13.5294805	3.4081893
H	-3.9062572	14.3270925	4.1377224
H	-4.6436983	12.7348925	3.9575649
C	-5.7014123	15.6783835	-6.1148541
H	-6.2424088	16.5164337	-6.5743180
H	-6.3290903	15.3121111	-5.2851688
C	-2.8067238	13.0032327	2.8220394
H	-3.0182326	12.1343042	2.1762853
H	-2.1522371	12.6408044	3.6258567
C	-2.9986314	14.6427073	0.9030049
H	-3.2242806	13.8455996	0.1782700
H	-2.4845459	15.4469278	0.3542093
C	-9.0806375	20.1560540	-3.6285838
H	-10.0586957	20.6271195	-3.4630334
H	-8.4925021	20.8613267	-4.2383849
C	-4.6807164	13.4029928	-6.5259134
H	-4.4962278	12.6231240	-7.2766327
H	-5.2626170	12.9297966	-5.7182542
C	-6.2891443	13.2195344	-2.6411123
H	-5.6571993	12.4774451	-3.1507183
H	-6.6133977	13.9412098	-3.4105919
C	-5.4893201	14.5530043	-7.1314967
H	-6.4572398	14.1856118	-7.4976204
H	-4.9563444	14.9529279	-8.0097979
C	-1.1629614	12.1759245	-1.9954624
H	-1.7790209	11.7025759	-1.2177216
H	-1.0416087	11.4281394	-2.7956205
C	-2.0902488	14.0814516	2.0022146
H	-1.7795981	14.9051777	2.6649832
H	-1.1722503	13.6780261	1.5516210
H	-0.8962599	17.0163306	-1.6061685
C	0.1460093	19.6021063	-3.5788404
H	0.4041730	20.3401362	-4.3568370
C	1.2377983	18.5178857	-3.5515004
H	1.3535412	18.0689903	-4.5489960
H	0.9314350	17.7150920	-2.8619248
C	0.3289478	14.5140933	-3.0451637
H	0.9435925	14.9904984	-3.8218612
H	0.2110006	15.2479649	-2.2331022
C	-1.0051420	16.4749502	-5.4478497
H	0.0385978	16.3381387	-5.1376453
H	-1.1253003	15.9440526	-6.4025601

C	-1.3073472	17.9728855	-5.6286594
H	-2.2482757	18.1108012	-6.1762956
H	-0.5175747	18.4447810	-6.2292266
C	-3.5661580	15.0177894	-4.9348326
H	-4.1508627	14.6146939	-4.0907480
C	-2.6097043	20.3295157	-4.4095443
H	-2.6491915	20.8919830	-3.4607607
C	-6.4692261	17.1627124	1.1709370
H	-7.1870991	16.5842588	1.7676437
H	-5.8252390	17.7205848	1.8651816
H	-4.9295107	23.3751099	-0.7609974
H	-3.2155959	23.0278437	-0.9951645
O	-3.4036223	18.3230524	0.7509333
C	-2.0939221	18.8397073	0.9162888
H	-1.3159184	18.1447801	0.5552496
H	-1.9191227	19.0184736	1.9874218
H	-1.9535345	19.8040949	0.3916721

SCF energy GEOOPT = -7372.004530091 H

ZPE = 3723. kJ/mol

FREEH energy = 3909.84 kJ/mol

FREEH entropy = 1.60252 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	13.67	0.00971	YES	YES
	8	a	16.77	0.03287	YES	YES
	9	a	22.29	0.21157	YES	YES
	10	a	25.92	0.04627	YES	YES
	11	a	28.34	0.01253	YES	YES
	12	a	31.10	0.03592	YES	YES
	13	a	31.72	0.00952	YES	YES
	14	a	33.97	0.04075	YES	YES
	15	a	37.00	0.00258	YES	YES
	16	a	37.45	0.03296	YES	YES
	17	a	40.87	0.09205	YES	YES
	18	a	45.65	0.16917	YES	YES
	19	a	48.41	0.13924	YES	YES
	20	a	49.07	0.30146	YES	YES
	21	a	51.62	0.08865	YES	YES
	22	a	52.39	0.28866	YES	YES
	23	a	55.08	0.08083	YES	YES
	24	a	56.56	0.52287	YES	YES
	25	a	61.74	0.04716	YES	YES
	26	a	64.10	0.01402	YES	YES
	27	a	66.42	0.08312	YES	YES
	28	a	67.59	0.05736	YES	YES
	29	a	70.19	0.38319	YES	YES
	30	a	74.29	0.34530	YES	YES
	31	a	75.64	0.01558	YES	YES
	32	a	76.89	0.03015	YES	YES

33	a	87.30	0.05203	YES	YES
34	a	89.72	0.36347	YES	YES
35	a	90.59	0.50448	YES	YES
36	a	100.56	0.23022	YES	YES
37	a	101.99	1.63297	YES	YES
38	a	105.46	0.35346	YES	YES
39	a	115.30	0.04324	YES	YES
40	a	122.74	0.74004	YES	YES
41	a	134.90	0.69249	YES	YES
42	a	135.60	1.42525	YES	YES
43	a	137.09	0.22789	YES	YES
44	a	140.24	0.25561	YES	YES
45	a	140.75	0.80586	YES	YES
46	a	149.00	13.35085	YES	YES
47	a	156.33	0.60313	YES	YES
48	a	159.09	2.01414	YES	YES
49	a	164.82	1.66219	YES	YES
50	a	166.85	0.09794	YES	YES
51	a	184.32	6.02239	YES	YES
52	a	188.05	9.21271	YES	YES
53	a	190.49	0.48172	YES	YES
54	a	193.80	0.82361	YES	YES
55	a	204.75	0.41398	YES	YES
56	a	210.19	0.72449	YES	YES
57	a	216.05	0.23875	YES	YES
58	a	219.15	0.13982	YES	YES
59	a	221.04	0.12856	YES	YES
60	a	223.97	0.01240	YES	YES
61	a	226.36	0.11709	YES	YES
62	a	227.73	0.44588	YES	YES
63	a	229.70	0.25470	YES	YES
64	a	231.84	0.55491	YES	YES
65	a	235.14	2.98040	YES	YES
66	a	236.67	0.08316	YES	YES
67	a	238.14	0.75935	YES	YES
68	a	240.11	7.70163	YES	YES
69	a	242.82	1.94168	YES	YES
70	a	244.06	0.44277	YES	YES
71	a	264.04	4.32160	YES	YES
72	a	281.22	1.22237	YES	YES
73	a	283.31	0.59140	YES	YES
74	a	285.99	0.25816	YES	YES
75	a	290.67	0.30674	YES	YES
76	a	303.60	1.87962	YES	YES
77	a	306.63	1.79620	YES	YES
78	a	310.02	0.46018	YES	YES
79	a	314.16	0.94563	YES	YES
80	a	329.62	0.71115	YES	YES
81	a	330.73	0.16843	YES	YES
82	a	334.46	0.31341	YES	YES
83	a	339.32	1.33027	YES	YES
84	a	340.35	1.28036	YES	YES
85	a	340.67	1.66968	YES	YES
86	a	370.26	5.65073	YES	YES
87	a	380.72	2.93075	YES	YES
88	a	381.50	0.75598	YES	YES
89	a	384.24	0.63871	YES	YES
90	a	394.50	0.49782	YES	YES

91	a	398.44	0.31866	YES	YES
92	a	406.17	0.38784	YES	YES
93	a	411.14	1.05609	YES	YES
94	a	419.52	0.75618	YES	YES
95	a	420.69	4.26226	YES	YES
96	a	425.20	3.77331	YES	YES
97	a	427.55	0.34446	YES	YES
98	a	429.73	0.07290	YES	YES
99	a	430.13	0.48961	YES	YES
100	a	430.59	0.06228	YES	YES
101	a	431.59	0.36110	YES	YES
102	a	433.24	0.12265	YES	YES
103	a	433.73	0.49263	YES	YES
104	a	435.75	1.17331	YES	YES
105	a	437.17	0.29415	YES	YES
106	a	445.51	2.26132	YES	YES
107	a	459.08	3.59002	YES	YES
108	a	460.27	4.86673	YES	YES
109	a	471.92	2.60237	YES	YES
110	a	492.22	11.72945	YES	YES
111	a	494.62	2.83101	YES	YES
112	a	496.65	10.55358	YES	YES
113	a	497.51	2.88098	YES	YES
114	a	499.15	2.74060	YES	YES
115	a	502.83	23.13260	YES	YES
116	a	508.37	11.04129	YES	YES
117	a	512.18	15.71572	YES	YES
118	a	514.62	11.80014	YES	YES
119	a	535.92	87.57757	YES	YES
120	a	593.10	87.93940	YES	YES
121	a	628.65	15.79248	YES	YES
122	a	633.07	24.23107	YES	YES
123	a	643.34	12.56273	YES	YES
124	a	661.97	12.18023	YES	YES
125	a	701.44	1.58488	YES	YES
126	a	718.36	1.95393	YES	YES
127	a	721.36	1.44313	YES	YES
128	a	732.52	10.56100	YES	YES
129	a	734.83	3.57795	YES	YES
130	a	735.26	4.27900	YES	YES
131	a	738.07	1.18874	YES	YES
132	a	741.83	4.62980	YES	YES
133	a	771.29	1.17445	YES	YES
134	a	773.27	0.06404	YES	YES
135	a	773.50	0.90531	YES	YES
136	a	774.04	0.44873	YES	YES
137	a	775.00	0.83359	YES	YES
138	a	776.26	0.76379	YES	YES
139	a	776.29	1.30173	YES	YES
140	a	776.36	1.03160	YES	YES
141	a	778.47	10.56374	YES	YES
142	a	787.93	13.77815	YES	YES
143	a	807.08	0.18150	YES	YES
144	a	809.42	2.54842	YES	YES
145	a	810.74	10.33254	YES	YES
146	a	810.89	5.31528	YES	YES
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149	a	815.02	2.53531	YES	YES
150	a	818.15	2.62075	YES	YES
151	a	832.56	6.06336	YES	YES
152	a	832.83	4.82516	YES	YES
153	a	837.01	5.99056	YES	YES
154	a	837.66	2.02235	YES	YES
155	a	838.32	0.64968	YES	YES
156	a	838.97	1.73538	YES	YES
157	a	839.22	4.23328	YES	YES
158	a	839.44	5.94719	YES	YES
159	a	848.54	12.34419	YES	YES
160	a	854.49	15.35280	YES	YES
161	a	872.38	3.24800	YES	YES
162	a	873.37	1.48229	YES	YES
163	a	873.64	2.00548	YES	YES
164	a	876.42	1.90593	YES	YES
165	a	877.33	3.98521	YES	YES
166	a	877.99	2.49155	YES	YES
167	a	878.55	3.13079	YES	YES
168	a	879.12	6.29623	YES	YES
169	a	879.72	1.51512	YES	YES
170	a	880.02	1.74880	YES	YES
171	a	880.68	2.15485	YES	YES
172	a	882.42	1.99042	YES	YES
173	a	883.26	5.37986	YES	YES
174	a	883.79	4.30122	YES	YES
175	a	885.88	0.72173	YES	YES
176	a	887.26	7.10020	YES	YES
177	a	903.90	1.58393	YES	YES
178	a	904.63	1.27805	YES	YES
179	a	904.79	1.43216	YES	YES
180	a	905.18	2.64559	YES	YES
181	a	907.88	2.03141	YES	YES
182	a	909.36	0.99123	YES	YES
183	a	909.96	0.79225	YES	YES
184	a	911.02	0.83106	YES	YES
185	a	980.58	1.20837	YES	YES
186	a	983.67	0.33769	YES	YES
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188	a	988.60	1.17845	YES	YES
189	a	989.38	12.63901	YES	YES
190	a	989.57	14.15640	YES	YES
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193	a	991.99	4.79839	YES	YES
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195	a	1013.59	0.35714	YES	YES
196	a	1014.66	0.58887	YES	YES
197	a	1016.65	0.11474	YES	YES
198	a	1017.04	1.18528	YES	YES
199	a	1017.82	1.07543	YES	YES
200	a	1018.44	0.34920	YES	YES
201	a	1019.22	1.26932	YES	YES
202	a	1021.89	0.51654	YES	YES
203	a	1030.37	0.81045	YES	YES
204	a	1031.33	2.59831	YES	YES
205	a	1031.82	0.57771	YES	YES
206	a	1033.29	0.92198	YES	YES

207	a	1037.11	2.93978	YES	YES
208	a	1039.22	4.04384	YES	YES
209	a	1039.46	0.74148	YES	YES
210	a	1040.07	1.93433	YES	YES
211	a	1050.25	142.45659	YES	YES
212	a	1056.77	3.48891	YES	YES
213	a	1057.86	2.54762	YES	YES
214	a	1059.51	3.19832	YES	YES
215	a	1061.01	1.27856	YES	YES
216	a	1061.40	1.75046	YES	YES
217	a	1064.82	0.74740	YES	YES
218	a	1065.20	1.80743	YES	YES
219	a	1067.93	1.26455	YES	YES
220	a	1070.23	0.06751	YES	YES
221	a	1071.34	0.27056	YES	YES
222	a	1071.83	0.10016	YES	YES
223	a	1072.01	0.26527	YES	YES
224	a	1072.55	0.14340	YES	YES
225	a	1073.37	0.12689	YES	YES
226	a	1073.38	0.23369	YES	YES
227	a	1074.44	0.03507	YES	YES
228	a	1082.47	2.70958	YES	YES
229	a	1083.44	3.22053	YES	YES
230	a	1092.96	1.38174	YES	YES
231	a	1093.87	4.92411	YES	YES
232	a	1094.45	5.53424	YES	YES
233	a	1097.47	7.76073	YES	YES
234	a	1101.88	1.23162	YES	YES
235	a	1104.73	1.81484	YES	YES
236	a	1109.07	9.61422	YES	YES
237	a	1116.33	8.10066	YES	YES
238	a	1122.01	0.82833	YES	YES
239	a	1130.93	1.68954	YES	YES
240	a	1133.87	0.29321	YES	YES
241	a	1145.50	1.72268	YES	YES
242	a	1159.39	10.38021	YES	YES
243	a	1160.71	1.01520	YES	YES
244	a	1161.77	14.37185	YES	YES
245	a	1165.12	6.64013	YES	YES
246	a	1167.21	7.37849	YES	YES
247	a	1167.73	5.84905	YES	YES
248	a	1169.42	13.75082	YES	YES
249	a	1170.72	2.46537	YES	YES
250	a	1177.78	10.56223	YES	YES
251	a	1180.57	10.30516	YES	YES
252	a	1181.46	4.82694	YES	YES
253	a	1181.56	5.05293	YES	YES
254	a	1187.23	0.53695	YES	YES
255	a	1188.82	1.48459	YES	YES
256	a	1192.97	1.92675	YES	YES
257	a	1213.33	2.85293	YES	YES
258	a	1239.35	0.26360	YES	YES
259	a	1241.54	0.29405	YES	YES
260	a	1243.07	0.81564	YES	YES
261	a	1245.82	0.08574	YES	YES
262	a	1246.50	1.50150	YES	YES
263	a	1247.30	0.58655	YES	YES
264	a	1247.73	0.36465	YES	YES

265	a	1248.49	0.45602	YES	YES
266	a	1250.07	0.40803	YES	YES
267	a	1250.61	0.03687	YES	YES
268	a	1252.30	1.30249	YES	YES
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274	a	1257.27	3.49200	YES	YES
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276	a	1258.77	2.40073	YES	YES
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278	a	1261.34	0.82972	YES	YES
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281	a	1263.97	0.75256	YES	YES
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289	a	1285.14	3.02992	YES	YES
290	a	1286.72	3.75650	YES	YES
291	a	1287.38	2.55108	YES	YES
292	a	1290.13	3.62474	YES	YES
293	a	1292.30	3.33301	YES	YES
294	a	1307.01	0.14317	YES	YES
295	a	1309.14	0.36093	YES	YES
296	a	1310.05	0.71172	YES	YES
297	a	1310.92	0.57161	YES	YES
298	a	1311.95	0.63642	YES	YES
299	a	1312.25	0.45150	YES	YES
300	a	1315.89	2.18233	YES	YES
301	a	1316.96	2.11873	YES	YES
302	a	1319.14	1.26254	YES	YES
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305	a	1322.35	0.75835	YES	YES
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307	a	1323.78	0.72493	YES	YES
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312	a	1325.83	6.10722	YES	YES
313	a	1326.80	1.53852	YES	YES
314	a	1329.84	3.27143	YES	YES
315	a	1330.13	3.35849	YES	YES
316	a	1330.39	6.40849	YES	YES
317	a	1333.21	3.13587	YES	YES
318	a	1336.60	0.23247	YES	YES
319	a	1336.70	0.36243	YES	YES
320	a	1336.88	0.37078	YES	YES
321	a	1337.60	0.11709	YES	YES
322	a	1337.82	0.54453	YES	YES

323	a	1338.47	0.17277	YES	YES
324	a	1338.77	0.02058	YES	YES
325	a	1339.44	0.31647	YES	YES
326	a	1343.85	1.59938	YES	YES
327	a	1344.72	1.08683	YES	YES
328	a	1345.04	1.06288	YES	YES
329	a	1346.22	1.45741	YES	YES
330	a	1346.43	0.27702	YES	YES
331	a	1347.39	2.44078	YES	YES
332	a	1347.87	1.66425	YES	YES
333	a	1350.06	1.21840	YES	YES
334	a	1399.80	5.80908	YES	YES
335	a	1403.95	8.07592	YES	YES
336	a	1404.28	7.77922	YES	YES
337	a	1407.56	11.63272	YES	YES
338	a	1424.66	4.62402	YES	YES
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341	a	1430.31	2.32282	YES	YES
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344	a	1432.10	3.29455	YES	YES
345	a	1433.22	2.77630	YES	YES
346	a	1433.39	6.45783	YES	YES
347	a	1434.52	0.51186	YES	YES
348	a	1435.93	0.16700	YES	YES
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351	a	1436.72	1.59054	YES	YES
352	a	1437.23	3.91169	YES	YES
353	a	1437.69	12.15745	YES	YES
354	a	1438.00	0.63549	YES	YES
355	a	1438.31	1.65602	YES	YES
356	a	1438.58	6.57113	YES	YES
357	a	1438.81	6.05648	YES	YES
358	a	1439.33	7.75234	YES	YES
359	a	1439.88	5.21921	YES	YES
360	a	1440.02	5.27888	YES	YES
361	a	1440.22	3.16411	YES	YES
362	a	1440.96	2.61958	YES	YES
363	a	1441.94	11.80994	YES	YES
364	a	1443.08	3.56343	YES	YES
365	a	1443.48	17.45311	YES	YES
366	a	1444.56	13.84874	YES	YES
367	a	1444.71	11.91952	YES	YES
368	a	1445.54	17.38057	YES	YES
369	a	1446.17	6.28639	YES	YES
370	a	1446.61	13.92127	YES	YES
371	a	1448.40	13.44967	YES	YES
372	a	1450.74	11.04633	YES	YES
373	a	1452.94	1.17700	YES	YES
374	a	1453.80	0.61294	YES	YES
375	a	1454.44	3.68781	YES	YES
376	a	1455.23	5.22411	YES	YES
377	a	1455.90	1.36592	YES	YES
378	a	1456.61	3.09951	YES	YES
379	a	1457.10	1.12465	YES	YES
380	a	1462.61	2.12343	YES	YES

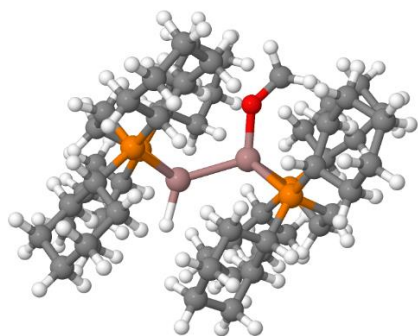
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388	a	2938.55	8.42888	YES	YES
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400	a	2945.75	12.08495	YES	YES
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405	a	2949.12	4.99893	YES	YES
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407	a	2950.89	10.68869	YES	YES
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414	a	2955.63	13.02183	YES	YES
415	a	2956.71	3.16816	YES	YES
416	a	2957.30	5.23603	YES	YES
417	a	2957.50	8.70705	YES	YES
418	a	2958.00	6.17297	YES	YES
419	a	2958.73	30.80892	YES	YES
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424	a	2961.52	41.72176	YES	YES
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435	a	2987.00	5.57897	YES	YES
436	a	2987.70	7.12929	YES	YES
437	a	2989.66	20.37846	YES	YES
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441	a	2994.25	26.74557	YES	YES
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443	a	2995.82	31.45671	YES	YES
444	a	2999.10	45.58245	YES	YES
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452	a	3007.96	19.87315	YES	YES
453	a	3010.51	12.15011	YES	YES
454	a	3011.79	18.93922	YES	YES
455	a	3012.34	15.05369	YES	YES
456	a	3012.78	22.57406	YES	YES
457	a	3013.26	18.90103	YES	YES
458	a	3013.72	16.56635	YES	YES
459	a	3014.05	31.55844	YES	YES
460	a	3015.07	12.90009	YES	YES
461	a	3015.78	22.80124	YES	YES
462	a	3016.06	20.77391	YES	YES
463	a	3016.42	33.74918	YES	YES
464	a	3017.00	18.53257	YES	YES
465	a	3017.05	10.90581	YES	YES
466	a	3017.21	10.38385	YES	YES
467	a	3017.30	44.13823	YES	YES
468	a	3017.78	24.93726	YES	YES
469	a	3018.27	22.23148	YES	YES
470	a	3018.71	23.02440	YES	YES
471	a	3018.87	28.09711	YES	YES
472	a	3019.25	32.86639	YES	YES
473	a	3019.46	12.82211	YES	YES
474	a	3019.48	36.94312	YES	YES
475	a	3019.88	22.25176	YES	YES
476	a	3020.86	27.58072	YES	YES
477	a	3032.00	1.01280	YES	YES
478	a	3032.13	0.39360	YES	YES
479	a	3040.52	0.42455	YES	YES
480	a	3045.90	0.33397	YES	YES

\$end

Double hybrid single point energy = -7364.706089042699 H
 COSMO energy + OC correction = -7372.1518871473 H (in oDFB)

6.2.24 [H{Ga(dcpe)}₂(OMe)]²⁺ (*anti*-periplanar)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-0.4456779	0.4751610	-1.8104128
P	-2.2353459	-0.8420844	-2.8723823
P	-1.7966751	2.4564738	-2.3957018
C	-1.7587144	-2.0742969	-4.1599087
H	-1.3510281	-2.9177435	-3.5759854
C	-0.6256943	-1.5382383	-5.0477971
H	-0.9667972	-0.6304669	-5.5747542
H	0.2234017	-1.2494053	-4.4151436
C	-0.1925927	-2.5891611	-6.0775198
H	0.5854898	-2.1668002	-6.7280748
H	0.2710701	-3.4363170	-5.5451355
C	-1.3768703	-3.0949919	-6.9058224
H	-1.0451573	-3.8723573	-7.6068071
H	-1.7735749	-2.2699854	-7.5206309
C	-2.4903900	-3.6365975	-6.0045981
H	-2.1276355	-4.5255948	-5.4629993
H	-3.3499829	-3.9647419	-6.6044044
C	-2.9517591	-2.5821529	-4.9883681
H	-3.7321568	-3.0015421	-4.3375978
H	-3.4051637	-1.7370133	-5.5307679
C	-3.3241518	-1.7480039	-1.6868659
H	-4.1089510	-2.2094650	-2.3114421
C	-2.5416942	-2.8651740	-0.9773913
H	-2.0906780	-3.5517815	-1.7071973
H	-1.7110675	-2.4093093	-0.4108421
C	-3.4504425	-3.6446598	-0.0196573
H	-4.2266215	-4.1633683	-0.6048933
H	-2.8698693	-4.4289059	0.4837965
C	-4.1151700	-2.7174309	1.0007003
H	-4.7810467	-3.2904623	1.6594861
H	-3.3436449	-2.2656731	1.6467694
C	-4.8927130	-1.6017543	0.2997817
H	-5.3293878	-0.9124576	1.0354866
H	-5.7358504	-2.0375266	-0.2601019
C	-4.0009383	-0.8145612	-0.6690207
H	-4.6116128	-0.0637003	-1.1875916
H	-3.2261155	-0.2763157	-0.0988598
C	-3.3057493	0.4148954	-3.7010487
H	-2.8632998	0.5768200	-4.6933178
H	-4.3067470	-0.0088827	-3.8629799
C	-3.4159795	1.7492463	-2.9411171

H	-4.0250436	1.6282971	-2.0372790
H	-3.9237732	2.4953513	-3.5681863
C	-1.2807140	3.5910350	-3.7566368
H	-2.1072782	4.3174100	-3.8447323
C	-0.0026286	4.3466396	-3.3639795
H	0.7847832	3.6173884	-3.1183263
H	-0.1789565	4.9371246	-2.4537856
C	0.4870920	5.2598952	-4.4931643
H	-0.2391942	6.0751079	-4.6421815
H	1.4316120	5.7341244	-4.1926515
C	0.6605578	4.4866884	-5.8027087
H	1.4569163	3.7332523	-5.6837828
H	0.9899400	5.1636548	-6.6017911
C	-0.6449736	3.7948787	-6.2035784
H	-0.5142975	3.2254628	-7.1338682
H	-1.4134457	4.5575522	-6.4090337
C	-1.1509924	2.8546604	-5.1011504
H	-0.4560181	2.0086023	-4.9940647
H	-2.1245523	2.4381162	-5.3960037
C	-2.1541614	3.5298694	-0.9339037
H	-1.1696867	3.9667497	-0.6925705
C	-2.6081123	2.7076418	0.2813451
H	-1.8903537	1.9017852	0.4925868
H	-3.5703525	2.2179477	0.0616378
C	-2.7749982	3.6039814	1.5129770
H	-3.1136402	2.9994036	2.3658358
H	-1.7900877	4.0179935	1.7899518
C	-3.7482702	4.7536852	1.2380921
H	-4.7563332	4.3419068	1.0665290
H	-3.8254231	5.4070494	2.1173978
C	-3.3133140	5.5639440	0.0135248
H	-2.3573203	6.0699022	0.2277413
H	-4.0425356	6.3556357	-0.2043078
C	-3.1382852	4.6755401	-1.2270256
H	-4.1146529	4.2535553	-1.5155626
H	-2.7903914	5.2853040	-2.0716541
Ga	-0.1466534	-0.0759411	0.5586913
P	1.4685320	1.3195417	1.6816957
P	1.2759277	-1.9414209	1.1126302
C	0.7725985	2.3860259	3.0204019
H	0.1491428	3.1151148	2.4727744
C	-0.1543688	1.5915276	3.9561453
H	0.4303017	0.8171709	4.4789764
H	-0.9254621	1.0691162	3.3730188
C	-0.7962639	2.5164999	4.9978593
H	-1.4320479	1.9249838	5.6708521
H	-1.4610364	3.2295870	4.4829474
C	0.2622481	3.2868222	5.7919321
H	-0.2187089	3.9683005	6.5061603
H	0.8577278	2.5777079	6.3904421
C	1.1909901	4.0685836	4.8592002
H	0.6158740	4.8531006	4.3398902
H	1.9735644	4.5833078	5.4327980
C	1.8447177	3.1545838	3.8126280
H	2.4765815	3.7524545	3.1416936
H	2.5070327	2.4350539	4.3211069
C	2.5110346	2.4123607	0.6288408
H	3.1857005	2.9230492	1.3379630

C	1.6623268	3.4746047	-0.0852303
H	1.0395847	4.0297043	0.6317328
H	0.9766637	2.9613899	-0.7822778
C	2.5627866	4.4419282	-0.8628419
H	3.1884354	4.9984761	-0.1467954
H	1.9482376	5.1906137	-1.3811164
C	3.4580746	3.6966859	-1.8562463
H	4.1304181	4.4014187	-2.3636189
H	2.8311676	3.2431532	-2.6405361
C	4.2683102	2.5941521	-1.1688342
H	4.8496624	2.0283106	-1.9095916
H	4.9988262	3.0522917	-0.4824426
C	3.3709137	1.6313700	-0.3781370
H	4.0030503	0.8993114	0.1432269
H	2.7141488	1.0763993	-1.0680240
C	2.6424939	0.1393329	2.4899869
H	2.2351343	-0.0590286	3.4890435
H	3.6080671	0.6442455	2.6330220
C	2.8449451	-1.1764578	1.7170735
H	3.4582065	-1.0013654	0.8242743
H	3.3831552	-1.9040062	2.3406435
C	0.6358442	-3.0015272	2.4802320
H	1.4334806	-3.7364100	2.6843733
C	-0.6266403	-3.7380705	2.0086394
H	-1.3739971	-2.9832177	1.7185504
H	-0.4125903	-4.3400659	1.1140333
C	-1.2124168	-4.6215518	3.1152023
H	-0.5035706	-5.4322600	3.3485909
H	-2.1296635	-5.1052067	2.7508701
C	-1.4973071	-3.8072580	4.3793450
H	-2.2822329	-3.0625940	4.1647875
H	-1.8904477	-4.4575879	5.1718007
C	-0.2335962	-3.0903737	4.8608309
H	-0.4481013	-2.4793680	5.7483822
H	0.5164867	-3.8367186	5.1685726
C	0.3631040	-2.1991067	3.7636412
H	-0.3373765	-1.3804581	3.5331363
H	1.2915380	-1.7417170	4.1322962
C	1.6894013	-3.0531695	-0.2988363
H	0.6937289	-3.3232813	-0.6961542
C	2.4446263	-2.3009496	-1.4056159
H	1.9460949	-1.3589659	-1.6729542
H	3.4533047	-2.0427016	-1.0438721
C	2.5828817	-3.1936358	-2.6444997
H	3.1289786	-2.6529923	-3.4298257
H	1.5766912	-3.4011164	-3.0489790
C	3.2874780	-4.5109699	-2.3048176
H	4.3304829	-4.2964686	-2.0198131
H	3.3358896	-5.1607367	-3.1891479
C	2.5886660	-5.2417686	-1.1534090
H	1.5897975	-5.5751168	-1.4819517
H	3.1441479	-6.1488915	-0.8798002
C	2.4242685	-4.3475329	0.0853470
H	3.4154525	-4.0952194	0.4959883
H	1.8833384	-4.8972090	0.8673423
H	-1.3856706	-0.2019092	1.5251757
O	1.1704618	0.3650755	-2.6845243
C	1.6657027	0.8898073	-3.8982912

H	2.6908815	0.5163962	-4.0425656
H	1.7085280	1.9910511	-3.8913881
H	1.0736735	0.5835860	-4.7763724

SCF energy GEOOPT = -7372.010905670 H

ZPE = 3726. kJ/mol

FREEH energy = 3911.68 kJ/mol

FREEH entropy = 1.59300 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	8.48	0.04936	YES	YES
8		a	14.89	0.08854	YES	YES
9		a	17.63	0.00701	YES	YES
10		a	24.14	0.01466	YES	YES
11		a	30.12	0.11460	YES	YES
12		a	32.15	0.03317	YES	YES
13		a	32.41	0.45213	YES	YES
14		a	34.08	0.04856	YES	YES
15		a	35.04	0.07867	YES	YES
16		a	38.32	0.04036	YES	YES
17		a	42.58	0.10129	YES	YES
18		a	44.33	0.04744	YES	YES
19		a	47.02	0.09557	YES	YES
20		a	49.80	0.19612	YES	YES
21		a	56.05	0.20461	YES	YES
22		a	56.70	0.20916	YES	YES
23		a	59.14	0.31883	YES	YES
24		a	64.13	0.91898	YES	YES
25		a	65.63	0.09683	YES	YES
26		a	67.45	0.03034	YES	YES
27		a	70.95	0.26819	YES	YES
28		a	73.57	0.20976	YES	YES
29		a	76.37	0.41931	YES	YES
30		a	78.00	0.52739	YES	YES
31		a	80.61	0.41129	YES	YES
32		a	84.27	0.86956	YES	YES
33		a	87.92	0.52482	YES	YES
34		a	89.22	0.38833	YES	YES
35		a	99.21	0.39471	YES	YES
36		a	109.00	4.66238	YES	YES
37		a	117.76	6.29863	YES	YES
38		a	127.21	0.90162	YES	YES
39		a	128.70	2.85107	YES	YES
40		a	135.16	3.41814	YES	YES
41		a	136.93	0.32856	YES	YES
42		a	139.85	7.48980	YES	YES
43		a	143.64	2.44170	YES	YES
44		a	148.10	2.03261	YES	YES
45		a	150.34	1.95029	YES	YES
46		a	151.46	0.04919	YES	YES

47	a	156.33	0.12454	YES	YES
48	a	163.50	1.20178	YES	YES
49	a	172.60	4.15603	YES	YES
50	a	180.10	3.61001	YES	YES
51	a	181.84	3.40159	YES	YES
52	a	186.14	0.07775	YES	YES
53	a	192.51	1.01204	YES	YES
54	a	200.99	0.60121	YES	YES
55	a	202.61	1.69135	YES	YES
56	a	207.52	3.81194	YES	YES
57	a	208.63	1.94701	YES	YES
58	a	213.59	0.09578	YES	YES
59	a	215.36	0.29438	YES	YES
60	a	216.45	0.43551	YES	YES
61	a	223.99	2.34974	YES	YES
62	a	230.04	0.71904	YES	YES
63	a	232.70	1.24403	YES	YES
64	a	234.79	3.51414	YES	YES
65	a	236.58	0.36540	YES	YES
66	a	238.64	1.09283	YES	YES
67	a	240.09	1.00109	YES	YES
68	a	244.00	0.01874	YES	YES
69	a	247.35	0.14879	YES	YES
70	a	248.16	2.46622	YES	YES
71	a	272.68	11.91526	YES	YES
72	a	277.39	2.90355	YES	YES
73	a	279.50	2.39438	YES	YES
74	a	287.19	0.39450	YES	YES
75	a	293.22	1.48567	YES	YES
76	a	305.27	0.41876	YES	YES
77	a	307.19	0.20962	YES	YES
78	a	313.99	0.11213	YES	YES
79	a	315.23	0.39370	YES	YES
80	a	329.53	0.62912	YES	YES
81	a	331.93	0.60798	YES	YES
82	a	335.15	0.26313	YES	YES
83	a	335.57	0.17789	YES	YES
84	a	342.78	0.66073	YES	YES
85	a	344.80	0.72129	YES	YES
86	a	370.02	1.34196	YES	YES
87	a	373.24	2.77780	YES	YES
88	a	375.30	2.08002	YES	YES
89	a	377.67	1.51988	YES	YES
90	a	394.19	0.15461	YES	YES
91	a	398.85	0.00869	YES	YES
92	a	411.93	1.17359	YES	YES
93	a	414.34	1.60562	YES	YES
94	a	422.66	6.25326	YES	YES
95	a	423.34	0.02725	YES	YES
96	a	424.97	1.34288	YES	YES
97	a	427.10	1.00235	YES	YES
98	a	429.81	0.07470	YES	YES
99	a	430.50	0.00912	YES	YES
100	a	431.10	0.48510	YES	YES
101	a	431.73	0.19035	YES	YES
102	a	432.50	0.72559	YES	YES
103	a	433.45	0.37911	YES	YES
104	a	434.13	0.93738	YES	YES

105	a	434.85	0.57315	YES	YES
106	a	443.25	4.30902	YES	YES
107	a	450.32	4.24208	YES	YES
108	a	467.15	1.72318	YES	YES
109	a	470.16	3.69328	YES	YES
110	a	489.71	2.73789	YES	YES
111	a	491.47	7.69657	YES	YES
112	a	493.06	2.89303	YES	YES
113	a	494.74	4.11827	YES	YES
114	a	498.92	17.09237	YES	YES
115	a	503.55	4.83682	YES	YES
116	a	505.25	4.18255	YES	YES
117	a	518.08	12.02334	YES	YES
118	a	519.43	17.77384	YES	YES
119	a	564.14	79.00738	YES	YES
120	a	579.52	114.85975	YES	YES
121	a	627.74	26.95999	YES	YES
122	a	628.61	2.45451	YES	YES
123	a	643.75	7.89807	YES	YES
124	a	645.30	9.45183	YES	YES
125	a	713.06	0.34076	YES	YES
126	a	716.13	1.11749	YES	YES
127	a	719.26	0.59804	YES	YES
128	a	724.59	0.91099	YES	YES
129	a	733.07	5.94769	YES	YES
130	a	735.41	10.00391	YES	YES
131	a	736.07	4.59507	YES	YES
132	a	736.18	4.57963	YES	YES
133	a	771.67	0.25308	YES	YES
134	a	772.21	0.24413	YES	YES
135	a	773.05	0.24319	YES	YES
136	a	773.44	0.50548	YES	YES
137	a	775.58	0.16187	YES	YES
138	a	775.99	0.46494	YES	YES
139	a	776.71	0.24165	YES	YES
140	a	778.28	0.19455	YES	YES
141	a	783.21	15.88498	YES	YES
142	a	785.69	8.10021	YES	YES
143	a	810.19	0.03639	YES	YES
144	a	810.34	0.76956	YES	YES
145	a	812.05	2.44689	YES	YES
146	a	812.36	0.47558	YES	YES
147	a	813.45	1.02449	YES	YES
148	a	814.23	0.99565	YES	YES
149	a	815.83	3.99690	YES	YES
150	a	816.49	7.97624	YES	YES
151	a	832.89	0.91490	YES	YES
152	a	833.97	0.39487	YES	YES
153	a	836.12	1.83532	YES	YES
154	a	837.07	1.34516	YES	YES
155	a	837.22	4.09565	YES	YES
156	a	837.54	5.98211	YES	YES
157	a	838.04	15.20416	YES	YES
158	a	839.19	7.10155	YES	YES
159	a	852.80	15.60341	YES	YES
160	a	854.41	2.91697	YES	YES
161	a	875.39	0.19507	YES	YES
162	a	875.58	0.21919	YES	YES

163	a	876.08	6.18139	YES	YES
164	a	876.79	4.60052	YES	YES
165	a	877.33	7.45190	YES	YES
166	a	877.86	2.75848	YES	YES
167	a	878.46	3.15316	YES	YES
168	a	879.72	0.18525	YES	YES
169	a	880.03	2.12936	YES	YES
170	a	880.30	5.89256	YES	YES
171	a	880.48	2.47176	YES	YES
172	a	881.97	1.52068	YES	YES
173	a	883.43	1.57286	YES	YES
174	a	884.85	1.13420	YES	YES
175	a	886.51	5.55840	YES	YES
176	a	888.01	0.20411	YES	YES
177	a	902.91	0.55783	YES	YES
178	a	903.81	3.64716	YES	YES
179	a	904.19	3.30892	YES	YES
180	a	905.04	0.92465	YES	YES
181	a	908.39	0.70486	YES	YES
182	a	908.97	4.14596	YES	YES
183	a	910.39	0.27488	YES	YES
184	a	911.15	1.39096	YES	YES
185	a	983.49	0.23413	YES	YES
186	a	984.98	0.34548	YES	YES
187	a	987.58	5.13368	YES	YES
188	a	987.75	5.40778	YES	YES
189	a	988.62	19.67645	YES	YES
190	a	989.98	11.92508	YES	YES
191	a	990.55	5.00946	YES	YES
192	a	990.66	14.67510	YES	YES
193	a	992.44	9.35783	YES	YES
194	a	993.36	2.82774	YES	YES
195	a	1016.02	0.26948	YES	YES
196	a	1016.19	1.42591	YES	YES
197	a	1016.69	1.38422	YES	YES
198	a	1016.97	0.15075	YES	YES
199	a	1018.64	1.09626	YES	YES
200	a	1020.81	0.96486	YES	YES
201	a	1021.58	0.31734	YES	YES
202	a	1021.95	1.46412	YES	YES
203	a	1031.12	2.23470	YES	YES
204	a	1032.02	1.57347	YES	YES
205	a	1033.16	1.57832	YES	YES
206	a	1034.52	2.31257	YES	YES
207	a	1038.84	2.73899	YES	YES
208	a	1039.78	1.09809	YES	YES
209	a	1040.45	1.36614	YES	YES
210	a	1042.04	0.60756	YES	YES
211	a	1059.15	0.60549	YES	YES
212	a	1059.99	2.89478	YES	YES
213	a	1060.44	0.83555	YES	YES
214	a	1061.00	1.37822	YES	YES
215	a	1064.72	3.59641	YES	YES
216	a	1067.05	1.50990	YES	YES
217	a	1068.48	0.70942	YES	YES
218	a	1069.48	0.34745	YES	YES
219	a	1070.31	0.52054	YES	YES
220	a	1071.44	0.15166	YES	YES

221	a	1072.02	44.90064	YES	YES
222	a	1072.41	13.36897	YES	YES
223	a	1072.90	75.99447	YES	YES
224	a	1074.11	5.14944	YES	YES
225	a	1074.56	7.59259	YES	YES
226	a	1074.98	1.43866	YES	YES
227	a	1077.34	0.19523	YES	YES
228	a	1082.77	2.43195	YES	YES
229	a	1084.85	3.02284	YES	YES
230	a	1093.80	9.81462	YES	YES
231	a	1095.76	3.61062	YES	YES
232	a	1095.99	8.10579	YES	YES
233	a	1099.31	2.20477	YES	YES
234	a	1103.23	1.56940	YES	YES
235	a	1105.23	3.80943	YES	YES
236	a	1107.45	5.95845	YES	YES
237	a	1108.86	7.85456	YES	YES
238	a	1127.74	0.34359	YES	YES
239	a	1130.00	4.58258	YES	YES
240	a	1132.14	0.69019	YES	YES
241	a	1144.19	5.85046	YES	YES
242	a	1160.52	2.05328	YES	YES
243	a	1160.59	14.92733	YES	YES
244	a	1161.48	2.15558	YES	YES
245	a	1161.89	1.06560	YES	YES
246	a	1170.30	6.69928	YES	YES
247	a	1171.26	1.38852	YES	YES
248	a	1172.20	26.52885	YES	YES
249	a	1172.64	1.66165	YES	YES
250	a	1178.07	20.37216	YES	YES
251	a	1180.26	11.37091	YES	YES
252	a	1182.40	4.21784	YES	YES
253	a	1187.74	8.54784	YES	YES
254	a	1188.98	0.47458	YES	YES
255	a	1190.39	3.05919	YES	YES
256	a	1193.75	1.17300	YES	YES
257	a	1194.53	5.50021	YES	YES
258	a	1242.58	0.15355	YES	YES
259	a	1243.50	0.05296	YES	YES
260	a	1244.12	1.33110	YES	YES
261	a	1245.01	0.20438	YES	YES
262	a	1245.58	0.25960	YES	YES
263	a	1246.27	0.45539	YES	YES
264	a	1246.95	0.44573	YES	YES
265	a	1247.92	0.36416	YES	YES
266	a	1249.43	0.36404	YES	YES
267	a	1250.71	0.26971	YES	YES
268	a	1254.05	1.65393	YES	YES
269	a	1256.56	8.76748	YES	YES
270	a	1256.76	2.10783	YES	YES
271	a	1256.97	2.43015	YES	YES
272	a	1257.55	6.47632	YES	YES
273	a	1257.87	3.06161	YES	YES
274	a	1258.44	0.86861	YES	YES
275	a	1258.66	3.01071	YES	YES
276	a	1258.93	3.50932	YES	YES
277	a	1259.47	2.07721	YES	YES
278	a	1260.20	8.61272	YES	YES

279	a	1261.56	2.97457	YES	YES
280	a	1262.99	0.38052	YES	YES
281	a	1264.48	1.16801	YES	YES
282	a	1266.00	4.54454	YES	YES
283	a	1267.20	0.72726	YES	YES
284	a	1269.87	2.28319	YES	YES
285	a	1271.11	0.33297	YES	YES
286	a	1280.51	2.24386	YES	YES
287	a	1282.86	2.33042	YES	YES
288	a	1284.62	0.88715	YES	YES
289	a	1287.15	3.92920	YES	YES
290	a	1288.32	5.61404	YES	YES
291	a	1290.44	3.22668	YES	YES
292	a	1291.60	4.85978	YES	YES
293	a	1293.66	2.18734	YES	YES
294	a	1309.13	1.00233	YES	YES
295	a	1309.94	0.86131	YES	YES
296	a	1310.70	3.20264	YES	YES
297	a	1310.82	3.31541	YES	YES
298	a	1312.70	0.43581	YES	YES
299	a	1312.77	2.22061	YES	YES
300	a	1316.44	0.82495	YES	YES
301	a	1317.46	0.75823	YES	YES
302	a	1320.73	0.18566	YES	YES
303	a	1321.90	0.25552	YES	YES
304	a	1322.76	3.42756	YES	YES
305	a	1323.38	0.43111	YES	YES
306	a	1323.70	2.03511	YES	YES
307	a	1324.25	0.43172	YES	YES
308	a	1324.93	1.64472	YES	YES
309	a	1325.47	3.35901	YES	YES
310	a	1325.86	0.80964	YES	YES
311	a	1326.19	0.30624	YES	YES
312	a	1326.53	0.43513	YES	YES
313	a	1327.01	8.29842	YES	YES
314	a	1327.24	0.96900	YES	YES
315	a	1327.62	3.59859	YES	YES
316	a	1330.10	2.66957	YES	YES
317	a	1336.18	0.08726	YES	YES
318	a	1336.76	0.10420	YES	YES
319	a	1337.40	0.33438	YES	YES
320	a	1338.35	0.96582	YES	YES
321	a	1338.66	0.20803	YES	YES
322	a	1339.11	0.55096	YES	YES
323	a	1339.41	0.29832	YES	YES
324	a	1340.85	1.28279	YES	YES
325	a	1340.97	0.44649	YES	YES
326	a	1345.22	2.30700	YES	YES
327	a	1347.49	1.06358	YES	YES
328	a	1347.89	2.52613	YES	YES
329	a	1348.22	0.54960	YES	YES
330	a	1348.49	1.48530	YES	YES
331	a	1350.33	2.86205	YES	YES
332	a	1350.47	0.20187	YES	YES
333	a	1351.21	0.42429	YES	YES
334	a	1400.87	7.17604	YES	YES
335	a	1402.89	8.90374	YES	YES
336	a	1405.50	7.82089	YES	YES

337	a	1407.94	7.15514	YES	YES
338	a	1421.57	4.03511	YES	YES
339	a	1426.49	1.99104	YES	YES
340	a	1427.95	3.88018	YES	YES
341	a	1428.84	8.31541	YES	YES
342	a	1429.50	2.28813	YES	YES
343	a	1430.23	1.45651	YES	YES
344	a	1432.11	3.29822	YES	YES
345	a	1432.51	1.85403	YES	YES
346	a	1434.67	4.41009	YES	YES
347	a	1435.16	8.93614	YES	YES
348	a	1435.45	6.46889	YES	YES
349	a	1436.10	1.10577	YES	YES
350	a	1436.68	1.76644	YES	YES
351	a	1436.84	3.80849	YES	YES
352	a	1437.71	4.15213	YES	YES
353	a	1437.80	3.53365	YES	YES
354	a	1438.29	1.87945	YES	YES
355	a	1438.60	3.24384	YES	YES
356	a	1439.01	5.02453	YES	YES
357	a	1439.25	9.76717	YES	YES
358	a	1439.86	3.74856	YES	YES
359	a	1440.51	11.82070	YES	YES
360	a	1440.74	4.28634	YES	YES
361	a	1440.82	5.43397	YES	YES
362	a	1442.20	10.63878	YES	YES
363	a	1442.89	31.49450	YES	YES
364	a	1443.31	8.19390	YES	YES
365	a	1443.49	8.90984	YES	YES
366	a	1444.27	10.76263	YES	YES
367	a	1444.98	8.89636	YES	YES
368	a	1446.65	4.41889	YES	YES
369	a	1446.91	14.43772	YES	YES
370	a	1447.47	35.92700	YES	YES
371	a	1449.80	6.29901	YES	YES
372	a	1452.61	2.13894	YES	YES
373	a	1453.15	1.65668	YES	YES
374	a	1454.21	1.90209	YES	YES
375	a	1454.89	1.75235	YES	YES
376	a	1455.85	1.95044	YES	YES
377	a	1456.53	1.07876	YES	YES
378	a	1458.08	1.86265	YES	YES
379	a	1462.04	2.34049	YES	YES
380	a	1465.52	3.24180	YES	YES
381	a	1862.36	115.80736	YES	YES
382	a	2918.40	79.56815	YES	YES
383	a	2921.15	2.04653	YES	YES
384	a	2925.03	16.82508	YES	YES
385	a	2927.27	11.26665	YES	YES
386	a	2929.14	15.85301	YES	YES
387	a	2930.33	2.65863	YES	YES
388	a	2931.31	9.28574	YES	YES
389	a	2934.48	18.96584	YES	YES
390	a	2938.15	20.14765	YES	YES
391	a	2939.45	12.18412	YES	YES
392	a	2939.76	4.20860	YES	YES
393	a	2941.54	6.89997	YES	YES
394	a	2941.67	3.52231	YES	YES

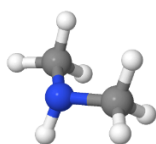
395	a	2941.71	4.63965	YES	YES
396	a	2941.98	14.16840	YES	YES
397	a	2942.64	8.18397	YES	YES
398	a	2943.32	6.09396	YES	YES
399	a	2944.53	7.34908	YES	YES
400	a	2945.02	10.08823	YES	YES
401	a	2946.21	8.89297	YES	YES
402	a	2946.28	12.66457	YES	YES
403	a	2946.34	12.73293	YES	YES
404	a	2948.52	3.36777	YES	YES
405	a	2950.45	20.88611	YES	YES
406	a	2951.88	10.44980	YES	YES
407	a	2952.36	15.56598	YES	YES
408	a	2952.97	18.67266	YES	YES
409	a	2953.96	14.73074	YES	YES
410	a	2954.14	1.60568	YES	YES
411	a	2955.21	2.07571	YES	YES
412	a	2955.61	10.66285	YES	YES
413	a	2956.00	5.45646	YES	YES
414	a	2956.13	3.67740	YES	YES
415	a	2956.35	5.69902	YES	YES
416	a	2957.69	7.33503	YES	YES
417	a	2958.28	4.63235	YES	YES
418	a	2958.55	2.23462	YES	YES
419	a	2960.16	1.40410	YES	YES
420	a	2960.25	65.26874	YES	YES
421	a	2960.83	14.25147	YES	YES
422	a	2961.12	23.53239	YES	YES
423	a	2961.21	56.95752	YES	YES
424	a	2961.53	25.98866	YES	YES
425	a	2962.02	30.78283	YES	YES
426	a	2963.88	36.47480	YES	YES
427	a	2964.30	54.87648	YES	YES
428	a	2964.94	15.74581	YES	YES
429	a	2965.32	52.44659	YES	YES
430	a	2968.88	37.72457	YES	YES
431	a	2973.46	16.41816	YES	YES
432	a	2982.42	6.59198	YES	YES
433	a	2986.66	5.44345	YES	YES
434	a	2989.82	3.62703	YES	YES
435	a	2989.92	2.19456	YES	YES
436	a	2991.50	25.92342	YES	YES
437	a	2992.18	25.18393	YES	YES
438	a	2995.34	36.88628	YES	YES
439	a	3001.70	23.95635	YES	YES
440	a	3004.34	17.30285	YES	YES
441	a	3004.51	34.44536	YES	YES
442	a	3004.92	8.57257	YES	YES
443	a	3005.09	26.38593	YES	YES
444	a	3005.93	6.31548	YES	YES
445	a	3006.64	23.80757	YES	YES
446	a	3006.97	35.70381	YES	YES
447	a	3007.60	13.24434	YES	YES
448	a	3008.05	19.98264	YES	YES
449	a	3008.48	22.42441	YES	YES
450	a	3009.60	12.59321	YES	YES
451	a	3009.92	8.12357	YES	YES
452	a	3010.32	21.98652	YES	YES

453	a	3010.95	20.11791	YES	YES
454	a	3011.19	10.47783	YES	YES
455	a	3011.26	16.97647	YES	YES
456	a	3011.84	22.26582	YES	YES
457	a	3012.02	24.11317	YES	YES
458	a	3012.28	16.49707	YES	YES
459	a	3012.55	31.16123	YES	YES
460	a	3013.05	24.86589	YES	YES
461	a	3013.59	28.58590	YES	YES
462	a	3014.72	21.39237	YES	YES
463	a	3015.12	31.64343	YES	YES
464	a	3015.55	33.91429	YES	YES
465	a	3015.95	20.18911	YES	YES
466	a	3016.48	23.11119	YES	YES
467	a	3016.98	11.37011	YES	YES
468	a	3017.02	19.62455	YES	YES
469	a	3017.52	28.36143	YES	YES
470	a	3017.67	42.71655	YES	YES
471	a	3018.09	37.43928	YES	YES
472	a	3018.32	13.23608	YES	YES
473	a	3018.51	22.18842	YES	YES
474	a	3019.13	29.52022	YES	YES
475	a	3020.56	30.76140	YES	YES
476	a	3023.59	8.75858	YES	YES
477	a	3029.02	0.13199	YES	YES
478	a	3033.76	0.07636	YES	YES
479	a	3046.82	0.79962	YES	YES
480	a	3047.73	0.20685	YES	YES

\$end

Double hybrid single point energy = -7364.706635170493 H
COSMO energy + OC correction = -7372.1585533757 H (in oDFB)

6.2.25 HNMe₂



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
Symmetry: cs

Cartesian coordinates in Ångström:

C	-0.0969023	0.0657129	-1.2133541
N	0.7117511	0.1035964	0.0000000
H	-0.8018585	-0.7916757	-1.2628324
H	0.5560872	0.0278495	-2.0950110
H	-0.6952222	0.9865342	-1.2801125
H	1.3639130	-0.6805431	0.0000000
C	-0.0969023	0.0657129	1.2133541
H	-0.6952222	0.9865342	1.2801125
H	0.5560872	0.0278495	2.0950110
H	-0.8018585	-0.7916757	1.2628324

SCF energy GEOPT = -135.2311371841 H

ZPE = 235.2 kJ/mol
 FREEH energy = 246.91 kJ/mol
 FREEH entropy = 0.27271 kJ/mol/K

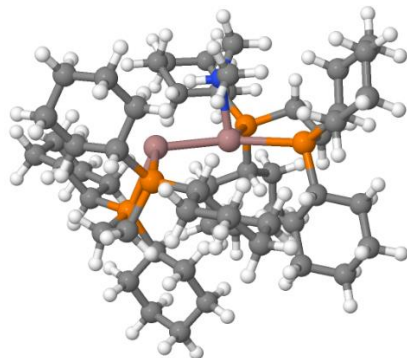
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	233.23	0.11153	YES	YES
8		a'	254.62	2.36465	YES	YES
9		a'	370.40	5.64611	YES	YES
10		a'	746.47	113.48381	YES	YES
11		a'	924.45	2.82346	YES	YES
12		a''	1000.70	7.68542	YES	YES
13		a''	1066.51	0.34888	YES	YES
14		a''	1138.20	30.28528	YES	YES
15		a'	1145.76	6.44304	YES	YES
16		a'	1227.54	0.05264	YES	YES
17		a''	1392.92	1.73733	YES	YES
18		a'	1418.20	0.97813	YES	YES
19		a''	1424.37	5.05181	YES	YES
20		a''	1437.53	4.00793	YES	YES
21		a'	1443.98	11.31507	YES	YES
22		a''	1468.85	11.50502	YES	YES
23		a'	1469.53	2.04840	YES	YES
24		a''	2846.93	54.30767	YES	YES
25		a'	2850.24	171.27428	YES	YES
26		a'	2977.24	48.55393	YES	YES
27		a''	2979.11	23.72549	YES	YES
28		a''	3031.76	25.87661	YES	YES
29		a'	3032.00	31.57215	YES	YES
30		a'	3436.51	0.02461	YES	YES

\$end

Double hybrid single point energy = -134.984427786201 H
 COSMO energy + OC correction = -135.2358620943 H (in oDFB)

6.2.26 [{Ga(dcpe)}₂(HNMe₂)]²⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-1.7258303	17.0346588	-2.2548376
Ga	-3.9345195	17.8363015	-1.2072985
P	-1.3018074	18.6806405	-4.1041886
P	-6.0566986	19.2243020	-0.7583028
P	-2.0167654	15.5039435	-4.1996961
P	-5.1097076	16.2387197	0.2998412
C	-4.6636462	21.1014218	-4.7965196
H	-4.6712646	21.6470233	-3.8372245
H	-5.7058399	20.8218118	-5.0108186
C	-1.0777293	13.9734356	-3.7411925
H	-0.9829010	13.3531276	-4.6472682
C	-4.1592851	15.2541655	1.5436604
H	-3.9549393	16.0018511	2.3316039
C	-4.3741265	16.0806758	-5.5953406
H	-3.7742403	16.5140707	-6.4117251
H	-4.5243699	16.8773710	-4.8505465
C	-6.9420654	19.3557229	-2.3813662
H	-6.2852125	20.0115562	-2.9763764
C	-7.1394183	18.1474796	0.3090928
H	-7.8130082	18.7946260	0.8870580
H	-7.7737444	17.5507401	-0.3600825
C	-2.6570585	22.3748407	-5.6460601
H	-2.2662104	22.9986278	-6.4612472
H	-2.5754470	22.9762975	-4.7253312
C	-1.7896169	21.1169763	-5.4999210
H	-0.7515369	21.4054705	-5.2883717
H	-1.7802111	20.5684102	-6.4557443
C	-3.8081291	19.8382793	-4.6461783
H	-3.8899301	19.2416050	-5.5689959
H	-4.1778217	19.2005967	-3.8270061
C	1.0577316	13.0450180	-2.7314234
H	1.2331125	12.3710206	-3.5856910
H	2.0476558	13.3217700	-2.3435788
C	-7.3748992	14.5247761	-0.2193446
H	-8.0158411	15.2852999	0.2486968
H	-7.0956819	13.8172042	0.5730753
C	-6.2430421	20.9139113	-0.0079540
H	-7.3358776	21.0704668	0.0115477
C	0.5193571	20.1412860	-2.5892033
H	-0.1626289	21.0030191	-2.6446664
H	0.1869005	19.5160713	-1.7410225
C	1.9520998	20.6218696	-2.3285908
H	2.2518832	21.3161212	-3.1302751
H	1.9848787	21.1950559	-1.3914020
C	-7.0158261	18.0007806	-3.1017944
H	-6.0101192	17.5529037	-3.1770917
H	-7.6356489	17.3052804	-2.5115025
C	-4.1250512	22.0212728	-5.8962138
H	-4.2185719	21.5138292	-6.8704099
H	-4.7322354	22.9343032	-5.9611884
C	-8.3323504	20.0081407	-2.2936417
H	-8.2727066	20.9961189	-1.8192458
H	-8.9895064	19.3885301	-1.6612754
C	-5.6200469	22.0052234	-0.8924088
H	-6.0480654	21.9687633	-1.9038005
H	-4.5399280	21.8181951	-1.0053041

C	-3.4118967	13.7583095	-5.9636316
H	-2.9120357	12.9074500	-5.4823441
H	-2.7573984	14.0872090	-6.7873727
C	2.8544693	18.6145548	-3.5610715
H	3.1952216	19.2243467	-4.4136278
H	3.5316315	17.7512066	-3.5044358
C	-5.9872327	22.3873747	2.0285642
H	-7.0719883	22.5687972	2.0957925
H	-5.5992464	22.4276866	3.0554697
C	-9.0229481	18.8079469	-4.4174948
H	-9.4347156	18.9409906	-5.4268681
H	-9.7173552	18.1379467	-3.8837573
C	-4.9226169	14.0942173	2.2070844
H	-5.8784716	14.4409101	2.6241301
H	-5.1582569	13.3335466	1.4476586
C	0.2453508	12.3100875	-1.6618409
H	0.7717574	11.4019968	-1.3389847
H	0.1506649	12.9542539	-0.7708259
C	-7.6436501	18.1482089	-4.4924029
H	-6.9748274	18.7542153	-5.1254568
H	-7.7165846	17.1617933	-4.9670891
C	2.9312443	19.4459392	-2.2779231
H	2.6892770	18.8057689	-1.4127423
H	3.9553446	19.8100185	-2.1214245
C	-5.3391371	23.4706576	1.1610913
H	-5.5415511	24.4643731	1.5817278
H	-4.2429299	23.3448801	1.1765445
C	-5.2287352	14.1263162	-1.5291599
H	-4.8479503	13.4005059	-0.7951665
H	-4.3487985	14.6218762	-1.9670670
C	-5.7448011	20.9904377	1.4415807
H	-4.6660562	20.7773283	1.4716754
H	-6.2388052	20.2278938	2.0623864
C	-6.1132204	15.1645905	-0.8212628
H	-6.4421295	15.8761942	-1.5990847
C	-5.8418817	23.3965063	-0.2835052
C	-7.2916342	12.7414612	-2.0191097
H	-7.8654150	12.2431725	-2.8118593
H	-7.0038969	11.9562042	-1.3011827
C	-8.1611882	13.7844342	-1.3104164
H	-9.0479032	13.3112546	-0.8677904
H	-8.5315303	14.5152711	-2.0493727
C	-1.8882077	13.2065667	-2.6810992
H	-2.8746681	12.9267080	-3.0780843
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C	-4.0622273	13.4551247	3.3067663
H	-3.9005154	14.1901710	4.1123622
H	-4.6097597	12.6157489	3.7563329
C	-5.7121758	15.6111829	-6.1779646
H	-6.2237097	16.4583376	-6.6548299
H	-6.3633660	15.2697033	-5.3556444
C	-2.7100727	12.9855533	2.7608974
H	-2.8733870	12.1723589	2.0341479
H	-2.1014309	12.5612169	3.5703369
C	-2.8076455	14.7794411	0.9784597
H	-2.9896257	14.0445611	0.1797304
H	-2.2651719	15.6122282	0.5026945
C	-8.9549353	20.1514179	-3.6892758

H	-9.9557320	20.5948791	-3.5999774
H	-8.3503210	20.8602812	-4.2788366
C	-4.7588282	13.3039913	-6.5436167
H	-4.5895018	12.5052272	-7.2783299
H	-5.3674741	12.8638839	-5.7368890
C	-6.0294969	13.3826468	-2.6029756
H	-5.3952645	12.6217010	-3.0807292
H	-6.3180658	14.0953165	-3.3938698
C	-5.5202854	14.4690201	-7.1789011
H	-6.4930749	14.1282013	-7.5582316
H	-4.9586102	14.8412432	-8.0516221
C	-1.1499341	11.9593155	-2.1837630
H	-1.7460578	11.4670086	-1.4020180
H	-1.0617709	11.2361599	-3.0105809
C	-1.9575747	14.1309668	2.0758259
H	-1.6891533	14.8941879	2.8255882
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H	-1.8130001	18.1814262	0.0162343
C	0.4286085	19.2981747	-3.8711689
H	0.6693420	19.9328191	-4.7400671
C	1.4257478	18.1267159	-3.8310543
H	1.3996828	17.5712079	-4.7791534
H	1.1199555	17.4244427	-3.0353572
C	0.3311927	14.3047204	-3.2185295
H	0.9282611	14.8003159	-3.9967207
H	0.2421706	15.0207482	-2.3822381
C	-1.0497315	16.2744722	-5.5811737
H	0.0058985	16.0693013	-5.3655927
H	-1.2873768	15.7544559	-6.5197085
C	-1.2776776	17.7858443	-5.7284655
H	-2.2499141	17.9799542	-6.1987553
H	-0.5105993	18.2267576	-6.3810510
C	-3.6023469	14.9114381	-4.9641203
H	-4.1925092	14.5398522	-4.1124734
C	-2.3359437	20.1982038	-4.3938466
H	-2.2853522	20.7428906	-3.4338254
C	-6.3437210	17.2289090	1.2460147
H	-7.0199679	16.5683500	1.8065507
H	-5.7795946	17.8162439	1.9843082
H	-6.9187837	23.6292934	-0.3072982
H	-5.3463064	24.1531690	-0.9069612
C	-2.2815466	20.1569621	-0.1048142
N	-2.6081191	18.7754133	0.3084661
H	-2.1481779	20.1839051	-1.1929324
H	-1.3603085	20.5130807	0.3776814
H	-3.1039693	20.8249254	0.1666805
C	-2.7579142	18.6452042	1.7724935
H	-3.7030645	19.0921368	2.0966380
H	-1.9334517	19.1461964	2.3014893
H	-2.7504981	17.5851036	2.0415767

SCF energy GEOOPT = -7391.428226926 H

ZPE = 3841. kJ/mol

FREEH energy = 4030.99 kJ/mol

FREEH entropy = 1.61213 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules

#		cm** (-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.66	0.14979	YES	YES
8	a	22.34	0.01017	YES	YES
9	a	25.53	0.05268	YES	YES
10	a	28.75	0.05300	YES	YES
11	a	29.59	0.04876	YES	YES
12	a	30.42	0.19426	YES	YES
13	a	33.19	0.46063	YES	YES
14	a	34.94	0.12526	YES	YES
15	a	36.76	0.36551	YES	YES
16	a	43.11	0.05738	YES	YES
17	a	44.44	0.09375	YES	YES
18	a	48.16	0.07110	YES	YES
19	a	49.86	0.14801	YES	YES
20	a	51.71	0.06836	YES	YES
21	a	56.48	0.04133	YES	YES
22	a	57.63	0.14580	YES	YES
23	a	61.94	0.17619	YES	YES
24	a	63.75	0.25773	YES	YES
25	a	65.92	0.20222	YES	YES
26	a	67.34	0.08439	YES	YES
27	a	71.38	0.00582	YES	YES
28	a	72.04	0.91230	YES	YES
29	a	76.60	0.41810	YES	YES
30	a	76.68	0.29042	YES	YES
31	a	77.96	0.03560	YES	YES
32	a	80.74	0.08201	YES	YES
33	a	86.42	0.24066	YES	YES
34	a	89.69	0.45159	YES	YES
35	a	97.38	0.09045	YES	YES
36	a	98.97	0.15795	YES	YES
37	a	101.45	0.21573	YES	YES
38	a	113.25	0.58810	YES	YES
39	a	116.94	1.68843	YES	YES
40	a	123.79	1.35533	YES	YES
41	a	128.04	0.88674	YES	YES
42	a	128.55	0.05934	YES	YES
43	a	134.32	0.78123	YES	YES
44	a	134.66	2.04414	YES	YES
45	a	138.01	0.75412	YES	YES
46	a	142.88	1.56577	YES	YES
47	a	146.39	0.35021	YES	YES
48	a	148.65	3.65529	YES	YES
49	a	169.93	0.43328	YES	YES
50	a	173.87	1.15587	YES	YES
51	a	178.65	1.32124	YES	YES
52	a	180.92	2.02199	YES	YES
53	a	182.06	2.72553	YES	YES
54	a	192.11	0.62156	YES	YES
55	a	199.57	0.20281	YES	YES
56	a	204.35	4.67018	YES	YES
57	a	209.24	0.29587	YES	YES

58	a	212.46	0.28784	YES	YES
59	a	214.63	1.03849	YES	YES
60	a	216.13	0.73653	YES	YES
61	a	217.27	0.88460	YES	YES
62	a	220.02	0.44937	YES	YES
63	a	222.31	0.91637	YES	YES
64	a	225.34	0.13382	YES	YES
65	a	226.51	0.10005	YES	YES
66	a	232.27	0.64292	YES	YES
67	a	235.00	0.17408	YES	YES
68	a	235.59	0.58273	YES	YES
69	a	238.81	0.17937	YES	YES
70	a	239.50	0.41971	YES	YES
71	a	241.60	2.98301	YES	YES
72	a	245.89	0.48364	YES	YES
73	a	254.07	1.14574	YES	YES
74	a	265.21	1.26297	YES	YES
75	a	277.06	1.31121	YES	YES
76	a	278.90	0.77856	YES	YES
77	a	287.27	0.49141	YES	YES
78	a	295.20	0.21816	YES	YES
79	a	301.90	0.80841	YES	YES
80	a	311.95	1.96025	YES	YES
81	a	313.26	0.48217	YES	YES
82	a	327.62	1.66673	YES	YES
83	a	329.91	1.06443	YES	YES
84	a	330.76	0.49890	YES	YES
85	a	334.29	0.70553	YES	YES
86	a	335.05	0.76359	YES	YES
87	a	337.88	0.71689	YES	YES
88	a	352.68	10.30649	YES	YES
89	a	364.71	9.44839	YES	YES
90	a	376.29	8.81088	YES	YES
91	a	379.51	3.18798	YES	YES
92	a	381.19	0.68686	YES	YES
93	a	388.55	1.36191	YES	YES
94	a	390.30	1.34853	YES	YES
95	a	407.96	0.28122	YES	YES
96	a	412.32	1.30471	YES	YES
97	a	413.19	2.30592	YES	YES
98	a	420.02	4.02498	YES	YES
99	a	422.84	3.62189	YES	YES
100	a	425.76	5.88927	YES	YES
101	a	429.19	2.34791	YES	YES
102	a	430.70	0.08840	YES	YES
103	a	431.04	0.29303	YES	YES
104	a	431.28	0.35083	YES	YES
105	a	433.03	0.57244	YES	YES
106	a	433.70	0.71435	YES	YES
107	a	433.88	1.03567	YES	YES
108	a	434.39	1.54326	YES	YES
109	a	438.27	0.23124	YES	YES
110	a	440.73	5.11308	YES	YES
111	a	456.60	5.91229	YES	YES
112	a	459.86	4.32480	YES	YES
113	a	469.93	3.05790	YES	YES
114	a	492.03	3.02986	YES	YES
115	a	492.68	4.73084	YES	YES

116	a	493.67	5.17796	YES	YES
117	a	496.36	0.84615	YES	YES
118	a	500.49	0.38292	YES	YES
119	a	501.07	1.67898	YES	YES
120	a	508.12	8.54312	YES	YES
121	a	511.48	9.96819	YES	YES
122	a	625.82	4.93595	YES	YES
123	a	626.61	26.94271	YES	YES
124	a	640.55	9.64961	YES	YES
125	a	662.76	11.74261	YES	YES
126	a	700.63	1.88155	YES	YES
127	a	711.25	8.24136	YES	YES
128	a	712.31	1.29671	YES	YES
129	a	726.40	4.71417	YES	YES
130	a	727.31	6.27768	YES	YES
131	a	729.64	2.91697	YES	YES
132	a	730.80	12.10351	YES	YES
133	a	732.42	6.13835	YES	YES
134	a	771.65	13.07358	YES	YES
135	a	772.72	3.41216	YES	YES
136	a	772.98	2.20721	YES	YES
137	a	773.72	0.23463	YES	YES
138	a	774.15	3.45197	YES	YES
139	a	775.16	0.85802	YES	YES
140	a	776.19	0.08390	YES	YES
141	a	776.31	0.49448	YES	YES
142	a	778.06	0.81117	YES	YES
143	a	785.81	16.68392	YES	YES
144	a	805.06	0.49758	YES	YES
145	a	808.02	1.44619	YES	YES
146	a	809.22	6.16303	YES	YES
147	a	810.11	7.15391	YES	YES
148	a	811.33	4.12460	YES	YES
149	a	812.33	2.47731	YES	YES
150	a	815.01	2.83481	YES	YES
151	a	816.91	1.87520	YES	YES
152	a	831.59	2.75723	YES	YES
153	a	832.23	6.43774	YES	YES
154	a	834.64	9.92299	YES	YES
155	a	837.19	2.19637	YES	YES
156	a	838.02	1.24460	YES	YES
157	a	838.68	1.84871	YES	YES
158	a	839.57	5.50798	YES	YES
159	a	839.74	4.86563	YES	YES
160	a	847.19	18.27678	YES	YES
161	a	851.32	15.35399	YES	YES
162	a	873.98	2.19495	YES	YES
163	a	875.04	8.25337	YES	YES
164	a	875.64	6.08716	YES	YES
165	a	875.95	5.10526	YES	YES
166	a	877.01	3.87825	YES	YES
167	a	877.24	19.32819	YES	YES
168	a	877.31	7.19934	YES	YES
169	a	878.04	9.20632	YES	YES
170	a	878.15	13.56387	YES	YES
171	a	879.26	4.27762	YES	YES
172	a	880.31	11.45761	YES	YES
173	a	881.04	2.09509	YES	YES

174	a	882.58	5.06544	YES	YES
175	a	883.32	0.55738	YES	YES
176	a	884.96	1.60732	YES	YES
177	a	885.17	2.31494	YES	YES
178	a	886.55	2.20124	YES	YES
179	a	903.17	3.68465	YES	YES
180	a	903.90	1.52852	YES	YES
181	a	904.18	3.40607	YES	YES
182	a	904.87	1.71341	YES	YES
183	a	908.83	0.75901	YES	YES
184	a	909.85	0.90112	YES	YES
185	a	910.26	0.35133	YES	YES
186	a	910.85	1.49291	YES	YES
187	a	984.37	1.89994	YES	YES
188	a	985.16	1.31055	YES	YES
189	a	986.48	7.95531	YES	YES
190	a	986.96	4.53844	YES	YES
191	a	988.29	12.17938	YES	YES
192	a	989.28	11.15557	YES	YES
193	a	990.12	16.25831	YES	YES
194	a	990.35	4.37912	YES	YES
195	a	991.25	2.55959	YES	YES
196	a	992.15	10.74737	YES	YES
197	a	997.88	7.01106	YES	YES
198	a	1014.06	1.70186	YES	YES
199	a	1015.51	2.52809	YES	YES
200	a	1016.02	2.62125	YES	YES
201	a	1017.25	1.34720	YES	YES
202	a	1018.03	0.57207	YES	YES
203	a	1019.44	0.09700	YES	YES
204	a	1020.81	0.49201	YES	YES
205	a	1022.38	0.79703	YES	YES
206	a	1024.71	60.56621	YES	YES
207	a	1030.87	1.13890	YES	YES
208	a	1031.97	1.95738	YES	YES
209	a	1034.74	1.50687	YES	YES
210	a	1035.44	1.19449	YES	YES
211	a	1038.75	2.95485	YES	YES
212	a	1039.22	0.91116	YES	YES
213	a	1040.41	0.79923	YES	YES
214	a	1042.33	0.79179	YES	YES
215	a	1044.05	2.87738	YES	YES
216	a	1056.33	1.49764	YES	YES
217	a	1056.94	0.56389	YES	YES
218	a	1057.41	2.80223	YES	YES
219	a	1058.16	2.09926	YES	YES
220	a	1060.74	0.71153	YES	YES
221	a	1063.09	0.74365	YES	YES
222	a	1064.63	0.72264	YES	YES
223	a	1066.35	2.46423	YES	YES
224	a	1070.17	0.50926	YES	YES
225	a	1071.30	0.84680	YES	YES
226	a	1072.45	0.21025	YES	YES
227	a	1072.74	0.65574	YES	YES
228	a	1073.32	0.21228	YES	YES
229	a	1074.11	0.29225	YES	YES
230	a	1074.62	0.14842	YES	YES
231	a	1074.92	0.32489	YES	YES

232	a	1075.71	2.66847	YES	YES
233	a	1077.88	4.06963	YES	YES
234	a	1088.79	6.31465	YES	YES
235	a	1090.06	7.29650	YES	YES
236	a	1090.97	4.23563	YES	YES
237	a	1092.84	16.21477	YES	YES
238	a	1098.24	1.55927	YES	YES
239	a	1104.13	8.63242	YES	YES
240	a	1104.32	1.45872	YES	YES
241	a	1113.35	3.19311	YES	YES
242	a	1113.88	16.45601	YES	YES
243	a	1122.34	3.84202	YES	YES
244	a	1126.75	2.71597	YES	YES
245	a	1158.34	5.38425	YES	YES
246	a	1159.74	5.70828	YES	YES
247	a	1160.38	9.23616	YES	YES
248	a	1165.64	10.07507	YES	YES
249	a	1168.06	17.54369	YES	YES
250	a	1168.95	3.61084	YES	YES
251	a	1169.98	7.42783	YES	YES
252	a	1170.61	17.22483	YES	YES
253	a	1173.84	5.25802	YES	YES
254	a	1177.05	3.48714	YES	YES
255	a	1177.65	22.65599	YES	YES
256	a	1180.66	5.72557	YES	YES
257	a	1182.74	3.68899	YES	YES
258	a	1185.83	0.98686	YES	YES
259	a	1187.32	10.70242	YES	YES
260	a	1192.91	1.22029	YES	YES
261	a	1212.15	1.27946	YES	YES
262	a	1229.59	21.18449	YES	YES
263	a	1234.83	0.94673	YES	YES
264	a	1236.52	0.51250	YES	YES
265	a	1244.13	0.77950	YES	YES
266	a	1244.81	0.83932	YES	YES
267	a	1245.41	0.22075	YES	YES
268	a	1245.81	0.30507	YES	YES
269	a	1246.94	2.33780	YES	YES
270	a	1248.58	1.99911	YES	YES
271	a	1250.16	0.24943	YES	YES
272	a	1250.56	0.88321	YES	YES
273	a	1251.23	3.06631	YES	YES
274	a	1253.49	0.74068	YES	YES
275	a	1254.32	1.84788	YES	YES
276	a	1255.29	6.50585	YES	YES
277	a	1255.92	3.32850	YES	YES
278	a	1256.30	5.77044	YES	YES
279	a	1256.48	4.53832	YES	YES
280	a	1257.13	1.91125	YES	YES
281	a	1257.73	2.99286	YES	YES
282	a	1258.57	5.28107	YES	YES
283	a	1259.41	2.35554	YES	YES
284	a	1260.56	1.76352	YES	YES
285	a	1261.12	1.52242	YES	YES
286	a	1263.33	0.15119	YES	YES
287	a	1264.18	2.37773	YES	YES
288	a	1264.85	1.38214	YES	YES
289	a	1269.20	0.96127	YES	YES

290	a	1269.65	3.68636	YES	YES
291	a	1281.65	1.25791	YES	YES
292	a	1282.47	3.74195	YES	YES
293	a	1283.41	1.08804	YES	YES
294	a	1284.19	1.28466	YES	YES
295	a	1289.81	4.00846	YES	YES
296	a	1290.11	3.16269	YES	YES
297	a	1291.25	3.36887	YES	YES
298	a	1291.81	5.20020	YES	YES
299	a	1306.03	0.93143	YES	YES
300	a	1307.42	1.79491	YES	YES
301	a	1309.37	1.84119	YES	YES
302	a	1310.31	0.58733	YES	YES
303	a	1311.82	2.81075	YES	YES
304	a	1313.01	0.41382	YES	YES
305	a	1314.41	0.57997	YES	YES
306	a	1316.10	1.99462	YES	YES
307	a	1318.58	3.30716	YES	YES
308	a	1319.31	0.65832	YES	YES
309	a	1320.40	1.90857	YES	YES
310	a	1320.71	0.67037	YES	YES
311	a	1322.59	5.52138	YES	YES
312	a	1322.94	1.54340	YES	YES
313	a	1323.08	0.11142	YES	YES
314	a	1323.64	4.29399	YES	YES
315	a	1324.19	0.73413	YES	YES
316	a	1324.29	0.54791	YES	YES
317	a	1324.60	3.27337	YES	YES
318	a	1324.90	1.36287	YES	YES
319	a	1325.03	1.94604	YES	YES
320	a	1326.33	4.18216	YES	YES
321	a	1327.11	9.64892	YES	YES
322	a	1331.17	3.31135	YES	YES
323	a	1335.79	0.63966	YES	YES
324	a	1335.90	0.12768	YES	YES
325	a	1336.49	0.08523	YES	YES
326	a	1336.70	0.02764	YES	YES
327	a	1337.28	0.22898	YES	YES
328	a	1338.14	0.14392	YES	YES
329	a	1338.28	0.02753	YES	YES
330	a	1338.69	0.14232	YES	YES
331	a	1344.50	2.28371	YES	YES
332	a	1345.04	0.57862	YES	YES
333	a	1345.67	0.44707	YES	YES
334	a	1346.78	1.47948	YES	YES
335	a	1347.78	1.90265	YES	YES
336	a	1348.00	2.56772	YES	YES
337	a	1348.63	0.51272	YES	YES
338	a	1349.17	1.35692	YES	YES
339	a	1388.80	1.89619	YES	YES
340	a	1400.74	4.86144	YES	YES
341	a	1405.95	6.72142	YES	YES
342	a	1407.32	10.90810	YES	YES
343	a	1411.23	5.07494	YES	YES
344	a	1415.05	0.87921	YES	YES
345	a	1419.53	1.14484	YES	YES
346	a	1424.98	2.24071	YES	YES
347	a	1426.40	3.88453	YES	YES

348	a	1428.48	4.95254	YES	YES
349	a	1429.40	1.29435	YES	YES
350	a	1430.71	0.84065	YES	YES
351	a	1432.70	1.28356	YES	YES
352	a	1433.28	3.36612	YES	YES
353	a	1433.37	4.40318	YES	YES
354	a	1433.83	2.21236	YES	YES
355	a	1435.30	4.54689	YES	YES
356	a	1436.38	9.18380	YES	YES
357	a	1436.99	4.50379	YES	YES
358	a	1437.48	12.95243	YES	YES
359	a	1437.94	5.24829	YES	YES
360	a	1438.10	2.88209	YES	YES
361	a	1438.21	9.29383	YES	YES
362	a	1438.29	2.37335	YES	YES
363	a	1438.70	4.61021	YES	YES
364	a	1438.88	6.05800	YES	YES
365	a	1439.35	1.93252	YES	YES
366	a	1439.49	0.63228	YES	YES
367	a	1439.89	10.40047	YES	YES
368	a	1440.65	6.70235	YES	YES
369	a	1441.00	3.36198	YES	YES
370	a	1441.53	4.64334	YES	YES
371	a	1443.13	14.35918	YES	YES
372	a	1443.78	11.79025	YES	YES
373	a	1444.18	2.04242	YES	YES
374	a	1444.42	0.98330	YES	YES
375	a	1445.20	37.02306	YES	YES
376	a	1445.94	6.96795	YES	YES
377	a	1446.35	19.09513	YES	YES
378	a	1447.32	10.79802	YES	YES
379	a	1451.33	3.97218	YES	YES
380	a	1452.74	1.59359	YES	YES
381	a	1454.05	2.58515	YES	YES
382	a	1454.36	4.21771	YES	YES
383	a	1455.07	2.38987	YES	YES
384	a	1455.92	4.06532	YES	YES
385	a	1456.19	4.41234	YES	YES
386	a	1456.75	0.21494	YES	YES
387	a	1457.74	0.80322	YES	YES
388	a	1462.40	11.01122	YES	YES
389	a	1464.85	11.42838	YES	YES
390	a	2917.56	18.26983	YES	YES
391	a	2917.89	14.65584	YES	YES
392	a	2919.90	38.19273	YES	YES
393	a	2923.42	17.28672	YES	YES
394	a	2924.43	3.44008	YES	YES
395	a	2924.64	6.00178	YES	YES
396	a	2927.94	13.96246	YES	YES
397	a	2934.00	2.58056	YES	YES
398	a	2935.31	18.44945	YES	YES
399	a	2936.16	22.17460	YES	YES
400	a	2937.17	12.87229	YES	YES
401	a	2938.49	8.24233	YES	YES
402	a	2938.93	5.15041	YES	YES
403	a	2939.19	9.78630	YES	YES
404	a	2940.29	12.10209	YES	YES
405	a	2940.75	8.25358	YES	YES

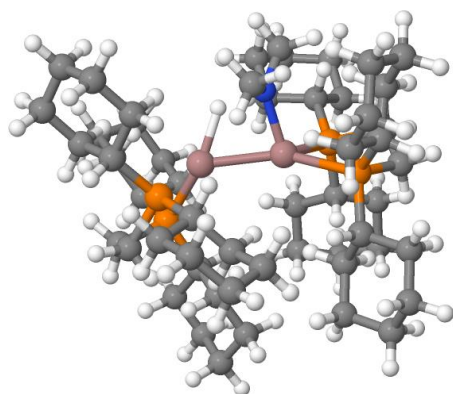
406	a	2941.33	18.37509	YES	YES
407	a	2942.06	9.99401	YES	YES
408	a	2943.31	5.76017	YES	YES
409	a	2944.58	8.77909	YES	YES
410	a	2944.86	8.94364	YES	YES
411	a	2945.39	22.65149	YES	YES
412	a	2946.13	4.65660	YES	YES
413	a	2947.81	12.36248	YES	YES
414	a	2948.05	11.24865	YES	YES
415	a	2950.24	5.84271	YES	YES
416	a	2952.39	5.43206	YES	YES
417	a	2954.06	12.07743	YES	YES
418	a	2954.15	8.92731	YES	YES
419	a	2955.17	4.44291	YES	YES
420	a	2955.27	5.04315	YES	YES
421	a	2955.65	6.20788	YES	YES
422	a	2957.45	20.25062	YES	YES
423	a	2957.79	20.51680	YES	YES
424	a	2958.08	20.41925	YES	YES
425	a	2958.98	34.02993	YES	YES
426	a	2959.07	50.70016	YES	YES
427	a	2959.20	20.80946	YES	YES
428	a	2960.09	1.01507	YES	YES
429	a	2960.30	15.66191	YES	YES
430	a	2960.44	28.33548	YES	YES
431	a	2961.23	42.83187	YES	YES
432	a	2962.04	35.63080	YES	YES
433	a	2962.68	4.27541	YES	YES
434	a	2964.12	37.57442	YES	YES
435	a	2965.42	17.86185	YES	YES
436	a	2967.76	35.25633	YES	YES
437	a	2970.03	12.67851	YES	YES
438	a	2975.39	33.53201	YES	YES
439	a	2977.84	3.53874	YES	YES
440	a	2978.15	20.34100	YES	YES
441	a	2978.69	16.87074	YES	YES
442	a	2980.56	15.21925	YES	YES
443	a	2981.38	3.24605	YES	YES
444	a	2985.71	4.24805	YES	YES
445	a	2986.91	30.25477	YES	YES
446	a	2989.40	4.49368	YES	YES
447	a	2992.10	9.91150	YES	YES
448	a	2993.35	37.51400	YES	YES
449	a	2993.99	14.71248	YES	YES
450	a	2994.46	14.92008	YES	YES
451	a	2997.26	34.13463	YES	YES
452	a	2998.30	25.88181	YES	YES
453	a	2999.85	24.88774	YES	YES
454	a	3001.86	29.50637	YES	YES
455	a	3003.77	26.49894	YES	YES
456	a	3004.34	24.64181	YES	YES
457	a	3006.07	20.52408	YES	YES
458	a	3007.00	15.70649	YES	YES
459	a	3007.54	17.70820	YES	YES
460	a	3009.11	23.89652	YES	YES
461	a	3010.04	18.63669	YES	YES
462	a	3010.70	15.59706	YES	YES
463	a	3011.47	30.36626	YES	YES

464	a	3013.22	12.83235	YES	YES
465	a	3013.31	28.01802	YES	YES
466	a	3013.47	28.14380	YES	YES
467	a	3014.07	20.82273	YES	YES
468	a	3014.26	31.08357	YES	YES
469	a	3014.34	13.21454	YES	YES
470	a	3015.24	36.60132	YES	YES
471	a	3015.37	30.45388	YES	YES
472	a	3015.96	22.40527	YES	YES
473	a	3016.07	27.06624	YES	YES
474	a	3016.37	8.73783	YES	YES
475	a	3016.40	35.12253	YES	YES
476	a	3016.76	35.80073	YES	YES
477	a	3016.81	38.90446	YES	YES
478	a	3017.06	17.10766	YES	YES
479	a	3018.40	17.12772	YES	YES
480	a	3018.63	25.32452	YES	YES
481	a	3019.59	31.54686	YES	YES
482	a	3022.93	6.89743	YES	YES
483	a	3026.03	28.18112	YES	YES
484	a	3026.87	14.20454	YES	YES
485	a	3030.02	1.55661	YES	YES
486	a	3034.95	2.57477	YES	YES
487	a	3045.10	4.67908	YES	YES
488	a	3046.30	1.08948	YES	YES
489	a	3051.29	2.63124	YES	YES
490	a	3081.73	4.24589	YES	YES
491	a	3089.95	1.89414	YES	YES
492	a	3190.84	102.14833	YES	YES

\$end

Double hybrid single point energy = -7384.056600270266 H
COSMO energy + OC correction = -7391.5761338392 H (in oDFB)

6.2.27 $[\{\text{Ga}(\text{dcpe})\}_2(\text{H-NMe}_2)]^{2+}$ (Transition State)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.0256823	17.2434061	-2.4121215
Ga	-4.0487714	17.8432785	-1.0786100
P	-1.3692115	18.8005491	-4.1497622
P	-6.1216389	19.1393855	-0.8116180

P	-1.9671263	15.5780233	-4.1448727
P	-5.2276509	16.1703847	0.2581906
C	-4.7808495	21.1123884	-4.9087987
H	-4.8058860	21.6793054	-3.9626378
H	-5.8149146	20.8034382	-5.1208417
C	-0.9936881	14.1146283	-3.5833382
H	-0.8243243	13.4671184	-4.4593531
C	-4.2926112	15.1766279	1.4992391
H	-4.0573756	15.9332431	2.2693406
C	-4.3444771	16.0917411	-5.5190929
H	-3.7604669	16.5172476	-6.3507025
H	-4.5009657	16.8998763	-4.7884619
C	-7.0001637	19.3398575	-2.4222615
H	-6.3270823	19.9925852	-3.0025855
C	-7.2314661	18.1038641	0.2606272
H	-7.8846488	18.7739748	0.8357891
H	-7.8822042	17.5224563	-0.4064810
C	-2.7998493	22.4149026	-5.7773756
H	-2.4199591	23.0292080	-6.6046969
H	-2.7382896	23.0387394	-4.8703485
C	-1.9020671	21.1830003	-5.5984042
H	-0.8726083	21.5003257	-5.3850610
H	-1.8728130	20.6138479	-6.5418683
C	-3.8974841	19.8728478	-4.7249147
H	-3.9603331	19.2535078	-5.6343107
H	-4.2552720	19.2468924	-3.8921436
C	1.1259094	13.3574251	-2.4104615
H	1.3863040	12.6513929	-3.2155490
H	2.0751760	13.7088691	-1.9838299
C	-7.5097819	14.5039414	-0.3093191
H	-8.1491340	15.2806378	0.1334615
H	-7.2619054	13.8018813	0.4988453
C	-6.1064218	20.8046595	-0.0195797
H	-7.1674349	21.1035408	0.0418171
C	0.4094154	20.3704926	-2.6743499
H	-0.2844843	21.2152029	-2.7956367
H	0.0802980	19.8055630	-1.7874664
C	1.8338346	20.8888570	-2.4414710
H	2.1352018	21.5207552	-3.2927289
H	1.8477818	21.5347021	-1.5526603
C	-7.1137639	18.0031981	-3.1721128
H	-6.1190208	17.5374366	-3.2685961
H	-7.7404377	17.3077399	-2.5887852
C	-4.2571841	22.0184801	-6.0270916
H	-4.3325180	21.4866141	-6.9898377
H	-4.8858797	22.9145690	-6.1165679
C	-8.3674267	20.0334882	-2.3012917
H	-8.2669632	21.0069229	-1.8027429
H	-9.0364287	19.4205774	-1.6750856
C	-5.3624398	21.8230196	-0.8995147
H	-5.8548250	21.9060153	-1.8788393
H	-4.3392739	21.4621521	-1.0893422
C	-3.3387667	13.7807972	-5.8537394
H	-2.8140601	12.9503654	-5.3625260
H	-2.7002920	14.1105283	-6.6895887
C	2.7709427	18.7979079	-3.4958596
H	3.1189297	19.3376973	-4.3915790
H	3.4525053	17.9468737	-3.3600539

C	-5.4909682	22.1271680	2.0523505
H	-6.5177885	22.4995465	2.1979765
H	-5.0420652	22.0506758	3.0519946
C	-9.1157561	18.8972562	-4.4404432
H	-9.5377589	19.0630054	-5.4406547
H	-9.8218794	18.2366613	-3.9104334
C	-5.0814947	14.0494850	2.1887670
H	-6.0256547	14.4279202	2.6048943
H	-5.3411672	13.2787825	1.4472358
C	0.2914476	12.6360940	-1.3488306
H	0.8443548	11.7766617	-0.9471275
H	0.1118660	13.3203176	-0.5019349
C	-7.7573186	18.1987274	-4.5498630
H	-7.0805438	18.7993706	-5.1796111
H	-7.8657199	17.2251895	-5.0453499
C	2.8248634	19.7325266	-2.2847446
H	2.5802720	19.1634812	-1.3721988
H	3.8435992	20.1191917	-2.1491884
C	-4.7108912	23.1168010	1.1823444
H	-4.7068938	24.1098362	1.6507366
H	-3.6562186	22.7995866	1.1185208
C	-5.3410868	14.0450923	-1.5518079
H	-5.0058442	13.3202410	-0.7952837
H	-4.4342116	14.5133911	-1.9629405
C	-5.5461956	20.7349265	1.4103403
H	-4.5363463	20.2989044	1.3835807
H	-6.1636535	20.0657958	2.0275742
C	-6.2216908	15.1135994	-0.8859854
H	-6.5131271	15.8236256	-1.6804137
C	-5.3066042	23.2001986	-0.2257711
C	-7.4141121	12.6968942	-2.0868483
H	-7.9766232	12.2027664	-2.8901991
H	-7.1628009	11.9129541	-1.3540209
C	-8.2809967	13.7643849	-1.4118072
H	-9.1873990	13.3126723	-0.9870691
H	-8.6187122	14.4935128	-2.1678676
C	-1.8251618	13.3559040	-2.5335433
H	-2.7676700	12.9987642	-2.9725139
H	-2.0927334	14.0652605	-1.7315798
C	-4.2285799	13.4153026	3.2974086
H	-4.0483709	14.1641444	4.0859417
H	-4.7905259	12.5967311	3.7670570
C	-5.6796705	15.5883505	-6.0781332
H	-6.2074969	16.4174904	-6.5685929
H	-6.3189627	15.2573147	-5.2428183
C	-2.8882000	12.9066454	2.7568299
H	-3.0709507	12.0783264	2.0519544
H	-2.2842117	12.4911580	3.5742896
C	-2.9604003	14.6534962	0.9293603
H	-3.1711479	13.8962052	0.1605345
H	-2.4041742	15.4611011	0.4280723
C	-9.0004795	20.2241418	-3.6864520
H	-9.9872168	20.6937032	-3.5773458
H	-8.3821467	20.9271324	-4.2686143
C	-4.6821448	13.2902059	-6.4125076
H	-4.5030342	12.4853536	-7.1380137
H	-5.2718317	12.8483538	-5.5934705
C	-6.1225041	13.3051137	-2.6412941

H	-5.4894042	12.5256229	-3.0897345
H	-6.3721607	14.0132240	-3.4488983
C	-5.4761016	14.4288997	-7.0574555
H	-6.4461125	14.0602371	-7.4170746
H	-4.9344082	14.7954132	-7.9450530
C	-1.0505957	12.1811496	-1.9267266
H	-1.6653640	11.7002155	-1.1523592
H	-0.8773804	11.4199602	-2.7043385
C	-2.1158491	14.0185359	2.0390001
H	-1.8271528	14.7966523	2.7649871
H	-1.1814661	13.6273396	1.6126770
H	-1.7003524	17.7075359	-0.7624499
C	0.3479935	19.4363417	-3.8919296
H	0.6014371	20.0070193	-4.8016934
C	1.3494506	18.2771838	-3.7446139
H	1.3441699	17.6481793	-4.6459227
H	1.0342799	17.6401884	-2.9006294
C	0.3642750	14.5490630	-3.0033317
H	0.9767711	15.0378468	-3.7738328
H	0.1874547	15.3000845	-2.2134012
C	-1.0224221	16.3451817	-5.5381520
H	0.0379747	16.1799452	-5.3120981
H	-1.2395938	15.7911440	-6.4619611
C	-1.2999425	17.8452126	-5.7348218
H	-2.2698476	17.9923765	-6.2260677
H	-0.5367598	18.2873747	-6.3907531
C	-3.5464789	14.9473536	-4.8731737
H	-4.1206510	14.5821114	-4.0074777
C	-2.4357657	20.2773117	-4.4754924
H	-2.4013758	20.8400441	-3.5254498
C	-6.4568785	17.1680809	1.1999165
H	-7.1480883	16.5154633	1.7507356
H	-5.8858130	17.7428644	1.9428152
H	-6.3265456	23.6132459	-0.1664450
H	-4.7270033	23.8911302	-0.8532578
C	-2.1954621	19.9322735	-0.1537631
N	-2.6369330	18.5803541	0.1693040
H	-2.2599876	20.0974036	-1.2403809
H	-1.1466070	20.0820694	0.1502028
H	-2.7955593	20.7125070	0.3409814
C	-2.4736031	18.2853730	1.5868589
H	-3.1910906	18.8270451	2.2295611
H	-1.4613341	18.5680346	1.9203884
H	-2.5907663	17.2123283	1.7682893

SCF energy GEOPT = -7391.395640946 H
 ZPE = 3824. kJ/mol
 FREEH energy = 4011.90 kJ/mol
 FREEH entropy = 1.58614 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1		a	-1003.77	0.00000	YES	YES
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-

6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	18.08	0.01380	YES	YES
9	a	24.73	0.00885	YES	YES
10	a	29.19	0.01476	YES	YES
11	a	31.43	0.07469	YES	YES
12	a	32.19	0.24835	YES	YES
13	a	34.48	0.00676	YES	YES
14	a	36.36	0.00426	YES	YES
15	a	36.61	0.05822	YES	YES
16	a	40.18	0.01818	YES	YES
17	a	42.03	0.06750	YES	YES
18	a	42.32	0.28864	YES	YES
19	a	48.60	0.14675	YES	YES
20	a	50.37	0.05779	YES	YES
21	a	53.44	0.03306	YES	YES
22	a	58.49	0.05571	YES	YES
23	a	58.93	0.32634	YES	YES
24	a	63.13	0.07042	YES	YES
25	a	65.61	0.23378	YES	YES
26	a	68.50	0.15551	YES	YES
27	a	70.72	0.24636	YES	YES
28	a	71.37	0.07209	YES	YES
29	a	74.08	0.00585	YES	YES
30	a	76.27	0.21764	YES	YES
31	a	77.63	0.08370	YES	YES
32	a	80.98	0.10425	YES	YES
33	a	84.96	0.38563	YES	YES
34	a	90.71	0.15634	YES	YES
35	a	93.78	0.21917	YES	YES
36	a	102.66	0.29652	YES	YES
37	a	107.87	0.72815	YES	YES
38	a	111.94	3.52961	YES	YES
39	a	119.45	0.47506	YES	YES
40	a	123.22	1.55184	YES	YES
41	a	129.15	0.19398	YES	YES
42	a	133.56	0.30463	YES	YES
43	a	136.98	2.12737	YES	YES
44	a	138.97	0.62098	YES	YES
45	a	141.64	1.04786	YES	YES
46	a	143.12	0.50798	YES	YES
47	a	148.81	2.33713	YES	YES
48	a	153.68	5.89137	YES	YES
49	a	162.24	1.21536	YES	YES
50	a	175.87	0.27516	YES	YES
51	a	178.71	0.78575	YES	YES
52	a	181.18	0.47646	YES	YES
53	a	185.83	0.43244	YES	YES
54	a	193.71	1.76101	YES	YES
55	a	198.67	1.09385	YES	YES
56	a	203.66	0.04192	YES	YES
57	a	215.15	0.35215	YES	YES
58	a	216.77	0.32098	YES	YES
59	a	217.72	0.37013	YES	YES
60	a	220.11	0.04433	YES	YES
61	a	224.03	0.42493	YES	YES
62	a	225.51	0.17910	YES	YES
63	a	228.46	0.60634	YES	YES

64	a	233.09	2.66520	YES	YES
65	a	236.37	0.63223	YES	YES
66	a	237.80	0.47436	YES	YES
67	a	238.50	0.46703	YES	YES
68	a	239.53	0.12121	YES	YES
69	a	241.94	1.32669	YES	YES
70	a	243.42	0.08947	YES	YES
71	a	251.20	0.24789	YES	YES
72	a	257.91	2.90135	YES	YES
73	a	259.13	1.99153	YES	YES
74	a	273.08	1.66472	YES	YES
75	a	281.18	1.94509	YES	YES
76	a	282.58	8.08458	YES	YES
77	a	284.93	0.27149	YES	YES
78	a	293.64	6.22395	YES	YES
79	a	298.59	1.17030	YES	YES
80	a	305.85	0.03665	YES	YES
81	a	313.29	0.11250	YES	YES
82	a	314.43	0.31899	YES	YES
83	a	329.87	0.28146	YES	YES
84	a	330.73	4.61159	YES	YES
85	a	332.60	6.11213	YES	YES
86	a	334.15	5.66281	YES	YES
87	a	336.40	7.55875	YES	YES
88	a	338.88	2.11558	YES	YES
89	a	339.98	0.51978	YES	YES
90	a	371.55	5.26539	YES	YES
91	a	379.89	2.59414	YES	YES
92	a	383.85	1.36796	YES	YES
93	a	385.82	0.55850	YES	YES
94	a	393.00	0.70122	YES	YES
95	a	397.02	0.75462	YES	YES
96	a	409.94	0.12325	YES	YES
97	a	413.93	0.46312	YES	YES
98	a	421.41	2.07416	YES	YES
99	a	422.24	3.13473	YES	YES
100	a	425.01	5.05845	YES	YES
101	a	429.23	0.83315	YES	YES
102	a	431.00	0.08499	YES	YES
103	a	431.21	0.46519	YES	YES
104	a	431.42	0.19798	YES	YES
105	a	431.55	0.03144	YES	YES
106	a	433.75	0.79190	YES	YES
107	a	434.15	0.46618	YES	YES
108	a	435.65	1.87384	YES	YES
109	a	438.98	0.51904	YES	YES
110	a	444.30	4.82853	YES	YES
111	a	459.93	6.65485	YES	YES
112	a	461.10	5.49638	YES	YES
113	a	472.57	2.98345	YES	YES
114	a	482.80	15.80817	YES	YES
115	a	493.07	6.71100	YES	YES
116	a	493.79	3.22385	YES	YES
117	a	495.63	1.88734	YES	YES
118	a	498.26	1.56642	YES	YES
119	a	502.74	2.09405	YES	YES
120	a	503.81	0.65265	YES	YES
121	a	512.10	7.45972	YES	YES

122	a	514.45	14.49791	YES	YES
123	a	631.30	5.96323	YES	YES
124	a	632.49	28.16366	YES	YES
125	a	643.07	10.04812	YES	YES
126	a	665.62	12.97772	YES	YES
127	a	703.13	1.77380	YES	YES
128	a	715.75	1.49607	YES	YES
129	a	719.97	4.07854	YES	YES
130	a	729.19	11.42723	YES	YES
131	a	731.37	2.16906	YES	YES
132	a	733.58	0.48378	YES	YES
133	a	734.05	5.06120	YES	YES
134	a	736.37	8.20017	YES	YES
135	a	771.42	0.78300	YES	YES
136	a	772.94	7.12861	YES	YES
137	a	773.33	1.59127	YES	YES
138	a	774.23	2.25697	YES	YES
139	a	775.46	11.48230	YES	YES
140	a	775.93	0.09780	YES	YES
141	a	777.25	0.96642	YES	YES
142	a	777.38	0.69449	YES	YES
143	a	777.98	0.38089	YES	YES
144	a	788.32	15.96222	YES	YES
145	a	805.83	0.76636	YES	YES
146	a	809.45	2.08691	YES	YES
147	a	810.25	4.85076	YES	YES
148	a	811.94	4.42130	YES	YES
149	a	812.62	3.35638	YES	YES
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151	a	814.55	2.52148	YES	YES
152	a	817.52	2.67459	YES	YES
153	a	832.44	2.78042	YES	YES
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156	a	837.64	1.46378	YES	YES
157	a	838.05	1.41296	YES	YES
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162	a	855.00	16.16191	YES	YES
163	a	873.39	1.67039	YES	YES
164	a	873.88	3.06088	YES	YES
165	a	875.92	0.11415	YES	YES
166	a	876.74	1.81483	YES	YES
167	a	877.12	3.68294	YES	YES
168	a	877.51	2.88517	YES	YES
169	a	878.31	2.10365	YES	YES
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171	a	879.67	9.02049	YES	YES
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173	a	881.29	0.31125	YES	YES
174	a	882.40	4.77061	YES	YES
175	a	883.20	2.05049	YES	YES
176	a	885.29	2.54379	YES	YES
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178	a	886.16	4.61398	YES	YES
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184	a	910.39	1.52038	YES	YES
185	a	910.47	0.18351	YES	YES
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189	a	983.30	0.97052	YES	YES
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203	a	1018.63	0.22030	YES	YES
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205	a	1020.32	0.47985	YES	YES
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211	a	1035.36	1.14039	YES	YES
212	a	1038.25	2.82401	YES	YES
213	a	1039.29	1.24885	YES	YES
214	a	1039.83	0.83773	YES	YES
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216	a	1057.73	1.58264	YES	YES
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221	a	1064.77	0.91998	YES	YES
222	a	1066.14	0.59314	YES	YES
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225	a	1070.27	0.47428	YES	YES
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227	a	1072.59	0.11654	YES	YES
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232	a	1075.98	0.42950	YES	YES
233	a	1077.69	3.50314	YES	YES
234	a	1080.33	3.63244	YES	YES
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253	a	1170.55	4.35107	YES	YES
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262	a	1210.70	4.17849	YES	YES
263	a	1213.37	1.79143	YES	YES
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269	a	1246.48	1.73578	YES	YES
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271	a	1248.77	1.31637	YES	YES
272	a	1249.93	0.35334	YES	YES
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276	a	1255.14	1.60775	YES	YES
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301	a	1305.44	12.21933	YES	YES
302	a	1309.97	0.82208	YES	YES
303	a	1310.44	0.55372	YES	YES
304	a	1310.73	1.91990	YES	YES
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386	a	1455.78	2.25218	YES	YES
387	a	1456.63	1.95877	YES	YES
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389	a	1459.67	6.11863	YES	YES
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393	a	2925.72	10.07298	YES	YES
394	a	2927.78	31.96957	YES	YES
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400	a	2938.02	2.49207	YES	YES
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415	a	2949.41	15.35664	YES	YES
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431	a	2960.67	23.78993	YES	YES
432	a	2960.72	58.81309	YES	YES
433	a	2960.85	26.18850	YES	YES
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447	a	2986.37	4.55571	YES	YES
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453	a	2999.22	52.94647	YES	YES
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466	a	3011.22	27.14267	YES	YES
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468	a	3012.44	16.48597	YES	YES
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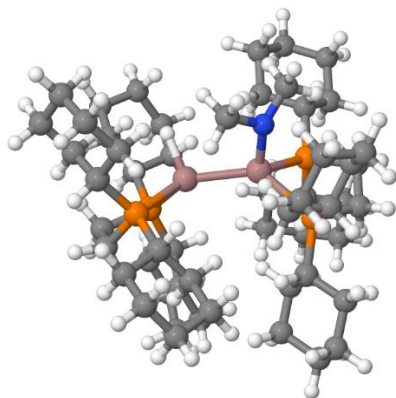
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483	a	3018.33	34.67332	YES	YES
484	a	3018.81	23.07596	YES	YES
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486	a	3019.79	25.08372	YES	YES
487	a	3022.68	31.52937	YES	YES
488	a	3026.74	4.13485	YES	YES
489	a	3032.25	1.16804	YES	YES
490	a	3036.27	2.13494	YES	YES
491	a	3047.92	0.64829	YES	YES
492	a	3065.35	10.47450	YES	YES

\$end

Double hybrid single point energy = -7384.020186848819 H

COSMO energy + OC correction = -7391.5418957544 H (in oDFB)

6.2.28 [H{Ga(dcpe)}₂(NMe₂)]²⁺ (*syn*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

```

Ga  -2.2612947   17.3197851  -2.4499839
Ga  -3.9591223   17.8820169  -0.7778190
P   -1.4583895   18.8840162  -4.1033400
P   -6.1088426   19.0941386  -0.8646001
P   -2.0892834   15.6264007  -4.1575050
P   -5.2472343   16.1862959   0.3610997
C   -4.8851483   21.1371128  -4.9473292
H   -4.9581765   21.7298272  -4.0203110
H   -5.9033831   20.7986329  -5.1869290
C   -1.0904247   14.1753542  -3.5987928

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H	-0.9854736	13.5141804	-4.4751947
C	-4.3191423	15.2165810	1.6220649
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C	-4.4100453	16.0889600	-5.6347781
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H	-4.6037425	16.9169070	-4.9351496
C	-6.9891149	19.2858330	-2.4742939
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C	-7.2573838	18.1108541	0.2155158
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H	-7.8864668	17.5075186	-0.4530738
C	-2.9067594	22.4682724	-5.7660029
H	-2.5102233	23.0821888	-6.5855953
H	-2.8979473	23.1040234	-4.8654445
C	-1.9862929	21.2622375	-5.5393088
H	-0.9734051	21.6073036	-5.2926449
H	-1.9092663	20.6861748	-6.4759510
C	-3.9831607	19.9214859	-4.6999026
H	-4.0172822	19.2750670	-5.5914500
H	-4.3553416	19.3159254	-3.8583236
C	1.0722295	13.3480237	-2.5764146
H	1.2527635	12.6391228	-3.4007484
H	2.0598507	13.6646852	-2.2147059
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H	-7.2039539	13.7669207	0.5283612
C	-5.9810761	20.7835334	-0.1378693
H	-6.9593546	21.2628706	-0.3140341
C	0.3380155	20.4241092	-2.6162752
H	-0.3739591	21.2578297	-2.7043704
H	0.0499513	19.8425854	-1.7275308
C	1.7610765	20.9624766	-2.4223493
H	2.0263402	21.6086845	-3.2749489
H	1.7922611	21.5972910	-1.5264050
C	-7.0487770	17.9553402	-3.2410107
H	-6.0387533	17.5246976	-3.3372252
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C	-4.3409129	22.0278476	-6.0672609
H	-4.3627320	21.4723049	-7.0193984
H	-4.9893568	22.9036490	-6.2025556
C	-8.3861080	19.9185206	-2.3487671
H	-8.3311731	20.8840909	-1.8288095
H	-9.0328701	19.2643669	-1.7417582
C	-4.8953892	21.5728122	-0.8913515
H	-5.1286597	21.6150837	-1.9654533
H	-3.9401279	21.0362775	-0.7832026
C	-3.3813557	13.7760774	-5.8705501
H	-2.8793346	12.9592229	-5.3353883
H	-2.7064089	14.0851217	-6.6857196
C	2.6970843	18.8974910	-3.5306835
H	3.0118868	19.4531134	-4.4289798
H	3.3942609	18.0550220	-3.4246455
C	-5.5739493	22.1882050	1.9203266
H	-6.5344760	22.7183284	1.8126384
H	-5.3579902	22.1480495	2.9966259
C	-9.0794894	18.7888654	-4.5071999
H	-9.5017345	18.9517935	-5.5077819
H	-9.7638530	18.0959804	-3.9900239

C	-5.0558552	14.0094750	2.2259837
H	-6.0304534	14.3116266	2.6345531
H	-5.2525816	13.2672613	1.4371253
C	0.2897100	12.6466003	-1.4629273
H	0.8415746	11.7678703	-1.1039018
H	0.1888563	13.3296524	-0.6024464
C	-7.6963927	18.1404967	-4.6184614
H	-7.0405287	18.7707081	-5.2414339
H	-7.7703105	17.1691868	-5.1237873
C	2.7722857	19.8183456	-2.3099244
H	2.5630345	19.2355318	-1.3974619
H	3.7890006	20.2180579	-2.1997387
C	-4.4792915	22.9625143	1.1800121
H	-4.4060560	23.9857348	1.5716797
H	-3.5037673	22.4827390	1.3664596
C	-5.2809634	14.1160970	-1.5194417
H	-4.9066049	13.3884661	-0.7839255
H	-4.3982517	14.6306159	-1.9277047
C	-5.7132322	20.7607177	1.3760911
H	-4.7810591	20.2060984	1.5520483
H	-6.5252382	20.2392439	1.9035027
C	-6.1944985	15.1353582	-0.8237349
H	-6.5033658	15.8621404	-1.5963066
C	-4.7499369	22.9910684	-0.3270848
C	-7.3115372	12.7091152	-2.0774062
H	-7.8561362	12.2092539	-2.8894816
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C	-8.2134747	13.7359162	-1.3862184
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C	-1.8767611	13.4389327	-2.4996059
H	-2.8557981	13.1130428	-2.8792080
H	-2.0700056	14.1499589	-1.6785105
C	-4.1967770	13.3598696	3.3202718
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H	-4.7227988	12.4851085	3.7257772
C	-5.7203346	15.5605906	-6.2299514
H	-6.2390769	16.3738708	-6.7550958
H	-6.3842393	15.2376716	-5.4107644
C	-2.8173081	12.9600500	2.7871431
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C	-2.9309361	14.8237982	1.0779218
H	-3.0557229	14.1210692	0.2397467
H	-2.4152214	15.7097632	0.6765262
C	-9.0176608	20.1085267	-3.7344592
H	-10.0221197	20.5386245	-3.6244039
H	-8.4234605	20.8430713	-4.3024529
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C	-6.0429305	13.3725130	-2.6210563
H	-5.3862536	12.6247243	-3.0896486
H	-6.3224911	14.0890534	-3.4120835
C	-5.4694654	14.3839479	-7.1764702
H	-6.4218441	14.0019958	-7.5675911
H	-4.8934280	14.7352162	-8.0484514
C	-1.1013244	12.2363301	-1.9511454

H	-1.6782031	11.7700427	-1.1397351
H	-1.0045864	11.4756071	-2.7424928
C	-2.0890917	14.1594955	2.1721525
H	-1.8717780	14.9015429	2.9577758
H	-1.1196261	13.8528716	1.7549930
H	-0.9423044	17.0023829	-1.6284749
C	0.2604639	19.5072686	-3.8470858
H	0.4904538	20.0972932	-4.7514498
C	1.2770049	18.3565303	-3.7466282
H	1.2563521	17.7452021	-4.6599741
H	0.9950042	17.7011362	-2.9073083
C	0.3138912	14.5707520	-3.1095340
H	0.8900963	15.0372595	-3.9206492
H	0.2191283	15.3211732	-2.3099334
C	-1.1304337	16.4334977	-5.5166173
H	-0.0733643	16.2745487	-5.2726193
H	-1.3233925	15.8964592	-6.4559636
C	-1.4159810	17.9333519	-5.6917554
H	-2.3921734	18.0826760	-6.1696065
H	-0.6633917	18.3851177	-6.3527659
C	-3.6314532	14.9662017	-4.9284689
H	-4.2380089	14.6176652	-4.0784538
C	-2.5323849	20.3523159	-4.4247966
H	-2.5208556	20.9105896	-3.4721791
C	-6.5221633	17.2050402	1.2180331
H	-7.2341876	16.5631811	1.7540472
H	-5.9960376	17.8077986	1.9709084
H	-5.6744567	23.5579412	-0.5237362
H	-3.9424666	23.5159395	-0.8566981
C	-1.8697156	19.5979851	0.1646023
N	-3.0433954	18.8543141	0.5785126
H	-1.9745774	19.9344565	-0.8775088
H	-0.9265804	19.0182845	0.2328791
H	-1.7406693	20.5056191	0.7831061
C	-2.9618446	18.4562117	1.9694331
H	-2.7192544	19.3263006	2.6060878
H	-2.1887499	17.6877825	2.1746322
H	-3.9241803	18.0668014	2.3288928

SCF energy GEOOPT = -7391.436447529 H

ZPE = 3828. kJ/mol

FREEH energy = 4017.63 kJ/mol

FREEH entropy = 1.59978 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	16.53	0.01412	YES	YES
	8	a	20.70	0.01592	YES	YES
	9	a	27.87	0.01660	YES	YES
	10	a	29.57	0.06911	YES	YES
	11	a	30.31	0.05954	YES	YES

12	a	32.62	0.00599	YES	YES
13	a	33.25	0.06466	YES	YES
14	a	36.25	0.01295	YES	YES
15	a	39.67	0.08195	YES	YES
16	a	41.72	0.00762	YES	YES
17	a	43.12	0.02144	YES	YES
18	a	47.50	0.03721	YES	YES
19	a	50.93	0.12058	YES	YES
20	a	51.59	0.01832	YES	YES
21	a	55.38	0.09815	YES	YES
22	a	59.57	0.29302	YES	YES
23	a	60.30	0.06459	YES	YES
24	a	64.37	0.28426	YES	YES
25	a	65.65	0.05342	YES	YES
26	a	68.90	0.20792	YES	YES
27	a	71.73	0.05530	YES	YES
28	a	73.54	0.20772	YES	YES
29	a	75.36	0.09285	YES	YES
30	a	79.11	0.04985	YES	YES
31	a	80.08	0.15056	YES	YES
32	a	86.03	0.23939	YES	YES
33	a	89.55	0.42411	YES	YES
34	a	91.25	0.41919	YES	YES
35	a	97.39	0.43250	YES	YES
36	a	105.16	0.22018	YES	YES
37	a	109.42	0.24660	YES	YES
38	a	113.93	0.12465	YES	YES
39	a	119.41	0.46399	YES	YES
40	a	124.64	1.16886	YES	YES
41	a	132.42	0.35069	YES	YES
42	a	135.67	0.06100	YES	YES
43	a	139.64	0.20396	YES	YES
44	a	140.20	2.49116	YES	YES
45	a	142.99	0.78952	YES	YES
46	a	150.18	6.89901	YES	YES
47	a	153.79	0.83942	YES	YES
48	a	156.91	0.35989	YES	YES
49	a	165.45	1.44843	YES	YES
50	a	174.90	2.04961	YES	YES
51	a	182.39	3.44573	YES	YES
52	a	184.95	4.17759	YES	YES
53	a	189.05	1.78265	YES	YES
54	a	200.96	0.47279	YES	YES
55	a	205.89	1.67717	YES	YES
56	a	215.00	0.15539	YES	YES
57	a	216.66	0.22739	YES	YES
58	a	220.20	0.04582	YES	YES
59	a	220.92	0.10604	YES	YES
60	a	225.35	0.14251	YES	YES
61	a	226.28	0.19903	YES	YES
62	a	227.67	0.06022	YES	YES
63	a	228.09	0.29994	YES	YES
64	a	234.85	1.33577	YES	YES
65	a	236.54	0.69792	YES	YES
66	a	238.43	0.64635	YES	YES
67	a	239.16	0.57344	YES	YES
68	a	239.49	0.69157	YES	YES
69	a	241.36	0.79176	YES	YES

70	a	246.16	4.98629	YES	YES
71	a	249.92	0.07885	YES	YES
72	a	265.94	6.88793	YES	YES
73	a	269.60	6.90911	YES	YES
74	a	280.56	1.86980	YES	YES
75	a	285.23	0.35938	YES	YES
76	a	286.83	0.77476	YES	YES
77	a	291.51	0.41875	YES	YES
78	a	300.52	6.21497	YES	YES
79	a	305.13	0.29451	YES	YES
80	a	312.79	0.19377	YES	YES
81	a	313.82	0.39262	YES	YES
82	a	321.64	7.01370	YES	YES
83	a	330.17	1.28734	YES	YES
84	a	331.46	0.03100	YES	YES
85	a	336.29	0.38301	YES	YES
86	a	336.67	0.32782	YES	YES
87	a	338.25	0.38795	YES	YES
88	a	340.23	1.49878	YES	YES
89	a	372.91	4.78591	YES	YES
90	a	377.05	2.75923	YES	YES
91	a	381.62	0.76693	YES	YES
92	a	384.09	0.46398	YES	YES
93	a	396.44	0.50819	YES	YES
94	a	397.59	0.81387	YES	YES
95	a	406.14	0.88456	YES	YES
96	a	412.25	0.88795	YES	YES
97	a	419.24	3.41129	YES	YES
98	a	420.57	1.89687	YES	YES
99	a	423.40	3.08003	YES	YES
100	a	428.45	0.41272	YES	YES
101	a	430.42	0.34787	YES	YES
102	a	430.96	0.34513	YES	YES
103	a	431.41	0.33576	YES	YES
104	a	431.51	0.09818	YES	YES
105	a	433.04	0.95618	YES	YES
106	a	433.79	0.44037	YES	YES
107	a	434.61	0.57058	YES	YES
108	a	437.20	0.10698	YES	YES
109	a	445.95	2.66855	YES	YES
110	a	458.61	5.02401	YES	YES
111	a	459.49	3.86615	YES	YES
112	a	470.52	2.62773	YES	YES
113	a	491.56	3.10891	YES	YES
114	a	493.86	7.59046	YES	YES
115	a	497.51	3.91555	YES	YES
116	a	499.38	1.34739	YES	YES
117	a	500.13	0.68424	YES	YES
118	a	504.70	0.78229	YES	YES
119	a	511.41	16.93639	YES	YES
120	a	511.88	2.02866	YES	YES
121	a	519.47	14.08933	YES	YES
122	a	543.64	98.78605	YES	YES
123	a	604.65	88.70916	YES	YES
124	a	630.39	11.41967	YES	YES
125	a	632.98	30.18241	YES	YES
126	a	645.30	12.28083	YES	YES
127	a	663.57	12.16345	YES	YES

128	a	701.38	1.18881	YES	YES
129	a	718.71	1.35273	YES	YES
130	a	720.06	1.41025	YES	YES
131	a	730.07	14.08577	YES	YES
132	a	732.78	2.04814	YES	YES
133	a	733.34	3.19573	YES	YES
134	a	736.60	2.69779	YES	YES
135	a	737.94	2.83431	YES	YES
136	a	771.52	0.99345	YES	YES
137	a	774.06	0.33866	YES	YES
138	a	774.17	0.27609	YES	YES
139	a	774.38	0.77779	YES	YES
140	a	775.14	0.13935	YES	YES
141	a	775.67	0.42998	YES	YES
142	a	777.05	0.49564	YES	YES
143	a	777.47	0.17555	YES	YES
144	a	779.36	14.27643	YES	YES
145	a	789.16	13.98312	YES	YES
146	a	806.89	0.72389	YES	YES
147	a	810.42	1.84002	YES	YES
148	a	811.03	3.47801	YES	YES
149	a	811.36	9.48879	YES	YES
150	a	813.06	2.67873	YES	YES
151	a	813.48	0.15612	YES	YES
152	a	814.19	4.69020	YES	YES
153	a	818.89	1.92006	YES	YES
154	a	833.78	3.94271	YES	YES
155	a	833.93	7.37934	YES	YES
156	a	836.97	6.58529	YES	YES
157	a	837.56	0.23329	YES	YES
158	a	838.36	0.92107	YES	YES
159	a	839.05	2.93748	YES	YES
160	a	839.56	6.00455	YES	YES
161	a	839.73	5.34326	YES	YES
162	a	850.73	14.43111	YES	YES
163	a	853.86	14.20203	YES	YES
164	a	874.21	2.88993	YES	YES
165	a	874.47	1.43498	YES	YES
166	a	876.34	3.09933	YES	YES
167	a	876.89	5.89994	YES	YES
168	a	877.08	1.93144	YES	YES
169	a	878.02	1.11764	YES	YES
170	a	878.27	2.87657	YES	YES
171	a	878.94	2.78829	YES	YES
172	a	879.68	4.09500	YES	YES
173	a	880.14	1.14086	YES	YES
174	a	880.99	2.59922	YES	YES
175	a	881.56	3.80291	YES	YES
176	a	883.73	3.66341	YES	YES
177	a	884.09	4.45706	YES	YES
178	a	885.94	2.53476	YES	YES
179	a	886.54	4.15893	YES	YES
180	a	904.28	1.19340	YES	YES
181	a	905.30	2.04731	YES	YES
182	a	905.90	3.41592	YES	YES
183	a	906.21	2.47708	YES	YES
184	a	908.99	0.62398	YES	YES
185	a	910.69	0.79362	YES	YES

186	a	910.74	0.64402	YES	YES
187	a	911.49	1.11878	YES	YES
188	a	953.62	74.17394	YES	YES
189	a	978.17	0.37533	YES	YES
190	a	985.48	1.94464	YES	YES
191	a	988.24	8.72641	YES	YES
192	a	988.57	9.05747	YES	YES
193	a	989.27	5.37462	YES	YES
194	a	989.74	15.36093	YES	YES
195	a	990.63	8.70407	YES	YES
196	a	991.42	8.66895	YES	YES
197	a	991.80	10.91108	YES	YES
198	a	993.51	4.07102	YES	YES
199	a	1014.78	0.38119	YES	YES
200	a	1016.17	0.46065	YES	YES
201	a	1017.58	0.26241	YES	YES
202	a	1018.12	0.18919	YES	YES
203	a	1018.51	0.43836	YES	YES
204	a	1019.18	0.38988	YES	YES
205	a	1019.70	0.38114	YES	YES
206	a	1021.87	0.53445	YES	YES
207	a	1031.15	1.21026	YES	YES
208	a	1031.91	0.65889	YES	YES
209	a	1033.20	1.53352	YES	YES
210	a	1034.27	0.70304	YES	YES
211	a	1038.29	3.35733	YES	YES
212	a	1039.17	1.15593	YES	YES
213	a	1040.92	1.25999	YES	YES
214	a	1041.39	0.97846	YES	YES
215	a	1047.49	4.18236	YES	YES
216	a	1058.16	2.05081	YES	YES
217	a	1059.02	1.96789	YES	YES
218	a	1059.73	0.22678	YES	YES
219	a	1061.48	1.19239	YES	YES
220	a	1062.19	1.64558	YES	YES
221	a	1065.03	1.52875	YES	YES
222	a	1066.06	0.06303	YES	YES
223	a	1068.27	1.19447	YES	YES
224	a	1070.75	0.06384	YES	YES
225	a	1071.55	0.16470	YES	YES
226	a	1072.11	0.91248	YES	YES
227	a	1072.58	0.13077	YES	YES
228	a	1072.89	0.14593	YES	YES
229	a	1073.35	0.17490	YES	YES
230	a	1074.18	0.11220	YES	YES
231	a	1074.53	0.02722	YES	YES
232	a	1077.06	2.07860	YES	YES
233	a	1077.96	0.78812	YES	YES
234	a	1082.73	2.94513	YES	YES
235	a	1091.38	1.01207	YES	YES
236	a	1094.75	4.18568	YES	YES
237	a	1095.37	4.05481	YES	YES
238	a	1096.56	8.81212	YES	YES
239	a	1100.95	3.74641	YES	YES
240	a	1104.42	1.73318	YES	YES
241	a	1106.43	8.35011	YES	YES
242	a	1111.77	1.23680	YES	YES
243	a	1114.39	6.25653	YES	YES

244	a	1122.44	1.54262	YES	YES
245	a	1132.09	2.23630	YES	YES
246	a	1160.01	8.34953	YES	YES
247	a	1161.21	0.19224	YES	YES
248	a	1162.33	12.68851	YES	YES
249	a	1166.52	5.56588	YES	YES
250	a	1168.74	9.25052	YES	YES
251	a	1169.70	13.27361	YES	YES
252	a	1170.52	7.80665	YES	YES
253	a	1171.60	2.70827	YES	YES
254	a	1176.29	46.02505	YES	YES
255	a	1178.66	20.71535	YES	YES
256	a	1180.07	13.88026	YES	YES
257	a	1181.64	14.34197	YES	YES
258	a	1182.30	6.47827	YES	YES
259	a	1187.23	0.39375	YES	YES
260	a	1189.49	1.15230	YES	YES
261	a	1192.27	2.02662	YES	YES
262	a	1211.42	1.14141	YES	YES
263	a	1227.52	11.97718	YES	YES
264	a	1238.80	0.03483	YES	YES
265	a	1242.06	0.33759	YES	YES
266	a	1244.55	0.83179	YES	YES
267	a	1246.25	0.49905	YES	YES
268	a	1246.49	0.03120	YES	YES
269	a	1247.19	1.01558	YES	YES
270	a	1247.87	1.22719	YES	YES
271	a	1248.36	2.03540	YES	YES
272	a	1250.48	0.26772	YES	YES
273	a	1251.01	0.72859	YES	YES
274	a	1251.70	0.12031	YES	YES
275	a	1255.07	1.67807	YES	YES
276	a	1255.39	5.64829	YES	YES
277	a	1256.34	4.68137	YES	YES
278	a	1256.69	4.93897	YES	YES
279	a	1257.34	1.59188	YES	YES
280	a	1257.90	5.75662	YES	YES
281	a	1258.25	2.54837	YES	YES
282	a	1259.53	3.94554	YES	YES
283	a	1261.22	0.90583	YES	YES
284	a	1261.81	1.71983	YES	YES
285	a	1262.86	1.69918	YES	YES
286	a	1263.33	0.79842	YES	YES
287	a	1264.42	0.64975	YES	YES
288	a	1266.31	0.17899	YES	YES
289	a	1267.32	1.93108	YES	YES
290	a	1269.77	1.50826	YES	YES
291	a	1272.69	2.10741	YES	YES
292	a	1281.85	2.69644	YES	YES
293	a	1282.95	0.90876	YES	YES
294	a	1284.89	4.40685	YES	YES
295	a	1285.50	1.81385	YES	YES
296	a	1288.03	4.07244	YES	YES
297	a	1290.10	4.03807	YES	YES
298	a	1290.93	2.59859	YES	YES
299	a	1294.02	3.32593	YES	YES
300	a	1305.59	1.12092	YES	YES
301	a	1309.21	0.28295	YES	YES

302	a	1311.32	1.03524	YES	YES
303	a	1311.57	0.50136	YES	YES
304	a	1313.73	1.28122	YES	YES
305	a	1314.51	0.28110	YES	YES
306	a	1316.89	2.85493	YES	YES
307	a	1317.88	0.66156	YES	YES
308	a	1320.06	1.47845	YES	YES
309	a	1321.25	1.27476	YES	YES
310	a	1322.67	0.65502	YES	YES
311	a	1322.92	0.64386	YES	YES
312	a	1323.40	0.16522	YES	YES
313	a	1324.29	0.89992	YES	YES
314	a	1324.52	2.90359	YES	YES
315	a	1324.65	1.38461	YES	YES
316	a	1324.83	0.33367	YES	YES
317	a	1324.91	0.63856	YES	YES
318	a	1325.44	0.35345	YES	YES
319	a	1325.99	5.81293	YES	YES
320	a	1327.07	2.15886	YES	YES
321	a	1329.86	0.02327	YES	YES
322	a	1330.19	10.23770	YES	YES
323	a	1331.48	3.55197	YES	YES
324	a	1336.50	0.23621	YES	YES
325	a	1336.83	0.48612	YES	YES
326	a	1337.19	0.21387	YES	YES
327	a	1337.26	0.18536	YES	YES
328	a	1338.02	0.45582	YES	YES
329	a	1338.64	0.18499	YES	YES
330	a	1338.99	0.01486	YES	YES
331	a	1339.49	0.34716	YES	YES
332	a	1344.79	2.10792	YES	YES
333	a	1345.69	0.15369	YES	YES
334	a	1346.61	1.00929	YES	YES
335	a	1346.68	1.29728	YES	YES
336	a	1347.10	0.78163	YES	YES
337	a	1348.09	3.04170	YES	YES
338	a	1348.27	0.24954	YES	YES
339	a	1350.67	1.05170	YES	YES
340	a	1392.38	1.00009	YES	YES
341	a	1401.22	5.38438	YES	YES
342	a	1406.22	7.40065	YES	YES
343	a	1407.77	11.22470	YES	YES
344	a	1409.65	6.90632	YES	YES
345	a	1417.20	3.30535	YES	YES
346	a	1421.96	0.57270	YES	YES
347	a	1425.82	3.95719	YES	YES
348	a	1426.91	5.40883	YES	YES
349	a	1427.70	17.49663	YES	YES
350	a	1428.40	0.74470	YES	YES
351	a	1431.98	1.98341	YES	YES
352	a	1432.69	1.67719	YES	YES
353	a	1433.36	0.60108	YES	YES
354	a	1433.78	8.61088	YES	YES
355	a	1434.41	1.68516	YES	YES
356	a	1435.25	6.29393	YES	YES
357	a	1435.85	2.20580	YES	YES
358	a	1437.10	4.38992	YES	YES
359	a	1437.46	8.39541	YES	YES

360	a	1437.63	4.26654	YES	YES
361	a	1438.22	2.77485	YES	YES
362	a	1438.28	1.14714	YES	YES
363	a	1438.69	5.11645	YES	YES
364	a	1438.85	8.21180	YES	YES
365	a	1439.02	9.19217	YES	YES
366	a	1439.55	6.37182	YES	YES
367	a	1439.76	4.05342	YES	YES
368	a	1440.14	4.89881	YES	YES
369	a	1440.39	3.18816	YES	YES
370	a	1440.94	2.86527	YES	YES
371	a	1441.34	3.74663	YES	YES
372	a	1442.18	13.81878	YES	YES
373	a	1443.68	5.61568	YES	YES
374	a	1444.15	17.18584	YES	YES
375	a	1444.92	15.81289	YES	YES
376	a	1445.49	26.38094	YES	YES
377	a	1446.45	13.50167	YES	YES
378	a	1446.90	17.29553	YES	YES
379	a	1447.09	7.42831	YES	YES
380	a	1452.77	1.60000	YES	YES
381	a	1453.18	8.45653	YES	YES
382	a	1454.44	2.56094	YES	YES
383	a	1454.67	0.53078	YES	YES
384	a	1455.07	1.68372	YES	YES
385	a	1456.04	1.42059	YES	YES
386	a	1456.40	0.40103	YES	YES
387	a	1457.28	11.59937	YES	YES
388	a	1458.21	0.56876	YES	YES
389	a	1470.69	7.25522	YES	YES
390	a	1833.27	127.02437	YES	YES
391	a	2860.01	74.03283	YES	YES
392	a	2862.96	111.20182	YES	YES
393	a	2912.84	68.44554	YES	YES
394	a	2925.65	19.04608	YES	YES
395	a	2930.28	32.69731	YES	YES
396	a	2933.82	1.19338	YES	YES
397	a	2935.79	2.40915	YES	YES
398	a	2937.38	16.41486	YES	YES
399	a	2937.62	2.43748	YES	YES
400	a	2938.96	16.69317	YES	YES
401	a	2940.51	11.84111	YES	YES
402	a	2940.81	10.06200	YES	YES
403	a	2941.66	5.84066	YES	YES
404	a	2941.80	7.91781	YES	YES
405	a	2942.33	19.77930	YES	YES
406	a	2942.36	10.88573	YES	YES
407	a	2942.68	8.81304	YES	YES
408	a	2944.43	6.11703	YES	YES
409	a	2944.79	31.99632	YES	YES
410	a	2945.45	7.08596	YES	YES
411	a	2945.64	1.75968	YES	YES
412	a	2946.72	13.54409	YES	YES
413	a	2948.36	12.84171	YES	YES
414	a	2948.89	4.32671	YES	YES
415	a	2949.26	9.55752	YES	YES
416	a	2951.92	12.88917	YES	YES
417	a	2952.53	15.26399	YES	YES

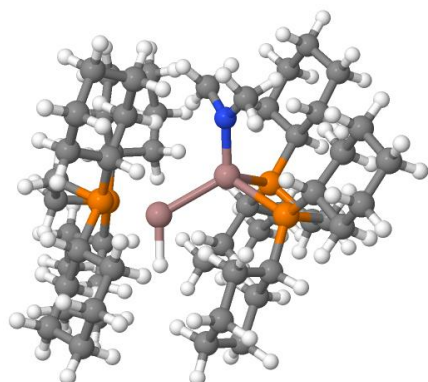
418	a	2952.69	22.44758	YES	YES
419	a	2952.71	9.61462	YES	YES
420	a	2953.72	4.19991	YES	YES
421	a	2953.81	5.15659	YES	YES
422	a	2955.24	4.12386	YES	YES
423	a	2956.06	20.54041	YES	YES
424	a	2956.43	4.25135	YES	YES
425	a	2957.52	4.79671	YES	YES
426	a	2958.12	37.77411	YES	YES
427	a	2959.01	31.49399	YES	YES
428	a	2959.27	0.15845	YES	YES
429	a	2960.14	30.56616	YES	YES
430	a	2960.56	33.62445	YES	YES
431	a	2961.01	29.17747	YES	YES
432	a	2961.18	26.72716	YES	YES
433	a	2961.39	37.01447	YES	YES
434	a	2961.65	8.49829	YES	YES
435	a	2963.55	25.56552	YES	YES
436	a	2963.70	25.82928	YES	YES
437	a	2964.39	26.57505	YES	YES
438	a	2965.51	15.15896	YES	YES
439	a	2967.54	8.45165	YES	YES
440	a	2968.97	20.02799	YES	YES
441	a	2979.51	7.87050	YES	YES
442	a	2980.28	36.45353	YES	YES
443	a	2981.60	10.06399	YES	YES
444	a	2984.87	25.97707	YES	YES
445	a	2986.20	2.44823	YES	YES
446	a	2987.53	6.86685	YES	YES
447	a	2988.39	4.51922	YES	YES
448	a	2990.44	30.74299	YES	YES
449	a	2990.90	4.01198	YES	YES
450	a	2992.88	18.39795	YES	YES
451	a	2995.71	29.19536	YES	YES
452	a	2996.78	15.25555	YES	YES
453	a	2999.78	28.08736	YES	YES
454	a	3001.50	19.60491	YES	YES
455	a	3001.94	24.43801	YES	YES
456	a	3004.08	0.99159	YES	YES
457	a	3004.20	44.15457	YES	YES
458	a	3004.60	39.78787	YES	YES
459	a	3007.55	8.61268	YES	YES
460	a	3007.78	0.69608	YES	YES
461	a	3008.54	30.30354	YES	YES
462	a	3009.33	5.97155	YES	YES
463	a	3009.40	35.49740	YES	YES
464	a	3009.95	38.59176	YES	YES
465	a	3011.56	15.74455	YES	YES
466	a	3012.02	4.52816	YES	YES
467	a	3012.05	27.64161	YES	YES
468	a	3014.11	20.04595	YES	YES
469	a	3014.21	36.20679	YES	YES
470	a	3014.30	14.60371	YES	YES
471	a	3015.07	13.65757	YES	YES
472	a	3015.53	22.82132	YES	YES
473	a	3015.56	18.24580	YES	YES
474	a	3016.17	26.88393	YES	YES
475	a	3016.66	15.00838	YES	YES

476	a	3016.68	30.98375	YES	YES
477	a	3017.15	30.57763	YES	YES
478	a	3017.41	23.73343	YES	YES
479	a	3017.42	32.71107	YES	YES
480	a	3017.98	18.59733	YES	YES
481	a	3018.27	33.86313	YES	YES
482	a	3018.59	20.49646	YES	YES
483	a	3019.09	9.53882	YES	YES
484	a	3019.17	16.59865	YES	YES
485	a	3019.21	48.86617	YES	YES
486	a	3023.97	22.03718	YES	YES
487	a	3025.17	25.36665	YES	YES
488	a	3025.84	8.26700	YES	YES
489	a	3030.91	1.45399	YES	YES
490	a	3034.79	0.41767	YES	YES
491	a	3038.87	1.16910	YES	YES
492	a	3049.81	0.24298	YES	YES

\$end

Double hybrid single point energy = -7384.071958556270 H
 COSMO energy + OC correction = -7391.5829919471 H (in oDFB)

6.2.29 [H{Ga(dcpe)}₂(NMe₂)]²⁺ (*anti*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-0.4319512	0.2874977	-2.0002729
P	-2.5051482	-0.7183509	-2.8853319
P	-1.5769251	2.4707777	-2.4372908
C	-2.4128390	-1.9507929	-4.2736453
H	-1.5771060	-2.6123144	-3.9873320
C	-2.0545197	-1.2758985	-5.6105533
H	-2.9092437	-0.6662713	-5.9430817
H	-1.1997097	-0.5973785	-5.4991655
C	-1.7770812	-2.3369872	-6.6817644
H	-1.5182694	-1.8446637	-7.6290378
H	-0.8978022	-2.9324587	-6.3853292
C	-2.9914292	-3.2528650	-6.8654138
H	-2.7685321	-4.0408441	-7.5969459
H	-3.8251407	-2.6659872	-7.2844778
C	-3.4284453	-3.8776960	-5.5371201
H	-2.6497875	-4.5744085	-5.1846498

H	-4.3408254	-4.4739803	-5.6733548
C	-3.6708467	-2.8213053	-4.4467343
H	-3.9421448	-3.3245343	-3.5097904
H	-4.5229609	-2.1818190	-4.7290325
C	-3.5062490	-1.4970484	-1.5495479
H	-4.4258256	-1.8552060	-2.0423043
C	-2.7519812	-2.7054707	-0.9725854
H	-2.5062854	-3.4257451	-1.7661500
H	-1.7919462	-2.3547551	-0.5556849
C	-3.5727055	-3.3841923	0.1294438
H	-4.4953718	-3.7966906	-0.3097335
H	-3.0169226	-4.2401827	0.5350999
C	-3.9304578	-2.3909991	1.2374337
H	-4.5284162	-2.8849546	2.0150239
H	-3.0044871	-2.0375172	1.7217865
C	-4.6911583	-1.1894144	0.6703229
H	-4.9108218	-0.4610861	1.4632343
H	-5.6637332	-1.5262684	0.2767422
C	-3.9065055	-0.4968274	-0.4520459
H	-4.5216325	0.3065031	-0.8800105
H	-3.0013384	-0.0330022	-0.0300673
C	-3.5209535	0.6802007	-3.5350893
H	-3.2410175	0.7911761	-4.5886163
H	-4.5790353	0.3813926	-3.5180078
C	-3.3328597	2.0127936	-2.8024793
H	-3.8428112	1.9930112	-1.8312899
H	-3.7898237	2.8244436	-3.3850965
C	-0.9691904	3.3890900	-3.9213263
H	-1.7631849	4.1129851	-4.1739717
C	0.3167115	4.1657908	-3.5903425
H	1.0734955	3.4661396	-3.2040701
H	0.1236333	4.8984353	-2.7943987
C	0.8729185	4.8820670	-4.8272758
H	0.1694440	5.6734771	-5.1326395
H	1.8131919	5.3855693	-4.5633612
C	1.0857691	3.9136734	-5.9936001
H	1.8661296	3.1814962	-5.7259920
H	1.4564730	4.4557985	-6.8735196
C	-0.2104222	3.1746229	-6.3342181
H	-0.0452518	2.4575724	-7.1501600
H	-0.9579786	3.8976678	-6.6989071
C	-0.7737768	2.4351505	-5.1147241
H	-0.0907810	1.6250830	-4.8146534
H	-1.7294207	1.9627363	-5.3818895
C	-1.7420539	3.7165696	-1.0800930
H	-0.7226529	4.1085834	-0.9421839
C	-2.1755333	3.0612020	0.2407669
H	-1.4694785	2.2614464	0.5168064
H	-3.1565427	2.5754400	0.1179471
C	-2.2773953	4.1023440	1.3621882
H	-2.6243669	3.6170325	2.2850659
H	-1.2718530	4.5051979	1.5741694
C	-3.1989298	5.2635796	0.9804811
H	-4.2290965	4.8895760	0.8611864
H	-3.2283725	6.0047198	1.7902466
C	-2.7386457	5.9171391	-0.3246054
H	-1.7453717	6.3730482	-0.1789555
H	-3.4174838	6.7316099	-0.6106449

C	-2.6621482	4.8910761	-1.4623289
H	-3.6758265	4.5138891	-1.6695908
H	-2.3067708	5.3749702	-2.3824584
Ga	-0.0241109	-0.1489400	0.4049604
P	1.3371784	1.2913427	1.8182660
P	1.4906804	-1.9355583	1.0625166
C	0.3879500	2.2295949	3.1009832
H	-0.2111137	2.9486512	2.5192686
C	-0.5865638	1.3159454	3.8663577
H	-0.0168534	0.5441876	4.4090458
H	-1.2422065	0.7865279	3.1620820
C	-1.4137140	2.1183722	4.8789690
H	-2.0724687	1.4358742	5.4333459
H	-2.0717713	2.8161922	4.3355778
C	-0.5201342	2.9074330	5.8389445
H	-1.1335724	3.5025457	6.5284409
H	0.0574503	2.2049781	6.4624642
C	0.4439496	3.8142966	5.0705128
H	-0.1286260	4.5833265	4.5260674
H	1.1081624	4.3500112	5.7620957
C	1.2909223	3.0183704	4.0669814
H	1.9503975	3.7038597	3.5176533
H	1.9408093	2.3183789	4.6167658
C	2.4566636	2.5060588	1.0011374
H	2.9288993	3.0694672	1.8234687
C	1.6423762	3.4827009	0.1415928
H	0.8617596	3.9674005	0.7460715
H	1.1235934	2.9060279	-0.6443114
C	2.5464304	4.5405077	-0.5003989
H	2.9809731	5.1682609	0.2938180
H	1.9451333	5.2106349	-1.1308230
C	3.6687155	3.8963641	-1.3190829
H	4.3412696	4.6702868	-1.7122626
H	3.2364984	3.3905398	-2.1968057
C	4.4665694	2.8884496	-0.4844062
H	5.2201692	2.3866535	-1.1065475
H	5.0206795	3.4277340	0.3006232
C	3.5699322	1.8345273	0.1828447
H	4.1869667	1.1966145	0.8306865
H	3.1221000	1.1784232	-0.5798326
C	2.4338183	0.1447853	2.7657548
H	1.8704755	-0.1372667	3.6637680
H	3.3177475	0.7019500	3.1064062
C	2.8618514	-1.1047441	1.9849648
H	3.6177552	-0.8436875	1.2337370
H	3.3230789	-1.8357878	2.6632144
C	0.7662145	-3.1624506	2.2379356
H	1.6168563	-3.7831325	2.5683681
C	-0.2536500	-4.0535260	1.5140198
H	-1.0529942	-3.4099405	1.1158360
H	0.2100789	-4.5587422	0.6549221
C	-0.8637787	-5.0888560	2.4662622
H	-0.0772622	-5.7891243	2.7909404
H	-1.6092177	-5.6902764	1.9269663
C	-1.4919267	-4.4188332	3.6908716
H	-2.3472331	-3.8012415	3.3711941
H	-1.8921338	-5.1776141	4.3762449
C	-0.4724112	-3.5364206	4.4155975

H	-0.9394007	-3.0264110	5.2693644
H	0.3304941	-4.1678935	4.8292900
C	0.1420961	-2.4926119	3.4736308
H	-0.6347330	-1.7840011	3.1449555
H	0.9001581	-1.9122826	4.0179748
C	2.3163190	-2.9011145	-0.2761866
H	1.4832309	-3.3934896	-0.8077937
C	3.0210412	-1.9678708	-1.2742871
H	2.2998951	-1.2433982	-1.6831304
H	3.8096113	-1.3980057	-0.7564424
C	3.6685894	-2.7758343	-2.4073084
H	4.1946865	-2.0933760	-3.0897467
H	2.8757087	-3.2628577	-2.9985455
C	4.6258820	-3.8420629	-1.8684952
H	5.4731927	-3.3511091	-1.3616600
H	5.0532033	-4.4234769	-2.6963697
C	3.9116443	-4.7700567	-0.8829846
H	3.1292716	-5.3378950	-1.4131767
H	4.6099070	-5.5109188	-0.4707986
C	3.2672516	-3.9833513	0.2664565
H	4.0597296	-3.5045930	0.8645087
H	2.7341095	-4.6726568	0.9352595
H	-1.2639688	-0.3961241	1.3525492
N	0.9958478	0.0143071	-3.1965964
C	1.0728735	-0.9310349	-4.2882967
C	2.1051330	0.9393743	-3.1922278
H	2.0640201	-1.4175339	-4.3079050
H	0.9348868	-0.4634866	-5.2849690
H	0.3265170	-1.7264446	-4.1805237
H	2.1580591	1.5584070	-4.1104986
H	3.0773252	0.4149089	-3.1083628
H	2.0295136	1.6286227	-2.3416010

SCF energy GEOOPT = -7391.442612933 H

ZPE = 3830. kJ/mol

FREEH energy = 4019.26 kJ/mol

FREEH entropy = 1.59770 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	9.05	0.01399	YES	YES
	8	a	9.84	0.00824	YES	YES
	9	a	19.79	0.03319	YES	YES
	10	a	25.84	0.02719	YES	YES
	11	a	29.44	0.01923	YES	YES
	12	a	32.78	0.06258	YES	YES
	13	a	37.81	0.03414	YES	YES
	14	a	42.28	0.12496	YES	YES
	15	a	45.03	0.03541	YES	YES
	16	a	46.82	0.02124	YES	YES
	17	a	51.31	0.03503	YES	YES

18	a	54.09	0.09223	YES	YES
19	a	56.75	0.44180	YES	YES
20	a	57.95	0.07058	YES	YES
21	a	62.02	0.26274	YES	YES
22	a	63.19	0.07373	YES	YES
23	a	63.81	0.09560	YES	YES
24	a	66.81	0.35266	YES	YES
25	a	70.12	0.05939	YES	YES
26	a	72.10	0.29088	YES	YES
27	a	73.40	0.73812	YES	YES
28	a	76.15	0.23688	YES	YES
29	a	79.03	0.01945	YES	YES
30	a	80.81	0.40115	YES	YES
31	a	85.56	0.02311	YES	YES
32	a	85.81	0.16380	YES	YES
33	a	90.37	0.59131	YES	YES
34	a	95.38	0.80932	YES	YES
35	a	95.91	0.09460	YES	YES
36	a	102.79	0.69369	YES	YES
37	a	118.45	5.48594	YES	YES
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52	a	182.29	0.61744	YES	YES
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66	a	239.68	0.09980	YES	YES
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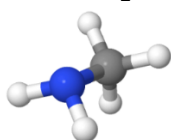
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451	a	3003.64	21.47018	YES	YES
452	a	3004.03	29.46031	YES	YES
453	a	3005.26	15.65401	YES	YES
454	a	3005.65	19.15109	YES	YES
455	a	3005.80	35.45882	YES	YES
456	a	3006.86	42.06148	YES	YES
457	a	3007.54	24.33928	YES	YES
458	a	3008.23	0.65096	YES	YES
459	a	3008.49	11.82922	YES	YES
460	a	3009.54	30.15516	YES	YES
461	a	3009.87	0.41960	YES	YES
462	a	3010.21	30.22052	YES	YES
463	a	3011.83	4.94159	YES	YES
464	a	3012.16	23.36343	YES	YES
465	a	3012.26	31.05064	YES	YES
466	a	3012.41	5.30443	YES	YES
467	a	3012.62	0.82356	YES	YES
468	a	3012.89	23.04754	YES	YES
469	a	3013.80	30.22432	YES	YES
470	a	3014.15	13.31669	YES	YES
471	a	3014.20	19.27561	YES	YES
472	a	3014.49	29.02720	YES	YES
473	a	3014.54	35.47919	YES	YES
474	a	3014.95	32.13051	YES	YES
475	a	3015.12	32.83340	YES	YES
476	a	3015.43	40.83230	YES	YES
477	a	3016.79	21.58312	YES	YES
478	a	3017.03	21.52214	YES	YES
479	a	3017.65	19.67203	YES	YES
480	a	3018.04	30.31175	YES	YES
481	a	3018.54	36.00476	YES	YES

482	a	3018.59	15.92670	YES	YES
483	a	3018.85	46.16208	YES	YES
484	a	3019.55	35.89690	YES	YES
485	a	3019.74	23.47137	YES	YES
486	a	3026.66	8.06505	YES	YES
487	a	3029.43	12.33665	YES	YES
488	a	3032.90	0.05092	YES	YES
489	a	3034.22	0.27472	YES	YES
490	a	3041.05	11.91545	YES	YES
491	a	3047.07	0.36222	YES	YES
492	a	3052.85	0.22714	YES	YES

\$end

Double hybrid single point energy = -7384.069502233423 H
 COSMO energy + OC correction = -7391.5848093672 H (in oDFB)

6.2.30 H₂NMe



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: cs

Cartesian coordinates in Ångström:

N	0.8114119	-0.4324804	0.0000000
H	0.7951481	-1.0462683	-0.8154029
H	0.7951481	-1.0462683	0.8154029
H	-0.3368083	1.0919505	-0.8832561
C	-0.3701413	0.4398886	0.0000000
H	-0.3368083	1.0919505	0.8832561
H	-1.3475198	-0.0791260	0.0000000

SCF energy GEOOPT = -95.908012557 H
 ZPE = 163.2 kJ/mol
 FREEH energy = 172.28 kJ/mol
 FREEH entropy = 0.24131 kJ/mol/K

\$vibrational spectrum

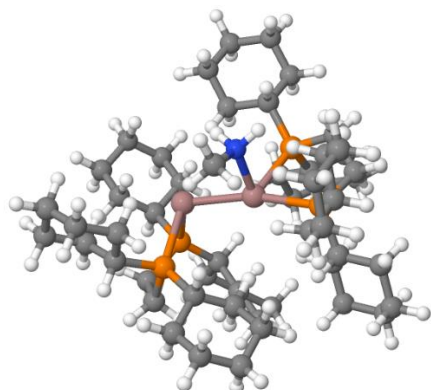
#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR RAMAN
1			-0.00	0.00000	- -
2			-0.00	0.00000	- -
3			-0.00	0.00000	- -
4			0.00	0.00000	- -
5			0.00	0.00000	- -
6			0.00	0.00000	- -
7		a''	294.96	34.07441	YES YES
8		a'	813.22	150.45328	YES YES
9		a''	947.78	0.11579	YES YES
10		a'	1032.70	7.78533	YES YES
11		a'	1135.50	5.17228	YES YES
12		a''	1308.43	0.09957	YES YES
13		a'	1409.23	1.81784	YES YES
14		a'	1448.62	6.85647	YES YES
15		a''	1470.62	3.74869	YES YES
16		a'	1614.08	18.01347	YES YES

17	a'	2890.88	98.57229	YES	YES
18	a'	2991.90	33.70520	YES	YES
19	a''	3030.35	29.67839	YES	YES
20	a'	3408.05	1.18933	YES	YES
21	a''	3485.24	0.12228	YES	YES

\$end

Double hybrid single point energy = -95.736887274557 H
 COSMO energy + OC correction = -95.9143077467 H (in oDFB)

6.2.31 $[\{\text{Ga}(\text{dcpe})\}_2(\text{H}_2\text{NMe})]^{2+}$



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-1.6948511	17.0992273	-2.1994605
Ga	-4.0025619	17.7956493	-1.3240355
P	-1.2894867	18.7293649	-4.0781792
P	-6.1204656	19.1686005	-0.8783539
P	-1.9911950	15.5513854	-4.1497530
P	-5.1966180	16.1925726	0.1608376
C	-4.6646780	21.1224957	-4.8222783
H	-4.7051063	21.6613720	-3.8604689
H	-5.6967421	20.8297341	-5.0668674
C	-1.0448804	14.0205184	-3.7088526
H	-0.9426572	13.4118495	-4.6221492
C	-4.1794163	15.3205405	1.4341067
H	-3.9115399	16.1490099	2.1195776
C	-4.3692830	16.1278446	-5.5094255
H	-3.7869396	16.5596516	-6.3392183
H	-4.4999762	16.9251682	-4.7615829
C	-7.0260494	19.3617623	-2.4772514
H	-6.3636489	20.0086867	-3.0757972
C	-7.2208321	18.1117594	0.1875387
H	-7.8866040	18.7637326	0.7693564
H	-7.8619441	17.5234497	-0.4828954
C	-2.6542707	22.4290778	-5.6033164
H	-2.2484688	23.0668012	-6.4002296
H	-2.6080026	23.0217682	-4.6744708
C	-1.7736196	21.1820217	-5.4451191
H	-0.7467041	21.4841156	-5.2013577
H	-1.7285923	20.6445345	-6.4063494
C	-3.7968291	19.8696216	-4.6584598

H	-3.8491392	19.2806883	-5.5881421
H	-4.1816633	19.2207189	-3.8550042
C	1.0974477	13.1023135	-2.7024851
H	1.2812829	12.4380944	-3.5625976
H	2.0837007	13.3847040	-2.3094131
C	-7.4350667	14.4158147	-0.2603095
H	-8.0904233	15.1842648	0.1737494
H	-7.1362438	13.7523770	0.5638774
C	-6.1840622	20.8402015	-0.0771873
H	-7.2605468	21.0800892	-0.0274264
C	0.5585916	20.2185782	-2.6139596
H	-0.1407930	21.0669077	-2.6559996
H	0.2702922	19.5979269	-1.7470056
C	1.9920714	20.7231687	-2.4079661
H	2.2580297	21.4032719	-3.2334294
H	2.0464110	21.3164932	-1.4845738
C	-7.1440777	18.0159058	-3.2114997
H	-6.1481494	17.5540810	-3.3218828
H	-7.7557193	17.3206273	-2.6122664
C	-4.1090567	22.0580894	-5.8997179
H	-4.1672049	21.5572360	-6.8800588
H	-4.7269583	22.9631232	-5.9750441
C	-8.3950311	20.0502253	-2.3471499
H	-8.2935577	21.0306667	-1.8629348
H	-9.0529401	19.4423536	-1.7043537
C	-5.4934132	21.9039376	-0.9445681
H	-5.9475996	21.9332098	-1.9446530
H	-4.4359051	21.6269273	-1.0933445
C	-3.4113576	13.8114983	-5.9053698
H	-2.8968862	12.9600004	-5.4408352
H	-2.7763140	14.1493293	-6.7405381
C	2.8789809	18.6951157	-3.6210072
H	3.1905328	19.2856283	-4.4979751
H	3.5646375	17.8386292	-3.5621105
C	-5.7573327	22.2284658	1.9936423
H	-6.8212962	22.4971786	2.0910820
H	-5.3459502	22.2061546	3.0119559
C	-9.1693741	18.8870147	-4.4602555
H	-9.6064437	19.0378966	-5.4563318
H	-9.8643318	18.2296049	-3.9117687
C	-4.9230312	14.2573152	2.2619959
H	-5.8518397	14.6648648	2.6851359
H	-5.2091118	13.4256395	1.5998366
C	0.2891873	12.3499270	-1.6420151
H	0.8233115	11.4440768	-1.3256210
H	0.1860572	12.9851801	-0.7454901
C	-7.8091268	18.1947464	-4.5815820
H	-7.1443787	18.7928038	-5.2265175
H	-7.9198129	17.2162310	-5.0655782
C	2.9859972	19.5592498	-2.3616857
H	2.7792333	18.9383610	-1.4737185
H	4.0104040	19.9377888	-2.2470039
C	-5.0386507	23.2781233	1.1407394
H	-5.1461888	24.2722373	1.5939837
H	-3.9569873	23.0598631	1.1260052
C	-5.2871537	13.9877541	-1.5455662
H	-4.9175596	13.2991784	-0.7708219
H	-4.4010829	14.4653760	-1.9898100

C	-5.6478612	20.8335555	1.3630020
H	-4.5864234	20.5378888	1.3606444
H	-6.1903003	20.0983650	1.9755218
C	-6.1884484	15.0497181	-0.8967241
H	-6.5298417	15.7175488	-1.7095393
C	-5.5781073	23.2901869	-0.2924067
C	-7.3233510	12.5558412	-1.9854033
H	-7.8909911	12.0203806	-2.7580122
H	-7.0245767	11.8017545	-1.2391255
C	-8.2090575	13.6111409	-1.3147728
H	-9.0838951	13.1391066	-0.8479973
H	-8.5978711	14.3032060	-2.0808709
C	-1.8509819	13.2341442	-2.6601537
H	-2.8314981	12.9458696	-3.0656221
H	-2.0426522	13.9026294	-1.8028122
C	-4.0171027	13.7240818	3.3812478
H	-3.8083280	14.5385378	4.0944685
H	-4.5511805	12.9468182	3.9442910
C	-5.7205776	15.6600499	-6.0602596
H	-6.2424167	16.5076065	-6.5246699
H	-6.3525467	15.3191054	-5.2224541
C	-2.6978478	13.1765191	2.8270386
H	-2.9041326	12.2885287	2.2067134
H	-2.0536300	12.8379552	3.6492589
C	-2.8693460	14.7537290	0.8571883
H	-3.1056402	13.9296981	0.1684371
H	-2.3407742	15.5115305	0.2542883
C	-9.0486429	20.2231163	-3.7248127
H	-10.0351775	20.6910255	-3.6067195
H	-8.4408615	20.9206881	-4.3244148
C	-4.7687058	13.3548176	-6.4590120
H	-4.6121495	12.5630323	-7.2040610
H	-5.3559778	12.9045457	-5.6423833
C	-6.0683639	13.1898204	-2.5934626
H	-5.4201661	12.4187584	-3.0343730
H	-6.3605838	13.8646946	-3.4154376
C	-5.5515448	14.5199451	-7.0682048
H	-6.5327653	14.1765229	-7.4228511
H	-5.0150529	14.8974058	-7.9543522
C	-1.1011587	11.9903883	-2.1710967
H	-1.6944337	11.4848785	-1.3955668
H	-1.0031890	11.2755567	-3.0040206
C	-1.9697447	14.2248379	1.9790498
H	-1.6554808	15.0649121	2.6212222
H	-1.0520598	13.8032885	1.5457156
H	-2.3213871	17.8595793	0.6741574
C	0.4423931	19.3548349	-3.8796708
H	0.6647725	19.9762988	-4.7629469
C	1.4471744	18.1900931	-3.8403920
H	1.4010174	17.6134201	-4.7749194
H	1.1676297	17.5033505	-3.0218647
C	0.3597370	14.3593398	-3.1792259
H	0.9536726	14.8691221	-3.9506762
H	0.2619556	15.0661507	-2.3359893
C	-1.0423349	16.3163606	-5.5468501
H	0.0159589	16.1147215	-5.3407902
H	-1.2877543	15.7912258	-6.4805073
C	-1.2755799	17.8261868	-5.6988925

H	-2.2509222	18.0148813	-6.1643679
H	-0.5138942	18.2667493	-6.3580072
C	-3.5861731	14.9578169	-4.8956490
H	-4.1644984	14.5810478	-4.0373804
C	-2.3350325	20.2418700	-4.3644656
H	-2.3113450	20.7681281	-3.3932939
C	-6.4290916	17.1806663	1.1140334
H	-7.1064535	16.5183485	1.6707781
H	-5.8657168	17.7586837	1.8614412
H	-6.6306114	23.6162529	-0.2831576
H	-5.0324429	24.0190488	-0.9070450
C	-2.2042563	19.8430475	0.1433139
N	-2.9777945	18.6172381	0.4560714
H	-1.5641163	19.6293650	-0.7204928
H	-1.5770079	20.1649883	0.9836730
H	-2.8959170	20.6490446	-0.1207840
H	-3.5611167	18.7679738	1.2829516

SCF energy GEOOPT = -7352.105335593 H

ZPE = 3767. kJ/mol

FREEH energy = 3954.72 kJ/mol

FREEH entropy = 1.59936 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	16.23	0.22135	YES	YES
	8	a	20.88	0.06237	YES	YES
	9	a	25.26	0.09180	YES	YES
	10	a	26.56	0.07986	YES	YES
	11	a	28.02	0.20497	YES	YES
	12	a	30.78	0.10174	YES	YES
	13	a	32.94	0.29996	YES	YES
	14	a	36.07	0.04715	YES	YES
	15	a	38.19	0.25691	YES	YES
	16	a	41.75	0.31886	YES	YES
	17	a	43.14	0.06384	YES	YES
	18	a	44.99	0.05934	YES	YES
	19	a	47.36	0.01611	YES	YES
	20	a	52.51	0.03330	YES	YES
	21	a	54.14	0.64127	YES	YES
	22	a	54.90	0.01028	YES	YES
	23	a	59.79	0.12703	YES	YES
	24	a	64.57	0.28157	YES	YES
	25	a	66.40	0.16393	YES	YES
	26	a	67.03	0.23916	YES	YES
	27	a	67.22	0.11051	YES	YES
	28	a	69.34	0.21062	YES	YES
	29	a	72.82	0.39113	YES	YES
	30	a	75.82	0.68630	YES	YES
	31	a	77.13	0.01907	YES	YES
	32	a	78.15	0.08544	YES	YES

33	a	85.39	0.19111	YES	YES
34	a	88.25	0.22431	YES	YES
35	a	95.90	0.13422	YES	YES
36	a	98.48	0.14151	YES	YES
37	a	106.23	0.06411	YES	YES
38	a	111.75	0.77487	YES	YES
39	a	122.52	0.39648	YES	YES
40	a	125.19	5.30601	YES	YES
41	a	126.85	1.04697	YES	YES
42	a	130.47	0.72721	YES	YES
43	a	134.63	0.67678	YES	YES
44	a	134.92	1.67292	YES	YES
45	a	138.53	1.94778	YES	YES
46	a	142.21	0.86226	YES	YES
47	a	145.78	0.37465	YES	YES
48	a	153.21	4.64600	YES	YES
49	a	171.25	0.40020	YES	YES
50	a	174.54	4.32645	YES	YES
51	a	176.68	0.17007	YES	YES
52	a	181.31	0.81268	YES	YES
53	a	188.58	0.39448	YES	YES
54	a	197.53	0.67351	YES	YES
55	a	200.85	1.58376	YES	YES
56	a	204.10	1.06001	YES	YES
57	a	212.30	0.41320	YES	YES
58	a	214.67	0.04285	YES	YES
59	a	215.18	0.08903	YES	YES
60	a	219.63	0.16622	YES	YES
61	a	220.44	0.17440	YES	YES
62	a	224.91	0.21053	YES	YES
63	a	225.90	0.06576	YES	YES
64	a	231.16	0.42753	YES	YES
65	a	233.34	1.35299	YES	YES
66	a	236.01	0.44157	YES	YES
67	a	236.94	0.02441	YES	YES
68	a	237.97	0.84043	YES	YES
69	a	240.06	2.34918	YES	YES
70	a	241.71	0.32926	YES	YES
71	a	251.61	2.30554	YES	YES
72	a	263.27	1.10406	YES	YES
73	a	277.58	1.74147	YES	YES
74	a	278.54	0.82877	YES	YES
75	a	284.97	0.38534	YES	YES
76	a	294.26	0.27435	YES	YES
77	a	302.29	0.51405	YES	YES
78	a	306.68	9.01597	YES	YES
79	a	311.43	0.72706	YES	YES
80	a	313.05	1.08363	YES	YES
81	a	329.54	0.97210	YES	YES
82	a	329.70	1.55374	YES	YES
83	a	330.85	0.11431	YES	YES
84	a	334.08	1.04019	YES	YES
85	a	334.95	0.80464	YES	YES
86	a	337.23	1.52812	YES	YES
87	a	364.40	9.58716	YES	YES
88	a	373.48	2.83747	YES	YES
89	a	379.18	1.97091	YES	YES
90	a	381.84	0.46839	YES	YES

91	a	388.17	2.95600	YES	YES
92	a	390.55	0.83345	YES	YES
93	a	408.23	0.48233	YES	YES
94	a	412.45	0.65741	YES	YES
95	a	418.12	3.03278	YES	YES
96	a	421.34	6.45582	YES	YES
97	a	422.93	2.38630	YES	YES
98	a	429.17	3.17502	YES	YES
99	a	430.12	0.05573	YES	YES
100	a	431.12	0.22648	YES	YES
101	a	431.45	0.22193	YES	YES
102	a	431.84	0.06423	YES	YES
103	a	432.58	0.42691	YES	YES
104	a	433.02	0.51144	YES	YES
105	a	434.50	1.33983	YES	YES
106	a	437.20	1.06762	YES	YES
107	a	440.67	3.89113	YES	YES
108	a	455.81	7.81970	YES	YES
109	a	460.09	4.37784	YES	YES
110	a	472.04	2.97626	YES	YES
111	a	490.78	4.62915	YES	YES
112	a	492.73	3.50336	YES	YES
113	a	494.20	6.71412	YES	YES
114	a	497.95	0.95050	YES	YES
115	a	500.73	1.48870	YES	YES
116	a	501.32	0.44628	YES	YES
117	a	509.20	7.61708	YES	YES
118	a	511.24	11.81022	YES	YES
119	a	543.35	60.35823	YES	YES
120	a	625.32	8.56712	YES	YES
121	a	626.74	23.32068	YES	YES
122	a	640.12	8.87224	YES	YES
123	a	661.92	14.16050	YES	YES
124	a	699.41	1.93120	YES	YES
125	a	712.22	1.41991	YES	YES
126	a	714.61	5.46094	YES	YES
127	a	726.83	9.03296	YES	YES
128	a	729.65	2.51270	YES	YES
129	a	730.63	2.14083	YES	YES
130	a	731.27	8.77528	YES	YES
131	a	732.41	8.39678	YES	YES
132	a	770.98	5.52112	YES	YES
133	a	771.83	13.22419	YES	YES
134	a	772.71	0.53778	YES	YES
135	a	773.92	2.02551	YES	YES
136	a	774.51	1.54069	YES	YES
137	a	775.46	0.42907	YES	YES
138	a	776.15	0.79582	YES	YES
139	a	777.21	0.31884	YES	YES
140	a	777.25	0.13001	YES	YES
141	a	783.71	17.82291	YES	YES
142	a	805.74	0.33856	YES	YES
143	a	808.30	0.72540	YES	YES
144	a	809.58	6.98341	YES	YES
145	a	810.59	6.31218	YES	YES
146	a	811.16	3.65436	YES	YES
147	a	812.41	2.88106	YES	YES
148	a	814.73	2.71554	YES	YES

149	a	816.72	3.08406	YES	YES
150	a	831.72	1.53955	YES	YES
151	a	832.04	7.04219	YES	YES
152	a	835.39	10.05322	YES	YES
153	a	837.43	1.90226	YES	YES
154	a	838.06	1.38050	YES	YES
155	a	838.47	0.88715	YES	YES
156	a	839.49	6.83283	YES	YES
157	a	840.07	3.88796	YES	YES
158	a	847.09	20.66483	YES	YES
159	a	851.42	17.13545	YES	YES
160	a	873.94	1.25220	YES	YES
161	a	875.30	0.51309	YES	YES
162	a	875.89	0.48227	YES	YES
163	a	876.05	2.92532	YES	YES
164	a	876.41	6.90804	YES	YES
165	a	877.15	1.66401	YES	YES
166	a	877.74	4.30663	YES	YES
167	a	878.27	4.16149	YES	YES
168	a	878.64	4.47533	YES	YES
169	a	879.23	0.86597	YES	YES
170	a	880.69	1.81098	YES	YES
171	a	882.18	2.97876	YES	YES
172	a	882.95	3.38914	YES	YES
173	a	884.20	2.76932	YES	YES
174	a	884.64	0.77332	YES	YES
175	a	886.08	6.15371	YES	YES
176	a	902.73	1.03771	YES	YES
177	a	903.10	2.00311	YES	YES
178	a	904.15	5.83441	YES	YES
179	a	904.87	0.82481	YES	YES
180	a	908.38	0.70121	YES	YES
181	a	909.60	1.08832	YES	YES
182	a	910.32	0.21906	YES	YES
183	a	910.63	1.17040	YES	YES
184	a	962.25	44.98869	YES	YES
185	a	980.98	34.50761	YES	YES
186	a	984.59	2.08445	YES	YES
187	a	985.96	1.41184	YES	YES
188	a	986.69	10.10111	YES	YES
189	a	987.22	3.25057	YES	YES
190	a	988.89	11.56024	YES	YES
191	a	989.49	17.38269	YES	YES
192	a	990.47	16.70270	YES	YES
193	a	991.22	4.69364	YES	YES
194	a	991.89	1.88321	YES	YES
195	a	992.50	7.27720	YES	YES
196	a	1008.99	4.05306	YES	YES
197	a	1013.56	0.91062	YES	YES
198	a	1015.22	1.42053	YES	YES
199	a	1016.47	1.32334	YES	YES
200	a	1017.25	0.58720	YES	YES
201	a	1017.68	0.43951	YES	YES
202	a	1018.80	0.15474	YES	YES
203	a	1020.15	0.25378	YES	YES
204	a	1022.54	0.46810	YES	YES
205	a	1030.78	1.21245	YES	YES
206	a	1031.84	0.66412	YES	YES

207	a	1032.03	2.71026	YES	YES
208	a	1034.77	0.79764	YES	YES
209	a	1038.39	1.10503	YES	YES
210	a	1038.57	2.66122	YES	YES
211	a	1039.32	1.08969	YES	YES
212	a	1042.04	1.20486	YES	YES
213	a	1054.99	1.63342	YES	YES
214	a	1056.27	1.55296	YES	YES
215	a	1056.87	0.78581	YES	YES
216	a	1058.03	2.48468	YES	YES
217	a	1059.41	1.43886	YES	YES
218	a	1062.35	1.02771	YES	YES
219	a	1063.92	0.68057	YES	YES
220	a	1066.25	2.56257	YES	YES
221	a	1069.05	0.76641	YES	YES
222	a	1070.22	1.04559	YES	YES
223	a	1072.33	0.49369	YES	YES
224	a	1072.76	0.08231	YES	YES
225	a	1073.47	1.05153	YES	YES
226	a	1073.61	0.69529	YES	YES
227	a	1073.83	0.84542	YES	YES
228	a	1074.70	0.07805	YES	YES
229	a	1075.09	0.60975	YES	YES
230	a	1077.71	3.43423	YES	YES
231	a	1088.46	5.54599	YES	YES
232	a	1089.68	6.00696	YES	YES
233	a	1091.59	6.61926	YES	YES
234	a	1092.67	9.46958	YES	YES
235	a	1098.28	2.31402	YES	YES
236	a	1102.85	3.36042	YES	YES
237	a	1104.20	6.11624	YES	YES
238	a	1113.98	9.83582	YES	YES
239	a	1121.83	4.65805	YES	YES
240	a	1126.95	2.65990	YES	YES
241	a	1157.85	5.61434	YES	YES
242	a	1159.43	3.10082	YES	YES
243	a	1159.68	12.77337	YES	YES
244	a	1165.59	9.64513	YES	YES
245	a	1167.84	17.55711	YES	YES
246	a	1168.41	2.75284	YES	YES
247	a	1169.49	2.32317	YES	YES
248	a	1169.65	14.46692	YES	YES
249	a	1173.82	5.65978	YES	YES
250	a	1177.64	4.73743	YES	YES
251	a	1178.39	20.26052	YES	YES
252	a	1179.35	12.63541	YES	YES
253	a	1182.88	8.22331	YES	YES
254	a	1183.32	5.27672	YES	YES
255	a	1185.80	0.29789	YES	YES
256	a	1192.17	1.11106	YES	YES
257	a	1210.36	1.48895	YES	YES
258	a	1234.56	1.15279	YES	YES
259	a	1235.32	0.61611	YES	YES
260	a	1242.34	0.57534	YES	YES
261	a	1245.40	0.35214	YES	YES
262	a	1245.46	0.58586	YES	YES
263	a	1245.74	0.59419	YES	YES
264	a	1246.25	1.92283	YES	YES

265	a	1247.91	0.36432	YES	YES
266	a	1249.07	1.21413	YES	YES
267	a	1250.45	1.27478	YES	YES
268	a	1250.84	1.83716	YES	YES
269	a	1253.29	0.92893	YES	YES
270	a	1253.91	0.90815	YES	YES
271	a	1255.20	2.70260	YES	YES
272	a	1255.48	1.47876	YES	YES
273	a	1256.38	1.10363	YES	YES
274	a	1256.45	4.34157	YES	YES
275	a	1256.81	2.21868	YES	YES
276	a	1257.53	8.84767	YES	YES
277	a	1258.02	4.25849	YES	YES
278	a	1258.23	4.63080	YES	YES
279	a	1259.93	3.53067	YES	YES
280	a	1260.83	1.30522	YES	YES
281	a	1262.26	0.98891	YES	YES
282	a	1263.03	1.34074	YES	YES
283	a	1263.94	1.74757	YES	YES
284	a	1267.68	3.08338	YES	YES
285	a	1269.32	1.68933	YES	YES
286	a	1281.02	2.91001	YES	YES
287	a	1281.94	0.78480	YES	YES
288	a	1282.39	1.51933	YES	YES
289	a	1283.84	2.29873	YES	YES
290	a	1288.30	2.92643	YES	YES
291	a	1289.97	2.64613	YES	YES
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293	a	1291.52	5.23339	YES	YES
294	a	1302.26	1.00534	YES	YES
295	a	1304.55	0.54009	YES	YES
296	a	1306.85	1.11876	YES	YES
297	a	1308.97	0.83993	YES	YES
298	a	1309.64	3.48028	YES	YES
299	a	1310.66	0.66958	YES	YES
300	a	1311.55	3.24953	YES	YES
301	a	1313.48	0.36143	YES	YES
302	a	1315.93	2.00209	YES	YES
303	a	1318.33	2.54954	YES	YES
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305	a	1320.01	0.51781	YES	YES
306	a	1321.29	0.93337	YES	YES
307	a	1321.92	6.30496	YES	YES
308	a	1322.29	0.87368	YES	YES
309	a	1323.05	2.40399	YES	YES
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311	a	1323.73	0.64890	YES	YES
312	a	1324.30	0.49382	YES	YES
313	a	1324.64	3.58500	YES	YES
314	a	1325.07	2.38454	YES	YES
315	a	1325.23	1.17778	YES	YES
316	a	1326.45	3.87035	YES	YES
317	a	1326.99	9.45711	YES	YES
318	a	1330.22	3.48892	YES	YES
319	a	1335.44	0.23100	YES	YES
320	a	1335.88	0.65997	YES	YES
321	a	1336.80	0.08528	YES	YES
322	a	1336.94	0.07916	YES	YES

323	a	1337.65	0.21335	YES	YES
324	a	1338.09	0.18982	YES	YES
325	a	1338.21	0.07739	YES	YES
326	a	1338.58	0.11328	YES	YES
327	a	1344.45	0.39732	YES	YES
328	a	1344.96	1.72762	YES	YES
329	a	1345.96	0.09664	YES	YES
330	a	1346.08	2.53739	YES	YES
331	a	1347.09	1.97982	YES	YES
332	a	1347.68	2.36176	YES	YES
333	a	1348.63	0.86353	YES	YES
334	a	1349.33	1.39427	YES	YES
335	a	1397.76	3.82370	YES	YES
336	a	1400.76	4.67439	YES	YES
337	a	1406.12	6.33701	YES	YES
338	a	1408.52	11.66183	YES	YES
339	a	1410.89	6.35539	YES	YES
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341	a	1426.74	5.18918	YES	YES
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343	a	1429.33	4.48892	YES	YES
344	a	1431.16	0.41443	YES	YES
345	a	1432.80	2.79017	YES	YES
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348	a	1433.99	0.47055	YES	YES
349	a	1435.26	0.92522	YES	YES
350	a	1435.53	14.68979	YES	YES
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352	a	1436.31	4.91830	YES	YES
353	a	1437.13	9.78807	YES	YES
354	a	1437.74	8.48982	YES	YES
355	a	1437.85	3.56906	YES	YES
356	a	1438.09	8.02981	YES	YES
357	a	1438.57	2.72392	YES	YES
358	a	1439.20	0.51910	YES	YES
359	a	1439.33	1.16714	YES	YES
360	a	1439.70	2.25090	YES	YES
361	a	1440.11	4.98978	YES	YES
362	a	1440.39	0.54143	YES	YES
363	a	1440.89	11.29145	YES	YES
364	a	1441.94	11.54227	YES	YES
365	a	1442.75	7.30038	YES	YES
366	a	1443.05	9.77779	YES	YES
367	a	1444.40	10.56642	YES	YES
368	a	1444.72	4.96265	YES	YES
369	a	1445.11	30.21774	YES	YES
370	a	1445.54	15.17975	YES	YES
371	a	1446.58	1.74281	YES	YES
372	a	1447.86	7.69779	YES	YES
373	a	1452.77	0.56791	YES	YES
374	a	1454.03	1.95297	YES	YES
375	a	1454.12	2.86234	YES	YES
376	a	1455.13	1.95140	YES	YES
377	a	1455.57	0.13302	YES	YES
378	a	1455.83	2.50312	YES	YES
379	a	1456.94	0.07442	YES	YES
380	a	1457.87	2.13802	YES	YES

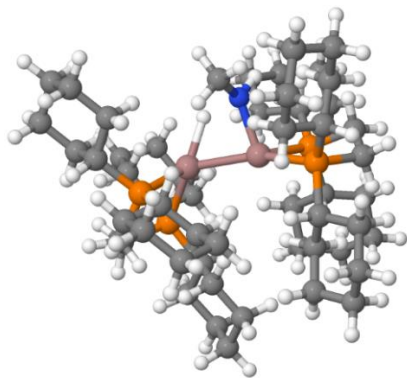
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382	a	1560.21	62.19501	YES	YES
383	a	2890.68	8.71050	YES	YES
384	a	2917.05	18.95698	YES	YES
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387	a	2923.77	39.02213	YES	YES
388	a	2924.46	23.93406	YES	YES
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391	a	2933.46	6.50771	YES	YES
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397	a	2939.33	23.14275	YES	YES
398	a	2941.31	9.33770	YES	YES
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406	a	2946.15	9.40827	YES	YES
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413	a	2955.23	5.48143	YES	YES
414	a	2955.29	6.23960	YES	YES
415	a	2956.15	22.60525	YES	YES
416	a	2957.56	22.99057	YES	YES
417	a	2957.78	4.82587	YES	YES
418	a	2959.05	29.26288	YES	YES
419	a	2959.20	29.03018	YES	YES
420	a	2959.32	33.14835	YES	YES
421	a	2959.60	32.06276	YES	YES
422	a	2960.02	32.20257	YES	YES
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425	a	2961.88	30.14222	YES	YES
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427	a	2963.61	26.26666	YES	YES
428	a	2963.74	33.60999	YES	YES
429	a	2972.94	5.64270	YES	YES
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431	a	2975.39	30.58596	YES	YES
432	a	2975.86	3.87282	YES	YES
433	a	2977.98	17.47017	YES	YES
434	a	2981.11	15.11457	YES	YES
435	a	2981.65	10.87421	YES	YES
436	a	2984.76	5.61968	YES	YES
437	a	2988.90	22.85045	YES	YES
438	a	2989.01	12.24120	YES	YES

439	a	2992.66	32.26213	YES	YES
440	a	2993.60	17.48344	YES	YES
441	a	2995.96	10.80779	YES	YES
442	a	2997.12	23.45433	YES	YES
443	a	2997.41	33.43826	YES	YES
444	a	2999.03	29.93624	YES	YES
445	a	2999.09	10.24735	YES	YES
446	a	2999.48	34.65296	YES	YES
447	a	3001.86	29.08028	YES	YES
448	a	3004.67	23.97699	YES	YES
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451	a	3008.17	3.07422	YES	YES
452	a	3009.24	32.07375	YES	YES
453	a	3010.24	23.22657	YES	YES
454	a	3010.60	20.74896	YES	YES
455	a	3011.57	29.08041	YES	YES
456	a	3012.49	21.00684	YES	YES
457	a	3012.87	28.28500	YES	YES
458	a	3013.06	12.26461	YES	YES
459	a	3013.12	31.73124	YES	YES
460	a	3013.40	20.12159	YES	YES
461	a	3013.95	18.85896	YES	YES
462	a	3014.57	21.72693	YES	YES
463	a	3015.34	35.84804	YES	YES
464	a	3015.78	28.80317	YES	YES
465	a	3015.95	23.34658	YES	YES
466	a	3016.02	20.62877	YES	YES
467	a	3016.80	17.89782	YES	YES
468	a	3016.83	41.01864	YES	YES
469	a	3017.30	37.09610	YES	YES
470	a	3017.35	12.95872	YES	YES
471	a	3017.40	26.83963	YES	YES
472	a	3018.79	31.63110	YES	YES
473	a	3019.22	11.82197	YES	YES
474	a	3020.16	27.79339	YES	YES
475	a	3020.61	22.69690	YES	YES
476	a	3025.23	17.29416	YES	YES
477	a	3030.56	1.20418	YES	YES
478	a	3033.66	2.64505	YES	YES
479	a	3046.30	1.30097	YES	YES
480	a	3056.81	2.90364	YES	YES
481	a	3076.35	0.87004	YES	YES
482	a	3351.88	4.26478	YES	YES
483	a	3437.06	11.90029	YES	YES

\$end

Double hybrid single point energy = -7344.811774872377 H
 COSMO energy + OC correction = -7352.2564056133 H (in oDFB)

6.2.32 $[\{\text{Ga}(\text{dcpe})\}_2(\text{H}-\text{NHMe})]^{2+}$ (Transition State)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.0531665	17.2450493	-2.4514219
Ga	-4.1289985	17.8199364	-1.1955610
P	-1.3831561	18.8123770	-4.1678759
P	-6.1614362	19.1351211	-0.8778519
P	-1.9788077	15.5890675	-4.1912354
P	-5.2802737	16.1641784	0.1549283
C	-4.7964182	21.1139823	-4.9643404
H	-4.8532989	21.6628575	-4.0088512
H	-5.8211373	20.8000759	-5.2112229
C	-1.0014541	14.1223936	-3.6462048
H	-0.8186570	13.4941046	-4.5336745
C	-4.2268885	15.3189732	1.4092706
H	-3.9700139	16.1563390	2.0871312
C	-4.3782210	16.1134842	-5.5234908
H	-3.8159551	16.5536448	-6.3626987
H	-4.5210760	16.9101873	-4.7777104
C	-7.0418251	19.3750658	-2.4796428
H	-6.3625495	20.0224103	-3.0586996
C	-7.2859765	18.0976416	0.1748768
H	-7.9415121	18.7618092	0.7542875
H	-7.9337087	17.5251832	-0.5030289
C	-2.8039019	22.4506383	-5.7470292
H	-2.4052064	23.0860917	-6.5491372
H	-2.7751799	23.0549917	-4.8252863
C	-1.9003386	21.2230580	-5.5682303
H	-0.8805786	21.5450098	-5.3185482
H	-1.8383590	20.6751451	-6.5226937
C	-3.9080963	19.8781531	-4.7789617
H	-3.9422178	19.2768618	-5.7017198
H	-4.2846022	19.2343903	-3.9685927
C	1.1178950	13.3592337	-2.4774011
H	1.3910490	12.6762500	-3.2979977
H	2.0605721	13.7095862	-2.0355010
C	-7.4773063	14.3403021	-0.2607091
H	-8.1464217	15.0890689	0.1863541
H	-7.1519758	13.6790211	0.5552987
C	-6.0636516	20.7811773	-0.0577674
H	-7.0948389	21.1744527	-0.0547565
C	0.3640045	20.3688964	-2.6502486
H	-0.3287152	21.2142308	-2.7742556

H	0.0203862	19.7921814	-1.7758325
C	1.7834405	20.8858865	-2.3850158
H	2.0980190	21.5301333	-3.2221121
H	1.7808071	21.5190789	-1.4871366
C	-7.1754831	18.0422287	-3.2356699
H	-6.1857240	17.5682785	-3.3446215
H	-7.8003448	17.3474964	-2.6493839
C	-4.2492359	22.0468763	-6.0485398
H	-4.2910034	21.5339890	-7.0235401
H	-4.8835161	22.9389411	-6.1386761
C	-8.3982279	20.0864852	-2.3449766
H	-8.2793100	21.0563808	-1.8432455
H	-9.0708348	19.4806975	-1.7157199
C	-5.1771019	21.7302444	-0.8826079
H	-5.5929141	21.8526832	-1.8931143
H	-4.1786855	21.2790717	-1.0036118
C	-3.3644387	13.8166884	-5.9175737
H	-2.8181200	12.9838915	-5.4546275
H	-2.7515496	14.1685569	-6.7634318
C	2.7437261	18.8111554	-3.4523361
H	3.1059410	19.3638839	-4.3343881
H	3.4249054	17.9599021	-3.3161786
C	-5.4551310	22.0377249	2.0553259
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H	-5.0725889	21.9208823	3.0783856
C	-9.1795617	18.9666938	-4.4800973
H	-9.6093970	19.1403216	-5.4756188
H	-9.8887927	18.3138804	-3.9446357
C	-4.9330657	14.2388404	2.2474422
H	-5.8648983	14.6250389	2.6839027
H	-5.2091960	13.3995148	1.5903753
C	0.2835950	12.6034556	-1.4399792
H	0.8419511	11.7391730	-1.0566694
H	0.0926252	13.2640477	-0.5770136
C	-7.8313842	18.2509529	-4.6057433
H	-7.1537639	18.8453830	-5.2404708
H	-7.9576953	17.2806641	-5.1034567
C	2.7739609	19.7291070	-2.2275850
H	2.5149693	19.1468763	-1.3274263
H	3.7892535	20.1160013	-2.0689112
C	-4.5466710	22.9629676	1.2404777
H	-4.4920996	23.9512260	1.7158147
H	-3.5186838	22.5631961	1.2381393
C	-5.3345703	13.9793336	-1.5752329
H	-4.9367497	13.2947008	-0.8110093
H	-4.4679537	14.4871725	-2.0246904
C	-5.5945912	20.6560742	1.4019321
H	-4.6292549	20.1262895	1.4319213
H	-6.3075624	20.0473728	1.9769586
C	-6.2547630	15.0113460	-0.9053989
H	-6.6212512	15.6809076	-1.7061376
C	-5.0457422	23.0979720	-0.2009060
C	-7.3370275	12.4977298	-2.0028953
H	-7.8997389	11.9535306	-2.7730246
H	-7.0090754	11.7459084	-1.2666592
C	-8.2420857	13.5236323	-1.3125945
H	-9.0981327	13.0240938	-0.8397237
H	-8.6587995	14.2111492	-2.0680030

C	-1.8333397	13.3334362	-2.6193644
H	-2.7696078	12.9778725	-3.0724855
H	-2.1124965	14.0207302	-1.8027124
C	-3.9977517	13.7294897	3.3534029
H	-3.8002626	14.5494593	4.0632379
H	-4.5028838	12.9384093	3.9238873
C	-5.7241935	15.6079056	-6.0536377
H	-6.2712288	16.4389687	-6.5188911
H	-6.3373343	15.2613602	-5.2046581
C	-2.6724207	13.2169999	2.7802360
H	-2.8640679	12.3230379	2.1634815
H	-2.0079303	12.8964058	3.5934937
C	-2.9119190	14.7867294	0.8104029
H	-3.1383617	13.9534378	0.1295328
H	-2.4129082	15.5623902	0.2091477
C	-9.0398113	20.2902907	-3.7242444
H	-10.0191240	20.7729242	-3.6058993
H	-8.4166129	20.9859933	-4.3098849
C	-4.7174785	13.3218173	-6.4485454
H	-4.5511006	12.5301237	-7.1913302
H	-5.2804124	12.8617177	-5.6206006
C	-6.1061218	13.1691108	-2.6205701
H	-5.4435327	12.4176842	-3.0742550
H	-6.4253138	13.8420962	-3.4341681
C	-5.5390675	14.4629074	-7.0538094
H	-6.5159156	14.0908250	-7.3907499
H	-5.0261993	14.8462069	-7.9513385
C	-1.0509423	12.1511910	-2.0371729
H	-1.6653608	11.6451846	-1.2788541
H	-0.8660206	11.4115804	-2.8327390
C	-1.9844068	14.2835286	1.9216214
H	-1.6845577	15.1339507	2.5562276
H	-1.0611384	13.8856110	1.4775233
H	-1.8210778	17.5408187	-0.7348835
C	0.3269275	19.4501949	-3.8816674
H	0.5938970	20.0335460	-4.7792526
C	1.3280276	18.2909688	-3.7327605
H	1.3383730	17.6735561	-4.6421752
H	1.0001255	17.6423420	-2.9024180
C	0.3478168	14.5571444	-3.0461205
H	0.9605176	15.0712896	-3.7998057
H	0.1572446	15.2864004	-2.2393196
C	-1.0329169	16.3681497	-5.5777465
H	0.0269060	16.1989195	-5.3511886
H	-1.2491119	15.8230962	-6.5070653
C	-1.3068590	17.8705039	-5.7613258
H	-2.2747774	18.0230965	-6.2549538
H	-0.5408833	18.3176368	-6.4104878
C	-3.5614634	14.9637754	-4.9127169
H	-4.1206325	14.5787996	-4.0449351
C	-2.4565042	20.2873564	-4.4810271
H	-2.4509603	20.8245028	-3.5157053
C	-6.5141095	17.1503290	1.1043865
H	-7.2054933	16.4926888	1.6486124
H	-5.9443472	17.7186498	1.8528791
H	-6.0284386	23.5965879	-0.2024446
H	-4.3713637	23.7368986	-0.7875394
C	-2.1525014	19.6656260	0.1762575

N	-2.7670660	18.3388059	0.2033590
H	-1.9703397	19.9466302	-0.8729373
H	-1.1815368	19.6693804	0.6926800
H	-2.7771391	20.4536958	0.6205728
H	-2.8489349	17.9886158	1.1593874

SCF energy GEOOPT = -7352.070844895 H

ZPE = 3750. kJ/mol

FREEH energy = 3935.62 kJ/mol

FREEH entropy = 1.57842 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1		a	-1046.19	0.00000	YES	YES
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			-0.00	0.00000	-	-
6			-0.00	0.00000	-	-
7			0.00	0.00000	-	-
8		a	16.43	0.02547	YES	YES
9		a	21.06	0.02424	YES	YES
10		a	25.88	0.13202	YES	YES
11		a	26.76	0.07917	YES	YES
12		a	28.21	0.03598	YES	YES
13		a	32.22	0.02795	YES	YES
14		a	32.78	0.02982	YES	YES
15		a	38.02	0.02038	YES	YES
16		a	38.81	0.09128	YES	YES
17		a	40.66	0.02383	YES	YES
18		a	41.17	0.02015	YES	YES
19		a	44.59	0.20055	YES	YES
20		a	46.16	0.18174	YES	YES
21		a	52.16	0.04118	YES	YES
22		a	55.62	0.08855	YES	YES
23		a	57.22	0.02278	YES	YES
24		a	60.86	0.20170	YES	YES
25		a	62.46	0.06022	YES	YES
26		a	63.51	0.03694	YES	YES
27		a	67.15	0.09590	YES	YES
28		a	68.46	0.25699	YES	YES
29		a	70.01	0.28283	YES	YES
30		a	71.68	0.02948	YES	YES
31		a	72.01	0.09523	YES	YES
32		a	75.80	0.07047	YES	YES
33		a	83.52	0.42742	YES	YES
34		a	86.24	0.11542	YES	YES
35		a	93.25	0.00067	YES	YES
36		a	96.56	0.03541	YES	YES
37		a	107.62	0.24511	YES	YES
38		a	114.87	5.33925	YES	YES
39		a	119.16	0.63287	YES	YES
40		a	129.63	0.18398	YES	YES
41		a	131.67	1.37365	YES	YES
42		a	136.61	0.28993	YES	YES
43		a	137.81	2.27813	YES	YES
44		a	139.03	3.24593	YES	YES

45	a	143.27	0.24076	YES	YES
46	a	146.83	0.24174	YES	YES
47	a	152.05	1.44997	YES	YES
48	a	158.12	5.66077	YES	YES
49	a	170.90	0.25166	YES	YES
50	a	176.97	1.07059	YES	YES
51	a	181.77	0.90270	YES	YES
52	a	187.08	0.65490	YES	YES
53	a	190.04	1.01062	YES	YES
54	a	199.68	1.40165	YES	YES
55	a	203.38	0.07640	YES	YES
56	a	214.51	0.51080	YES	YES
57	a	215.60	0.24660	YES	YES
58	a	216.47	0.26918	YES	YES
59	a	219.47	0.06919	YES	YES
60	a	224.34	0.21194	YES	YES
61	a	225.20	1.97534	YES	YES
62	a	225.83	0.51869	YES	YES
63	a	230.45	2.00776	YES	YES
64	a	234.40	0.04678	YES	YES
65	a	236.43	0.44468	YES	YES
66	a	237.74	0.03996	YES	YES
67	a	239.77	0.74669	YES	YES
68	a	240.65	1.12925	YES	YES
69	a	242.57	0.53943	YES	YES
70	a	249.19	1.25677	YES	YES
71	a	258.16	0.82161	YES	YES
72	a	273.58	0.83254	YES	YES
73	a	280.50	0.13681	YES	YES
74	a	283.80	0.61166	YES	YES
75	a	288.31	0.58700	YES	YES
76	a	297.18	1.64256	YES	YES
77	a	305.21	0.64130	YES	YES
78	a	309.61	9.55543	YES	YES
79	a	312.28	0.37725	YES	YES
80	a	314.10	0.63785	YES	YES
81	a	329.31	0.63731	YES	YES
82	a	330.75	0.37770	YES	YES
83	a	333.15	0.92994	YES	YES
84	a	336.00	1.09250	YES	YES
85	a	338.71	1.35850	YES	YES
86	a	340.09	0.49491	YES	YES
87	a	371.72	4.62928	YES	YES
88	a	381.60	2.78260	YES	YES
89	a	383.07	1.58579	YES	YES
90	a	384.55	1.04137	YES	YES
91	a	394.34	1.04848	YES	YES
92	a	396.93	1.13867	YES	YES
93	a	408.29	0.02313	YES	YES
94	a	413.27	0.42972	YES	YES
95	a	419.05	1.57532	YES	YES
96	a	421.19	3.54438	YES	YES
97	a	422.88	3.49170	YES	YES
98	a	428.56	1.99110	YES	YES
99	a	430.45	0.06278	YES	YES
100	a	430.72	0.50762	YES	YES
101	a	431.31	0.07211	YES	YES
102	a	432.22	0.13538	YES	YES

103	a	432.70	0.32875	YES	YES
104	a	433.75	0.44346	YES	YES
105	a	435.42	2.75932	YES	YES
106	a	437.98	0.79189	YES	YES
107	a	443.86	8.57315	YES	YES
108	a	457.09	17.57950	YES	YES
109	a	459.90	21.87072	YES	YES
110	a	460.51	15.32680	YES	YES
111	a	473.38	3.12916	YES	YES
112	a	492.98	6.53204	YES	YES
113	a	493.67	3.24644	YES	YES
114	a	495.76	1.93132	YES	YES
115	a	499.14	1.64548	YES	YES
116	a	502.32	1.88688	YES	YES
117	a	503.99	1.41439	YES	YES
118	a	512.23	6.84789	YES	YES
119	a	513.85	14.70729	YES	YES
120	a	598.81	44.70600	YES	YES
121	a	629.86	7.12861	YES	YES
122	a	631.17	27.87278	YES	YES
123	a	642.20	9.87434	YES	YES
124	a	664.76	15.71267	YES	YES
125	a	701.26	1.78848	YES	YES
126	a	716.04	1.55631	YES	YES
127	a	721.65	3.78280	YES	YES
128	a	729.69	11.19535	YES	YES
129	a	732.65	2.50134	YES	YES
130	a	733.66	0.25849	YES	YES
131	a	735.85	5.00178	YES	YES
132	a	736.56	8.29960	YES	YES
133	a	769.49	0.31082	YES	YES
134	a	771.98	7.84043	YES	YES
135	a	772.47	0.50174	YES	YES
136	a	774.03	2.47018	YES	YES
137	a	774.80	9.75771	YES	YES
138	a	775.54	0.27339	YES	YES
139	a	776.59	1.90407	YES	YES
140	a	777.26	0.95337	YES	YES
141	a	777.62	0.13281	YES	YES
142	a	787.02	18.02917	YES	YES
143	a	806.85	0.45398	YES	YES
144	a	809.42	1.76733	YES	YES
145	a	810.28	5.60838	YES	YES
146	a	811.83	6.90053	YES	YES
147	a	812.42	0.67069	YES	YES
148	a	812.51	6.49502	YES	YES
149	a	814.78	2.93124	YES	YES
150	a	817.87	3.32159	YES	YES
151	a	831.84	4.31783	YES	YES
152	a	832.69	3.41114	YES	YES
153	a	834.79	11.58587	YES	YES
154	a	837.43	0.66935	YES	YES
155	a	837.83	2.10898	YES	YES
156	a	838.47	1.62693	YES	YES
157	a	839.18	3.40763	YES	YES
158	a	840.32	6.53387	YES	YES
159	a	848.39	21.70145	YES	YES
160	a	854.67	18.50930	YES	YES

161	a	872.68	3.31255	YES	YES
162	a	873.34	1.30084	YES	YES
163	a	875.66	0.35086	YES	YES
164	a	875.90	1.68813	YES	YES
165	a	876.74	5.05051	YES	YES
166	a	877.17	1.08198	YES	YES
167	a	878.45	2.63461	YES	YES
168	a	879.04	10.11234	YES	YES
169	a	879.37	1.40623	YES	YES
170	a	879.64	2.53659	YES	YES
171	a	881.73	0.96605	YES	YES
172	a	882.20	5.08248	YES	YES
173	a	883.23	2.64980	YES	YES
174	a	884.76	4.16394	YES	YES
175	a	885.36	0.56864	YES	YES
176	a	886.47	5.40907	YES	YES
177	a	903.03	1.67509	YES	YES
178	a	903.17	1.76562	YES	YES
179	a	904.32	5.80780	YES	YES
180	a	905.22	1.20546	YES	YES
181	a	907.96	0.74850	YES	YES
182	a	909.15	1.31653	YES	YES
183	a	910.33	0.83201	YES	YES
184	a	910.91	0.78888	YES	YES
185	a	960.27	55.64081	YES	YES
186	a	983.30	1.50320	YES	YES
187	a	983.55	0.09965	YES	YES
188	a	986.52	12.20726	YES	YES
189	a	987.46	2.52428	YES	YES
190	a	988.48	5.55337	YES	YES
191	a	989.39	15.45875	YES	YES
192	a	989.66	9.78165	YES	YES
193	a	990.83	1.75324	YES	YES
194	a	991.79	12.56933	YES	YES
195	a	991.84	13.46162	YES	YES
196	a	1013.99	0.98245	YES	YES
197	a	1015.33	1.35467	YES	YES
198	a	1016.19	0.92281	YES	YES
199	a	1017.29	1.64990	YES	YES
200	a	1018.47	0.37728	YES	YES
201	a	1019.46	0.61889	YES	YES
202	a	1019.94	0.40284	YES	YES
203	a	1020.26	2.26891	YES	YES
204	a	1022.15	0.47557	YES	YES
205	a	1029.99	1.30840	YES	YES
206	a	1031.55	0.87260	YES	YES
207	a	1032.76	2.30068	YES	YES
208	a	1033.91	1.68606	YES	YES
209	a	1037.70	2.15088	YES	YES
210	a	1038.90	1.55028	YES	YES
211	a	1039.18	0.43428	YES	YES
212	a	1040.61	0.72835	YES	YES
213	a	1043.13	29.73353	YES	YES
214	a	1056.64	1.29175	YES	YES
215	a	1057.38	2.32292	YES	YES
216	a	1058.53	2.31050	YES	YES
217	a	1059.40	1.25613	YES	YES
218	a	1060.83	1.83054	YES	YES

219	a	1064.42	0.24943	YES	YES
220	a	1065.03	0.66881	YES	YES
221	a	1067.67	2.14121	YES	YES
222	a	1069.39	0.06045	YES	YES
223	a	1071.18	0.41805	YES	YES
224	a	1072.22	0.21263	YES	YES
225	a	1072.71	0.13381	YES	YES
226	a	1073.18	0.12360	YES	YES
227	a	1073.62	0.11102	YES	YES
228	a	1074.40	0.09475	YES	YES
229	a	1075.12	0.23311	YES	YES
230	a	1076.83	3.13070	YES	YES
231	a	1080.37	3.65900	YES	YES
232	a	1090.55	3.51650	YES	YES
233	a	1092.49	4.17840	YES	YES
234	a	1093.45	4.62450	YES	YES
235	a	1094.38	7.86730	YES	YES
236	a	1099.60	1.65246	YES	YES
237	a	1099.85	5.25678	YES	YES
238	a	1103.15	2.69137	YES	YES
239	a	1106.60	8.05722	YES	YES
240	a	1115.07	8.72900	YES	YES
241	a	1121.45	4.56881	YES	YES
242	a	1129.63	2.26988	YES	YES
243	a	1158.92	5.67239	YES	YES
244	a	1160.70	6.08412	YES	YES
245	a	1161.52	9.72025	YES	YES
246	a	1165.82	8.49460	YES	YES
247	a	1167.94	7.43908	YES	YES
248	a	1169.29	13.91376	YES	YES
249	a	1170.16	1.99938	YES	YES
250	a	1170.58	9.79873	YES	YES
251	a	1176.07	10.17433	YES	YES
252	a	1178.08	18.51323	YES	YES
253	a	1179.24	5.96339	YES	YES
254	a	1179.48	2.68016	YES	YES
255	a	1186.01	0.75528	YES	YES
256	a	1188.51	0.54307	YES	YES
257	a	1191.52	0.81527	YES	YES
258	a	1210.49	2.26112	YES	YES
259	a	1236.88	2.28995	YES	YES
260	a	1239.10	0.97532	YES	YES
261	a	1242.93	0.81540	YES	YES
262	a	1245.21	0.50694	YES	YES
263	a	1245.50	0.34832	YES	YES
264	a	1245.91	2.11624	YES	YES
265	a	1246.48	0.04058	YES	YES
266	a	1248.67	1.91204	YES	YES
267	a	1249.44	0.66246	YES	YES
268	a	1250.44	1.08231	YES	YES
269	a	1252.66	1.05673	YES	YES
270	a	1254.04	0.85833	YES	YES
271	a	1254.68	1.51679	YES	YES
272	a	1255.94	3.17916	YES	YES
273	a	1256.75	3.91810	YES	YES
274	a	1257.36	2.63558	YES	YES
275	a	1257.63	3.48334	YES	YES
276	a	1258.01	27.91069	YES	YES

277	a	1258.44	5.55269	YES	YES
278	a	1259.24	10.04352	YES	YES
279	a	1260.76	0.54116	YES	YES
280	a	1261.05	8.41523	YES	YES
281	a	1261.60	3.30753	YES	YES
282	a	1262.96	6.05882	YES	YES
283	a	1264.74	10.06762	YES	YES
284	a	1265.39	3.96324	YES	YES
285	a	1267.35	98.52854	YES	YES
286	a	1269.31	31.41225	YES	YES
287	a	1271.07	26.41526	YES	YES
288	a	1280.85	3.40239	YES	YES
289	a	1282.30	0.91586	YES	YES
290	a	1282.45	1.36042	YES	YES
291	a	1284.34	2.84114	YES	YES
292	a	1288.68	3.93567	YES	YES
293	a	1289.26	1.69772	YES	YES
294	a	1290.99	3.23699	YES	YES
295	a	1291.33	4.09502	YES	YES
296	a	1300.45	2.88269	YES	YES
297	a	1307.33	0.79216	YES	YES
298	a	1309.01	0.70428	YES	YES
299	a	1310.40	2.12377	YES	YES
300	a	1310.66	0.68586	YES	YES
301	a	1311.53	0.49528	YES	YES
302	a	1314.44	0.99463	YES	YES
303	a	1314.78	1.63351	YES	YES
304	a	1317.21	1.93731	YES	YES
305	a	1318.74	1.00737	YES	YES
306	a	1320.44	0.49845	YES	YES
307	a	1321.75	0.80548	YES	YES
308	a	1322.20	0.97015	YES	YES
309	a	1322.86	1.05550	YES	YES
310	a	1323.43	0.62656	YES	YES
311	a	1323.77	4.13879	YES	YES
312	a	1324.07	1.95411	YES	YES
313	a	1324.52	0.41549	YES	YES
314	a	1324.76	0.82846	YES	YES
315	a	1325.22	3.98632	YES	YES
316	a	1326.12	1.38082	YES	YES
317	a	1326.60	0.89575	YES	YES
318	a	1327.29	7.21782	YES	YES
319	a	1329.29	7.30623	YES	YES
320	a	1330.38	3.41472	YES	YES
321	a	1335.99	0.28557	YES	YES
322	a	1336.62	0.74750	YES	YES
323	a	1336.93	0.12338	YES	YES
324	a	1337.34	0.17120	YES	YES
325	a	1337.81	0.30593	YES	YES
326	a	1338.21	0.12627	YES	YES
327	a	1338.38	0.05332	YES	YES
328	a	1338.81	0.15885	YES	YES
329	a	1344.69	0.31105	YES	YES
330	a	1345.05	1.58979	YES	YES
331	a	1345.90	0.27795	YES	YES
332	a	1346.18	2.04993	YES	YES
333	a	1347.56	1.64850	YES	YES
334	a	1348.16	1.61604	YES	YES

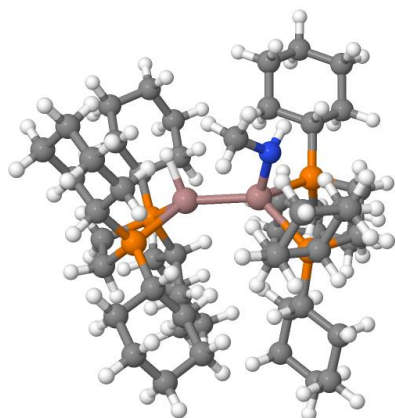
335	a	1348.83	1.04759	YES	YES
336	a	1349.60	0.94660	YES	YES
337	a	1401.62	4.54861	YES	YES
338	a	1403.83	4.87302	YES	YES
339	a	1406.28	7.18507	YES	YES
340	a	1407.22	10.91900	YES	YES
341	a	1410.14	6.29248	YES	YES
342	a	1425.00	2.30875	YES	YES
343	a	1426.51	7.59813	YES	YES
344	a	1427.39	5.69530	YES	YES
345	a	1430.32	4.75325	YES	YES
346	a	1431.70	4.78263	YES	YES
347	a	1433.23	1.97670	YES	YES
348	a	1433.70	0.30597	YES	YES
349	a	1434.01	4.25045	YES	YES
350	a	1434.43	3.85039	YES	YES
351	a	1434.85	4.09462	YES	YES
352	a	1435.69	2.89871	YES	YES
353	a	1436.06	8.04994	YES	YES
354	a	1436.51	9.92217	YES	YES
355	a	1437.51	11.89256	YES	YES
356	a	1437.57	3.99946	YES	YES
357	a	1438.11	3.23517	YES	YES
358	a	1438.48	7.37153	YES	YES
359	a	1438.70	2.82439	YES	YES
360	a	1439.19	3.50697	YES	YES
361	a	1439.41	5.82995	YES	YES
362	a	1439.78	10.90425	YES	YES
363	a	1439.86	1.56970	YES	YES
364	a	1440.22	0.71880	YES	YES
365	a	1440.55	0.51905	YES	YES
366	a	1442.01	16.46946	YES	YES
367	a	1442.39	5.89422	YES	YES
368	a	1443.26	10.55799	YES	YES
369	a	1443.86	6.07051	YES	YES
370	a	1444.47	37.96068	YES	YES
371	a	1444.75	7.20540	YES	YES
372	a	1445.80	12.94878	YES	YES
373	a	1446.27	14.65566	YES	YES
374	a	1447.41	3.65083	YES	YES
375	a	1452.70	0.86803	YES	YES
376	a	1453.61	2.14538	YES	YES
377	a	1454.06	1.67959	YES	YES
378	a	1454.73	0.92821	YES	YES
379	a	1455.04	4.17342	YES	YES
380	a	1456.28	1.71049	YES	YES
381	a	1456.84	0.32084	YES	YES
382	a	1457.03	3.09514	YES	YES
383	a	1467.82	3.20028	YES	YES
384	a	2898.72	6.60381	YES	YES
385	a	2916.42	0.81922	YES	YES
386	a	2927.22	11.94831	YES	YES
387	a	2928.20	31.44495	YES	YES
388	a	2929.57	1.89406	YES	YES
389	a	2933.83	8.43966	YES	YES
390	a	2937.64	18.62938	YES	YES
391	a	2938.64	10.17110	YES	YES
392	a	2938.74	34.81137	YES	YES

393	a	2939.37	9.09783	YES	YES
394	a	2940.58	14.19675	YES	YES
395	a	2941.10	2.34714	YES	YES
396	a	2941.25	16.20021	YES	YES
397	a	2942.27	20.27313	YES	YES
398	a	2942.48	13.54146	YES	YES
399	a	2943.23	13.34716	YES	YES
400	a	2943.25	13.89362	YES	YES
401	a	2943.68	5.16651	YES	YES
402	a	2944.02	6.90746	YES	YES
403	a	2944.22	9.03494	YES	YES
404	a	2946.27	8.62206	YES	YES
405	a	2946.77	7.96218	YES	YES
406	a	2947.01	10.45747	YES	YES
407	a	2948.98	14.50956	YES	YES
408	a	2949.58	13.29585	YES	YES
409	a	2951.48	2.84455	YES	YES
410	a	2951.87	21.08139	YES	YES
411	a	2952.57	6.52021	YES	YES
412	a	2953.48	10.41425	YES	YES
413	a	2954.97	5.48076	YES	YES
414	a	2955.96	2.94916	YES	YES
415	a	2956.11	13.14969	YES	YES
416	a	2956.97	5.10942	YES	YES
417	a	2957.38	9.55009	YES	YES
418	a	2958.24	4.08415	YES	YES
419	a	2958.41	0.45486	YES	YES
420	a	2959.54	29.05626	YES	YES
421	a	2959.60	12.71473	YES	YES
422	a	2959.89	20.87491	YES	YES
423	a	2960.11	2.32410	YES	YES
424	a	2960.20	56.20132	YES	YES
425	a	2960.65	36.77762	YES	YES
426	a	2961.25	40.69386	YES	YES
427	a	2962.40	43.65838	YES	YES
428	a	2962.55	27.80517	YES	YES
429	a	2963.57	27.42760	YES	YES
430	a	2963.67	8.46950	YES	YES
431	a	2972.65	0.47374	YES	YES
432	a	2973.87	9.69142	YES	YES
433	a	2976.09	37.23628	YES	YES
434	a	2982.14	5.87877	YES	YES
435	a	2982.99	17.03971	YES	YES
436	a	2984.62	16.51861	YES	YES
437	a	2986.16	5.35004	YES	YES
438	a	2990.95	2.99947	YES	YES
439	a	2994.23	3.27455	YES	YES
440	a	2994.94	39.34386	YES	YES
441	a	2996.15	17.65098	YES	YES
442	a	2997.26	19.56592	YES	YES
443	a	2998.80	26.67392	YES	YES
444	a	2999.63	30.23685	YES	YES
445	a	2999.79	26.12256	YES	YES
446	a	3000.47	48.06044	YES	YES
447	a	3000.59	19.66116	YES	YES
448	a	3001.65	9.14461	YES	YES
449	a	3002.38	13.03577	YES	YES
450	a	3003.52	19.03990	YES	YES

451	a	3004.80	29.43485	YES	YES
452	a	3007.20	7.37226	YES	YES
453	a	3007.98	12.06132	YES	YES
454	a	3009.81	18.74131	YES	YES
455	a	3010.03	18.60788	YES	YES
456	a	3010.66	26.00725	YES	YES
457	a	3010.72	20.49506	YES	YES
458	a	3011.49	12.50265	YES	YES
459	a	3011.69	20.78231	YES	YES
460	a	3012.05	30.18189	YES	YES
461	a	3013.29	18.78409	YES	YES
462	a	3013.63	18.72037	YES	YES
463	a	3013.87	17.93605	YES	YES
464	a	3014.92	29.62980	YES	YES
465	a	3015.04	22.53125	YES	YES
466	a	3015.24	25.55326	YES	YES
467	a	3015.93	19.61403	YES	YES
468	a	3016.38	26.95114	YES	YES
469	a	3017.21	20.81423	YES	YES
470	a	3017.33	0.42908	YES	YES
471	a	3017.34	29.15247	YES	YES
472	a	3017.47	42.63310	YES	YES
473	a	3018.12	17.96137	YES	YES
474	a	3018.15	58.73378	YES	YES
475	a	3018.45	22.36869	YES	YES
476	a	3018.55	29.48580	YES	YES
477	a	3019.29	26.38023	YES	YES
478	a	3020.26	25.37807	YES	YES
479	a	3027.86	4.43886	YES	YES
480	a	3032.00	0.98483	YES	YES
481	a	3036.77	2.79732	YES	YES
482	a	3047.34	0.68772	YES	YES
483	a	3426.56	1.84873	YES	YES
\$end					

Double hybrid single point energy = -7344.774077423213 H
COSMO energy + OC correction = -7352.2183821669 H (in oDFB)

6.2.33 [H{Ga(dcpe)}₂(NHMe)]²⁺ (*syn*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.2404231	17.3527965	-2.5024946
Ga	-3.9384769	17.8124576	-0.8264875
P	-1.5198820	18.9345226	-4.1588329
P	-6.0235467	19.0968101	-0.9057996
P	-2.0427539	15.6620429	-4.1927030
P	-5.2552851	16.1445058	0.2898787
C	-5.0026325	21.0570142	-5.1053997
H	-5.1182909	21.6503023	-4.1825330
H	-6.0027416	20.6825706	-5.3659617
C	-1.0555195	14.2100012	-3.6191397
H	-0.9400076	13.5446237	-4.4909558
C	-4.2894758	15.2201477	1.5563731
H	-4.0640036	16.0072157	2.3007764
C	-4.3845548	16.1242744	-5.6398948
H	-3.7892398	16.5486654	-6.4642289
H	-4.5730826	16.9405313	-4.9257858
C	-6.9452785	19.2696748	-2.4938106
H	-6.3078639	19.9342803	-3.0987076
C	-7.1708954	18.1760613	0.2281006
H	-7.7807574	18.8970186	0.7878587
H	-7.8606830	17.6082491	-0.4115956
C	-3.0514738	22.4508668	-5.8874313
H	-2.6581811	23.0734043	-6.7020417
H	-3.0820147	23.0909687	-4.9904140
C	-2.0968110	21.2767520	-5.6346244
H	-1.1010723	21.6567478	-5.3702938
H	-1.9820901	20.6974214	-6.5653638
C	-4.0639014	19.8746215	-4.8344012
H	-4.0525038	19.2273115	-5.7256620
H	-4.4338770	19.2555435	-4.0018226
C	1.0860083	13.3817061	-2.5526867
H	1.2768267	12.6636663	-3.3666884
H	2.0689401	13.6972795	-2.1775979
C	-7.5084336	14.4256874	-0.2228102
H	-8.1465929	15.1778919	0.2625136
H	-7.2163318	13.7086001	0.5569794
C	-5.7836365	20.8038161	-0.2543383
H	-6.7132015	21.3541767	-0.4790854
C	0.0797224	20.4165989	-2.4611778
H	-0.6652623	21.2234648	-2.5260621
H	-0.2528731	19.7326034	-1.6638401
C	1.4514133	20.9940923	-2.0915336
H	1.7414878	21.7507564	-2.8384506
H	1.3794148	21.5166840	-1.1278808
C	-7.0617949	17.9223138	-3.2238398
H	-6.0661444	17.4652206	-3.3444030
H	-7.6587538	17.2278232	-2.6088888
C	-4.4640678	21.9627185	-6.2161579
H	-4.4480779	21.4040908	-7.1665454
H	-5.1378413	22.8163904	-6.3678972
C	-8.3233231	19.9368150	-2.3368281
H	-8.2295058	20.9130332	-1.8427057
H	-8.9631832	19.3126434	-1.6922385
C	-4.6244480	21.4564915	-1.0312333
H	-4.8397611	21.4591790	-2.1105275
H	-3.7175217	20.8467000	-0.8864423

C	-3.3353872	13.8276332	-5.9259642
H	-2.8116905	13.0097908	-5.4134737
H	-2.6812241	14.1591377	-6.7491413
C	2.5879298	19.1296913	-3.3571483
H	2.9245684	19.8088169	-4.1571977
H	3.3313586	18.3229565	-3.2988848
C	-5.2804336	22.2768869	1.7322927
H	-6.1870530	22.8856720	1.5807078
H	-5.0815130	22.2770146	2.8125492
C	-9.1187364	18.7683061	-4.4382304
H	-9.5733567	18.9147414	-5.4270887
H	-9.7995513	18.1059308	-3.8781870
C	-5.0438673	14.0914259	2.2793530
H	-5.9890291	14.4599238	2.7022222
H	-5.3005457	13.3063370	1.5512135
C	0.2812319	12.6955349	-1.4456533
H	0.8232417	11.8188927	-1.0670460
H	0.1678438	13.3887484	-0.5948168
C	-7.7558745	18.0843061	-4.5813780
H	-7.1096081	18.6808133	-5.2459038
H	-7.8702182	17.1010267	-5.0556461
C	2.5171021	19.8962762	-2.0335550
H	2.2755527	19.1956423	-1.2169008
H	3.4969348	20.3303706	-1.7946271
C	-4.1111104	22.9103153	0.9718874
H	-3.9520546	23.9427184	1.3105330
H	-3.1851268	22.3568772	1.1998989
C	-5.3690563	14.0544379	-1.5506585
H	-4.9880520	13.3191880	-0.8256311
H	-4.4895151	14.5596777	-1.9777110
C	-5.5424255	20.8394122	1.2645939
H	-4.6765368	20.1990696	1.4953977
H	-6.4133829	20.4294856	1.7969598
C	-6.2560928	15.0793896	-0.8273138
H	-6.5938903	15.8010914	-1.5927888
C	-4.3587553	22.8837165	-0.5394166
C	-7.4280229	12.6742216	-2.0579313
H	-8.0059250	12.1909346	-2.8569115
H	-7.1337038	11.8747276	-1.3587613
C	-8.2977846	13.6983561	-1.3208563
H	-9.1769057	13.2093879	-0.8805177
H	-8.6807058	14.4403778	-2.0420274
C	-1.8647689	13.4829901	-2.5293603
H	-2.8355628	13.1534664	-2.9265994
H	-2.0763247	14.2010470	-1.7190587
C	-4.1640296	13.4851849	3.3815910
H	-3.9819314	14.2462119	4.1578732
H	-4.7051565	12.6639989	3.8705922
C	-5.7005166	15.5907342	-6.2168487
H	-6.2381319	16.4048730	-6.7212374
H	-6.3441642	15.2513830	-5.3881371
C	-2.8257287	12.9908628	2.8230672
H	-3.0081296	12.1540979	2.1280171
H	-2.2020980	12.5910001	3.6335138
C	-2.9483863	14.7238064	0.9814301
H	-3.1458004	13.9635230	0.2106851
H	-2.4160806	15.5517390	0.4875290
C	-8.9988392	20.1061584	-3.7042876

H	-9.9886927	20.5625774	-3.5706526
H	-8.4087109	20.8112198	-4.3122860
C	-4.6577474	13.3095388	-6.5084748
H	-4.4502402	12.4993824	-7.2201779
H	-5.2577093	12.8675776	-5.6964573
C	-6.1682486	13.3271896	-2.6363461
H	-5.5340565	12.5740163	-3.1265118
H	-6.4579821	14.0528020	-3.4156349
C	-5.4565263	14.4276805	-7.1820583
H	-6.4126412	14.0394737	-7.5576192
H	-4.9030163	14.7953339	-8.0618026
C	-1.1022684	12.2846185	-1.9541268
H	-1.6950712	11.8285402	-1.1482767
H	-0.9937106	11.5149540	-2.7351817
C	-2.0815232	14.1088545	2.0854626
H	-1.7966419	14.8974772	2.8010707
H	-1.1462608	13.7297269	1.6501200
H	-0.8875651	17.0935471	-1.7162480
C	0.1435833	19.6311720	-3.7830646
H	0.3815599	20.3239059	-4.6080485
C	1.2246177	18.5370149	-3.7377352
H	1.3002078	18.0353780	-4.7135635
H	0.9345684	17.7751129	-2.9967998
C	0.3424981	14.6026965	-3.1099844
H	0.9338742	15.0589087	-3.9161812
H	0.2385773	15.3609101	-2.3188228
C	-1.0630727	16.4812765	-5.5309527
H	-0.0119355	16.3549051	-5.2433386
H	-1.2042610	15.9298179	-6.4711161
C	-1.3774501	17.9731831	-5.7346960
H	-2.3340379	18.0953068	-6.2580607
H	-0.6067959	18.4366214	-6.3660206
C	-3.5841311	15.0001149	-4.9623843
H	-4.1771677	14.6322575	-4.1089778
C	-2.6376302	20.3575665	-4.5251099
H	-2.6697662	20.9238371	-3.5780054
C	-6.4377716	17.2308668	1.1938400
H	-7.1570970	16.6334723	1.7700343
H	-5.8326868	17.8054641	1.9095944
H	-5.2264955	23.5183364	-0.7820595
H	-3.5009591	23.3062034	-1.0818803
C	-1.8742136	19.2851738	0.6504671
N	-3.1392568	18.5561858	0.7466058
H	-1.9688098	20.0998562	-0.0827303
H	-1.0089417	18.6695977	0.3418573
H	-1.6229071	19.7571558	1.6123003
H	-3.0897945	17.8877873	1.5145886

SCF energy GEOOPT = -7352.112926291 H

ZPE = 3755. kJ/mol

FREEH energy = 3941.71 kJ/mol

FREEH entropy = 1.59813 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.06	0.01524	YES	YES
8	a	19.06	0.01838	YES	YES
9	a	19.55	0.05192	YES	YES
10	a	25.69	0.10762	YES	YES
11	a	28.30	0.05892	YES	YES
12	a	30.60	0.00777	YES	YES
13	a	31.73	0.03825	YES	YES
14	a	34.64	0.01312	YES	YES
15	a	35.70	0.02247	YES	YES
16	a	40.07	0.04126	YES	YES
17	a	42.88	0.03613	YES	YES
18	a	43.74	0.02572	YES	YES
19	a	46.25	0.14204	YES	YES
20	a	48.50	0.17445	YES	YES
21	a	52.05	0.04204	YES	YES
22	a	55.25	0.01713	YES	YES
23	a	56.84	0.26223	YES	YES
24	a	60.28	0.31486	YES	YES
25	a	63.98	0.06028	YES	YES
26	a	65.74	0.08230	YES	YES
27	a	68.04	0.18140	YES	YES
28	a	68.94	0.04797	YES	YES
29	a	72.79	0.10657	YES	YES
30	a	77.08	0.08317	YES	YES
31	a	77.31	0.00403	YES	YES
32	a	86.62	0.69970	YES	YES
33	a	88.07	0.26467	YES	YES
34	a	93.16	0.21131	YES	YES
35	a	99.60	0.54662	YES	YES
36	a	104.39	0.46239	YES	YES
37	a	109.51	0.87505	YES	YES
38	a	113.06	0.44949	YES	YES
39	a	121.54	0.16880	YES	YES
40	a	128.96	0.90864	YES	YES
41	a	134.26	0.58806	YES	YES
42	a	135.07	1.98248	YES	YES
43	a	138.29	0.35899	YES	YES
44	a	140.27	0.11306	YES	YES
45	a	142.80	0.22085	YES	YES
46	a	155.10	1.09477	YES	YES
47	a	157.03	3.23679	YES	YES
48	a	164.56	0.99407	YES	YES
49	a	168.86	0.28709	YES	YES
50	a	173.80	0.68491	YES	YES
51	a	184.68	4.30860	YES	YES
52	a	187.42	8.19623	YES	YES
53	a	189.39	0.35808	YES	YES
54	a	195.42	0.20854	YES	YES
55	a	206.98	0.22842	YES	YES
56	a	211.18	0.61002	YES	YES
57	a	216.15	0.41162	YES	YES
58	a	219.40	0.01412	YES	YES
59	a	221.63	0.09547	YES	YES
60	a	224.00	0.80961	YES	YES

61	a	225.66	0.28437	YES	YES
62	a	227.12	0.23839	YES	YES
63	a	229.72	0.37811	YES	YES
64	a	231.73	0.74709	YES	YES
65	a	233.73	7.88959	YES	YES
66	a	235.65	0.07567	YES	YES
67	a	238.49	3.15040	YES	YES
68	a	239.30	2.29245	YES	YES
69	a	242.81	3.99481	YES	YES
70	a	245.45	0.65035	YES	YES
71	a	264.90	4.77958	YES	YES
72	a	280.92	0.92344	YES	YES
73	a	284.13	0.39886	YES	YES
74	a	286.44	0.39698	YES	YES
75	a	290.49	0.04329	YES	YES
76	a	301.69	3.46518	YES	YES
77	a	305.04	1.20697	YES	YES
78	a	311.15	0.06724	YES	YES
79	a	313.78	0.61086	YES	YES
80	a	329.76	0.86536	YES	YES
81	a	330.40	0.07368	YES	YES
82	a	334.57	0.37232	YES	YES
83	a	338.14	0.40888	YES	YES
84	a	338.76	0.87022	YES	YES
85	a	339.23	1.86346	YES	YES
86	a	370.12	6.79023	YES	YES
87	a	379.81	3.28856	YES	YES
88	a	380.99	0.96305	YES	YES
89	a	382.90	0.32559	YES	YES
90	a	394.97	0.57025	YES	YES
91	a	397.42	1.64887	YES	YES
92	a	406.27	0.18389	YES	YES
93	a	411.47	1.02712	YES	YES
94	a	418.86	12.63003	YES	YES
95	a	420.33	1.73457	YES	YES
96	a	424.60	14.02239	YES	YES
97	a	425.53	11.48983	YES	YES
98	a	427.97	1.59789	YES	YES
99	a	430.34	0.11775	YES	YES
100	a	430.59	0.64365	YES	YES
101	a	431.15	0.68704	YES	YES
102	a	432.02	0.58134	YES	YES
103	a	433.57	2.69814	YES	YES
104	a	434.21	2.72091	YES	YES
105	a	435.00	1.55539	YES	YES
106	a	437.75	0.03462	YES	YES
107	a	445.21	2.91807	YES	YES
108	a	459.51	3.58027	YES	YES
109	a	459.84	4.81412	YES	YES
110	a	472.37	3.15435	YES	YES
111	a	490.79	20.97163	YES	YES
112	a	492.73	3.97891	YES	YES
113	a	496.32	1.50305	YES	YES
114	a	497.64	5.35982	YES	YES
115	a	499.39	1.11598	YES	YES
116	a	505.47	1.56171	YES	YES
117	a	511.18	17.84261	YES	YES
118	a	513.18	4.76922	YES	YES

119	a	522.53	73.39220	YES	YES
120	a	568.13	18.71127	YES	YES
121	a	595.51	92.34724	YES	YES
122	a	629.75	15.07885	YES	YES
123	a	633.16	25.66810	YES	YES
124	a	644.17	13.13525	YES	YES
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126	a	702.52	1.27118	YES	YES
127	a	718.68	1.90348	YES	YES
128	a	720.54	1.53852	YES	YES
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130	a	734.31	3.03793	YES	YES
131	a	734.62	4.46768	YES	YES
132	a	737.09	0.45953	YES	YES
133	a	739.97	4.73044	YES	YES
134	a	771.23	1.26002	YES	YES
135	a	773.71	0.19052	YES	YES
136	a	774.23	0.88793	YES	YES
137	a	774.50	1.01344	YES	YES
138	a	775.18	0.29386	YES	YES
139	a	775.67	0.30158	YES	YES
140	a	776.10	0.82998	YES	YES
141	a	776.88	0.10653	YES	YES
142	a	778.31	13.49558	YES	YES
143	a	786.79	14.34061	YES	YES
144	a	806.99	0.44905	YES	YES
145	a	809.94	1.78057	YES	YES
146	a	810.47	7.45756	YES	YES
147	a	811.48	7.63385	YES	YES
148	a	812.32	1.42424	YES	YES
149	a	813.61	1.81123	YES	YES
150	a	814.72	2.64992	YES	YES
151	a	818.28	2.28661	YES	YES
152	a	832.94	2.66903	YES	YES
153	a	833.37	8.69537	YES	YES
154	a	836.43	7.41936	YES	YES
155	a	837.91	1.65029	YES	YES
156	a	838.21	0.04859	YES	YES
157	a	838.90	4.47371	YES	YES
158	a	839.25	0.97177	YES	YES
159	a	839.90	7.53164	YES	YES
160	a	849.52	13.27580	YES	YES
161	a	854.77	13.32904	YES	YES
162	a	872.06	3.23690	YES	YES
163	a	874.13	1.37229	YES	YES
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166	a	876.91	6.06761	YES	YES
167	a	877.84	1.37480	YES	YES
168	a	878.94	2.18887	YES	YES
169	a	879.51	5.74080	YES	YES
170	a	879.82	0.80946	YES	YES
171	a	880.06	2.03234	YES	YES
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173	a	881.92	3.29492	YES	YES
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181	a	905.57	2.05072	YES	YES
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189	a	988.77	1.35521	YES	YES
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206	a	1032.14	0.38835	YES	YES
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227	a	1073.46	0.21152	YES	YES
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229	a	1074.45	0.02735	YES	YES
230	a	1081.15	2.14223	YES	YES
231	a	1083.17	3.32355	YES	YES
232	a	1091.91	0.55531	YES	YES
233	a	1094.67	3.73907	YES	YES
234	a	1094.80	6.97107	YES	YES

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236	a	1096.84	6.09489	YES	YES
237	a	1101.43	1.62336	YES	YES
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239	a	1107.84	9.35838	YES	YES
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241	a	1122.38	1.02380	YES	YES
242	a	1130.93	2.16160	YES	YES
243	a	1159.70	9.53899	YES	YES
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246	a	1166.03	8.34633	YES	YES
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254	a	1181.50	5.05089	YES	YES
255	a	1187.28	0.61978	YES	YES
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259	a	1239.63	0.10810	YES	YES
260	a	1241.74	0.33125	YES	YES
261	a	1244.43	0.47552	YES	YES
262	a	1245.89	0.37637	YES	YES
263	a	1246.35	0.06283	YES	YES
264	a	1247.11	2.38286	YES	YES
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266	a	1248.06	1.12308	YES	YES
267	a	1250.27	0.47844	YES	YES
268	a	1251.31	0.05074	YES	YES
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270	a	1254.31	1.55424	YES	YES
271	a	1254.72	6.87572	YES	YES
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283	a	1266.50	0.72751	YES	YES
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285	a	1270.77	1.67145	YES	YES
286	a	1272.46	1.68568	YES	YES
287	a	1282.07	2.09707	YES	YES
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314	a	1327.82	2.47051	YES	YES
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319	a	1336.53	0.77798	YES	YES
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324	a	1338.53	0.26582	YES	YES
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326	a	1339.44	0.40676	YES	YES
327	a	1339.90	4.87912	YES	YES
328	a	1344.65	1.00302	YES	YES
329	a	1345.63	0.47804	YES	YES
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332	a	1346.65	0.71212	YES	YES
333	a	1347.98	2.56569	YES	YES
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335	a	1350.49	1.16860	YES	YES
336	a	1399.34	6.19625	YES	YES
337	a	1404.85	6.15291	YES	YES
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343	a	1427.66	3.46430	YES	YES
344	a	1430.83	0.44813	YES	YES
345	a	1431.80	6.44166	YES	YES
346	a	1432.54	0.07969	YES	YES
347	a	1433.19	9.01860	YES	YES
348	a	1433.82	2.14040	YES	YES
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352	a	1436.64	3.04412	YES	YES
353	a	1437.08	7.29205	YES	YES
354	a	1437.94	1.81063	YES	YES
355	a	1437.96	3.04950	YES	YES
356	a	1438.23	2.78077	YES	YES
357	a	1438.43	5.42380	YES	YES
358	a	1438.62	8.63649	YES	YES
359	a	1438.99	5.43230	YES	YES
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361	a	1439.70	4.69702	YES	YES
362	a	1439.81	11.29393	YES	YES
363	a	1440.17	2.62606	YES	YES
364	a	1440.93	5.47087	YES	YES
365	a	1441.65	10.53512	YES	YES
366	a	1443.09	4.09481	YES	YES
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373	a	1448.75	8.62222	YES	YES
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382	a	1466.01	9.20408	YES	YES
383	a	1833.13	133.87607	YES	YES
384	a	2893.70	71.75160	YES	YES
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386	a	2930.76	34.00797	YES	YES
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391	a	2939.57	6.09448	YES	YES
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407	a	2950.81	15.33211	YES	YES
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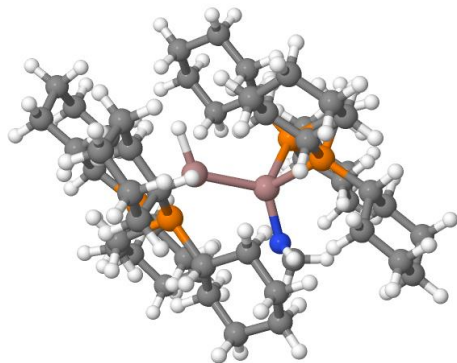
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424	a	2960.84	37.50457	YES	YES
425	a	2961.58	39.97150	YES	YES
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433	a	2975.67	11.35782	YES	YES
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437	a	2987.41	8.18373	YES	YES
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441	a	2993.04	12.86274	YES	YES
442	a	2994.10	37.48991	YES	YES
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444	a	2997.75	32.49980	YES	YES
445	a	2998.98	27.20066	YES	YES
446	a	3000.01	14.03837	YES	YES
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462	a	3014.86	16.76990	YES	YES
463	a	3014.92	13.17261	YES	YES
464	a	3015.80	20.96909	YES	YES
465	a	3016.37	26.00309	YES	YES
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469	a	3017.54	19.66513	YES	YES
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471	a	3017.95	14.82439	YES	YES
472	a	3018.18	31.86835	YES	YES
473	a	3018.87	27.18620	YES	YES
474	a	3018.96	26.34761	YES	YES
475	a	3019.03	23.31033	YES	YES
476	a	3019.38	23.73948	YES	YES
477	a	3020.58	28.07251	YES	YES
478	a	3022.74	28.99436	YES	YES
479	a	3030.82	1.32532	YES	YES
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483	a	3449.44	1.85490	YES	YES

\$end

Double hybrid single point energy = -7344.826402651739 H
 COSMO energy + OC correction = -7352.2602829504 H (in oDFB)

6.2.34 [H{Ga(dcpe)}₂(NHMe)]²⁺ (*anti*-periplanar)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-0.4142791	0.4626268	-1.8559953
P	-2.2574730	-0.7467801	-2.9294231
P	-1.7697999	2.4803512	-2.2749942
C	-1.8506332	-1.8721661	-4.3480381
H	-0.9534140	-2.4132043	-3.9983810
C	-1.4619962	-1.0745551	-5.6051027
H	-2.3553211	-0.5621491	-5.9958337
H	-0.7244845	-0.2983691	-5.3668262
C	-0.9300745	-2.0169808	-6.6908169
H	-0.6568640	-1.4353538	-7.5817969
H	-0.0048332	-2.4976031	-6.3321448
C	-1.9704530	-3.0848598	-7.0429163
H	-1.5636219	-3.7843039	-7.7852075
H	-2.8397794	-2.5996748	-7.5161522
C	-2.4313797	-3.8486011	-5.7979351
H	-1.5920453	-4.4427376	-5.3996540
H	-3.2241348	-4.5638566	-6.0556955

C	-2.9353300	-2.9079024	-4.6917324
H	-3.2154634	-3.5008173	-3.8113147
H	-3.8445275	-2.3857273	-5.0319074
C	-3.2614481	-1.7334192	-1.7399249
H	-4.0566563	-2.1848909	-2.3579563
C	-2.4292057	-2.8630459	-1.1152232
H	-1.9561027	-3.4791218	-1.8939366
H	-1.6109674	-2.4138157	-0.5256858
C	-3.3071340	-3.7333372	-0.2075081
H	-4.0671033	-4.2390593	-0.8247264
H	-2.7010526	-4.5288919	0.2457868
C	-4.0015593	-2.8964550	0.8713956
H	-4.6536259	-3.5331659	1.4840341
H	-3.2459706	-2.4722923	1.5532632
C	-4.8061050	-1.7495259	0.2559057
H	-5.2528571	-1.1268500	1.0430801
H	-5.6430676	-2.1602180	-0.3316399
C	-3.9365889	-0.8755744	-0.6575729
H	-4.5657686	-0.1028217	-1.1188621
H	-3.1664248	-0.3630714	-0.0584750
C	-3.4156278	0.5430792	-3.5756119
H	-3.1020499	0.7466382	-4.6053898
H	-4.4261850	0.1132866	-3.6297833
C	-3.4375812	1.8483161	-2.7641869
H	-3.9924825	1.7103339	-1.8277335
H	-3.9592954	2.6316488	-3.3313735
C	-1.1869750	3.5312379	-3.6789841
H	-1.9979287	4.2518821	-3.8806552
C	0.0759476	4.3019428	-3.2647772
H	0.8359001	3.5792660	-2.9270041
H	-0.1392163	4.9565683	-2.4088047
C	0.6540383	5.1220746	-4.4223024
H	-0.0535620	5.9232667	-4.6895986
H	1.5769375	5.6184770	-4.0912843
C	0.9184905	4.2442238	-5.6474466
H	1.6944323	3.4980788	-5.4044912
H	1.3155865	4.8502927	-6.4722276
C	-0.3606525	3.5262322	-6.0833851
H	-0.1676383	2.8779513	-6.9491815
H	-1.1046724	4.2708830	-6.4094204
C	-0.9485408	2.6859305	-4.9435727
H	-0.2562145	1.8661910	-4.6948807
H	-1.8890551	2.2263174	-5.2757961
C	-2.0751332	3.6099508	-0.8467360
H	-1.0822857	4.0404939	-0.6320516
C	-2.5224091	2.8295641	0.3993673
H	-1.7962433	2.0377680	0.6371917
H	-3.4795019	2.3208402	0.2005063
C	-2.6992349	3.7690607	1.5973335
H	-3.0451680	3.1942621	2.4675621
H	-1.7171794	4.1931603	1.8685643
C	-3.6667618	4.9125167	1.2798613
H	-4.6746064	4.4998980	1.1087340
H	-3.7502928	5.5895223	2.1404999
C	-3.2149731	5.6861948	0.0381120
H	-2.2544700	6.1866442	0.2450900
H	-3.9338078	6.4797894	-0.2058138
C	-3.0458129	4.7585657	-1.1730382

H	-4.0275793	4.3404715	-1.4476057
H	-2.6899037	5.3335688	-2.0390224
Ga	-0.1569887	-0.1000656	0.5293830
P	1.4328812	1.3085398	1.7029803
P	1.2734177	-1.9484945	1.1713810
C	0.7040265	2.4180787	2.9885253
H	0.0906227	3.1289404	2.4077706
C	-0.2398004	1.6454394	3.9271446
H	0.3325793	0.8766422	4.4712954
H	-1.0047759	1.1157198	3.3424451
C	-0.8911561	2.5885866	4.9467892
H	-1.5312640	2.0073749	5.6246597
H	-1.5525892	3.2916999	4.4152437
C	0.1581550	3.3762816	5.7356145
H	-0.3313085	4.0682374	6.4338103
H	0.7526024	2.6809676	6.3511432
C	1.0897287	4.1448831	4.7950968
H	0.5133770	4.9126531	4.2525308
H	1.8626341	4.6787888	5.3642855
C	1.7605903	3.2115550	3.7773003
H	2.3970317	3.7971099	3.0996425
H	2.4212963	2.5090083	4.3108961
C	2.5419371	2.3507187	0.6648930
H	3.2249917	2.8439465	1.3778842
C	1.7460919	3.4344918	-0.0757458
H	1.1628275	4.0426210	0.6310092
H	1.0193267	2.9406861	-0.7448697
C	2.6823087	4.3313365	-0.8942727
H	3.3423403	4.8800735	-0.2037073
H	2.0983181	5.0916248	-1.4300547
C	3.5350630	3.5149508	-1.8689289
H	4.2288868	4.1725476	-2.4094615
H	2.8841357	3.0622172	-2.6371673
C	4.3076095	2.4091719	-1.1451408
H	4.8624715	1.7931214	-1.8658438
H	5.0590978	2.8684814	-0.4829420
C	3.3823461	1.5115178	-0.3119357
H	3.9939673	0.7850676	0.2400327
H	2.7145973	0.9424613	-0.9814496
C	2.5594750	0.1479116	2.6006154
H	2.0952540	-0.0302816	3.5784694
H	3.5150217	0.6571439	2.7884642
C	2.8029094	-1.1829405	1.8709300
H	3.4852116	-1.0348842	1.0251111
H	3.2816112	-1.9045591	2.5474035
C	0.5918766	-3.0240330	2.5075560
H	1.4127603	-3.7069150	2.7865122
C	-0.5872446	-3.8408308	1.9620496
H	-1.3442240	-3.1362679	1.5860162
H	-0.2692494	-4.4569522	1.1089017
C	-1.2181178	-4.7232160	3.0445694
H	-0.4942892	-5.4946629	3.3530122
H	-2.0815406	-5.2573573	2.6235931
C	-1.6360453	-3.8956844	4.2623967
H	-2.4355986	-3.1938834	3.9712608
H	-2.0584610	-4.5470580	5.0388069
C	-0.4474021	-3.1086445	4.8194677
H	-0.7565384	-2.4920885	5.6746601

H	0.3125086	-3.8111842	5.1982054
C	0.1836976	-2.2102850	3.7479627
H	-0.5372546	-1.4334448	3.4467821
H	1.0580542	-1.6965970	4.1712362
C	1.8087378	-3.0544550	-0.2019213
H	0.8544371	-3.4217446	-0.6206799
C	2.5325314	-2.2665065	-1.3057745
H	1.9487137	-1.3875734	-1.6190231
H	3.4867127	-1.8799319	-0.9123543
C	2.8346775	-3.1818506	-2.4989853
H	3.3680202	-2.6146838	-3.2736457
H	1.8826946	-3.5123797	-2.9494312
C	3.6514874	-4.4053836	-2.0717589
H	4.6460484	-4.0732695	-1.7312993
H	3.8234138	-5.0682254	-2.9304332
C	2.9593892	-5.1733234	-0.9420502
H	2.0187508	-5.6108232	-1.3162476
H	3.5824583	-6.0140299	-0.6085574
C	2.6410659	-4.2647743	0.2540557
H	3.5812428	-3.9092587	0.7065641
H	2.1117755	-4.8395477	1.0260038
H	-1.3883801	-0.2212259	1.5106832
N	1.1724095	0.5783629	-2.8815773
C	1.5489027	-0.1893099	-4.0600464
H	1.5297627	1.5297918	-2.9407049
H	2.6442042	-0.2849299	-4.1313303
H	1.2017534	0.2367572	-5.0200071
H	1.1463823	-1.2088625	-3.9936487

SCF energy GEOOPT = -7352.121960061 H

ZPE = 3757. kJ/mol

FREEH energy = 3943.07 kJ/mol

FREEH entropy = 1.57436 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	13.18	0.05696	YES	YES
	8	a	18.88	0.06316	YES	YES
	9	a	20.92	0.03706	YES	YES
	10	a	31.27	0.07194	YES	YES
	11	a	31.51	0.04055	YES	YES
	12	a	34.07	0.01710	YES	YES
	13	a	36.29	0.03634	YES	YES
	14	a	39.02	0.11667	YES	YES
	15	a	40.27	0.16775	YES	YES
	16	a	44.74	0.01836	YES	YES
	17	a	45.69	0.01110	YES	YES
	18	a	46.83	0.05664	YES	YES
	19	a	51.88	0.01390	YES	YES
	20	a	52.68	0.22944	YES	YES
	21	a	55.79	0.27861	YES	YES

22	a	59.95	0.04516	YES	YES
23	a	65.32	0.05601	YES	YES
24	a	66.82	0.58411	YES	YES
25	a	68.88	0.73118	YES	YES
26	a	70.04	0.05000	YES	YES
27	a	73.65	0.58385	YES	YES
28	a	75.36	0.36792	YES	YES
29	a	79.57	0.40187	YES	YES
30	a	80.94	0.10087	YES	YES
31	a	86.14	0.05058	YES	YES
32	a	87.51	0.37687	YES	YES
33	a	90.79	0.10978	YES	YES
34	a	93.09	0.48269	YES	YES
35	a	97.89	0.39707	YES	YES
36	a	99.05	0.12956	YES	YES
37	a	114.18	1.04532	YES	YES
38	a	125.44	0.54767	YES	YES
39	a	131.02	0.61563	YES	YES
40	a	134.90	3.54586	YES	YES
41	a	138.86	2.25605	YES	YES
42	a	141.47	3.46410	YES	YES
43	a	145.40	1.11562	YES	YES
44	a	149.76	4.57283	YES	YES
45	a	149.96	1.04205	YES	YES
46	a	152.57	0.36129	YES	YES
47	a	157.77	2.80824	YES	YES
48	a	168.66	2.30062	YES	YES
49	a	176.32	4.33584	YES	YES
50	a	179.56	0.83876	YES	YES
51	a	183.08	0.15312	YES	YES
52	a	188.25	0.46298	YES	YES
53	a	196.99	1.18955	YES	YES
54	a	200.00	0.90093	YES	YES
55	a	204.94	1.01368	YES	YES
56	a	206.58	6.88632	YES	YES
57	a	209.18	5.95326	YES	YES
58	a	215.85	0.22121	YES	YES
59	a	218.82	1.03447	YES	YES
60	a	222.67	0.18222	YES	YES
61	a	225.45	1.13603	YES	YES
62	a	225.91	4.37486	YES	YES
63	a	229.71	0.15653	YES	YES
64	a	237.36	0.49025	YES	YES
65	a	239.47	0.14519	YES	YES
66	a	240.97	0.21270	YES	YES
67	a	243.05	0.88357	YES	YES
68	a	245.45	0.56933	YES	YES
69	a	246.57	1.76251	YES	YES
70	a	256.98	0.48095	YES	YES
71	a	264.03	9.84299	YES	YES
72	a	275.93	2.41544	YES	YES
73	a	278.96	0.83434	YES	YES
74	a	284.32	1.82211	YES	YES
75	a	290.93	0.43303	YES	YES
76	a	305.33	0.56860	YES	YES
77	a	309.27	0.13286	YES	YES
78	a	315.87	0.22799	YES	YES
79	a	316.92	0.22867	YES	YES

80	a	331.33	1.09608	YES	YES
81	a	331.53	0.06482	YES	YES
82	a	334.01	0.11619	YES	YES
83	a	335.43	0.22498	YES	YES
84	a	344.05	0.26051	YES	YES
85	a	345.27	0.14057	YES	YES
86	a	365.62	11.14694	YES	YES
87	a	371.63	6.25412	YES	YES
88	a	374.03	1.42440	YES	YES
89	a	374.71	1.19899	YES	YES
90	a	391.74	8.06072	YES	YES
91	a	395.75	8.66266	YES	YES
92	a	402.02	23.66808	YES	YES
93	a	413.32	2.50033	YES	YES
94	a	414.20	0.77553	YES	YES
95	a	423.22	3.46773	YES	YES
96	a	423.53	3.40708	YES	YES
97	a	424.59	0.58347	YES	YES
98	a	426.51	1.25347	YES	YES
99	a	429.56	0.07507	YES	YES
100	a	430.97	0.09033	YES	YES
101	a	431.30	0.15889	YES	YES
102	a	432.56	0.32512	YES	YES
103	a	432.64	1.28103	YES	YES
104	a	433.32	0.14006	YES	YES
105	a	434.14	0.20576	YES	YES
106	a	436.12	1.91953	YES	YES
107	a	447.06	4.30747	YES	YES
108	a	449.68	2.40821	YES	YES
109	a	468.98	3.62109	YES	YES
110	a	472.39	3.17455	YES	YES
111	a	490.83	5.02148	YES	YES
112	a	492.65	0.00828	YES	YES
113	a	493.24	2.72018	YES	YES
114	a	494.60	3.28494	YES	YES
115	a	503.63	6.27547	YES	YES
116	a	506.78	0.33012	YES	YES
117	a	518.96	25.23624	YES	YES
118	a	519.59	1.10579	YES	YES
119	a	557.90	109.58800	YES	YES
120	a	559.91	24.51131	YES	YES
121	a	580.01	93.64282	YES	YES
122	a	623.93	18.34388	YES	YES
123	a	630.00	15.41247	YES	YES
124	a	641.21	7.80246	YES	YES
125	a	645.64	9.53860	YES	YES
126	a	715.54	1.00589	YES	YES
127	a	717.39	0.63783	YES	YES
128	a	722.70	1.04674	YES	YES
129	a	723.99	0.94078	YES	YES
130	a	731.14	5.07921	YES	YES
131	a	734.85	4.76378	YES	YES
132	a	735.08	11.44074	YES	YES
133	a	736.73	3.71671	YES	YES
134	a	771.93	1.08358	YES	YES
135	a	772.70	0.13946	YES	YES
136	a	772.88	0.22021	YES	YES
137	a	773.77	0.17863	YES	YES

138	a	774.23	0.75622	YES	YES
139	a	775.36	0.33160	YES	YES
140	a	775.82	0.40730	YES	YES
141	a	776.72	3.87919	YES	YES
142	a	780.32	14.34438	YES	YES
143	a	782.16	7.40993	YES	YES
144	a	808.78	0.97292	YES	YES
145	a	810.27	1.31372	YES	YES
146	a	810.96	2.07448	YES	YES
147	a	812.12	0.93073	YES	YES
148	a	812.94	0.63719	YES	YES
149	a	813.49	1.08407	YES	YES
150	a	815.90	2.59229	YES	YES
151	a	816.42	9.49127	YES	YES
152	a	833.28	0.34614	YES	YES
153	a	834.12	0.83263	YES	YES
154	a	836.52	5.28193	YES	YES
155	a	837.63	5.26132	YES	YES
156	a	837.82	2.34000	YES	YES
157	a	838.27	4.34033	YES	YES
158	a	839.06	15.61576	YES	YES
159	a	839.71	3.32589	YES	YES
160	a	851.26	11.41990	YES	YES
161	a	855.21	6.98213	YES	YES
162	a	874.82	0.57198	YES	YES
163	a	875.34	3.62131	YES	YES
164	a	875.73	9.47763	YES	YES
165	a	876.06	0.26152	YES	YES
166	a	876.94	4.52538	YES	YES
167	a	878.05	2.18530	YES	YES
168	a	878.35	2.78633	YES	YES
169	a	878.88	0.71326	YES	YES
170	a	879.08	3.63562	YES	YES
171	a	880.03	5.77626	YES	YES
172	a	880.54	3.22706	YES	YES
173	a	880.86	1.33211	YES	YES
174	a	882.24	0.39595	YES	YES
175	a	883.49	2.53666	YES	YES
176	a	886.02	4.91578	YES	YES
177	a	887.79	0.17765	YES	YES
178	a	902.96	0.62947	YES	YES
179	a	903.43	3.89479	YES	YES
180	a	904.78	1.68437	YES	YES
181	a	905.57	1.57520	YES	YES
182	a	908.64	0.66255	YES	YES
183	a	909.12	2.40653	YES	YES
184	a	910.84	1.20925	YES	YES
185	a	911.34	1.79063	YES	YES
186	a	986.91	2.23578	YES	YES
187	a	987.77	2.50933	YES	YES
188	a	988.27	7.70608	YES	YES
189	a	988.75	4.13736	YES	YES
190	a	989.75	0.38287	YES	YES
191	a	990.30	29.11852	YES	YES
192	a	991.00	24.89025	YES	YES
193	a	991.74	6.83956	YES	YES
194	a	993.49	1.09459	YES	YES
195	a	995.05	0.25206	YES	YES

196	a	1014.26	1.49383	YES	YES
197	a	1016.94	0.52609	YES	YES
198	a	1017.35	0.98510	YES	YES
199	a	1017.71	0.29060	YES	YES
200	a	1017.85	0.58544	YES	YES
201	a	1020.48	0.94291	YES	YES
202	a	1021.68	0.58413	YES	YES
203	a	1022.92	0.87809	YES	YES
204	a	1030.00	2.63012	YES	YES
205	a	1031.76	2.02435	YES	YES
206	a	1032.18	0.42416	YES	YES
207	a	1033.28	3.00082	YES	YES
208	a	1038.99	2.95138	YES	YES
209	a	1039.82	2.04481	YES	YES
210	a	1040.64	0.31976	YES	YES
211	a	1041.39	1.36733	YES	YES
212	a	1049.44	4.23801	YES	YES
213	a	1058.45	1.55275	YES	YES
214	a	1059.98	3.60312	YES	YES
215	a	1060.65	1.06778	YES	YES
216	a	1061.69	0.72970	YES	YES
217	a	1064.10	3.54344	YES	YES
218	a	1066.35	0.67717	YES	YES
219	a	1067.83	0.41798	YES	YES
220	a	1069.15	0.52407	YES	YES
221	a	1070.95	0.22540	YES	YES
222	a	1071.57	0.11172	YES	YES
223	a	1072.29	0.18734	YES	YES
224	a	1072.86	0.11764	YES	YES
225	a	1073.81	0.15777	YES	YES
226	a	1075.99	0.31293	YES	YES
227	a	1076.35	0.06327	YES	YES
228	a	1076.74	0.26887	YES	YES
229	a	1079.47	49.79106	YES	YES
230	a	1085.09	4.34676	YES	YES
231	a	1085.89	8.71019	YES	YES
232	a	1092.09	5.74019	YES	YES
233	a	1096.18	8.46435	YES	YES
234	a	1096.48	11.83959	YES	YES
235	a	1098.11	5.51692	YES	YES
236	a	1100.49	1.67294	YES	YES
237	a	1101.74	0.52782	YES	YES
238	a	1102.45	3.51342	YES	YES
239	a	1107.01	1.09751	YES	YES
240	a	1107.68	16.38346	YES	YES
241	a	1132.89	4.97365	YES	YES
242	a	1135.18	1.01760	YES	YES
243	a	1159.36	4.67753	YES	YES
244	a	1160.40	4.77478	YES	YES
245	a	1160.83	6.05294	YES	YES
246	a	1161.91	4.50430	YES	YES
247	a	1169.85	3.21983	YES	YES
248	a	1170.54	0.88851	YES	YES
249	a	1171.07	19.35950	YES	YES
250	a	1172.04	9.53170	YES	YES
251	a	1175.88	14.41953	YES	YES
252	a	1179.68	9.39865	YES	YES
253	a	1185.73	3.96394	YES	YES

254	a	1186.92	10.10942	YES	YES
255	a	1188.97	3.82505	YES	YES
256	a	1191.08	0.26614	YES	YES
257	a	1193.29	2.76085	YES	YES
258	a	1197.07	1.72009	YES	YES
259	a	1242.25	0.10378	YES	YES
260	a	1242.61	0.10476	YES	YES
261	a	1244.10	0.11191	YES	YES
262	a	1244.46	1.21337	YES	YES
263	a	1245.14	0.55798	YES	YES
264	a	1245.83	0.88716	YES	YES
265	a	1247.10	0.17938	YES	YES
266	a	1247.48	0.41091	YES	YES
267	a	1249.75	0.21608	YES	YES
268	a	1250.61	0.20803	YES	YES
269	a	1254.92	1.43007	YES	YES
270	a	1256.37	3.44881	YES	YES
271	a	1256.99	5.82021	YES	YES
272	a	1257.46	2.68309	YES	YES
273	a	1257.73	1.69063	YES	YES
274	a	1257.89	3.21610	YES	YES
275	a	1258.51	3.60833	YES	YES
276	a	1259.19	4.05894	YES	YES
277	a	1259.56	3.19429	YES	YES
278	a	1259.95	2.90055	YES	YES
279	a	1260.14	8.92403	YES	YES
280	a	1260.39	0.08837	YES	YES
281	a	1262.18	4.10683	YES	YES
282	a	1263.53	2.12841	YES	YES
283	a	1265.66	2.63314	YES	YES
284	a	1268.22	1.07840	YES	YES
285	a	1269.31	1.14326	YES	YES
286	a	1271.71	0.28337	YES	YES
287	a	1281.25	2.95741	YES	YES
288	a	1283.62	1.72921	YES	YES
289	a	1283.67	2.20628	YES	YES
290	a	1285.79	4.83743	YES	YES
291	a	1289.43	4.59400	YES	YES
292	a	1290.22	1.45543	YES	YES
293	a	1291.06	2.05548	YES	YES
294	a	1291.34	5.08737	YES	YES
295	a	1307.36	3.85204	YES	YES
296	a	1310.21	0.16558	YES	YES
297	a	1310.75	2.37981	YES	YES
298	a	1311.47	1.00567	YES	YES
299	a	1312.74	2.79435	YES	YES
300	a	1313.62	0.53697	YES	YES
301	a	1315.14	2.97121	YES	YES
302	a	1318.95	1.51285	YES	YES
303	a	1321.74	0.55630	YES	YES
304	a	1322.12	1.02250	YES	YES
305	a	1322.55	4.08926	YES	YES
306	a	1323.36	0.14761	YES	YES
307	a	1323.58	0.70979	YES	YES
308	a	1323.96	1.15996	YES	YES
309	a	1324.98	1.08925	YES	YES
310	a	1325.25	0.38232	YES	YES
311	a	1325.84	0.03511	YES	YES

312	a	1326.19	0.40371	YES	YES
313	a	1326.76	3.88293	YES	YES
314	a	1327.18	5.17627	YES	YES
315	a	1327.76	4.10502	YES	YES
316	a	1328.96	1.85044	YES	YES
317	a	1329.98	3.80078	YES	YES
318	a	1333.78	0.68120	YES	YES
319	a	1336.01	0.21863	YES	YES
320	a	1337.45	0.59458	YES	YES
321	a	1337.72	1.82100	YES	YES
322	a	1337.98	0.33205	YES	YES
323	a	1338.65	0.23739	YES	YES
324	a	1339.09	0.83313	YES	YES
325	a	1340.25	0.18846	YES	YES
326	a	1342.31	0.46625	YES	YES
327	a	1345.29	2.76383	YES	YES
328	a	1347.11	5.05841	YES	YES
329	a	1347.27	0.51000	YES	YES
330	a	1348.13	2.30226	YES	YES
331	a	1348.28	0.68133	YES	YES
332	a	1349.40	0.94815	YES	YES
333	a	1349.62	0.62961	YES	YES
334	a	1350.70	0.22653	YES	YES
335	a	1351.00	1.26936	YES	YES
336	a	1400.65	7.27909	YES	YES
337	a	1402.46	6.71721	YES	YES
338	a	1405.28	9.35745	YES	YES
339	a	1407.22	7.51114	YES	YES
340	a	1412.39	7.91367	YES	YES
341	a	1423.49	2.86220	YES	YES
342	a	1426.31	6.70967	YES	YES
343	a	1427.52	5.85706	YES	YES
344	a	1427.80	4.77295	YES	YES
345	a	1429.27	4.13259	YES	YES
346	a	1429.82	7.15112	YES	YES
347	a	1433.03	2.83753	YES	YES
348	a	1434.21	1.50307	YES	YES
349	a	1434.95	10.12951	YES	YES
350	a	1436.24	2.61546	YES	YES
351	a	1436.48	2.52136	YES	YES
352	a	1437.22	1.70915	YES	YES
353	a	1437.55	6.44797	YES	YES
354	a	1437.87	1.32266	YES	YES
355	a	1437.99	3.79083	YES	YES
356	a	1438.37	6.38451	YES	YES
357	a	1438.62	5.74157	YES	YES
358	a	1439.04	2.45811	YES	YES
359	a	1439.11	1.56585	YES	YES
360	a	1439.87	2.07312	YES	YES
361	a	1440.25	17.45951	YES	YES
362	a	1440.78	6.85760	YES	YES
363	a	1441.32	10.55094	YES	YES
364	a	1441.56	2.35474	YES	YES
365	a	1441.89	3.94042	YES	YES
366	a	1443.30	42.69597	YES	YES
367	a	1443.63	9.39922	YES	YES
368	a	1444.65	7.03402	YES	YES
369	a	1445.25	8.89473	YES	YES

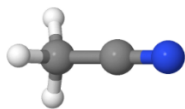
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374	a	1452.90	1.12424	YES	YES
375	a	1454.07	3.01550	YES	YES
376	a	1454.33	0.24374	YES	YES
377	a	1454.75	0.32539	YES	YES
378	a	1456.34	1.17562	YES	YES
379	a	1456.83	1.16136	YES	YES
380	a	1457.77	0.87404	YES	YES
381	a	1460.89	1.36208	YES	YES
382	a	1475.18	9.13092	YES	YES
383	a	1850.65	128.76158	YES	YES
384	a	2887.74	97.27812	YES	YES
385	a	2924.31	10.80559	YES	YES
386	a	2927.08	10.11451	YES	YES
387	a	2927.41	6.15867	YES	YES
388	a	2929.20	12.54097	YES	YES
389	a	2929.52	1.91347	YES	YES
390	a	2931.66	37.33274	YES	YES
391	a	2932.61	18.74660	YES	YES
392	a	2934.51	20.13013	YES	YES
393	a	2938.30	9.97860	YES	YES
394	a	2938.37	5.15675	YES	YES
395	a	2941.20	3.55331	YES	YES
396	a	2941.74	2.51351	YES	YES
397	a	2941.93	10.72545	YES	YES
398	a	2943.70	10.99582	YES	YES
399	a	2943.89	7.38341	YES	YES
400	a	2944.32	6.38397	YES	YES
401	a	2944.57	9.40848	YES	YES
402	a	2944.68	7.44135	YES	YES
403	a	2946.04	16.19604	YES	YES
404	a	2946.19	9.93202	YES	YES
405	a	2946.45	8.37807	YES	YES
406	a	2946.78	8.15968	YES	YES
407	a	2948.51	15.25829	YES	YES
408	a	2948.94	8.38645	YES	YES
409	a	2951.91	7.78619	YES	YES
410	a	2953.00	25.99473	YES	YES
411	a	2953.36	18.93662	YES	YES
412	a	2954.07	7.45101	YES	YES
413	a	2954.60	25.98856	YES	YES
414	a	2955.22	1.54096	YES	YES
415	a	2955.53	0.75927	YES	YES
416	a	2956.93	3.12134	YES	YES
417	a	2957.94	2.93914	YES	YES
418	a	2958.04	8.14540	YES	YES
419	a	2958.37	1.96615	YES	YES
420	a	2958.76	10.39753	YES	YES
421	a	2959.13	17.57008	YES	YES
422	a	2959.20	4.33785	YES	YES
423	a	2959.55	7.02952	YES	YES
424	a	2960.15	36.27481	YES	YES
425	a	2960.93	44.22231	YES	YES
426	a	2961.34	14.01919	YES	YES
427	a	2962.62	16.90774	YES	YES

428	a	2962.99	38.04725	YES	YES
429	a	2963.57	45.13520	YES	YES
430	a	2963.88	38.37826	YES	YES
431	a	2964.62	88.43989	YES	YES
432	a	2965.74	12.97536	YES	YES
433	a	2967.24	24.01887	YES	YES
434	a	2985.38	5.08838	YES	YES
435	a	2987.08	6.13730	YES	YES
436	a	2989.41	0.99116	YES	YES
437	a	2990.07	5.16179	YES	YES
438	a	2990.36	42.69260	YES	YES
439	a	2991.16	5.47570	YES	YES
440	a	2992.95	6.54320	YES	YES
441	a	2992.98	49.04665	YES	YES
442	a	3004.56	34.85778	YES	YES
443	a	3005.36	33.45883	YES	YES
444	a	3005.65	5.39509	YES	YES
445	a	3006.20	13.80717	YES	YES
446	a	3007.05	20.22608	YES	YES
447	a	3007.93	19.87746	YES	YES
448	a	3008.48	25.81059	YES	YES
449	a	3009.57	23.04022	YES	YES
450	a	3009.74	10.86644	YES	YES
451	a	3010.71	17.64337	YES	YES
452	a	3011.07	26.29329	YES	YES
453	a	3011.18	16.61707	YES	YES
454	a	3011.58	14.98764	YES	YES
455	a	3011.74	5.59400	YES	YES
456	a	3012.19	22.79574	YES	YES
457	a	3012.29	16.01065	YES	YES
458	a	3012.35	24.54931	YES	YES
459	a	3013.38	30.36500	YES	YES
460	a	3013.90	24.59655	YES	YES
461	a	3014.15	30.47819	YES	YES
462	a	3014.47	27.30404	YES	YES
463	a	3014.83	38.88035	YES	YES
464	a	3014.91	25.03679	YES	YES
465	a	3015.30	31.65112	YES	YES
466	a	3015.41	15.05351	YES	YES
467	a	3016.03	29.09563	YES	YES
468	a	3016.17	18.80169	YES	YES
469	a	3016.33	21.27225	YES	YES
470	a	3016.58	20.51668	YES	YES
471	a	3017.16	16.42660	YES	YES
472	a	3017.28	38.86483	YES	YES
473	a	3017.94	32.05939	YES	YES
474	a	3018.23	20.25547	YES	YES
475	a	3018.95	31.92498	YES	YES
476	a	3019.46	22.89707	YES	YES
477	a	3019.58	29.52935	YES	YES
478	a	3031.74	6.53947	YES	YES
479	a	3034.60	0.01085	YES	YES
480	a	3035.29	0.20344	YES	YES
481	a	3049.61	0.35914	YES	YES
482	a	3054.92	0.19877	YES	YES
483	a	3458.78	8.66488	YES	YES

\$end

Double hybrid single point energy = -7344.830305190681 H
 COSMO energy + OC correction = -7352.2689154038 H (in oDFB)

6.2.35 H₃CCN



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c3v

Cartesian coordinates in Ångström:

N	0.0000000	0.0000000	-2.1284736
C	0.0000000	0.0000000	-0.9665286
C	0.0000000	0.0000000	0.4884740
H	0.5147647	0.8915986	0.8688108
H	0.5147647	-0.8915986	0.8688108
H	-1.0295294	0.0000000	0.8688108

SCF energy GEOOPT = -132.8168663825 H

ZPE = 115.3 kJ/mol

FREEH energy = 124.93 kJ/mol

FREEH entropy = 0.24344 kJ/mol/K

\$vibrational spectrum

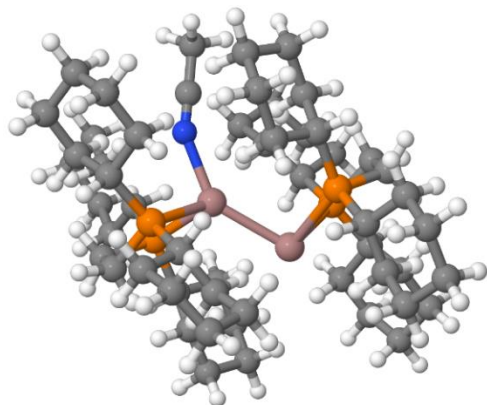
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#			cm ⁻¹	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
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3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	370.13	0.15852	YES	YES
8		e	370.13	0.15852	YES	YES
9		a1	919.25	0.42873	YES	YES
10		e	1021.94	2.03865	YES	YES
11		e	1021.94	2.03865	YES	YES
12		a1	1360.91	2.99554	YES	YES
13		e	1425.33	10.59818	YES	YES
14		e	1425.33	10.59818	YES	YES
15		a1	2278.74	9.01912	YES	YES
16		a1	2982.13	2.81479	YES	YES
17		e	3054.39	0.66764	YES	YES
18		e	3054.39	0.66764	YES	YES

\$end

Double hybrid single point energy = -132.585848102054 H

COSMO energy + OC correction = -132.8271645470 H (in oDFB)

6.2.36 $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_3)]^{2+}$ (Adduct)



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

H	3.8327870	-5.9231862	1.2048901
H	4.0369300	-5.3225199	-1.2284679
C	3.1039520	-5.2509532	0.7324309
C	3.7219330	-4.5700295	-0.4929734
H	2.2581246	-5.8817755	0.4131005
H	4.6337065	-4.0294297	-0.1880471
H	1.0574737	-4.6638004	-6.3890685
H	0.0860716	-5.1159353	-4.1536618
C	2.7375181	-3.5820192	-1.1279402
C	2.6039308	-4.2263017	1.7613500
H	-1.1639671	-5.2980441	-5.3836499
H	1.8707671	-4.1368808	-1.5262756
H	2.1352665	-4.7455672	2.6081667
C	-0.5132481	-4.5607036	-4.8945480
H	3.1983455	-3.0717339	-1.9880560
C	0.4193237	-3.9051078	-5.9167353
H	3.4636037	-3.6678963	2.1657762
H	1.9663780	-3.2754098	-4.5362106
C	1.2781510	-2.8164492	-5.2661678
C	1.6168996	-3.2422475	1.1127252
H	-0.1813626	-3.4563646	-6.7247397
H	1.9018812	-2.3165543	-6.0206015
C	2.2405155	-2.5545647	-0.1068512
H	0.7411075	-3.8109410	0.7552918
H	-1.2327983	-5.4366679	4.4133880
C	-1.3773808	-3.5277509	-4.1555194
H	-0.6626965	-4.5517885	2.1686326
H	3.0815895	-1.9175558	0.2186562
H	-1.9991083	-4.0401057	-3.4100332
H	0.1759453	-2.9609766	-2.7678159
H	-1.3639024	-3.8529593	-1.1408962
H	-2.6805486	-4.7468760	0.7811730
H	0.7876171	-3.7124503	4.0075316
C	-1.8857782	-4.6767005	3.9544228
H	-2.6909770	-5.2243070	3.4443316
C	-0.4870901	-2.4603888	-3.4963638
H	-3.6798004	-4.6291530	-0.6639926
C	0.4047883	-1.7796355	-4.5484804
C	-1.0835239	-3.8740504	2.9248285

H	1.4993539	-1.8785081	-0.5586228
C	-3.1470458	-4.0302058	0.0924067
H	4.4312211	-0.5362516	-3.5292408
H	-2.0640863	-3.0407793	-4.8670774
C	0.0273936	-3.0389137	3.5767714
C	-2.0632833	-3.1969255	-0.6017390
H	2.6598224	-1.9187645	3.9732423
P	0.8780830	-2.0098146	2.2894072
H	-0.6627938	-3.6576686	6.2473919
H	1.0239250	-1.0028606	-4.0846099
C	2.3053271	-1.2372087	3.1864422
H	-0.2312074	-1.2771732	-5.2945144
C	4.2679327	-0.0388482	-2.5637038
H	-1.4741012	-2.6518040	0.1565851
H	3.1145676	-1.1482998	2.4496487
C	-2.4569103	-3.7674021	5.0445892
H	-3.0050916	-4.3605828	5.7885266
H	-1.7638093	-3.1857473	2.3967957
H	-3.2473607	-2.7162497	-2.3433777
C	-1.3412528	-2.9671307	5.7203691
H	4.7432356	0.9508389	-2.5880126
C	-2.6975255	-2.1729184	-1.5555935
C	-4.1459199	-3.1364944	0.8327741
C	-0.5377168	-2.1513819	4.7003269
H	-4.9284890	-3.7476334	1.3018023
C	2.8538393	0.1076935	-2.3135560
P	-1.3966546	-1.2235489	-2.4554870
H	4.7322228	-0.6382138	-1.7686918
H	0.2767132	-1.6231263	5.2148583
N	1.7113864	0.2196234	-2.1224077
H	-3.6281961	-2.6048546	1.6488158
H	2.8829318	0.7224564	0.3438068
H	-3.1863389	-3.0720683	4.5960296
H	5.2076079	1.5648623	-0.0762535
H	3.8581704	0.6744732	1.8183037
H	-5.3831176	-2.6243554	-0.8674958
C	1.9706220	0.1395785	3.7820183
H	-1.7540245	-2.2922087	6.4828606
C	-4.7710840	-2.1064002	-0.1111578
Ga	-0.7701968	-0.2197092	1.5583652
C	3.3899882	1.3533211	1.0931605
Ga	-0.0703444	0.1861247	-0.8756856
C	-3.6989652	-1.2675216	-0.8185139
H	-1.1905765	-1.3814890	4.2523217
H	2.8883441	0.6554503	4.0980695
H	1.3477043	0.0253019	4.6778898
C	-2.3296106	-0.1005434	-3.5947993
H	-1.7176987	0.0052323	-4.4981817
H	0.7602262	1.2345443	-4.2231069
H	-3.2671192	-0.5892167	-3.8962342
C	4.4772397	2.2111537	0.4329276
H	1.3700097	2.1863360	-6.4153975
H	-3.1598382	-0.6573453	-0.0738068
H	2.9105362	2.7479347	-4.5234529
C	0.1873603	2.0913070	-4.6073953
P	1.0182116	1.2314266	2.6231964
H	-4.1845196	-0.5791243	-1.5240045
H	-0.6965223	1.6851384	-5.1178363

H	3.4180949	2.7143518	-1.3876271
H	-5.4506175	-1.4413957	0.4392364
H	5.0403431	2.7397143	1.2183260
C	1.0450101	2.8663507	-5.6158380
C	3.8858686	3.2381674	-0.5359923
C	2.3394860	2.2324556	1.7847715
C	2.2486868	3.5278896	-4.9403575
C	-2.6235209	1.2815708	-2.9848125
H	4.6799980	3.8708835	-0.9553157
H	1.5713168	2.9652701	-2.2734601
P	-1.1693510	2.0454412	-2.1326022
H	2.8444632	4.0808703	-5.6784280
H	2.8404467	2.7872361	2.5961773
H	1.1863465	2.6814544	0.0236322
C	-0.2463536	2.9839459	-3.4325360
H	-0.5580642	1.0419422	5.2006089
H	-3.4145833	1.2060405	-2.2277474
C	1.7351273	3.2423173	0.8023428
H	0.4290573	3.6422288	-6.0980649
C	0.9425415	3.7099444	-2.7854875
H	-1.6417967	1.2093399	3.8139607
C	2.8260159	4.1022737	0.1536271
C	-0.9899213	1.7745531	4.4988684
C	0.1412918	2.4555793	3.7089084
H	-2.9873337	1.9704619	-3.7601555
C	1.7919283	4.4598293	-3.8159652
H	1.5612510	2.5922920	5.3392622
H	-2.1060517	1.8427559	0.6367865
H	2.6547948	4.9189531	-3.3132747
C	1.0487547	3.2741530	4.6410135
H	-0.9593103	3.7343540	-3.8149464
H	3.3081484	4.7167475	0.9303484
H	2.3775848	4.8058998	-0.5605040
H	0.9995225	3.8841981	1.3082798
C	-2.6672434	2.6618041	0.1582309
C	-1.8396413	3.3092526	-0.9635965
H	-0.3335887	3.1447627	2.9862088
H	0.5855255	4.4056886	-2.0137380
H	1.8315400	3.7954447	4.0727114
H	-3.5781254	2.2086931	-0.2660323
H	-0.9292234	3.7296221	-0.5010272
H	1.2035798	5.2870164	-4.2440308
C	-1.8037101	2.8044150	5.2910872
H	-0.4801899	2.9680376	6.9935706
H	-2.5894415	2.2928914	5.8639923
C	-0.9070095	3.6279819	6.2201896
C	0.2288531	4.2969231	5.4413385
C	-2.6185028	4.4541591	-1.6322574
C	-3.0697233	3.7081143	1.2028006
H	-2.3166800	3.4765312	4.5831786
H	-3.5164257	4.0460801	-2.1240770
H	-3.6708180	3.2313837	1.9894639
H	-2.0166510	4.9376879	-2.4139563
H	-2.1581058	4.0928416	1.6922562
H	0.8925733	4.8477983	6.1217045
H	-0.1927924	5.0405701	4.7445958
H	-1.5005101	4.3846993	6.7507253
C	-3.8357071	4.8690168	0.5612148

C	-3.0365962	5.4972452	-0.5848163
H	-4.7983318	4.4963405	0.1743666
H	-2.1299467	5.9776070	-0.1805447
H	-3.6191527	6.2913757	-1.0708659
H	-4.0781295	5.6302229	1.3149251

SCF energy GEOOPT = -7389.015250247 H

ZPE = 3713. kJ/mol

FREEH energy = 3904.02 kJ/mol

FREEH entropy = 1.64445 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.04	0.17045	YES	YES
8		a	16.32	0.15208	YES	YES
9		a	17.54	0.11819	YES	YES
10		a	18.95	0.01731	YES	YES
11		a	26.98	0.15613	YES	YES
12		a	29.22	0.01719	YES	YES
13		a	30.20	0.05451	YES	YES
14		a	31.01	0.01518	YES	YES
15		a	32.71	0.72630	YES	YES
16		a	39.18	0.91399	YES	YES
17		a	40.63	1.57450	YES	YES
18		a	41.12	0.34352	YES	YES
19		a	43.77	0.43168	YES	YES
20		a	47.15	0.25658	YES	YES
21		a	50.14	0.03738	YES	YES
22		a	52.70	0.34492	YES	YES
23		a	54.73	0.37656	YES	YES
24		a	57.97	0.03109	YES	YES
25		a	60.25	0.26230	YES	YES
26		a	62.46	0.36001	YES	YES
27		a	66.25	0.45064	YES	YES
28		a	67.93	0.23453	YES	YES
29		a	70.71	0.93116	YES	YES
30		a	71.32	1.47860	YES	YES
31		a	73.28	0.26025	YES	YES
32		a	77.35	0.40620	YES	YES
33		a	78.70	1.21327	YES	YES
34		a	83.03	0.18218	YES	YES
35		a	85.94	0.30696	YES	YES
36		a	88.32	0.13052	YES	YES
37		a	92.54	1.50831	YES	YES
38		a	99.24	0.10139	YES	YES
39		a	115.93	1.75986	YES	YES
40		a	121.62	0.22429	YES	YES
41		a	122.88	0.04690	YES	YES
42		a	134.22	0.85096	YES	YES
43		a	136.36	1.59996	YES	YES
44		a	137.84	1.11617	YES	YES

45	a	140.17	2.39376	YES	YES
46	a	143.09	5.84359	YES	YES
47	a	144.77	0.84082	YES	YES
48	a	146.93	10.17361	YES	YES
49	a	151.86	2.33326	YES	YES
50	a	156.49	4.70701	YES	YES
51	a	167.96	2.04806	YES	YES
52	a	173.36	9.16797	YES	YES
53	a	178.57	6.11277	YES	YES
54	a	179.93	2.64277	YES	YES
55	a	185.67	5.25842	YES	YES
56	a	192.81	1.09153	YES	YES
57	a	196.44	0.38573	YES	YES
58	a	201.32	4.10800	YES	YES
59	a	206.80	3.83860	YES	YES
60	a	212.41	0.40264	YES	YES
61	a	212.94	3.88114	YES	YES
62	a	214.71	0.15692	YES	YES
63	a	217.52	1.89979	YES	YES
64	a	222.26	5.88319	YES	YES
65	a	224.67	2.13769	YES	YES
66	a	228.01	1.65892	YES	YES
67	a	237.42	0.12255	YES	YES
68	a	238.02	1.08845	YES	YES
69	a	239.53	0.56656	YES	YES
70	a	242.26	1.14816	YES	YES
71	a	244.09	0.17446	YES	YES
72	a	245.57	0.44825	YES	YES
73	a	275.89	1.48622	YES	YES
74	a	277.33	0.25900	YES	YES
75	a	284.53	2.40615	YES	YES
76	a	285.58	0.57121	YES	YES
77	a	301.60	0.13424	YES	YES
78	a	304.07	0.33098	YES	YES
79	a	313.59	0.65336	YES	YES
80	a	315.11	0.24616	YES	YES
81	a	328.11	0.79246	YES	YES
82	a	331.00	0.87656	YES	YES
83	a	332.86	0.30096	YES	YES
84	a	334.74	0.28206	YES	YES
85	a	337.61	1.13706	YES	YES
86	a	342.53	0.58078	YES	YES
87	a	361.60	8.07565	YES	YES
88	a	366.51	0.97584	YES	YES
89	a	373.36	0.81210	YES	YES
90	a	374.88	0.53638	YES	YES
91	a	383.14	12.63024	YES	YES
92	a	387.69	4.89915	YES	YES
93	a	390.39	0.16375	YES	YES
94	a	391.67	0.68134	YES	YES
95	a	411.93	1.44290	YES	YES
96	a	412.45	1.45777	YES	YES
97	a	420.94	4.96436	YES	YES
98	a	422.22	5.06264	YES	YES
99	a	422.76	1.09740	YES	YES
100	a	423.58	1.21618	YES	YES
101	a	428.84	0.11955	YES	YES
102	a	430.03	0.33348	YES	YES

103	a	430.56	0.08246	YES	YES
104	a	431.52	0.33218	YES	YES
105	a	431.70	1.04034	YES	YES
106	a	431.83	0.08586	YES	YES
107	a	432.16	0.63116	YES	YES
108	a	432.66	0.31761	YES	YES
109	a	440.10	7.15937	YES	YES
110	a	446.55	2.28896	YES	YES
111	a	462.79	3.41953	YES	YES
112	a	467.03	3.98920	YES	YES
113	a	489.10	5.81351	YES	YES
114	a	490.65	2.39762	YES	YES
115	a	491.26	0.65030	YES	YES
116	a	492.72	4.68429	YES	YES
117	a	499.87	0.74035	YES	YES
118	a	503.51	0.49111	YES	YES
119	a	512.05	13.47999	YES	YES
120	a	516.46	9.28730	YES	YES
121	a	622.43	25.36394	YES	YES
122	a	623.52	4.45110	YES	YES
123	a	638.87	11.91122	YES	YES
124	a	641.13	7.67969	YES	YES
125	a	707.03	0.62582	YES	YES
126	a	713.53	0.45330	YES	YES
127	a	717.49	4.85351	YES	YES
128	a	721.52	1.68133	YES	YES
129	a	729.98	3.52772	YES	YES
130	a	730.93	9.44736	YES	YES
131	a	731.31	6.66421	YES	YES
132	a	734.40	6.39204	YES	YES
133	a	770.99	0.26264	YES	YES
134	a	771.59	0.67557	YES	YES
135	a	771.90	0.20835	YES	YES
136	a	772.41	0.58460	YES	YES
137	a	773.16	0.36483	YES	YES
138	a	773.91	0.95177	YES	YES
139	a	774.81	0.57613	YES	YES
140	a	775.18	2.34013	YES	YES
141	a	776.96	22.80596	YES	YES
142	a	779.27	10.34266	YES	YES
143	a	808.74	0.36445	YES	YES
144	a	810.48	2.49583	YES	YES
145	a	810.52	0.11502	YES	YES
146	a	811.32	1.15814	YES	YES
147	a	812.36	1.63075	YES	YES
148	a	813.40	0.40968	YES	YES
149	a	813.99	6.63603	YES	YES
150	a	815.61	7.29276	YES	YES
151	a	831.87	2.19264	YES	YES
152	a	832.80	1.30739	YES	YES
153	a	834.98	4.96372	YES	YES
154	a	835.95	2.71548	YES	YES
155	a	836.56	3.21609	YES	YES
156	a	837.27	1.71049	YES	YES
157	a	838.04	13.73575	YES	YES
158	a	839.45	8.25296	YES	YES
159	a	850.37	27.27812	YES	YES
160	a	852.34	1.30023	YES	YES

161	a	873.45	1.17193	YES	YES
162	a	875.62	3.90918	YES	YES
163	a	876.39	0.88578	YES	YES
164	a	876.51	6.75812	YES	YES
165	a	876.80	3.13342	YES	YES
166	a	878.05	0.94586	YES	YES
167	a	878.33	5.86233	YES	YES
168	a	878.95	1.31628	YES	YES
169	a	879.37	2.34908	YES	YES
170	a	879.93	1.24101	YES	YES
171	a	880.15	5.84410	YES	YES
172	a	880.27	3.30428	YES	YES
173	a	882.46	2.41413	YES	YES
174	a	883.77	0.64970	YES	YES
175	a	885.38	4.03002	YES	YES
176	a	887.81	1.10722	YES	YES
177	a	902.30	2.36985	YES	YES
178	a	902.83	3.52526	YES	YES
179	a	903.50	2.60865	YES	YES
180	a	904.32	0.83550	YES	YES
181	a	907.56	1.19126	YES	YES
182	a	909.34	1.54656	YES	YES
183	a	910.38	1.72970	YES	YES
184	a	910.67	0.34938	YES	YES
185	a	932.17	0.43422	YES	YES
186	a	982.13	0.14147	YES	YES
187	a	984.31	0.94694	YES	YES
188	a	986.40	4.75739	YES	YES
189	a	988.15	13.75894	YES	YES
190	a	989.12	0.83541	YES	YES
191	a	989.72	20.80771	YES	YES
192	a	989.87	12.22206	YES	YES
193	a	990.71	4.85598	YES	YES
194	a	991.61	6.86562	YES	YES
195	a	992.65	4.55477	YES	YES
196	a	1002.23	0.89821	YES	YES
197	a	1007.44	5.42490	YES	YES
198	a	1013.24	3.31561	YES	YES
199	a	1014.46	1.40880	YES	YES
200	a	1016.75	1.29445	YES	YES
201	a	1018.19	0.53754	YES	YES
202	a	1018.52	0.68631	YES	YES
203	a	1020.43	0.27087	YES	YES
204	a	1022.88	0.68101	YES	YES
205	a	1023.41	0.36632	YES	YES
206	a	1031.71	3.07133	YES	YES
207	a	1032.59	0.26412	YES	YES
208	a	1033.18	0.93755	YES	YES
209	a	1034.12	2.96976	YES	YES
210	a	1039.22	2.91094	YES	YES
211	a	1040.44	0.21525	YES	YES
212	a	1040.52	2.09336	YES	YES
213	a	1041.20	0.67474	YES	YES
214	a	1058.08	2.85228	YES	YES
215	a	1058.87	1.43348	YES	YES
216	a	1059.57	1.69961	YES	YES
217	a	1059.92	1.39199	YES	YES
218	a	1062.30	3.04161	YES	YES

219	a	1065.74	0.51069	YES	YES
220	a	1067.11	0.11708	YES	YES
221	a	1069.75	0.16830	YES	YES
222	a	1070.59	0.12167	YES	YES
223	a	1072.22	0.05840	YES	YES
224	a	1072.59	0.00682	YES	YES
225	a	1073.04	0.31122	YES	YES
226	a	1073.68	0.48004	YES	YES
227	a	1074.73	1.13909	YES	YES
228	a	1076.56	0.21897	YES	YES
229	a	1077.51	0.29882	YES	YES
230	a	1078.17	1.13672	YES	YES
231	a	1082.06	2.69488	YES	YES
232	a	1090.12	7.79223	YES	YES
233	a	1091.91	12.23608	YES	YES
234	a	1093.57	8.03715	YES	YES
235	a	1098.39	2.05766	YES	YES
236	a	1100.34	0.93264	YES	YES
237	a	1101.64	0.97704	YES	YES
238	a	1104.49	5.36447	YES	YES
239	a	1107.21	11.03337	YES	YES
240	a	1124.07	11.63256	YES	YES
241	a	1127.04	1.35806	YES	YES
242	a	1158.35	7.42808	YES	YES
243	a	1159.54	6.83392	YES	YES
244	a	1159.85	3.22663	YES	YES
245	a	1161.79	5.95514	YES	YES
246	a	1168.15	10.65917	YES	YES
247	a	1168.57	1.00158	YES	YES
248	a	1170.25	10.04213	YES	YES
249	a	1172.12	7.96248	YES	YES
250	a	1174.59	9.73472	YES	YES
251	a	1176.88	11.24920	YES	YES
252	a	1179.45	9.75179	YES	YES
253	a	1183.26	6.95754	YES	YES
254	a	1189.06	2.72511	YES	YES
255	a	1191.55	0.63133	YES	YES
256	a	1194.31	1.64600	YES	YES
257	a	1198.25	2.32678	YES	YES
258	a	1234.18	0.41521	YES	YES
259	a	1237.77	0.39402	YES	YES
260	a	1243.45	0.04152	YES	YES
261	a	1244.27	0.15548	YES	YES
262	a	1244.82	0.39815	YES	YES
263	a	1245.42	0.40421	YES	YES
264	a	1245.54	0.46982	YES	YES
265	a	1247.16	0.45115	YES	YES
266	a	1247.89	1.34272	YES	YES
267	a	1250.24	0.15418	YES	YES
268	a	1252.05	1.28962	YES	YES
269	a	1253.77	7.97641	YES	YES
270	a	1254.32	3.95728	YES	YES
271	a	1255.91	2.70525	YES	YES
272	a	1256.69	5.39216	YES	YES
273	a	1256.93	4.04681	YES	YES
274	a	1257.06	2.15039	YES	YES
275	a	1257.83	7.69904	YES	YES
276	a	1258.68	0.92121	YES	YES

277	a	1259.09	1.39188	YES	YES
278	a	1260.14	1.42491	YES	YES
279	a	1260.22	0.94037	YES	YES
280	a	1261.12	2.66522	YES	YES
281	a	1261.70	0.21682	YES	YES
282	a	1264.77	3.19777	YES	YES
283	a	1266.52	1.89847	YES	YES
284	a	1267.06	1.37175	YES	YES
285	a	1268.37	1.86610	YES	YES
286	a	1278.86	1.87667	YES	YES
287	a	1281.54	0.71697	YES	YES
288	a	1283.92	3.06850	YES	YES
289	a	1284.21	1.61503	YES	YES
290	a	1289.38	1.90572	YES	YES
291	a	1290.34	0.07081	YES	YES
292	a	1290.73	5.79364	YES	YES
293	a	1291.93	3.17407	YES	YES
294	a	1308.59	2.04245	YES	YES
295	a	1309.38	2.04030	YES	YES
296	a	1310.31	0.90135	YES	YES
297	a	1312.20	2.82115	YES	YES
298	a	1312.41	1.13888	YES	YES
299	a	1314.83	1.81148	YES	YES
300	a	1315.66	3.96219	YES	YES
301	a	1319.55	1.44840	YES	YES
302	a	1320.33	0.33170	YES	YES
303	a	1320.58	2.25934	YES	YES
304	a	1322.13	0.27325	YES	YES
305	a	1322.79	1.00106	YES	YES
306	a	1323.21	2.02243	YES	YES
307	a	1323.44	1.51742	YES	YES
308	a	1323.77	3.17285	YES	YES
309	a	1324.64	0.87178	YES	YES
310	a	1324.93	1.31225	YES	YES
311	a	1325.49	2.29581	YES	YES
312	a	1325.99	4.12602	YES	YES
313	a	1326.28	3.10543	YES	YES
314	a	1326.69	0.20691	YES	YES
315	a	1327.16	5.55126	YES	YES
316	a	1328.23	0.54560	YES	YES
317	a	1328.62	1.22676	YES	YES
318	a	1333.06	0.16355	YES	YES
319	a	1333.49	0.55111	YES	YES
320	a	1336.49	0.31666	YES	YES
321	a	1337.25	1.58991	YES	YES
322	a	1337.59	0.37003	YES	YES
323	a	1337.92	0.33741	YES	YES
324	a	1338.36	0.21048	YES	YES
325	a	1340.70	1.09588	YES	YES
326	a	1340.97	1.08275	YES	YES
327	a	1346.82	3.27231	YES	YES
328	a	1347.08	0.94191	YES	YES
329	a	1347.37	2.69850	YES	YES
330	a	1348.00	1.15520	YES	YES
331	a	1348.24	1.28145	YES	YES
332	a	1350.00	0.76104	YES	YES
333	a	1350.34	0.51318	YES	YES
334	a	1353.63	6.34592	YES	YES

335	a	1400.48	8.51202	YES	YES
336	a	1400.71	12.89912	YES	YES
337	a	1401.06	10.73491	YES	YES
338	a	1405.42	13.60924	YES	YES
339	a	1405.79	7.61343	YES	YES
340	a	1407.04	5.52467	YES	YES
341	a	1422.83	3.21318	YES	YES
342	a	1424.33	3.26873	YES	YES
343	a	1425.97	4.97678	YES	YES
344	a	1427.32	2.14480	YES	YES
345	a	1429.03	0.64849	YES	YES
346	a	1429.74	5.57236	YES	YES
347	a	1430.76	3.97042	YES	YES
348	a	1432.68	0.56241	YES	YES
349	a	1433.20	2.14272	YES	YES
350	a	1434.10	7.09930	YES	YES
351	a	1434.53	6.10331	YES	YES
352	a	1434.99	1.44202	YES	YES
353	a	1435.49	4.11297	YES	YES
354	a	1437.15	5.05355	YES	YES
355	a	1437.21	5.11225	YES	YES
356	a	1437.81	3.51687	YES	YES
357	a	1437.94	10.04702	YES	YES
358	a	1438.09	1.37502	YES	YES
359	a	1438.50	1.56461	YES	YES
360	a	1438.66	2.73257	YES	YES
361	a	1439.42	2.21633	YES	YES
362	a	1440.23	2.04055	YES	YES
363	a	1440.50	2.51062	YES	YES
364	a	1441.59	6.55677	YES	YES
365	a	1441.90	6.11511	YES	YES
366	a	1442.38	43.16783	YES	YES
367	a	1442.73	21.62341	YES	YES
368	a	1443.36	9.80062	YES	YES
369	a	1444.44	0.42610	YES	YES
370	a	1444.69	14.33882	YES	YES
371	a	1446.43	2.58603	YES	YES
372	a	1446.62	21.51272	YES	YES
373	a	1452.18	5.21164	YES	YES
374	a	1452.37	0.61299	YES	YES
375	a	1453.24	9.15532	YES	YES
376	a	1453.53	0.54686	YES	YES
377	a	1454.60	1.35437	YES	YES
378	a	1455.63	2.32705	YES	YES
379	a	1455.81	0.49203	YES	YES
380	a	1457.90	1.25697	YES	YES
381	a	2242.26	20.31840	YES	YES
382	a	2911.62	16.82176	YES	YES
383	a	2916.85	2.00186	YES	YES
384	a	2922.93	10.57171	YES	YES
385	a	2923.17	8.28668	YES	YES
386	a	2923.46	15.33175	YES	YES
387	a	2924.47	23.35140	YES	YES
388	a	2925.24	18.67567	YES	YES
389	a	2926.66	7.61476	YES	YES
390	a	2927.53	1.14034	YES	YES
391	a	2931.48	15.22161	YES	YES
392	a	2933.07	18.01906	YES	YES

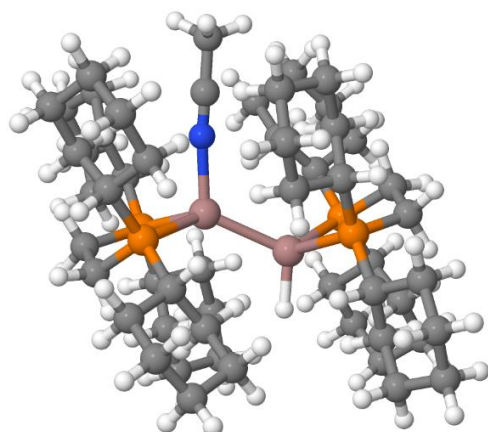
393	a	2933.61	26.37113	YES	YES
394	a	2936.35	13.36636	YES	YES
395	a	2936.43	14.96044	YES	YES
396	a	2940.19	10.69268	YES	YES
397	a	2940.84	3.25615	YES	YES
398	a	2941.27	4.07313	YES	YES
399	a	2942.47	12.23144	YES	YES
400	a	2942.49	9.05098	YES	YES
401	a	2942.54	11.93925	YES	YES
402	a	2942.60	1.24862	YES	YES
403	a	2942.81	4.46334	YES	YES
404	a	2943.61	9.88514	YES	YES
405	a	2943.79	12.42787	YES	YES
406	a	2944.90	7.48269	YES	YES
407	a	2945.53	10.65785	YES	YES
408	a	2946.23	6.35159	YES	YES
409	a	2951.99	10.43736	YES	YES
410	a	2952.02	12.61697	YES	YES
411	a	2953.54	3.28905	YES	YES
412	a	2953.92	2.36763	YES	YES
413	a	2955.43	3.84467	YES	YES
414	a	2955.56	9.06041	YES	YES
415	a	2956.00	6.35357	YES	YES
416	a	2956.37	3.28986	YES	YES
417	a	2957.64	27.05426	YES	YES
418	a	2958.11	14.68455	YES	YES
419	a	2958.91	25.88212	YES	YES
420	a	2959.16	53.43262	YES	YES
421	a	2959.32	12.36222	YES	YES
422	a	2959.70	20.75652	YES	YES
423	a	2960.69	48.27405	YES	YES
424	a	2961.10	25.01620	YES	YES
425	a	2961.12	19.88236	YES	YES
426	a	2963.66	38.64074	YES	YES
427	a	2963.70	30.17184	YES	YES
428	a	2966.48	22.51114	YES	YES
429	a	2973.13	28.85297	YES	YES
430	a	2973.58	17.40027	YES	YES
431	a	2973.85	40.92784	YES	YES
432	a	2975.77	4.91662	YES	YES
433	a	2975.90	14.11282	YES	YES
434	a	2978.32	31.17717	YES	YES
435	a	2980.97	39.35276	YES	YES
436	a	2983.83	6.05436	YES	YES
437	a	2984.57	11.80997	YES	YES
438	a	2987.69	7.34172	YES	YES
439	a	2989.42	26.04757	YES	YES
440	a	2993.93	17.07463	YES	YES
441	a	2995.58	32.50940	YES	YES
442	a	3000.80	47.32400	YES	YES
443	a	3002.19	8.17463	YES	YES
444	a	3002.62	24.55513	YES	YES
445	a	3004.17	19.00315	YES	YES
446	a	3004.39	31.57926	YES	YES
447	a	3005.40	14.99110	YES	YES
448	a	3005.83	29.03149	YES	YES
449	a	3006.45	16.81195	YES	YES
450	a	3008.29	25.08170	YES	YES

451	a	3008.90	27.28031	YES	YES
452	a	3009.03	22.17084	YES	YES
453	a	3009.41	12.17312	YES	YES
454	a	3009.77	28.32911	YES	YES
455	a	3011.35	13.21771	YES	YES
456	a	3011.47	20.83219	YES	YES
457	a	3011.75	47.52653	YES	YES
458	a	3012.18	14.30558	YES	YES
459	a	3012.62	19.90995	YES	YES
460	a	3013.60	41.76386	YES	YES
461	a	3013.66	23.18659	YES	YES
462	a	3014.76	21.78947	YES	YES
463	a	3014.91	24.88707	YES	YES
464	a	3015.19	30.65217	YES	YES
465	a	3015.35	30.07934	YES	YES
466	a	3016.20	37.72091	YES	YES
467	a	3016.51	3.50030	YES	YES
468	a	3016.52	30.46247	YES	YES
469	a	3016.66	38.64847	YES	YES
470	a	3016.81	31.72181	YES	YES
471	a	3017.21	18.03515	YES	YES
472	a	3018.93	21.80220	YES	YES
473	a	3020.34	26.40154	YES	YES
474	a	3023.94	2.41472	YES	YES
475	a	3032.53	0.13029	YES	YES
476	a	3037.42	14.26913	YES	YES
477	a	3041.49	1.61676	YES	YES
478	a	3049.71	4.61990	YES	YES
479	a	3049.98	0.27075	YES	YES
480	a	3055.60	2.36994	YES	YES

\$end

Double hybrid single point energy = -7381.656574387431 H
 COSMO energy + OC correction = -7389.1647565056 H (in oDFB)

6.2.37 [H{Ga(dcpe)}₂(NCCH₃)]³⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:
 H 4.1188786 -5.7757600 1.2725987

H	4.1636458	-5.2676800	-1.1878541
C	3.3171391	-5.1860870	0.8097278
C	3.8204953	-4.5116032	-0.4698988
H	2.5112396	-5.8955047	0.5621926
H	4.6970456	-3.8856381	-0.2332486
H	0.9871171	-4.7132818	-6.4374935
H	-0.0422708	-5.1787089	-4.2300284
C	2.7274686	-3.6418513	-1.1003257
C	2.7929500	-4.1570999	1.8215036
H	-1.2754355	-5.2791582	-5.4849631
H	1.8958198	-4.2858942	-1.4325249
H	2.4106188	-4.6677697	2.7159207
C	-0.6030021	-4.5819251	-4.9684186
H	3.1042565	-3.1335905	-2.0014455
C	0.3719023	-3.9406226	-5.9589162
H	3.6272650	-3.5165659	2.1492002
H	1.9205670	-3.4097533	-4.5380663
C	1.2655020	-2.9058068	-5.2686774
C	1.6960671	-3.2853386	1.1826523
H	-0.1938873	-3.4502588	-6.7674109
H	1.9219386	-2.4157178	-6.0009413
C	2.1849104	-2.6098438	-0.1054880
H	0.8447669	-3.9349203	0.9163903
H	-1.3864951	-5.3632216	4.3771306
C	-1.4421211	-3.5319593	-4.2234956
H	-0.7636142	-4.4588008	2.1561619
H	2.9719192	-1.8745494	0.1371954
H	-2.0963422	-4.0325307	-3.4977932
H	0.1003363	-3.0493481	-2.7851314
H	-1.4520798	-3.8870454	-1.1531621
H	-2.7574469	-4.7040218	0.8100729
H	0.7215689	-3.7553787	4.0256788
C	-1.9951173	-4.5565723	3.9388201
H	-2.8273047	-5.0454864	3.4138694
C	-0.5188708	-2.5139130	-3.5273563
H	-3.7762480	-4.5688257	-0.6161769
C	0.4244818	-1.8459948	-4.5433409
C	-1.1486073	-3.7757597	2.9263920
H	1.3538022	-2.0464496	-0.5567490
C	-3.2115135	-3.9786538	0.1227145
H	4.1335338	-0.3953198	-3.8136948
H	-2.0946566	-3.0042064	-4.9377303
C	0.0047157	-3.0255179	3.6102233
C	-2.1097369	-3.1968671	-0.6050280
H	2.7253390	-1.9079495	4.0206110
P	0.9586354	-2.0673489	2.3561031
H	-0.7223225	-3.6609114	6.2587370
H	1.0692451	-1.1085018	-4.0474478
C	2.3528568	-1.2336655	3.2369013
H	-0.1707755	-1.2966355	-5.2893907
C	4.1235700	0.0948817	-2.8298675
H	-1.4792984	-2.6690188	0.1330390
H	3.1606848	-1.1273998	2.5006784
C	-2.5164841	-3.6424038	5.0492072
H	-3.0956445	-4.2230573	5.7783854
H	-1.7874583	-3.0367165	2.4166843
H	-3.3201881	-2.6949262	-2.3224627
C	-1.3602235	-2.9231436	5.7465513

H	4.5080831	1.1191355	-2.9349495
C	-2.7317776	-2.1615728	-1.5558167
C	-4.1671889	-3.0438804	0.8693909
C	-0.5069106	-2.1261706	4.7501868
H	-4.9664873	-3.6243088	1.3477473
C	2.7774922	0.1335354	-2.3201147
P	-1.4358796	-1.2738483	-2.5103488
H	4.7715225	-0.4654002	-2.1422332
H	0.3374223	-1.6674598	5.2829087
N	1.6852120	0.1642907	-1.9335571
H	-3.6252243	-2.5297074	1.6807995
H	2.9409126	0.7155449	0.4283489
H	-3.2085886	-2.8985472	4.6196963
H	5.2351911	1.5810069	-0.0319642
H	3.9212448	0.7183636	1.9016900
H	-5.4133229	-2.4900506	-0.8118334
C	1.9944415	0.1330650	3.8494157
H	-1.7351576	-2.2436360	6.5235759
C	-4.7671683	-1.9954842	-0.0694070
Ga	-0.2332692	-0.2234258	1.3755388
C	3.4372771	1.3716046	1.1637764
Ga	-0.1567291	0.1711132	-1.0515268
C	-3.6767769	-1.2058997	-0.8065773
H	-1.1118723	-1.3098106	4.3215805
H	2.9054625	0.6378410	4.2001165
H	1.3484540	0.0026573	4.7262736
C	-2.3164313	-0.1071220	-3.6393132
H	-1.6904505	-0.0111304	-4.5344010
H	0.7927447	1.2043058	-4.2320437
H	-3.2587612	-0.5748360	-3.9579604
C	4.5077908	2.2302527	0.4763928
H	1.4436926	2.1425896	-6.4171985
H	-3.0979991	-0.6090723	-0.0805098
H	2.9720929	2.6962924	-4.5109340
C	0.2372342	2.0708687	-4.6246679
P	1.0865629	1.2692320	2.7106912
H	-4.1517807	-0.5063325	-1.5073973
H	-0.6460342	1.6764225	-5.1449473
H	3.4284341	2.7033807	-1.3421679
H	-5.4090245	-1.2992497	0.4865860
H	5.0770986	2.7717343	1.2475302
C	1.1189707	2.8303672	-5.6248668
C	3.8974872	3.2401903	-0.4983513
C	2.3776392	2.2545902	1.8415864
C	2.3207076	3.4814848	-4.9371811
C	-2.6014666	1.2796765	-3.0322281
H	4.6831373	3.8739016	-0.9301869
H	1.6059624	2.9471196	-2.2670863
P	-1.1635839	2.0659525	-2.1811845
H	2.9310793	4.0235500	-5.6704650
H	2.8737237	2.8299838	2.6417653
H	1.2040487	2.6728487	0.0756226
C	-0.1957848	2.9778296	-3.4587783
H	-0.5927732	0.9934027	5.2052714
H	-3.4024843	1.2185237	-2.2844158
C	1.7516544	3.2442431	0.8477199
H	0.5177149	3.6094449	-6.1189072
C	0.9918807	3.6934993	-2.7963778

H	-1.6489278	1.1316944	3.7912780
C	2.8354800	4.1043972	0.1867426
C	-1.0308542	1.7106268	4.4924025
C	0.0979901	2.4374423	3.7390876
H	-2.9532098	1.9643982	-3.8166168
C	1.8633517	4.4247365	-3.8230972
H	1.4780667	2.6139974	5.4044143
H	-1.8488474	1.8698610	0.6742406
H	2.7246623	4.8769399	-3.3125282
C	0.9629953	3.2809854	4.6941968
H	-0.8964565	3.7355994	-3.8504720
H	3.3148317	4.7298891	0.9555756
H	2.3785912	4.7990198	-0.5299646
H	1.0137855	3.8853699	1.3503542
C	-2.5225804	2.6040959	0.2055939
C	-1.8284526	3.2924457	-0.9809189
H	-0.3703929	3.1080235	2.9960646
H	0.6316230	4.4014018	-2.0376257
H	1.7409774	3.8285846	4.1441680
H	-3.4018193	2.0421680	-0.1488402
H	-0.9235736	3.7949762	-0.5967300
H	1.2909709	5.2569757	-4.2612986
C	-1.8929453	2.7164628	5.2676387
H	-0.6187435	2.9158267	7.0050230
H	-2.6752384	2.1767269	5.8178712
C	-1.0454320	3.5627529	6.2212146
C	0.0858252	4.2727979	5.4737454
C	-2.7392879	4.3495218	-1.6327892
C	-2.9732852	3.6414115	1.2414832
H	-2.4096472	3.3741011	4.5493403
H	-3.6239067	3.8540442	-2.0638711
H	-3.4877711	3.1335266	2.0687261
H	-2.2218465	4.8598181	-2.4568896
H	-2.0803321	4.1267743	1.6722109
H	0.7163979	4.8400054	6.1709559
H	-0.3391777	5.0059826	4.7685692
H	-1.6761389	4.2979387	6.7373663
C	-3.8763102	4.7052987	0.6098379
C	-3.1928771	5.3769200	-0.5844889
H	-4.8164659	4.2345916	0.2796722
H	-2.3157560	5.9476206	-0.2379369
H	-3.8680031	6.1016531	-1.0576454
H	-4.1544901	5.4583680	1.3583787
H	-1.7122031	-0.2441420	1.8963738

SCF energy GEOPT = -7389.282422237 H
 ZPE = 3737. kJ/mol
 FREEH energy = 3927.11 kJ/mol
 FREEH entropy = 1.65571 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	a	2.69	0.10980	YES	YES
8	a	10.91	0.11068	YES	YES
9	a	17.28	0.01268	YES	YES
10	a	20.79	0.14548	YES	YES
11	a	23.01	0.11202	YES	YES
12	a	24.02	0.01023	YES	YES
13	a	28.48	0.09094	YES	YES
14	a	30.91	0.59768	YES	YES
15	a	32.27	0.01015	YES	YES
16	a	38.10	0.56407	YES	YES
17	a	38.80	0.23526	YES	YES
18	a	41.69	0.35775	YES	YES
19	a	45.27	0.77405	YES	YES
20	a	46.47	0.19549	YES	YES
21	a	48.09	0.53787	YES	YES
22	a	50.18	0.71096	YES	YES
23	a	52.54	0.43739	YES	YES
24	a	54.38	0.55758	YES	YES
25	a	56.95	0.16974	YES	YES
26	a	60.11	0.22225	YES	YES
27	a	62.61	1.90390	YES	YES
28	a	66.33	0.36761	YES	YES
29	a	68.77	0.41876	YES	YES
30	a	69.60	0.22589	YES	YES
31	a	77.11	0.84634	YES	YES
32	a	77.47	0.64284	YES	YES
33	a	80.42	0.51804	YES	YES
34	a	85.21	0.11242	YES	YES
35	a	88.43	0.63852	YES	YES
36	a	91.41	0.32132	YES	YES
37	a	92.31	0.11825	YES	YES
38	a	97.50	0.10281	YES	YES
39	a	126.98	1.00825	YES	YES
40	a	129.85	0.80450	YES	YES
41	a	133.31	0.32762	YES	YES
42	a	140.90	0.51658	YES	YES
43	a	144.26	0.25997	YES	YES
44	a	146.04	1.94283	YES	YES
45	a	147.39	1.44931	YES	YES
46	a	150.08	0.60602	YES	YES
47	a	152.26	2.82430	YES	YES
48	a	155.77	1.87918	YES	YES
49	a	167.39	6.18944	YES	YES
50	a	172.83	0.08065	YES	YES
51	a	182.33	7.36120	YES	YES
52	a	184.31	3.95930	YES	YES
53	a	186.95	7.78444	YES	YES
54	a	188.77	2.01591	YES	YES
55	a	196.47	0.61719	YES	YES
56	a	198.11	0.10042	YES	YES
57	a	198.38	3.05677	YES	YES
58	a	207.23	4.73707	YES	YES
59	a	210.28	0.92336	YES	YES
60	a	212.45	0.04082	YES	YES
61	a	215.12	0.12514	YES	YES
62	a	223.34	1.84805	YES	YES
63	a	225.09	0.11688	YES	YES

64	a	225.96	1.91828	YES	YES
65	a	236.39	1.48879	YES	YES
66	a	236.88	0.04817	YES	YES
67	a	238.06	0.40940	YES	YES
68	a	240.18	0.71465	YES	YES
69	a	242.10	0.09455	YES	YES
70	a	242.84	0.81896	YES	YES
71	a	247.02	1.88941	YES	YES
72	a	270.67	2.09640	YES	YES
73	a	276.31	1.65678	YES	YES
74	a	278.75	1.06980	YES	YES
75	a	287.97	2.15973	YES	YES
76	a	295.51	0.19714	YES	YES
77	a	306.73	0.43757	YES	YES
78	a	307.61	0.14928	YES	YES
79	a	315.06	0.23598	YES	YES
80	a	315.81	0.37124	YES	YES
81	a	329.31	0.66066	YES	YES
82	a	331.16	0.50460	YES	YES
83	a	335.93	0.16035	YES	YES
84	a	336.31	0.33670	YES	YES
85	a	345.57	0.37325	YES	YES
86	a	347.06	0.46212	YES	YES
87	a	370.24	1.97341	YES	YES
88	a	375.06	3.19456	YES	YES
89	a	376.74	2.12502	YES	YES
90	a	379.33	1.18304	YES	YES
91	a	392.52	3.33800	YES	YES
92	a	394.50	0.26650	YES	YES
93	a	396.08	0.91113	YES	YES
94	a	397.64	8.77844	YES	YES
95	a	410.72	1.61465	YES	YES
96	a	413.06	1.09479	YES	YES
97	a	419.35	0.88215	YES	YES
98	a	420.19	4.95365	YES	YES
99	a	421.12	2.50939	YES	YES
100	a	424.60	1.49718	YES	YES
101	a	428.04	0.17195	YES	YES
102	a	428.67	0.34977	YES	YES
103	a	429.77	0.13099	YES	YES
104	a	430.79	0.11289	YES	YES
105	a	431.37	0.01450	YES	YES
106	a	431.79	0.34693	YES	YES
107	a	432.42	0.76770	YES	YES
108	a	433.89	0.91483	YES	YES
109	a	444.17	6.09477	YES	YES
110	a	446.80	1.16022	YES	YES
111	a	466.07	2.48567	YES	YES
112	a	466.91	4.72608	YES	YES
113	a	489.96	3.30614	YES	YES
114	a	491.44	0.08357	YES	YES
115	a	492.50	0.76949	YES	YES
116	a	493.92	4.74816	YES	YES
117	a	501.98	7.22879	YES	YES
118	a	505.73	0.88560	YES	YES
119	a	516.80	26.43094	YES	YES
120	a	520.65	9.57280	YES	YES
121	a	549.12	49.29588	YES	YES

122	a	563.33	120.26402	YES	YES
123	a	624.66	19.45455	YES	YES
124	a	628.69	10.66223	YES	YES
125	a	641.73	7.82588	YES	YES
126	a	645.04	8.00806	YES	YES
127	a	713.40	0.56187	YES	YES
128	a	714.81	0.25352	YES	YES
129	a	720.68	1.12976	YES	YES
130	a	721.15	1.14509	YES	YES
131	a	732.82	6.10507	YES	YES
132	a	735.23	6.65538	YES	YES
133	a	736.26	2.28959	YES	YES
134	a	736.91	7.39179	YES	YES
135	a	768.73	0.18200	YES	YES
136	a	770.13	0.51607	YES	YES
137	a	770.97	0.36476	YES	YES
138	a	772.22	0.82707	YES	YES
139	a	774.00	0.32698	YES	YES
140	a	774.09	0.28135	YES	YES
141	a	774.74	0.46106	YES	YES
142	a	774.99	0.11488	YES	YES
143	a	780.27	16.53449	YES	YES
144	a	783.97	8.98794	YES	YES
145	a	807.19	1.67729	YES	YES
146	a	808.55	0.53925	YES	YES
147	a	809.46	2.91225	YES	YES
148	a	810.23	0.91629	YES	YES
149	a	811.33	0.55224	YES	YES
150	a	813.39	2.07537	YES	YES
151	a	814.86	4.32840	YES	YES
152	a	815.47	9.53925	YES	YES
153	a	831.62	0.82155	YES	YES
154	a	833.02	1.02348	YES	YES
155	a	834.40	2.22362	YES	YES
156	a	835.50	1.33656	YES	YES
157	a	836.00	0.90176	YES	YES
158	a	836.24	6.00929	YES	YES
159	a	836.80	9.42485	YES	YES
160	a	838.83	8.93812	YES	YES
161	a	850.94	13.65923	YES	YES
162	a	852.96	3.08177	YES	YES
163	a	871.39	3.11961	YES	YES
164	a	873.22	3.21313	YES	YES
165	a	873.40	1.74934	YES	YES
166	a	874.41	3.97709	YES	YES
167	a	875.00	4.13656	YES	YES
168	a	876.14	4.76623	YES	YES
169	a	876.54	1.81927	YES	YES
170	a	877.86	1.46700	YES	YES
171	a	878.68	1.94501	YES	YES
172	a	879.00	2.76445	YES	YES
173	a	879.25	3.43352	YES	YES
174	a	881.40	1.52946	YES	YES
175	a	882.28	3.35719	YES	YES
176	a	883.25	1.99138	YES	YES
177	a	885.74	6.82372	YES	YES
178	a	887.47	0.55817	YES	YES
179	a	901.76	2.41806	YES	YES

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181	a	903.27	1.00119	YES	YES
182	a	904.21	2.45030	YES	YES
183	a	907.57	0.66674	YES	YES
184	a	908.04	4.34551	YES	YES
185	a	909.19	0.47269	YES	YES
186	a	910.46	1.27499	YES	YES
187	a	951.64	3.37034	YES	YES
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191	a	987.00	3.69872	YES	YES
192	a	987.21	26.84156	YES	YES
193	a	988.05	25.24001	YES	YES
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201	a	1012.96	0.87861	YES	YES
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203	a	1014.82	1.23601	YES	YES
204	a	1016.62	1.39184	YES	YES
205	a	1018.99	0.91762	YES	YES
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207	a	1020.98	1.32277	YES	YES
208	a	1030.10	3.92577	YES	YES
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210	a	1032.71	0.75251	YES	YES
211	a	1033.12	3.61027	YES	YES
212	a	1038.06	3.82851	YES	YES
213	a	1039.29	0.50716	YES	YES
214	a	1039.74	2.42329	YES	YES
215	a	1040.16	0.39987	YES	YES
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217	a	1058.10	1.10714	YES	YES
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220	a	1062.67	4.14489	YES	YES
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223	a	1068.40	0.92207	YES	YES
224	a	1069.32	0.28342	YES	YES
225	a	1069.65	0.38753	YES	YES
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232	a	1084.21	1.21120	YES	YES
233	a	1085.87	1.31492	YES	YES
234	a	1093.29	13.38399	YES	YES
235	a	1094.97	3.02032	YES	YES
236	a	1097.42	9.70465	YES	YES
237	a	1098.57	1.38705	YES	YES

238	a	1100.86	1.61118	YES	YES
239	a	1102.99	0.40429	YES	YES
240	a	1106.34	1.02704	YES	YES
241	a	1107.31	15.30181	YES	YES
242	a	1132.59	3.92706	YES	YES
243	a	1134.83	0.47359	YES	YES
244	a	1159.42	4.57156	YES	YES
245	a	1161.01	13.33008	YES	YES
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247	a	1161.91	2.27479	YES	YES
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249	a	1170.19	7.39722	YES	YES
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251	a	1172.22	9.55930	YES	YES
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257	a	1191.81	2.18098	YES	YES
258	a	1192.47	1.26583	YES	YES
259	a	1195.87	2.43710	YES	YES
260	a	1241.53	0.57079	YES	YES
261	a	1242.71	0.16898	YES	YES
262	a	1243.24	0.26521	YES	YES
263	a	1244.39	0.44107	YES	YES
264	a	1244.88	0.41437	YES	YES
265	a	1245.50	0.96055	YES	YES
266	a	1246.05	0.10643	YES	YES
267	a	1246.93	0.28574	YES	YES
268	a	1247.06	0.23500	YES	YES
269	a	1248.40	0.28396	YES	YES
270	a	1252.11	0.54172	YES	YES
271	a	1253.04	5.79266	YES	YES
272	a	1255.02	9.27971	YES	YES
273	a	1255.38	3.79953	YES	YES
274	a	1255.81	1.76846	YES	YES
275	a	1256.14	2.93954	YES	YES
276	a	1257.05	5.33330	YES	YES
277	a	1257.93	12.35897	YES	YES
278	a	1258.00	6.27695	YES	YES
279	a	1258.82	3.32009	YES	YES
280	a	1259.06	2.45572	YES	YES
281	a	1259.17	2.26119	YES	YES
282	a	1261.13	1.80692	YES	YES
283	a	1261.57	1.12764	YES	YES
284	a	1264.78	3.59799	YES	YES
285	a	1266.86	1.87253	YES	YES
286	a	1268.85	0.08387	YES	YES
287	a	1269.26	2.88430	YES	YES
288	a	1279.77	1.15507	YES	YES
289	a	1280.53	3.11175	YES	YES
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326	a	1340.92	0.32633	YES	YES
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328	a	1344.54	2.34873	YES	YES
329	a	1346.01	3.05589	YES	YES
330	a	1347.25	3.32458	YES	YES
331	a	1348.28	15.48195	YES	YES
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334	a	1350.86	0.09647	YES	YES
335	a	1351.16	2.05863	YES	YES
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337	a	1392.83	19.46811	YES	YES
338	a	1394.34	13.00949	YES	YES
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347	a	1428.31	5.68162	YES	YES
348	a	1429.49	1.20930	YES	YES
349	a	1430.05	4.64516	YES	YES
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351	a	1433.91	0.75411	YES	YES
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356	a	1437.06	4.65995	YES	YES
357	a	1437.28	8.76531	YES	YES
358	a	1437.67	5.57947	YES	YES
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360	a	1438.04	9.75867	YES	YES
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364	a	1440.16	10.04165	YES	YES
365	a	1440.60	5.62710	YES	YES
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367	a	1442.64	40.35143	YES	YES
368	a	1443.13	7.96470	YES	YES
369	a	1443.38	24.76266	YES	YES
370	a	1443.53	8.33493	YES	YES
371	a	1444.50	2.84819	YES	YES
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373	a	1445.97	16.65999	YES	YES
374	a	1446.66	21.84109	YES	YES
375	a	1452.03	0.58467	YES	YES
376	a	1452.61	6.06900	YES	YES
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378	a	1453.27	1.26798	YES	YES
379	a	1454.44	3.48251	YES	YES
380	a	1455.23	0.30224	YES	YES
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382	a	1456.49	0.81234	YES	YES
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384	a	2293.84	73.58213	YES	YES
385	a	2910.49	29.03188	YES	YES
386	a	2914.67	37.48746	YES	YES
387	a	2919.93	30.74067	YES	YES
388	a	2924.84	47.90194	YES	YES
389	a	2925.42	30.95678	YES	YES
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391	a	2929.23	1.68929	YES	YES
392	a	2933.13	16.02234	YES	YES
393	a	2933.28	20.05101	YES	YES
394	a	2938.20	11.48184	YES	YES
395	a	2938.47	18.78221	YES	YES
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397	a	2939.64	6.48630	YES	YES
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406	a	2948.05	6.69941	YES	YES
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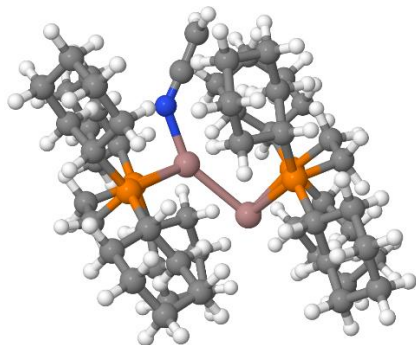
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418	a	2960.50	11.14519	YES	YES
419	a	2962.41	18.05911	YES	YES
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424	a	2966.27	22.82924	YES	YES
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426	a	2967.03	23.59368	YES	YES
427	a	2967.50	15.39093	YES	YES
428	a	2967.85	38.17229	YES	YES
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431	a	2971.31	30.89530	YES	YES
432	a	2972.57	13.01138	YES	YES
433	a	2974.32	45.87219	YES	YES
434	a	2975.09	49.27940	YES	YES
435	a	2984.92	39.77438	YES	YES
436	a	2985.34	42.79219	YES	YES
437	a	2987.20	4.13205	YES	YES
438	a	2989.66	3.60730	YES	YES
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444	a	3004.26	28.32797	YES	YES
445	a	3005.13	22.43274	YES	YES
446	a	3007.24	22.31279	YES	YES
447	a	3007.37	15.88113	YES	YES
448	a	3009.20	20.23619	YES	YES
449	a	3009.96	14.62171	YES	YES
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468	a	3024.09	14.91420	YES	YES
469	a	3024.28	7.71537	YES	YES

470	a	3024.93	19.87233	YES	YES
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472	a	3026.20	15.70653	YES	YES
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474	a	3026.58	16.69208	YES	YES
475	a	3027.07	17.28520	YES	YES
476	a	3027.59	11.30923	YES	YES
477	a	3027.91	10.98590	YES	YES
478	a	3032.00	0.70264	YES	YES
479	a	3035.86	1.17796	YES	YES
480	a	3047.52	0.48495	YES	YES
481	a	3051.13	0.71917	YES	YES
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\$end

Double hybrid single point energy = -7381.932133400864 H
 COSMO energy + OC correction = -7389.6084596274 H (in oDFB)

6.2.38 $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_2)]^+$



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

H	4.2060833	-5.6009288	1.1513931
H	4.0229966	-5.2802880	-1.3350992
C	3.3302005	-5.0978517	0.7177284
C	3.6787217	-4.4951751	-0.6473819
H	2.5543454	-5.8712280	0.5900715
H	4.5167153	-3.7881496	-0.5297092
H	1.0212229	-4.5941597	-6.4578179
H	0.0171062	-5.0985900	-4.2459427
C	2.4787530	-3.7511810	-1.2411187
C	2.8166828	-4.0245416	1.6883741
H	-1.2251518	-5.2013259	-5.4953108
H	1.6741110	-4.4750775	-1.4600001
H	2.5554634	-4.4810394	2.6539925
C	-0.5593071	-4.5007027	-4.9718433
H	2.7479486	-3.2803840	-2.1980317
C	0.4052848	-3.8340341	-5.9572631
H	3.6283338	-3.3058132	1.8830673
H	1.9549549	-3.3182314	-4.5347350
C	1.2923718	-2.8047629	-5.2511637
C	1.6112783	-3.2803614	1.0922945

H	-0.1745078	-3.3301677	-6.7488095
H	1.9467604	-2.2960482	-5.9727607
C	1.9506606	-2.6869712	-0.2768648
H	0.7929533	-4.0074087	0.9507003
H	-1.3145092	-5.4116737	4.3053668
C	-1.3986275	-3.4695948	-4.2029216
H	-0.8752328	-4.3880955	2.0849318
H	2.7030959	-1.8888370	-0.1691378
H	-2.0458137	-3.9901724	-3.4843269
H	0.1446742	-3.0015747	-2.7717674
H	-1.3703905	-3.8612982	-1.1327771
H	-2.7237467	-4.7584672	0.7670995
H	0.7922893	-3.8067442	3.8393114
C	-1.9439268	-4.5744199	3.9608638
H	-2.8296512	-5.0218986	3.4867545
C	-0.4878409	-2.4550800	-3.4936339
H	-3.6973837	-4.6266492	-0.6963773
C	0.4525112	-1.7667689	-4.4984364
C	-1.1729691	-3.7483030	2.9273245
H	1.0540206	-2.2056936	-0.6953286
C	-3.1727822	-4.0354189	0.0727090
H	4.4162783	-1.3018952	-2.3549180
H	-2.0618971	-2.9363639	-4.9041765
C	0.0529536	-3.0477872	3.5285952
C	-2.0735585	-3.2046493	-0.5991225
H	2.6933787	-1.8983997	3.8614048
P	0.8633717	-1.9981208	2.2203513
H	-0.4581913	-3.8256907	6.1995879
H	1.0945737	-1.0427163	-3.9829764
C	2.2940450	-1.2115016	3.1002544
H	-0.1485808	-1.2025614	-5.2302408
C	4.0783944	-0.3144696	-2.0508787
H	-1.4913724	-2.6695898	0.1703693
H	3.0744252	-1.0805467	2.3391081
C	-2.3504213	-3.7151262	5.1602904
H	-2.8791880	-4.3230136	5.9075630
H	-1.8382560	-2.9701195	2.5171242
H	-3.2317204	-2.7041550	-2.3509970
C	-1.1227676	-3.0487896	5.7861181
H	4.8190521	0.4472174	-1.8242989
C	-2.6843869	-2.1694001	-1.5552663
C	-4.1798185	-3.1414486	0.8025276
C	-0.3471949	-2.2161837	4.7578233
H	-4.9746276	-3.7516369	1.2536883
C	2.7807635	-0.0157545	-2.0617903
P	-1.3631516	-1.2149193	-2.4260333
H	0.5460896	-1.7903793	5.2349620
N	1.6046199	0.2581612	-2.1318763
H	-3.6717034	-2.6186493	1.6290310
H	2.9710963	0.7748466	0.3776873
H	-3.0573407	-2.9369720	4.8265779
H	5.2433165	1.7041616	0.0570097
H	3.8632611	0.7847182	1.9028764
H	-5.3827416	-2.6052745	-0.9153626
C	1.9353250	0.1433884	3.7281892
H	-1.4173524	-2.4077880	6.6293297
C	-4.7801630	-2.0981537	-0.1431601
Ga	-0.8252823	-0.2256753	1.5087606

C	3.3969788	1.4346489	1.1501430
Ga	0.0665655	0.1735444	-0.8772133
C	-3.6878117	-1.2635992	-0.8228167
H	-0.9726789	-1.3707136	4.4233933
H	2.8451483	0.6710961	4.0486497
H	1.3154645	0.0002411	4.6215577
C	-2.3101422	-0.0987333	-3.5642758
H	-1.7029712	0.0020378	-4.4712799
H	0.7732505	1.1897627	-4.1926217
H	-3.2512355	-0.5867539	-3.8567416
C	4.4745497	2.3310643	0.5297647
H	1.3783415	2.0925004	-6.4144914
H	-3.1526900	-0.6684187	-0.0628736
H	2.9360876	2.6327317	-4.5364521
C	0.2074711	2.0403491	-4.5989886
P	0.9638362	1.2278347	2.5775225
H	-4.1540079	-0.5611026	-1.5274672
H	-0.6858165	1.6428920	-5.1009884
H	3.4679843	2.7441549	-1.3334190
H	-5.4640381	-1.4332128	0.4031143
H	4.9794493	2.8965008	1.3307371
C	1.0716844	2.7887932	-5.6210815
C	3.8775448	3.3115141	-0.4819713
C	2.2838411	2.2747487	1.7878012
C	2.2964595	3.4253169	-4.9588440
C	-2.5912880	1.2878626	-2.9592439
H	4.6598511	3.9676150	-0.8885027
H	1.6195116	2.8873628	-2.3026894
P	-1.1202920	2.0312887	-2.1125224
H	2.9009581	3.9588989	-5.7052925
H	2.7315574	2.8560840	2.6117037
H	1.1849742	2.6652831	-0.0196438
C	-0.2070560	2.9551926	-3.4335281
H	-0.5866486	1.0130345	5.1868529
H	-3.3791360	1.2201531	-2.1976940
C	1.6803359	3.2525479	0.7736948
H	0.4706590	3.5755977	-6.1073770
C	1.0066431	3.6524129	-2.8016886
H	-1.6767962	1.1598435	3.8052433
C	2.7629777	4.1457334	0.1566570
C	-1.0357224	1.7383755	4.4875067
C	0.0811171	2.4343600	3.6922246
H	-2.9522206	1.9774801	-3.7355364
C	1.8653375	4.3780139	-3.8412663
H	1.5010347	2.5788401	5.3206251
H	-1.9610391	1.9301750	0.6838582
H	2.7422273	4.8183618	-3.3451363
C	0.9785610	3.2590385	4.6276887
H	-0.9051546	3.7193719	-3.8178024
H	3.1923839	4.7843191	0.9462370
H	2.3161032	4.8253876	-0.5817820
H	0.9004595	3.8697175	1.2453506
C	-2.5660925	2.7079917	0.1911133
C	-1.7988581	3.3316232	-0.9844084
H	-0.4069270	3.1249035	2.9796029
H	0.6756214	4.3592780	-2.0281109
H	1.7542096	3.7932398	4.0625750
H	-3.4698970	2.1986540	-0.1827876

H	-0.8897697	3.8011800	-0.5697115
H	1.2928636	5.2159123	-4.2728628
C	-1.8620237	2.7527878	5.2854085
H	-0.5382746	2.9284334	6.9852597
H	-2.6404460	2.2293804	5.8587459
C	-0.9759351	3.5864901	6.2157850
C	0.1510372	4.2693823	5.4357030
C	-2.6359807	4.4225901	-1.6698698
C	-2.9784325	3.7808723	1.2030482
H	-2.3853076	3.4210743	4.5810483
H	-3.5347576	3.9656452	-2.1156235
H	-3.5383046	3.3170394	2.0275210
H	-2.0749697	4.8900171	-2.4909154
H	-2.0686106	4.2196413	1.6483531
H	0.8097881	4.8271915	6.1164334
H	-0.2824998	5.0095422	4.7422017
H	-1.5771472	4.3352064	6.7506211
C	-3.8039789	4.8870595	0.5386027
C	-3.0593814	5.4947058	-0.6550561
H	-4.7615602	4.4633070	0.1926000
H	-2.1580740	6.0185076	-0.2949672
H	-3.6821405	6.2510914	-1.1529724
H	-4.0548825	5.6699235	1.2680027

SCF energy GEOOPT = -7388.658098428 H

ZPE = 3682. kJ/mol

FREEH energy = 3869.39 kJ/mol

FREEH entropy = 1.60240 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	8.36	0.01238	YES	YES
	8	a	19.00	0.03842	YES	YES
	9	a	21.11	0.01550	YES	YES
	10	a	24.33	0.10127	YES	YES
	11	a	27.97	0.03512	YES	YES
	12	a	30.10	0.04731	YES	YES
	13	a	33.07	0.04188	YES	YES
	14	a	34.60	0.01031	YES	YES
	15	a	37.59	0.02700	YES	YES
	16	a	41.20	0.02008	YES	YES
	17	a	46.03	0.13906	YES	YES
	18	a	47.63	0.02666	YES	YES
	19	a	49.19	0.23283	YES	YES
	20	a	51.77	0.00711	YES	YES
	21	a	53.27	0.15932	YES	YES
	22	a	55.57	0.07191	YES	YES
	23	a	58.31	0.21820	YES	YES
	24	a	62.30	0.30818	YES	YES
	25	a	65.75	0.09454	YES	YES
	26	a	66.60	0.35787	YES	YES

27	a	71.45	0.44835	YES	YES
28	a	74.66	0.11105	YES	YES
29	a	77.98	0.09238	YES	YES
30	a	81.38	0.29176	YES	YES
31	a	84.45	0.45010	YES	YES
32	a	87.27	0.14690	YES	YES
33	a	88.83	0.46635	YES	YES
34	a	93.36	0.06790	YES	YES
35	a	96.50	0.27750	YES	YES
36	a	101.77	0.14987	YES	YES
37	a	106.72	0.76448	YES	YES
38	a	120.35	1.90824	YES	YES
39	a	121.40	0.82824	YES	YES
40	a	127.46	4.48056	YES	YES
41	a	131.53	6.93188	YES	YES
42	a	136.71	0.67787	YES	YES
43	a	138.93	0.74282	YES	YES
44	a	142.08	4.89232	YES	YES
45	a	145.82	0.61032	YES	YES
46	a	148.88	0.53943	YES	YES
47	a	154.49	2.03495	YES	YES
48	a	156.55	0.89917	YES	YES
49	a	164.18	4.03260	YES	YES
50	a	171.23	0.23384	YES	YES
51	a	172.96	2.15207	YES	YES
52	a	176.13	10.76303	YES	YES
53	a	180.69	6.85801	YES	YES
54	a	193.71	1.71419	YES	YES
55	a	194.53	0.04865	YES	YES
56	a	194.89	0.64021	YES	YES
57	a	209.64	7.64374	YES	YES
58	a	211.66	0.18368	YES	YES
59	a	212.52	0.05689	YES	YES
60	a	216.36	0.16673	YES	YES
61	a	218.03	1.12153	YES	YES
62	a	225.19	0.48167	YES	YES
63	a	229.45	0.07234	YES	YES
64	a	231.71	0.01633	YES	YES
65	a	236.61	0.34023	YES	YES
66	a	238.00	0.14018	YES	YES
67	a	239.93	0.14477	YES	YES
68	a	241.84	0.22889	YES	YES
69	a	245.68	0.06159	YES	YES
70	a	250.36	1.01456	YES	YES
71	a	274.54	1.70342	YES	YES
72	a	279.37	4.69241	YES	YES
73	a	284.37	1.02950	YES	YES
74	a	285.47	1.03375	YES	YES
75	a	293.40	0.67302	YES	YES
76	a	299.99	0.79917	YES	YES
77	a	302.69	0.59879	YES	YES
78	a	315.34	0.54393	YES	YES
79	a	316.50	0.12198	YES	YES
80	a	329.57	0.82912	YES	YES
81	a	332.44	0.63706	YES	YES
82	a	334.43	0.44585	YES	YES
83	a	336.27	0.31422	YES	YES
84	a	339.17	2.12832	YES	YES

85	a	342.71	1.22910	YES	YES
86	a	353.02	49.68105	YES	YES
87	a	360.73	2.88552	YES	YES
88	a	368.01	1.93345	YES	YES
89	a	374.53	1.81363	YES	YES
90	a	376.48	1.03263	YES	YES
91	a	390.21	0.92831	YES	YES
92	a	390.42	0.13054	YES	YES
93	a	411.86	1.34120	YES	YES
94	a	414.79	1.02058	YES	YES
95	a	422.25	3.80011	YES	YES
96	a	423.12	5.86940	YES	YES
97	a	424.44	2.45413	YES	YES
98	a	428.96	1.14272	YES	YES
99	a	429.75	0.01456	YES	YES
100	a	430.75	0.05740	YES	YES
101	a	431.87	0.03494	YES	YES
102	a	432.91	2.96812	YES	YES
103	a	433.23	0.32998	YES	YES
104	a	433.55	1.10524	YES	YES
105	a	434.64	0.67169	YES	YES
106	a	434.74	0.79516	YES	YES
107	a	437.11	3.27061	YES	YES
108	a	441.76	7.93086	YES	YES
109	a	445.44	3.05305	YES	YES
110	a	465.99	3.05010	YES	YES
111	a	466.35	3.63454	YES	YES
112	a	490.56	9.18240	YES	YES
113	a	491.88	1.78813	YES	YES
114	a	492.68	3.07325	YES	YES
115	a	493.65	6.68367	YES	YES
116	a	500.34	0.38848	YES	YES
117	a	502.87	0.59134	YES	YES
118	a	511.12	12.14257	YES	YES
119	a	513.75	70.98069	YES	YES
120	a	515.02	8.71459	YES	YES
121	a	572.02	6.95182	YES	YES
122	a	622.63	17.29078	YES	YES
123	a	627.81	7.83157	YES	YES
124	a	641.54	15.99571	YES	YES
125	a	642.52	7.08046	YES	YES
126	a	704.01	0.54944	YES	YES
127	a	712.65	0.77736	YES	YES
128	a	714.51	5.12142	YES	YES
129	a	722.67	2.65273	YES	YES
130	a	727.97	7.06944	YES	YES
131	a	731.40	3.87697	YES	YES
132	a	731.56	11.70064	YES	YES
133	a	734.71	9.81970	YES	YES
134	a	772.18	0.46728	YES	YES
135	a	774.13	0.17985	YES	YES
136	a	774.27	0.61226	YES	YES
137	a	774.94	0.40276	YES	YES
138	a	776.26	1.64375	YES	YES
139	a	776.67	0.14034	YES	YES
140	a	777.17	0.31517	YES	YES
141	a	777.27	0.42708	YES	YES
142	a	780.26	35.73009	YES	YES

143	a	780.98	0.37201	YES	YES
144	a	809.85	0.11112	YES	YES
145	a	811.51	1.78503	YES	YES
146	a	811.70	0.85294	YES	YES
147	a	812.63	0.82061	YES	YES
148	a	814.26	1.19354	YES	YES
149	a	814.88	0.42464	YES	YES
150	a	815.21	5.70451	YES	YES
151	a	816.70	4.88090	YES	YES
152	a	833.40	1.28291	YES	YES
153	a	833.89	3.43393	YES	YES
154	a	836.50	4.36143	YES	YES
155	a	837.19	1.50411	YES	YES
156	a	837.94	2.84639	YES	YES
157	a	838.50	5.35820	YES	YES
158	a	839.89	13.58608	YES	YES
159	a	840.31	10.82938	YES	YES
160	a	851.51	28.70672	YES	YES
161	a	853.08	0.20090	YES	YES
162	a	876.66	2.79129	YES	YES
163	a	876.85	4.11505	YES	YES
164	a	877.49	2.20812	YES	YES
165	a	877.71	3.01792	YES	YES
166	a	878.92	3.68171	YES	YES
167	a	879.43	2.78543	YES	YES
168	a	879.91	3.08613	YES	YES
169	a	880.38	2.46198	YES	YES
170	a	881.15	1.03925	YES	YES
171	a	881.54	8.96426	YES	YES
172	a	882.11	2.93745	YES	YES
173	a	882.76	2.11941	YES	YES
174	a	883.55	1.68606	YES	YES
175	a	885.25	1.62257	YES	YES
176	a	887.17	2.25474	YES	YES
177	a	889.60	1.11989	YES	YES
178	a	902.54	2.89789	YES	YES
179	a	903.36	0.97476	YES	YES
180	a	903.87	3.85706	YES	YES
181	a	904.40	1.08880	YES	YES
182	a	908.70	1.07625	YES	YES
183	a	909.60	1.73332	YES	YES
184	a	910.98	0.87330	YES	YES
185	a	912.65	1.57215	YES	YES
186	a	960.07	0.17067	YES	YES
187	a	981.97	0.15206	YES	YES
188	a	985.81	0.55182	YES	YES
189	a	989.67	4.98939	YES	YES
190	a	989.97	13.93376	YES	YES
191	a	990.22	10.68666	YES	YES
192	a	990.63	5.04033	YES	YES
193	a	991.52	3.96756	YES	YES
194	a	992.42	17.53034	YES	YES
195	a	993.69	7.63572	YES	YES
196	a	994.84	2.72562	YES	YES
197	a	1016.02	1.58893	YES	YES
198	a	1017.46	0.60827	YES	YES
199	a	1017.83	1.53613	YES	YES
200	a	1019.20	0.80389	YES	YES

201	a	1020.19	0.29597	YES	YES
202	a	1021.95	0.65387	YES	YES
203	a	1024.17	0.39784	YES	YES
204	a	1025.04	0.01570	YES	YES
205	a	1031.45	1.92852	YES	YES
206	a	1032.64	0.61037	YES	YES
207	a	1033.48	0.65147	YES	YES
208	a	1034.01	2.21483	YES	YES
209	a	1039.34	2.69002	YES	YES
210	a	1039.68	1.23939	YES	YES
211	a	1040.39	0.26867	YES	YES
212	a	1041.74	1.10701	YES	YES
213	a	1058.01	3.33407	YES	YES
214	a	1058.55	1.08899	YES	YES
215	a	1058.81	1.04893	YES	YES
216	a	1059.32	1.07407	YES	YES
217	a	1063.46	3.25100	YES	YES
218	a	1066.15	0.68848	YES	YES
219	a	1067.78	0.11300	YES	YES
220	a	1070.61	0.00755	YES	YES
221	a	1071.29	0.09451	YES	YES
222	a	1072.69	0.22468	YES	YES
223	a	1072.95	0.04536	YES	YES
224	a	1074.15	0.60789	YES	YES
225	a	1074.59	0.37788	YES	YES
226	a	1075.94	0.61511	YES	YES
227	a	1076.78	0.56102	YES	YES
228	a	1077.92	0.29003	YES	YES
229	a	1079.90	1.09534	YES	YES
230	a	1081.54	1.96213	YES	YES
231	a	1088.61	3.67067	YES	YES
232	a	1091.87	16.37181	YES	YES
233	a	1094.23	4.50247	YES	YES
234	a	1098.77	3.00091	YES	YES
235	a	1101.23	1.54035	YES	YES
236	a	1102.36	0.57925	YES	YES
237	a	1105.29	2.03966	YES	YES
238	a	1107.01	10.39354	YES	YES
239	a	1120.78	10.76792	YES	YES
240	a	1124.04	2.56564	YES	YES
241	a	1159.32	3.44152	YES	YES
242	a	1159.47	4.61985	YES	YES
243	a	1159.89	15.41339	YES	YES
244	a	1160.55	3.60660	YES	YES
245	a	1161.27	4.64051	YES	YES
246	a	1167.56	7.40924	YES	YES
247	a	1168.27	4.00385	YES	YES
248	a	1170.32	12.27034	YES	YES
249	a	1171.00	3.04172	YES	YES
250	a	1174.51	10.30460	YES	YES
251	a	1176.92	11.19188	YES	YES
252	a	1180.01	12.84548	YES	YES
253	a	1183.60	7.20032	YES	YES
254	a	1190.60	1.88566	YES	YES
255	a	1193.31	2.98764	YES	YES
256	a	1193.45	0.68197	YES	YES
257	a	1197.08	2.33382	YES	YES
258	a	1232.77	0.83812	YES	YES

259	a	1235.13	0.41073	YES	YES
260	a	1244.01	1.30001	YES	YES
261	a	1244.34	0.18825	YES	YES
262	a	1245.39	0.38450	YES	YES
263	a	1246.75	0.88597	YES	YES
264	a	1247.81	0.17648	YES	YES
265	a	1248.17	0.17837	YES	YES
266	a	1249.35	1.96108	YES	YES
267	a	1251.31	0.21794	YES	YES
268	a	1252.98	7.56795	YES	YES
269	a	1253.47	0.37801	YES	YES
270	a	1255.13	6.51139	YES	YES
271	a	1256.24	2.34094	YES	YES
272	a	1256.40	2.65545	YES	YES
273	a	1256.78	1.70170	YES	YES
274	a	1257.83	1.01738	YES	YES
275	a	1258.21	1.64767	YES	YES
276	a	1259.18	1.67558	YES	YES
277	a	1259.35	0.96178	YES	YES
278	a	1260.28	5.34496	YES	YES
279	a	1261.19	1.94981	YES	YES
280	a	1261.65	1.58937	YES	YES
281	a	1262.82	0.46980	YES	YES
282	a	1265.75	3.40902	YES	YES
283	a	1268.40	0.30481	YES	YES
284	a	1269.33	1.83063	YES	YES
285	a	1272.29	2.08553	YES	YES
286	a	1280.33	1.84192	YES	YES
287	a	1282.54	0.55252	YES	YES
288	a	1284.96	2.35444	YES	YES
289	a	1285.89	0.55464	YES	YES
290	a	1289.84	1.19984	YES	YES
291	a	1291.17	3.59592	YES	YES
292	a	1292.13	2.13917	YES	YES
293	a	1293.55	2.38058	YES	YES
294	a	1309.03	1.67912	YES	YES
295	a	1309.40	1.83804	YES	YES
296	a	1312.83	1.58024	YES	YES
297	a	1313.18	0.57929	YES	YES
298	a	1314.71	0.77900	YES	YES
299	a	1317.88	0.84639	YES	YES
300	a	1319.33	3.00659	YES	YES
301	a	1320.31	2.49449	YES	YES
302	a	1321.27	0.41242	YES	YES
303	a	1321.50	0.09460	YES	YES
304	a	1322.15	0.58538	YES	YES
305	a	1322.48	0.07224	YES	YES
306	a	1322.65	1.03679	YES	YES
307	a	1323.25	1.70501	YES	YES
308	a	1323.78	0.61461	YES	YES
309	a	1324.25	0.25662	YES	YES
310	a	1325.43	1.11881	YES	YES
311	a	1326.42	1.79149	YES	YES
312	a	1327.38	3.83447	YES	YES
313	a	1327.52	8.55380	YES	YES
314	a	1328.18	5.57987	YES	YES
315	a	1329.26	1.02985	YES	YES
316	a	1330.31	0.55438	YES	YES

317	a	1332.68	0.06767	YES	YES
318	a	1333.07	0.16055	YES	YES
319	a	1334.25	0.59946	YES	YES
320	a	1334.62	0.79896	YES	YES
321	a	1335.78	0.03913	YES	YES
322	a	1336.51	0.29498	YES	YES
323	a	1337.53	1.82755	YES	YES
324	a	1339.09	0.80082	YES	YES
325	a	1340.24	1.38907	YES	YES
326	a	1341.05	1.54172	YES	YES
327	a	1345.57	2.35582	YES	YES
328	a	1346.62	0.33136	YES	YES
329	a	1346.71	0.05409	YES	YES
330	a	1347.02	2.21338	YES	YES
331	a	1348.91	0.87945	YES	YES
332	a	1349.23	1.20449	YES	YES
333	a	1349.58	0.10978	YES	YES
334	a	1381.53	11.58657	YES	YES
335	a	1400.73	8.18573	YES	YES
336	a	1401.48	4.46362	YES	YES
337	a	1407.51	8.33116	YES	YES
338	a	1407.85	3.92834	YES	YES
339	a	1424.39	2.53724	YES	YES
340	a	1426.36	6.61957	YES	YES
341	a	1428.55	3.38746	YES	YES
342	a	1429.70	7.51180	YES	YES
343	a	1429.87	0.65096	YES	YES
344	a	1431.57	2.96681	YES	YES
345	a	1433.02	1.17213	YES	YES
346	a	1433.32	0.55123	YES	YES
347	a	1434.78	4.99678	YES	YES
348	a	1435.08	0.57740	YES	YES
349	a	1435.51	0.64270	YES	YES
350	a	1435.79	5.35100	YES	YES
351	a	1436.02	4.80703	YES	YES
352	a	1436.61	7.22181	YES	YES
353	a	1436.80	1.99155	YES	YES
354	a	1437.40	2.10805	YES	YES
355	a	1437.68	3.57367	YES	YES
356	a	1437.80	5.32060	YES	YES
357	a	1438.41	3.23729	YES	YES
358	a	1438.83	4.03039	YES	YES
359	a	1439.31	3.22146	YES	YES
360	a	1439.41	18.67496	YES	YES
361	a	1439.82	2.53694	YES	YES
362	a	1441.67	10.62463	YES	YES
363	a	1442.12	11.78374	YES	YES
364	a	1442.50	10.89927	YES	YES
365	a	1442.83	30.39603	YES	YES
366	a	1444.20	1.92727	YES	YES
367	a	1444.68	12.77868	YES	YES
368	a	1445.99	4.11053	YES	YES
369	a	1446.48	20.31315	YES	YES
370	a	1447.58	12.26820	YES	YES
371	a	1452.72	3.23056	YES	YES
372	a	1453.31	0.06922	YES	YES
373	a	1453.56	1.51732	YES	YES
374	a	1454.32	4.54150	YES	YES

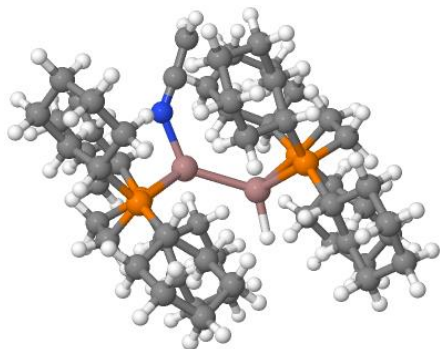
375	a	1455.17	1.18986	YES	YES
376	a	1456.17	1.28453	YES	YES
377	a	1456.71	0.75146	YES	YES
378	a	1460.50	0.47860	YES	YES
379	a	2071.47	607.14620	YES	YES
380	a	2916.01	1.34859	YES	YES
381	a	2919.60	6.58325	YES	YES
382	a	2920.22	13.32571	YES	YES
383	a	2926.75	20.16079	YES	YES
384	a	2926.95	5.97164	YES	YES
385	a	2927.02	1.45124	YES	YES
386	a	2928.96	11.26390	YES	YES
387	a	2931.02	14.91110	YES	YES
388	a	2931.12	16.10228	YES	YES
389	a	2933.48	3.37728	YES	YES
390	a	2934.71	19.34369	YES	YES
391	a	2935.65	5.73534	YES	YES
392	a	2936.65	8.26467	YES	YES
393	a	2938.12	6.56213	YES	YES
394	a	2938.42	18.80177	YES	YES
395	a	2939.18	11.50739	YES	YES
396	a	2939.36	4.99288	YES	YES
397	a	2939.87	13.65561	YES	YES
398	a	2940.19	13.90757	YES	YES
399	a	2940.49	27.38354	YES	YES
400	a	2941.27	11.31462	YES	YES
401	a	2941.74	41.21185	YES	YES
402	a	2941.94	9.98226	YES	YES
403	a	2943.31	18.40214	YES	YES
404	a	2943.54	0.06405	YES	YES
405	a	2943.62	16.55639	YES	YES
406	a	2943.99	12.47996	YES	YES
407	a	2944.33	26.11666	YES	YES
408	a	2945.13	16.17696	YES	YES
409	a	2947.03	12.08899	YES	YES
410	a	2947.99	6.46032	YES	YES
411	a	2948.06	10.74664	YES	YES
412	a	2949.41	7.62176	YES	YES
413	a	2950.34	6.03208	YES	YES
414	a	2950.88	16.16445	YES	YES
415	a	2951.43	3.15391	YES	YES
416	a	2951.84	14.32265	YES	YES
417	a	2952.60	61.03961	YES	YES
418	a	2952.92	33.50585	YES	YES
419	a	2954.00	25.87531	YES	YES
420	a	2954.67	17.22058	YES	YES
421	a	2956.77	19.18730	YES	YES
422	a	2957.38	16.68750	YES	YES
423	a	2957.86	13.14760	YES	YES
424	a	2957.93	78.36515	YES	YES
425	a	2962.72	15.36136	YES	YES
426	a	2966.94	20.56729	YES	YES
427	a	2967.74	18.76208	YES	YES
428	a	2968.51	16.77617	YES	YES
429	a	2970.85	32.89411	YES	YES
430	a	2977.03	9.23395	YES	YES
431	a	2979.82	8.64386	YES	YES
432	a	2981.06	31.81130	YES	YES

433	a	2981.72	16.82592	YES	YES
434	a	2982.58	28.23065	YES	YES
435	a	2982.97	45.69970	YES	YES
436	a	2990.08	28.67169	YES	YES
437	a	2992.50	16.88197	YES	YES
438	a	2995.59	35.79485	YES	YES
439	a	2998.04	36.79890	YES	YES
440	a	2999.55	29.08118	YES	YES
441	a	2999.88	20.12157	YES	YES
442	a	3000.24	11.78404	YES	YES
443	a	3000.42	32.84976	YES	YES
444	a	3000.75	13.51836	YES	YES
445	a	3001.12	32.71348	YES	YES
446	a	3001.21	31.82124	YES	YES
447	a	3001.43	68.81630	YES	YES
448	a	3001.93	54.06008	YES	YES
449	a	3002.55	39.83597	YES	YES
450	a	3003.21	49.24012	YES	YES
451	a	3003.37	18.11529	YES	YES
452	a	3003.95	11.83994	YES	YES
453	a	3004.23	80.80571	YES	YES
454	a	3004.42	11.45543	YES	YES
455	a	3004.55	11.95875	YES	YES
456	a	3004.69	54.68585	YES	YES
457	a	3005.26	52.83435	YES	YES
458	a	3006.62	39.24522	YES	YES
459	a	3006.84	8.18055	YES	YES
460	a	3007.14	30.71010	YES	YES
461	a	3007.22	26.21482	YES	YES
462	a	3007.54	46.73533	YES	YES
463	a	3007.62	67.23811	YES	YES
464	a	3007.76	41.44485	YES	YES
465	a	3007.95	18.85769	YES	YES
466	a	3009.19	39.24496	YES	YES
467	a	3009.75	31.14506	YES	YES
468	a	3012.36	34.58718	YES	YES
469	a	3015.30	19.37585	YES	YES
470	a	3020.17	10.39010	YES	YES
471	a	3022.77	4.15877	YES	YES
472	a	3027.48	1.27586	YES	YES
473	a	3033.57	3.04408	YES	YES
474	a	3041.89	1.99891	YES	YES
475	a	3048.10	0.73069	YES	YES
476	a	3103.00	5.09220	YES	YES
477	a	3187.44	0.04737	YES	YES

\$end

Double hybrid single point energy = -7381.294959206796 H
 COSMO energy + OC correction = -7388.7022664540 H (in oDFB)

6.2.39 [H{Ga(dcpe)}₂(NCCH₂)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

H	4.2808739	-5.5815338	1.1275304
H	4.0255017	-5.2702199	-1.3525707
C	3.3871276	-5.0937917	0.7160191
C	3.6896304	-4.4885499	-0.6583477
H	2.6200074	-5.8787684	0.6141868
H	4.5217501	-3.7712153	-0.5657639
H	0.9324843	-4.6628959	-6.4982749
H	-0.0866674	-5.1460991	-4.2890946
C	2.4626207	-3.7670745	-1.2238067
C	2.8905605	-4.0250999	1.6999639
H	-1.3290385	-5.2166275	-5.5390809
H	1.6644827	-4.5039059	-1.4190590
H	2.6610180	-4.4813158	2.6737225
C	-0.6461978	-4.5336716	-5.0158288
H	2.6977445	-3.2950717	-2.1888206
C	0.3333964	-3.8888744	-6.0003778
H	3.6976822	-3.2948127	1.8675227
H	1.8953986	-3.4077400	-4.5778907
C	1.2448231	-2.8805891	-5.2954722
C	1.6568125	-3.3019192	1.1309864
H	-0.2323918	-3.3742870	-6.7944415
H	1.9102648	-2.3876027	-6.0170619
C	1.9396208	-2.7060197	-0.2521244
H	0.8414114	-4.0381977	1.0265083
H	-1.4143390	-5.3187375	4.2970336
C	-1.4649815	-3.4837362	-4.2496173
H	-0.9145987	-4.2927477	2.0935572
H	2.6788694	-1.8925275	-0.1695486
H	-2.1242180	-3.9871244	-3.5294891
H	0.0879860	-3.0450000	-2.8128607
H	-1.4252077	-3.8578895	-1.1491058
H	-2.7604270	-4.6998883	0.7880314
H	0.7447151	-3.8014026	3.8857672
C	-2.0088371	-4.4550342	3.9584475
H	-2.9047428	-4.8638883	3.4706601
C	-0.5273197	-2.4895912	-3.5431404
H	-3.7562140	-4.5539134	-0.6549581
C	0.4298532	-1.8194185	-4.5458556
C	-1.1992586	-3.6491814	2.9373576
H	1.0183905	-2.2540261	-0.6500673
C	-3.2039313	-3.9694224	0.0984081

H	4.4685316	-1.3183699	-2.1657596
H	-2.1138423	-2.9364570	-4.9529429
C	0.0449221	-3.0072406	3.5699659
C	-2.0956567	-3.1764458	-0.6055113
H	2.8045863	-1.8777823	3.8623810
P	0.9518924	-2.0397490	2.2827303
H	-0.5175986	-3.7770239	6.2219574
H	1.0901088	-1.1094700	-4.0322082
C	2.3694351	-1.1981924	3.1166065
H	-0.1575387	-1.2438384	-5.2793939
C	4.1038600	-0.3297823	-1.8970940
H	-1.4788286	-2.6523891	0.1451268
H	3.1296641	-1.0466561	2.3382286
C	-2.3942818	-3.5923403	5.1620827
H	-2.9478778	-4.1895867	5.8984106
H	-1.8307683	-2.8441829	2.5288139
H	-3.2908570	-2.6670316	-2.3273506
C	-1.1509380	-2.9761859	5.8073584
H	4.8260638	0.4439491	-1.6511649
C	-2.7054690	-2.1356970	-1.5570053
C	-4.1752899	-3.0455499	0.8393094
C	-0.3328345	-2.1613977	4.7964637
H	-4.9811753	-3.6330881	1.2988940
C	2.8145714	-0.0409266	-2.0034095
P	-1.4010638	-1.2405439	-2.4994409
H	0.5712288	-1.7769995	5.2883485
N	1.6447601	0.2294497	-2.1746737
H	-3.6464425	-2.5392127	1.6632394
H	3.0491627	0.8168773	0.4394127
H	-3.0743111	-2.7885312	4.8332616
H	5.2900726	1.8217706	0.1180168
H	3.9344388	0.8782901	1.9711158
H	-5.3949778	-2.4737513	-0.8545007
C	1.9980276	0.1440617	3.7720741
H	-1.4299360	-2.3309651	6.6516105
C	-4.7605203	-1.9860796	-0.0968910
Ga	-0.2553249	-0.2067347	1.2690768
C	3.4490231	1.5000278	1.2066528
Ga	0.0257186	0.1844336	-1.1368210
C	-3.6586396	-1.1895878	-0.8079335
H	-0.9243029	-1.2926622	4.4636777
H	2.9063765	0.6611700	4.1114372
H	1.3726623	-0.0183165	4.6580177
C	-2.3116077	-0.0897311	-3.6224151
H	-1.6970815	0.0039654	-4.5255238
H	0.7560734	1.1902861	-4.2990440
H	-3.2581567	-0.5599775	-3.9241712
C	4.4963950	2.4264994	0.5769272
H	1.3405369	2.1180309	-6.5135456
H	-3.0879399	-0.6024575	-0.0692548
H	2.9456264	2.6012965	-4.6607672
C	0.1989381	2.0585227	-4.6811250
P	1.0460185	1.2712768	2.6597773
H	-4.1224035	-0.4803840	-1.5064294
H	-0.7104714	1.6879026	-5.1747065
H	3.4852999	2.7847094	-1.2983493
H	-5.4114274	-1.2974874	0.4590257
H	4.9782377	3.0165504	1.3731940

C	1.0616638	2.8076410	-5.7051059
C	3.8698212	3.3730404	-0.4490769
C	2.3083557	2.3209607	1.8258346
C	2.3086481	3.4108885	-5.0539484
C	-2.5808765	1.2999539	-3.0166718
H	4.6317950	4.0504729	-0.8566521
H	1.6670664	2.8407339	-2.3902840
P	-1.1141069	2.0646267	-2.1924078
H	2.9056651	3.9483900	-5.8023759
H	2.7353527	2.9389121	2.6344809
H	1.2037686	2.6393234	-0.0015052
C	-0.1753729	2.9696349	-3.4978530
H	-0.6348710	0.9153824	5.1529854
H	-3.3669228	1.2435319	-2.2524729
C	1.6659805	3.2550727	0.7901175
H	0.4659099	3.6105826	-6.1691692
C	1.0624364	3.6268044	-2.8676122
H	-1.6831468	1.0756793	3.7370063
C	2.7245623	4.1772197	0.1729274
C	-1.0784262	1.6455304	4.4563059
C	0.0476060	2.3997280	3.7287167
H	-2.9428146	1.9848092	-3.7960898
C	1.9175367	4.3516249	-3.9120670
H	1.4091796	2.5371883	5.4109185
H	-1.6204342	2.0062996	0.7013631
H	2.8110905	4.7655060	-3.4240673
C	0.8953872	3.2214112	4.7160455
H	-0.8593705	3.7573227	-3.8599807
H	3.1240028	4.8380551	0.9589337
H	2.2602343	4.8339380	-0.5741637
H	0.8599265	3.8489763	1.2463591
C	-2.3594411	2.6782968	0.2397764
C	-1.7677360	3.3288589	-1.0198350
H	-0.4222234	3.0907965	3.0060538
H	0.7571957	4.3299489	-2.0804684
H	1.6749054	3.7892182	4.1901475
H	-3.2222771	2.0482395	-0.0323662
H	-0.8660718	3.8879408	-0.7156724
H	1.3549090	5.2087748	-4.3161032
C	-1.9566464	2.6188357	5.2528197
H	-0.6972895	2.7811673	7.0037000
H	-2.7386108	2.0575764	5.7823782
C	-1.1249526	3.4470709	6.2360051
C	0.0069342	4.1851383	5.5164451
C	-2.7583436	4.3155715	-1.6619379
C	-2.8066797	3.7430393	1.2470556
H	-2.4739000	3.2924335	4.5497289
H	-3.6449614	3.7651030	-2.0154131
H	-3.2538987	3.2556772	2.1248738
H	-2.3109199	4.8007626	-2.5403831
H	-1.9174624	4.2901044	1.6059049
H	0.6264839	4.7395299	6.2341847
H	-0.4201800	4.9327828	4.8278209
H	-1.7656548	4.1627391	6.7680742
C	-3.7887001	4.7357021	0.6172708
C	-3.1973874	5.3759871	-0.6422661
H	-4.7209256	4.2079236	0.3569574
H	-2.3265260	5.9939736	-0.3682474

H	-3.9257426	6.0528731	-1.1083457
H	-4.0635765	5.5113107	1.3444603
H	-1.7060317	-0.2532995	1.8807152

SCF energy GEOOPT = -7389.022242704 H

ZPE = 3707. kJ/mol

FREEH energy = 3894.43 kJ/mol

FREEH entropy = 1.60092 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			-0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.23	0.00549	YES	YES
8		a	16.73	0.03494	YES	YES
9		a	17.88	0.07428	YES	YES
10		a	21.85	0.01761	YES	YES
11		a	25.42	0.05421	YES	YES
12		a	26.91	0.08986	YES	YES
13		a	32.98	0.02932	YES	YES
14		a	33.59	0.05959	YES	YES
15		a	37.61	0.01558	YES	YES
16		a	41.79	0.04525	YES	YES
17		a	43.54	0.00885	YES	YES
18		a	47.29	0.02278	YES	YES
19		a	48.13	0.38920	YES	YES
20		a	49.19	0.00324	YES	YES
21		a	52.65	0.10861	YES	YES
22		a	53.09	0.00872	YES	YES
23		a	57.26	0.22952	YES	YES
24		a	59.32	0.01888	YES	YES
25		a	62.58	0.38008	YES	YES
26		a	65.81	0.19576	YES	YES
27		a	73.03	0.20475	YES	YES
28		a	74.80	0.43853	YES	YES
29		a	78.65	0.14656	YES	YES
30		a	81.49	0.22634	YES	YES
31		a	87.31	0.66956	YES	YES
32		a	88.65	0.13545	YES	YES
33		a	91.68	0.29426	YES	YES
34		a	94.17	0.53041	YES	YES
35		a	95.81	0.13429	YES	YES
36		a	101.75	0.19909	YES	YES
37		a	109.38	0.41685	YES	YES
38		a	126.00	1.55360	YES	YES
39		a	127.58	8.90352	YES	YES
40		a	131.65	1.63863	YES	YES
41		a	136.24	0.16664	YES	YES
42		a	141.77	0.87605	YES	YES
43		a	143.73	0.18714	YES	YES
44		a	146.83	2.53194	YES	YES
45		a	148.83	0.46852	YES	YES
46		a	151.17	1.70521	YES	YES

47	a	156.97	0.06847	YES	YES
48	a	159.67	2.46826	YES	YES
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51	a	182.13	10.84525	YES	YES
52	a	185.09	4.42864	YES	YES
53	a	187.43	1.24288	YES	YES
54	a	193.08	0.69328	YES	YES
55	a	196.94	0.57825	YES	YES
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59	a	214.69	1.19107	YES	YES
60	a	216.33	0.81127	YES	YES
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63	a	229.56	0.03693	YES	YES
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65	a	238.32	0.39008	YES	YES
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67	a	242.50	0.59175	YES	YES
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71	a	277.76	1.09913	YES	YES
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133	a	736.42	4.25239	YES	YES
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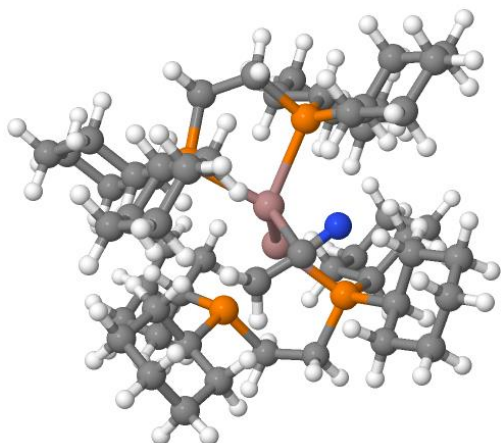
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477	a	3048.55	0.42539	YES	YES
478	a	3050.04	0.12071	YES	YES
479	a	3102.08	12.81029	YES	YES
480	a	3186.53	1.44490	YES	YES

\$end

Double hybrid single point energy = -7381.665875854929 H
COSMO energy + OC correction = -7389.1715293695 H (in oDFB)

6.2.40 $[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_2)]^{2+}/[\text{H}\{\text{Ga}(\text{dcpe})\}_2(\text{CH}_2\text{CN})]^{2+}$ Transition State



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

H	5.2915549	-3.2460622	-0.3110634
H	4.1049615	-5.0150475	-1.6584701

C	4.3567741	-3.7005312	0.0448585
C	3.5370039	-4.2368656	-1.1311961
H	4.6473914	-4.5341409	0.7050132
H	3.3545590	-3.4270148	-1.8531589
H	-0.0817156	-5.0506955	-6.6053857
H	-0.7993063	-5.3257524	-4.2502537
C	2.1908036	-4.7913963	-0.6588945
C	3.5787244	-2.6689213	0.8755135
H	-2.2156901	-5.3631507	-5.3014215
H	2.3501477	-5.6945768	-0.0469032
H	4.2004257	-2.3526121	1.7235338
C	-1.4146153	-4.7108395	-4.9278053
H	1.5812918	-5.1014181	-1.5196079
C	-0.5481909	-4.2039603	-6.0842989
H	3.3767403	-1.7736634	0.2632800
H	1.2400822	-3.7498889	-4.9387313
C	0.5229678	-3.2266629	-5.5915355
C	2.2432534	-3.2597886	1.3605481
H	-1.1891065	-3.6976578	-6.8249689
H	1.0998419	-2.8280000	-6.4373352
C	1.4126843	-3.7542509	0.1590838
H	2.4573428	-4.1110082	2.0317216
H	-0.7034318	-5.5622400	4.5638908
C	-2.0308293	-3.5574564	-4.1209365
H	0.1639957	-4.8943752	2.3577318
H	1.1848506	-2.8919057	-0.4841801
H	-2.6105658	-3.9684023	-3.2835784
H	-0.2277670	-3.1719816	-2.9758623
H	-1.7561201	-3.8340961	-1.1459169
H	-2.8813685	-4.4506425	0.9926734
H	0.9964186	-3.5387241	4.2444037
C	-1.3735528	-5.0300139	3.8696396
H	-1.9292753	-5.8035929	3.3216886
C	-0.9232054	-2.6126564	-3.6234415
H	-4.0733140	-4.1760861	-0.2717895
C	-0.1038409	-2.0677372	-4.8069844
C	-0.5296136	-4.2213329	2.8763318
H	0.4545997	-4.1733439	0.4853959
C	-3.3226262	-3.6706472	0.3568117
H	3.3525038	0.7434511	-0.8080478
H	-2.7364056	-2.9967107	-4.7559311
C	0.2415515	-3.0892377	3.5737451
C	-2.2431890	-3.0570107	-0.5405185
H	2.8119737	-1.7756767	4.2312676
P	1.2489862	-2.0782651	2.3806798
H	-0.8829642	-3.4892948	6.1399519
H	0.6761110	-1.3833724	-4.4520627
C	2.4347242	-1.1210278	3.4324845
H	-0.7661115	-1.5032922	-5.4834904
C	2.6853396	0.7066550	-1.6660081
H	-1.4550979	-2.6097082	0.0890627
H	3.2869402	-0.8843694	2.7835299
C	-2.3255528	-4.1356329	4.6644853
H	-2.8989916	-4.7331933	5.3852703
H	-1.1904387	-3.7817224	2.1124984
H	-3.5687706	-2.4256094	-2.1263831
C	-1.5462145	-3.0355144	5.3859074
H	2.8413474	1.4600555	-2.4338031

C	-2.8383574	-1.9618879	-1.4416617
C	-4.0028343	-2.5942269	1.2055875
C	-0.7072024	-2.2073761	4.4046265
H	-4.7805224	-3.0399714	1.8402294
C	2.2601670	-0.5375549	-2.0608040
P	-1.5180218	-1.2551389	-2.5196286
H	-0.1389643	-1.4550273	4.9658857
N	1.6739981	-1.5652007	-2.2558733
H	-3.2579107	-2.1421537	1.8826933
H	3.4893018	0.9912663	1.0810160
H	-3.0586761	-3.6774606	3.9800255
H	5.5697417	2.3435295	1.0397109
H	4.0480293	1.3026278	2.7266861
H	-5.4222030	-1.9357822	-0.2854997
C	1.8655986	0.1761636	4.0262762
H	-2.2272011	-2.3668672	5.9305444
C	-4.6085523	-1.5026734	0.3181696
Ga	0.0442114	-0.3417470	1.2216177
C	3.6318951	1.7847557	1.8310022
Ga	0.2308223	-0.0193940	-1.2062241
C	-3.5628110	-0.8827220	-0.6189420
H	-1.3742415	-1.6606258	3.7194742
H	2.6698488	0.7559987	4.4999440
H	1.1283117	-0.0355005	4.8093564
C	-2.3462722	-0.0017006	-3.5896217
H	-1.8012935	0.0007812	-4.5411369
H	1.3650508	1.0247833	-4.0648203
H	-3.3728458	-0.3246083	-3.8133569
C	4.6268600	2.8354156	1.3146704
H	1.9727958	1.5626186	-6.3852564
H	-2.8262623	-0.3241535	-0.0194744
H	3.3706873	2.6567258	-4.6271622
C	0.7272563	1.7239272	-4.6271970
P	1.0172409	1.2454642	2.7803022
H	-4.0573166	-0.1645133	-1.2879582
H	-0.0899715	1.1247288	-5.0517022
H	3.9711708	2.9810510	-0.7460360
H	-5.0626974	-0.7120558	0.9315780
H	4.8659570	3.5257728	2.1395230
C	1.5478397	2.3569496	-5.7568487
C	4.0748564	3.6382379	0.1308980
C	2.2779708	2.4342981	2.1498993
C	2.6506959	3.2624832	-5.2036818
C	-2.3617286	1.4106262	-2.9821571
H	4.7912772	4.4205932	-0.1526684
H	1.9071139	3.2339469	-2.4564133
P	-0.7551779	1.9970695	-2.2785248
H	3.2181564	3.7156026	-6.0270660
H	2.4333761	3.1479422	2.9768583
H	1.5215591	2.4821174	0.1294012
C	0.1609801	2.7923675	-3.6717655
H	-1.1008518	0.6571347	4.8579813
H	-3.0829231	1.4603201	-2.1560694
C	1.7189488	3.2018749	0.9421432
H	0.8802653	2.9474714	-6.4048891
C	1.2397817	3.7615974	-3.1539441
H	-1.8902299	0.9690129	3.3120024
C	2.7156438	4.2620209	0.4610910

C	-1.4236911	1.4603428	4.1763474
C	-0.1955785	2.2715854	3.7306647
H	-2.6916348	2.1399616	-3.7346683
C	2.0594814	4.3535122	-4.3073987
H	0.8345709	2.2535789	5.6415109
H	-1.2827431	2.0447930	0.6382547
H	2.8522662	4.9935517	-3.8966864
C	0.4514503	2.9980683	4.9253166
H	-0.5974821	3.3784182	-4.2196534
H	2.8392905	5.0249698	1.2463681
H	2.3079132	4.7833824	-0.4166437
H	0.7604919	3.6738326	1.2034854
C	-1.9378319	2.7785869	0.1418463
C	-1.2480850	3.3411465	-1.1112735
H	-0.5304747	3.0277838	3.0007200
H	0.7698558	4.5730341	-2.5810717
H	1.3092992	3.6045795	4.6042786
H	-2.8520595	2.2336004	-0.1421654
H	-0.2932191	3.7927994	-0.7987772
H	1.4111894	5.0083068	-4.9118908
C	-2.4374534	2.3514659	4.9056822
H	-1.4924576	2.3552247	6.8518326
H	-3.2855123	1.7391530	5.2417229
C	-1.7987968	3.0871354	6.0861895
C	-0.5766578	3.8905928	5.6352728
C	-2.1036661	4.4271224	-1.7904940
C	-2.3124812	3.9031002	1.1144160
H	-2.8458019	3.0890992	4.1953784
H	-3.0370491	3.9791643	-2.1656465
H	-2.8398101	3.4787697	1.9800050
H	-1.5780883	4.8452502	-2.6600850
H	-1.3892208	4.3682606	1.5010357
H	-0.0982317	4.3839355	6.4920448
H	-0.8937175	4.6921212	4.9479749
H	-2.5331046	3.7484692	6.5649109
C	-3.1620902	4.9824407	0.4381951
C	-2.4525468	5.5427799	-0.7969194
H	-4.1319238	4.5510447	0.1405297
H	-1.5277575	6.0586479	-0.4902342
H	-3.0791617	6.2941285	-1.2956272
H	-3.3851055	5.7885768	1.1496643
H	-1.4494762	-0.4624652	1.7043705

SCF energy GEOPT = -7388.976138557 H

ZPE = 3708. kJ/mol

FREEH energy = 3893.01 kJ/mol

FREEH entropy = 1.55326 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1	a	-228.98	0.00000	YES	YES	
2		-0.00	0.00000	-	-	
3		-0.00	0.00000	-	-	
4		0.00	0.00000	-	-	
5		0.00	0.00000	-	-	
6		0.00	0.00000	-	-	
7		0.00	0.00000	-	-	

8	a	16.58	0.05439	YES	YES
9	a	18.07	0.01092	YES	YES
10	a	25.32	0.01540	YES	YES
11	a	28.83	0.01172	YES	YES
12	a	33.46	0.02270	YES	YES
13	a	35.75	0.02350	YES	YES
14	a	36.85	0.04538	YES	YES
15	a	42.03	0.03745	YES	YES
16	a	46.97	0.12346	YES	YES
17	a	48.36	0.02026	YES	YES
18	a	50.16	0.30591	YES	YES
19	a	54.23	0.22881	YES	YES
20	a	57.20	0.17441	YES	YES
21	a	59.69	0.11637	YES	YES
22	a	60.03	0.26627	YES	YES
23	a	63.33	0.22653	YES	YES
24	a	64.37	0.05589	YES	YES
25	a	66.49	0.38451	YES	YES
26	a	70.92	0.05081	YES	YES
27	a	72.14	0.26966	YES	YES
28	a	73.85	0.12105	YES	YES
29	a	77.36	0.55656	YES	YES
30	a	79.83	0.02897	YES	YES
31	a	80.86	0.13635	YES	YES
32	a	84.69	0.14067	YES	YES
33	a	89.33	0.03911	YES	YES
34	a	93.28	0.24551	YES	YES
35	a	99.48	0.40428	YES	YES
36	a	106.12	0.44873	YES	YES
37	a	119.15	1.95722	YES	YES
38	a	126.32	1.13894	YES	YES
39	a	132.04	3.85191	YES	YES
40	a	135.04	2.44264	YES	YES
41	a	136.37	4.01668	YES	YES
42	a	137.86	4.96993	YES	YES
43	a	144.22	2.46148	YES	YES
44	a	148.73	0.71857	YES	YES
45	a	150.64	0.05754	YES	YES
46	a	153.28	1.59094	YES	YES
47	a	162.60	0.32474	YES	YES
48	a	167.74	3.99140	YES	YES
49	a	173.22	1.30775	YES	YES
50	a	177.74	1.03006	YES	YES
51	a	178.19	2.65693	YES	YES
52	a	182.11	0.33127	YES	YES
53	a	186.23	1.08204	YES	YES
54	a	197.26	1.57062	YES	YES
55	a	205.34	2.73413	YES	YES
56	a	212.12	1.05044	YES	YES
57	a	213.01	0.43204	YES	YES
58	a	215.28	0.15189	YES	YES
59	a	216.31	1.43961	YES	YES
60	a	222.60	0.76969	YES	YES
61	a	224.86	0.68799	YES	YES
62	a	227.87	0.08683	YES	YES
63	a	229.69	4.74695	YES	YES
64	a	235.32	1.80574	YES	YES
65	a	238.67	13.30771	YES	YES

66	a	241.05	0.98600	YES	YES
67	a	242.80	2.29745	YES	YES
68	a	250.84	1.90377	YES	YES
69	a	253.75	0.07359	YES	YES
70	a	259.18	0.76829	YES	YES
71	a	267.03	11.25898	YES	YES
72	a	272.20	4.27052	YES	YES
73	a	281.85	2.75414	YES	YES
74	a	291.07	1.80282	YES	YES
75	a	295.78	0.18072	YES	YES
76	a	304.06	0.43689	YES	YES
77	a	305.41	0.40840	YES	YES
78	a	312.88	0.23472	YES	YES
79	a	317.25	0.37029	YES	YES
80	a	330.62	0.43181	YES	YES
81	a	331.69	0.76989	YES	YES
82	a	333.34	0.09396	YES	YES
83	a	335.32	0.39137	YES	YES
84	a	340.70	0.20174	YES	YES
85	a	342.70	0.24853	YES	YES
86	a	362.29	1.78170	YES	YES
87	a	368.37	2.58502	YES	YES
88	a	373.13	0.77181	YES	YES
89	a	376.80	7.71845	YES	YES
90	a	388.17	12.24959	YES	YES
91	a	395.49	0.53455	YES	YES
92	a	397.97	0.77708	YES	YES
93	a	402.71	8.72768	YES	YES
94	a	414.62	1.17221	YES	YES
95	a	419.46	0.53869	YES	YES
96	a	422.27	0.99750	YES	YES
97	a	424.07	4.70756	YES	YES
98	a	424.42	0.84945	YES	YES
99	a	428.18	0.91599	YES	YES
100	a	428.49	2.84953	YES	YES
101	a	429.26	0.77253	YES	YES
102	a	430.68	0.67901	YES	YES
103	a	430.85	1.17378	YES	YES
104	a	432.53	0.25392	YES	YES
105	a	433.79	0.62429	YES	YES
106	a	434.99	0.78329	YES	YES
107	a	436.32	8.32842	YES	YES
108	a	440.93	0.70134	YES	YES
109	a	446.13	1.37144	YES	YES
110	a	462.19	5.32299	YES	YES
111	a	469.85	4.72845	YES	YES
112	a	490.12	2.22231	YES	YES
113	a	491.42	10.19027	YES	YES
114	a	494.07	3.43781	YES	YES
115	a	495.13	1.76617	YES	YES
116	a	498.29	5.94146	YES	YES
117	a	505.33	0.15801	YES	YES
118	a	513.40	15.57864	YES	YES
119	a	519.35	9.15554	YES	YES
120	a	530.77	66.07700	YES	YES
121	a	547.03	2.15148	YES	YES
122	a	607.09	99.83427	YES	YES
123	a	623.30	15.94097	YES	YES

124	a	633.48	19.46049	YES	YES
125	a	641.79	7.33998	YES	YES
126	a	647.36	82.34632	YES	YES
127	a	654.69	9.04490	YES	YES
128	a	713.99	1.31070	YES	YES
129	a	716.41	0.24381	YES	YES
130	a	717.57	1.56693	YES	YES
131	a	720.94	1.75363	YES	YES
132	a	730.47	2.96733	YES	YES
133	a	732.90	7.00383	YES	YES
134	a	735.02	3.87573	YES	YES
135	a	736.27	5.37152	YES	YES
136	a	768.00	0.09934	YES	YES
137	a	770.54	0.56004	YES	YES
138	a	771.76	0.10626	YES	YES
139	a	772.61	0.34640	YES	YES
140	a	773.50	0.73675	YES	YES
141	a	774.53	0.16101	YES	YES
142	a	775.49	1.31788	YES	YES
143	a	776.53	0.11871	YES	YES
144	a	782.84	14.36521	YES	YES
145	a	785.73	9.98678	YES	YES
146	a	808.16	2.11561	YES	YES
147	a	809.31	0.19734	YES	YES
148	a	809.97	1.52397	YES	YES
149	a	810.22	5.10458	YES	YES
150	a	811.28	0.66119	YES	YES
151	a	812.96	0.45547	YES	YES
152	a	814.52	4.67721	YES	YES
153	a	815.44	5.47672	YES	YES
154	a	832.06	1.85099	YES	YES
155	a	835.18	0.66928	YES	YES
156	a	836.58	1.03296	YES	YES
157	a	837.15	8.22161	YES	YES
158	a	838.09	4.25016	YES	YES
159	a	838.84	9.43402	YES	YES
160	a	839.72	1.55026	YES	YES
161	a	840.96	8.78715	YES	YES
162	a	850.78	11.83575	YES	YES
163	a	853.44	5.28595	YES	YES
164	a	872.31	2.66158	YES	YES
165	a	874.17	0.16602	YES	YES
166	a	874.67	3.97741	YES	YES
167	a	875.42	5.79281	YES	YES
168	a	876.50	3.02104	YES	YES
169	a	877.55	1.47554	YES	YES
170	a	878.03	1.94981	YES	YES
171	a	878.90	5.10208	YES	YES
172	a	879.23	4.85748	YES	YES
173	a	879.66	3.50267	YES	YES
174	a	880.56	3.87456	YES	YES
175	a	881.92	0.32739	YES	YES
176	a	882.45	1.43922	YES	YES
177	a	884.00	0.41656	YES	YES
178	a	884.85	4.71661	YES	YES
179	a	886.06	0.93085	YES	YES
180	a	902.66	1.87217	YES	YES
181	a	903.87	2.76485	YES	YES

182	a	904.74	0.90471	YES	YES
183	a	907.37	2.81041	YES	YES
184	a	908.40	2.92474	YES	YES
185	a	908.73	0.70340	YES	YES
186	a	910.32	0.50761	YES	YES
187	a	912.52	0.58433	YES	YES
188	a	985.35	9.49039	YES	YES
189	a	986.41	1.31399	YES	YES
190	a	987.53	5.42192	YES	YES
191	a	987.94	11.00392	YES	YES
192	a	989.50	0.90989	YES	YES
193	a	989.69	18.39010	YES	YES
194	a	991.01	23.23180	YES	YES
195	a	992.83	1.63162	YES	YES
196	a	994.32	6.77948	YES	YES
197	a	995.14	0.70125	YES	YES
198	a	1006.78	0.85315	YES	YES
199	a	1015.73	0.82286	YES	YES
200	a	1016.52	1.62297	YES	YES
201	a	1017.61	0.16392	YES	YES
202	a	1019.07	1.80805	YES	YES
203	a	1019.59	0.59221	YES	YES
204	a	1019.90	0.64717	YES	YES
205	a	1021.30	0.60236	YES	YES
206	a	1025.10	0.91692	YES	YES
207	a	1028.57	0.37349	YES	YES
208	a	1029.37	1.73760	YES	YES
209	a	1032.09	2.46103	YES	YES
210	a	1032.82	1.70620	YES	YES
211	a	1035.18	0.53110	YES	YES
212	a	1038.65	1.34951	YES	YES
213	a	1039.19	0.74326	YES	YES
214	a	1040.11	2.34457	YES	YES
215	a	1057.46	1.11772	YES	YES
216	a	1059.75	2.62705	YES	YES
217	a	1060.91	1.93739	YES	YES
218	a	1063.18	1.50015	YES	YES
219	a	1064.00	0.73251	YES	YES
220	a	1066.84	0.51767	YES	YES
221	a	1068.42	0.19579	YES	YES
222	a	1069.93	0.70176	YES	YES
223	a	1072.07	0.11876	YES	YES
224	a	1072.32	0.35904	YES	YES
225	a	1072.35	0.32645	YES	YES
226	a	1074.22	0.36243	YES	YES
227	a	1074.27	0.40255	YES	YES
228	a	1075.47	0.17530	YES	YES
229	a	1075.63	0.07348	YES	YES
230	a	1077.42	0.09364	YES	YES
231	a	1082.93	4.15086	YES	YES
232	a	1084.22	5.05216	YES	YES
233	a	1091.30	1.90231	YES	YES
234	a	1092.04	7.55948	YES	YES
235	a	1095.66	0.98652	YES	YES
236	a	1097.92	4.79352	YES	YES
237	a	1099.24	3.74300	YES	YES
238	a	1101.00	4.48948	YES	YES
239	a	1103.80	4.30261	YES	YES

240	a	1106.41	1.00773	YES	YES
241	a	1108.19	7.36071	YES	YES
242	a	1131.66	4.80161	YES	YES
243	a	1133.97	1.23953	YES	YES
244	a	1159.12	2.73973	YES	YES
245	a	1160.48	4.11680	YES	YES
246	a	1162.69	3.64619	YES	YES
247	a	1164.06	3.06934	YES	YES
248	a	1169.59	5.03028	YES	YES
249	a	1170.83	3.72159	YES	YES
250	a	1171.23	11.09583	YES	YES
251	a	1171.67	3.66521	YES	YES
252	a	1177.70	16.32450	YES	YES
253	a	1179.33	3.13655	YES	YES
254	a	1182.46	7.48657	YES	YES
255	a	1187.71	19.19518	YES	YES
256	a	1189.19	4.06182	YES	YES
257	a	1190.59	3.48929	YES	YES
258	a	1191.52	12.15455	YES	YES
259	a	1201.92	1.91956	YES	YES
260	a	1242.67	0.48884	YES	YES
261	a	1243.47	0.29721	YES	YES
262	a	1243.94	0.29080	YES	YES
263	a	1245.36	0.22652	YES	YES
264	a	1246.00	0.31164	YES	YES
265	a	1247.66	0.67033	YES	YES
266	a	1248.03	1.72578	YES	YES
267	a	1249.09	1.00348	YES	YES
268	a	1250.12	0.22506	YES	YES
269	a	1250.78	0.26930	YES	YES
270	a	1253.62	8.98142	YES	YES
271	a	1255.03	1.78151	YES	YES
272	a	1256.83	5.99769	YES	YES
273	a	1257.27	7.19603	YES	YES
274	a	1258.10	2.75965	YES	YES
275	a	1258.32	1.15331	YES	YES
276	a	1259.07	9.05650	YES	YES
277	a	1259.86	1.23705	YES	YES
278	a	1260.26	5.56089	YES	YES
279	a	1260.56	6.82994	YES	YES
280	a	1261.28	1.93827	YES	YES
281	a	1261.82	2.22868	YES	YES
282	a	1262.89	4.05567	YES	YES
283	a	1264.72	2.01121	YES	YES
284	a	1266.93	0.75497	YES	YES
285	a	1269.06	0.20598	YES	YES
286	a	1269.81	1.61847	YES	YES
287	a	1270.15	2.15520	YES	YES
288	a	1280.95	2.60946	YES	YES
289	a	1282.18	5.02016	YES	YES
290	a	1285.19	1.05624	YES	YES
291	a	1289.03	0.60532	YES	YES
292	a	1289.88	5.30254	YES	YES
293	a	1290.15	1.87570	YES	YES
294	a	1291.52	3.11196	YES	YES
295	a	1294.38	3.95774	YES	YES
296	a	1306.06	1.22692	YES	YES
297	a	1309.31	0.95473	YES	YES

298	a	1310.28	0.36749	YES	YES
299	a	1310.98	2.10207	YES	YES
300	a	1313.43	0.46809	YES	YES
301	a	1314.74	2.21768	YES	YES
302	a	1316.48	1.69003	YES	YES
303	a	1320.10	2.50681	YES	YES
304	a	1322.20	0.29237	YES	YES
305	a	1323.00	3.38206	YES	YES
306	a	1323.36	2.10145	YES	YES
307	a	1323.57	1.21803	YES	YES
308	a	1323.89	0.24615	YES	YES
309	a	1324.53	3.10598	YES	YES
310	a	1325.23	1.09643	YES	YES
311	a	1325.43	3.74716	YES	YES
312	a	1325.94	0.38234	YES	YES
313	a	1326.38	0.58019	YES	YES
314	a	1326.50	0.69125	YES	YES
315	a	1326.93	1.99245	YES	YES
316	a	1328.18	3.06753	YES	YES
317	a	1328.94	2.20503	YES	YES
318	a	1329.84	2.03397	YES	YES
319	a	1330.12	1.38200	YES	YES
320	a	1336.09	0.05756	YES	YES
321	a	1336.63	1.04156	YES	YES
322	a	1338.05	0.38751	YES	YES
323	a	1338.42	0.19332	YES	YES
324	a	1338.72	0.33758	YES	YES
325	a	1339.12	0.58592	YES	YES
326	a	1340.58	0.04769	YES	YES
327	a	1344.81	1.13048	YES	YES
328	a	1345.06	1.38750	YES	YES
329	a	1347.03	1.45854	YES	YES
330	a	1347.33	2.79588	YES	YES
331	a	1348.76	0.27337	YES	YES
332	a	1348.92	0.60509	YES	YES
333	a	1350.01	1.13078	YES	YES
334	a	1350.61	0.88754	YES	YES
335	a	1352.97	0.21285	YES	YES
336	a	1373.97	11.64455	YES	YES
337	a	1402.56	6.27073	YES	YES
338	a	1405.16	8.28182	YES	YES
339	a	1406.01	10.53186	YES	YES
340	a	1409.15	6.41648	YES	YES
341	a	1421.91	2.08641	YES	YES
342	a	1424.21	7.44658	YES	YES
343	a	1425.38	1.88942	YES	YES
344	a	1429.70	4.86024	YES	YES
345	a	1431.10	3.97963	YES	YES
346	a	1432.04	2.73451	YES	YES
347	a	1433.14	2.98676	YES	YES
348	a	1434.60	4.62765	YES	YES
349	a	1435.52	1.35850	YES	YES
350	a	1435.63	2.36077	YES	YES
351	a	1436.89	5.36742	YES	YES
352	a	1437.46	10.78074	YES	YES
353	a	1437.73	1.13539	YES	YES
354	a	1437.76	17.23381	YES	YES
355	a	1438.00	4.61736	YES	YES

356	a	1438.18	3.90856	YES	YES
357	a	1438.34	0.55100	YES	YES
358	a	1438.65	5.45014	YES	YES
359	a	1439.66	0.23992	YES	YES
360	a	1440.05	3.70395	YES	YES
361	a	1441.14	8.80207	YES	YES
362	a	1441.72	8.67844	YES	YES
363	a	1441.82	4.27126	YES	YES
364	a	1442.89	7.44974	YES	YES
365	a	1443.23	21.55321	YES	YES
366	a	1443.84	4.89833	YES	YES
367	a	1444.29	7.82911	YES	YES
368	a	1445.35	30.85699	YES	YES
369	a	1446.33	8.51947	YES	YES
370	a	1446.57	4.88195	YES	YES
371	a	1447.80	8.36316	YES	YES
372	a	1448.87	9.38718	YES	YES
373	a	1453.27	0.43702	YES	YES
374	a	1453.75	2.69591	YES	YES
375	a	1454.78	6.20617	YES	YES
376	a	1454.92	0.46243	YES	YES
377	a	1455.68	0.86834	YES	YES
378	a	1457.06	1.07241	YES	YES
379	a	1458.13	0.92432	YES	YES
380	a	1461.11	0.36640	YES	YES
381	a	1880.40	110.69460	YES	YES
382	a	2029.99	190.33166	YES	YES
383	a	2925.97	4.04183	YES	YES
384	a	2928.62	3.37066	YES	YES
385	a	2930.58	3.22346	YES	YES
386	a	2932.23	22.07006	YES	YES
387	a	2935.35	7.59021	YES	YES
388	a	2936.42	4.16421	YES	YES
389	a	2938.59	16.25524	YES	YES
390	a	2939.24	6.20425	YES	YES
391	a	2942.58	36.70198	YES	YES
392	a	2943.47	8.03407	YES	YES
393	a	2944.46	14.50900	YES	YES
394	a	2944.84	6.99054	YES	YES
395	a	2945.01	4.85441	YES	YES
396	a	2945.58	14.63007	YES	YES
397	a	2946.42	6.15302	YES	YES
398	a	2948.06	5.53857	YES	YES
399	a	2948.10	10.19987	YES	YES
400	a	2948.47	15.04220	YES	YES
401	a	2948.55	13.35249	YES	YES
402	a	2948.60	21.04498	YES	YES
403	a	2948.90	2.90618	YES	YES
404	a	2953.99	10.41242	YES	YES
405	a	2954.52	11.82686	YES	YES
406	a	2955.05	34.61624	YES	YES
407	a	2955.92	15.51649	YES	YES
408	a	2956.11	7.36957	YES	YES
409	a	2956.23	6.92118	YES	YES
410	a	2956.95	9.28403	YES	YES
411	a	2957.80	8.46302	YES	YES
412	a	2958.33	3.21930	YES	YES
413	a	2958.99	10.09542	YES	YES

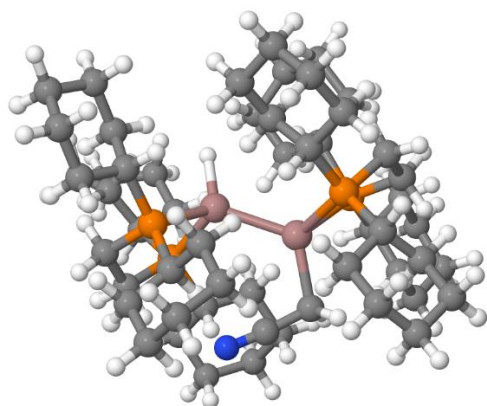
414	a	2959.62	20.81588	YES	YES
415	a	2960.51	2.00653	YES	YES
416	a	2960.54	25.98376	YES	YES
417	a	2961.62	29.77778	YES	YES
418	a	2962.40	41.03785	YES	YES
419	a	2962.75	25.83954	YES	YES
420	a	2963.20	31.92540	YES	YES
421	a	2964.16	21.44231	YES	YES
422	a	2965.97	15.96271	YES	YES
423	a	2967.29	26.58282	YES	YES
424	a	2968.39	30.22383	YES	YES
425	a	2969.03	7.49894	YES	YES
426	a	2970.30	18.29627	YES	YES
427	a	2973.22	4.90060	YES	YES
428	a	2974.48	5.27788	YES	YES
429	a	2974.63	26.94765	YES	YES
430	a	2982.04	11.51414	YES	YES
431	a	2984.05	6.80874	YES	YES
432	a	2984.41	2.42252	YES	YES
433	a	2986.34	21.08734	YES	YES
434	a	2987.81	14.77380	YES	YES
435	a	2992.87	4.26869	YES	YES
436	a	2994.33	16.87775	YES	YES
437	a	3002.94	33.06273	YES	YES
438	a	3003.12	15.68172	YES	YES
439	a	3004.57	26.65347	YES	YES
440	a	3005.38	19.31742	YES	YES
441	a	3005.70	18.88408	YES	YES
442	a	3007.08	15.20663	YES	YES
443	a	3007.78	17.47990	YES	YES
444	a	3008.74	13.19730	YES	YES
445	a	3009.09	25.69844	YES	YES
446	a	3009.55	26.75927	YES	YES
447	a	3009.88	27.63994	YES	YES
448	a	3010.01	29.01149	YES	YES
449	a	3010.05	24.25302	YES	YES
450	a	3010.57	6.78388	YES	YES
451	a	3010.75	20.51854	YES	YES
452	a	3010.88	24.26646	YES	YES
453	a	3011.39	21.12291	YES	YES
454	a	3011.56	4.54373	YES	YES
455	a	3011.80	31.48693	YES	YES
456	a	3012.64	21.08601	YES	YES
457	a	3012.91	37.95109	YES	YES
458	a	3013.79	39.33653	YES	YES
459	a	3015.06	15.39724	YES	YES
460	a	3015.54	3.22864	YES	YES
461	a	3016.00	28.31340	YES	YES
462	a	3017.05	22.87534	YES	YES
463	a	3017.27	36.33760	YES	YES
464	a	3017.64	15.82221	YES	YES
465	a	3018.87	33.57349	YES	YES
466	a	3019.33	28.07003	YES	YES
467	a	3019.46	15.99799	YES	YES
468	a	3019.93	36.65678	YES	YES
469	a	3021.86	15.82313	YES	YES
470	a	3022.06	51.69754	YES	YES
471	a	3022.72	28.81721	YES	YES

472	a	3028.04	14.76083	YES	YES
473	a	3030.24	0.34917	YES	YES
474	a	3031.06	11.29452	YES	YES
475	a	3036.49	1.00838	YES	YES
476	a	3046.04	8.08065	YES	YES
477	a	3046.71	0.46992	YES	YES
478	a	3051.78	0.67159	YES	YES
479	a	3084.28	3.59878	YES	YES
480	a	3170.42	1.74430	YES	YES

\$end

Double hybrid single point energy = -7381.619781965132 H
 COSMO energy + OC correction = -7389.1253556530 H (in oDFB)

6.2.41 [H{Ga(dcpe)}₂(CH₂CN)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	0.0199873	-0.0612427	-1.3450973
Ga	-0.3302978	0.0476855	1.0856514
H	0.7041359	0.8507132	1.9624954
N	-3.2099155	-1.8367576	-0.9866473
C	-2.4876837	-1.3175793	-1.7428988
C	-1.5381803	-0.6311238	-2.5666329
H	-2.0005441	0.2703448	-2.9884595
H	-1.2053950	-1.2669977	-3.3942253
P	-2.5363604	0.7732642	1.7439526
P	-0.8042075	-2.0292114	2.2259281
C	-2.6293400	2.0499099	3.0727474
H	-3.7004016	2.0944059	3.3323552
C	-1.8420607	1.6735366	4.3377236
H	-2.0740534	0.6542663	4.6672376
H	-0.7678819	1.6898820	4.0999807
C	-2.1707357	2.6555283	5.4861142
H	-3.0238073	2.2731622	6.0631755
H	-1.3163576	2.6831926	6.1764220
C	-2.4817109	4.0768069	4.9737411
H	-2.2445043	4.8175374	5.7472934
H	-3.5588259	4.1829600	4.7711387
C	-1.6988511	4.3573115	3.6909369

H	-1.8047434	5.4046679	3.3795595
H	-0.6269909	4.1964556	3.8825264
C	-2.1705296	3.4334859	2.5486829
H	-1.3535310	3.3067715	1.8244188
H	-3.0014917	3.9050505	2.0066711
C	-3.6383013	1.2794454	0.3564356
H	-3.8037422	0.3226696	-0.1653785
C	-5.0064430	1.8200321	0.8049986
H	-5.4950154	1.1166345	1.4943281
H	-4.8718776	2.7665619	1.3517149
C	-5.9019577	2.0625224	-0.4187806
H	-6.1244234	1.0952202	-0.8972471
H	-6.8639013	2.4806372	-0.0933377
C	-5.2311203	2.9937966	-1.4338004
H	-5.1103219	3.9953380	-0.9888598
H	-5.8745020	3.1196493	-2.3148078
C	-3.8561116	2.4622912	-1.8550444
H	-3.3722133	3.1605909	-2.5531042
H	-3.9851280	1.5089630	-2.3949612
C	-2.9556992	2.2342251	-0.6370513
H	-1.9807998	1.8202088	-0.9433999
H	-2.7458527	3.1988240	-0.1515765
C	-3.3086236	-0.7682419	2.4133787
H	-4.1696416	-0.5031779	3.0425194
H	-3.6917425	-1.3120442	1.5367728
C	-2.3220673	-1.6465023	3.1975807
H	-2.8039331	-2.5846137	3.5003574
H	-1.9880060	-1.1493999	4.1155972
C	0.4989309	-2.5364340	3.4301837
H	1.3639859	-2.7856790	2.7911117
C	0.9046227	-1.3511010	4.3269800
H	0.0401371	-1.0403480	4.9362429
H	1.1844364	-0.4854346	3.7110948
C	2.0533679	-1.7435862	5.2643643
H	2.9516054	-1.9582804	4.6620652
H	2.3052485	-0.8916898	5.9109042
C	1.6978520	-2.9737406	6.1035072
H	0.8654277	-2.7248250	6.7823009
H	2.5451634	-3.2572678	6.7419552
C	1.2915354	-4.1483785	5.2104749
H	2.1576307	-4.4675050	4.6068911
H	0.9987593	-5.0152130	5.8182092
C	0.1382103	-3.7756408	4.2682678
H	-0.7664470	-3.5653739	4.8612839
H	-0.0982909	-4.6266972	3.6172276
C	-1.2368484	-3.4251345	1.0967439
H	-1.7443312	-2.9202643	0.2590448
C	0.0409679	-4.0814126	0.5507438
H	0.6822701	-3.3095480	0.0942880
H	0.6202374	-4.5273477	1.3744873
C	-0.2982516	-5.1723052	-0.4721855
H	0.6264546	-5.6553275	-0.8198160
H	-0.7687504	-4.7061067	-1.3524469
C	-1.2606783	-6.2078664	0.1139757
H	-1.5019215	-6.9682898	-0.6407749
H	-0.7697467	-6.7382194	0.9466954
C	-2.5389176	-5.5319802	0.6146974
H	-3.2257795	-6.2723422	1.0461859

H	-3.0660713	-5.0660167	-0.2332170
C	-2.2320207	-4.4537871	1.6625658
H	-3.1678999	-3.9551665	1.9485799
H	-1.8288921	-4.9282446	2.5689796
P	2.0965431	-1.1068465	-2.1204522
P	1.0477063	2.0036030	-2.1109876
C	1.9242499	-2.2389910	-3.5655832
H	2.9376337	-2.6225239	-3.7740419
C	1.4260742	-1.4996670	-4.8211106
H	2.1618028	-0.7432681	-5.1287540
H	0.4920257	-0.9604528	-4.5930533
C	1.1789325	-2.4752372	-5.9794701
H	0.7800680	-1.9226307	-6.8408861
H	2.1422628	-2.9028153	-6.3008157
C	0.2324382	-3.6077777	-5.5733155
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H	5.0613866	-1.4788084	-1.5654039
H	4.4384529	-2.9881037	-2.2447182
C	5.2377922	-3.1733465	-0.2344965
H	4.7248237	-4.1343546	-0.0656698
H	6.2486787	-3.4167177	-0.5877334
C	5.3000675	-2.3875514	1.0782100
H	5.9037099	-1.4765754	0.9324571
H	5.8103957	-2.9779115	1.8507478
C	3.8976835	-1.9959101	1.5516303
H	3.3299685	-2.9099430	1.7958992
H	3.9476440	-1.3995410	2.4731802
C	3.1357787	-1.2140388	0.4758629
H	3.6364070	-0.2449226	0.3113448
H	2.1179064	-0.9808981	0.8225066
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H	3.7484422	0.6140562	-1.7875005
H	3.9023482	-0.0860773	-3.3997734
C	2.3903013	1.4753023	-3.2519917
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H	3.0625163	2.3201449	-3.4531201
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C	-0.5968280	2.7003486	-4.2439514
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H	0.1844444	2.3631088	-4.9438244
C	-1.4757137	3.7408950	-4.9499417
H	-1.9083228	3.2977784	-5.8572302
H	-2.3223378	4.0022637	-4.2941204
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H	0.0950630	4.7657885	-6.0286145
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C	-0.0311420	5.5955082	-4.0344316

H	-0.8134104	5.9347202	-3.3353566
H	0.5665379	6.4813785	-4.2878893
C	0.8618863	4.5681351	-3.3249042
H	1.2877193	5.0103685	-2.4154370
H	1.7075464	4.3059498	-3.9807511
C	1.8883350	2.6910826	-0.6158975
H	2.1213746	1.7874407	-0.0216540
C	0.8842848	3.5137132	0.2074826
H	0.5840185	4.4075992	-0.3607922
H	-0.0302525	2.9234431	0.3748588
C	1.4995306	3.9377151	1.5442688
H	0.7863843	4.5654690	2.0953319
H	1.6691959	3.0362067	2.1560075
C	2.8210173	4.6851375	1.3403772
H	3.2648550	4.9399000	2.3119942
H	2.6250570	5.6412517	0.8278494
C	3.8074855	3.8593452	0.5091335
H	4.7365653	4.4206451	0.3422058
H	4.0850183	2.9487898	1.0665562
C	3.2025208	3.4541972	-0.8424886
H	3.0196609	4.3540714	-1.4469676
H	3.9223342	2.8404966	-1.4026912

SCF energy GEOOPT = -7389.023362915 H
ZPE = 3710. kJ/mol
FREEH energy = 3895.05 kJ/mol
FREEH entropy = 1.58077 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1	a	-10.47	0.00000	YES	YES
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		-0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7		0.00	0.00000	-	-
	8	a	11.13	0.08455	YES	YES
	9	a	13.96	0.12439	YES	YES
	10	a	22.23	0.03388	YES	YES
	11	a	23.71	0.28455	YES	YES
	12	a	28.69	0.02911	YES	YES
	13	a	30.29	0.07123	YES	YES
	14	a	34.68	0.01816	YES	YES
	15	a	36.45	0.17222	YES	YES
	16	a	39.27	0.07820	YES	YES
	17	a	40.95	0.21247	YES	YES
	18	a	43.60	0.81858	YES	YES
	19	a	50.39	0.04783	YES	YES
	20	a	53.44	0.12709	YES	YES
	21	a	53.85	0.04676	YES	YES
	22	a	54.71	0.07015	YES	YES
	23	a	58.25	0.13116	YES	YES
	24	a	59.72	0.13099	YES	YES
	25	a	62.02	0.18066	YES	YES
	26	a	65.98	0.05522	YES	YES
	27	a	67.17	0.55673	YES	YES

28	a	69.92	0.61878	YES	YES
29	a	74.81	0.22388	YES	YES
30	a	78.55	0.11105	YES	YES
31	a	79.58	0.12076	YES	YES
32	a	84.51	0.35526	YES	YES
33	a	89.06	0.49323	YES	YES
34	a	92.39	1.64375	YES	YES
35	a	96.01	3.34835	YES	YES
36	a	103.42	1.32246	YES	YES
37	a	105.58	5.88786	YES	YES
38	a	116.93	0.71250	YES	YES
39	a	118.06	1.00136	YES	YES
40	a	129.94	1.27381	YES	YES
41	a	134.36	1.36442	YES	YES
42	a	136.44	0.71643	YES	YES
43	a	138.02	2.02268	YES	YES
44	a	140.97	0.40926	YES	YES
45	a	148.56	1.68006	YES	YES
46	a	151.62	0.73842	YES	YES
47	a	155.24	0.77378	YES	YES
48	a	160.53	0.67750	YES	YES
49	a	160.88	2.43685	YES	YES
50	a	161.64	0.63294	YES	YES
51	a	179.31	2.64260	YES	YES
52	a	185.11	1.64012	YES	YES
53	a	187.17	5.07442	YES	YES
54	a	191.93	5.08994	YES	YES
55	a	194.76	0.02181	YES	YES
56	a	200.09	1.71458	YES	YES
57	a	202.87	1.85663	YES	YES
58	a	208.82	0.38559	YES	YES
59	a	213.89	0.23541	YES	YES
60	a	219.43	0.68460	YES	YES
61	a	223.59	0.31407	YES	YES
62	a	226.07	0.86823	YES	YES
63	a	228.95	0.00906	YES	YES
64	a	232.00	0.24515	YES	YES
65	a	233.45	1.43775	YES	YES
66	a	236.65	0.35845	YES	YES
67	a	237.78	0.01276	YES	YES
68	a	239.29	0.37449	YES	YES
69	a	241.55	0.63427	YES	YES
70	a	256.47	0.16693	YES	YES
71	a	261.07	0.25803	YES	YES
72	a	275.38	1.02539	YES	YES
73	a	292.93	0.29772	YES	YES
74	a	297.33	0.36096	YES	YES
75	a	306.09	0.61988	YES	YES
76	a	307.72	0.05854	YES	YES
77	a	312.61	0.14829	YES	YES
78	a	313.26	0.25703	YES	YES
79	a	327.59	0.45036	YES	YES
80	a	330.13	0.54591	YES	YES
81	a	332.33	0.31850	YES	YES
82	a	335.83	0.25589	YES	YES
83	a	337.18	0.01415	YES	YES
84	a	341.94	0.54365	YES	YES
85	a	344.96	1.31853	YES	YES

86	a	374.06	0.31937	YES	YES
87	a	376.66	0.82423	YES	YES
88	a	379.84	1.11721	YES	YES
89	a	385.03	0.84863	YES	YES
90	a	387.47	0.61311	YES	YES
91	a	390.69	0.62303	YES	YES
92	a	402.94	1.93259	YES	YES
93	a	408.42	3.14689	YES	YES
94	a	411.71	2.19376	YES	YES
95	a	416.92	1.72292	YES	YES
96	a	421.08	3.25693	YES	YES
97	a	424.02	0.72109	YES	YES
98	a	426.02	0.59719	YES	YES
99	a	428.90	0.43274	YES	YES
100	a	430.40	0.15733	YES	YES
101	a	431.07	0.07016	YES	YES
102	a	431.72	0.07078	YES	YES
103	a	431.92	0.07955	YES	YES
104	a	434.17	3.12873	YES	YES
105	a	436.62	2.67659	YES	YES
106	a	449.82	1.44674	YES	YES
107	a	453.44	3.74704	YES	YES
108	a	464.07	0.42414	YES	YES
109	a	465.04	8.38768	YES	YES
110	a	469.88	1.66073	YES	YES
111	a	491.32	2.46765	YES	YES
112	a	495.98	0.51558	YES	YES
113	a	498.53	2.72194	YES	YES
114	a	502.28	1.42980	YES	YES
115	a	503.64	4.37536	YES	YES
116	a	514.12	17.28476	YES	YES
117	a	514.79	2.38378	YES	YES
118	a	525.10	14.46596	YES	YES
119	a	536.47	83.71877	YES	YES
120	a	563.90	82.22459	YES	YES
121	a	583.74	25.88896	YES	YES
122	a	628.62	3.89062	YES	YES
123	a	631.95	33.25149	YES	YES
124	a	633.97	8.06655	YES	YES
125	a	644.99	8.07147	YES	YES
126	a	654.77	9.42883	YES	YES
127	a	697.12	6.53588	YES	YES
128	a	708.95	3.25577	YES	YES
129	a	716.62	4.12345	YES	YES
130	a	726.30	5.51461	YES	YES
131	a	727.91	7.49798	YES	YES
132	a	733.37	10.18336	YES	YES
133	a	737.06	1.14423	YES	YES
134	a	740.44	0.96315	YES	YES
135	a	758.18	1.30682	YES	YES
136	a	768.38	0.39226	YES	YES
137	a	769.84	0.31009	YES	YES
138	a	770.34	0.11026	YES	YES
139	a	772.83	0.35587	YES	YES
140	a	774.00	0.13488	YES	YES
141	a	774.41	0.03474	YES	YES
142	a	775.98	0.21666	YES	YES
143	a	788.23	22.95114	YES	YES

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145	a	806.86	0.82134	YES	YES
146	a	809.12	1.23768	YES	YES
147	a	809.97	1.08165	YES	YES
148	a	810.32	2.90723	YES	YES
149	a	812.26	3.76578	YES	YES
150	a	815.21	0.69785	YES	YES
151	a	815.67	4.12627	YES	YES
152	a	819.36	5.85401	YES	YES
153	a	833.65	2.88794	YES	YES
154	a	834.37	2.57588	YES	YES
155	a	835.28	6.87645	YES	YES
156	a	836.27	0.82939	YES	YES
157	a	837.06	1.25534	YES	YES
158	a	837.70	4.74145	YES	YES
159	a	839.86	6.49324	YES	YES
160	a	843.20	4.25273	YES	YES
161	a	852.22	14.86251	YES	YES
162	a	859.30	10.90356	YES	YES
163	a	871.86	2.37132	YES	YES
164	a	871.95	3.28022	YES	YES
165	a	872.99	4.36333	YES	YES
166	a	874.69	2.10272	YES	YES
167	a	875.76	4.81552	YES	YES
168	a	876.35	3.30608	YES	YES
169	a	877.73	4.00245	YES	YES
170	a	878.48	1.41167	YES	YES
171	a	879.33	1.90990	YES	YES
172	a	880.44	0.55574	YES	YES
173	a	881.49	3.85956	YES	YES
174	a	881.94	2.62274	YES	YES
175	a	882.56	1.10092	YES	YES
176	a	885.20	2.26973	YES	YES
177	a	885.86	0.68694	YES	YES
178	a	896.29	1.26542	YES	YES
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183	a	905.89	1.26973	YES	YES
184	a	906.68	0.58285	YES	YES
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186	a	910.27	0.58552	YES	YES
187	a	969.30	3.26640	YES	YES
188	a	970.62	3.28542	YES	YES
189	a	985.34	12.16884	YES	YES
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191	a	986.49	1.11663	YES	YES
192	a	986.99	14.57976	YES	YES
193	a	988.17	7.33692	YES	YES
194	a	991.00	3.97136	YES	YES
195	a	992.34	15.15368	YES	YES
196	a	992.64	7.22690	YES	YES
197	a	993.36	0.82341	YES	YES
198	a	1013.99	1.02946	YES	YES
199	a	1014.85	1.05884	YES	YES
200	a	1016.27	0.86289	YES	YES
201	a	1016.48	0.52123	YES	YES

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204	a	1020.49	1.83688	YES	YES
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206	a	1030.97	3.62095	YES	YES
207	a	1032.03	1.84090	YES	YES
208	a	1033.14	3.06160	YES	YES
209	a	1037.01	24.96528	YES	YES
210	a	1038.52	4.46223	YES	YES
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213	a	1042.58	0.66729	YES	YES
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226	a	1071.97	0.05557	YES	YES
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234	a	1093.97	7.04545	YES	YES
235	a	1095.62	6.22755	YES	YES
236	a	1100.83	0.18860	YES	YES
237	a	1101.86	17.25973	YES	YES
238	a	1105.20	1.85525	YES	YES
239	a	1107.62	3.75270	YES	YES
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241	a	1112.38	0.89606	YES	YES
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253	a	1184.77	6.77345	YES	YES
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274	a	1256.48	9.96820	YES	YES
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276	a	1257.34	3.27718	YES	YES
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279	a	1259.79	2.34126	YES	YES
280	a	1260.34	2.02385	YES	YES
281	a	1261.61	0.61562	YES	YES
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283	a	1264.87	2.52622	YES	YES
284	a	1265.11	0.32143	YES	YES
285	a	1268.78	2.18208	YES	YES
286	a	1270.22	4.32669	YES	YES
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291	a	1283.61	0.85033	YES	YES
292	a	1286.06	1.82584	YES	YES
293	a	1287.30	7.43350	YES	YES
294	a	1289.33	2.59232	YES	YES
295	a	1292.73	2.23733	YES	YES
296	a	1305.99	1.62170	YES	YES
297	a	1308.52	2.62105	YES	YES
298	a	1309.24	0.78395	YES	YES
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301	a	1311.58	0.47699	YES	YES
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312	a	1324.34	1.66257	YES	YES
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319	a	1329.64	4.89310	YES	YES
320	a	1335.59	0.50023	YES	YES
321	a	1335.97	0.10953	YES	YES
322	a	1336.14	0.34072	YES	YES
323	a	1336.65	0.24297	YES	YES
324	a	1337.72	0.06388	YES	YES
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331	a	1344.48	1.42002	YES	YES
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333	a	1345.67	0.67160	YES	YES
334	a	1347.03	1.06061	YES	YES
335	a	1349.21	0.77411	YES	YES
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361	a	1439.87	7.83737	YES	YES
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364	a	1442.93	10.02272	YES	YES
365	a	1443.00	18.83950	YES	YES
366	a	1444.15	6.46514	YES	YES
367	a	1444.51	8.18514	YES	YES
368	a	1445.11	10.94470	YES	YES
369	a	1445.52	19.19745	YES	YES
370	a	1446.11	2.42204	YES	YES
371	a	1447.08	7.15596	YES	YES
372	a	1453.50	0.30102	YES	YES
373	a	1453.90	3.50259	YES	YES
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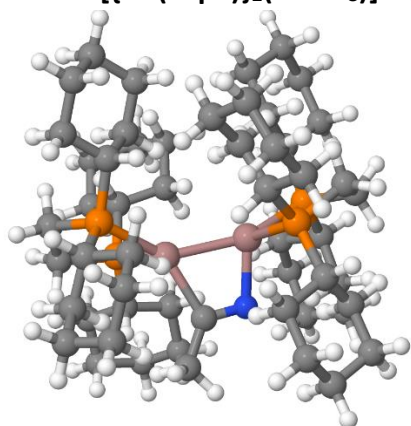
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389	a	2940.99	31.76515	YES	YES
390	a	2941.52	5.36939	YES	YES
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392	a	2942.41	0.37801	YES	YES
393	a	2942.71	27.97717	YES	YES
394	a	2943.58	14.12530	YES	YES
395	a	2945.11	5.63420	YES	YES
396	a	2945.47	5.62989	YES	YES
397	a	2945.72	9.42568	YES	YES
398	a	2946.14	8.06996	YES	YES
399	a	2947.92	11.85030	YES	YES
400	a	2948.07	10.69535	YES	YES
401	a	2948.27	8.10865	YES	YES
402	a	2948.92	19.38412	YES	YES
403	a	2950.79	20.26057	YES	YES
404	a	2951.01	10.73189	YES	YES
405	a	2952.29	3.30903	YES	YES
406	a	2954.33	12.04411	YES	YES
407	a	2954.61	5.61825	YES	YES
408	a	2954.79	6.21382	YES	YES
409	a	2957.05	5.84647	YES	YES
410	a	2958.01	18.02697	YES	YES
411	a	2958.50	5.36679	YES	YES
412	a	2958.94	4.75452	YES	YES
413	a	2959.20	9.15696	YES	YES
414	a	2959.38	24.53555	YES	YES
415	a	2959.48	20.50944	YES	YES
416	a	2959.60	11.59604	YES	YES
417	a	2960.96	5.78084	YES	YES
418	a	2962.82	23.65998	YES	YES
419	a	2963.26	34.22165	YES	YES
420	a	2963.58	45.78461	YES	YES
421	a	2963.75	52.96193	YES	YES
422	a	2964.92	38.85302	YES	YES
423	a	2965.27	31.71324	YES	YES
424	a	2966.94	1.39211	YES	YES
425	a	2969.69	16.64651	YES	YES
426	a	2972.65	9.59786	YES	YES
427	a	2973.02	21.98947	YES	YES
428	a	2973.73	17.90642	YES	YES
429	a	2975.86	28.43609	YES	YES
430	a	2976.16	7.27809	YES	YES
431	a	2979.35	17.16803	YES	YES
432	a	2982.47	2.04425	YES	YES
433	a	2985.25	47.86327	YES	YES

434	a	2986.21	18.55400	YES	YES
435	a	2991.34	35.56827	YES	YES
436	a	2992.43	15.09761	YES	YES
437	a	2995.16	3.07094	YES	YES
438	a	3002.90	7.91160	YES	YES
439	a	3003.18	27.33745	YES	YES
440	a	3003.54	8.70260	YES	YES
441	a	3003.60	20.18948	YES	YES
442	a	3003.82	2.38001	YES	YES
443	a	3006.48	25.42453	YES	YES
444	a	3006.85	14.87199	YES	YES
445	a	3007.84	17.90801	YES	YES
446	a	3010.20	31.12294	YES	YES
447	a	3010.39	14.02503	YES	YES
448	a	3010.92	1.23269	YES	YES
449	a	3010.95	34.23985	YES	YES
450	a	3011.13	21.78044	YES	YES
451	a	3011.32	11.64393	YES	YES
452	a	3013.33	14.41469	YES	YES
453	a	3013.73	19.46109	YES	YES
454	a	3014.23	32.62825	YES	YES
455	a	3014.32	10.71102	YES	YES
456	a	3014.86	9.93301	YES	YES
457	a	3014.96	18.44706	YES	YES
458	a	3015.84	21.05623	YES	YES
459	a	3016.21	13.67480	YES	YES
460	a	3016.29	23.52738	YES	YES
461	a	3016.51	39.58563	YES	YES
462	a	3016.67	17.12743	YES	YES
463	a	3017.16	16.66026	YES	YES
464	a	3017.73	30.38357	YES	YES
465	a	3018.37	38.65352	YES	YES
466	a	3019.45	18.86425	YES	YES
467	a	3019.52	19.78499	YES	YES
468	a	3019.94	23.24554	YES	YES
469	a	3020.33	13.31013	YES	YES
470	a	3020.74	26.94753	YES	YES
471	a	3023.61	26.84224	YES	YES
472	a	3025.03	54.79850	YES	YES
473	a	3025.15	6.06383	YES	YES
474	a	3027.00	3.51489	YES	YES
475	a	3028.99	1.68146	YES	YES
476	a	3029.14	17.40739	YES	YES
477	a	3036.87	25.11073	YES	YES
478	a	3048.19	0.26798	YES	YES
479	a	3052.09	1.05950	YES	YES
480	a	3059.79	1.05876	YES	YES

\$end

Double hybrid single point energy = -7381.673797476506 H
 COSMO energy + OC correction = -7389.1728423134 H (in oDFB)

6.2.42 $[\{\text{Ga}(\text{dcpe})\}_2(\text{NCCH}_3)]^{2+}$ (Cycloadduct)



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.5834570	17.2714063	-2.7598019
Ga	-4.1137959	17.8080044	-0.9661316
P	-1.6836030	18.9272054	-4.2632371
P	-6.1013092	19.1454404	-0.8396918
P	-1.9733328	15.6297384	-4.3807046
P	-5.3730103	16.1819797	0.2722999
C	-5.1788785	20.9089881	-5.4322688
H	-5.3791270	21.4459691	-4.4885870
H	-6.1434565	20.5111605	-5.7774343
C	-0.9842700	14.2625659	-3.6503505
H	-0.6752760	13.5865987	-4.4651986
C	-4.3203994	15.3526485	1.5339900
H	-3.7593520	16.2128949	1.9457844
C	-4.3558563	16.0457371	-5.7628236
H	-3.8191668	16.6169958	-6.5376046
H	-4.5988445	16.7526533	-4.9533725
C	-6.9699211	19.3048086	-2.4537488
H	-6.2617599	19.8747851	-3.0778699
C	-7.2621331	18.2861899	0.3239928
H	-7.7872468	19.0267948	0.9425499
H	-8.0255658	17.8012248	-0.2993275
C	-3.2379243	22.4183332	-6.0156772
H	-2.8188819	23.0899615	-6.7767117
H	-3.3530934	23.0182916	-5.0977347
C	-2.2548670	21.2719888	-5.7433293
H	-1.2952117	21.6750606	-5.3920221
H	-2.0511388	20.7355663	-6.6844279
C	-4.2095508	19.7533530	-5.1554581
H	-4.0993863	19.1553715	-6.0742134
H	-4.6108447	19.0763647	-4.3847665
C	1.0241504	13.7201241	-2.2018783
H	1.4175989	12.9887063	-2.9263213
H	1.8938484	14.1584457	-1.6941017
C	-7.1281580	13.9191502	0.0133633
H	-7.6994959	14.3288430	0.8582871
H	-6.3872393	13.2233152	0.4350258
C	-5.6882632	20.8157324	-0.1966072
H	-6.6089163	21.4208707	-0.1590603
C	-0.4492312	20.5998933	-2.4398949

H	-1.1365274	21.4071819	-2.7312437
H	-0.9600817	19.9935067	-1.6754206
C	0.8309474	21.1966509	-1.8420078
H	1.2830408	21.8901729	-2.5696699
H	0.5734264	21.7962817	-0.9578240
C	-2.1491013	17.8578505	-0.2404696
C	-7.1536272	17.9186719	-3.0968425
H	-6.1828767	17.4013510	-3.1614930
H	-7.8022607	17.3006074	-2.4538391
C	-4.6060873	21.8920647	-6.4576262
H	-4.5064065	21.3834287	-7.4305839
H	-5.3032371	22.7261689	-6.6131296
C	-8.2943056	20.0808347	-2.3795514
H	-8.1309841	21.0833586	-1.9598094
H	-8.9884628	19.5596304	-1.7000913
C	-4.6797095	21.4663956	-1.1650257
H	-5.1372776	21.6081661	-2.1550689
H	-3.8288502	20.7732725	-1.3024289
C	-3.1110187	13.8961469	-6.3198956
H	-2.4922309	13.0856888	-5.9098420
H	-2.5197916	14.3786551	-7.1152302
C	2.1753768	19.2464610	-2.7044857
H	2.6751756	19.8675579	-3.4657297
H	2.8819779	18.4490622	-2.4366272
C	-4.5776877	22.0301929	1.7394900
H	-5.4229363	22.7250947	1.8677601
H	-4.1345658	21.8903934	2.7347860
C	-9.1246488	18.8087385	-4.4123533
H	-9.5532481	18.9145184	-5.4178984
H	-9.8555837	18.2310999	-3.8225635
C	-5.0464193	14.6679190	2.7042047
H	-5.7523673	15.3599969	3.1842497
H	-5.6345447	13.8179546	2.3315110
C	0.1152738	13.0092932	-1.1965082
H	0.6678490	12.2170615	-0.6740407
H	-0.2061921	13.7332120	-0.4291810
C	-7.8051306	18.0327169	-4.4790705
H	-7.1085255	18.5444420	-5.1626394
H	-7.9679110	17.0278103	-4.8925397
C	1.8418498	20.1048862	-1.4814019
H	1.4198997	19.4616360	-0.6917465
H	2.7557077	20.5548804	-1.0713745
C	-3.5577499	22.6399869	0.7736410
H	-3.2081217	23.6091811	1.1527852
H	-2.6703742	21.9862210	0.7165798
C	-5.5960138	14.4647827	-1.9364439
H	-4.8053870	13.7987671	-1.5584606
H	-5.0874784	15.2822245	-2.4706526
C	-5.1016687	20.6853610	1.2218373
H	-4.2697062	19.9589406	1.1950167
H	-5.8571775	20.2826411	1.9121966
C	-6.3940992	15.0331823	-0.7494519
H	-7.1564898	15.7148849	-1.1702057
C	-4.1572204	22.8022566	-0.6256182
C	-7.2841174	12.5834680	-2.1335552
H	-7.9704333	12.0683767	-2.8188483
H	-6.5698694	11.8231364	-1.7768900
C	-8.0559850	13.1509404	-0.9379563

H	-8.5605043	12.3446154	-0.3889878
H	-8.8482431	13.8285995	-1.2971911
C	-1.8902805	13.4992547	-2.6632228
H	-2.7393885	13.0438607	-3.1925821
H	-2.3116504	14.2245958	-1.9459380
C	-4.0212294	14.1641296	3.7304290
H	-3.5023994	15.0279354	4.1780417
H	-4.5450088	13.6550944	4.5506816
C	-5.6350445	15.4635634	-6.3741214
H	-6.2513632	16.2758042	-6.7837055
H	-6.2273157	14.9880307	-5.5756648
C	-2.9942286	13.2283996	3.0847313
H	-3.5037860	12.3159144	2.7330750
H	-2.2562522	12.9039257	3.8303207
C	-3.2951922	14.4180138	0.8677720
H	-3.8234960	13.5636821	0.4153653
H	-2.7721232	14.9467481	0.0567443
C	-8.9333990	20.1872094	-3.7716591
H	-9.8949032	20.7121254	-3.6949370
H	-8.2884787	20.8072001	-4.4152228
C	-4.4003035	13.3233140	-6.9259543
H	-4.1472994	12.6138520	-7.7250136
H	-4.9338670	12.7459288	-6.1527555
C	-6.5191645	13.6835939	-2.8769986
H	-5.9329994	13.2507838	-3.7012729
H	-7.2362753	14.3842207	-3.3377111
C	-5.3142621	14.4307395	-7.4596648
H	-6.2423929	13.9978219	-7.8559617
H	-4.8200498	14.9347084	-8.3066589
C	-1.1149402	12.4240591	-1.8937422
H	-1.7864099	11.9456203	-1.1663205
H	-0.7997322	11.6332214	-2.5931139
C	-2.2891198	13.9020551	1.9031695
H	-1.6844754	14.7495026	2.2656486
H	-1.5908202	13.2038046	1.4217407
C	-1.6475158	18.3168475	1.0962370
N	-1.4094893	17.3633908	-1.1532249
C	-0.1304652	19.7017997	-3.6521629
H	0.2613535	20.3265223	-4.4733655
C	0.9090008	18.6205411	-3.3011372
H	1.1688471	18.0394901	-4.1983355
H	0.4682534	17.9293475	-2.5651558
C	0.2649306	14.8260128	-2.9443166
H	0.9320477	15.3093553	-3.6717187
H	-0.0434995	15.5999834	-2.2216736
C	-0.9304567	16.5235472	-5.6186015
H	0.0968177	16.4479621	-5.2399136
H	-0.9563399	15.9873660	-6.5773178
C	-1.3089378	18.0043844	-5.8264815
H	-2.2106326	18.0825268	-6.4481869
H	-0.5045671	18.5212976	-6.3676306
C	-3.4445416	14.9264676	-5.2308608
H	-3.9875635	14.4139050	-4.4181123
C	-2.8391045	20.2899686	-4.7142004
H	-2.9841966	20.8245033	-3.7589965
C	-6.5583169	17.2447701	1.2138614
H	-7.3009787	16.6231857	1.7325411
H	-5.9592986	17.7432580	1.9897168

H	-4.9841936	23.5292913	-0.5899439
H	-3.4122553	23.2112255	-1.3226914
H	-0.5816117	18.0840829	1.2242410
H	-2.2253819	17.8623014	1.9141540
H	-1.7905340	19.4051611	1.1858095

SCF energy GEOOPT = -7389.017622100 H

ZPE = 3716. kJ/mol

FREEH energy = 3903.63 kJ/mol

FREEH entropy = 1.61005 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.64	0.04883	YES	YES
8		a	18.41	0.05663	YES	YES
9		a	21.52	0.07816	YES	YES
10		a	22.56	0.01737	YES	YES
11		a	26.88	0.01137	YES	YES
12		a	28.74	0.05278	YES	YES
13		a	30.10	0.18842	YES	YES
14		a	33.62	0.06499	YES	YES
15		a	36.52	0.01367	YES	YES
16		a	36.90	0.02061	YES	YES
17		a	38.84	0.04729	YES	YES
18		a	44.13	0.04945	YES	YES
19		a	45.04	0.07364	YES	YES
20		a	45.96	0.01488	YES	YES
21		a	49.75	0.09731	YES	YES
22		a	51.24	0.11849	YES	YES
23		a	55.61	0.41745	YES	YES
24		a	55.92	0.06585	YES	YES
25		a	59.80	0.29108	YES	YES
26		a	62.30	0.20116	YES	YES
27		a	63.19	0.29464	YES	YES
28		a	66.15	0.05564	YES	YES
29		a	68.65	0.15890	YES	YES
30		a	73.53	0.16444	YES	YES
31		a	75.77	0.21415	YES	YES
32		a	77.51	0.30471	YES	YES
33		a	85.75	0.74210	YES	YES
34		a	87.45	0.48940	YES	YES
35		a	91.53	0.19794	YES	YES
36		a	94.28	1.12795	YES	YES
37		a	101.24	0.26515	YES	YES
38		a	115.91	0.33491	YES	YES
39		a	124.07	1.00492	YES	YES
40		a	129.60	0.39453	YES	YES
41		a	134.33	0.29132	YES	YES
42		a	135.30	1.52134	YES	YES
43		a	137.78	1.79887	YES	YES
44		a	140.25	0.31831	YES	YES

45	a	142.48	0.52844	YES	YES
46	a	152.83	0.15218	YES	YES
47	a	156.72	1.60496	YES	YES
48	a	165.35	0.22765	YES	YES
49	a	170.99	0.31276	YES	YES
50	a	179.10	2.62641	YES	YES
51	a	182.92	0.18755	YES	YES
52	a	187.07	0.37662	YES	YES
53	a	195.83	2.31462	YES	YES
54	a	206.57	7.78124	YES	YES
55	a	209.25	1.81686	YES	YES
56	a	211.14	1.08994	YES	YES
57	a	216.57	1.80918	YES	YES
58	a	216.88	0.07632	YES	YES
59	a	220.38	1.09136	YES	YES
60	a	222.23	2.62803	YES	YES
61	a	224.29	0.55063	YES	YES
62	a	225.32	0.82179	YES	YES
63	a	228.67	0.08217	YES	YES
64	a	230.37	6.28211	YES	YES
65	a	232.64	1.09148	YES	YES
66	a	236.79	0.69141	YES	YES
67	a	239.76	0.66549	YES	YES
68	a	242.85	0.19815	YES	YES
69	a	246.37	0.83440	YES	YES
70	a	255.52	1.92106	YES	YES
71	a	275.91	2.12425	YES	YES
72	a	279.20	0.28839	YES	YES
73	a	283.40	0.17379	YES	YES
74	a	292.15	8.04355	YES	YES
75	a	294.68	20.28974	YES	YES
76	a	302.51	6.05629	YES	YES
77	a	305.14	2.10399	YES	YES
78	a	311.42	0.18314	YES	YES
79	a	314.42	0.82262	YES	YES
80	a	328.78	0.48296	YES	YES
81	a	329.82	0.91340	YES	YES
82	a	333.53	0.23195	YES	YES
83	a	336.30	0.20017	YES	YES
84	a	340.63	0.37825	YES	YES
85	a	342.90	1.22076	YES	YES
86	a	371.86	0.72960	YES	YES
87	a	374.20	1.98574	YES	YES
88	a	375.70	3.44159	YES	YES
89	a	380.29	1.28208	YES	YES
90	a	393.46	0.43381	YES	YES
91	a	394.68	1.20676	YES	YES
92	a	404.47	7.98572	YES	YES
93	a	407.11	0.85185	YES	YES
94	a	410.46	2.18055	YES	YES
95	a	413.13	0.80890	YES	YES
96	a	420.62	3.68634	YES	YES
97	a	422.77	1.94610	YES	YES
98	a	424.31	2.39302	YES	YES
99	a	427.33	0.33749	YES	YES
100	a	429.48	0.01243	YES	YES
101	a	429.89	0.20643	YES	YES
102	a	430.18	0.13319	YES	YES

103	a	430.53	0.26534	YES	YES
104	a	432.02	0.46596	YES	YES
105	a	432.36	0.73197	YES	YES
106	a	434.98	0.95184	YES	YES
107	a	438.34	0.20933	YES	YES
108	a	445.28	2.14306	YES	YES
109	a	456.43	4.02726	YES	YES
110	a	461.35	5.21779	YES	YES
111	a	471.14	4.00949	YES	YES
112	a	491.64	3.50925	YES	YES
113	a	493.24	4.44995	YES	YES
114	a	494.80	4.83915	YES	YES
115	a	496.21	0.26583	YES	YES
116	a	502.83	1.85369	YES	YES
117	a	503.90	0.59769	YES	YES
118	a	513.64	6.52394	YES	YES
119	a	514.93	14.05281	YES	YES
120	a	620.44	60.47473	YES	YES
121	a	625.48	10.88697	YES	YES
122	a	631.60	20.49765	YES	YES
123	a	640.49	10.75620	YES	YES
124	a	656.33	12.50079	YES	YES
125	a	699.29	2.13160	YES	YES
126	a	718.30	1.82624	YES	YES
127	a	725.90	1.59696	YES	YES
128	a	729.23	4.12438	YES	YES
129	a	732.89	8.74392	YES	YES
130	a	736.91	1.83415	YES	YES
131	a	739.69	3.44434	YES	YES
132	a	741.68	3.46878	YES	YES
133	a	770.22	1.44274	YES	YES
134	a	771.05	0.99663	YES	YES
135	a	772.22	0.57036	YES	YES
136	a	772.95	1.42184	YES	YES
137	a	773.88	0.03860	YES	YES
138	a	775.28	0.26823	YES	YES
139	a	776.17	11.34837	YES	YES
140	a	776.26	0.77799	YES	YES
141	a	777.19	3.33710	YES	YES
142	a	778.46	12.12734	YES	YES
143	a	805.73	0.24284	YES	YES
144	a	808.15	4.01350	YES	YES
145	a	808.81	9.93945	YES	YES
146	a	810.96	3.80589	YES	YES
147	a	811.72	0.10916	YES	YES
148	a	813.05	3.35571	YES	YES
149	a	814.88	1.66549	YES	YES
150	a	816.58	4.48479	YES	YES
151	a	830.34	4.68730	YES	YES
152	a	831.32	5.81545	YES	YES
153	a	836.19	1.06114	YES	YES
154	a	837.71	3.01418	YES	YES
155	a	838.07	1.75566	YES	YES
156	a	838.62	0.89778	YES	YES
157	a	838.93	6.64348	YES	YES
158	a	839.92	5.67576	YES	YES
159	a	847.54	15.12049	YES	YES
160	a	852.50	13.94880	YES	YES

161	a	868.99	3.76531	YES	YES
162	a	870.92	1.37949	YES	YES
163	a	872.91	3.09562	YES	YES
164	a	875.80	0.48271	YES	YES
165	a	876.51	1.56802	YES	YES
166	a	877.66	3.12820	YES	YES
167	a	878.07	3.68536	YES	YES
168	a	878.99	2.68405	YES	YES
169	a	879.11	2.43245	YES	YES
170	a	880.51	0.77731	YES	YES
171	a	880.83	3.84672	YES	YES
172	a	881.26	0.82880	YES	YES
173	a	882.47	3.93982	YES	YES
174	a	883.39	11.88328	YES	YES
175	a	884.92	5.85091	YES	YES
176	a	886.33	0.26103	YES	YES
177	a	901.93	2.63465	YES	YES
178	a	902.95	0.84110	YES	YES
179	a	903.79	0.85107	YES	YES
180	a	904.26	4.49654	YES	YES
181	a	906.67	3.52487	YES	YES
182	a	908.94	1.21146	YES	YES
183	a	910.37	2.01090	YES	YES
184	a	911.06	0.48362	YES	YES
185	a	934.72	19.88313	YES	YES
186	a	969.23	4.37165	YES	YES
187	a	977.07	0.39112	YES	YES
188	a	977.70	0.06903	YES	YES
189	a	986.95	2.29292	YES	YES
190	a	987.35	14.55294	YES	YES
191	a	988.24	11.16761	YES	YES
192	a	988.59	8.03933	YES	YES
193	a	989.23	2.99420	YES	YES
194	a	990.08	10.46381	YES	YES
195	a	991.09	9.01993	YES	YES
196	a	991.91	22.08582	YES	YES
197	a	1013.18	0.44136	YES	YES
198	a	1014.79	2.46083	YES	YES
199	a	1015.46	0.07175	YES	YES
200	a	1016.49	0.67777	YES	YES
201	a	1017.23	0.22193	YES	YES
202	a	1019.76	1.11092	YES	YES
203	a	1019.91	0.40207	YES	YES
204	a	1022.30	0.47809	YES	YES
205	a	1027.63	1.28919	YES	YES
206	a	1028.53	0.91838	YES	YES
207	a	1030.28	0.98566	YES	YES
208	a	1035.43	1.59409	YES	YES
209	a	1037.72	3.60574	YES	YES
210	a	1038.06	1.69660	YES	YES
211	a	1039.73	2.92895	YES	YES
212	a	1040.24	0.39369	YES	YES
213	a	1054.35	9.02646	YES	YES
214	a	1057.50	11.81945	YES	YES
215	a	1059.68	1.99364	YES	YES
216	a	1060.10	7.36869	YES	YES
217	a	1060.38	7.25884	YES	YES
218	a	1062.29	32.89306	YES	YES

219	a	1064.99	7.19078	YES	YES
220	a	1066.47	2.04223	YES	YES
221	a	1069.62	0.52206	YES	YES
222	a	1069.98	0.50998	YES	YES
223	a	1071.74	0.18915	YES	YES
224	a	1071.82	0.08648	YES	YES
225	a	1071.90	0.46554	YES	YES
226	a	1072.54	0.32464	YES	YES
227	a	1072.71	0.32999	YES	YES
228	a	1073.37	0.03068	YES	YES
229	a	1073.94	0.12033	YES	YES
230	a	1077.35	5.50797	YES	YES
231	a	1081.65	3.10621	YES	YES
232	a	1087.42	6.61228	YES	YES
233	a	1091.29	4.78125	YES	YES
234	a	1093.81	0.79464	YES	YES
235	a	1095.03	4.66224	YES	YES
236	a	1102.12	0.83567	YES	YES
237	a	1102.52	3.40850	YES	YES
238	a	1110.75	9.35711	YES	YES
239	a	1115.08	8.44616	YES	YES
240	a	1121.97	1.06202	YES	YES
241	a	1129.82	3.78224	YES	YES
242	a	1158.50	4.23515	YES	YES
243	a	1159.58	1.52537	YES	YES
244	a	1160.90	7.34004	YES	YES
245	a	1165.83	7.14365	YES	YES
246	a	1166.61	7.89086	YES	YES
247	a	1167.34	10.12959	YES	YES
248	a	1168.89	12.33977	YES	YES
249	a	1170.16	3.93332	YES	YES
250	a	1172.41	7.03849	YES	YES
251	a	1174.37	9.06243	YES	YES
252	a	1178.05	5.92831	YES	YES
253	a	1179.13	7.14767	YES	YES
254	a	1186.99	0.36300	YES	YES
255	a	1188.62	1.54203	YES	YES
256	a	1191.33	0.95365	YES	YES
257	a	1210.19	1.19245	YES	YES
258	a	1236.27	0.70496	YES	YES
259	a	1240.76	0.35702	YES	YES
260	a	1241.30	0.35680	YES	YES
261	a	1245.38	0.20002	YES	YES
262	a	1246.63	0.07369	YES	YES
263	a	1247.16	0.58296	YES	YES
264	a	1248.29	0.16263	YES	YES
265	a	1249.02	1.88257	YES	YES
266	a	1249.66	0.72900	YES	YES
267	a	1252.24	1.42641	YES	YES
268	a	1252.63	0.40892	YES	YES
269	a	1254.75	3.06917	YES	YES
270	a	1255.56	2.53107	YES	YES
271	a	1255.73	5.79036	YES	YES
272	a	1256.05	0.33122	YES	YES
273	a	1256.26	1.50557	YES	YES
274	a	1256.95	3.91914	YES	YES
275	a	1257.21	2.59761	YES	YES
276	a	1258.47	1.62621	YES	YES

277	a	1258.95	0.27685	YES	YES
278	a	1260.52	1.43049	YES	YES
279	a	1261.26	3.96993	YES	YES
280	a	1262.30	2.10936	YES	YES
281	a	1263.53	0.31881	YES	YES
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283	a	1267.26	1.60679	YES	YES
284	a	1269.60	1.02687	YES	YES
285	a	1272.32	1.85443	YES	YES
286	a	1280.29	1.67195	YES	YES
287	a	1281.48	0.49510	YES	YES
288	a	1283.29	3.67597	YES	YES
289	a	1284.10	7.17397	YES	YES
290	a	1284.62	0.88898	YES	YES
291	a	1287.14	4.24037	YES	YES
292	a	1289.37	3.00596	YES	YES
293	a	1291.77	3.31856	YES	YES
294	a	1304.57	0.47937	YES	YES
295	a	1309.65	1.66302	YES	YES
296	a	1310.14	1.09657	YES	YES
297	a	1311.14	0.93730	YES	YES
298	a	1312.86	1.87702	YES	YES
299	a	1313.29	0.68876	YES	YES
300	a	1317.99	0.20683	YES	YES
301	a	1319.53	3.32505	YES	YES
302	a	1320.44	0.77630	YES	YES
303	a	1320.74	0.47853	YES	YES
304	a	1321.78	0.75437	YES	YES
305	a	1321.96	0.14792	YES	YES
306	a	1323.58	1.66583	YES	YES
307	a	1323.97	1.55751	YES	YES
308	a	1324.27	1.09512	YES	YES
309	a	1324.50	1.35778	YES	YES
310	a	1325.07	2.96560	YES	YES
311	a	1325.33	1.90501	YES	YES
312	a	1325.85	1.53331	YES	YES
313	a	1326.48	3.65094	YES	YES
314	a	1327.52	7.40155	YES	YES
315	a	1329.11	1.41456	YES	YES
316	a	1331.88	9.49989	YES	YES
317	a	1336.13	0.29362	YES	YES
318	a	1336.34	0.06874	YES	YES
319	a	1336.78	0.16597	YES	YES
320	a	1337.28	0.50013	YES	YES
321	a	1337.75	0.43464	YES	YES
322	a	1338.57	0.22034	YES	YES
323	a	1338.84	0.67371	YES	YES
324	a	1339.05	0.48232	YES	YES
325	a	1340.00	0.30231	YES	YES
326	a	1342.13	1.08958	YES	YES
327	a	1343.83	0.13193	YES	YES
328	a	1344.86	0.66695	YES	YES
329	a	1345.37	1.49325	YES	YES
330	a	1345.61	0.96377	YES	YES
331	a	1346.64	2.65293	YES	YES
332	a	1347.01	0.50245	YES	YES
333	a	1347.47	0.88242	YES	YES
334	a	1350.01	0.95150	YES	YES

335	a	1400.47	7.40521	YES	YES
336	a	1404.44	7.58656	YES	YES
337	a	1404.66	8.31742	YES	YES
338	a	1406.93	17.30723	YES	YES
339	a	1409.16	11.69148	YES	YES
340	a	1415.63	11.40858	YES	YES
341	a	1423.34	5.25614	YES	YES
342	a	1426.79	5.32552	YES	YES
343	a	1426.98	0.73240	YES	YES
344	a	1429.40	1.71175	YES	YES
345	a	1431.14	1.94379	YES	YES
346	a	1431.70	1.73698	YES	YES
347	a	1432.20	3.32962	YES	YES
348	a	1433.31	2.76844	YES	YES
349	a	1435.16	3.72702	YES	YES
350	a	1435.47	2.56385	YES	YES
351	a	1435.82	4.28664	YES	YES
352	a	1436.56	6.12995	YES	YES
353	a	1436.72	4.77669	YES	YES
354	a	1436.91	8.18518	YES	YES
355	a	1437.63	2.77624	YES	YES
356	a	1438.17	14.26703	YES	YES
357	a	1438.33	5.81959	YES	YES
358	a	1438.69	4.84349	YES	YES
359	a	1438.82	2.26762	YES	YES
360	a	1438.96	4.10287	YES	YES
361	a	1439.55	2.54551	YES	YES
362	a	1439.98	8.53234	YES	YES
363	a	1440.17	3.98706	YES	YES
364	a	1441.90	9.10643	YES	YES
365	a	1442.69	14.19176	YES	YES
366	a	1443.30	6.40466	YES	YES
367	a	1443.83	23.19729	YES	YES
368	a	1444.23	13.73167	YES	YES
369	a	1444.53	18.53765	YES	YES
370	a	1444.87	0.99718	YES	YES
371	a	1445.24	2.35466	YES	YES
372	a	1447.77	10.07392	YES	YES
373	a	1452.69	3.31411	YES	YES
374	a	1453.56	2.05996	YES	YES
375	a	1453.75	1.05667	YES	YES
376	a	1453.92	1.02397	YES	YES
377	a	1455.31	1.39905	YES	YES
378	a	1455.99	3.59897	YES	YES
379	a	1456.60	2.31805	YES	YES
380	a	1459.29	1.34333	YES	YES
381	a	1570.28	146.99778	YES	YES
382	a	2909.35	19.22158	YES	YES
383	a	2912.87	3.40088	YES	YES
384	a	2920.28	3.04743	YES	YES
385	a	2923.79	13.00602	YES	YES
386	a	2929.76	21.51867	YES	YES
387	a	2934.00	29.63977	YES	YES
388	a	2934.19	12.50547	YES	YES
389	a	2936.36	4.21166	YES	YES
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391	a	2937.53	11.53104	YES	YES
392	a	2938.28	6.83827	YES	YES

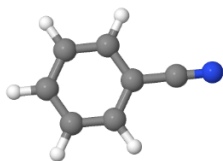
393	a	2938.98	34.98136	YES	YES
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396	a	2944.60	8.48432	YES	YES
397	a	2945.21	12.79226	YES	YES
398	a	2946.12	3.84136	YES	YES
399	a	2946.13	12.19369	YES	YES
400	a	2946.52	0.94840	YES	YES
401	a	2946.66	15.65936	YES	YES
402	a	2946.85	6.90356	YES	YES
403	a	2947.73	14.81066	YES	YES
404	a	2948.29	11.08144	YES	YES
405	a	2948.42	18.15623	YES	YES
406	a	2948.79	2.90097	YES	YES
407	a	2949.61	32.83775	YES	YES
408	a	2951.45	11.90182	YES	YES
409	a	2951.65	7.46363	YES	YES
410	a	2953.53	3.00920	YES	YES
411	a	2953.94	1.79586	YES	YES
412	a	2955.28	2.72302	YES	YES
413	a	2955.96	4.97095	YES	YES
414	a	2956.12	7.45572	YES	YES
415	a	2957.27	18.63838	YES	YES
416	a	2957.82	1.95141	YES	YES
417	a	2958.70	3.51228	YES	YES
418	a	2959.09	10.52463	YES	YES
419	a	2959.49	26.54050	YES	YES
420	a	2959.65	20.45039	YES	YES
421	a	2959.90	4.77894	YES	YES
422	a	2960.57	32.96611	YES	YES
423	a	2960.70	17.45429	YES	YES
424	a	2961.37	33.50358	YES	YES
425	a	2961.78	59.60477	YES	YES
426	a	2962.47	18.96868	YES	YES
427	a	2962.58	29.12400	YES	YES
428	a	2964.74	1.47168	YES	YES
429	a	2965.17	20.87522	YES	YES
430	a	2978.06	7.59093	YES	YES
431	a	2979.97	34.22705	YES	YES
432	a	2980.24	4.95763	YES	YES
433	a	2984.13	15.79671	YES	YES
434	a	2985.82	4.56028	YES	YES
435	a	2986.25	6.97892	YES	YES
436	a	2987.62	39.27811	YES	YES
437	a	2987.75	29.71745	YES	YES
438	a	2989.66	11.45682	YES	YES
439	a	2990.99	24.62464	YES	YES
440	a	2994.55	20.48665	YES	YES
441	a	2995.88	17.56796	YES	YES
442	a	2997.44	35.23137	YES	YES
443	a	2999.81	22.07126	YES	YES
444	a	3000.23	31.80287	YES	YES
445	a	3002.76	7.53422	YES	YES
446	a	3003.43	22.21170	YES	YES
447	a	3003.72	30.78953	YES	YES
448	a	3005.02	21.09763	YES	YES
449	a	3005.71	21.90740	YES	YES
450	a	3006.20	20.62735	YES	YES

451	a	3006.69	15.93016	YES	YES
452	a	3009.13	16.32788	YES	YES
453	a	3009.18	21.75649	YES	YES
454	a	3009.25	21.89816	YES	YES
455	a	3010.18	17.31359	YES	YES
456	a	3010.23	11.34524	YES	YES
457	a	3010.87	21.45153	YES	YES
458	a	3012.33	29.04403	YES	YES
459	a	3012.44	20.51608	YES	YES
460	a	3014.47	19.86286	YES	YES
461	a	3015.01	19.46602	YES	YES
462	a	3015.33	17.80355	YES	YES
463	a	3016.32	19.65524	YES	YES
464	a	3016.45	28.57043	YES	YES
465	a	3016.86	28.16573	YES	YES
466	a	3017.06	25.94595	YES	YES
467	a	3017.29	23.17833	YES	YES
468	a	3017.57	24.33446	YES	YES
469	a	3018.14	20.79165	YES	YES
470	a	3018.39	25.53827	YES	YES
471	a	3018.44	8.94328	YES	YES
472	a	3018.57	39.11859	YES	YES
473	a	3019.09	24.00755	YES	YES
474	a	3019.20	33.03766	YES	YES
475	a	3024.31	20.64434	YES	YES
476	a	3025.68	11.62290	YES	YES
477	a	3029.67	0.47216	YES	YES
478	a	3036.43	1.18054	YES	YES
479	a	3038.76	10.67019	YES	YES
480	a	3043.87	0.27687	YES	YES

\$end

Double hybrid single point energy = -7381.660502283365 H
 COSMO energy + OC correction = -7389.1667075968 H (in oDFB)

6.2.43 PhCN



Method: /def2-TZVPP
 Symmetry: c2v

Cartesian coordinates in Ångström:

N	0.0000000	0.0000000	-3.6582627
C	0.0000000	0.0000000	1.7296030
C	0.0000000	0.0000000	-2.4927647
C	-1.2113566	0.0000000	1.0321792
C	1.2113566	0.0000000	1.0321792
C	-1.2185765	0.0000000	-0.3605540
C	1.2185765	0.0000000	-0.3605540
C	0.0000000	0.0000000	-1.0634635
H	0.0000000	0.0000000	2.8192397

H	-2.1554361	0.0000000	1.5757986
H	2.1554361	0.0000000	1.5757986
H	-2.1559489	0.0000000	-0.9141959
H	2.1559489	0.0000000	-0.9141959

SCF energy GEOOPT = -324.6460562709 H

ZPE = 253.2 kJ/mol

FREEH energy = 269.61 kJ/mol

FREEH entropy = 0.32567 kJ/mol/K

\$vibrational spectrum

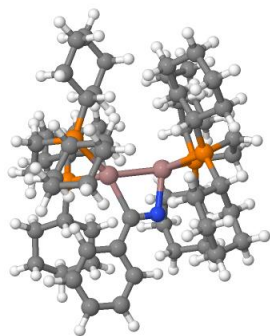
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#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b2	138.99	1.70591	YES	YES
8		b1	160.11	4.11861	YES	YES
9		b2	374.94	0.42485	YES	YES
10		a2	392.80	0.00000	NO	YES
11		a1	454.45	0.00079	YES	YES
12		b1	551.14	0.11741	YES	YES
13		b2	551.53	16.48498	YES	YES
14		b1	621.31	0.13006	YES	YES
15		b2	686.21	35.42973	YES	YES
16		b2	754.65	36.42336	YES	YES
17		a1	757.11	1.74200	YES	YES
18		a2	831.75	0.00000	NO	YES
19		b2	914.93	3.27362	YES	YES
20		a2	958.30	0.00000	NO	YES
21		b2	980.33	0.05600	YES	YES
22		a1	994.20	0.26028	YES	YES
23		a1	1025.33	3.62139	YES	YES
24		b1	1077.25	4.54144	YES	YES
25		b1	1155.83	0.04640	YES	YES
26		a1	1168.45	0.72867	YES	YES
27		a1	1195.11	0.48480	YES	YES
28		b1	1301.83	0.05302	YES	YES
29		b1	1337.25	1.28358	YES	YES
30		b1	1437.06	6.27502	YES	YES
31		a1	1480.55	7.40501	YES	YES
32		b1	1570.04	1.11182	YES	YES
33		a1	1596.68	0.67923	YES	YES
34		a1	2244.73	24.68242	YES	YES
35		a1	3106.37	0.01611	YES	YES
36		b1	3116.29	3.85991	YES	YES
37		a1	3124.49	8.65743	YES	YES
38		b1	3133.31	7.45263	YES	YES
39		a1	3136.05	2.73495	YES	YES

\$end

Double hybrid single point energy = -324.058476872803 H

COSMO energy + OC correction = -324.6556969616 H (in oDFB)

6.2.44 $\{[Ga(dcpe)]_2(NCPh)\}^{2+}$ (Cycloadduct)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.6146066	17.2977245	-2.8358805
Ga	-4.0171652	17.8008193	-0.9181935
P	-1.6946771	18.9507195	-4.3222075
P	-5.9901436	19.1732293	-0.7851658
P	-2.0204154	15.6569466	-4.4652595
P	-5.2984871	16.1834038	0.3161008
C	-5.1922988	20.9174197	-5.4917933
H	-5.4067317	21.4370364	-4.5415497
H	-6.1491880	20.5132905	-5.8509989
C	-1.0538266	14.2788812	-3.7183955
H	-0.8123914	13.5569378	-4.5163896
C	-4.2340206	15.3661608	1.5716640
H	-3.6791365	16.2348941	1.9710942
C	-4.4087033	16.0667524	-5.8446826
H	-3.8820059	16.6620833	-6.6084475
H	-4.6628212	16.7537776	-5.0217827
C	-6.8519986	19.2675532	-2.4129537
H	-6.1424769	19.8188769	-3.0520920
C	-7.1526825	18.3236009	0.3861963
H	-7.6602704	19.0701551	1.0120122
H	-7.9295870	17.8525608	-0.2310245
C	-3.2611992	22.4549437	-6.0392825
H	-2.8445616	23.1417847	-6.7879660
H	-3.3881255	23.0403497	-5.1135168
C	-2.2679141	21.3149027	-5.7766475
H	-1.3146838	21.7220462	-5.4125064
H	-2.0521377	20.7936069	-6.7235882
C	-4.2115491	19.7695182	-5.2257000
H	-4.0878342	19.1873824	-6.1528615
H	-4.6109037	19.0753801	-4.4693176
C	0.9754112	13.6964748	-2.3132584
H	1.3037432	12.9086167	-3.0105323
H	1.8852796	14.1120385	-1.8591501
C	-7.0524864	13.9190915	0.0897527
H	-7.6225331	14.3318506	0.9340718
H	-6.3033904	13.2337927	0.5141092
C	-5.6592973	20.8919872	-0.2240014
H	-6.6081434	21.4523359	-0.2619462
C	-0.5111549	20.5423670	-2.4125675
H	-1.1895716	21.3647648	-2.6819743
H	-1.0456183	19.8972772	-1.6971306

C	0.7462556	21.1036003	-1.7377181
H	1.2224135	21.8391841	-2.4062728
H	0.4558246	21.6478416	-0.8284129
C	-2.0249977	17.6418403	-0.2943698
C	-7.0356622	17.8653155	-3.0164747
H	-6.0665282	17.3437210	-3.0606096
H	-7.6910186	17.2686432	-2.3607303
C	-4.6216730	21.9219604	-6.4976760
H	-4.5107808	21.4294030	-7.4776695
H	-5.3257274	22.7517198	-6.6451229
C	-8.1781226	20.0437598	-2.3669417
H	-8.0190908	21.0593524	-1.9789541
H	-8.8729406	19.5425572	-1.6731521
C	-4.6456346	21.5303727	-1.1951189
H	-5.0588631	21.5668261	-2.2139037
H	-3.7476615	20.8869280	-1.2363398
C	-3.1304256	13.9488780	-6.4436439
H	-2.4974761	13.1410825	-6.0505546
H	-2.5488948	14.4573376	-7.2298954
C	2.1267773	19.2148900	-2.6709947
H	2.6477752	19.8866137	-3.3726724
H	2.8300486	18.4054241	-2.4314942
C	-4.7332670	22.3138725	1.6583419
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C	-9.0012250	18.7134424	-4.3660766
H	-9.4260806	18.7907208	-5.3758601
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C	-4.9353724	14.6862184	2.7584808
H	-5.6661870	15.3632614	3.2228974
H	-5.4904139	13.8024274	2.4138519
C	0.0677856	13.0871723	-1.2422555
H	0.5986602	12.2981302	-0.6930058
H	-0.1970372	13.8665762	-0.5081078
C	-7.6788333	17.9412007	-4.4051528
H	-6.9803874	18.4378434	-5.0981872
H	-7.8354948	16.9253201	-4.7932054
C	1.7450527	19.9915156	-1.4079744
H	1.2929991	19.3012680	-0.6763902
H	2.6414427	20.4147291	-0.9354889
C	-3.7113651	22.9289378	0.6974589
H	-3.4584929	23.9493780	1.0139994
H	-2.7765118	22.3450190	0.7386695
C	-5.5353621	14.4567614	-1.8718142
H	-4.7427484	13.7966893	-1.4879223
H	-5.0288416	15.2702247	-2.4143100
C	-5.1237988	20.8981830	1.2170051
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C	-6.3321524	15.0319380	-0.6871885
H	-7.1007801	15.7061038	-1.1073757
C	-4.2422030	22.9373122	-0.7388956
C	-7.2115977	12.5656165	-2.0480632
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H	-8.7794761	13.8047047	-1.2095941

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C	-3.8827406	14.2592278	3.7925514
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H	-4.3775921	13.7576568	4.6351724
C	-5.6786787	15.4732582	-6.4645431
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H	-6.2585747	14.9702530	-5.6732290
C	-2.8222895	13.3451513	3.1695970
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H	-2.0650948	13.0795232	3.9194506
C	-3.1923125	14.4433188	0.9170426
H	-3.6967500	13.5566265	0.5003308
H	-2.6960843	14.9607379	0.0828959
C	-8.8159602	20.1088341	-3.7621469
H	-9.7793510	20.6323499	-3.7002646
H	-8.1726004	20.7135321	-4.4213432
C	-4.4100962	13.3657511	-7.0599357
H	-4.1455447	12.6766118	-7.8729446
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C	-6.4570060	13.6647278	-2.8041452
H	-5.8714257	13.2290280	-3.6276203
H	-7.1798215	14.3580331	-3.2670568
C	-5.3428569	14.4679501	-7.5709760
H	-6.2644811	14.0278103	-7.9744446
H	-4.8584155	14.9968685	-8.4083792
C	-1.2088966	12.5268043	-1.8724750
H	-1.8780399	12.1163933	-1.1024972
H	-0.9525599	11.6897352	-2.5414216
C	-2.1555315	14.0046770	1.9581032
H	-1.5859237	14.8910475	2.2817031
H	-1.4334261	13.3186185	1.4942900
N	-1.3610527	17.2111870	-1.2987242
C	-0.1552253	19.7114068	-3.6632849
H	0.2431872	20.3807174	-4.4448555
C	0.8867031	18.6206241	-3.3491976
H	1.1792251	18.1007071	-4.2735343
H	0.4320898	17.8797356	-2.6723988
C	0.2491696	14.8044484	-3.0852836
H	0.9144381	15.2116721	-3.8593917
H	0.0057748	15.6249603	-2.3904796
C	-0.9518484	16.5499589	-5.6833126
H	0.0681480	16.4646055	-5.2876609
H	-0.9654660	16.0202123	-6.6457508
C	-1.3130613	18.0356913	-5.8882571
H	-2.2092386	18.1262043	-6.5165432
H	-0.4991013	18.5464897	-6.4208411
C	-3.4796886	14.9524326	-5.3344336
H	-4.0160507	14.4153475	-4.5325824
C	-2.8504319	20.3138755	-4.7656766
H	-3.0081845	20.8338131	-3.8044591
C	-6.4571351	17.2688308	1.2663480
H	-7.2044095	16.6611477	1.7948395
H	-5.8400677	17.7556468	2.0358594
H	-5.1170047	23.6039273	-0.8049859
H	-3.4883915	23.3428573	-1.4284856
H	-2.4466665	18.7447924	4.2085264

C	-1.8119027	18.3580000	3.4119399
C	-2.2927738	18.2745200	2.1058292
H	-3.3108252	18.5908086	1.8678785
C	-1.4873690	17.7825492	1.0696614
C	-0.1738132	17.3723301	1.3647281
H	0.4412472	16.9839370	0.5534320
C	0.3080149	17.4485574	2.6681850
H	1.3235227	17.1235628	2.8930524
C	-0.5088298	17.9398215	3.6949003
H	-0.1274742	17.9970841	4.7137933

SCF energy GEOOPT = -7580.864035474 H

ZPE = 3854. kJ/mol

FREEH energy = 4049.59 kJ/mol

FREEH entropy = 1.67928 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	7.75	0.00619	YES	YES
	8	a	13.40	0.09086	YES	YES
	9	a	18.43	0.00352	YES	YES
	10	a	20.89	0.03009	YES	YES
	11	a	24.74	0.02910	YES	YES
	12	a	26.38	0.12933	YES	YES
	13	a	27.78	0.02095	YES	YES
	14	a	30.05	0.02127	YES	YES
	15	a	33.33	0.02486	YES	YES
	16	a	35.83	0.04031	YES	YES
	17	a	38.22	0.01987	YES	YES
	18	a	40.52	0.02642	YES	YES
	19	a	42.20	0.04865	YES	YES
	20	a	45.63	0.18416	YES	YES
	21	a	46.46	0.18356	YES	YES
	22	a	48.69	0.03436	YES	YES
	23	a	52.81	0.16873	YES	YES
	24	a	55.01	0.08504	YES	YES
	25	a	55.70	0.11780	YES	YES
	26	a	57.05	0.03195	YES	YES
	27	a	59.97	0.41309	YES	YES
	28	a	63.61	0.09653	YES	YES
	29	a	65.60	0.08564	YES	YES
	30	a	65.98	0.04874	YES	YES
	31	a	70.22	0.18271	YES	YES
	32	a	71.60	0.05726	YES	YES
	33	a	75.46	0.10575	YES	YES
	34	a	77.19	0.03395	YES	YES
	35	a	81.75	0.36612	YES	YES
	36	a	86.85	0.24274	YES	YES
	37	a	92.76	0.11737	YES	YES
	38	a	96.41	0.40643	YES	YES
	39	a	113.09	3.26649	YES	YES

40	a	118.10	1.22642	YES	YES
41	a	125.66	0.95438	YES	YES
42	a	130.18	0.88873	YES	YES
43	a	134.53	0.87259	YES	YES
44	a	137.20	3.56828	YES	YES
45	a	140.75	7.18866	YES	YES
46	a	141.10	0.32798	YES	YES
47	a	142.60	1.00126	YES	YES
48	a	154.44	0.38677	YES	YES
49	a	159.51	0.63061	YES	YES
50	a	166.23	0.04489	YES	YES
51	a	169.89	0.24687	YES	YES
52	a	177.31	2.40164	YES	YES
53	a	183.68	0.17317	YES	YES
54	a	185.32	1.77338	YES	YES
55	a	196.07	1.40303	YES	YES
56	a	208.69	0.22794	YES	YES
57	a	208.75	0.76648	YES	YES
58	a	214.03	7.66613	YES	YES
59	a	215.74	2.39558	YES	YES
60	a	218.24	1.32669	YES	YES
61	a	218.32	1.05743	YES	YES
62	a	222.45	2.00970	YES	YES
63	a	225.08	0.63814	YES	YES
64	a	225.92	1.21017	YES	YES
65	a	227.32	2.93720	YES	YES
66	a	228.84	2.31464	YES	YES
67	a	232.37	0.39843	YES	YES
68	a	236.06	2.74666	YES	YES
69	a	238.29	1.30823	YES	YES
70	a	242.42	4.61060	YES	YES
71	a	243.08	0.77607	YES	YES
72	a	250.80	0.77389	YES	YES
73	a	258.81	1.12669	YES	YES
74	a	277.11	2.01187	YES	YES
75	a	280.36	1.42892	YES	YES
76	a	284.54	2.34507	YES	YES
77	a	293.51	0.19973	YES	YES
78	a	302.77	1.05196	YES	YES
79	a	305.85	0.84726	YES	YES
80	a	310.62	0.11076	YES	YES
81	a	316.18	0.43289	YES	YES
82	a	328.74	0.43756	YES	YES
83	a	330.21	0.74291	YES	YES
84	a	333.63	0.51183	YES	YES
85	a	337.04	0.15885	YES	YES
86	a	341.46	0.62057	YES	YES
87	a	343.70	0.71282	YES	YES
88	a	372.07	0.49329	YES	YES
89	a	374.09	3.01619	YES	YES
90	a	377.15	2.00344	YES	YES
91	a	381.94	0.73794	YES	YES
92	a	393.36	0.01771	YES	YES
93	a	395.89	1.87321	YES	YES
94	a	399.03	0.57088	YES	YES
95	a	408.91	0.02117	YES	YES
96	a	410.50	1.03481	YES	YES
97	a	411.98	2.46471	YES	YES

98	a	419.26	0.86001	YES	YES
99	a	420.70	3.25155	YES	YES
100	a	423.69	2.16842	YES	YES
101	a	427.52	0.17604	YES	YES
102	a	429.21	0.08798	YES	YES
103	a	429.92	0.13045	YES	YES
104	a	430.53	0.18695	YES	YES
105	a	431.35	0.12593	YES	YES
106	a	431.54	0.34676	YES	YES
107	a	432.54	0.31461	YES	YES
108	a	434.71	1.45114	YES	YES
109	a	437.94	0.22064	YES	YES
110	a	441.16	0.43239	YES	YES
111	a	450.59	19.80895	YES	YES
112	a	455.02	1.47501	YES	YES
113	a	461.46	6.92356	YES	YES
114	a	471.88	3.14021	YES	YES
115	a	492.45	3.37499	YES	YES
116	a	494.04	2.33118	YES	YES
117	a	495.50	7.27456	YES	YES
118	a	496.60	0.89371	YES	YES
119	a	502.24	0.79951	YES	YES
120	a	504.01	0.95649	YES	YES
121	a	512.41	7.83587	YES	YES
122	a	515.39	12.20482	YES	YES
123	a	547.53	19.43559	YES	YES
124	a	558.25	4.35939	YES	YES
125	a	615.36	1.74054	YES	YES
126	a	623.85	18.24916	YES	YES
127	a	630.36	15.45684	YES	YES
128	a	640.05	11.15209	YES	YES
129	a	654.88	13.03229	YES	YES
130	a	677.47	64.87221	YES	YES
131	a	692.90	24.67630	YES	YES
132	a	699.92	2.21139	YES	YES
133	a	718.66	1.79618	YES	YES
134	a	724.92	1.52062	YES	YES
135	a	728.13	4.18842	YES	YES
136	a	734.16	7.14905	YES	YES
137	a	736.37	5.90203	YES	YES
138	a	739.62	1.83136	YES	YES
139	a	740.25	2.00920	YES	YES
140	a	761.67	39.24727	YES	YES
141	a	771.82	0.82684	YES	YES
142	a	772.32	2.69888	YES	YES
143	a	772.86	2.16813	YES	YES
144	a	773.64	0.83576	YES	YES
145	a	773.91	0.86694	YES	YES
146	a	775.48	0.50646	YES	YES
147	a	775.90	0.60856	YES	YES
148	a	776.45	18.04967	YES	YES
149	a	776.64	3.41854	YES	YES
150	a	779.75	1.81880	YES	YES
151	a	805.90	0.29737	YES	YES
152	a	807.63	3.90388	YES	YES
153	a	809.64	4.53317	YES	YES
154	a	809.74	10.05368	YES	YES
155	a	811.25	1.35726	YES	YES

156	a	812.84	2.31984	YES	YES
157	a	815.06	1.59693	YES	YES
158	a	816.47	3.44464	YES	YES
159	a	829.84	3.94835	YES	YES
160	a	831.61	5.69926	YES	YES
161	a	836.17	2.11903	YES	YES
162	a	836.98	3.90211	YES	YES
163	a	837.56	1.55645	YES	YES
164	a	838.04	2.40473	YES	YES
165	a	839.14	0.17792	YES	YES
166	a	839.95	3.43391	YES	YES
167	a	841.16	4.35342	YES	YES
168	a	847.44	16.28606	YES	YES
169	a	851.38	33.03518	YES	YES
170	a	861.07	48.87098	YES	YES
171	a	871.60	3.60070	YES	YES
172	a	872.13	1.80952	YES	YES
173	a	873.03	3.13287	YES	YES
174	a	875.52	0.23154	YES	YES
175	a	876.56	2.72459	YES	YES
176	a	877.19	2.98020	YES	YES
177	a	878.07	3.74296	YES	YES
178	a	879.23	1.96440	YES	YES
179	a	880.04	0.98904	YES	YES
180	a	880.26	5.76146	YES	YES
181	a	880.81	4.13725	YES	YES
182	a	881.88	0.46927	YES	YES
183	a	883.23	7.47484	YES	YES
184	a	883.61	12.17288	YES	YES
185	a	886.15	1.29105	YES	YES
186	a	886.71	5.52181	YES	YES
187	a	902.35	2.02339	YES	YES
188	a	903.04	0.72675	YES	YES
189	a	904.38	0.78992	YES	YES
190	a	904.61	2.24217	YES	YES
191	a	907.06	3.07922	YES	YES
192	a	909.31	1.96699	YES	YES
193	a	910.75	1.26788	YES	YES
194	a	912.67	1.47855	YES	YES
195	a	922.15	3.84523	YES	YES
196	a	966.37	0.38273	YES	YES
197	a	976.92	0.11731	YES	YES
198	a	977.62	0.19619	YES	YES
199	a	987.16	2.58752	YES	YES
200	a	988.11	18.62243	YES	YES
201	a	988.66	11.02424	YES	YES
202	a	988.92	0.59983	YES	YES
203	a	989.68	1.26238	YES	YES
204	a	990.10	7.53218	YES	YES
205	a	990.77	2.79475	YES	YES
206	a	991.79	30.13130	YES	YES
207	a	992.91	8.16639	YES	YES
208	a	996.45	3.63655	YES	YES
209	a	1012.48	0.23897	YES	YES
210	a	1014.82	0.74251	YES	YES
211	a	1015.46	1.50738	YES	YES
212	a	1015.91	0.88440	YES	YES
213	a	1017.40	0.20708	YES	YES

214	a	1018.44	4.24246	YES	YES
215	a	1019.16	0.76220	YES	YES
216	a	1020.44	0.65390	YES	YES
217	a	1023.17	0.47302	YES	YES
218	a	1028.93	1.08971	YES	YES
219	a	1029.04	0.78920	YES	YES
220	a	1029.98	1.23402	YES	YES
221	a	1035.63	1.06116	YES	YES
222	a	1038.33	2.30037	YES	YES
223	a	1039.19	3.02584	YES	YES
224	a	1039.98	0.52029	YES	YES
225	a	1040.78	0.67748	YES	YES
226	a	1054.85	0.70151	YES	YES
227	a	1058.46	1.52020	YES	YES
228	a	1059.21	0.65266	YES	YES
229	a	1060.19	1.21661	YES	YES
230	a	1060.98	2.36292	YES	YES
231	a	1063.96	0.97734	YES	YES
232	a	1067.38	0.61967	YES	YES
233	a	1068.77	3.55444	YES	YES
234	a	1069.35	0.44096	YES	YES
235	a	1070.95	0.79285	YES	YES
236	a	1071.23	0.38378	YES	YES
237	a	1071.39	0.20614	YES	YES
238	a	1072.10	0.21593	YES	YES
239	a	1072.53	0.23286	YES	YES
240	a	1072.93	0.04083	YES	YES
241	a	1073.39	0.06669	YES	YES
242	a	1075.20	0.51386	YES	YES
243	a	1076.96	3.59787	YES	YES
244	a	1082.74	3.93471	YES	YES
245	a	1090.50	6.50011	YES	YES
246	a	1091.11	5.06570	YES	YES
247	a	1093.76	5.83315	YES	YES
248	a	1096.26	1.64644	YES	YES
249	a	1101.89	0.74791	YES	YES
250	a	1103.36	3.00626	YES	YES
251	a	1110.94	9.14587	YES	YES
252	a	1115.98	6.94657	YES	YES
253	a	1121.38	1.97734	YES	YES
254	a	1128.52	7.18736	YES	YES
255	a	1145.23	19.98258	YES	YES
256	a	1155.35	1.92773	YES	YES
257	a	1158.70	3.78938	YES	YES
258	a	1159.87	2.40481	YES	YES
259	a	1161.14	8.54352	YES	YES
260	a	1164.51	7.40356	YES	YES
261	a	1167.18	8.44408	YES	YES
262	a	1167.93	14.67776	YES	YES
263	a	1168.46	10.30549	YES	YES
264	a	1169.95	4.57379	YES	YES
265	a	1173.45	8.73594	YES	YES
266	a	1174.70	5.65400	YES	YES
267	a	1178.20	6.59271	YES	YES
268	a	1182.30	4.79712	YES	YES
269	a	1188.33	0.50008	YES	YES
270	a	1188.58	1.51232	YES	YES
271	a	1191.31	1.15508	YES	YES

272	a	1198.12	51.34478	YES	YES
273	a	1215.62	1.18459	YES	YES
274	a	1235.70	0.60771	YES	YES
275	a	1240.21	0.25872	YES	YES
276	a	1242.24	0.60219	YES	YES
277	a	1246.28	0.10469	YES	YES
278	a	1246.82	0.04362	YES	YES
279	a	1247.98	0.93438	YES	YES
280	a	1248.18	0.32633	YES	YES
281	a	1249.48	0.30301	YES	YES
282	a	1251.89	1.86251	YES	YES
283	a	1252.07	1.07059	YES	YES
284	a	1252.51	0.17172	YES	YES
285	a	1254.18	3.74640	YES	YES
286	a	1255.23	1.86181	YES	YES
287	a	1255.69	3.88035	YES	YES
288	a	1255.86	2.88307	YES	YES
289	a	1256.09	1.17923	YES	YES
290	a	1257.64	4.63260	YES	YES
291	a	1257.74	1.04150	YES	YES
292	a	1258.84	0.61862	YES	YES
293	a	1259.18	2.52084	YES	YES
294	a	1260.11	0.58726	YES	YES
295	a	1261.12	2.92843	YES	YES
296	a	1261.63	2.49624	YES	YES
297	a	1264.23	0.58929	YES	YES
298	a	1266.09	2.16610	YES	YES
299	a	1270.16	1.01967	YES	YES
300	a	1272.84	0.78097	YES	YES
301	a	1274.93	1.18489	YES	YES
302	a	1280.24	2.27100	YES	YES
303	a	1281.87	0.55278	YES	YES
304	a	1283.00	4.71648	YES	YES
305	a	1284.11	0.86511	YES	YES
306	a	1286.63	9.47215	YES	YES
307	a	1287.91	11.03541	YES	YES
308	a	1288.40	3.12807	YES	YES
309	a	1289.11	3.36356	YES	YES
310	a	1293.52	3.25697	YES	YES
311	a	1305.48	0.45301	YES	YES
312	a	1308.51	0.99636	YES	YES
313	a	1310.20	1.02961	YES	YES
314	a	1310.70	2.57067	YES	YES
315	a	1311.43	0.43827	YES	YES
316	a	1312.65	1.72763	YES	YES
317	a	1319.79	4.25458	YES	YES
318	a	1320.83	0.42689	YES	YES
319	a	1321.16	0.80493	YES	YES
320	a	1321.62	1.19298	YES	YES
321	a	1321.79	0.55191	YES	YES
322	a	1322.19	0.31810	YES	YES
323	a	1323.21	1.77555	YES	YES
324	a	1323.68	0.22227	YES	YES
325	a	1324.16	1.69058	YES	YES
326	a	1324.30	1.05858	YES	YES
327	a	1324.52	2.25509	YES	YES
328	a	1325.67	5.43485	YES	YES
329	a	1326.08	1.98298	YES	YES

330	a	1326.64	0.85297	YES	YES
331	a	1327.48	7.67735	YES	YES
332	a	1329.93	2.54177	YES	YES
333	a	1335.99	0.27131	YES	YES
334	a	1336.16	0.05289	YES	YES
335	a	1337.22	0.28531	YES	YES
336	a	1337.43	0.80618	YES	YES
337	a	1337.82	0.05870	YES	YES
338	a	1338.80	0.14625	YES	YES
339	a	1340.18	0.21180	YES	YES
340	a	1340.31	0.28693	YES	YES
341	a	1340.64	0.54078	YES	YES
342	a	1343.09	0.46939	YES	YES
343	a	1343.85	0.61881	YES	YES
344	a	1345.16	0.72569	YES	YES
345	a	1345.59	1.74650	YES	YES
346	a	1346.12	1.36931	YES	YES
347	a	1346.46	0.19674	YES	YES
348	a	1346.95	0.59747	YES	YES
349	a	1347.41	2.04985	YES	YES
350	a	1347.81	0.39519	YES	YES
351	a	1350.96	0.98199	YES	YES
352	a	1399.11	8.17730	YES	YES
353	a	1404.82	5.09856	YES	YES
354	a	1405.04	8.49429	YES	YES
355	a	1406.79	8.80585	YES	YES
356	a	1422.43	4.94901	YES	YES
357	a	1426.42	5.74802	YES	YES
358	a	1428.24	1.69749	YES	YES
359	a	1429.99	1.95426	YES	YES
360	a	1430.92	1.84559	YES	YES
361	a	1431.54	1.66806	YES	YES
362	a	1432.48	2.34334	YES	YES
363	a	1433.40	5.02661	YES	YES
364	a	1434.12	1.35605	YES	YES
365	a	1435.49	13.23432	YES	YES
366	a	1435.54	2.18751	YES	YES
367	a	1436.26	7.09974	YES	YES
368	a	1436.75	6.44417	YES	YES
369	a	1437.12	12.14075	YES	YES
370	a	1437.56	1.59732	YES	YES
371	a	1437.81	18.93916	YES	YES
372	a	1438.29	13.12858	YES	YES
373	a	1438.39	5.85883	YES	YES
374	a	1438.64	1.62179	YES	YES
375	a	1438.95	4.10754	YES	YES
376	a	1439.20	1.49616	YES	YES
377	a	1439.67	1.10215	YES	YES
378	a	1440.07	9.53426	YES	YES
379	a	1440.14	0.28935	YES	YES
380	a	1441.73	7.61241	YES	YES
381	a	1442.59	13.09108	YES	YES
382	a	1443.14	7.60383	YES	YES
383	a	1444.26	19.14151	YES	YES
384	a	1444.41	24.28871	YES	YES
385	a	1444.83	10.01835	YES	YES
386	a	1445.31	3.00283	YES	YES
387	a	1445.52	1.89464	YES	YES

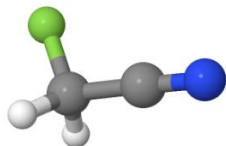
388	a	1447.16	7.01395	YES	YES
389	a	1452.64	2.99373	YES	YES
390	a	1453.71	0.89146	YES	YES
391	a	1454.28	1.30738	YES	YES
392	a	1454.39	1.58652	YES	YES
393	a	1455.31	0.65185	YES	YES
394	a	1455.50	1.69826	YES	YES
395	a	1456.48	2.28440	YES	YES
396	a	1457.97	2.89634	YES	YES
397	a	1470.15	6.58998	YES	YES
398	a	1532.69	204.55797	YES	YES
399	a	1570.09	3.29367	YES	YES
400	a	1591.40	3.64772	YES	YES
401	a	2915.15	17.81610	YES	YES
402	a	2923.20	6.97812	YES	YES
403	a	2925.67	3.90415	YES	YES
404	a	2930.20	21.08774	YES	YES
405	a	2935.37	16.19873	YES	YES
406	a	2936.72	29.31586	YES	YES
407	a	2936.86	9.70919	YES	YES
408	a	2937.19	4.51753	YES	YES
409	a	2937.79	11.68794	YES	YES
410	a	2939.64	4.61418	YES	YES
411	a	2941.15	29.07998	YES	YES
412	a	2941.86	23.20970	YES	YES
413	a	2944.14	5.42600	YES	YES
414	a	2944.33	14.85713	YES	YES
415	a	2944.83	6.18690	YES	YES
416	a	2944.98	0.84031	YES	YES
417	a	2945.03	6.89373	YES	YES
418	a	2945.10	20.13895	YES	YES
419	a	2945.53	8.96280	YES	YES
420	a	2946.00	10.46734	YES	YES
421	a	2947.03	9.18594	YES	YES
422	a	2947.84	3.31432	YES	YES
423	a	2948.11	11.99320	YES	YES
424	a	2948.42	10.51576	YES	YES
425	a	2948.62	36.92738	YES	YES
426	a	2949.52	6.15745	YES	YES
427	a	2950.36	15.91153	YES	YES
428	a	2953.61	2.38302	YES	YES
429	a	2954.32	5.16578	YES	YES
430	a	2955.42	4.11694	YES	YES
431	a	2955.58	3.23634	YES	YES
432	a	2955.60	8.52831	YES	YES
433	a	2956.82	9.27851	YES	YES
434	a	2957.03	6.80251	YES	YES
435	a	2957.28	10.49631	YES	YES
436	a	2957.51	10.83631	YES	YES
437	a	2958.38	10.86317	YES	YES
438	a	2958.53	7.62423	YES	YES
439	a	2959.83	38.61263	YES	YES
440	a	2960.03	18.37519	YES	YES
441	a	2960.49	26.33113	YES	YES
442	a	2960.75	27.46290	YES	YES
443	a	2961.18	50.48096	YES	YES
444	a	2961.87	31.80652	YES	YES
445	a	2963.18	21.23101	YES	YES

446	a	2965.50	2.44056	YES	YES
447	a	2965.71	18.79355	YES	YES
448	a	2975.29	9.32380	YES	YES
449	a	2977.63	6.62752	YES	YES
450	a	2982.22	28.07900	YES	YES
451	a	2983.09	9.00082	YES	YES
452	a	2985.42	3.05829	YES	YES
453	a	2985.68	39.01598	YES	YES
454	a	2986.90	7.34201	YES	YES
455	a	2987.15	48.27328	YES	YES
456	a	2990.36	20.99202	YES	YES
457	a	2990.43	11.70657	YES	YES
458	a	2998.04	11.44414	YES	YES
459	a	2998.14	38.78326	YES	YES
460	a	2998.51	21.36786	YES	YES
461	a	2998.83	18.03067	YES	YES
462	a	3000.27	33.78475	YES	YES
463	a	3001.63	11.02408	YES	YES
464	a	3002.79	11.32667	YES	YES
465	a	3002.87	37.96063	YES	YES
466	a	3005.37	17.20145	YES	YES
467	a	3005.47	25.66549	YES	YES
468	a	3007.29	15.86372	YES	YES
469	a	3008.11	16.60747	YES	YES
470	a	3009.24	7.97941	YES	YES
471	a	3009.35	18.07402	YES	YES
472	a	3009.41	28.93645	YES	YES
473	a	3009.90	21.95604	YES	YES
474	a	3010.55	17.71222	YES	YES
475	a	3011.26	15.60025	YES	YES
476	a	3011.86	38.46661	YES	YES
477	a	3012.60	21.81239	YES	YES
478	a	3012.98	21.10047	YES	YES
479	a	3015.10	17.96490	YES	YES
480	a	3015.62	29.33294	YES	YES
481	a	3015.73	17.19967	YES	YES
482	a	3015.88	20.00029	YES	YES
483	a	3016.22	28.05243	YES	YES
484	a	3016.78	27.48328	YES	YES
485	a	3016.92	27.87592	YES	YES
486	a	3017.41	32.28939	YES	YES
487	a	3017.77	16.72226	YES	YES
488	a	3018.34	4.66958	YES	YES
489	a	3018.45	39.49187	YES	YES
490	a	3018.85	24.58698	YES	YES
491	a	3019.57	32.30783	YES	YES
492	a	3021.48	34.99377	YES	YES
493	a	3024.25	4.36706	YES	YES
494	a	3029.77	0.56138	YES	YES
495	a	3036.09	1.26717	YES	YES
496	a	3044.41	0.21472	YES	YES
497	a	3072.26	8.36753	YES	YES
498	a	3108.45	0.43096	YES	YES
499	a	3115.43	0.87896	YES	YES
500	a	3122.79	7.13447	YES	YES
501	a	3132.02	7.28845	YES	YES

\$end

Double hybrid single point energy = -7573.145370452997 H
 COSMO energy + OC correction = -7581.0105805499 H (in oDFB)

6.2.45 H₂FCCN



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: cs

Cartesian coordinates in Ångström:

N	-0.0600457	-2.1499227	0.0000000
C	-0.0391259	-0.9886156	0.0000000
C	-0.0414465	0.4763755	0.0000000
F	1.2600929	0.9710033	0.0000000
H	-0.5597374	0.8455798	0.8976042
H	-0.5597374	0.8455798	-0.8976042

SCF energy GEOOPT = -232.0867825213 H
 ZPE = 97.52 kJ/mol
 FREEH energy = 108.25 kJ/mol
 FREEH entropy = 0.27596 kJ/mol/K

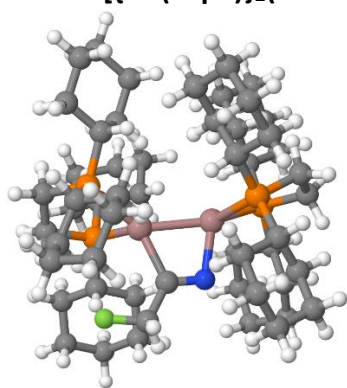
\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a'	214.83	8.08432	YES	YES
8		a''	339.26	0.57497	YES	YES
9		a'	556.41	1.34017	YES	YES
10		a'	906.66	15.43937	YES	YES
11		a''	994.26	1.31910	YES	YES
12		a'	1025.25	122.97639	YES	YES
13		a''	1219.37	0.41011	YES	YES
14		a'	1349.71	14.43360	YES	YES
15		a'	1432.49	5.21986	YES	YES
16		a'	2274.65	1.60430	YES	YES
17		a'	2973.94	11.90277	YES	YES
18		a''	3017.98	3.26866	YES	YES

\$end

Double hybrid single point energy = -231.741278146058 H
 COSMO energy + OC correction = -232.0965627414 H (in oDFB)

6.2.46 $\{[Ga(dcpe)]_2(NCCH_2F)\}^{2+}$ (Cycloadduct)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-2.5521115	17.3150639	-2.7691630
Ga	-4.1244429	17.7255718	-0.9651381
P	-1.6899779	18.9662100	-4.2961851
P	-6.0515547	19.1329047	-0.8218948
P	-1.9392492	15.6643324	-4.3785231
P	-5.3920394	16.1375517	0.2958301
C	-5.2072895	20.9049292	-5.4647284
H	-5.4055227	21.4494370	-4.5249071
H	-6.1708335	20.4954148	-5.7988055
C	-0.9453558	14.3064476	-3.6384378
H	-0.6297108	13.6263169	-4.4471077
C	-4.3468883	15.2824605	1.5424883
H	-3.7787398	16.1335862	1.9595940
C	-4.3327670	16.0614038	-5.7494171
H	-3.8027927	16.6237861	-6.5351575
H	-4.5716597	16.7777131	-4.9471034
C	-6.9288296	19.2829998	-2.4335375
H	-6.2229441	19.8479491	-3.0648970
C	-7.2161051	18.3010023	0.3573281
H	-7.7160832	19.0554387	0.9796839
H	-7.9979633	17.8321546	-0.2555491
C	-3.2822665	22.4232009	-6.0798323
H	-2.8746457	23.0892368	-6.8518732
H	-3.3942248	23.0325921	-5.1677896
C	-2.2879521	21.2875371	-5.8029116
H	-1.3288055	21.7019980	-5.4636151
H	-2.0876093	20.7418900	-6.7393899
C	-4.2261436	19.7603809	-5.1840048
H	-4.1169151	19.1541154	-6.0974074
H	-4.6162681	19.0874773	-4.4039716
C	1.0574698	13.7897940	-2.1711494
H	1.4593598	13.0516764	-2.8840142
H	1.9216663	14.2386110	-1.6631627
C	-7.1927268	13.9138446	0.0227347
H	-7.7547316	14.3253598	0.8729594
H	-6.4621061	13.2024899	0.4361648
C	-5.6053626	20.8116119	-0.2258776
H	-6.5058003	21.4465945	-0.2649090
C	-0.4780132	20.6398923	-2.4623089
H	-1.1796566	21.4381652	-2.7441289

H	-0.9776951	20.0168098	-1.7033495
C	0.7926415	21.2518050	-1.8596954
H	1.2324964	21.9597824	-2.5807779
H	0.5260671	21.8389321	-0.9697819
C	-2.1818545	17.8148707	-0.2425798
C	-7.1272940	17.8968668	-3.0706691
H	-6.1613411	17.3713772	-3.1409478
H	-7.7759115	17.2864782	-2.4206115
C	-4.6500420	21.8818138	-6.5045916
H	-4.5546925	21.3640239	-7.4731406
H	-5.3547161	22.7090297	-6.6626728
C	-8.2490142	20.0662779	-2.3521487
H	-8.0783396	21.0691698	-1.9366004
H	-8.9407946	19.5503094	-1.6663527
C	-4.5327234	21.3798405	-1.1783160
H	-4.9388047	21.4819325	-2.1958286
H	-3.6984685	20.6565568	-1.2383092
C	-3.0880275	13.9075417	-6.2889627
H	-2.4645681	13.1033497	-5.8736582
H	-2.5034005	14.3818335	-7.0940949
C	2.1677109	19.3328767	-2.7432915
H	2.6554636	19.9701422	-3.4988844
H	2.8883255	18.5450544	-2.4847667
C	-4.5515840	22.0920974	1.6938688
H	-5.3781772	22.8189827	1.7442770
H	-4.1602365	21.9911764	2.7149734
C	-9.1024032	18.7934395	-4.3749427
H	-9.5375764	18.8988159	-5.3777049
H	-9.8323149	18.2215922	-3.7783285
C	-5.0835457	14.5962479	2.7058025
H	-5.7766700	15.2955206	3.1938986
H	-5.6851167	13.7577189	2.3285664
C	0.1452740	13.0862700	-1.1635370
H	0.6987038	12.3039417	-0.6272820
H	-0.1868539	13.8169676	-0.4070608
C	-7.7878574	18.0098199	-4.4486186
H	-7.0933198	18.5152058	-5.1390134
H	-7.9592758	17.0044279	-4.8573680
C	1.8217082	20.1731734	-1.5111262
H	1.4117310	19.5141519	-0.7278837
H	2.7285322	20.6336957	-1.0973239
C	-3.4671553	22.6191345	0.7497085
H	-3.1037862	23.5959115	1.0951684
H	-2.6010082	21.9356635	0.7700895
C	-5.6576368	14.4539489	-1.9275085
H	-4.8748302	13.7735428	-1.5583642
H	-5.1392701	15.2683922	-2.4572353
C	-5.0916420	20.7361162	1.2231086
H	-4.2872619	19.9848502	1.2851653
H	-5.8948076	20.3980884	1.8940250
C	-6.4431735	15.0233604	-0.7314516
H	-7.1958993	15.7215870	-1.1416438
C	-3.9935507	22.7262985	-0.6839392
C	-7.3749611	12.6005912	-2.1359941
H	-8.0708881	12.1022932	-2.8239984
H	-6.6717820	11.8261491	-1.7878470
C	-8.1348913	13.1696161	-0.9334393
H	-8.6511011	12.3664697	-0.3907635

H	-8.9170158	13.8630972	-1.2846662
C	-1.8529013	13.5461105	-2.6498747
H	-2.6941377	13.0785263	-3.1809818
H	-2.2864708	14.2750443	-1.9432910
C	-4.0631535	14.0697728	3.7255568
H	-3.5316389	14.9227942	4.1779519
H	-4.5922864	13.5607880	4.5424161
C	-5.6153087	15.4694568	-6.3439998
H	-6.2361520	16.2754735	-6.7589260
H	-6.2007279	15.0029666	-5.5352578
C	-3.0514436	13.1245957	3.0695152
H	-3.5745553	12.2232503	2.7089741
H	-2.3172178	12.7818315	3.8106420
C	-3.3382511	14.3387347	0.8646355
H	-3.8760415	13.4951779	0.4030537
H	-2.8090224	14.8679216	0.0571814
C	-8.8984431	20.1723670	-3.7394228
H	-9.8564358	20.7026329	-3.6560407
H	-8.2555792	20.7873608	-4.3896928
C	-4.3804274	13.3248765	-6.8787117
H	-4.1317402	12.6062840	-7.6709145
H	-4.9069812	12.7558012	-6.0945997
C	-6.5949084	13.6950450	-2.8722518
H	-6.0170991	13.2608885	-3.7016721
H	-7.3025888	14.4106104	-3.3245801
C	-5.3006298	14.4238831	-7.4190433
H	-6.2308878	13.9843377	-7.8028242
H	-4.8139754	14.9182069	-8.2760276
C	-1.0756996	12.4849871	-1.8631205
H	-1.7494908	12.0100845	-1.1356169
H	-0.7498898	11.6887645	-2.5513982
C	-2.3376971	13.7995132	1.8937253
H	-1.7237058	14.6357980	2.2664796
H	-1.6480315	13.0970918	1.4056818
C	-1.7195026	18.1866991	1.1378931
N	-1.3800345	17.4207620	-1.1545487
C	-0.1468227	19.7585613	-3.6835339
H	0.2326058	20.3969685	-4.4999051
C	0.9113038	18.6915352	-3.3448399
H	1.1797696	18.1243051	-4.2482323
H	0.4842634	17.9856663	-2.6149489
C	0.2977367	14.8828266	-2.9318661
H	0.9664416	15.3609394	-3.6613671
H	-0.0177315	15.6637392	-2.2196722
C	-0.9081743	16.5552567	-5.6280434
H	0.1206706	16.4935748	-5.2508657
H	-0.9306114	16.0105409	-6.5819976
C	-1.3026506	18.0305352	-5.8489683
H	-2.2045118	18.0935211	-6.4721736
H	-0.5034624	18.5514718	-6.3940024
C	-3.4159590	14.9503143	-5.2101340
H	-3.9526734	14.4473473	-4.3870215
C	-2.8576362	20.3136281	-4.7580126
H	-3.0007943	20.8589886	-3.8088166
C	-6.5251052	17.2481491	1.2441100
H	-7.2757649	16.6569145	1.7861609
H	-5.8894280	17.7351954	1.9977018
H	-4.7969751	23.4789130	-0.7265725

H	-3.2030723	23.0747403	-1.3640531
H	-1.0042421	17.4528352	1.5353313
F	-2.8180683	18.2429620	2.0274046
H	-1.2538923	19.1842786	1.1337748

SCF energy GEOOPT = -7488.302837555 H

ZPE = 3699. kJ/mol

FREEH energy = 3887.69 kJ/mol

FREEH entropy = 1.62124 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.04	0.04657	YES	YES
8		a	19.01	0.02054	YES	YES
9		a	21.18	0.07094	YES	YES
10		a	25.81	0.07839	YES	YES
11		a	27.57	0.00798	YES	YES
12		a	29.75	0.10162	YES	YES
13		a	33.03	0.09048	YES	YES
14		a	34.30	0.06264	YES	YES
15		a	36.10	0.00486	YES	YES
16		a	36.84	0.01987	YES	YES
17		a	38.90	0.08083	YES	YES
18		a	44.48	0.02804	YES	YES
19		a	44.57	0.11666	YES	YES
20		a	47.61	0.14258	YES	YES
21		a	50.20	0.17083	YES	YES
22		a	51.17	0.09446	YES	YES
23		a	54.56	0.45560	YES	YES
24		a	56.04	0.06377	YES	YES
25		a	60.56	0.18380	YES	YES
26		a	62.42	0.02893	YES	YES
27		a	62.60	0.25701	YES	YES
28		a	64.54	0.13095	YES	YES
29		a	69.65	0.02303	YES	YES
30		a	73.41	0.14117	YES	YES
31		a	74.29	0.07196	YES	YES
32		a	75.97	0.15662	YES	YES
33		a	79.22	0.87701	YES	YES
34		a	85.09	1.05198	YES	YES
35		a	87.43	1.27958	YES	YES
36		a	89.35	2.62818	YES	YES
37		a	94.37	1.75938	YES	YES
38		a	100.08	0.40083	YES	YES
39		a	116.63	0.89660	YES	YES
40		a	121.08	2.38122	YES	YES
41		a	128.45	0.81147	YES	YES
42		a	133.62	0.12681	YES	YES
43		a	136.35	1.10313	YES	YES
44		a	138.74	0.63274	YES	YES
45		a	141.02	1.08176	YES	YES

46	a	145.88	0.81124	YES	YES
47	a	151.58	0.74003	YES	YES
48	a	157.22	1.04059	YES	YES
49	a	169.05	0.10018	YES	YES
50	a	174.62	1.05325	YES	YES
51	a	179.81	4.87393	YES	YES
52	a	181.78	0.50883	YES	YES
53	a	188.97	2.03496	YES	YES
54	a	195.69	2.04836	YES	YES
55	a	203.25	16.50382	YES	YES
56	a	210.68	0.21181	YES	YES
57	a	210.99	0.74236	YES	YES
58	a	216.31	0.35232	YES	YES
59	a	218.16	0.72211	YES	YES
60	a	220.03	0.90581	YES	YES
61	a	222.29	0.89488	YES	YES
62	a	225.37	0.14558	YES	YES
63	a	226.23	0.97301	YES	YES
64	a	228.27	0.54445	YES	YES
65	a	232.07	0.46106	YES	YES
66	a	235.62	3.36270	YES	YES
67	a	239.41	11.44549	YES	YES
68	a	240.51	3.79904	YES	YES
69	a	243.80	1.47100	YES	YES
70	a	246.77	1.80963	YES	YES
71	a	255.22	3.68381	YES	YES
72	a	276.33	2.15434	YES	YES
73	a	280.83	0.45677	YES	YES
74	a	286.45	4.26987	YES	YES
75	a	293.30	0.53426	YES	YES
76	a	300.67	0.13113	YES	YES
77	a	304.99	0.73241	YES	YES
78	a	311.52	0.07235	YES	YES
79	a	313.97	0.20627	YES	YES
80	a	328.89	0.56967	YES	YES
81	a	329.89	0.78250	YES	YES
82	a	333.64	0.47187	YES	YES
83	a	336.73	0.24057	YES	YES
84	a	341.34	0.50041	YES	YES
85	a	343.92	1.11945	YES	YES
86	a	372.64	1.73448	YES	YES
87	a	373.54	1.22898	YES	YES
88	a	377.10	2.51088	YES	YES
89	a	380.81	1.64066	YES	YES
90	a	390.47	3.24006	YES	YES
91	a	394.11	0.15230	YES	YES
92	a	395.50	1.09697	YES	YES
93	a	407.70	0.03172	YES	YES
94	a	410.29	2.22757	YES	YES
95	a	413.18	0.89031	YES	YES
96	a	417.56	2.61846	YES	YES
97	a	421.61	4.49483	YES	YES
98	a	423.47	1.55824	YES	YES
99	a	427.39	0.32617	YES	YES
100	a	429.24	0.06926	YES	YES
101	a	429.90	0.18830	YES	YES
102	a	430.40	0.11883	YES	YES
103	a	430.88	0.13885	YES	YES

104	a	432.09	0.55920	YES	YES
105	a	432.40	0.49226	YES	YES
106	a	435.28	1.07877	YES	YES
107	a	438.33	0.15359	YES	YES
108	a	445.29	2.09526	YES	YES
109	a	456.44	2.77022	YES	YES
110	a	461.96	5.26678	YES	YES
111	a	471.11	3.48836	YES	YES
112	a	491.54	3.45433	YES	YES
113	a	494.36	1.03947	YES	YES
114	a	495.09	4.63276	YES	YES
115	a	497.01	1.28770	YES	YES
116	a	502.87	2.30888	YES	YES
117	a	503.93	0.34942	YES	YES
118	a	513.41	7.67307	YES	YES
119	a	514.92	17.64458	YES	YES
120	a	520.99	20.61261	YES	YES
121	a	606.87	40.11725	YES	YES
122	a	625.32	14.54826	YES	YES
123	a	632.07	18.73891	YES	YES
124	a	640.32	10.67507	YES	YES
125	a	656.48	12.27509	YES	YES
126	a	700.00	2.03304	YES	YES
127	a	718.27	1.79974	YES	YES
128	a	725.55	1.42758	YES	YES
129	a	729.43	4.01786	YES	YES
130	a	732.95	8.52051	YES	YES
131	a	737.29	2.01283	YES	YES
132	a	739.91	2.98774	YES	YES
133	a	742.14	3.18440	YES	YES
134	a	769.67	1.34280	YES	YES
135	a	771.69	0.36136	YES	YES
136	a	772.63	0.28845	YES	YES
137	a	773.51	1.92108	YES	YES
138	a	774.24	0.21068	YES	YES
139	a	775.67	6.35646	YES	YES
140	a	775.83	0.76139	YES	YES
141	a	776.76	6.33322	YES	YES
142	a	776.94	1.34446	YES	YES
143	a	779.28	13.05515	YES	YES
144	a	806.14	0.28681	YES	YES
145	a	807.93	4.65098	YES	YES
146	a	809.59	9.03000	YES	YES
147	a	810.64	3.86132	YES	YES
148	a	811.67	0.55682	YES	YES
149	a	813.12	2.90886	YES	YES
150	a	815.09	1.71304	YES	YES
151	a	816.48	4.27359	YES	YES
152	a	830.41	4.61857	YES	YES
153	a	831.18	5.58577	YES	YES
154	a	836.16	0.71900	YES	YES
155	a	837.94	2.38294	YES	YES
156	a	838.13	2.17121	YES	YES
157	a	838.46	0.15102	YES	YES
158	a	839.54	9.64054	YES	YES
159	a	839.77	3.99700	YES	YES
160	a	847.22	14.66472	YES	YES
161	a	853.52	12.94217	YES	YES

162	a	870.02	1.35649	YES	YES
163	a	870.27	4.51746	YES	YES
164	a	872.36	3.09281	YES	YES
165	a	876.32	0.80112	YES	YES
166	a	877.09	0.67772	YES	YES
167	a	877.81	2.85575	YES	YES
168	a	878.13	3.78912	YES	YES
169	a	878.98	0.61217	YES	YES
170	a	879.66	3.58359	YES	YES
171	a	880.54	0.25346	YES	YES
172	a	880.70	4.87685	YES	YES
173	a	881.26	0.60219	YES	YES
174	a	882.90	3.66972	YES	YES
175	a	883.39	13.16561	YES	YES
176	a	884.62	5.36428	YES	YES
177	a	886.26	0.50193	YES	YES
178	a	902.26	3.14353	YES	YES
179	a	902.90	0.80348	YES	YES
180	a	904.16	3.77421	YES	YES
181	a	905.08	1.00476	YES	YES
182	a	907.55	3.11901	YES	YES
183	a	908.92	0.73722	YES	YES
184	a	910.26	2.01023	YES	YES
185	a	910.88	0.57899	YES	YES
186	a	913.93	8.75965	YES	YES
187	a	964.91	39.70716	YES	YES
188	a	976.66	0.12321	YES	YES
189	a	976.81	1.05981	YES	YES
190	a	987.20	7.39540	YES	YES
191	a	987.68	10.31316	YES	YES
192	a	988.31	3.17486	YES	YES
193	a	988.89	14.25355	YES	YES
194	a	989.03	5.35307	YES	YES
195	a	990.12	8.98375	YES	YES
196	a	991.79	28.19100	YES	YES
197	a	992.08	5.54762	YES	YES
198	a	1012.99	0.31585	YES	YES
199	a	1014.84	2.74412	YES	YES
200	a	1015.25	0.59961	YES	YES
201	a	1016.33	0.79062	YES	YES
202	a	1017.22	0.37342	YES	YES
203	a	1019.75	0.95742	YES	YES
204	a	1020.20	0.71403	YES	YES
205	a	1022.21	0.40005	YES	YES
206	a	1028.28	0.88263	YES	YES
207	a	1028.41	1.88952	YES	YES
208	a	1030.00	2.10841	YES	YES
209	a	1034.85	14.99987	YES	YES
210	a	1037.17	8.17843	YES	YES
211	a	1039.67	6.83955	YES	YES
212	a	1040.00	30.95353	YES	YES
213	a	1040.18	2.23442	YES	YES
214	a	1040.94	23.80902	YES	YES
215	a	1055.49	0.83361	YES	YES
216	a	1058.36	1.05195	YES	YES
217	a	1059.70	0.30245	YES	YES
218	a	1060.50	1.31524	YES	YES
219	a	1062.36	1.87588	YES	YES

220	a	1065.65	1.09873	YES	YES
221	a	1066.32	0.86192	YES	YES
222	a	1069.54	0.93002	YES	YES
223	a	1070.44	0.00074	YES	YES
224	a	1071.82	0.08711	YES	YES
225	a	1071.86	0.13581	YES	YES
226	a	1072.07	0.26512	YES	YES
227	a	1072.58	0.10590	YES	YES
228	a	1073.05	0.25646	YES	YES
229	a	1073.24	0.12428	YES	YES
230	a	1073.65	0.06797	YES	YES
231	a	1078.50	3.27039	YES	YES
232	a	1081.76	3.86986	YES	YES
233	a	1087.90	7.25058	YES	YES
234	a	1090.96	4.50832	YES	YES
235	a	1094.50	4.63006	YES	YES
236	a	1096.04	0.72434	YES	YES
237	a	1102.40	0.70843	YES	YES
238	a	1103.18	3.51713	YES	YES
239	a	1111.09	8.96747	YES	YES
240	a	1116.19	10.23880	YES	YES
241	a	1122.01	0.99429	YES	YES
242	a	1129.77	3.41844	YES	YES
243	a	1158.56	4.48129	YES	YES
244	a	1159.55	2.37934	YES	YES
245	a	1160.97	7.73403	YES	YES
246	a	1165.60	5.77571	YES	YES
247	a	1166.41	9.46561	YES	YES
248	a	1167.41	10.00385	YES	YES
249	a	1168.75	12.88994	YES	YES
250	a	1170.18	3.55211	YES	YES
251	a	1172.86	9.01239	YES	YES
252	a	1174.49	9.66305	YES	YES
253	a	1178.87	7.73827	YES	YES
254	a	1181.41	5.00557	YES	YES
255	a	1185.88	0.13053	YES	YES
256	a	1187.20	0.42703	YES	YES
257	a	1189.08	1.80617	YES	YES
258	a	1192.16	0.84020	YES	YES
259	a	1215.37	2.17140	YES	YES
260	a	1237.00	0.67301	YES	YES
261	a	1240.94	0.34187	YES	YES
262	a	1241.84	0.82418	YES	YES
263	a	1245.70	0.20176	YES	YES
264	a	1246.41	0.06121	YES	YES
265	a	1246.77	0.46986	YES	YES
266	a	1248.94	0.86805	YES	YES
267	a	1249.21	1.37881	YES	YES
268	a	1252.15	1.21377	YES	YES
269	a	1252.85	0.86159	YES	YES
270	a	1253.80	0.20390	YES	YES
271	a	1254.52	3.38976	YES	YES
272	a	1255.14	2.65831	YES	YES
273	a	1255.46	4.49090	YES	YES
274	a	1256.10	0.76303	YES	YES
275	a	1256.44	2.55854	YES	YES
276	a	1257.06	4.03779	YES	YES
277	a	1257.55	1.01668	YES	YES

278	a	1258.72	1.50209	YES	YES
279	a	1259.40	1.60586	YES	YES
280	a	1260.66	2.41872	YES	YES
281	a	1261.34	3.16593	YES	YES
282	a	1262.71	1.73945	YES	YES
283	a	1263.51	0.70717	YES	YES
284	a	1265.42	1.02140	YES	YES
285	a	1269.22	1.25366	YES	YES
286	a	1270.91	2.14242	YES	YES
287	a	1272.13	1.77136	YES	YES
288	a	1280.84	2.42288	YES	YES
289	a	1281.18	0.89839	YES	YES
290	a	1283.23	4.43186	YES	YES
291	a	1284.96	1.03343	YES	YES
292	a	1286.55	5.57863	YES	YES
293	a	1288.18	3.77221	YES	YES
294	a	1288.66	3.28858	YES	YES
295	a	1291.73	3.27273	YES	YES
296	a	1299.35	6.24905	YES	YES
297	a	1305.85	0.75811	YES	YES
298	a	1309.69	1.21552	YES	YES
299	a	1311.43	0.85361	YES	YES
300	a	1312.48	2.15842	YES	YES
301	a	1314.79	0.56317	YES	YES
302	a	1316.19	2.31929	YES	YES
303	a	1317.87	0.55244	YES	YES
304	a	1319.77	2.66425	YES	YES
305	a	1320.53	1.34236	YES	YES
306	a	1321.12	0.55601	YES	YES
307	a	1321.53	0.04636	YES	YES
308	a	1321.82	0.82882	YES	YES
309	a	1323.56	1.21777	YES	YES
310	a	1324.04	1.62471	YES	YES
311	a	1324.24	0.97246	YES	YES
312	a	1324.42	1.36407	YES	YES
313	a	1325.18	1.78126	YES	YES
314	a	1325.44	4.13329	YES	YES
315	a	1325.84	2.13479	YES	YES
316	a	1327.23	6.40042	YES	YES
317	a	1330.01	2.30616	YES	YES
318	a	1332.29	1.12655	YES	YES
319	a	1336.17	0.17266	YES	YES
320	a	1336.41	0.26667	YES	YES
321	a	1336.63	0.16672	YES	YES
322	a	1337.14	0.39307	YES	YES
323	a	1337.42	1.00644	YES	YES
324	a	1338.17	0.10700	YES	YES
325	a	1338.34	0.24778	YES	YES
326	a	1338.76	0.42202	YES	YES
327	a	1339.94	0.18980	YES	YES
328	a	1341.43	1.11965	YES	YES
329	a	1343.63	0.13894	YES	YES
330	a	1344.59	2.14134	YES	YES
331	a	1344.89	0.61633	YES	YES
332	a	1345.36	0.41884	YES	YES
333	a	1346.59	2.90252	YES	YES
334	a	1347.03	0.67953	YES	YES
335	a	1347.35	0.87868	YES	YES

336	a	1349.86	0.96861	YES	YES
337	a	1400.70	6.63602	YES	YES
338	a	1403.85	8.87075	YES	YES
339	a	1404.60	8.01749	YES	YES
340	a	1407.30	9.71820	YES	YES
341	a	1412.67	10.04530	YES	YES
342	a	1423.67	5.30208	YES	YES
343	a	1427.05	4.44249	YES	YES
344	a	1428.35	1.62968	YES	YES
345	a	1430.33	2.07207	YES	YES
346	a	1430.47	3.64805	YES	YES
347	a	1431.89	3.02089	YES	YES
348	a	1432.54	1.36521	YES	YES
349	a	1433.39	3.22049	YES	YES
350	a	1434.71	2.42577	YES	YES
351	a	1435.07	5.84985	YES	YES
352	a	1435.93	7.14829	YES	YES
353	a	1436.34	6.89878	YES	YES
354	a	1436.61	5.16285	YES	YES
355	a	1436.76	4.80711	YES	YES
356	a	1437.70	0.91540	YES	YES
357	a	1438.06	11.02221	YES	YES
358	a	1438.14	3.27803	YES	YES
359	a	1438.70	3.80005	YES	YES
360	a	1439.08	4.09397	YES	YES
361	a	1439.53	1.95599	YES	YES
362	a	1439.99	9.41174	YES	YES
363	a	1440.18	8.23962	YES	YES
364	a	1440.33	1.63138	YES	YES
365	a	1441.44	7.61258	YES	YES
366	a	1442.65	12.46337	YES	YES
367	a	1443.46	10.97033	YES	YES
368	a	1443.66	21.09438	YES	YES
369	a	1444.42	12.04306	YES	YES
370	a	1444.79	19.18149	YES	YES
371	a	1444.89	5.71627	YES	YES
372	a	1445.03	2.31336	YES	YES
373	a	1447.61	10.23565	YES	YES
374	a	1452.57	4.14909	YES	YES
375	a	1453.53	0.27959	YES	YES
376	a	1454.11	0.61372	YES	YES
377	a	1454.67	2.93586	YES	YES
378	a	1455.25	0.78177	YES	YES
379	a	1456.30	3.93426	YES	YES
380	a	1456.60	2.31104	YES	YES
381	a	1458.88	1.57548	YES	YES
382	a	1558.53	110.99801	YES	YES
383	a	2912.34	21.36487	YES	YES
384	a	2922.60	3.63564	YES	YES
385	a	2929.49	21.21774	YES	YES
386	a	2932.31	16.88844	YES	YES
387	a	2935.29	28.00346	YES	YES
388	a	2935.97	7.94119	YES	YES
389	a	2936.90	10.93507	YES	YES
390	a	2938.27	22.93360	YES	YES
391	a	2938.64	10.33116	YES	YES
392	a	2939.04	13.74503	YES	YES
393	a	2939.44	4.58042	YES	YES

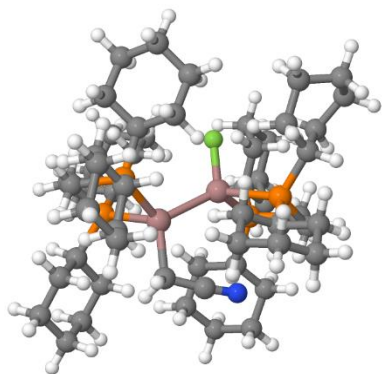
394	a	2941.19	10.97826	YES	YES
395	a	2942.82	17.51430	YES	YES
396	a	2944.55	11.35046	YES	YES
397	a	2944.97	4.74586	YES	YES
398	a	2945.15	6.97742	YES	YES
399	a	2945.46	8.42599	YES	YES
400	a	2946.07	12.98743	YES	YES
401	a	2946.21	3.86888	YES	YES
402	a	2947.22	7.98334	YES	YES
403	a	2947.97	15.59569	YES	YES
404	a	2948.58	8.19608	YES	YES
405	a	2948.89	5.60544	YES	YES
406	a	2949.50	8.26514	YES	YES
407	a	2950.46	31.81641	YES	YES
408	a	2951.00	22.20218	YES	YES
409	a	2951.49	9.94434	YES	YES
410	a	2953.04	1.83296	YES	YES
411	a	2954.95	2.47691	YES	YES
412	a	2955.28	2.31368	YES	YES
413	a	2956.06	2.70482	YES	YES
414	a	2956.48	7.50830	YES	YES
415	a	2957.29	10.38425	YES	YES
416	a	2957.40	20.42551	YES	YES
417	a	2958.08	7.08116	YES	YES
418	a	2958.10	2.77590	YES	YES
419	a	2958.45	3.66110	YES	YES
420	a	2959.40	1.86921	YES	YES
421	a	2960.04	19.47679	YES	YES
422	a	2960.15	38.47447	YES	YES
423	a	2960.80	23.93108	YES	YES
424	a	2961.46	37.97970	YES	YES
425	a	2961.66	63.86324	YES	YES
426	a	2961.81	17.17821	YES	YES
427	a	2962.91	21.14058	YES	YES
428	a	2963.91	12.57410	YES	YES
429	a	2964.34	1.92759	YES	YES
430	a	2966.15	20.60434	YES	YES
431	a	2978.33	8.10029	YES	YES
432	a	2980.56	31.93261	YES	YES
433	a	2981.23	4.66322	YES	YES
434	a	2984.35	12.71779	YES	YES
435	a	2985.62	5.51430	YES	YES
436	a	2986.70	24.53379	YES	YES
437	a	2987.12	50.76129	YES	YES
438	a	2987.34	11.83979	YES	YES
439	a	2987.45	13.56269	YES	YES
440	a	2989.63	9.21686	YES	YES
441	a	2991.04	31.96067	YES	YES
442	a	2997.76	21.68391	YES	YES
443	a	2998.39	32.59202	YES	YES
444	a	3000.23	31.97986	YES	YES
445	a	3001.66	14.62855	YES	YES
446	a	3002.71	8.00225	YES	YES
447	a	3003.20	25.16282	YES	YES
448	a	3003.84	9.69151	YES	YES
449	a	3004.04	32.17444	YES	YES
450	a	3004.26	38.95748	YES	YES
451	a	3006.52	16.68191	YES	YES

452	a	3007.32	15.35457	YES	YES
453	a	3008.57	18.19159	YES	YES
454	a	3009.38	32.65254	YES	YES
455	a	3009.91	2.17467	YES	YES
456	a	3010.33	37.66731	YES	YES
457	a	3010.48	18.00753	YES	YES
458	a	3010.74	23.43234	YES	YES
459	a	3013.04	16.01405	YES	YES
460	a	3014.72	22.07104	YES	YES
461	a	3015.10	21.08720	YES	YES
462	a	3016.46	16.72450	YES	YES
463	a	3016.53	34.59639	YES	YES
464	a	3017.08	14.14342	YES	YES
465	a	3017.25	21.03488	YES	YES
466	a	3017.31	51.30093	YES	YES
467	a	3017.41	12.86176	YES	YES
468	a	3017.83	20.20198	YES	YES
469	a	3018.42	20.20915	YES	YES
470	a	3018.54	27.92990	YES	YES
471	a	3018.64	16.92846	YES	YES
472	a	3018.92	26.18963	YES	YES
473	a	3019.05	28.46485	YES	YES
474	a	3019.41	22.64386	YES	YES
475	a	3022.63	6.62352	YES	YES
476	a	3024.70	26.22837	YES	YES
477	a	3027.37	4.44302	YES	YES
478	a	3029.46	0.43871	YES	YES
479	a	3037.63	0.82462	YES	YES
480	a	3043.60	0.26242	YES	YES

\$end

Double hybrid single point energy = -7480.832967431653 H
 COSMO energy + OC correction = -7488.4523583825 H (in oDFB)

6.2.47 [F{Ga(dcpe)}₂(CH₂CN)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	0.0523128	-0.0611468	-1.4363081
Ga	-0.4675508	-0.0577757	0.9659102
F	0.7627414	0.8759795	1.9567170
N	-3.2844698	-1.5128843	-0.9568105

C	-2.4955561	-1.2088434	-1.7620902
C	-1.4398079	-0.8109386	-2.6437100
H	-1.7903145	-0.0521451	-3.3527200
H	-1.0761332	-1.6733460	-3.2148335
P	-2.5943668	0.7493809	1.7997769
P	-0.9179814	-2.1320087	2.1521298
C	-2.5299213	1.9821496	3.1663745
H	-3.5875843	2.1444382	3.4342595
C	-1.7846327	1.4897388	4.4168485
H	-2.1433169	0.5031679	4.7321609
H	-0.7189551	1.3812819	4.1686041
C	-1.9887793	2.4842345	5.5847605
H	-2.8641602	2.1829766	6.1762712
H	-1.1214190	2.4147688	6.2556035
C	-2.1627218	3.9371630	5.0991776
H	-1.8531029	4.6368203	5.8853809
H	-3.2253298	4.1506078	4.9039872
C	-1.3583255	4.1645521	3.8194623
H	-1.3668139	5.2229751	3.5280638
H	-0.3063852	3.8997195	4.0027067
C	-1.9132353	3.3091443	2.6606420
H	-1.1005914	3.0885432	1.9557964
H	-2.6761676	3.8738687	2.1072993
C	-3.7267061	1.3657216	0.4821357
H	-4.0280895	0.4338063	-0.0236043
C	-4.9906191	2.0623472	1.0127120
H	-5.5159211	1.4175131	1.7320290
H	-4.7122109	2.9833609	1.5485949
C	-5.9233006	2.4183527	-0.1541629
H	-6.2876436	1.4887244	-0.6199363
H	-6.8071408	2.9448607	0.2301949
C	-5.2080859	3.2722805	-1.2062678
H	-4.9405339	4.2472618	-0.7661007
H	-5.8845714	3.4839813	-2.0450249
C	-3.9368140	2.5824824	-1.7141103
H	-3.4149914	3.2247921	-2.4383009
H	-4.2091325	1.6565418	-2.2472193
C	-2.9959576	2.2333220	-0.5571008
H	-2.1069165	1.6979971	-0.9306048
H	-2.6288491	3.1580497	-0.0857826
C	-3.3823916	-0.7902927	2.4522934
H	-4.2089832	-0.5203204	3.1241648
H	-3.8167506	-1.2922129	1.5755187
C	-2.3953308	-1.7245513	3.1742588
H	-2.9000047	-2.6540880	3.4669102
H	-2.0153032	-1.2658182	4.0940883
C	0.4147020	-2.6914758	3.2945177
H	1.2571990	-2.9271970	2.6199346
C	0.8512707	-1.5284538	4.2085283
H	0.0025130	-1.2297573	4.8451944
H	1.1232158	-0.6496388	3.6083701
C	2.0132151	-1.9548486	5.1145321
H	2.8998533	-2.1587224	4.4923564
H	2.2818967	-1.1205982	5.7770389
C	1.6644122	-3.2032711	5.9287772
H	0.8447086	-2.9676856	6.6275675
H	2.5203465	-3.5081066	6.5455631
C	1.2369110	-4.3532304	5.0134399

H	2.0900892	-4.6587653	4.3848868
H	0.9527108	-5.2351673	5.6032739
C	0.0665569	-3.9527593	4.1041309
H	-0.8256032	-3.7565094	4.7204862
H	-0.1850617	-4.7848841	3.4341494
C	-1.4273693	-3.4672152	0.9853775
H	-1.9753852	-2.9169792	0.2029230
C	-0.1885929	-4.1049679	0.3355160
H	0.4463529	-3.3188164	-0.1072042
H	0.4204975	-4.6093122	1.1022425
C	-0.6004558	-5.1247217	-0.7330472
H	0.2953824	-5.6000966	-1.1562186
H	-1.1042134	-4.5963868	-1.5595051
C	-1.5508415	-6.1808049	-0.1631241
H	-1.8502026	-6.8834217	-0.9522770
H	-1.0226301	-6.7751743	0.6005977
C	-2.7849414	-5.5243925	0.4597652
H	-3.4542475	-6.2840865	0.8850779
H	-3.3576961	-4.9996693	-0.3219613
C	-2.3958915	-4.5198804	1.5526734
H	-3.3030590	-4.0343617	1.9369219
H	-1.9355525	-5.0547734	2.3957948
P	2.1873046	-1.0310820	-2.0765617
P	1.0060268	2.0362554	-2.1703428
C	2.1471265	-2.2544570	-3.4527841
H	3.1998918	-2.5285688	-3.6382578
C	1.5790252	-1.6359469	-4.7438541
H	2.2207734	-0.8094559	-5.0804805
H	0.5838248	-1.2059028	-4.5459924
C	1.4658551	-2.6855388	-5.8574313
H	1.0153404	-2.2248653	-6.7469461
H	2.4772221	-3.0096679	-6.1508236
C	0.6544362	-3.9022079	-5.4048349
H	0.6006354	-4.6428421	-6.2132968
H	-0.3848985	-3.5960716	-5.1944833
C	1.2662072	-4.5305613	-4.1504706
H	2.2691405	-4.9206132	-4.3871394
H	0.6685983	-5.3881112	-3.8126192
C	1.3781261	-3.5098461	-3.0131128
H	0.3664401	-3.2207937	-2.6843921
H	1.8672971	-3.9661922	-2.1409758
C	3.1083178	-1.7759483	-0.6642370
H	2.4382869	-2.5781127	-0.3073337
C	4.4550116	-2.4031235	-1.0623061
H	5.1162813	-1.6203387	-1.4686363
H	4.3199719	-3.1517788	-1.8548692
C	5.1229116	-3.0539883	0.1580636
H	4.5074829	-3.9079752	0.4868315
H	6.0970409	-3.4670143	-0.1359115
C	5.2832319	-2.0642154	1.3158120
H	5.9917965	-1.2714003	1.0249255
H	5.7234918	-2.5685764	2.1864019
C	3.9418830	-1.4289913	1.6908839
H	3.2650443	-2.2065442	2.0835246
H	4.0660692	-0.6891239	2.4929512
C	3.2791668	-0.7630955	0.4801917
H	3.9188246	0.0693179	0.1436555
H	2.3169781	-0.3207263	0.7747767

C	3.2039602	0.3866077	-2.6904141
H	3.7787141	0.7621427	-1.8336928
H	3.9310959	0.0081230	-3.4217855
C	2.3635315	1.5166864	-3.3014849
H	1.8945956	1.1961905	-4.2409818
H	3.0006606	2.3806934	-3.5320327
C	-0.0069003	3.2875183	-3.0693411
H	-0.7377917	3.6313311	-2.3175674
C	-0.7852206	2.6339214	-4.2265234
H	-1.4159545	1.8212919	-3.8410699
H	-0.0791151	2.1827425	-4.9426120
C	-1.6555477	3.6632130	-4.9600978
H	-2.1644531	3.1756419	-5.8026991
H	-2.4465464	4.0139208	-4.2769596
C	-0.8344613	4.8624059	-5.4396581
H	-0.1113898	4.5322397	-6.2036853
H	-1.4886903	5.5966598	-5.9278110
C	-0.0838415	5.5115700	-4.2747264
H	-0.8074051	5.9304322	-3.5560861
H	0.5292913	6.3519120	-4.6269766
C	0.8137802	4.4983447	-3.5519394
H	1.3204118	4.9809619	-2.7063364
H	1.5994896	4.1558101	-4.2439315
C	1.8104314	2.7865874	-0.6852708
H	2.0041047	1.9223952	-0.0252515
C	0.8031799	3.6859900	0.0505986
H	0.5564889	4.5547839	-0.5794978
H	-0.1358933	3.1372751	0.2188969
C	1.3888425	4.1681993	1.3816109
H	0.6762035	4.8456920	1.8705811
H	1.5135889	3.2970782	2.0432081
C	2.7332837	4.8729028	1.1771781
H	3.1557134	5.1681005	2.1469286
H	2.5773796	5.8049168	0.6091872
C	3.7224561	3.9813699	0.4207984
H	4.6680634	4.5125335	0.2474471
H	3.9628600	3.0967760	1.0337445
C	3.1429539	3.5151583	-0.9222854
H	2.9879034	4.3853830	-1.5769394
H	3.8672487	2.8642793	-1.4320713

SCF energy GEOOPT = -7488.371066174 H

ZPE = 3699. kJ/mol

FREEH energy = 3889.25 kJ/mol

FREEH entropy = 1.62075 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	8.19	0.25380	YES	YES
	8	a	17.77	0.18374	YES	YES
	9	a	22.37	0.01370	YES	YES

10	a	26.50	0.18655	YES	YES
11	a	28.28	0.01829	YES	YES
12	a	31.39	0.03500	YES	YES
13	a	33.09	0.10348	YES	YES
14	a	35.05	0.03976	YES	YES
15	a	38.99	0.19782	YES	YES
16	a	42.59	0.03348	YES	YES
17	a	43.42	0.26720	YES	YES
18	a	45.22	0.11617	YES	YES
19	a	50.18	0.01243	YES	YES
20	a	51.84	0.25191	YES	YES
21	a	55.16	0.19058	YES	YES
22	a	56.19	0.04764	YES	YES
23	a	58.77	0.10960	YES	YES
24	a	60.59	0.13406	YES	YES
25	a	65.69	0.21966	YES	YES
26	a	66.37	0.29034	YES	YES
27	a	68.86	0.45061	YES	YES
28	a	73.11	0.17902	YES	YES
29	a	75.45	0.12209	YES	YES
30	a	78.73	0.40498	YES	YES
31	a	80.96	0.34750	YES	YES
32	a	82.24	0.82107	YES	YES
33	a	84.89	1.09657	YES	YES
34	a	91.07	1.18113	YES	YES
35	a	96.96	1.40001	YES	YES
36	a	98.92	2.14479	YES	YES
37	a	107.80	2.06718	YES	YES
38	a	112.30	4.97500	YES	YES
39	a	120.52	0.27270	YES	YES
40	a	124.28	0.47097	YES	YES
41	a	133.31	0.57413	YES	YES
42	a	134.35	10.84920	YES	YES
43	a	136.63	1.53407	YES	YES
44	a	138.31	0.64870	YES	YES
45	a	141.50	3.65389	YES	YES
46	a	145.70	0.66451	YES	YES
47	a	149.29	1.75406	YES	YES
48	a	154.67	23.43716	YES	YES
49	a	157.24	3.39992	YES	YES
50	a	162.39	5.20780	YES	YES
51	a	163.10	2.90105	YES	YES
52	a	165.79	2.98678	YES	YES
53	a	179.54	2.80361	YES	YES
54	a	185.29	1.02191	YES	YES
55	a	188.12	4.56231	YES	YES
56	a	191.96	8.27372	YES	YES
57	a	195.28	3.40283	YES	YES
58	a	205.70	2.05613	YES	YES
59	a	206.85	0.44875	YES	YES
60	a	209.04	0.34941	YES	YES
61	a	217.72	2.19188	YES	YES
62	a	221.98	0.40939	YES	YES
63	a	224.37	1.01377	YES	YES
64	a	224.89	1.08318	YES	YES
65	a	230.61	0.17201	YES	YES
66	a	231.89	0.65457	YES	YES
67	a	233.45	1.58254	YES	YES

68	a	237.14	0.47228	YES	YES
69	a	239.25	0.02813	YES	YES
70	a	240.65	0.17074	YES	YES
71	a	242.48	1.04636	YES	YES
72	a	252.42	0.08238	YES	YES
73	a	266.53	0.79249	YES	YES
74	a	276.98	1.05972	YES	YES
75	a	291.69	0.74123	YES	YES
76	a	295.16	0.36458	YES	YES
77	a	306.12	0.37206	YES	YES
78	a	307.19	0.63249	YES	YES
79	a	311.77	0.48419	YES	YES
80	a	314.40	0.30561	YES	YES
81	a	329.89	0.65916	YES	YES
82	a	330.33	0.68091	YES	YES
83	a	331.71	1.70331	YES	YES
84	a	336.64	0.14403	YES	YES
85	a	338.49	1.43836	YES	YES
86	a	341.45	0.28758	YES	YES
87	a	349.57	3.42887	YES	YES
88	a	370.51	0.16228	YES	YES
89	a	378.42	0.91924	YES	YES
90	a	381.16	0.71376	YES	YES
91	a	386.85	1.00989	YES	YES
92	a	388.61	1.79929	YES	YES
93	a	390.25	0.10024	YES	YES
94	a	403.18	2.04781	YES	YES
95	a	408.49	2.73048	YES	YES
96	a	414.38	2.64052	YES	YES
97	a	417.09	3.14654	YES	YES
98	a	424.28	1.51184	YES	YES
99	a	425.06	1.65655	YES	YES
100	a	427.04	0.09366	YES	YES
101	a	429.88	0.64396	YES	YES
102	a	430.60	0.17615	YES	YES
103	a	430.94	0.06081	YES	YES
104	a	431.60	0.05371	YES	YES
105	a	432.38	0.00130	YES	YES
106	a	435.27	1.45117	YES	YES
107	a	436.19	3.36931	YES	YES
108	a	448.53	0.43789	YES	YES
109	a	457.13	3.79996	YES	YES
110	a	465.40	0.95053	YES	YES
111	a	466.78	5.18802	YES	YES
112	a	469.56	1.30836	YES	YES
113	a	492.13	2.55476	YES	YES
114	a	497.73	0.36520	YES	YES
115	a	499.37	0.31496	YES	YES
116	a	503.25	1.32462	YES	YES
117	a	504.62	0.43496	YES	YES
118	a	514.43	12.52952	YES	YES
119	a	516.24	4.94661	YES	YES
120	a	525.67	1.08589	YES	YES
121	a	547.15	46.28633	YES	YES
122	a	576.43	5.60555	YES	YES
123	a	628.29	3.65725	YES	YES
124	a	629.24	29.88220	YES	YES
125	a	633.48	16.90612	YES	YES

126	a	644.93	9.01299	YES	YES
127	a	653.60	8.68930	YES	YES
128	a	701.14	4.37901	YES	YES
129	a	710.99	3.55426	YES	YES
130	a	715.48	5.59097	YES	YES
131	a	728.74	11.25163	YES	YES
132	a	729.59	3.74708	YES	YES
133	a	732.76	9.91982	YES	YES
134	a	738.32	1.61807	YES	YES
135	a	740.55	1.20429	YES	YES
136	a	760.20	1.20740	YES	YES
137	a	770.33	0.16069	YES	YES
138	a	771.33	0.15714	YES	YES
139	a	773.58	0.11898	YES	YES
140	a	773.88	0.08189	YES	YES
141	a	775.15	0.02981	YES	YES
142	a	775.77	0.26180	YES	YES
143	a	776.58	0.05069	YES	YES
144	a	787.40	22.14841	YES	YES
145	a	790.94	15.14475	YES	YES
146	a	808.17	0.79425	YES	YES
147	a	808.58	0.45040	YES	YES
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152	a	815.84	4.08620	YES	YES
153	a	819.81	6.56057	YES	YES
154	a	834.00	2.80715	YES	YES
155	a	834.13	2.44898	YES	YES
156	a	836.10	4.03590	YES	YES
157	a	836.82	3.26224	YES	YES
158	a	837.18	3.58750	YES	YES
159	a	838.55	4.83510	YES	YES
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161	a	842.85	3.12030	YES	YES
162	a	853.19	18.50714	YES	YES
163	a	857.75	9.72857	YES	YES
164	a	872.96	2.24542	YES	YES
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166	a	874.27	5.09883	YES	YES
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175	a	881.73	1.11849	YES	YES
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182	a	904.37	1.84342	YES	YES
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208	a	1032.24	3.54864	YES	YES
209	a	1033.80	10.40113	YES	YES
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212	a	1039.42	1.70798	YES	YES
213	a	1040.64	0.66268	YES	YES
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215	a	1046.38	2.06981	YES	YES
216	a	1059.07	0.74978	YES	YES
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229	a	1074.80	0.27975	YES	YES
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239	a	1106.17	0.73506	YES	YES
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243	a	1125.88	5.64191	YES	YES
244	a	1128.35	2.76797	YES	YES
245	a	1160.96	9.09199	YES	YES
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252	a	1171.08	6.28559	YES	YES
253	a	1177.95	13.63029	YES	YES
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255	a	1186.94	3.72221	YES	YES
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260	a	1209.25	3.97394	YES	YES
261	a	1222.94	2.26784	YES	YES
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263	a	1244.01	0.10376	YES	YES
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266	a	1245.27	0.68092	YES	YES
267	a	1247.62	0.44490	YES	YES
268	a	1248.86	0.62240	YES	YES
269	a	1250.29	0.67470	YES	YES
270	a	1251.71	0.61093	YES	YES
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279	a	1259.45	2.09295	YES	YES
280	a	1260.23	1.47355	YES	YES
281	a	1260.80	0.79099	YES	YES
282	a	1260.89	2.65481	YES	YES
283	a	1266.47	1.41675	YES	YES
284	a	1266.57	4.27314	YES	YES
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293	a	1287.83	0.60196	YES	YES
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317	a	1327.02	1.50254	YES	YES
318	a	1327.86	4.95600	YES	YES
319	a	1328.75	0.45490	YES	YES
320	a	1329.76	5.07738	YES	YES
321	a	1336.02	0.86282	YES	YES
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323	a	1336.58	0.23010	YES	YES
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334	a	1347.17	1.84908	YES	YES
335	a	1349.65	0.52872	YES	YES
336	a	1350.97	0.24163	YES	YES
337	a	1385.48	5.62842	YES	YES
338	a	1405.31	7.44008	YES	YES
339	a	1407.68	5.47027	YES	YES
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348	a	1434.83	1.28618	YES	YES
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352	a	1437.34	3.33190	YES	YES
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354	a	1438.05	2.06533	YES	YES
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361	a	1439.91	10.85779	YES	YES
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364	a	1442.53	5.76258	YES	YES
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366	a	1443.65	9.24418	YES	YES
367	a	1444.77	9.66047	YES	YES
368	a	1445.11	7.88105	YES	YES
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370	a	1446.20	1.90405	YES	YES
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372	a	1449.50	3.10971	YES	YES
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376	a	1454.93	1.19151	YES	YES
377	a	1456.49	14.12508	YES	YES
378	a	1457.10	2.81312	YES	YES
379	a	1457.89	2.14374	YES	YES
380	a	1458.67	0.75134	YES	YES
381	a	1466.93	1.08934	YES	YES
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387	a	2935.45	3.67204	YES	YES
388	a	2937.33	10.19922	YES	YES
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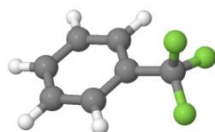
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422	a	2964.32	14.65401	YES	YES
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434	a	2988.28	2.98643	YES	YES
435	a	2992.52	1.58100	YES	YES
436	a	2994.52	29.79771	YES	YES
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448	a	3010.89	20.26606	YES	YES
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457	a	3016.15	18.23043	YES	YES
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471	a	3022.74	39.94889	YES	YES
472	a	3024.97	27.83245	YES	YES
473	a	3028.08	18.89936	YES	YES

474	a	3028.40	20.89781	YES	YES
475	a	3029.81	1.20114	YES	YES
476	a	3033.98	0.71745	YES	YES
477	a	3038.28	22.06289	YES	YES
478	a	3044.76	0.37350	YES	YES
479	a	3053.73	1.48818	YES	YES
480	a	3060.18	1.20992	YES	YES

\$end

Double hybrid single point energy = -7480.928580306914 H
 COSMO energy + OC correction = -7488.5208407909 H (in oDFB)

6.2.48 PhCF₃



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: cs

Cartesian coordinates in Ångström:

H	0.2910558	3.1833279	0.0000000
C	0.1992900	2.0974380	0.0000000
C	0.1421281	1.4014188	-1.2098584
H	0.1897234	1.9415917	-2.1548306
C	0.0271671	0.0111957	-1.2132341
H	-0.0125869	-0.5368621	-2.1529977
C	-0.0279844	-0.6824439	0.0000000
C	-0.2024647	-2.1788288	0.0000000
C	0.0271671	0.0111957	1.2132341
H	-0.0125869	-0.5368621	2.1529977
C	0.1421281	1.4014188	1.2098584
H	0.1897234	1.9415917	2.1548306
F	0.3550461	-2.7630774	-1.0949976
F	-1.5234809	-2.5303479	0.0000000
F	0.3550461	-2.7630774	1.0949976

SCF energy GEOOPT = -569.5771654083 H

ZPE = 267.9 kJ/mol

FREEH energy = 289.23 kJ/mol

FREEH entropy = 0.38620 kJ/mol/K

\$vibrational spectrum

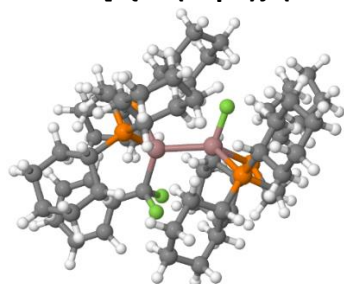
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15	a''	550.54	0.24497	YES	YES
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17	a''	614.45	0.13361	YES	YES
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21	a'	761.06	42.25706	YES	YES
22	a''	833.35	0.15703	YES	YES
23	a'	915.26	9.33371	YES	YES
24	a''	957.63	0.12081	YES	YES
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30	a'	1065.36	228.14582	YES	YES
31	a''	1118.57	112.95958	YES	YES
32	a''	1155.09	0.00004	YES	YES
33	a'	1172.90	4.63586	YES	YES
34	a'	1279.42	304.47713	YES	YES
35	a''	1310.44	2.52929	YES	YES
36	a''	1346.62	0.00110	YES	YES
37	a''	1443.93	15.18811	YES	YES
38	a'	1488.03	0.00372	YES	YES
39	a''	1587.47	0.06439	YES	YES
40	a'	1603.67	4.02029	YES	YES
41	a'	3104.04	0.15539	YES	YES
42	a''	3114.81	6.27986	YES	YES
43	a'	3123.57	11.16749	YES	YES
44	a''	3133.52	7.60687	YES	YES
45	a'	3135.72	2.32210	YES	YES

\$end

Double hybrid single point energy = -568.722549723201 H
COSMO energy + OC correction = -569.5796058811 H (in oDFB)

6.2.49 [F{Ga(dcpe)}₂(CF₂Ph)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

H	10.6218165	12.1116328	3.4682765
H	11.7929127	10.8954102	3.9793082
C	10.9192142	11.0587691	3.3336167
H	11.9422566	8.0090661	7.9496918
H	12.0781181	11.5027162	1.5539175
H	9.5084396	10.4101711	4.8320678
C	11.2820225	10.8139202	1.8667981
C	11.8402865	6.9122121	7.9926040
H	12.7434915	6.5341049	8.4897926
C	9.7730406	10.1476299	3.7987592
H	10.6425195	6.9758191	9.8087555
H	9.3517049	8.1418591	8.0541656
H	9.7017317	12.0237937	1.0082324
H	8.6185321	9.1820895	6.0746129
H	10.5280343	7.8993386	5.6840835
H	6.8057113	10.6796790	5.2833554
H	12.6218439	6.6457187	5.9780813
C	10.5930681	6.5467245	8.7990382
H	8.1565095	11.3241651	2.9815157
H	11.6753164	9.7905952	1.7624339
C	10.0537085	10.9801462	0.9693772
H	7.2207173	9.0057821	7.1346362
C	11.7460033	6.3528958	6.5719846
C	7.5813285	8.8283238	6.1125804
C	9.3206018	7.0420836	8.0999186
C	8.5498264	10.2950612	2.8837844
H	10.1168593	9.1024774	3.7818768
C	10.4728191	6.8126857	5.8539208
C	6.7106461	9.5978185	5.1116765
H	13.5269085	9.1596818	0.1129849
H	10.3049053	10.7788841	-0.0810135
H	4.8042480	11.1765291	3.8565327
H	14.4504052	9.2941479	-1.3863185
C	8.9180381	10.0500799	1.4104382
H	8.4390770	6.7720458	8.6964755
H	10.5388096	5.4529234	8.9244249
C	9.2194587	6.4734865	6.6693574
H	4.0111300	9.6204809	3.5881581
C	13.6312028	8.7453007	-0.9032442
H	12.0601992	10.0153774	-1.7146069
H	5.6522358	9.3443576	5.2565769
H	11.7504663	5.2504890	6.6264030
H	10.4139150	6.3541705	4.8561785
C	4.5054724	10.4604466	3.0786816
H	15.3361674	6.2493776	3.7196960
P	7.1024794	9.2373001	3.3412115
H	14.4045123	5.7581353	5.1332160
P	7.6582493	7.0056045	5.8223850
C	12.3264088	8.9497280	-1.6736349
H	2.6128666	11.4328724	2.6967283
H	8.0433051	10.1866311	0.7591590
C	14.6851736	5.4557232	4.1113894
H	9.2407491	9.0017969	1.3015219
H	6.7412834	6.1884016	7.8486473
H	10.9661691	8.5664673	-0.0360749
C	3.4979884	11.1210214	2.1257005
H	14.8882590	7.0979276	-0.2356392

H	12.8788510	6.3171126	3.2348065
H	9.1279744	5.3755342	6.7323992
C	5.7349875	9.9685399	2.2956045
C	13.9675807	7.2563499	-0.8142442
H	5.1941362	8.0214023	7.2942952
C	6.3201992	6.2151771	6.8289127
C	11.1687398	8.1675273	-1.0413060
H	16.3084114	4.2014196	4.8247618
H	12.7017311	6.7782280	0.8770063
C	13.4232553	5.3640055	3.2432768
H	12.4597637	8.6224189	-2.7174889
C	15.4310363	4.1209977	4.1692597
H	3.9431259	12.0407155	1.7123922
Ga	9.7227287	6.2259376	2.2650558
C	5.0133592	7.0168699	6.8852882
Ga	7.5764530	6.8363907	3.3712293
C	12.8266180	6.4600127	-0.1681167
H	6.2228730	10.8634540	1.8713506
H	2.5816142	9.3035030	1.3868862
H	10.2629999	8.3115235	-1.6433817
H	4.9259825	8.1120832	1.5063720
C	3.1039222	10.1851956	0.9798097
H	14.1615876	6.8627928	-1.8253385
H	4.3093191	6.2740576	8.7925642
H	13.7322096	5.1652040	2.2049085
C	5.3554928	9.0475742	1.1244290
H	7.0441853	4.2118980	6.3781258
H	15.8128817	3.8694533	3.1658411
H	12.1465609	4.4743144	4.7327124
C	6.0961630	4.7681867	6.3630810
C	11.4957712	6.6702279	-0.9079876
H	14.2010473	3.2022648	5.6954848
C	3.9695227	6.2894259	7.7440489
C	12.5017318	4.2274195	3.7193639
C	14.5074832	3.0019132	4.6554699
H	5.4392944	3.9582082	8.2618567
H	4.6136307	7.1384031	5.8702921
H	2.3947452	10.6878854	0.3091045
H	13.0950667	5.3957401	-0.1667656
C	4.3389490	9.7255796	0.2000380
H	9.1378170	6.0876705	-2.2757110
C	5.0512774	4.0650650	7.2356116
H	6.2578147	8.7686263	0.5646814
P	10.0894041	5.7514407	-0.1170199
H	3.0295565	6.8580257	7.7287994
H	5.7459613	4.7734627	5.3226538
P	10.9509617	4.1279276	2.7121798
H	11.5687775	6.2263668	-1.9180293
H	8.6764267	4.0535586	4.6252344
C	13.2531758	2.8834958	3.7774864
H	10.1618424	3.5684414	5.4644239
H	15.0341745	2.0380119	4.6647589
C	3.7395831	4.8546328	7.2601709
C	8.6646248	5.9299893	-1.2899469
H	4.8086711	10.5944872	-0.2902196
C	9.3639945	3.2080155	4.7976936
H	4.0533891	9.0285812	-0.5999392
H	8.4730295	8.0683177	-0.8641433

H	7.1668407	7.6089614	-2.9423882
H	12.4975497	3.9148084	0.8949702
H	4.8848032	3.0480015	6.8545976
H	13.5540353	2.5871056	2.7596525
H	7.0404131	5.0036285	-3.3865439
H	8.3407306	3.8094164	-1.6934315
H	3.0055153	4.3529655	7.9045861
C	11.4810090	3.5345209	1.0448354
C	7.8357358	7.1783191	-0.9326757
H	12.6074052	2.0849781	4.1666318
H	8.1806125	2.3763723	6.4160522
C	9.9513981	2.7674769	3.4474961
C	7.7619570	4.6867899	-1.3753587
H	3.3094055	4.8755850	6.2459958
C	10.5568540	3.9623356	-0.1059252
C	6.7184028	7.4004044	-1.9572039
C	8.6032838	2.0508684	5.4546365
C	6.6160786	4.9157270	-2.3730688
H	8.1899417	3.0481267	2.2103045
H	11.0108749	3.7049069	-1.0738734
H	6.7403258	2.3011857	4.3900654
H	10.6710841	1.9522277	3.6325542
C	8.8683187	2.2327561	2.4978391
H	6.1406402	8.2951802	-1.6869547
H	11.5532765	2.4383480	1.0729595
C	5.8061249	6.1753372	-2.0522783
H	7.3969634	7.0222609	0.0635122
H	9.6094370	3.4120894	-0.0421950
C	7.5023441	1.5199421	4.5322121
H	9.3144450	1.2426614	5.6901039
H	7.3466270	4.4669178	-0.3793641
H	5.9658051	4.0304289	-2.3839847
H	5.0369205	6.3315340	-2.8205283
H	9.3290501	1.8480392	1.5769235
C	8.0715494	1.1042296	3.1707469
H	6.9971826	0.6649695	5.0012175
H	5.2780958	6.0394005	-1.0955689
H	7.2648761	0.7783248	2.5001724
H	8.7346365	0.2343445	3.3064254
F	11.0502247	7.4693041	2.5274624
C	6.0540757	5.5954319	2.7420869
C	4.6264866	5.6600221	3.1956724
C	4.0742302	6.8755504	3.5985252
H	4.7157695	7.7531736	3.6501348
C	2.7240153	6.9752028	3.9342449
H	2.3046701	7.9323472	4.2435792
C	1.9160916	5.8381589	3.8861928
H	0.8623841	5.9047858	4.1536183
C	2.4644273	4.6106185	3.4987324
H	1.8358196	3.7216700	3.4646774
C	3.8105212	4.5195166	3.1474103
H	4.2323952	3.5657221	2.8361596
F	6.0550873	5.6681215	1.3293899
F	6.5499209	4.3025569	3.0009163

SCF energy GEOOPT = -7825.823699134 H
ZPE = 3873. kJ/mol
FREEH energy = 4073.69 kJ/mol

FREEH entropy = 1.67067 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			-0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	19.96	0.02023	YES	YES
8		a	21.18	0.02784	YES	YES
9		a	24.16	0.21327	YES	YES
10		a	27.97	0.15694	YES	YES
11		a	30.20	0.10534	YES	YES
12		a	32.44	0.01504	YES	YES
13		a	35.29	0.20832	YES	YES
14		a	38.17	0.46469	YES	YES
15		a	43.64	0.31631	YES	YES
16		a	45.37	0.29239	YES	YES
17		a	46.53	0.09207	YES	YES
18		a	48.42	0.41836	YES	YES
19		a	51.16	0.07086	YES	YES
20		a	54.44	0.06640	YES	YES
21		a	54.93	0.37636	YES	YES
22		a	58.43	0.18580	YES	YES
23		a	61.66	0.33108	YES	YES
24		a	62.12	0.22022	YES	YES
25		a	65.93	0.31718	YES	YES
26		a	68.73	0.40070	YES	YES
27		a	70.28	0.24320	YES	YES
28		a	71.69	0.01533	YES	YES
29		a	73.98	1.06352	YES	YES
30		a	76.35	0.26340	YES	YES
31		a	77.69	0.27796	YES	YES
32		a	80.29	0.13869	YES	YES
33		a	84.54	0.17184	YES	YES
34		a	88.62	0.50805	YES	YES
35		a	90.65	0.04085	YES	YES
36		a	94.03	0.03840	YES	YES
37		a	95.83	0.04033	YES	YES
38		a	98.21	0.26322	YES	YES
39		a	105.95	2.14146	YES	YES
40		a	116.56	1.66424	YES	YES
41		a	124.72	0.70318	YES	YES
42		a	132.64	2.51567	YES	YES
43		a	133.92	0.25727	YES	YES
44		a	135.98	0.95105	YES	YES
45		a	138.14	2.57217	YES	YES
46		a	139.55	1.99600	YES	YES
47		a	145.95	11.09043	YES	YES
48		a	147.71	11.88490	YES	YES
49		a	155.19	2.94868	YES	YES
50		a	158.98	0.97633	YES	YES
51		a	162.71	5.43749	YES	YES
52		a	163.85	3.77627	YES	YES
53		a	171.13	7.06300	YES	YES

54	a	172.11	0.18426	YES	YES
55	a	176.41	7.05075	YES	YES
56	a	182.18	0.32211	YES	YES
57	a	184.48	11.07904	YES	YES
58	a	196.37	1.47196	YES	YES
59	a	206.58	0.65764	YES	YES
60	a	210.20	1.54930	YES	YES
61	a	212.31	1.00270	YES	YES
62	a	216.18	1.22472	YES	YES
63	a	217.50	0.36842	YES	YES
64	a	221.24	0.96629	YES	YES
65	a	224.82	0.10353	YES	YES
66	a	226.81	0.79998	YES	YES
67	a	229.49	1.06268	YES	YES
68	a	231.20	0.35729	YES	YES
69	a	232.33	1.18637	YES	YES
70	a	237.40	1.94311	YES	YES
71	a	238.77	0.35645	YES	YES
72	a	246.86	0.93850	YES	YES
73	a	248.53	0.17612	YES	YES
74	a	250.13	1.73592	YES	YES
75	a	255.21	1.27692	YES	YES
76	a	265.63	10.42489	YES	YES
77	a	268.23	1.08263	YES	YES
78	a	288.51	3.22834	YES	YES
79	a	293.14	0.06925	YES	YES
80	a	294.00	0.76610	YES	YES
81	a	296.96	0.47246	YES	YES
82	a	305.42	0.75175	YES	YES
83	a	307.24	0.01726	YES	YES
84	a	308.91	1.02678	YES	YES
85	a	317.67	0.22316	YES	YES
86	a	324.79	4.86414	YES	YES
87	a	330.22	0.28241	YES	YES
88	a	332.06	1.49063	YES	YES
89	a	335.20	0.56995	YES	YES
90	a	337.79	0.14701	YES	YES
91	a	343.82	0.93069	YES	YES
92	a	345.36	0.34979	YES	YES
93	a	361.86	2.96794	YES	YES
94	a	362.16	1.09391	YES	YES
95	a	376.71	1.47401	YES	YES
96	a	378.71	1.01692	YES	YES
97	a	383.97	6.22287	YES	YES
98	a	388.55	0.20784	YES	YES
99	a	394.72	1.60285	YES	YES
100	a	402.59	0.57406	YES	YES
101	a	412.66	1.72182	YES	YES
102	a	417.57	1.16667	YES	YES
103	a	420.12	3.40600	YES	YES
104	a	423.18	0.96979	YES	YES
105	a	427.33	4.18024	YES	YES
106	a	428.41	0.98607	YES	YES
107	a	428.50	0.08972	YES	YES
108	a	430.51	0.12865	YES	YES
109	a	430.91	0.10126	YES	YES
110	a	431.05	0.42793	YES	YES
111	a	431.92	0.48950	YES	YES

112	a	434.18	3.04486	YES	YES
113	a	434.83	0.66271	YES	YES
114	a	438.30	3.61332	YES	YES
115	a	439.72	0.35973	YES	YES
116	a	441.13	5.01798	YES	YES
117	a	463.05	2.64441	YES	YES
118	a	465.33	4.06584	YES	YES
119	a	490.11	2.44868	YES	YES
120	a	492.45	3.96304	YES	YES
121	a	493.56	4.68638	YES	YES
122	a	496.83	5.31252	YES	YES
123	a	500.59	0.23742	YES	YES
124	a	502.86	1.30560	YES	YES
125	a	512.24	9.46436	YES	YES
126	a	515.02	4.76749	YES	YES
127	a	532.56	2.02783	YES	YES
128	a	542.18	48.29741	YES	YES
129	a	550.76	2.39581	YES	YES
130	a	616.92	0.30295	YES	YES
131	a	630.80	21.01384	YES	YES
132	a	631.53	14.47184	YES	YES
133	a	651.58	10.79893	YES	YES
134	a	653.92	9.38973	YES	YES
135	a	663.70	11.45993	YES	YES
136	a	700.09	32.75912	YES	YES
137	a	706.36	1.06533	YES	YES
138	a	710.57	1.34977	YES	YES
139	a	712.59	1.17774	YES	YES
140	a	719.04	1.78025	YES	YES
141	a	728.68	1.31338	YES	YES
142	a	729.76	1.98607	YES	YES
143	a	734.90	8.05891	YES	YES
144	a	735.29	4.59893	YES	YES
145	a	758.64	57.98659	YES	YES
146	a	771.45	0.09696	YES	YES
147	a	771.62	0.52748	YES	YES
148	a	772.06	0.33064	YES	YES
149	a	773.09	0.13413	YES	YES
150	a	773.19	0.16349	YES	YES
151	a	773.95	0.14421	YES	YES
152	a	776.25	0.37322	YES	YES
153	a	779.22	0.24458	YES	YES
154	a	784.30	17.93154	YES	YES
155	a	786.14	9.50639	YES	YES
156	a	807.09	2.60510	YES	YES
157	a	808.16	0.40248	YES	YES
158	a	810.60	3.66346	YES	YES
159	a	810.94	1.08578	YES	YES
160	a	812.06	1.16280	YES	YES
161	a	812.62	0.62357	YES	YES
162	a	814.13	2.94495	YES	YES
163	a	815.89	4.44690	YES	YES
164	a	834.71	6.77724	YES	YES
165	a	835.66	0.88792	YES	YES
166	a	836.02	0.44044	YES	YES
167	a	837.20	2.95191	YES	YES
168	a	837.59	1.61922	YES	YES
169	a	838.46	0.51259	YES	YES

170	a	838.68	5.70112	YES	YES
171	a	839.83	7.46091	YES	YES
172	a	840.77	7.77272	YES	YES
173	a	851.01	11.55142	YES	YES
174	a	853.22	5.80855	YES	YES
175	a	869.80	82.40759	YES	YES
176	a	873.85	1.78313	YES	YES
177	a	874.23	4.19043	YES	YES
178	a	875.10	4.98542	YES	YES
179	a	876.15	3.34806	YES	YES
180	a	877.48	1.60922	YES	YES
181	a	878.59	4.64180	YES	YES
182	a	879.09	2.84340	YES	YES
183	a	879.69	0.14920	YES	YES
184	a	880.18	9.32778	YES	YES
185	a	881.32	5.13925	YES	YES
186	a	881.50	2.64032	YES	YES
187	a	881.68	10.27362	YES	YES
188	a	884.49	1.46251	YES	YES
189	a	884.95	1.08066	YES	YES
190	a	887.20	2.81344	YES	YES
191	a	889.73	3.21402	YES	YES
192	a	896.90	17.78564	YES	YES
193	a	903.93	1.88751	YES	YES
194	a	904.44	0.28432	YES	YES
195	a	906.71	2.28103	YES	YES
196	a	907.13	2.24892	YES	YES
197	a	908.45	1.02408	YES	YES
198	a	909.09	1.09321	YES	YES
199	a	911.07	0.67166	YES	YES
200	a	912.71	0.92274	YES	YES
201	a	919.39	7.95168	YES	YES
202	a	961.57	9.30839	YES	YES
203	a	967.58	82.76431	YES	YES
204	a	985.49	8.58221	YES	YES
205	a	986.71	2.02721	YES	YES
206	a	987.94	18.61945	YES	YES
207	a	988.32	2.73944	YES	YES
208	a	989.63	8.64232	YES	YES
209	a	990.04	14.99640	YES	YES
210	a	990.35	0.30778	YES	YES
211	a	993.62	6.08660	YES	YES
212	a	995.13	1.78563	YES	YES
213	a	996.18	4.81309	YES	YES
214	a	999.05	1.17497	YES	YES
215	a	1001.60	4.04964	YES	YES
216	a	1017.01	1.20353	YES	YES
217	a	1017.47	0.47529	YES	YES
218	a	1018.20	0.55424	YES	YES
219	a	1018.93	1.38132	YES	YES
220	a	1019.39	0.63821	YES	YES
221	a	1019.73	0.96426	YES	YES
222	a	1020.29	1.13617	YES	YES
223	a	1024.29	1.04821	YES	YES
224	a	1029.43	0.41155	YES	YES
225	a	1029.68	1.06843	YES	YES
226	a	1030.63	3.92666	YES	YES
227	a	1033.51	1.46312	YES	YES

228	a	1034.80	0.50573	YES	YES
229	a	1037.68	0.86277	YES	YES
230	a	1039.20	0.93092	YES	YES
231	a	1039.86	1.41927	YES	YES
232	a	1040.13	0.38076	YES	YES
233	a	1061.13	1.42585	YES	YES
234	a	1061.97	0.91431	YES	YES
235	a	1063.18	0.25674	YES	YES
236	a	1064.33	0.07441	YES	YES
237	a	1064.68	0.43412	YES	YES
238	a	1066.46	1.26605	YES	YES
239	a	1070.55	0.49723	YES	YES
240	a	1071.83	0.54041	YES	YES
241	a	1072.08	0.00919	YES	YES
242	a	1072.51	0.09931	YES	YES
243	a	1073.18	0.12827	YES	YES
244	a	1073.82	0.17956	YES	YES
245	a	1074.18	0.50610	YES	YES
246	a	1074.49	0.09198	YES	YES
247	a	1074.56	0.62985	YES	YES
248	a	1076.39	0.11537	YES	YES
249	a	1082.88	0.61601	YES	YES
250	a	1086.93	0.71109	YES	YES
251	a	1088.56	5.07823	YES	YES
252	a	1095.52	0.25491	YES	YES
253	a	1096.27	5.93709	YES	YES
254	a	1098.89	2.14037	YES	YES
255	a	1099.94	12.68094	YES	YES
256	a	1105.52	5.11860	YES	YES
257	a	1105.80	0.99917	YES	YES
258	a	1107.43	2.05824	YES	YES
259	a	1108.27	1.66868	YES	YES
260	a	1130.87	1.31912	YES	YES
261	a	1134.35	3.20560	YES	YES
262	a	1156.54	0.59480	YES	YES
263	a	1160.85	7.34982	YES	YES
264	a	1162.22	4.61928	YES	YES
265	a	1164.57	2.18653	YES	YES
266	a	1165.89	0.85791	YES	YES
267	a	1168.17	2.99878	YES	YES
268	a	1169.28	4.52612	YES	YES
269	a	1169.78	11.66695	YES	YES
270	a	1171.26	3.06966	YES	YES
271	a	1171.60	7.15709	YES	YES
272	a	1178.71	9.26095	YES	YES
273	a	1184.78	12.50544	YES	YES
274	a	1185.10	12.27089	YES	YES
275	a	1186.60	0.44965	YES	YES
276	a	1187.57	15.90778	YES	YES
277	a	1189.59	6.67561	YES	YES
278	a	1193.35	17.76332	YES	YES
279	a	1201.59	14.37314	YES	YES
280	a	1220.04	59.46689	YES	YES
281	a	1243.63	0.36846	YES	YES
282	a	1245.13	0.73109	YES	YES
283	a	1246.45	0.28104	YES	YES
284	a	1246.93	0.27194	YES	YES
285	a	1249.12	0.47102	YES	YES

286	a	1250.52	2.97498	YES	YES
287	a	1250.92	1.22552	YES	YES
288	a	1251.22	1.23384	YES	YES
289	a	1252.10	2.14398	YES	YES
290	a	1252.95	5.48571	YES	YES
291	a	1254.12	1.20702	YES	YES
292	a	1255.34	1.51079	YES	YES
293	a	1256.71	5.56689	YES	YES
294	a	1257.04	15.72258	YES	YES
295	a	1257.55	5.28365	YES	YES
296	a	1258.18	1.94187	YES	YES
297	a	1258.67	7.44947	YES	YES
298	a	1259.69	3.33734	YES	YES
299	a	1259.85	5.89458	YES	YES
300	a	1261.07	8.09957	YES	YES
301	a	1262.75	5.27787	YES	YES
302	a	1264.13	0.10678	YES	YES
303	a	1266.82	1.07145	YES	YES
304	a	1267.75	1.92140	YES	YES
305	a	1270.64	0.36953	YES	YES
306	a	1272.50	2.41391	YES	YES
307	a	1272.57	1.01967	YES	YES
308	a	1273.60	0.47877	YES	YES
309	a	1284.13	3.82581	YES	YES
310	a	1286.51	0.58787	YES	YES
311	a	1287.44	0.95694	YES	YES
312	a	1287.98	3.40272	YES	YES
313	a	1290.45	2.39948	YES	YES
314	a	1292.03	3.34813	YES	YES
315	a	1292.46	2.50074	YES	YES
316	a	1293.94	2.66959	YES	YES
317	a	1302.96	5.90392	YES	YES
318	a	1310.98	1.53511	YES	YES
319	a	1313.02	1.53558	YES	YES
320	a	1313.11	0.36068	YES	YES
321	a	1313.93	1.19548	YES	YES
322	a	1314.85	1.06380	YES	YES
323	a	1316.46	2.72889	YES	YES
324	a	1317.43	2.75396	YES	YES
325	a	1319.03	0.43767	YES	YES
326	a	1322.48	0.84104	YES	YES
327	a	1323.29	2.22040	YES	YES
328	a	1323.65	0.12471	YES	YES
329	a	1324.14	0.94206	YES	YES
330	a	1324.37	0.45820	YES	YES
331	a	1324.63	1.21319	YES	YES
332	a	1325.92	0.42063	YES	YES
333	a	1326.38	1.25867	YES	YES
334	a	1326.99	1.71797	YES	YES
335	a	1327.28	0.77718	YES	YES
336	a	1328.65	2.66857	YES	YES
337	a	1328.78	0.99610	YES	YES
338	a	1329.32	0.93016	YES	YES
339	a	1330.04	8.99639	YES	YES
340	a	1332.13	1.08473	YES	YES
341	a	1334.18	1.07425	YES	YES
342	a	1336.34	0.17405	YES	YES
343	a	1338.86	0.09910	YES	YES

344	a	1339.06	0.04797	YES	YES
345	a	1339.27	0.11939	YES	YES
346	a	1339.33	0.63557	YES	YES
347	a	1340.68	1.29987	YES	YES
348	a	1341.16	0.49943	YES	YES
349	a	1344.69	0.64215	YES	YES
350	a	1345.50	1.34673	YES	YES
351	a	1346.43	0.49219	YES	YES
352	a	1346.86	1.47402	YES	YES
353	a	1347.45	0.26297	YES	YES
354	a	1347.90	0.59817	YES	YES
355	a	1349.49	0.21604	YES	YES
356	a	1349.90	0.73973	YES	YES
357	a	1350.83	0.45909	YES	YES
358	a	1352.88	0.08670	YES	YES
359	a	1401.34	11.91138	YES	YES
360	a	1404.73	9.10457	YES	YES
361	a	1404.94	5.93526	YES	YES
362	a	1410.10	7.28904	YES	YES
363	a	1419.92	6.39259	YES	YES
364	a	1422.73	2.95018	YES	YES
365	a	1429.97	2.98655	YES	YES
366	a	1431.53	1.23841	YES	YES
367	a	1432.56	1.44624	YES	YES
368	a	1433.04	1.21014	YES	YES
369	a	1434.83	2.48100	YES	YES
370	a	1435.15	4.65592	YES	YES
371	a	1435.60	1.93704	YES	YES
372	a	1436.79	7.43168	YES	YES
373	a	1437.10	5.56699	YES	YES
374	a	1437.38	3.66717	YES	YES
375	a	1437.67	2.64438	YES	YES
376	a	1437.94	8.85756	YES	YES
377	a	1438.17	6.88349	YES	YES
378	a	1438.46	7.11981	YES	YES
379	a	1438.67	2.13570	YES	YES
380	a	1438.94	3.12669	YES	YES
381	a	1439.17	1.54314	YES	YES
382	a	1439.62	4.08911	YES	YES
383	a	1440.26	4.71428	YES	YES
384	a	1441.84	0.77099	YES	YES
385	a	1442.31	8.05496	YES	YES
386	a	1442.49	14.27439	YES	YES
387	a	1442.97	24.21906	YES	YES
388	a	1443.92	8.88301	YES	YES
389	a	1444.42	31.56291	YES	YES
390	a	1444.70	9.49763	YES	YES
391	a	1444.91	9.51986	YES	YES
392	a	1445.74	29.01911	YES	YES
393	a	1446.33	11.00349	YES	YES
394	a	1447.18	11.56143	YES	YES
395	a	1448.91	9.59701	YES	YES
396	a	1453.77	0.27132	YES	YES
397	a	1454.16	1.97062	YES	YES
398	a	1454.99	1.94122	YES	YES
399	a	1455.61	1.39426	YES	YES
400	a	1455.92	1.16415	YES	YES
401	a	1457.59	0.27567	YES	YES

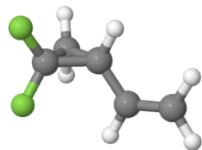
402	a	1458.73	0.56428	YES	YES
403	a	1461.97	0.99090	YES	YES
404	a	1484.11	5.08500	YES	YES
405	a	1579.28	3.68132	YES	YES
406	a	1600.19	0.69459	YES	YES
407	a	2916.42	6.26900	YES	YES
408	a	2921.53	5.80532	YES	YES
409	a	2930.23	5.39184	YES	YES
410	a	2931.03	14.68870	YES	YES
411	a	2934.43	24.34805	YES	YES
412	a	2935.73	3.65902	YES	YES
413	a	2942.09	4.25525	YES	YES
414	a	2944.39	9.12798	YES	YES
415	a	2944.63	7.40503	YES	YES
416	a	2946.60	1.22474	YES	YES
417	a	2947.35	14.55492	YES	YES
418	a	2948.39	10.09445	YES	YES
419	a	2949.48	12.51999	YES	YES
420	a	2949.53	9.06485	YES	YES
421	a	2950.12	14.75979	YES	YES
422	a	2950.47	28.77868	YES	YES
423	a	2951.28	22.02048	YES	YES
424	a	2951.47	17.45057	YES	YES
425	a	2952.00	10.55388	YES	YES
426	a	2952.38	10.64340	YES	YES
427	a	2952.89	12.98691	YES	YES
428	a	2953.75	4.88542	YES	YES
429	a	2954.14	21.51476	YES	YES
430	a	2954.20	10.68850	YES	YES
431	a	2954.98	11.61924	YES	YES
432	a	2956.99	17.28655	YES	YES
433	a	2958.85	13.05062	YES	YES
434	a	2959.16	14.04582	YES	YES
435	a	2960.04	13.26468	YES	YES
436	a	2960.13	27.32202	YES	YES
437	a	2961.01	32.32756	YES	YES
438	a	2962.68	37.28332	YES	YES
439	a	2965.60	11.47064	YES	YES
440	a	2965.92	23.96285	YES	YES
441	a	2966.52	11.48127	YES	YES
442	a	2966.60	19.83569	YES	YES
443	a	2968.12	15.00274	YES	YES
444	a	2968.77	17.43134	YES	YES
445	a	2972.77	24.00161	YES	YES
446	a	2973.73	13.40606	YES	YES
447	a	2973.84	8.46544	YES	YES
448	a	2974.02	4.89759	YES	YES
449	a	2975.04	20.38527	YES	YES
450	a	2975.44	21.76460	YES	YES
451	a	2977.09	11.90684	YES	YES
452	a	2981.53	3.11857	YES	YES
453	a	2981.80	15.93722	YES	YES
454	a	2982.10	1.77942	YES	YES
455	a	2984.56	15.91794	YES	YES
456	a	2989.47	23.81538	YES	YES
457	a	2992.13	4.53885	YES	YES
458	a	2992.23	8.11560	YES	YES
459	a	2994.71	3.07570	YES	YES

460	a	2997.54	40.66999	YES	YES
461	a	3000.44	42.63464	YES	YES
462	a	3004.13	28.64358	YES	YES
463	a	3005.25	16.50109	YES	YES
464	a	3007.94	18.93529	YES	YES
465	a	3008.39	23.82699	YES	YES
466	a	3008.63	4.42454	YES	YES
467	a	3009.15	30.87450	YES	YES
468	a	3009.33	48.40169	YES	YES
469	a	3010.11	13.91074	YES	YES
470	a	3010.68	22.29604	YES	YES
471	a	3010.94	28.08929	YES	YES
472	a	3011.31	23.13389	YES	YES
473	a	3011.52	10.18581	YES	YES
474	a	3011.77	9.97046	YES	YES
475	a	3012.15	23.51934	YES	YES
476	a	3014.24	44.10720	YES	YES
477	a	3014.45	11.69304	YES	YES
478	a	3015.70	12.59335	YES	YES
479	a	3015.90	7.77179	YES	YES
480	a	3016.59	20.41196	YES	YES
481	a	3017.43	27.36356	YES	YES
482	a	3017.53	9.15752	YES	YES
483	a	3018.00	22.14882	YES	YES
484	a	3018.18	34.46607	YES	YES
485	a	3019.10	25.38566	YES	YES
486	a	3019.46	33.21120	YES	YES
487	a	3019.55	27.90664	YES	YES
488	a	3020.10	22.52043	YES	YES
489	a	3020.25	23.89822	YES	YES
490	a	3021.06	28.75777	YES	YES
491	a	3025.31	23.38345	YES	YES
492	a	3025.96	6.80841	YES	YES
493	a	3027.28	9.19989	YES	YES
494	a	3029.14	16.88608	YES	YES
495	a	3029.63	2.64335	YES	YES
496	a	3031.97	1.04749	YES	YES
497	a	3034.17	5.38219	YES	YES
498	a	3034.39	11.74576	YES	YES
499	a	3036.01	10.78933	YES	YES
500	a	3036.25	6.92957	YES	YES
501	a	3048.72	0.64949	YES	YES
502	a	3053.52	0.60454	YES	YES
503	a	3106.23	3.16567	YES	YES
504	a	3117.31	3.05842	YES	YES
505	a	3120.54	10.24956	YES	YES
506	a	3131.25	1.79720	YES	YES
507	a	3138.09	2.07155	YES	YES

\$end

Double hybrid single point energy = -7817.865624002791 H
COSMO energy + OC correction = -7825.9709651389 H (in oDFB)

6.2.50 C₅H₆F₂



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

C	0.0630981	0.0484875	0.4454405
C	1.2402205	0.9378405	0.2018589
C	1.5220016	-0.5062340	0.2863503
F	1.3644021	1.5772606	-0.9950855
F	1.6570946	1.7667589	1.2009047
H	1.7437404	-1.0297111	-0.6420663
H	2.0083795	-0.8862641	1.1820349
H	-0.3081269	0.0603374	1.4711462
C	-0.9365941	-0.2041923	-0.6058872
C	-2.2277632	-0.4600502	-0.3694101
H	-0.5716341	-0.1691482	-1.6358137
H	-2.6275409	-0.4969885	0.6450966
H	-2.9272778	-0.6380965	-1.1845694

SCF energy GEOOPT = -393.9597861465 H

ZPE = 250.5 kJ/mol

FREEH energy = 268.79 kJ/mol

FREEH entropy = 0.34387 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	95.73	0.68681	YES	YES
8		a	156.29	0.83744	YES	YES
9		a	200.76	0.95789	YES	YES
10		a	348.65	0.72032	YES	YES
11		a	375.11	4.05481	YES	YES
12		a	407.28	0.24746	YES	YES
13		a	457.85	4.34406	YES	YES
14		a	555.59	8.26735	YES	YES
15		a	650.23	0.17736	YES	YES
16		a	715.28	14.51155	YES	YES
17		a	805.32	12.62452	YES	YES
18		a	876.62	22.32296	YES	YES
19		a	897.22	32.04832	YES	YES
20		a	913.46	30.16554	YES	YES
21		a	954.27	68.15588	YES	YES
22		a	985.43	12.77619	YES	YES
23		a	993.99	11.26182	YES	YES
24		a	1012.55	39.45598	YES	YES
25		a	1071.16	38.33327	YES	YES

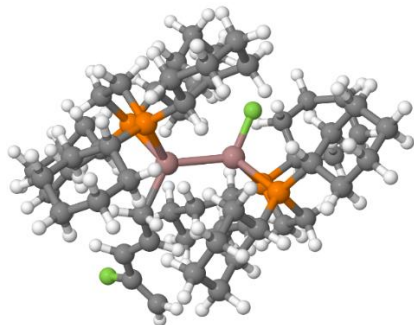
26	a	1170.62	57.54495	YES	YES
27	a	1190.01	54.65603	YES	YES
28	a	1261.03	61.02189	YES	YES
29	a	1293.06	12.53054	YES	YES
30	a	1345.76	68.56078	YES	YES
31	a	1415.67	17.96741	YES	YES
32	a	1441.68	93.73265	YES	YES
33	a	1650.90	28.75189	YES	YES
34	a	3069.26	6.64961	YES	YES
35	a	3073.63	3.58023	YES	YES
36	a	3076.13	0.72833	YES	YES
37	a	3091.71	4.81359	YES	YES
38	a	3159.42	10.32249	YES	YES
39	a	3171.36	0.62730	YES	YES

\$end

Double hybrid single point energy = -393.357223642735 H

COSMO energy + OC correction = -393.9649753282 H (in oDFB)

6.2.51 [F{Ga(dcpe)}₂(C₅H₆F)]²⁺



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

C	4.6080890	5.2873209	1.4044631
C	4.2712120	4.8593627	0.0552994
C	4.7071632	3.8019664	-0.6388574
F	3.3641013	5.7017952	-0.5317675
H	5.3682321	3.0783765	-0.1699037
H	4.3653469	3.6183468	-1.6539730
H	3.8416895	5.8782628	1.9095465
C	5.7672542	5.0037497	2.0285078
C	6.1360580	5.3894983	3.4021654
H	6.5113400	4.4282188	1.4709201
H	5.2763774	5.7753166	3.9600855
H	6.5196521	4.5201962	3.9549043
H	9.8433068	12.4135336	2.8109565
H	11.2775784	11.5637879	3.3875931
C	10.3710954	11.4464409	2.7784336
H	12.0703967	8.3695315	8.3057495
H	11.3364484	11.9231133	0.8944828
H	9.1964702	10.6781892	4.4161231
C	10.7421843	11.1099201	1.3322127
C	12.0922601	7.2962658	8.0555895
H	13.0525116	6.9118175	8.4251297
C	9.4738052	10.3669061	3.4003583

H	10.9774802	6.7586387	9.8456065
H	9.4064970	8.1018718	8.4687191
H	8.9150557	11.7784859	0.3755515
H	8.6099949	9.5107264	5.9233135
H	10.5400424	8.6858069	6.2171635
H	6.6870797	10.7153054	4.9616940
H	12.8022892	7.6878055	6.0308022
C	10.9334527	6.5860063	8.7618930
H	7.6794819	11.1293215	2.4980803
H	11.3791787	10.2132365	1.3319656
C	9.4976891	10.8485816	0.4778540
H	7.2525213	9.3192080	7.0344103
C	11.9991649	7.1344846	6.5360018
C	7.6162197	9.0604670	6.0300380
C	9.5655470	7.0381458	8.2276546
C	8.2196311	10.1671096	2.5357744
H	10.0290840	9.4187113	3.4761537
C	10.6407241	7.6085713	6.0083533
C	6.6537213	9.6165054	4.9638500
H	14.5718612	8.1446025	0.3322543
H	9.7819585	10.5540419	-0.5426450
H	5.9841591	11.0583244	1.2526922
H	15.1673437	8.5176835	-1.2864121
C	8.6030477	9.7708876	1.1025163
H	8.7716483	6.4721007	8.7327743
H	11.0266616	5.4966288	8.6156963
C	9.5024034	6.8468419	6.7031438
H	4.9788610	11.2732600	2.6923735
C	14.3335353	8.0566910	-0.7406852
H	13.1046696	9.8533953	-0.7170534
H	5.6222891	9.3274913	5.1987817
H	12.1345903	6.0716650	6.2693664
H	10.6011025	7.4942520	4.9174052
C	5.1355061	10.6358916	1.8064950
H	15.4161161	5.7323821	3.7305814
P	6.9849198	9.0013506	3.2509943
H	14.3675498	5.4681030	5.1236874
P	7.8642029	7.2312781	5.9387541
C	13.0289392	8.8032521	-1.0313997
H	3.6699041	11.7061389	0.6282329
H	7.7088795	9.6085616	0.4832871
C	14.6671224	5.0469200	4.1500889
H	9.1480948	8.8118562	1.1392916
H	6.8212014	6.8741894	8.0496478
H	11.9793383	8.2095156	0.7742119
C	3.8825720	10.6683899	0.9184145
H	15.1365269	6.0368334	-0.8689717
H	13.0089303	6.0042275	3.1013975
H	9.6329742	5.7720731	6.4821499
C	5.4324483	9.1956824	2.2581949
C	14.2120990	6.5770367	-1.1152013
H	5.0690414	8.0314854	6.8036529
C	6.5843185	6.4884975	7.0430537
C	11.8457194	8.1434372	-0.3159201
H	16.1151028	3.6970319	5.0454685
H	13.2097094	5.9154103	0.6829423
C	13.4429464	5.0029596	3.2267674
H	12.8425523	8.8131256	-2.1176974
C	15.2641665	3.6517623	4.3528379
H	4.0948884	10.1186130	-0.0134444
Ga	9.8490825	6.2806103	2.4804616
C	5.1559401	6.9412748	6.6950033

Ga	7.6789329	6.7104221	3.5633549
C	13.0285935	5.9077468	-0.4017369
H	5.6244379	8.5790161	1.3620721
H	2.3863110	10.6593772	2.4817042
H	10.9168027	8.6780794	-0.5591205
H	4.0048398	9.1813429	3.8919963
C	2.6709451	10.0423135	1.6136223
H	14.0760244	6.4828580	-2.2048695
H	4.2578697	6.6035374	8.6329697
H	13.7680447	4.6528205	2.2338809
C	4.2190139	8.5919252	2.9864402
H	7.7398785	4.6774199	7.3912233
H	15.6629721	3.2828376	3.3933996
H	12.0641140	4.4097277	4.7616090
C	6.7297754	4.9577790	7.0592846
C	11.7248867	6.6587120	-0.6965318
H	13.8958067	2.9744807	5.8873583
C	4.1228356	6.2530097	7.5970159
C	12.3895765	4.0270152	3.7770521
C	14.2119099	2.6699613	4.8757320
H	5.8621343	4.5827862	9.0053731
H	4.9337366	6.7056490	5.6432430
H	1.8063726	10.0390806	0.9368806
H	12.9543502	4.8593582	-0.7241139
C	2.9808899	8.6176940	2.0812297
H	9.1395564	7.6213641	-1.1535088
C	5.6759203	4.3002669	7.9567142
H	4.4383910	7.5676301	3.3160301
P	10.2041255	5.9541732	0.0886463
H	3.1129893	6.5602299	7.2929406
H	6.6151538	4.5753224	6.0335977
P	10.8307500	4.0640838	2.7887821
H	11.5201590	6.5812288	-1.7796924
H	8.7905305	4.1328179	4.9518230
C	12.9752028	2.6172051	3.9659138
H	10.2398226	3.3375734	5.5809553
H	14.6356564	1.6611763	4.9718071
C	4.2623769	4.7289204	7.5549394
C	8.8508091	6.5647533	-1.0060785
H	3.1570629	7.9738563	1.2046691
C	9.3397099	3.1747929	4.9708584
H	2.1230334	8.1913730	2.6195716
H	7.5172468	7.0002977	0.6586787
H	6.7231796	8.3259835	-1.3005097
H	12.2373960	3.7126559	0.8715665
H	5.7812490	3.2077033	7.9038138
H	13.2586799	2.2069286	2.9826361
H	8.1123212	7.6174597	-3.4801854
H	9.7828738	5.8928659	-2.8726698
H	3.5209843	4.2629914	8.2171137
C	11.1854144	3.4759972	1.0694539
C	7.4721372	6.5426346	-0.3414476
H	12.2317076	1.9328676	4.3968220
H	8.1849680	2.3820569	6.6248341
C	9.7192026	2.7963552	3.5307670
C	8.7974726	5.8849059	-2.3853460
H	4.0444018	4.3664982	6.5360128
C	10.2829933	4.1102208	-0.0119545
C	6.4441855	7.2612103	-1.2190432
C	8.4642023	2.0867701	5.6042639
C	7.7642416	6.5915425	-3.2761434
H	7.9131785	3.4895458	2.5762826

H	10.6293339	3.8119970	-1.0111273
H	6.5520005	2.6864245	4.7874458
H	10.3132512	1.8668824	3.5549470
C	8.4695713	2.5454694	2.6761355
H	5.4561234	7.2254017	-0.7405011
H	11.0932605	2.3814298	1.0388092
C	6.3820583	6.6357261	-2.6160060
H	7.1501080	5.5002042	-0.2017312
H	9.2482626	3.7511718	0.0867015
C	7.2150837	1.8057239	4.7645977
H	9.0584510	1.1641310	5.7008339
H	8.5082621	4.8295599	-2.2563795
H	7.7090851	6.0820145	-4.2475192
H	5.6762757	7.1888774	-3.2494697
H	8.7512431	2.2295598	1.6617322
C	7.5721885	1.4747530	3.3120783
H	6.6393573	0.9815073	5.2060863
H	5.9863249	5.6117629	-2.5248587
H	6.6604340	1.3547447	2.7110657
H	8.0980473	0.5072810	3.2778261
F	11.2356352	7.4193067	2.8648808

SCF energy GEOOPT = -7650.249603044 H
 ZPE = 3853. kJ/mol
 FREEH energy = 4051.07 kJ/mol
 FREEH entropy = 1.66502 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	12.02	0.02844	YES	YES
	8	a	19.62	0.05988	YES	YES
	9	a	24.17	0.07743	YES	YES
	10	a	25.20	0.07423	YES	YES
	11	a	27.90	0.12297	YES	YES
	12	a	28.91	0.51728	YES	YES
	13	a	33.79	0.36760	YES	YES
	14	a	35.76	0.15572	YES	YES
	15	a	39.73	0.17464	YES	YES
	16	a	43.49	0.35141	YES	YES
	17	a	45.55	0.05829	YES	YES
	18	a	46.38	0.07758	YES	YES
	19	a	48.15	0.00820	YES	YES
	20	a	49.98	0.28106	YES	YES
	21	a	53.62	0.27630	YES	YES
	22	a	55.56	0.28718	YES	YES
	23	a	59.29	0.12628	YES	YES
	24	a	63.47	0.47769	YES	YES
	25	a	64.08	0.44776	YES	YES
	26	a	67.36	0.22219	YES	YES
	27	a	68.57	0.20645	YES	YES
	28	a	69.86	0.31632	YES	YES
	29	a	73.74	0.26816	YES	YES
	30	a	77.88	0.02525	YES	YES
	31	a	78.63	0.10270	YES	YES
	32	a	81.76	0.34186	YES	YES

33	a	82.40	0.25033	YES	YES
34	a	89.51	0.17921	YES	YES
35	a	90.11	0.43953	YES	YES
36	a	91.56	0.01467	YES	YES
37	a	93.85	0.46626	YES	YES
38	a	97.33	0.38513	YES	YES
39	a	111.79	0.37989	YES	YES
40	a	122.89	0.89179	YES	YES
41	a	130.67	0.18615	YES	YES
42	a	134.84	0.14664	YES	YES
43	a	137.65	0.34757	YES	YES
44	a	140.12	7.14779	YES	YES
45	a	143.27	6.85818	YES	YES
46	a	144.93	7.66518	YES	YES
47	a	147.24	2.86560	YES	YES
48	a	150.25	3.50589	YES	YES
49	a	156.55	0.19789	YES	YES
50	a	159.03	1.68978	YES	YES
51	a	164.13	2.18239	YES	YES
52	a	166.42	12.28945	YES	YES
53	a	170.28	5.51077	YES	YES
54	a	180.36	2.38014	YES	YES
55	a	184.54	1.12332	YES	YES
56	a	188.32	4.24404	YES	YES
57	a	190.52	1.43057	YES	YES
58	a	193.84	3.06661	YES	YES
59	a	201.56	2.85233	YES	YES
60	a	202.68	1.31977	YES	YES
61	a	211.15	5.05122	YES	YES
62	a	212.99	0.75648	YES	YES
63	a	215.54	0.12793	YES	YES
64	a	216.53	1.07504	YES	YES
65	a	219.12	0.35281	YES	YES
66	a	227.96	1.49246	YES	YES
67	a	232.64	0.15231	YES	YES
68	a	234.33	1.04272	YES	YES
69	a	238.47	0.29042	YES	YES
70	a	240.29	1.24877	YES	YES
71	a	241.45	0.74015	YES	YES
72	a	244.30	0.09988	YES	YES
73	a	247.94	0.17804	YES	YES
74	a	253.32	0.53177	YES	YES
75	a	257.29	1.45338	YES	YES
76	a	265.39	12.29263	YES	YES
77	a	278.83	1.39344	YES	YES
78	a	279.30	0.36444	YES	YES
79	a	287.95	0.89642	YES	YES
80	a	291.78	1.43839	YES	YES
81	a	303.41	0.68434	YES	YES
82	a	304.24	0.73778	YES	YES
83	a	312.24	0.51046	YES	YES
84	a	314.79	0.16021	YES	YES
85	a	328.76	0.65496	YES	YES
86	a	330.31	1.36792	YES	YES
87	a	335.48	0.65370	YES	YES
88	a	336.20	0.00701	YES	YES
89	a	341.39	2.10462	YES	YES
90	a	343.85	0.06420	YES	YES
91	a	359.34	1.03740	YES	YES
92	a	374.57	1.86555	YES	YES
93	a	375.49	0.20783	YES	YES
94	a	380.82	0.63341	YES	YES

95	a	383.52	0.87641	YES	YES
96	a	395.10	0.31147	YES	YES
97	a	396.69	0.32679	YES	YES
98	a	410.86	1.28442	YES	YES
99	a	414.91	1.58545	YES	YES
100	a	421.96	2.20149	YES	YES
101	a	425.59	2.42926	YES	YES
102	a	426.88	0.85070	YES	YES
103	a	429.66	0.09425	YES	YES
104	a	430.41	0.27234	YES	YES
105	a	431.36	0.70643	YES	YES
106	a	431.76	0.08336	YES	YES
107	a	432.00	0.47612	YES	YES
108	a	432.61	0.09398	YES	YES
109	a	434.82	0.76240	YES	YES
110	a	435.42	0.74533	YES	YES
111	a	439.16	1.08415	YES	YES
112	a	448.36	1.39764	YES	YES
113	a	451.00	7.54860	YES	YES
114	a	452.17	1.08865	YES	YES
115	a	468.80	2.09679	YES	YES
116	a	470.99	3.21691	YES	YES
117	a	472.93	4.73280	YES	YES
118	a	490.80	2.79114	YES	YES
119	a	493.29	2.30362	YES	YES
120	a	495.57	1.09031	YES	YES
121	a	496.84	2.91457	YES	YES
122	a	506.11	0.68981	YES	YES
123	a	506.65	0.20996	YES	YES
124	a	518.79	14.10855	YES	YES
125	a	519.49	0.43671	YES	YES
126	a	545.95	49.67543	YES	YES
127	a	553.50	2.72576	YES	YES
128	a	599.72	9.89931	YES	YES
129	a	624.34	19.57719	YES	YES
130	a	625.98	14.12693	YES	YES
131	a	642.68	16.13822	YES	YES
132	a	643.22	1.15793	YES	YES
133	a	692.12	27.94458	YES	YES
134	a	696.53	9.03930	YES	YES
135	a	708.18	0.06592	YES	YES
136	a	714.62	0.48742	YES	YES
137	a	720.01	1.98125	YES	YES
138	a	721.85	2.19388	YES	YES
139	a	731.55	6.35416	YES	YES
140	a	732.94	4.97740	YES	YES
141	a	733.95	6.11371	YES	YES
142	a	738.02	5.82761	YES	YES
143	a	771.90	0.17735	YES	YES
144	a	773.01	0.46019	YES	YES
145	a	773.54	0.60354	YES	YES
146	a	774.61	1.02126	YES	YES
147	a	777.55	0.13948	YES	YES
148	a	779.16	0.16268	YES	YES
149	a	780.57	0.73233	YES	YES
150	a	781.84	0.16351	YES	YES
151	a	783.61	19.06807	YES	YES
152	a	785.44	5.49884	YES	YES
153	a	809.84	0.95886	YES	YES
154	a	810.06	2.00276	YES	YES
155	a	811.64	1.81578	YES	YES
156	a	812.30	1.68422	YES	YES

157	a	813.02	0.71868	YES	YES
158	a	813.49	0.31422	YES	YES
159	a	815.48	6.26166	YES	YES
160	a	816.80	8.12653	YES	YES
161	a	817.29	48.45005	YES	YES
162	a	830.83	10.60165	YES	YES
163	a	832.59	1.04987	YES	YES
164	a	833.25	1.55245	YES	YES
165	a	836.24	3.20087	YES	YES
166	a	836.64	4.06280	YES	YES
167	a	837.59	7.16825	YES	YES
168	a	837.91	0.60088	YES	YES
169	a	838.46	9.79789	YES	YES
170	a	838.89	8.71788	YES	YES
171	a	850.79	16.95102	YES	YES
172	a	852.68	4.59367	YES	YES
173	a	875.30	3.66622	YES	YES
174	a	875.82	4.14325	YES	YES
175	a	877.29	2.18540	YES	YES
176	a	877.89	1.11338	YES	YES
177	a	878.12	4.83708	YES	YES
178	a	878.48	10.00352	YES	YES
179	a	878.78	2.04331	YES	YES
180	a	879.57	4.20074	YES	YES
181	a	880.42	0.69554	YES	YES
182	a	880.95	1.36778	YES	YES
183	a	882.52	3.70347	YES	YES
184	a	884.06	2.21653	YES	YES
185	a	885.01	2.05185	YES	YES
186	a	885.86	3.88346	YES	YES
187	a	888.97	1.20165	YES	YES
188	a	890.28	3.08210	YES	YES
189	a	892.79	41.74373	YES	YES
190	a	903.36	1.83942	YES	YES
191	a	904.41	2.92604	YES	YES
192	a	905.62	1.37332	YES	YES
193	a	906.93	3.45398	YES	YES
194	a	908.54	2.79989	YES	YES
195	a	909.58	2.48188	YES	YES
196	a	911.20	0.52519	YES	YES
197	a	912.52	0.06997	YES	YES
198	a	942.63	1.64654	YES	YES
199	a	955.69	32.04286	YES	YES
200	a	970.99	0.09073	YES	YES
201	a	982.32	0.12866	YES	YES
202	a	987.92	2.60495	YES	YES
203	a	988.58	6.56471	YES	YES
204	a	989.00	11.89114	YES	YES
205	a	989.99	28.29702	YES	YES
206	a	990.66	11.72583	YES	YES
207	a	991.09	11.82776	YES	YES
208	a	992.67	6.79615	YES	YES
209	a	993.72	1.12508	YES	YES
210	a	1013.44	1.01085	YES	YES
211	a	1015.31	1.22856	YES	YES
212	a	1016.54	0.89648	YES	YES
213	a	1017.16	0.84454	YES	YES
214	a	1017.40	1.44272	YES	YES
215	a	1019.96	0.92548	YES	YES
216	a	1020.24	1.15754	YES	YES
217	a	1020.43	0.45271	YES	YES
218	a	1031.92	5.19693	YES	YES

219	a	1032.28	0.17996	YES	YES
220	a	1033.44	1.28044	YES	YES
221	a	1033.66	6.49774	YES	YES
222	a	1036.92	26.45030	YES	YES
223	a	1038.88	1.25835	YES	YES
224	a	1040.23	3.80247	YES	YES
225	a	1041.73	1.33397	YES	YES
226	a	1042.47	3.91554	YES	YES
227	a	1059.12	3.15856	YES	YES
228	a	1060.22	0.71720	YES	YES
229	a	1060.65	2.16950	YES	YES
230	a	1060.79	1.42351	YES	YES
231	a	1064.13	3.96972	YES	YES
232	a	1066.43	1.95896	YES	YES
233	a	1067.18	14.36446	YES	YES
234	a	1068.70	0.06746	YES	YES
235	a	1069.08	1.04981	YES	YES
236	a	1070.61	0.08651	YES	YES
237	a	1070.74	0.07434	YES	YES
238	a	1071.27	0.28905	YES	YES
239	a	1071.41	0.42835	YES	YES
240	a	1073.21	0.26887	YES	YES
241	a	1074.46	0.38335	YES	YES
242	a	1075.68	0.08850	YES	YES
243	a	1076.96	0.45900	YES	YES
244	a	1080.83	2.12153	YES	YES
245	a	1085.69	2.53577	YES	YES
246	a	1095.19	7.51068	YES	YES
247	a	1097.46	2.33434	YES	YES
248	a	1100.30	3.26508	YES	YES
249	a	1101.38	3.53240	YES	YES
250	a	1106.91	4.35333	YES	YES
251	a	1107.76	0.82775	YES	YES
252	a	1108.29	5.28698	YES	YES
253	a	1111.89	5.30189	YES	YES
254	a	1122.24	38.11547	YES	YES
255	a	1126.31	2.29612	YES	YES
256	a	1130.82	3.26073	YES	YES
257	a	1159.81	3.40712	YES	YES
258	a	1160.81	9.17624	YES	YES
259	a	1162.66	8.87383	YES	YES
260	a	1163.18	1.08610	YES	YES
261	a	1170.49	8.68719	YES	YES
262	a	1170.98	3.08931	YES	YES
263	a	1171.50	2.38977	YES	YES
264	a	1173.24	13.40238	YES	YES
265	a	1180.83	18.05658	YES	YES
266	a	1182.81	9.20185	YES	YES
267	a	1185.74	12.99800	YES	YES
268	a	1190.20	1.90109	YES	YES
269	a	1190.37	4.70803	YES	YES
270	a	1191.69	36.51603	YES	YES
271	a	1193.87	0.64794	YES	YES
272	a	1197.79	4.91029	YES	YES
273	a	1200.25	3.57572	YES	YES
274	a	1242.19	0.17324	YES	YES
275	a	1242.69	0.12905	YES	YES
276	a	1242.97	0.35847	YES	YES
277	a	1244.23	0.42950	YES	YES
278	a	1244.89	1.06985	YES	YES
279	a	1245.94	0.50427	YES	YES
280	a	1246.83	0.89970	YES	YES

281	a	1247.59	0.59607	YES	YES
282	a	1248.10	0.23120	YES	YES
283	a	1250.39	3.55819	YES	YES
284	a	1251.92	1.00380	YES	YES
285	a	1254.46	3.05115	YES	YES
286	a	1255.80	2.67534	YES	YES
287	a	1256.35	6.25736	YES	YES
288	a	1257.16	6.64035	YES	YES
289	a	1258.18	4.73826	YES	YES
290	a	1258.42	4.01383	YES	YES
291	a	1258.52	7.57073	YES	YES
292	a	1258.80	1.42402	YES	YES
293	a	1259.80	0.80169	YES	YES
294	a	1260.56	1.83034	YES	YES
295	a	1261.82	0.14899	YES	YES
296	a	1262.47	4.58994	YES	YES
297	a	1263.02	0.93905	YES	YES
298	a	1264.52	2.75045	YES	YES
299	a	1269.00	4.02208	YES	YES
300	a	1269.13	0.07456	YES	YES
301	a	1269.97	1.77400	YES	YES
302	a	1279.11	1.70540	YES	YES
303	a	1282.96	0.93498	YES	YES
304	a	1284.11	1.71257	YES	YES
305	a	1286.28	3.44643	YES	YES
306	a	1288.19	2.36423	YES	YES
307	a	1289.76	2.33921	YES	YES
308	a	1291.83	3.84717	YES	YES
309	a	1292.68	5.86955	YES	YES
310	a	1297.04	0.62383	YES	YES
311	a	1306.31	2.24996	YES	YES
312	a	1307.30	0.25357	YES	YES
313	a	1307.54	1.68378	YES	YES
314	a	1309.41	2.78053	YES	YES
315	a	1311.83	12.74760	YES	YES
316	a	1313.35	11.93775	YES	YES
317	a	1314.33	3.75744	YES	YES
318	a	1315.78	10.91006	YES	YES
319	a	1316.53	0.59541	YES	YES
320	a	1319.37	1.36248	YES	YES
321	a	1320.49	0.37532	YES	YES
322	a	1321.40	2.80855	YES	YES
323	a	1322.58	1.08688	YES	YES
324	a	1322.95	2.74687	YES	YES
325	a	1323.45	0.17500	YES	YES
326	a	1324.00	0.38006	YES	YES
327	a	1324.23	2.08893	YES	YES
328	a	1324.53	0.69971	YES	YES
329	a	1325.48	0.38943	YES	YES
330	a	1326.35	1.91842	YES	YES
331	a	1326.73	0.85604	YES	YES
332	a	1326.82	4.67625	YES	YES
333	a	1327.75	1.50871	YES	YES
334	a	1328.45	1.73304	YES	YES
335	a	1333.38	2.22885	YES	YES
336	a	1335.78	0.09623	YES	YES
337	a	1336.40	0.50452	YES	YES
338	a	1337.40	0.22585	YES	YES
339	a	1338.74	0.81551	YES	YES
340	a	1338.87	0.06380	YES	YES
341	a	1339.51	0.39798	YES	YES
342	a	1339.95	0.58863	YES	YES

343	a	1340.93	1.03203	YES	YES
344	a	1343.13	0.07007	YES	YES
345	a	1346.85	3.25532	YES	YES
346	a	1347.93	4.02812	YES	YES
347	a	1348.71	0.59361	YES	YES
348	a	1348.80	1.31478	YES	YES
349	a	1349.21	0.80625	YES	YES
350	a	1350.49	0.03795	YES	YES
351	a	1351.69	0.54408	YES	YES
352	a	1369.83	3.75693	YES	YES
353	a	1396.73	6.57649	YES	YES
354	a	1400.27	7.47413	YES	YES
355	a	1401.06	7.90017	YES	YES
356	a	1404.41	8.61236	YES	YES
357	a	1405.09	7.74705	YES	YES
358	a	1420.38	4.56207	YES	YES
359	a	1427.77	1.46984	YES	YES
360	a	1429.86	2.84527	YES	YES
361	a	1430.68	2.42949	YES	YES
362	a	1431.37	7.59001	YES	YES
363	a	1434.74	1.34814	YES	YES
364	a	1434.99	5.01307	YES	YES
365	a	1436.07	1.68892	YES	YES
366	a	1436.78	1.50782	YES	YES
367	a	1437.10	0.72180	YES	YES
368	a	1437.45	4.12620	YES	YES
369	a	1437.79	7.73437	YES	YES
370	a	1437.94	4.57422	YES	YES
371	a	1438.04	1.66312	YES	YES
372	a	1438.50	3.28289	YES	YES
373	a	1438.80	6.17878	YES	YES
374	a	1438.89	3.01629	YES	YES
375	a	1439.40	4.91811	YES	YES
376	a	1440.39	0.55421	YES	YES
377	a	1440.85	8.07722	YES	YES
378	a	1441.11	3.36986	YES	YES
379	a	1441.45	6.02004	YES	YES
380	a	1442.00	10.63582	YES	YES
381	a	1442.96	25.03742	YES	YES
382	a	1443.42	16.46464	YES	YES
383	a	1444.04	3.49105	YES	YES
384	a	1445.31	16.12042	YES	YES
385	a	1445.86	21.25124	YES	YES
386	a	1446.19	17.40735	YES	YES
387	a	1447.01	26.58493	YES	YES
388	a	1447.17	6.33259	YES	YES
389	a	1447.47	7.09445	YES	YES
390	a	1453.11	0.29011	YES	YES
391	a	1453.32	2.65548	YES	YES
392	a	1454.46	1.21989	YES	YES
393	a	1456.56	0.77821	YES	YES
394	a	1456.97	3.15046	YES	YES
395	a	1458.40	1.22528	YES	YES
396	a	1459.50	2.91119	YES	YES
397	a	1462.23	7.37402	YES	YES
398	a	1637.42	72.65404	YES	YES
399	a	1649.78	33.76049	YES	YES
400	a	2922.54	4.13181	YES	YES
401	a	2926.44	16.53061	YES	YES
402	a	2926.76	6.25940	YES	YES
403	a	2927.46	2.63631	YES	YES
404	a	2928.06	1.74709	YES	YES

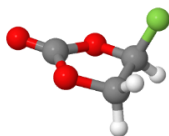
405	a	2929.72	7.35077	YES	YES
406	a	2931.02	24.75051	YES	YES
407	a	2933.44	2.89606	YES	YES
408	a	2935.80	16.23027	YES	YES
409	a	2941.34	19.95874	YES	YES
410	a	2941.73	4.55101	YES	YES
411	a	2942.14	9.20750	YES	YES
412	a	2942.49	4.12740	YES	YES
413	a	2943.88	8.51816	YES	YES
414	a	2945.55	8.26399	YES	YES
415	a	2946.43	7.92611	YES	YES
416	a	2946.88	14.02275	YES	YES
417	a	2947.32	10.10665	YES	YES
418	a	2947.71	3.47569	YES	YES
419	a	2948.85	27.08007	YES	YES
420	a	2950.83	8.70520	YES	YES
421	a	2951.98	13.86471	YES	YES
422	a	2952.81	15.45741	YES	YES
423	a	2953.79	9.89498	YES	YES
424	a	2954.42	7.75598	YES	YES
425	a	2955.06	25.35318	YES	YES
426	a	2955.52	4.36649	YES	YES
427	a	2956.10	1.50322	YES	YES
428	a	2956.30	12.29188	YES	YES
429	a	2957.13	14.25851	YES	YES
430	a	2957.15	7.85164	YES	YES
431	a	2958.14	9.38444	YES	YES
432	a	2959.11	7.00886	YES	YES
433	a	2960.21	8.01920	YES	YES
434	a	2960.67	34.43881	YES	YES
435	a	2961.15	21.26149	YES	YES
436	a	2961.45	67.23545	YES	YES
437	a	2962.49	37.75386	YES	YES
438	a	2964.29	42.62618	YES	YES
439	a	2964.63	6.32462	YES	YES
440	a	2965.06	4.76746	YES	YES
441	a	2965.80	54.48352	YES	YES
442	a	2966.11	14.64602	YES	YES
443	a	2966.61	21.49687	YES	YES
444	a	2968.27	27.27178	YES	YES
445	a	2969.57	10.98726	YES	YES
446	a	2971.98	19.77763	YES	YES
447	a	2977.26	4.23381	YES	YES
448	a	2979.08	3.01680	YES	YES
449	a	2979.92	2.72338	YES	YES
450	a	2986.32	4.22744	YES	YES
451	a	2990.71	3.95553	YES	YES
452	a	2991.33	5.29617	YES	YES
453	a	2995.82	21.04796	YES	YES
454	a	2996.82	24.72266	YES	YES
455	a	2999.85	26.11970	YES	YES
456	a	3000.46	36.07859	YES	YES
457	a	3003.85	19.98177	YES	YES
458	a	3003.86	24.19053	YES	YES
459	a	3008.25	24.65930	YES	YES
460	a	3008.40	18.77258	YES	YES
461	a	3008.53	21.92365	YES	YES
462	a	3010.10	20.25917	YES	YES
463	a	3010.41	8.73021	YES	YES
464	a	3011.37	11.44996	YES	YES
465	a	3011.59	11.07319	YES	YES
466	a	3011.99	5.13840	YES	YES

467	a	3012.05	30.89320	YES	YES
468	a	3012.09	28.08250	YES	YES
469	a	3013.02	20.30990	YES	YES
470	a	3013.12	8.99018	YES	YES
471	a	3013.34	31.98237	YES	YES
472	a	3014.50	26.55582	YES	YES
473	a	3014.73	32.34274	YES	YES
474	a	3014.92	17.87148	YES	YES
475	a	3015.80	26.54429	YES	YES
476	a	3015.88	13.29563	YES	YES
477	a	3016.15	17.58725	YES	YES
478	a	3016.30	38.47670	YES	YES
479	a	3016.47	14.94836	YES	YES
480	a	3016.68	15.17172	YES	YES
481	a	3017.35	13.62849	YES	YES
482	a	3017.90	25.76995	YES	YES
483	a	3017.97	21.40578	YES	YES
484	a	3018.35	14.40793	YES	YES
485	a	3019.39	45.15321	YES	YES
486	a	3019.54	26.04398	YES	YES
487	a	3020.48	30.67400	YES	YES
488	a	3020.80	22.25748	YES	YES
489	a	3021.57	3.28102	YES	YES
490	a	3021.93	19.09253	YES	YES
491	a	3022.22	8.28591	YES	YES
492	a	3024.87	29.37357	YES	YES
493	a	3026.44	0.63393	YES	YES
494	a	3038.66	0.03147	YES	YES
495	a	3047.17	1.54317	YES	YES
496	a	3050.29	0.42850	YES	YES
497	a	3052.96	0.05031	YES	YES
498	a	3064.45	14.33180	YES	YES
499	a	3096.93	5.44369	YES	YES
500	a	3108.50	4.68921	YES	YES
501	a	3202.45	0.68883	YES	YES

\$end

Double hybrid single point energy = -7642.543931570848 H
 COSMO energy + OC correction = -7650.4002375445 H (in oDFB)

6.2.52 FEC



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

O	0.5817457	0.5302533	1.0706794
C	-0.5636870	-0.1845406	1.4087580
O	-0.9499657	-0.3483472	2.5247825
O	-1.1720424	-0.6409267	0.2765452
C	-0.4653763	-0.1532809	-0.8769602
C	0.8490530	0.3745658	-0.2995605
H	-1.0560358	0.6403365	-1.3542362
H	-0.2986483	-0.9799518	-1.5752858

H 1.2117472 1.3240592 -0.7097489
F 1.8632095 -0.5621677 -0.4649736

SCF energy GEOOPT = -441.8789275718 H
ZPE = 169.8 kJ/mol
FREEH energy = 184.48 kJ/mol
FREEH entropy = 0.32062 kJ/mol/K

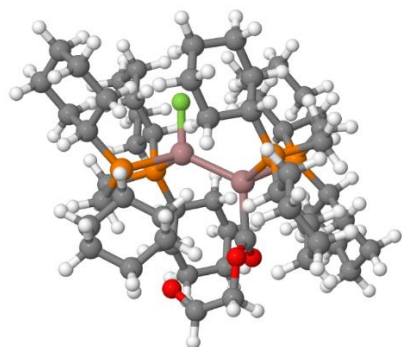
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		112.85	2.37579	YES	YES
8	a		171.86	1.33920	YES	YES
9	a		378.25	4.61397	YES	YES
10	a		459.98	3.22752	YES	YES
11	a		528.56	2.92681	YES	YES
12	a		709.94	8.10293	YES	YES
13	a		726.59	9.28333	YES	YES
14	a		792.52	17.06851	YES	YES
15	a		835.97	34.11829	YES	YES
16	a		860.23	11.45584	YES	YES
17	a		968.09	196.48061	YES	YES
18	a		1025.52	168.71195	YES	YES
19	a		1035.18	26.82360	YES	YES
20	a		1077.86	48.93653	YES	YES
21	a		1102.45	225.12134	YES	YES
22	a		1195.56	21.96222	YES	YES
23	a		1311.51	21.29545	YES	YES
24	a		1325.85	24.46421	YES	YES
25	a		1351.85	12.81199	YES	YES
26	a		1453.37	8.56791	YES	YES
27	a		1863.71	552.09850	YES	YES
28	a		2996.20	17.30453	YES	YES
29	a		3042.79	22.38991	YES	YES
30	a		3068.89	4.87759	YES	YES

\$end

Double hybrid single point energy = -441.230407350209 H
COSMO energy + OC correction = -441.8917367036 H (in oDFB)

6.2.53 [F{Ga(dcpe)}₂(COOCH₂CHO)]²⁺



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

C	4.4376790	5.0496805	1.5649686
C	5.0301972	3.8462729	0.8635642
O	6.2127898	3.6928459	0.6391868
H	4.2734928	3.0907378	0.5465040
H	3.7704771	5.5780066	0.8683094
O	5.4330760	6.0002101	1.9791975
C	6.1619057	5.6384268	3.0878099
H	10.1451690	12.4437708	3.0515063
H	11.4946710	11.4666657	3.6319481
C	10.6002540	11.4414977	2.9948536
H	11.9619543	8.1869780	8.3126718
H	11.6560047	11.9110195	1.1583895
H	9.3219867	10.6997923	4.5691852
C	10.9855995	11.1324052	1.5461042
C	11.9336662	7.0979253	8.1443204
H	12.8540375	6.6918037	8.5849870
C	9.6093900	10.4085220	3.5496940
H	10.7164601	6.7505914	9.9145659
H	9.3029659	8.0906581	8.3809804
H	9.2363322	11.9848095	0.5904809
H	8.6646692	9.4144979	6.0260379
H	10.5635497	8.4297895	6.1058729
H	6.8516254	10.7948057	5.0988039
H	12.7547953	7.2851607	6.1321939
C	10.7067472	6.5059204	8.8439870
H	7.8754699	11.3106923	2.6419928
H	11.5464371	10.1858044	1.5236463
C	9.7468696	11.0100723	0.6535899
H	7.2666658	9.2324397	7.0877518
C	11.8967410	6.8226281	6.6387043
C	7.6429792	9.0185200	6.0777497
C	9.3959339	7.0045539	8.2182332
C	8.3686936	10.3227254	2.6453702
H	10.0970590	9.4219926	3.6019565
C	10.5963281	7.3327661	6.0078420
C	6.7474609	9.7026522	5.0302136
H	14.4265628	8.2849117	0.1512185
H	10.0331288	10.7470874	-0.3741713
H	6.1628012	11.2747838	1.3080531
H	15.0097345	8.6242583	-1.4794491
C	8.7642997	9.9685862	1.2032399

H	8.5420393	6.5301605	8.7202175
H	10.7383577	5.4058207	8.7744238
C	9.3789361	6.7117835	6.7073630
H	5.1239099	11.5103808	2.7199704
C	14.1894599	8.1578046	-0.9180743
H	12.9131943	9.9209083	-0.9462775
H	5.6940264	9.4682039	5.2229073
H	11.9761915	5.7350656	6.4665196
H	10.5912751	7.1232278	4.9299353
C	5.2921346	10.8688183	1.8396133
H	15.4172097	5.8244491	3.5748386
P	7.0846334	9.1742348	3.2922394
H	14.4001181	5.5716079	4.9936877
P	7.7949286	7.1846179	5.8881508
C	12.8649238	8.8600710	-1.2288319
H	3.8707501	11.9555865	0.6193826
H	7.8777723	9.8960982	0.5562565
C	14.6796162	5.1414618	4.0180137
H	9.2456901	8.9758147	1.2050245
H	6.5488030	6.8670782	7.8914137
H	11.8382879	8.2957937	0.5964167
C	4.0634666	10.9164119	0.9180904
H	15.0469342	6.1578244	-0.9870776
H	12.9968740	6.0832883	2.9971494
H	9.4268398	5.6191576	6.5622348
C	5.5450429	9.4231675	2.2986749
C	14.1073521	6.6645312	-1.2466693
H	4.9170971	7.9258888	6.3950640
C	6.4321869	6.4375362	6.8809032
C	11.7013108	8.1910334	-0.4905252
H	16.1513040	3.8056189	4.8957564
H	13.1286296	6.0313828	0.5750395
C	13.4352882	5.0840102	3.1227529
H	12.6767036	8.8318424	-2.3144341
C	15.2851110	3.7503037	4.2229756
H	4.2959162	10.3625961	-0.0068252
Ga	9.8733374	6.3417637	2.4139046
C	5.0450263	6.8352321	6.3467025
Ga	7.7346484	6.8706723	3.4879764
C	12.9447054	5.9858663	-0.5086431
H	5.7199051	8.7964407	1.4067426
H	2.5143737	10.9393048	2.4283870
H	10.7567990	8.6927867	-0.7453425
H	4.0844725	9.4886030	3.9001308
C	2.8223864	10.3085258	1.5786135
H	13.9711546	6.5332506	-2.3324619
H	3.9307542	6.5369174	8.1776461
H	13.7389877	4.7253368	2.1260055
C	4.3077873	8.8624966	3.0218668
H	7.5775560	4.6686592	7.4249205
H	15.6631520	3.3716366	3.2589027
H	12.0909369	4.5026917	4.6934897
C	6.6121226	4.9118245	6.9591908
C	11.6188459	6.6904971	-0.8196528
H	13.9524990	3.0877724	5.7947578
C	3.9278835	6.1509057	7.1453478
C	12.3967636	4.1114633	3.7065945
C	14.2472106	2.7721837	4.7800796

H	5.5254098	4.5707005	8.8023602
H	4.9640140	6.5424603	5.2896862
H	1.9811599	10.3074813	0.8727236
H	12.8965078	4.9263122	-0.7973116
C	3.0960618	8.8879585	2.0831308
H	9.0578150	7.5503013	-1.3644775
C	5.4734021	4.2548381	7.7476175
H	4.4942215	7.8446085	3.3863183
P	10.1343377	5.9840011	0.0237595
H	2.9548400	6.4228261	6.7133556
H	6.6252473	4.5059228	5.9375610
P	10.8188889	4.1282834	2.7492811
H	11.3997352	6.5662283	-1.8961690
H	8.7278859	4.1762554	4.9070367
C	12.9910712	2.7054461	3.8984123
H	10.2338200	3.4904653	5.5471093
H	14.6756987	1.7656244	4.8786802
C	4.1071407	4.6306125	7.1685784
C	8.7300095	6.5489292	-1.0337822
H	3.2930638	8.2214333	1.2264741
C	9.3398646	3.2588642	4.9489297
H	2.2154613	8.4863263	2.6030905
H	7.6073559	7.3633316	0.6309311
H	6.5516668	8.2848655	-1.4056194
H	12.1954287	3.7795850	0.8073040
H	5.6112424	3.1647564	7.7399141
H	13.2540327	2.2841277	2.9140908
H	7.6983319	7.2315663	-3.5398965
H	9.4453506	5.5911576	-2.8656160
H	3.3042334	4.1641995	7.7546071
C	11.1510385	3.5324576	1.0306335
C	7.4361546	6.6998749	-0.2301828
H	12.2592717	2.0247724	4.3538334
H	8.2500270	2.4308149	6.6291658
C	9.7234786	2.8658848	3.5149991
C	8.5175878	5.6721624	-2.2806186
H	4.0251238	4.2352670	6.1429716
C	10.2112989	4.1399639	-0.0318589
C	6.3056158	7.2530739	-1.1016089
C	8.5360424	2.1328720	5.6109211
C	7.3909466	6.2474413	-3.1501993
H	7.8605590	3.4670569	2.5804696
H	10.5197642	3.8160673	-1.0352662
H	6.5925353	2.6152973	4.7991054
H	10.3426198	1.9525501	3.5543675
C	8.4757810	2.5610697	2.6757419
H	5.3821517	7.3139048	-0.5069631
H	11.0691829	2.4368011	1.0153476
C	6.0910295	6.3942224	-2.3524101
H	7.1451136	5.7230067	0.1785635
H	9.1794042	3.7886153	0.1171644
C	7.2953974	1.7706952	4.7886000
H	9.1866759	1.2497314	5.7175527
H	8.2412010	4.6540086	-1.9654226
H	7.2356780	5.5996824	-4.0233668
H	5.3052801	6.8291721	-2.9845865
H	8.7533279	2.2532989	1.6583597
C	7.6550235	1.4438626	3.3352130

H	6.7782626	0.9171356	5.2473884
H	5.7384222	5.3939706	-2.0515052
H	6.7450027	1.2689371	2.7457892
H	8.2363216	0.5078821	3.2991739
F	11.2426303	7.5012351	2.7888297
O	5.8992199	4.6265959	3.7112602
H	3.8365975	4.6981264	2.4177939

SCF energy GEOOPT = -7698.133629778 H

ZPE = 3764. kJ/mol

FREEH energy = 3961.56 kJ/mol

FREEH entropy = 1.67005 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		-0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	8.00	0.11045	YES	YES
	8	a	12.13	0.09012	YES	YES
	9	a	19.37	0.17570	YES	YES
	10	a	25.75	0.02735	YES	YES
	11	a	28.88	0.03589	YES	YES
	12	a	32.56	0.32476	YES	YES
	13	a	34.66	0.23236	YES	YES
	14	a	35.64	0.12259	YES	YES
	15	a	39.86	0.23032	YES	YES
	16	a	41.54	0.14922	YES	YES
	17	a	45.13	0.15870	YES	YES
	18	a	48.77	0.06473	YES	YES
	19	a	50.06	0.44913	YES	YES
	20	a	51.45	0.14460	YES	YES
	21	a	54.86	0.03111	YES	YES
	22	a	56.62	0.23650	YES	YES
	23	a	58.85	0.60398	YES	YES
	24	a	62.25	0.04736	YES	YES
	25	a	65.16	0.82205	YES	YES
	26	a	67.53	0.10166	YES	YES
	27	a	68.95	0.07714	YES	YES
	28	a	71.64	0.05914	YES	YES
	29	a	72.02	0.64482	YES	YES
	30	a	75.32	0.19777	YES	YES
	31	a	76.93	0.03840	YES	YES
	32	a	78.12	0.72638	YES	YES
	33	a	83.13	0.60614	YES	YES
	34	a	87.33	0.72366	YES	YES
	35	a	90.97	0.13226	YES	YES
	36	a	91.77	0.74448	YES	YES
	37	a	92.66	0.15406	YES	YES
	38	a	100.82	0.54889	YES	YES
	39	a	106.70	2.13984	YES	YES
	40	a	113.57	6.01343	YES	YES
	41	a	128.82	3.20338	YES	YES
	42	a	131.64	0.50699	YES	YES

43	a	137.65	0.26122	YES	YES
44	a	140.38	3.93184	YES	YES
45	a	142.45	3.11413	YES	YES
46	a	145.61	13.21490	YES	YES
47	a	149.68	0.56410	YES	YES
48	a	152.47	5.49308	YES	YES
49	a	153.86	3.32520	YES	YES
50	a	157.99	10.07889	YES	YES
51	a	162.31	9.81272	YES	YES
52	a	163.95	17.30609	YES	YES
53	a	167.52	0.95503	YES	YES
54	a	174.45	0.47497	YES	YES
55	a	180.43	0.60235	YES	YES
56	a	183.48	2.79373	YES	YES
57	a	190.71	5.55201	YES	YES
58	a	191.19	4.07739	YES	YES
59	a	198.21	1.63327	YES	YES
60	a	205.91	1.72395	YES	YES
61	a	209.65	2.37929	YES	YES
62	a	212.97	1.44225	YES	YES
63	a	214.00	6.24860	YES	YES
64	a	216.38	0.80431	YES	YES
65	a	217.40	1.34977	YES	YES
66	a	227.37	1.52565	YES	YES
67	a	229.08	0.94382	YES	YES
68	a	235.70	0.79508	YES	YES
69	a	238.88	0.82062	YES	YES
70	a	240.81	0.88724	YES	YES
71	a	242.77	2.06036	YES	YES
72	a	245.30	0.02503	YES	YES
73	a	249.81	3.28730	YES	YES
74	a	253.63	0.24885	YES	YES
75	a	257.10	3.16416	YES	YES
76	a	277.31	1.97804	YES	YES
77	a	280.70	0.37492	YES	YES
78	a	283.03	3.11240	YES	YES
79	a	286.56	1.59121	YES	YES
80	a	292.43	0.27259	YES	YES
81	a	302.53	0.86192	YES	YES
82	a	305.20	2.29217	YES	YES
83	a	308.49	0.93467	YES	YES
84	a	312.01	0.37615	YES	YES
85	a	316.03	0.60023	YES	YES
86	a	330.40	0.47364	YES	YES
87	a	331.91	1.55936	YES	YES
88	a	335.88	0.94930	YES	YES
89	a	336.99	0.24263	YES	YES
90	a	337.86	14.69255	YES	YES
91	a	342.38	1.69712	YES	YES
92	a	345.18	0.10130	YES	YES
93	a	374.44	2.41774	YES	YES
94	a	377.05	0.85984	YES	YES
95	a	379.72	1.26025	YES	YES
96	a	381.80	0.92547	YES	YES
97	a	396.21	0.30052	YES	YES
98	a	397.07	0.82714	YES	YES
99	a	413.25	0.70721	YES	YES
100	a	414.84	1.07968	YES	YES

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102	a	423.68	6.62842	YES	YES
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104	a	429.40	0.09008	YES	YES
105	a	430.41	0.22052	YES	YES
106	a	430.79	0.09736	YES	YES
107	a	431.58	0.53792	YES	YES
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109	a	432.83	0.89341	YES	YES
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111	a	436.83	0.94995	YES	YES
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114	a	450.94	1.83292	YES	YES
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116	a	471.50	4.61495	YES	YES
117	a	492.05	4.80750	YES	YES
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121	a	506.42	0.39434	YES	YES
122	a	507.58	0.67944	YES	YES
123	a	518.65	7.93595	YES	YES
124	a	520.94	8.92977	YES	YES
125	a	542.40	16.10770	YES	YES
126	a	551.32	32.91799	YES	YES
127	a	625.37	17.88440	YES	YES
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129	a	643.31	10.58623	YES	YES
130	a	646.14	6.42869	YES	YES
131	a	647.74	3.66353	YES	YES
132	a	710.84	0.01655	YES	YES
133	a	717.39	0.45833	YES	YES
134	a	721.72	1.99980	YES	YES
135	a	723.81	1.47759	YES	YES
136	a	732.53	17.52948	YES	YES
137	a	733.71	16.20925	YES	YES
138	a	734.50	5.23952	YES	YES
139	a	735.20	4.51084	YES	YES
140	a	740.07	7.84905	YES	YES
141	a	771.39	0.23883	YES	YES
142	a	771.97	0.24533	YES	YES
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161	a	833.84	0.51442	YES	YES
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173	a	876.98	1.67780	YES	YES
174	a	877.72	1.66340	YES	YES
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176	a	878.92	8.25192	YES	YES
177	a	879.50	2.26354	YES	YES
178	a	879.94	2.27381	YES	YES
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182	a	883.78	2.04792	YES	YES
183	a	884.13	2.92716	YES	YES
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186	a	889.06	2.02452	YES	YES
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190	a	907.79	2.40256	YES	YES
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225	a	1060.76	1.08327	YES	YES
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269	a	1244.11	0.28976	YES	YES
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368	a	1438.98	3.87316	YES	YES
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375	a	1442.57	36.05818	YES	YES
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382	a	1446.73	3.84609	YES	YES
383	a	1447.29	4.53143	YES	YES
384	a	1452.78	3.68581	YES	YES
385	a	1454.14	2.36117	YES	YES
386	a	1455.08	0.43992	YES	YES
387	a	1455.46	2.10367	YES	YES
388	a	1457.19	1.16338	YES	YES
389	a	1457.74	2.21520	YES	YES
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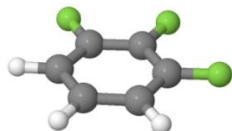
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410	a	2946.17	10.06175	YES	YES
411	a	2946.53	10.54129	YES	YES
412	a	2947.28	10.42229	YES	YES
413	a	2948.60	13.75533	YES	YES
414	a	2949.40	13.15102	YES	YES
415	a	2951.97	19.83320	YES	YES
416	a	2952.53	12.77274	YES	YES
417	a	2953.77	10.85592	YES	YES
418	a	2953.98	14.37309	YES	YES
419	a	2954.23	10.00204	YES	YES
420	a	2955.26	14.45047	YES	YES
421	a	2955.46	16.00935	YES	YES
422	a	2955.71	0.82908	YES	YES
423	a	2956.11	5.74783	YES	YES
424	a	2957.10	2.61219	YES	YES
425	a	2957.51	14.54261	YES	YES
426	a	2959.11	15.20298	YES	YES
427	a	2959.97	12.06408	YES	YES
428	a	2960.34	36.43101	YES	YES
429	a	2960.68	30.23658	YES	YES
430	a	2961.04	22.32403	YES	YES
431	a	2961.48	18.01780	YES	YES
432	a	2961.73	20.33328	YES	YES
433	a	2961.95	73.51704	YES	YES
434	a	2964.76	46.80189	YES	YES
435	a	2964.99	20.39142	YES	YES
436	a	2965.27	20.92681	YES	YES
437	a	2966.56	14.60931	YES	YES
438	a	2968.77	27.81104	YES	YES
439	a	2972.98	19.89147	YES	YES
440	a	2974.02	8.00472	YES	YES
441	a	2975.97	16.17209	YES	YES
442	a	2977.03	5.60000	YES	YES
443	a	2979.90	12.48551	YES	YES
444	a	2985.48	10.12404	YES	YES
445	a	2987.27	4.39903	YES	YES
446	a	2989.93	29.96213	YES	YES
447	a	2990.88	5.22581	YES	YES
448	a	2991.09	38.98294	YES	YES

449	a	2992.12	3.57581	YES	YES
450	a	2993.99	28.20045	YES	YES
451	a	3004.00	21.48782	YES	YES
452	a	3006.26	28.12389	YES	YES
453	a	3006.63	41.23760	YES	YES
454	a	3007.11	12.74200	YES	YES
455	a	3007.18	38.40905	YES	YES
456	a	3008.62	6.76709	YES	YES
457	a	3009.62	26.28832	YES	YES
458	a	3010.18	9.05561	YES	YES
459	a	3010.29	11.93389	YES	YES
460	a	3010.82	25.16326	YES	YES
461	a	3011.41	23.38174	YES	YES
462	a	3011.83	12.85598	YES	YES
463	a	3012.90	12.66963	YES	YES
464	a	3013.36	23.82913	YES	YES
465	a	3013.40	23.27549	YES	YES
466	a	3014.36	30.55119	YES	YES
467	a	3014.61	34.44640	YES	YES
468	a	3014.75	22.73835	YES	YES
469	a	3015.08	13.56894	YES	YES
470	a	3015.37	26.70463	YES	YES
471	a	3015.49	22.26594	YES	YES
472	a	3015.62	11.87713	YES	YES
473	a	3016.11	19.43399	YES	YES
474	a	3016.72	15.99665	YES	YES
475	a	3017.22	36.68421	YES	YES
476	a	3017.51	17.98108	YES	YES
477	a	3018.09	18.03530	YES	YES
478	a	3018.55	25.52106	YES	YES
479	a	3018.72	26.10117	YES	YES
480	a	3019.31	20.18773	YES	YES
481	a	3020.59	10.17101	YES	YES
482	a	3022.47	9.63627	YES	YES
483	a	3022.79	15.14078	YES	YES
484	a	3022.81	28.12927	YES	YES
485	a	3024.32	7.10647	YES	YES
486	a	3025.01	0.14704	YES	YES
487	a	3026.18	20.32989	YES	YES
488	a	3027.55	0.38371	YES	YES
489	a	3032.10	26.00099	YES	YES
490	a	3036.66	0.06324	YES	YES
491	a	3050.64	0.49840	YES	YES
492	a	3051.81	0.02822	YES	YES

\$end

Double hybrid single point energy = -7690.386609477206 H
 COSMO energy + OC correction = -7698.2834970422 H (in oDFB)

6.2.54 1,2,3-C₆F₃H₃ (3FB)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c2v

Cartesian coordinates in Ångström:

H	2.1711364	0.0000000	1.2689662
C	1.2148251	0.0000000	0.7497252
C	0.0000000	0.0000000	1.4385189
H	0.0000000	0.0000000	2.5269849
C	-1.2148251	0.0000000	0.7497252
H	-2.1711364	0.0000000	1.2689662
C	-1.2023417	0.0000000	-0.6408303
F	-2.3582127	0.0000000	-1.3361296
C	0.0000000	0.0000000	-1.3530881
F	0.0000000	0.0000000	-2.6958826
C	1.2023417	0.0000000	-0.6408303
F	2.3582127	0.0000000	-1.3361296

SCF energy GEOOPT = -530.2114836135 H

ZPE = 193.6 kJ/mol

FREEH energy = 212.08 kJ/mol

FREEH entropy = 0.34268 kJ/mol/K

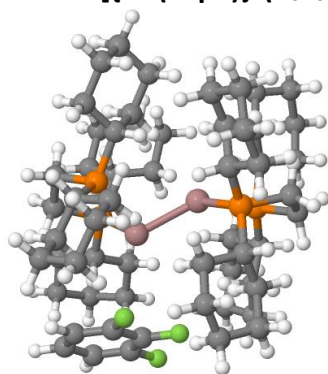
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b2	146.42	0.14589	YES	YES
8		a2	243.97	0.00000	NO	YES
9		b1	269.71	0.02798	YES	YES
10		b2	289.90	0.19644	YES	YES
11		a1	296.51	1.11042	YES	YES
12		a1	469.94	0.11890	YES	YES
13		b1	492.45	1.98853	YES	YES
14		b2	529.24	0.10970	YES	YES
15		a2	559.45	0.00000	NO	YES
16		b1	563.72	2.75268	YES	YES
17		b2	664.54	7.33420	YES	YES
18		a1	683.65	21.71400	YES	YES
19		b2	740.73	61.09867	YES	YES
20		a1	816.41	11.30959	YES	YES
21		a2	846.13	0.00000	NO	YES
22		b2	911.60	0.42367	YES	YES
23		b1	1005.56	136.78447	YES	YES
24		a1	1054.02	10.34000	YES	YES
25		b1	1144.05	2.07489	YES	YES
26		a1	1211.93	21.24624	YES	YES

27	b1	1230.29	42.40523	YES	YES
28	a1	1287.96	94.82304	YES	YES
29	b1	1341.64	0.45147	YES	YES
30	b1	1467.47	85.82427	YES	YES
31	a1	1497.54	196.98206	YES	YES
32	b1	1596.81	71.66679	YES	YES
33	a1	1601.97	0.09224	YES	YES
34	a1	3124.28	3.48167	YES	YES
35	b1	3138.97	1.04163	YES	YES
36	a1	3145.00	0.19411	YES	YES
§end					

Double hybrid single point energy = -529.424581590831 H
COSMO energy + OC correction = -530.2158225968 H (in 3FB)

6.2.55 $[\{\text{Ga}(\text{dcpe})\}_2(\text{C}_6\text{F}_3\text{H}_3)]^{2+}$ (Adduct)



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

```

Ga  -0.4899183    0.2404897   -1.0682031
Ga   0.6611474    0.0273380    1.0322014
P   -0.4561479    2.3605827   -2.2797401
P   -1.1857843    0.7751259    2.5041997
P   -0.1966905   -0.7552641   -3.2660672
P    0.2190203   -2.1124589    2.1465993
C   -4.2797998    3.5504808   -1.1073975
H   -4.0432956    3.7572072   -0.0496185
H   -5.2302440    2.9986579   -1.1147400
C    1.2542210   -1.8496668   -3.5634953
H    1.2631486   -2.0987482   -4.6385104
C    1.7611922   -3.1152978    2.3053011
H    2.5401539   -2.3371926    2.4074775
C   -2.9805598   -0.8732962   -3.2366454
H   -3.0423731   -0.0299111   -3.9435452
H   -2.8921830   -0.4373799   -2.2253840
C   -2.9232092    1.0245749    1.8867630
H   -2.8083056    1.7930551    1.1027675
C   -1.3147051   -0.4931296    3.8569916
H   -1.3720884    0.0192377    4.8269379
H   -2.2715733   -1.0138421    3.7203457
C   -3.0872037    5.6309585   -1.9134924
H   -3.1894205    6.5537695   -2.4999230

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H	-2.8028904	5.9382016	-0.8933873
C	-1.9625401	4.7685325	-2.5042168
H	-1.0152015	5.3244375	-2.4840612
H	-2.1842594	4.5499462	-3.5615113
C	-3.1682164	2.6815190	-1.7046787
H	-3.4511004	2.3927342	-2.7296707
H	-3.0541263	1.7442164	-1.1353179
C	3.7755603	-2.0251590	-3.3617540
H	3.8976587	-2.2838472	-4.4259169
H	4.6798828	-1.4778535	-3.0641977
C	-1.4376737	-4.4559655	2.4153983
H	-1.3653606	-4.3063074	3.5017823
H	-0.6326174	-5.1510091	2.1332094
C	-0.7023416	2.3613582	3.3098133
H	-1.4474910	2.5936330	4.0877604
C	1.3560385	3.9012391	-0.8270599
H	0.4966279	4.4718279	-0.4477073
H	1.4964665	3.0347525	-0.1579071
C	2.6145165	4.7777352	-0.7969611
H	2.4304377	5.6923214	-1.3838000
H	2.8054854	5.1020586	0.2354408
C	-3.4945861	-0.2370538	1.2261843
H	-2.8074700	-0.5890680	0.4404639
H	-3.5668665	-1.0418802	1.9766689
C	-4.4180420	4.8741222	-1.8667872
H	-4.7587324	4.6680141	-2.8947106
H	-5.1931962	5.4978838	-1.4021786
C	-3.8746417	1.5587527	2.9714161
H	-3.4878093	2.4909997	3.4042169
H	-3.9374792	0.8274627	3.7938831
C	-0.7050811	3.4687770	2.2423945
H	-1.7212633	3.6117972	1.8455166
H	-0.0740448	3.1363499	1.4005037
C	-1.8377352	-2.3735177	-4.9422700
H	-0.9582052	-3.0020840	-5.1412056
H	-1.8518750	-1.5898541	-5.7172555
C	3.5508419	3.4990940	-2.7665815
H	3.4159834	4.3400779	-3.4661828
H	4.4092043	2.9208116	-3.1350322
C	1.2007714	3.5477166	4.5043846
H	0.5578103	3.8839661	5.3337250
H	2.2050645	3.4078183	4.9285291
C	-5.8464369	0.5433752	1.7302964
H	-6.8328717	0.7563897	1.2968504
H	-6.0035193	-0.2378555	2.4923066
C	1.8454712	-4.0302493	3.5396812
H	1.7083691	-3.4470338	4.4605140
H	1.0396088	-4.7770193	3.5108804
C	3.6258264	-3.3027681	-2.5330314
H	4.4929258	-3.9592077	-2.6845688
H	3.6205740	-3.0360885	-1.4642046
C	-4.8940689	0.0134766	0.6544700
H	-4.8249716	0.7440993	-0.1676211
H	-5.2829067	-0.9161246	0.2149320
C	3.8301689	4.0375345	-1.3607041
H	4.0840975	3.1994176	-0.6951649
H	4.7031441	4.7034771	-1.3786279
C	1.2254186	4.6171410	3.4084860

H	1.5825905	5.5716428	3.8171219
H	1.9423177	4.3185163	2.6263658
C	-1.3719024	-3.3301680	0.1436167
H	-0.5585178	-3.9813313	-0.2089250
H	-1.2498142	-2.3599892	-0.3662198
C	0.6800563	2.2103363	3.9652266
H	1.3843615	1.8254811	3.2082434
H	0.6393440	1.4639142	4.7727476
C	-1.2537884	-3.1279179	1.6619256
H	-2.0839680	-2.4617782	1.9551883
C	-0.1619929	4.7944365	2.7864044
C	-2.9421893	-5.2755290	0.5443648
H	-3.9324102	-5.6888069	0.3101243
H	-2.2041715	-6.0189470	0.2007744
C	-2.7946141	-5.0795634	2.0565292
H	-2.9091284	-6.0378463	2.5809552
H	-3.6012198	-4.4232745	2.4237225
C	1.1032776	-3.1397560	-2.7388783
H	0.1984192	-3.6881298	-3.0350011
H	0.9737837	-2.8616247	-1.6792422
C	3.1990460	-4.7528560	3.5784207
H	3.9998242	-4.0092467	3.7214468
H	3.2323247	-5.4194996	4.4507657
C	-4.2568629	-1.7140971	-3.3452540
H	-5.1347566	-1.0837478	-3.1470560
H	-4.2401167	-2.4891490	-2.5618962
C	3.4544506	-5.5389528	2.2892666
H	2.7054645	-6.3431915	2.1991473
H	4.4348573	-6.0320891	2.3316541
C	2.0364838	-3.8837287	1.0013100
H	1.2299094	-4.6139179	0.8319573
H	2.0225007	-3.1884355	0.1479538
C	-5.2798042	1.7983551	2.3990252
H	-5.9460373	2.1420743	3.2017962
H	-5.2303363	2.6158644	1.6618543
C	-3.1220815	-3.2094246	-5.0463111
H	-3.1987607	-3.6417764	-6.0528345
H	-3.0543910	-4.0579662	-4.3455174
C	-2.7216670	-3.9609056	-0.2118094
H	-2.7797331	-4.1299025	-1.2975071
H	-3.5273561	-3.2503033	0.0391082
C	-4.3669557	-2.3765759	-4.7232242
H	-5.2657224	-3.0058520	-4.7687304
H	-4.4940495	-1.5970690	-5.4925208
C	2.3334324	-4.0435949	-2.8835822
H	2.2080594	-4.9300550	-2.2455395
H	2.3888486	-4.4129876	-3.9200915
C	3.3746746	-4.6279981	1.0609301
H	4.1952498	-3.8957212	1.0893061
H	3.5116710	-5.2096836	0.1387577
F	4.0830974	0.5995711	-0.4166631
C	1.0801577	3.3837731	-2.2469610
H	0.8702518	4.2408538	-2.9107980
C	2.2944383	2.6186759	-2.7956272
H	2.1061897	2.2821992	-3.8250108
H	2.4575696	1.7197548	-2.1800245
C	2.5552313	-1.1124878	-3.1979641
H	2.6774996	-0.2093121	-3.8115408

H	2.4897556	-0.7762772	-2.1485204
C	-0.1291276	0.6113994	-4.5117101
H	0.9376818	0.7746952	-4.7102931
H	-0.5788199	0.2697213	-5.4544522
C	-0.7937828	1.9215107	-4.0484370
H	-1.8853636	1.8449618	-4.1382519
H	-0.4788357	2.7537094	-4.6931598
C	-1.7376003	-1.7227369	-3.5556367
H	-1.6810700	-2.5215405	-2.7953682
C	-1.8369079	3.4485384	-1.7270134
H	-1.5698638	3.6810697	-0.6805574
C	-0.1561259	-1.5003327	3.8494580
H	-0.3729774	-2.3424628	4.5201944
H	0.7707051	-1.0297721	4.2095138
H	-0.8582387	5.1879595	3.5443572
H	-0.1309469	5.5381728	1.9771168
H	3.7637212	1.2939681	4.0433015
C	4.0679634	0.6272358	3.2393023
C	3.8797457	1.0240725	1.9203456
F	3.3282732	2.2254817	1.6373210
C	4.2750695	0.2103798	0.8569001
C	4.8941775	-1.0088998	1.1371663
F	5.2896555	-1.7743409	0.1009327
C	5.1044364	-1.4234885	2.4477425
H	5.6148862	-2.3668047	2.6295075
C	4.6814133	-0.6015565	3.4948969
H	4.8552134	-0.9115272	4.5235028

SCF energy GEOOPT = -7786.399948175 H

ZPE = 3792. kJ/mol

FREEH energy = 3992.89 kJ/mol

FREEH entropy = 1.71264 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	13.82	0.07364	YES	YES
	8	a	18.60	0.06536	YES	YES
	9	a	22.37	0.03251	YES	YES
	10	a	24.29	0.03738	YES	YES
	11	a	26.63	0.52926	YES	YES
	12	a	31.25	0.23155	YES	YES
	13	a	32.02	0.09428	YES	YES
	14	a	35.50	0.42678	YES	YES
	15	a	37.40	0.53564	YES	YES
	16	a	38.00	0.52064	YES	YES
	17	a	40.10	0.01692	YES	YES
	18	a	42.21	0.44892	YES	YES
	19	a	43.20	1.35327	YES	YES
	20	a	46.31	0.14886	YES	YES
	21	a	47.19	0.11618	YES	YES
	22	a	48.40	0.08747	YES	YES

23	a	49.82	0.65420	YES	YES
24	a	51.21	0.16145	YES	YES
25	a	54.04	0.66327	YES	YES
26	a	56.38	0.36059	YES	YES
27	a	59.18	0.14537	YES	YES
28	a	60.83	0.09323	YES	YES
29	a	63.74	0.01338	YES	YES
30	a	64.33	0.13724	YES	YES
31	a	66.67	0.16129	YES	YES
32	a	68.05	0.08057	YES	YES
33	a	69.14	0.08772	YES	YES
34	a	71.09	0.43829	YES	YES
35	a	71.86	0.24739	YES	YES
36	a	74.84	0.24549	YES	YES
37	a	77.01	0.23929	YES	YES
38	a	81.92	0.31438	YES	YES
39	a	84.58	0.67268	YES	YES
40	a	89.58	1.14860	YES	YES
41	a	97.47	0.43360	YES	YES
42	a	113.72	0.38896	YES	YES
43	a	119.48	0.27907	YES	YES
44	a	126.69	1.05442	YES	YES
45	a	133.20	0.16402	YES	YES
46	a	134.94	0.41049	YES	YES
47	a	139.23	0.75101	YES	YES
48	a	141.28	0.10522	YES	YES
49	a	145.09	1.48460	YES	YES
50	a	152.42	0.55273	YES	YES
51	a	157.97	1.33678	YES	YES
52	a	159.04	5.29189	YES	YES
53	a	168.37	0.08160	YES	YES
54	a	174.37	1.86575	YES	YES
55	a	182.04	1.00933	YES	YES
56	a	184.08	2.07451	YES	YES
57	a	191.13	0.61820	YES	YES
58	a	195.38	1.69012	YES	YES
59	a	212.69	0.40824	YES	YES
60	a	213.34	0.04128	YES	YES
61	a	215.62	0.46516	YES	YES
62	a	217.63	0.10892	YES	YES
63	a	220.83	0.43689	YES	YES
64	a	224.31	0.07694	YES	YES
65	a	226.95	0.13266	YES	YES
66	a	227.92	0.76298	YES	YES
67	a	231.25	0.11557	YES	YES
68	a	234.17	0.27411	YES	YES
69	a	241.10	0.18193	YES	YES
70	a	243.71	0.04500	YES	YES
71	a	245.61	0.51152	YES	YES
72	a	246.56	1.14314	YES	YES
73	a	251.22	0.15704	YES	YES
74	a	251.57	0.10723	YES	YES
75	a	271.23	0.82643	YES	YES
76	a	273.05	0.66746	YES	YES
77	a	278.97	0.26917	YES	YES
78	a	282.29	0.37343	YES	YES
79	a	290.38	6.84414	YES	YES
80	a	294.06	1.57701	YES	YES

81	a	296.90	0.65919	YES	YES
82	a	299.17	0.46582	YES	YES
83	a	301.19	0.09464	YES	YES
84	a	309.18	0.53520	YES	YES
85	a	312.65	0.75335	YES	YES
86	a	328.46	2.28795	YES	YES
87	a	328.87	0.11364	YES	YES
88	a	332.46	0.40608	YES	YES
89	a	333.11	0.26592	YES	YES
90	a	338.77	5.01345	YES	YES
91	a	339.91	0.21184	YES	YES
92	a	367.01	2.66491	YES	YES
93	a	373.10	6.70221	YES	YES
94	a	376.14	5.34559	YES	YES
95	a	376.89	0.41957	YES	YES
96	a	388.19	4.96552	YES	YES
97	a	394.90	0.06013	YES	YES
98	a	409.35	0.45299	YES	YES
99	a	412.81	1.12419	YES	YES
100	a	416.89	0.81242	YES	YES
101	a	422.16	4.56653	YES	YES
102	a	423.79	0.97311	YES	YES
103	a	429.06	0.41783	YES	YES
104	a	429.46	1.11052	YES	YES
105	a	430.69	0.38347	YES	YES
106	a	430.96	0.05545	YES	YES
107	a	431.53	0.23962	YES	YES
108	a	432.72	0.56550	YES	YES
109	a	433.08	0.48577	YES	YES
110	a	434.28	1.31251	YES	YES
111	a	437.66	0.35321	YES	YES
112	a	441.52	3.73634	YES	YES
113	a	454.69	5.05073	YES	YES
114	a	461.05	8.84081	YES	YES
115	a	467.22	3.68430	YES	YES
116	a	471.62	0.06916	YES	YES
117	a	492.33	0.27578	YES	YES
118	a	492.61	2.23009	YES	YES
119	a	492.88	5.91932	YES	YES
120	a	494.28	5.86912	YES	YES
121	a	495.43	4.59841	YES	YES
122	a	498.08	1.54977	YES	YES
123	a	502.94	0.66631	YES	YES
124	a	508.48	15.16806	YES	YES
125	a	513.41	10.55653	YES	YES
126	a	529.09	0.01138	YES	YES
127	a	553.46	0.33370	YES	YES
128	a	562.89	2.70682	YES	YES
129	a	624.84	23.07206	YES	YES
130	a	634.60	12.63261	YES	YES
131	a	639.91	11.89811	YES	YES
132	a	656.24	11.02699	YES	YES
133	a	683.38	21.42813	YES	YES
134	a	685.89	17.31273	YES	YES
135	a	695.97	4.47917	YES	YES
136	a	715.48	1.84625	YES	YES
137	a	720.26	4.74160	YES	YES
138	a	723.62	4.31126	YES	YES

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140	a	733.71	5.02470	YES	YES
141	a	735.44	0.67406	YES	YES
142	a	736.91	4.24518	YES	YES
143	a	759.07	71.75391	YES	YES
144	a	768.78	1.14913	YES	YES
145	a	769.99	1.25324	YES	YES
146	a	770.17	11.25731	YES	YES
147	a	771.58	3.52917	YES	YES
148	a	771.99	1.05462	YES	YES
149	a	773.65	2.86353	YES	YES
150	a	775.70	0.18018	YES	YES
151	a	776.93	16.63089	YES	YES
152	a	777.77	0.05285	YES	YES
153	a	779.28	0.29306	YES	YES
154	a	806.52	1.71134	YES	YES
155	a	807.68	2.27186	YES	YES
156	a	809.04	5.33120	YES	YES
157	a	810.30	6.96310	YES	YES
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160	a	814.17	2.57013	YES	YES
161	a	814.90	6.80555	YES	YES
162	a	815.96	6.27226	YES	YES
163	a	831.34	5.70750	YES	YES
164	a	831.64	6.34133	YES	YES
165	a	836.13	0.58933	YES	YES
166	a	837.35	1.16247	YES	YES
167	a	838.23	1.89685	YES	YES
168	a	838.47	5.11491	YES	YES
169	a	838.81	0.37479	YES	YES
170	a	839.89	6.75768	YES	YES
171	a	847.87	18.31447	YES	YES
172	a	853.07	8.26678	YES	YES
173	a	860.74	1.10345	YES	YES
174	a	871.65	1.65964	YES	YES
175	a	873.53	2.79199	YES	YES
176	a	875.31	0.08796	YES	YES
177	a	876.55	3.64685	YES	YES
178	a	876.91	5.89798	YES	YES
179	a	877.22	1.26033	YES	YES
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182	a	878.93	4.09007	YES	YES
183	a	879.64	6.42884	YES	YES
184	a	880.73	0.80055	YES	YES
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187	a	882.11	2.48159	YES	YES
188	a	884.65	6.74062	YES	YES
189	a	885.57	0.24492	YES	YES
190	a	902.39	0.67939	YES	YES
191	a	902.58	2.89883	YES	YES
192	a	903.87	0.83576	YES	YES
193	a	904.14	2.77345	YES	YES
194	a	906.56	4.00806	YES	YES
195	a	909.75	1.97914	YES	YES
196	a	909.96	1.17585	YES	YES

197	a	910.38	0.91093	YES	YES
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213	a	1016.65	0.63845	YES	YES
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230	a	1059.68	1.52838	YES	YES
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248	a	1095.52	8.61655	YES	YES
249	a	1100.64	2.31652	YES	YES
250	a	1102.09	3.70556	YES	YES
251	a	1109.08	12.27781	YES	YES
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253	a	1124.09	2.95119	YES	YES
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256	a	1158.08	7.59712	YES	YES
257	a	1158.68	1.61646	YES	YES
258	a	1160.50	6.12638	YES	YES
259	a	1165.25	10.81855	YES	YES
260	a	1166.64	7.02136	YES	YES
261	a	1167.37	6.51811	YES	YES
262	a	1168.87	17.85515	YES	YES
263	a	1170.12	3.60429	YES	YES
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266	a	1178.93	15.47291	YES	YES
267	a	1179.83	2.74198	YES	YES
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288	a	1255.61	2.48661	YES	YES
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293	a	1258.06	4.17809	YES	YES
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306	a	1284.63	34.38267	YES	YES
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313	a	1309.48	0.62993	YES	YES
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343	a	1342.78	0.28024	YES	YES
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346	a	1344.79	1.87666	YES	YES
347	a	1345.08	1.72385	YES	YES
348	a	1346.06	0.50204	YES	YES
349	a	1347.25	0.96089	YES	YES
350	a	1348.94	0.72199	YES	YES
351	a	1350.15	0.42149	YES	YES
352	a	1401.08	5.21632	YES	YES
353	a	1404.81	6.10689	YES	YES
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356	a	1419.64	3.18844	YES	YES
357	a	1425.26	5.76167	YES	YES
358	a	1427.67	3.37461	YES	YES
359	a	1429.26	4.40269	YES	YES
360	a	1430.13	2.25649	YES	YES
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368	a	1436.01	2.95877	YES	YES
369	a	1436.45	1.48500	YES	YES
370	a	1436.83	10.60773	YES	YES

371	a	1437.20	14.15485	YES	YES
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374	a	1439.06	3.37378	YES	YES
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376	a	1439.44	4.13037	YES	YES
377	a	1439.88	3.60098	YES	YES
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379	a	1441.45	10.67172	YES	YES
380	a	1442.26	11.53659	YES	YES
381	a	1442.45	0.97896	YES	YES
382	a	1443.25	5.79672	YES	YES
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384	a	1443.79	2.84544	YES	YES
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386	a	1444.72	6.86648	YES	YES
387	a	1445.26	6.99984	YES	YES
388	a	1452.20	4.08383	YES	YES
389	a	1452.83	5.36981	YES	YES
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393	a	1454.97	1.80201	YES	YES
394	a	1455.97	2.13369	YES	YES
395	a	1457.59	0.15540	YES	YES
396	a	1467.13	59.96759	YES	YES
397	a	1493.37	102.18542	YES	YES
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402	a	2925.69	25.81122	YES	YES
403	a	2926.94	15.57237	YES	YES
404	a	2930.58	8.02371	YES	YES
405	a	2932.25	5.27004	YES	YES
406	a	2932.31	9.45373	YES	YES
407	a	2935.65	24.40571	YES	YES
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411	a	2939.00	20.62902	YES	YES
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425	a	2951.83	3.23530	YES	YES
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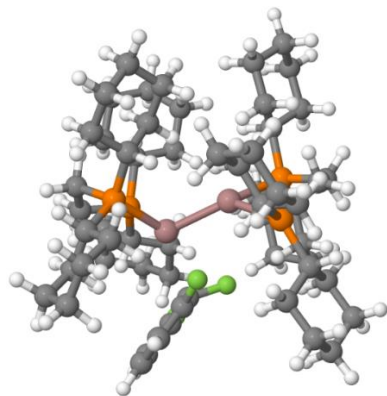
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441	a	2962.01	15.41602	YES	YES
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443	a	2965.37	21.98298	YES	YES
444	a	2967.90	32.77388	YES	YES
445	a	2973.24	43.22628	YES	YES
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447	a	2974.12	12.70932	YES	YES
448	a	2976.56	3.81890	YES	YES
449	a	2978.37	61.18297	YES	YES
450	a	2979.05	5.56606	YES	YES
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453	a	2986.01	19.99754	YES	YES
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461	a	3001.70	21.03987	YES	YES
462	a	3002.82	21.75911	YES	YES
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464	a	3004.58	16.12583	YES	YES
465	a	3004.86	23.99746	YES	YES
466	a	3005.25	31.08476	YES	YES
467	a	3005.68	9.44777	YES	YES
468	a	3006.12	28.80285	YES	YES
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480	a	3016.77	26.53832	YES	YES
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487	a	3019.08	14.37036	YES	YES
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489	a	3020.87	32.88084	YES	YES
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491	a	3025.91	7.61648	YES	YES
492	a	3026.04	29.09705	YES	YES
493	a	3028.97	0.33402	YES	YES
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495	a	3043.60	0.61988	YES	YES
496	a	3130.10	0.85223	YES	YES
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498	a	3148.05	0.97311	YES	YES

\$end

Double hybrid single point energy = -7778.505759193832 H
 COSMO energy + OC correction = -7786.5541536446 H (in 3FB)

6.2.56 $\{[\text{Ga}(\text{dcpe})]_2(\text{F}-\text{C}_6\text{F}_2\text{H}_3)\}^{2+}$ Transition State



Method: (RI-)BP86 (D3BJ) /def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-3.0405172	17.4565679	-2.9570182
Ga	-3.8177700	17.7773865	-0.6776452
P	-1.5441436	18.8702763	-4.2679258
P	-5.9314611	19.0492445	-0.6777892
P	-2.1491963	15.5999253	-4.2487806
P	-5.1899030	16.0192742	0.3275407
C	-4.7630186	21.3688178	-5.1991148
H	-4.7761844	21.9332783	-4.2513035
H	-5.8082175	21.1228818	-5.4362978
C	-1.1199006	14.2608409	-3.5050151
H	-0.8007016	13.6050699	-4.3332240
C	-4.2614913	15.0363071	1.5773264
H	-3.8762560	15.8337641	2.2411236
C	-4.4273451	15.8733957	-5.8325347
H	-3.8149996	16.2923304	-6.6474901
H	-4.6841449	16.7116948	-5.1618628
C	-6.7418474	19.2968006	-2.3258559
H	-6.0179759	19.9265113	-2.8715257
C	-7.1057255	18.0332095	0.3439100
H	-7.7433899	18.7160889	0.9218560

H	-7.7652349	17.4900892	-0.3460679
C	-2.6739602	22.5314787	-6.0319369
H	-2.2393203	23.1092976	-6.8585702
H	-2.5851456	23.1595719	-5.1303143
C	-1.8629408	21.2442405	-5.8221800
H	-0.8190248	21.4952199	-5.5908861
H	-1.8542337	20.6600984	-6.7567570
C	-3.9578861	20.0804714	-5.0001111
H	-4.0272143	19.4669076	-5.9135949
H	-4.3851155	19.4714201	-4.1850159
C	0.9386279	13.7501642	-2.1206524
H	1.3427965	13.0610341	-2.8797079
H	1.8032787	14.2040491	-1.6176757
C	-7.4558132	14.3070045	-0.1930889
H	-8.0612361	15.0032682	0.4039508
H	-7.1116351	13.5194757	0.4914784
C	-5.9448900	20.6904122	0.1618506
H	-7.0169992	20.9336676	0.2704929
C	0.3471805	20.5301467	-2.9234295
H	-0.3155409	21.3727781	-3.1612879
H	0.0418476	20.1426039	-1.9426128
C	1.8026025	21.0089123	-2.8365939
H	2.1030430	21.4537329	-3.7995596
H	1.8762221	21.8079778	-2.0861840
C	-6.9058971	17.9825795	-3.1035175
H	-5.9405176	17.4533286	-3.1589853
H	-7.6077385	17.3245419	-2.5637788
C	-4.1519177	22.2356653	-6.3058004
H	-4.2471012	21.7093419	-7.2697908
H	-4.7142003	23.1735906	-6.4070488
C	-8.0799412	20.0519309	-2.2415200
H	-7.9599642	21.0062391	-1.7122177
H	-8.8017986	19.4525355	-1.6628885
C	-5.2797603	21.7942080	-0.6721802
H	-5.7458274	21.8628411	-1.6658140
H	-4.2213827	21.5435988	-0.8329731
C	-3.2556779	13.6239544	-5.9725269
H	-2.7075348	12.8575568	-5.4075402
H	-2.5888168	13.9585124	-6.7841197
C	2.5996870	18.7101787	-3.4957991
H	2.9526003	19.0473650	-4.4841564
H	3.2342955	17.8592476	-3.2116187
C	-5.4311365	21.9482012	2.2889207
H	-6.4928841	22.1713037	2.4828090
H	-4.9431567	21.8760858	3.2705647
C	-8.7843970	19.0113582	-4.4505210
H	-9.1429779	19.2306944	-5.4651943
H	-9.5521909	18.3753747	-3.9798483
C	-5.1074268	14.0682150	2.4217537
H	-5.9793665	14.5773908	2.8555871
H	-5.4920075	13.2668455	1.7726597
C	0.0827637	12.9693524	-1.1209139
H	0.6749961	12.1736807	-0.6497247
H	-0.2341033	13.6488206	-0.3125333
C	-7.4609143	18.2423323	-4.5081198
H	-6.7200661	18.8208717	-5.0842429
H	-7.5914144	17.2866221	-5.0348101
C	2.7423573	19.8522892	-2.4869759

H	2.5012871	19.4812582	-1.4771818
H	3.7832751	20.2005322	-2.4537996
C	-4.8139312	23.0834167	1.4661405
H	-4.9658347	24.0432744	1.9776077
H	-3.7255427	22.9331624	1.4038118
C	-5.4108415	14.0679266	-1.6811728
H	-4.9813190	13.2751849	-1.0508098
H	-4.5652067	14.6169299	-2.1225312
C	-5.3301365	20.5968572	1.5679211
H	-4.2736587	20.2957393	1.4840543
H	-5.8397728	19.8256473	2.1642398
C	-6.2457580	15.0210234	-0.8174128
H	-6.6333856	15.8008255	-1.4967013
C	-5.3977371	23.1433405	0.0510798
C	-7.5019233	12.7295358	-2.1784763
H	-8.1304343	12.3188582	-2.9799571
H	-7.1676878	11.8713236	-1.5731432
C	-8.3184568	13.6821335	-1.2994645
H	-9.1696434	13.1549007	-0.8482283
H	-8.7431135	14.4859208	-1.9244388
C	-1.9763378	13.4581064	-2.5120782
H	-2.8382048	13.0033736	-3.0204284
H	-2.3784205	14.1567444	-1.7603941
C	-4.2481303	13.4435400	3.5296717
H	-3.9271806	14.2343048	4.2273479
H	-4.8578244	12.7399753	4.1126037
C	-5.6937167	15.2562155	-6.4355766
H	-6.2445427	16.0209894	-7.0004399
H	-6.3567156	14.9258508	-5.6190731
C	-3.0179384	12.7391945	2.9493110
H	-3.3451900	11.8787566	2.3419062
H	-2.3984094	12.3302814	3.7585335
C	-3.0397015	14.3233157	0.9713943
H	-3.3821201	13.5347051	0.2844522
H	-2.4389437	15.0329090	0.3838110
C	-8.6397630	20.3077601	-3.6486903
H	-9.6070858	20.8217941	-3.5693857
H	-7.9622788	20.9966290	-4.1796428
C	-4.5270106	13.0155457	-6.5827604
H	-4.2525528	12.1887980	-7.2514668
H	-5.1364234	12.5765066	-5.7759741
C	-6.2786674	13.4343993	-2.7729018
H	-5.6785064	12.7273287	-3.3642914
H	-6.6121339	14.2240343	-3.4678103
C	-5.3541299	14.0626184	-7.3343894
H	-6.2743212	13.6092479	-7.7264065
H	-4.7853853	14.4180532	-8.2094166
C	-1.1536397	12.3770477	-1.8017834
H	-1.7895742	11.8584506	-1.0699641
H	-0.8420203	11.6170723	-2.5362163
C	-2.1896898	13.6903731	2.0796656
H	-1.7654435	14.4914419	2.7048592
H	-1.3386728	13.1586262	1.6324184
F	-1.0532487	17.9629918	-0.8723778
C	0.2130598	19.4094526	-3.9618861
H	0.5063219	19.8093743	-4.9503089
C	1.1438725	18.2377277	-3.6172707
H	1.0846168	17.4552617	-4.3851464

H	0.8142074	17.7910017	-2.6675077
C	0.1216475	14.8472940	-2.8131871
H	0.7526267	15.3792057	-3.5370434
H	-0.2029904	15.5915563	-2.0664034
C	-1.1639756	16.3753695	-5.6086900
H	-0.1095374	16.2232222	-5.3504343
H	-1.3444943	15.8167968	-6.5381052
C	-1.4562283	17.8711483	-5.8265411
H	-2.4244214	17.9978492	-6.3289676
H	-0.6940487	18.3088576	-6.4859338
C	-3.6078600	14.8163714	-5.0698455
H	-4.2272519	14.4523459	-4.2340163
C	-2.4853023	20.4003556	-4.6979871
H	-2.4548486	20.9838126	-3.7620089
C	-6.3824487	17.0526283	1.2760671
H	-7.1033322	16.4184285	1.8087408
H	-5.7987193	17.5901911	2.0369996
H	-6.4612345	23.4283934	0.1045028
H	-4.8964745	23.9231109	-0.5387529
H	-1.8173989	22.0755633	0.7770395
C	-1.7127323	21.0156173	0.9993352
C	-1.8325088	20.1001645	-0.0245267
F	-2.1966781	20.5298574	-1.2749225
C	-1.7438350	18.6964542	0.1608306
C	-1.4425657	18.2975879	1.4892819
F	-1.3291211	16.9624684	1.7123440
C	-1.3419230	19.1839444	2.5444061
H	-1.1433518	18.7976708	3.5428087
C	-1.4536102	20.5586293	2.2987959
H	-1.3303551	21.2699636	3.1119156

SCF energy GEOOPT = -7786.367203851 H

ZPE = 3789. kJ/mol

FREEH energy = 3987.74 kJ/mol

FREEH entropy = 1.69946 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1	a	-149.44	0.00000	YES	YES
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		-0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7		0.00	0.00000	-	-
	8	a	5.14	0.04811	YES	YES
	9	a	11.38	0.06585	YES	YES
	10	a	15.96	0.06286	YES	YES
	11	a	19.57	0.42664	YES	YES
	12	a	25.31	0.02685	YES	YES
	13	a	28.92	0.16692	YES	YES
	14	a	31.38	0.07138	YES	YES
	15	a	32.46	0.51913	YES	YES
	16	a	33.98	0.61527	YES	YES
	17	a	39.18	0.52285	YES	YES
	18	a	41.46	0.44010	YES	YES
	19	a	42.96	0.51115	YES	YES

20	a	44.33	0.15345	YES	YES
21	a	49.64	0.08414	YES	YES
22	a	51.12	0.19748	YES	YES
23	a	52.18	2.17137	YES	YES
24	a	53.51	0.11163	YES	YES
25	a	56.32	0.32102	YES	YES
26	a	58.76	0.56001	YES	YES
27	a	60.39	0.28484	YES	YES
28	a	61.36	0.02557	YES	YES
29	a	65.33	1.07441	YES	YES
30	a	69.77	0.42308	YES	YES
31	a	71.67	0.07706	YES	YES
32	a	72.43	0.08690	YES	YES
33	a	73.24	0.02758	YES	YES
34	a	76.34	2.86011	YES	YES
35	a	78.48	0.85151	YES	YES
36	a	80.88	0.42040	YES	YES
37	a	84.79	0.25687	YES	YES
38	a	87.36	0.12720	YES	YES
39	a	93.55	0.59056	YES	YES
40	a	100.96	1.56296	YES	YES
41	a	108.43	0.41276	YES	YES
42	a	115.71	0.27824	YES	YES
43	a	120.62	1.23667	YES	YES
44	a	130.63	1.02476	YES	YES
45	a	133.86	1.69206	YES	YES
46	a	136.37	0.15343	YES	YES
47	a	138.86	0.89584	YES	YES
48	a	146.74	0.17521	YES	YES
49	a	148.19	2.42335	YES	YES
50	a	155.05	0.98369	YES	YES
51	a	161.96	4.23693	YES	YES
52	a	170.33	0.73811	YES	YES
53	a	177.39	0.94250	YES	YES
54	a	182.52	0.39133	YES	YES
55	a	185.48	1.81879	YES	YES
56	a	187.88	3.50293	YES	YES
57	a	191.60	0.73284	YES	YES
58	a	195.96	1.17161	YES	YES
59	a	212.10	0.59527	YES	YES
60	a	215.39	0.20870	YES	YES
61	a	216.61	0.23715	YES	YES
62	a	218.36	0.24355	YES	YES
63	a	220.96	0.22556	YES	YES
64	a	225.67	0.13717	YES	YES
65	a	227.34	0.77935	YES	YES
66	a	233.36	0.82256	YES	YES
67	a	236.56	1.05759	YES	YES
68	a	238.90	0.84310	YES	YES
69	a	240.52	0.23986	YES	YES
70	a	242.03	2.28975	YES	YES
71	a	244.26	5.66321	YES	YES
72	a	245.76	0.08899	YES	YES
73	a	249.09	9.01947	YES	YES
74	a	252.35	1.29733	YES	YES
75	a	255.56	0.19337	YES	YES
76	a	261.90	12.50184	YES	YES
77	a	271.51	0.65823	YES	YES

78	a	276.75	0.19982	YES	YES
79	a	285.45	0.46319	YES	YES
80	a	290.16	0.86927	YES	YES
81	a	293.91	3.73673	YES	YES
82	a	299.76	47.38744	YES	YES
83	a	304.63	0.49117	YES	YES
84	a	310.79	2.13126	YES	YES
85	a	312.06	0.21147	YES	YES
86	a	329.61	0.37685	YES	YES
87	a	329.86	4.93162	YES	YES
88	a	331.94	0.23829	YES	YES
89	a	332.35	1.47099	YES	YES
90	a	335.83	3.01978	YES	YES
91	a	338.36	0.87426	YES	YES
92	a	373.61	15.93649	YES	YES
93	a	374.80	0.93686	YES	YES
94	a	380.19	0.67655	YES	YES
95	a	382.67	0.13224	YES	YES
96	a	391.07	3.28055	YES	YES
97	a	396.98	1.47093	YES	YES
98	a	403.81	1.23393	YES	YES
99	a	414.08	3.49376	YES	YES
100	a	417.00	1.77487	YES	YES
101	a	422.36	5.33945	YES	YES
102	a	424.44	3.32921	YES	YES
103	a	428.01	4.48618	YES	YES
104	a	428.25	25.53819	YES	YES
105	a	430.46	0.41083	YES	YES
106	a	430.95	0.18715	YES	YES
107	a	431.74	2.09222	YES	YES
108	a	432.67	5.86298	YES	YES
109	a	433.25	18.44762	YES	YES
110	a	434.06	34.20768	YES	YES
111	a	435.17	1.01774	YES	YES
112	a	439.34	0.98945	YES	YES
113	a	442.12	11.93535	YES	YES
114	a	459.29	8.20557	YES	YES
115	a	461.17	4.65384	YES	YES
116	a	472.16	8.58703	YES	YES
117	a	478.12	44.96379	YES	YES
118	a	489.24	8.02209	YES	YES
119	a	491.48	6.80334	YES	YES
120	a	493.38	2.54210	YES	YES
121	a	494.96	1.89657	YES	YES
122	a	495.18	4.45044	YES	YES
123	a	500.24	3.67476	YES	YES
124	a	502.03	1.57620	YES	YES
125	a	511.13	3.30243	YES	YES
126	a	512.05	17.19318	YES	YES
127	a	535.15	1.39228	YES	YES
128	a	566.94	5.09832	YES	YES
129	a	606.83	22.89780	YES	YES
130	a	627.13	22.26769	YES	YES
131	a	633.08	12.80131	YES	YES
132	a	641.50	14.89177	YES	YES
133	a	652.84	93.28984	YES	YES
134	a	663.74	12.33404	YES	YES
135	a	697.69	3.77228	YES	YES

136	a	706.24	5.89367	YES	YES
137	a	721.06	10.55964	YES	YES
138	a	721.73	2.44552	YES	YES
139	a	725.93	4.56390	YES	YES
140	a	730.29	16.34611	YES	YES
141	a	731.26	1.43670	YES	YES
142	a	734.25	3.40261	YES	YES
143	a	744.38	60.44258	YES	YES
144	a	747.75	0.85171	YES	YES
145	a	771.45	0.25750	YES	YES
146	a	772.81	3.60524	YES	YES
147	a	773.25	0.08249	YES	YES
148	a	773.36	0.93971	YES	YES
149	a	774.94	0.64726	YES	YES
150	a	776.37	6.89962	YES	YES
151	a	776.67	4.55419	YES	YES
152	a	779.03	1.64768	YES	YES
153	a	780.17	0.01951	YES	YES
154	a	787.42	17.17656	YES	YES
155	a	807.20	0.60665	YES	YES
156	a	808.17	3.73019	YES	YES
157	a	809.54	2.57695	YES	YES
158	a	810.40	2.60208	YES	YES
159	a	811.58	1.85049	YES	YES
160	a	812.02	6.22297	YES	YES
161	a	812.26	5.91823	YES	YES
162	a	817.60	4.87135	YES	YES
163	a	831.14	6.95938	YES	YES
164	a	833.33	3.33995	YES	YES
165	a	833.65	9.42972	YES	YES
166	a	836.25	2.75121	YES	YES
167	a	837.21	1.31908	YES	YES
168	a	838.10	5.19506	YES	YES
169	a	840.00	3.62669	YES	YES
170	a	840.65	3.42700	YES	YES
171	a	848.02	15.57644	YES	YES
172	a	854.23	16.34644	YES	YES
173	a	862.97	0.96770	YES	YES
174	a	874.68	3.94379	YES	YES
175	a	876.17	2.19129	YES	YES
176	a	876.57	2.31929	YES	YES
177	a	876.74	2.49335	YES	YES
178	a	878.18	4.06717	YES	YES
179	a	878.44	4.11355	YES	YES
180	a	879.08	1.78268	YES	YES
181	a	879.29	6.29807	YES	YES
182	a	880.03	3.33874	YES	YES
183	a	880.36	1.03902	YES	YES
184	a	881.26	0.46363	YES	YES
185	a	882.33	8.63225	YES	YES
186	a	882.73	2.42015	YES	YES
187	a	883.56	5.39853	YES	YES
188	a	883.99	1.02540	YES	YES
189	a	887.78	7.43431	YES	YES
190	a	902.12	0.77654	YES	YES
191	a	903.27	1.72536	YES	YES
192	a	904.38	2.74154	YES	YES
193	a	905.02	1.14643	YES	YES

194	a	908.19	1.85629	YES	YES
195	a	909.42	3.35115	YES	YES
196	a	910.60	2.13702	YES	YES
197	a	911.15	1.05661	YES	YES
198	a	922.54	9.40379	YES	YES
199	a	964.43	66.73125	YES	YES
200	a	982.78	0.64485	YES	YES
201	a	984.81	3.07999	YES	YES
202	a	987.71	9.44236	YES	YES
203	a	987.82	8.56475	YES	YES
204	a	988.25	7.41958	YES	YES
205	a	988.66	3.45903	YES	YES
206	a	989.66	21.46842	YES	YES
207	a	989.79	4.48137	YES	YES
208	a	991.68	17.58193	YES	YES
209	a	992.08	8.20394	YES	YES
210	a	1001.00	4.94449	YES	YES
211	a	1012.40	1.67654	YES	YES
212	a	1014.86	2.07115	YES	YES
213	a	1015.30	0.75162	YES	YES
214	a	1016.51	0.91408	YES	YES
215	a	1016.91	0.47731	YES	YES
216	a	1018.26	1.18133	YES	YES
217	a	1018.57	1.21149	YES	YES
218	a	1021.93	0.63742	YES	YES
219	a	1030.77	1.17479	YES	YES
220	a	1032.50	1.20794	YES	YES
221	a	1033.57	0.97394	YES	YES
222	a	1034.27	0.26296	YES	YES
223	a	1038.23	2.89181	YES	YES
224	a	1040.21	1.33879	YES	YES
225	a	1040.75	2.97247	YES	YES
226	a	1041.82	0.98345	YES	YES
227	a	1055.95	0.41821	YES	YES
228	a	1056.93	2.11367	YES	YES
229	a	1058.12	1.14709	YES	YES
230	a	1058.26	6.79761	YES	YES
231	a	1058.82	1.58094	YES	YES
232	a	1062.83	1.76059	YES	YES
233	a	1064.30	0.04843	YES	YES
234	a	1065.09	1.40852	YES	YES
235	a	1067.33	1.98631	YES	YES
236	a	1069.58	0.16241	YES	YES
237	a	1070.33	0.15865	YES	YES
238	a	1070.68	0.27247	YES	YES
239	a	1071.00	0.14725	YES	YES
240	a	1072.10	0.11898	YES	YES
241	a	1072.27	1.08907	YES	YES
242	a	1075.35	0.25381	YES	YES
243	a	1075.82	0.15458	YES	YES
244	a	1076.37	2.37005	YES	YES
245	a	1079.35	2.33313	YES	YES
246	a	1090.05	13.30763	YES	YES
247	a	1091.60	2.50431	YES	YES
248	a	1096.05	15.88035	YES	YES
249	a	1098.77	7.03481	YES	YES
250	a	1101.53	5.51952	YES	YES
251	a	1103.23	2.20027	YES	YES

252	a	1106.75	10.60698	YES	YES
253	a	1116.49	12.42936	YES	YES
254	a	1123.40	1.34610	YES	YES
255	a	1130.86	9.51299	YES	YES
256	a	1137.44	1.02171	YES	YES
257	a	1157.77	5.60152	YES	YES
258	a	1159.41	4.17320	YES	YES
259	a	1160.56	8.19828	YES	YES
260	a	1166.33	6.56346	YES	YES
261	a	1168.19	14.22542	YES	YES
262	a	1169.27	8.35762	YES	YES
263	a	1170.48	5.09376	YES	YES
264	a	1171.24	6.28468	YES	YES
265	a	1172.61	20.27545	YES	YES
266	a	1178.36	2.19617	YES	YES
267	a	1179.54	40.22246	YES	YES
268	a	1185.17	10.24642	YES	YES
269	a	1188.45	2.00990	YES	YES
270	a	1188.73	0.32359	YES	YES
271	a	1192.77	1.60246	YES	YES
272	a	1202.46	19.00034	YES	YES
273	a	1212.22	1.73811	YES	YES
274	a	1226.47	45.19314	YES	YES
275	a	1237.58	0.97917	YES	YES
276	a	1240.61	0.23494	YES	YES
277	a	1241.65	0.63625	YES	YES
278	a	1244.68	1.21778	YES	YES
279	a	1246.21	0.28557	YES	YES
280	a	1247.08	0.62674	YES	YES
281	a	1247.76	1.85792	YES	YES
282	a	1248.58	0.98539	YES	YES
283	a	1251.00	1.21374	YES	YES
284	a	1251.81	1.69147	YES	YES
285	a	1252.41	0.98231	YES	YES
286	a	1253.09	5.01688	YES	YES
287	a	1254.00	0.40924	YES	YES
288	a	1254.88	4.83232	YES	YES
289	a	1255.46	5.44246	YES	YES
290	a	1256.35	6.73982	YES	YES
291	a	1257.10	2.68335	YES	YES
292	a	1257.97	6.75608	YES	YES
293	a	1258.41	1.18140	YES	YES
294	a	1259.06	1.01054	YES	YES
295	a	1259.41	10.96197	YES	YES
296	a	1261.42	3.00575	YES	YES
297	a	1261.79	0.87001	YES	YES
298	a	1262.61	3.61246	YES	YES
299	a	1264.05	1.43383	YES	YES
300	a	1264.49	1.22370	YES	YES
301	a	1268.00	2.03914	YES	YES
302	a	1269.87	1.46876	YES	YES
303	a	1280.32	2.76638	YES	YES
304	a	1280.78	2.92477	YES	YES
305	a	1282.24	2.82851	YES	YES
306	a	1283.45	3.63931	YES	YES
307	a	1286.56	5.94521	YES	YES
308	a	1286.99	1.96813	YES	YES
309	a	1290.21	4.90720	YES	YES

310	a	1290.73	3.86342	YES	YES
311	a	1304.03	0.02677	YES	YES
312	a	1307.14	1.55662	YES	YES
313	a	1309.90	0.59046	YES	YES
314	a	1310.44	2.78469	YES	YES
315	a	1312.97	2.36351	YES	YES
316	a	1313.97	1.53434	YES	YES
317	a	1315.15	1.98774	YES	YES
318	a	1317.38	2.49577	YES	YES
319	a	1318.25	1.76098	YES	YES
320	a	1320.45	1.34332	YES	YES
321	a	1321.03	1.53622	YES	YES
322	a	1321.67	1.77419	YES	YES
323	a	1322.56	1.39780	YES	YES
324	a	1322.96	2.46140	YES	YES
325	a	1323.37	3.98200	YES	YES
326	a	1323.68	3.71926	YES	YES
327	a	1324.47	4.43036	YES	YES
328	a	1325.21	0.31294	YES	YES
329	a	1325.39	2.29154	YES	YES
330	a	1326.34	0.72500	YES	YES
331	a	1326.63	1.17325	YES	YES
332	a	1327.69	1.86472	YES	YES
333	a	1330.82	1.08548	YES	YES
334	a	1332.09	2.94623	YES	YES
335	a	1335.58	0.82215	YES	YES
336	a	1335.74	0.27614	YES	YES
337	a	1336.43	0.43266	YES	YES
338	a	1337.17	0.32783	YES	YES
339	a	1337.94	0.88156	YES	YES
340	a	1338.42	0.38658	YES	YES
341	a	1339.02	0.51614	YES	YES
342	a	1339.37	0.46549	YES	YES
343	a	1341.97	11.41899	YES	YES
344	a	1343.37	0.44898	YES	YES
345	a	1343.82	1.05559	YES	YES
346	a	1345.22	1.57128	YES	YES
347	a	1346.14	2.73810	YES	YES
348	a	1347.13	1.11503	YES	YES
349	a	1348.41	0.89344	YES	YES
350	a	1349.52	0.29182	YES	YES
351	a	1350.55	0.77261	YES	YES
352	a	1386.03	2.40556	YES	YES
353	a	1402.54	4.14435	YES	YES
354	a	1406.26	7.35164	YES	YES
355	a	1407.63	9.40696	YES	YES
356	a	1409.63	8.91475	YES	YES
357	a	1421.48	4.09446	YES	YES
358	a	1423.19	3.85962	YES	YES
359	a	1425.66	5.27491	YES	YES
360	a	1428.12	4.90203	YES	YES
361	a	1429.48	0.29926	YES	YES
362	a	1431.19	2.73928	YES	YES
363	a	1432.72	7.65330	YES	YES
364	a	1433.31	6.85453	YES	YES
365	a	1433.99	1.47464	YES	YES
366	a	1434.58	4.02614	YES	YES
367	a	1435.08	3.12712	YES	YES

368	a	1435.27	1.06835	YES	YES
369	a	1436.34	10.23732	YES	YES
370	a	1436.66	10.58684	YES	YES
371	a	1436.73	3.16952	YES	YES
372	a	1438.10	10.65596	YES	YES
373	a	1438.35	2.18539	YES	YES
374	a	1438.50	1.21473	YES	YES
375	a	1438.68	5.23856	YES	YES
376	a	1439.98	11.77509	YES	YES
377	a	1440.21	2.79508	YES	YES
378	a	1440.25	0.95838	YES	YES
379	a	1440.77	1.99553	YES	YES
380	a	1441.04	7.98539	YES	YES
381	a	1441.55	6.11898	YES	YES
382	a	1442.61	7.57857	YES	YES
383	a	1443.64	3.93980	YES	YES
384	a	1444.11	26.90438	YES	YES
385	a	1445.04	12.81260	YES	YES
386	a	1445.76	12.11694	YES	YES
387	a	1446.12	25.70348	YES	YES
388	a	1446.62	11.39076	YES	YES
389	a	1451.77	50.35413	YES	YES
390	a	1452.35	4.19711	YES	YES
391	a	1453.57	11.77305	YES	YES
392	a	1454.07	3.36613	YES	YES
393	a	1454.58	2.15797	YES	YES
394	a	1455.53	4.22482	YES	YES
395	a	1456.79	3.50328	YES	YES
396	a	1457.66	1.15722	YES	YES
397	a	1458.17	1.50995	YES	YES
398	a	1536.93	12.02578	YES	YES
399	a	1572.07	6.27392	YES	YES
400	a	2913.14	2.95698	YES	YES
401	a	2917.59	78.41114	YES	YES
402	a	2919.07	1.89094	YES	YES
403	a	2919.27	11.05924	YES	YES
404	a	2919.90	64.90231	YES	YES
405	a	2929.35	4.58384	YES	YES
406	a	2935.49	2.23724	YES	YES
407	a	2936.89	15.57665	YES	YES
408	a	2938.11	8.98854	YES	YES
409	a	2939.31	4.42667	YES	YES
410	a	2942.22	3.38822	YES	YES
411	a	2942.36	11.92898	YES	YES
412	a	2944.81	12.11083	YES	YES
413	a	2945.25	11.77649	YES	YES
414	a	2945.65	2.44059	YES	YES
415	a	2945.89	13.83335	YES	YES
416	a	2946.06	16.04890	YES	YES
417	a	2946.34	5.45277	YES	YES
418	a	2947.33	12.01463	YES	YES
419	a	2947.95	7.53270	YES	YES
420	a	2948.53	6.73614	YES	YES
421	a	2948.57	1.00605	YES	YES
422	a	2951.57	10.83062	YES	YES
423	a	2952.18	21.11595	YES	YES
424	a	2952.50	4.08934	YES	YES
425	a	2952.90	11.27811	YES	YES

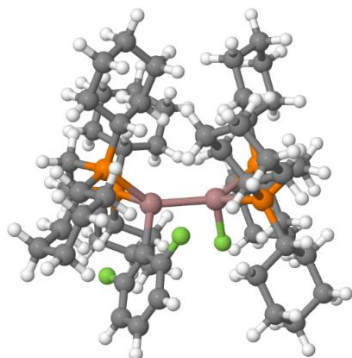
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427	a	2955.32	22.48248	YES	YES
428	a	2956.86	2.22453	YES	YES
429	a	2956.89	1.86422	YES	YES
430	a	2957.46	12.19842	YES	YES
431	a	2957.62	16.53669	YES	YES
432	a	2958.26	3.28597	YES	YES
433	a	2959.68	29.29745	YES	YES
434	a	2959.72	24.42843	YES	YES
435	a	2960.49	13.81432	YES	YES
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438	a	2961.65	29.07013	YES	YES
439	a	2962.86	38.75410	YES	YES
440	a	2965.04	16.92164	YES	YES
441	a	2965.63	14.77587	YES	YES
442	a	2966.66	13.67397	YES	YES
443	a	2969.41	31.43174	YES	YES
444	a	2970.59	50.25149	YES	YES
445	a	2972.33	16.05704	YES	YES
446	a	2974.07	13.97298	YES	YES
447	a	2974.61	13.08948	YES	YES
448	a	2978.07	12.73935	YES	YES
449	a	2980.44	27.67560	YES	YES
450	a	2982.26	2.64376	YES	YES
451	a	2983.43	4.84150	YES	YES
452	a	2984.46	8.02731	YES	YES
453	a	2985.55	6.22243	YES	YES
454	a	2987.46	7.68271	YES	YES
455	a	2992.07	22.13477	YES	YES
456	a	2998.57	27.26198	YES	YES
457	a	2999.46	21.19911	YES	YES
458	a	3000.80	28.09124	YES	YES
459	a	3002.01	7.40965	YES	YES
460	a	3006.22	35.28654	YES	YES
461	a	3006.46	17.45248	YES	YES
462	a	3006.92	26.72857	YES	YES
463	a	3007.85	24.92404	YES	YES
464	a	3008.25	19.01957	YES	YES
465	a	3008.50	8.29969	YES	YES
466	a	3009.16	33.01192	YES	YES
467	a	3009.28	14.20836	YES	YES
468	a	3010.97	11.36308	YES	YES
469	a	3012.18	15.36962	YES	YES
470	a	3013.41	16.84390	YES	YES
471	a	3013.84	19.55684	YES	YES
472	a	3014.56	25.09808	YES	YES
473	a	3014.76	28.24371	YES	YES
474	a	3014.92	19.20022	YES	YES
475	a	3015.40	18.51967	YES	YES
476	a	3015.68	25.53449	YES	YES
477	a	3015.82	20.61505	YES	YES
478	a	3016.20	23.47197	YES	YES
479	a	3016.38	22.04685	YES	YES
480	a	3016.77	26.46980	YES	YES
481	a	3017.16	26.72171	YES	YES
482	a	3017.99	14.39976	YES	YES
483	a	3018.14	16.51174	YES	YES

484	a	3018.30	25.32623	YES	YES
485	a	3018.42	42.37943	YES	YES
486	a	3018.92	15.21071	YES	YES
487	a	3019.11	15.78008	YES	YES
488	a	3021.87	23.16229	YES	YES
489	a	3023.50	28.64355	YES	YES
490	a	3023.97	35.88206	YES	YES
491	a	3028.30	4.60709	YES	YES
492	a	3029.52	1.47139	YES	YES
493	a	3034.36	13.56738	YES	YES
494	a	3037.06	1.25476	YES	YES
495	a	3047.19	0.59201	YES	YES
496	a	3130.42	0.68829	YES	YES
497	a	3135.61	0.45851	YES	YES
498	a	3150.37	1.18726	YES	YES

§end

Double hybrid single point energy = -7778.466427138916 H
 COSMO energy + OC correction = -7786.5209100887 H (in 3FB)

6.2.57 [F{Ga(dcpe)}₂(C₆F₂H₃)]²⁺ (*syn*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Ga	0.5442265	0.2060604	-1.1454217
Ga	0.3126102	0.0421497	1.2935460
P	0.2803816	2.2649656	-2.4194931
P	-1.4630293	0.5749113	2.8894687
P	-0.1138980	-0.9760975	-3.1852066
P	0.2375358	-2.1670839	2.2363857
C	-2.9171949	3.8821162	-0.2826805
H	-2.3470517	4.3278394	0.5488697
H	-3.7937725	3.3880123	0.1622552
C	1.0947084	-2.2419480	-3.7735841
H	0.7026820	-2.6055017	-4.7392021
C	1.7949074	-3.1455003	2.2567399
H	2.3791765	-2.6535766	3.0490758
C	-2.8754849	-0.7088116	-2.8822382
H	-2.8851976	0.0467144	-3.6838903
H	-2.6511020	-0.1774996	-1.9428587
C	-3.1300421	0.8838065	2.1665076
H	-2.9970588	1.8444633	1.6404474

C	-1.5836735	-0.9532082	3.9425838
H	-1.8490794	-0.6434901	4.9623492
H	-2.4238037	-1.5514308	3.5650626
C	-2.1634998	5.6491229	-1.9286868
H	-2.5008436	6.4093833	-2.6457700
H	-1.5561082	6.1758375	-1.1748244
C	-1.2858333	4.6161708	-2.6491928
H	-0.4165338	5.1102847	-3.1052341
H	-1.8650161	4.1630612	-3.4696165
C	-2.0348574	2.8433046	-0.9849211
H	-2.6369079	2.3071314	-1.7381583
H	-1.6759886	2.0883959	-0.2675659
C	3.4810435	-2.7640320	-4.4231644
H	3.1816246	-3.1638284	-5.4058986
H	4.4804836	-2.3276277	-4.5541981
C	-1.7734869	-4.2043136	2.4095578
H	-2.0209780	-3.8158671	3.4071667
H	-1.0270920	-4.9960803	2.5576915
C	-1.1813907	1.9336859	4.1129215
H	-2.0349350	1.8320741	4.8075627
C	2.6575583	3.4272021	-1.5948547
H	2.0697617	4.0995745	-0.9565788
H	2.8295421	2.5008171	-1.0241331
C	4.0076372	4.0691953	-1.9332312
H	3.8400124	5.0449838	-2.4179131
H	4.5531636	4.2710402	-1.0008713
C	-3.5101528	-0.1714880	1.1183992
H	-2.7062917	-0.2741295	0.3709269
H	-3.6196634	-1.1528806	1.6096774
C	-3.3642617	4.9852975	-1.2475204
H	-4.0253044	4.5503781	-2.0155139
H	-3.9609034	5.7364077	-0.7128601
C	-4.2424285	1.0560882	3.2147095
H	-3.9778709	1.8379447	3.9387139
H	-4.3592757	0.1186553	3.7828108
C	-1.2558902	3.3200906	3.4545556
H	-2.2276510	3.4544009	2.9576256
H	-0.4869183	3.3968373	2.6748175
C	-2.0960531	-2.5469186	-4.4600229
H	-1.3392131	-3.3256948	-4.6229508
H	-2.0547189	-1.8743118	-5.3324042
C	4.0541220	2.8466700	-4.1351990
H	3.8859090	3.7724070	-4.7095225
H	4.6345371	2.1770720	-4.7847789
C	0.2866307	2.8655334	5.9485184
H	-0.5178433	2.8116597	6.7001140
H	1.2316653	2.7182648	6.4886525
C	-5.9565692	0.3739695	1.4746070
H	-6.8879500	0.6697025	0.9735840
H	-6.1608438	-0.5916630	1.9661962
C	1.6503875	-4.6326150	2.6215391
H	1.1318159	-4.7516433	3.5834133
H	1.0427381	-5.1446524	1.8598684
C	3.5211263	-3.9029393	-3.4008262
H	4.2167412	-4.6868015	-3.7285805
H	3.9064520	-3.5172908	-2.4420806
C	-4.8392322	0.1868250	0.4438128
H	-4.7082149	1.1161579	-0.1350693

H	-5.1102703	-0.5967449	-0.2749730
C	4.8332647	3.1720486	-2.8583849
H	5.0811568	2.2357629	-2.3322163
H	5.7861379	3.6566026	-3.1095631
C	0.2591603	4.2363240	5.2677901
H	0.3802900	5.0337525	6.0128461
H	1.1144727	4.3152318	4.5759584
C	-0.8921813	-3.5998345	0.0987352
H	-0.0908168	-4.3525637	0.1290398
H	-0.5164479	-2.7686791	-0.5168343
C	0.1101794	1.7367555	4.9249764
H	0.9723473	1.7291368	4.2459229
H	0.0944132	0.7655783	5.4410520
C	-1.1897601	-3.0947543	1.5167481
H	-1.9604386	-2.3116016	1.4133866
C	-1.0456832	4.4320853	4.4912546
C	-2.7328597	-5.3255930	0.3527911
H	-3.6457512	-5.7300240	-0.1043717
H	-2.0172210	-6.1613739	0.4147971
C	-3.0284148	-4.8031349	1.7610462
H	-3.4223636	-5.6071626	2.3968517
H	-3.8151633	-4.0312215	1.7080471
C	1.1240376	-3.4062773	-2.7693076
H	0.1219465	-3.8438039	-2.6532242
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C	3.0352414	-5.2939688	2.6792697
H	3.6150042	-4.8467679	3.5028651
H	2.9196342	-6.3594506	2.9201458
C	-4.2608838	-1.3630570	-2.8162492
H	-5.0234092	-0.5923358	-2.6398396
H	-4.2950063	-2.0482027	-1.9528282
C	3.7967735	-5.1173096	1.3617462
H	3.2631058	-5.6529730	0.5582094
H	4.7908852	-5.5779418	1.4352046
C	2.5532836	-2.9553617	0.9279084
H	1.9650223	-3.4014905	0.1109308
H	2.6656104	-1.8877496	0.6900896
C	-5.5714215	1.4099100	2.5332379
H	-6.3605197	1.4987511	3.2917512
H	-5.4778972	2.4023043	2.0620247
C	-3.4892696	-3.1861240	-4.3823161
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H	-3.4916480	-3.9473308	-3.5851052
C	-2.1463819	-4.2190567	-0.5278486
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H	-2.9056939	-3.4305088	-0.6678707
C	-4.5723565	-2.1439319	-4.0957494
H	-5.5548756	-2.6274459	-4.0140074
H	-4.6401511	-1.4422143	-4.9434166
C	2.1242332	-4.4898693	-3.1863705
H	2.1452245	-5.2787990	-2.4209719
H	1.7769989	-4.9666766	-4.1172313
C	3.9233850	-3.6374521	0.9877998
H	4.5480690	-3.1189909	1.7327560
H	4.4309746	-3.5224873	0.0198499
F	2.3602717	-0.0602091	-1.2512322
C	1.8703525	3.0793486	-2.8716632
H	1.5969119	4.0108920	-3.3982040

C	2.7017135	2.1948258	-3.8187448
H	2.1543267	2.0202408	-4.7561568
H	2.8688190	1.2192521	-3.3367479
C	2.5034783	-1.6612869	-3.9957172
H	2.4803374	-0.8762496	-4.7644380
H	2.8509223	-1.1951596	-3.0626033
C	-0.1512782	0.3421451	-4.4794368
H	0.8611050	0.3744110	-4.8987361
H	-0.8200884	0.0194473	-5.2897348
C	-0.5607673	1.7360985	-3.9776140
H	-1.6374309	1.7670430	-3.7636426
H	-0.3715062	2.4857031	-4.7584388
C	-1.7858282	-1.7538959	-3.1790267
H	-1.7566945	-2.4588496	-2.3346322
C	-0.8342228	3.5220368	-1.6669781
H	-0.2180904	3.9872596	-0.8825825
C	-0.2913862	-1.7896570	3.9570981
H	-0.4381099	-2.7138273	4.5319495
H	0.5350205	-1.2376464	4.4250522
H	-1.8931171	4.4377348	5.1960605
H	-1.0552462	5.4067982	3.9842014
H	2.7282525	4.4654320	1.7655581
C	2.8045142	3.4213619	2.0616612
C	1.8505860	2.5004833	1.6559324
F	0.7997570	2.9644934	0.8890208
C	1.8399123	1.1485339	1.9848864
C	2.9067633	0.7598332	2.7907743
F	2.9576319	-0.5416930	3.2119382
C	3.9102282	1.6120540	3.2369254
H	4.7093421	1.2286959	3.8682301
C	3.8507423	2.9559237	2.8630508
H	4.6208372	3.6462084	3.2027044

SCF energy GEOOPT = -7786.496718414 H

ZPE = 3798. kJ/mol

FREEH energy = 3996.20 kJ/mol

FREEH entropy = 1.66860 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	14.29	0.01854	YES	YES
	8	a	21.58	0.00057	YES	YES
	9	a	24.37	0.01619	YES	YES
	10	a	25.74	0.05350	YES	YES
	11	a	31.98	0.06187	YES	YES
	12	a	32.62	0.00486	YES	YES
	13	a	34.82	0.01171	YES	YES
	14	a	35.71	0.03088	YES	YES
	15	a	38.04	0.06232	YES	YES
	16	a	40.42	0.02464	YES	YES
	17	a	43.47	0.03024	YES	YES

18	a	45.93	0.03881	YES	YES
19	a	47.80	0.04216	YES	YES
20	a	49.93	0.03929	YES	YES
21	a	50.49	0.04892	YES	YES
22	a	54.15	0.02313	YES	YES
23	a	56.13	0.18098	YES	YES
24	a	58.08	0.15066	YES	YES
25	a	60.70	0.24253	YES	YES
26	a	64.60	0.13459	YES	YES
27	a	66.35	0.53536	YES	YES
28	a	67.28	0.27107	YES	YES
29	a	69.01	0.33232	YES	YES
30	a	72.00	0.16564	YES	YES
31	a	73.43	0.29025	YES	YES
32	a	75.79	0.57808	YES	YES
33	a	80.31	0.30629	YES	YES
34	a	84.17	0.12258	YES	YES
35	a	92.27	0.41907	YES	YES
36	a	93.66	0.17512	YES	YES
37	a	94.18	0.02214	YES	YES
38	a	103.61	0.01282	YES	YES
39	a	105.74	0.72842	YES	YES
40	a	117.81	3.02022	YES	YES
41	a	118.57	0.46418	YES	YES
42	a	123.98	7.03255	YES	YES
43	a	130.99	1.13293	YES	YES
44	a	132.43	1.50673	YES	YES
45	a	138.12	1.76317	YES	YES
46	a	141.92	3.99881	YES	YES
47	a	143.86	3.72324	YES	YES
48	a	147.16	7.76889	YES	YES
49	a	153.50	2.58727	YES	YES
50	a	158.84	3.41354	YES	YES
51	a	161.48	26.24452	YES	YES
52	a	171.96	2.25829	YES	YES
53	a	176.09	0.93528	YES	YES
54	a	182.83	6.65762	YES	YES
55	a	185.08	8.68697	YES	YES
56	a	188.37	1.96106	YES	YES
57	a	195.88	1.71390	YES	YES
58	a	199.60	3.65987	YES	YES
59	a	214.30	0.50794	YES	YES
60	a	215.40	0.09954	YES	YES
61	a	217.92	0.11891	YES	YES
62	a	221.23	0.20129	YES	YES
63	a	223.19	0.69098	YES	YES
64	a	223.73	0.81950	YES	YES
65	a	228.66	0.34970	YES	YES
66	a	230.30	2.89458	YES	YES
67	a	234.24	3.03431	YES	YES
68	a	235.89	2.81866	YES	YES
69	a	236.33	2.91746	YES	YES
70	a	239.45	1.93926	YES	YES
71	a	241.33	1.10545	YES	YES
72	a	244.31	0.39735	YES	YES
73	a	245.54	1.83443	YES	YES
74	a	249.87	3.40229	YES	YES
75	a	260.96	1.90325	YES	YES

76	a	276.80	9.17427	YES	YES
77	a	280.11	1.35572	YES	YES
78	a	285.18	1.91864	YES	YES
79	a	286.62	0.92576	YES	YES
80	a	293.26	0.84563	YES	YES
81	a	299.43	0.38823	YES	YES
82	a	304.07	1.08283	YES	YES
83	a	313.49	0.75988	YES	YES
84	a	316.47	0.20728	YES	YES
85	a	331.16	0.89782	YES	YES
86	a	332.07	0.23751	YES	YES
87	a	336.17	0.06901	YES	YES
88	a	337.32	0.56969	YES	YES
89	a	339.90	0.72780	YES	YES
90	a	341.38	1.13054	YES	YES
91	a	368.72	0.21914	YES	YES
92	a	377.65	2.43839	YES	YES
93	a	380.11	2.36771	YES	YES
94	a	382.58	0.38974	YES	YES
95	a	387.08	0.05798	YES	YES
96	a	395.52	0.99992	YES	YES
97	a	398.03	0.16472	YES	YES
98	a	406.01	0.83643	YES	YES
99	a	412.48	1.47081	YES	YES
100	a	418.90	1.77541	YES	YES
101	a	422.32	3.80105	YES	YES
102	a	423.34	1.91189	YES	YES
103	a	429.11	0.43571	YES	YES
104	a	429.57	0.05191	YES	YES
105	a	430.67	0.38686	YES	YES
106	a	431.61	0.06078	YES	YES
107	a	431.89	0.06621	YES	YES
108	a	433.32	0.04304	YES	YES
109	a	435.28	1.35301	YES	YES
110	a	435.49	0.96480	YES	YES
111	a	437.81	0.06464	YES	YES
112	a	445.20	1.76359	YES	YES
113	a	460.02	3.30232	YES	YES
114	a	460.71	4.62827	YES	YES
115	a	469.81	2.89710	YES	YES
116	a	488.43	3.58931	YES	YES
117	a	491.60	3.62226	YES	YES
118	a	492.82	1.89283	YES	YES
119	a	496.15	2.90715	YES	YES
120	a	498.01	0.65614	YES	YES
121	a	499.19	0.73505	YES	YES
122	a	503.58	0.31280	YES	YES
123	a	505.31	0.52233	YES	YES
124	a	514.08	5.68759	YES	YES
125	a	515.21	12.57645	YES	YES
126	a	534.91	5.79461	YES	YES
127	a	543.16	45.08466	YES	YES
128	a	548.68	2.92306	YES	YES
129	a	592.97	0.06760	YES	YES
130	a	629.87	20.25023	YES	YES
131	a	634.99	15.42537	YES	YES
132	a	645.44	9.51900	YES	YES
133	a	667.96	13.28744	YES	YES

134	a	691.61	3.44994	YES	YES
135	a	701.87	1.42836	YES	YES
136	a	717.57	3.51196	YES	YES
137	a	718.26	0.50169	YES	YES
138	a	729.81	7.58923	YES	YES
139	a	731.34	2.70685	YES	YES
140	a	733.88	5.38747	YES	YES
141	a	734.58	3.61543	YES	YES
142	a	739.80	4.23161	YES	YES
143	a	742.43	9.82298	YES	YES
144	a	770.37	7.83008	YES	YES
145	a	771.74	42.41666	YES	YES
146	a	772.45	2.13720	YES	YES
147	a	773.72	0.18091	YES	YES
148	a	774.41	0.48651	YES	YES
149	a	775.12	0.65301	YES	YES
150	a	777.03	0.14389	YES	YES
151	a	777.68	0.64065	YES	YES
152	a	779.73	1.33567	YES	YES
153	a	781.79	12.74440	YES	YES
154	a	792.24	13.93851	YES	YES
155	a	806.07	0.93503	YES	YES
156	a	810.41	2.98490	YES	YES
157	a	811.96	1.49315	YES	YES
158	a	812.20	7.56518	YES	YES
159	a	813.21	1.85722	YES	YES
160	a	814.00	1.38249	YES	YES
161	a	815.61	3.93904	YES	YES
162	a	818.98	1.80254	YES	YES
163	a	833.49	4.89512	YES	YES
164	a	833.81	5.70580	YES	YES
165	a	835.86	5.44471	YES	YES
166	a	837.24	3.16451	YES	YES
167	a	837.66	0.77985	YES	YES
168	a	838.36	2.25106	YES	YES
169	a	839.41	5.48929	YES	YES
170	a	840.57	1.72871	YES	YES
171	a	849.54	12.56540	YES	YES
172	a	856.99	15.84330	YES	YES
173	a	868.01	0.24272	YES	YES
174	a	874.19	2.15120	YES	YES
175	a	875.04	2.25587	YES	YES
176	a	875.88	2.29584	YES	YES
177	a	877.16	3.34929	YES	YES
178	a	877.80	3.15004	YES	YES
179	a	878.58	3.94213	YES	YES
180	a	879.15	5.92224	YES	YES
181	a	880.42	4.50100	YES	YES
182	a	880.69	6.12069	YES	YES
183	a	881.36	1.04150	YES	YES
184	a	881.80	2.43933	YES	YES
185	a	882.28	3.07366	YES	YES
186	a	883.83	6.23734	YES	YES
187	a	885.79	0.62833	YES	YES
188	a	887.28	3.26062	YES	YES
189	a	888.04	1.52466	YES	YES
190	a	903.80	2.62781	YES	YES
191	a	904.94	1.23809	YES	YES

192	a	905.09	1.93834	YES	YES
193	a	906.31	2.62049	YES	YES
194	a	909.33	1.50101	YES	YES
195	a	911.21	0.58115	YES	YES
196	a	911.32	1.90415	YES	YES
197	a	911.92	0.75752	YES	YES
198	a	942.76	71.03066	YES	YES
199	a	957.51	0.47905	YES	YES
200	a	975.39	0.39770	YES	YES
201	a	986.63	2.38914	YES	YES
202	a	987.96	9.24864	YES	YES
203	a	989.26	8.74248	YES	YES
204	a	989.83	16.46326	YES	YES
205	a	990.30	3.09160	YES	YES
206	a	991.50	20.90005	YES	YES
207	a	991.58	5.12789	YES	YES
208	a	992.17	4.42108	YES	YES
209	a	995.34	2.96469	YES	YES
210	a	1015.12	0.25111	YES	YES
211	a	1015.60	0.77031	YES	YES
212	a	1015.80	0.20251	YES	YES
213	a	1018.15	0.07009	YES	YES
214	a	1019.18	0.12207	YES	YES
215	a	1020.05	0.70560	YES	YES
216	a	1020.44	0.93650	YES	YES
217	a	1021.23	0.58041	YES	YES
218	a	1030.58	1.04467	YES	YES
219	a	1031.09	2.66151	YES	YES
220	a	1031.67	0.93872	YES	YES
221	a	1034.66	0.95672	YES	YES
222	a	1036.21	1.11558	YES	YES
223	a	1039.02	3.07000	YES	YES
224	a	1040.28	1.37633	YES	YES
225	a	1042.94	1.34895	YES	YES
226	a	1043.97	1.19990	YES	YES
227	a	1058.34	1.56177	YES	YES
228	a	1059.11	1.03795	YES	YES
229	a	1059.39	1.11865	YES	YES
230	a	1060.86	0.76142	YES	YES
231	a	1061.85	1.30290	YES	YES
232	a	1067.55	0.88694	YES	YES
233	a	1068.17	0.33954	YES	YES
234	a	1070.41	0.76889	YES	YES
235	a	1070.80	0.08876	YES	YES
236	a	1071.55	0.11408	YES	YES
237	a	1072.38	0.22405	YES	YES
238	a	1072.98	0.06977	YES	YES
239	a	1073.12	0.04174	YES	YES
240	a	1073.99	0.15535	YES	YES
241	a	1074.23	1.20739	YES	YES
242	a	1074.84	0.75711	YES	YES
243	a	1076.59	12.84528	YES	YES
244	a	1078.24	2.64804	YES	YES
245	a	1085.50	3.67302	YES	YES
246	a	1092.22	1.12004	YES	YES
247	a	1096.59	2.97533	YES	YES
248	a	1098.04	4.97540	YES	YES
249	a	1098.49	8.22835	YES	YES

250	a	1103.92	1.31469	YES	YES
251	a	1105.74	2.72433	YES	YES
252	a	1109.34	10.14496	YES	YES
253	a	1114.78	7.46541	YES	YES
254	a	1121.99	1.12009	YES	YES
255	a	1133.11	2.78814	YES	YES
256	a	1143.86	1.17627	YES	YES
257	a	1160.10	8.59767	YES	YES
258	a	1161.56	0.41004	YES	YES
259	a	1162.59	12.61558	YES	YES
260	a	1166.49	5.53334	YES	YES
261	a	1169.45	11.17065	YES	YES
262	a	1169.85	5.36257	YES	YES
263	a	1171.44	2.91275	YES	YES
264	a	1172.31	6.78709	YES	YES
265	a	1179.66	17.40290	YES	YES
266	a	1182.38	4.26589	YES	YES
267	a	1183.78	24.92495	YES	YES
268	a	1184.96	4.21602	YES	YES
269	a	1187.58	30.08364	YES	YES
270	a	1189.51	9.57147	YES	YES
271	a	1193.05	2.01925	YES	YES
272	a	1195.76	6.24742	YES	YES
273	a	1212.04	27.29383	YES	YES
274	a	1214.41	0.40356	YES	YES
275	a	1239.91	0.26748	YES	YES
276	a	1244.45	0.56449	YES	YES
277	a	1246.10	0.22048	YES	YES
278	a	1246.64	1.24899	YES	YES
279	a	1247.45	0.05759	YES	YES
280	a	1248.19	2.12825	YES	YES
281	a	1249.23	1.04182	YES	YES
282	a	1250.34	0.21646	YES	YES
283	a	1250.57	0.13098	YES	YES
284	a	1252.34	0.86782	YES	YES
285	a	1254.36	0.39630	YES	YES
286	a	1254.58	4.52278	YES	YES
287	a	1255.48	2.57403	YES	YES
288	a	1256.34	5.50154	YES	YES
289	a	1257.26	4.24174	YES	YES
290	a	1257.65	9.32334	YES	YES
291	a	1257.98	4.69496	YES	YES
292	a	1258.63	0.60311	YES	YES
293	a	1259.43	4.03013	YES	YES
294	a	1261.60	2.76131	YES	YES
295	a	1262.00	1.42113	YES	YES
296	a	1263.22	1.95522	YES	YES
297	a	1263.90	2.66236	YES	YES
298	a	1265.85	0.39989	YES	YES
299	a	1267.92	0.80235	YES	YES
300	a	1270.16	1.32660	YES	YES
301	a	1270.91	1.09582	YES	YES
302	a	1274.48	0.75234	YES	YES
303	a	1282.70	2.99275	YES	YES
304	a	1284.16	2.88335	YES	YES
305	a	1286.41	1.18337	YES	YES
306	a	1286.61	4.89244	YES	YES
307	a	1289.98	1.44949	YES	YES

308	a	1291.71	4.11444	YES	YES
309	a	1292.90	4.20056	YES	YES
310	a	1293.14	1.85763	YES	YES
311	a	1306.59	1.84392	YES	YES
312	a	1309.81	1.62694	YES	YES
313	a	1310.47	0.64313	YES	YES
314	a	1313.65	0.59199	YES	YES
315	a	1314.31	2.00242	YES	YES
316	a	1318.26	2.26184	YES	YES
317	a	1319.36	0.78765	YES	YES
318	a	1320.64	0.39255	YES	YES
319	a	1321.57	1.24088	YES	YES
320	a	1321.87	1.11372	YES	YES
321	a	1322.02	1.43232	YES	YES
322	a	1323.02	0.20209	YES	YES
323	a	1323.46	0.21312	YES	YES
324	a	1324.27	1.76412	YES	YES
325	a	1324.33	0.23298	YES	YES
326	a	1324.47	1.82159	YES	YES
327	a	1325.46	4.39448	YES	YES
328	a	1326.17	1.22064	YES	YES
329	a	1326.39	2.84235	YES	YES
330	a	1327.05	1.12887	YES	YES
331	a	1328.57	2.42088	YES	YES
332	a	1331.44	2.58788	YES	YES
333	a	1334.95	0.92079	YES	YES
334	a	1336.63	0.35751	YES	YES
335	a	1336.78	0.52518	YES	YES
336	a	1337.10	0.55801	YES	YES
337	a	1337.79	0.22472	YES	YES
338	a	1338.01	0.73009	YES	YES
339	a	1338.15	1.76674	YES	YES
340	a	1339.30	0.48951	YES	YES
341	a	1339.39	0.22203	YES	YES
342	a	1340.02	6.23453	YES	YES
343	a	1340.25	3.06934	YES	YES
344	a	1344.13	0.45248	YES	YES
345	a	1345.64	0.33672	YES	YES
346	a	1346.53	0.66198	YES	YES
347	a	1346.94	2.72938	YES	YES
348	a	1348.26	1.85989	YES	YES
349	a	1349.22	1.26239	YES	YES
350	a	1349.27	0.18212	YES	YES
351	a	1349.85	0.64817	YES	YES
352	a	1400.73	5.49041	YES	YES
353	a	1405.39	5.58853	YES	YES
354	a	1407.74	5.82291	YES	YES
355	a	1413.20	17.78197	YES	YES
356	a	1420.09	28.40459	YES	YES
357	a	1422.99	7.19985	YES	YES
358	a	1426.65	4.86412	YES	YES
359	a	1430.49	19.10681	YES	YES
360	a	1430.98	13.58918	YES	YES
361	a	1432.18	10.58459	YES	YES
362	a	1432.95	14.62039	YES	YES
363	a	1433.96	1.78167	YES	YES
364	a	1435.41	4.05958	YES	YES
365	a	1435.57	14.67225	YES	YES

366	a	1436.43	1.12739	YES	YES
367	a	1436.57	2.21689	YES	YES
368	a	1437.30	7.98711	YES	YES
369	a	1437.41	10.51015	YES	YES
370	a	1437.53	7.54880	YES	YES
371	a	1437.73	6.58893	YES	YES
372	a	1437.90	2.53109	YES	YES
373	a	1438.42	3.62741	YES	YES
374	a	1439.03	5.26232	YES	YES
375	a	1439.13	8.62817	YES	YES
376	a	1439.73	4.62035	YES	YES
377	a	1439.91	0.56079	YES	YES
378	a	1440.55	7.22506	YES	YES
379	a	1440.84	5.16944	YES	YES
380	a	1441.65	3.85368	YES	YES
381	a	1442.15	3.14436	YES	YES
382	a	1442.86	10.17495	YES	YES
383	a	1444.00	9.47328	YES	YES
384	a	1444.27	18.73414	YES	YES
385	a	1444.93	28.74590	YES	YES
386	a	1445.08	19.55036	YES	YES
387	a	1446.15	17.85016	YES	YES
388	a	1446.91	3.44667	YES	YES
389	a	1447.30	18.33421	YES	YES
390	a	1453.99	1.14354	YES	YES
391	a	1454.70	2.29350	YES	YES
392	a	1454.85	4.97332	YES	YES
393	a	1455.10	3.06451	YES	YES
394	a	1455.91	0.74649	YES	YES
395	a	1456.47	0.32023	YES	YES
396	a	1457.75	0.28124	YES	YES
397	a	1460.09	4.29257	YES	YES
398	a	1563.88	37.29682	YES	YES
399	a	1595.47	63.97794	YES	YES
400	a	2925.74	5.57821	YES	YES
401	a	2929.00	33.67914	YES	YES
402	a	2933.47	33.20744	YES	YES
403	a	2933.53	2.42486	YES	YES
404	a	2934.29	16.66830	YES	YES
405	a	2939.37	16.07112	YES	YES
406	a	2939.98	3.23828	YES	YES
407	a	2940.09	9.66993	YES	YES
408	a	2940.67	33.24031	YES	YES
409	a	2942.28	13.64033	YES	YES
410	a	2943.29	5.05478	YES	YES
411	a	2943.66	8.32814	YES	YES
412	a	2944.38	10.66563	YES	YES
413	a	2944.65	7.95621	YES	YES
414	a	2945.76	8.49341	YES	YES
415	a	2946.07	5.39048	YES	YES
416	a	2947.53	8.55238	YES	YES
417	a	2947.64	12.23615	YES	YES
418	a	2948.94	13.41793	YES	YES
419	a	2949.78	3.15012	YES	YES
420	a	2951.06	11.18948	YES	YES
421	a	2951.55	28.39032	YES	YES
422	a	2953.24	7.35574	YES	YES
423	a	2953.45	6.10926	YES	YES

424	a	2953.80	3.83293	YES	YES
425	a	2954.27	6.81839	YES	YES
426	a	2955.25	19.08781	YES	YES
427	a	2957.67	5.90087	YES	YES
428	a	2958.50	21.11542	YES	YES
429	a	2958.68	33.63360	YES	YES
430	a	2959.59	32.01845	YES	YES
431	a	2959.86	12.75555	YES	YES
432	a	2960.26	29.87773	YES	YES
433	a	2960.43	14.90320	YES	YES
434	a	2960.60	16.44578	YES	YES
435	a	2961.02	15.59923	YES	YES
436	a	2961.59	22.06054	YES	YES
437	a	2961.84	33.07961	YES	YES
438	a	2962.16	13.64120	YES	YES
439	a	2963.21	29.59381	YES	YES
440	a	2964.51	22.87108	YES	YES
441	a	2971.86	5.49005	YES	YES
442	a	2972.48	46.25842	YES	YES
443	a	2973.34	14.96234	YES	YES
444	a	2975.58	40.70541	YES	YES
445	a	2978.19	34.48623	YES	YES
446	a	2978.47	17.85120	YES	YES
447	a	2982.36	11.73001	YES	YES
448	a	2984.73	4.88299	YES	YES
449	a	2987.74	3.63022	YES	YES
450	a	2988.30	1.68454	YES	YES
451	a	2989.24	4.57922	YES	YES
452	a	2989.32	9.25278	YES	YES
453	a	2989.96	6.65594	YES	YES
454	a	2990.29	22.78032	YES	YES
455	a	2995.31	24.85344	YES	YES
456	a	2995.61	11.10194	YES	YES
457	a	3000.41	29.16850	YES	YES
458	a	3003.90	9.63478	YES	YES
459	a	3004.88	37.32459	YES	YES
460	a	3005.72	17.35579	YES	YES
461	a	3006.67	39.02924	YES	YES
462	a	3008.04	4.94330	YES	YES
463	a	3008.24	0.84640	YES	YES
464	a	3008.26	22.47389	YES	YES
465	a	3008.80	20.97811	YES	YES
466	a	3011.33	16.69363	YES	YES
467	a	3011.79	21.85593	YES	YES
468	a	3012.58	8.76612	YES	YES
469	a	3012.72	13.30177	YES	YES
470	a	3013.19	24.17639	YES	YES
471	a	3014.22	22.64913	YES	YES
472	a	3015.45	29.95619	YES	YES
473	a	3015.74	17.82379	YES	YES
474	a	3015.82	17.04889	YES	YES
475	a	3016.16	24.85390	YES	YES
476	a	3016.73	30.65125	YES	YES
477	a	3017.19	13.86589	YES	YES
478	a	3017.30	38.46557	YES	YES
479	a	3017.35	51.76945	YES	YES
480	a	3017.76	30.30393	YES	YES
481	a	3017.85	12.05389	YES	YES

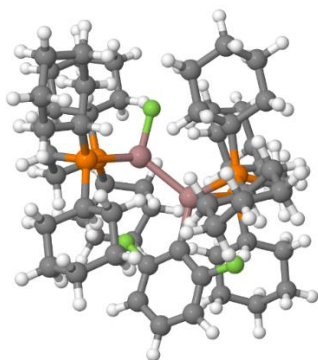
482	a	3017.85	27.96259	YES	YES
483	a	3018.37	17.28963	YES	YES
484	a	3018.86	18.67870	YES	YES
485	a	3019.18	28.46936	YES	YES
486	a	3021.35	17.77788	YES	YES
487	a	3022.79	10.34082	YES	YES
488	a	3026.49	17.81714	YES	YES
489	a	3028.75	22.19647	YES	YES
490	a	3030.14	0.85826	YES	YES
491	a	3031.89	3.40370	YES	YES
492	a	3034.88	2.14184	YES	YES
493	a	3038.77	8.58521	YES	YES
494	a	3041.31	0.90115	YES	YES
495	a	3049.49	0.01605	YES	YES
496	a	3128.30	0.70443	YES	YES
497	a	3139.72	0.08159	YES	YES
498	a	3146.35	0.50251	YES	YES

\$end

Double hybrid single point energy = -7778.618007731069 H

COSMO energy + OC correction = -7786.6514250075 H (in 3FB)

6.2.58 [F{Ga(dcpe)}₂(C₆F₂H₃)]²⁺ (*anti*-periplanar)



Method: (RI-)BP86(D3BJ)/def2-TZVPP

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	15.5057854	5.0189822	43.3936472
Ga	13.6247904	5.4753221	41.9146561
F	11.7767433	7.2987352	40.0144176
F	16.2198428	5.6628057	40.2203165
F	15.0792802	4.2328426	44.9940404
C	13.9866319	6.4634362	40.2147589
C	13.0580848	7.2402576	39.5236125
C	15.5956023	7.1014265	38.4534156
H	16.6024938	7.0169307	38.0499339
C	14.6147379	7.8760194	37.8277836
H	14.8550941	8.4188855	36.9153946
C	13.3257673	7.9511411	38.3600300
H	12.5430898	8.5388600	37.8846484
C	15.2431400	6.4289691	39.6148371
P	12.2614909	3.5732168	41.2599838
P	11.6503228	6.2521513	43.0602144
C	11.9987699	3.7707045	39.4475006

H	11.9133230	4.8656876	39.3406699
C	10.7421171	3.1532059	38.8179544
H	9.8358170	3.4768102	39.3494028
H	10.7805238	2.0566216	38.8877662
C	10.6587016	3.5696344	37.3410414
H	9.7728929	3.1121867	36.8803417
H	10.5139637	4.6612696	37.2854021
C	11.9252235	3.1811070	36.5696532
H	12.0036911	2.0821221	36.5299574
H	11.8523896	3.5240158	35.5289391
C	13.1859989	3.7527351	37.2275582
H	13.1743738	4.8536966	37.1681216
H	14.0859247	3.4170301	36.6938657
C	13.2747924	3.3419387	38.7010460
H	13.3873616	2.2483480	38.7744171
H	14.1646422	3.7895845	39.1687330
C	12.8089747	1.8731444	41.7011959
H	13.7163472	1.7113887	41.0995365
C	11.7872339	0.7784133	41.3431454
H	10.8392811	0.9689383	41.8709404
H	11.5644655	0.7991648	40.2691162
C	12.3172446	-0.6058579	41.7410136
H	11.5641391	-1.3673865	41.4979535
H	13.2068671	-0.8390455	41.1326497
C	12.6844472	-0.6627379	43.2255766
H	11.7753252	-0.5247882	43.8338765
H	13.0826075	-1.6535987	43.4817219
C	13.7028701	0.4239521	43.5791438
H	14.6479420	0.2199198	43.0488558
H	13.9360921	0.4075498	44.6526058
C	13.1983930	1.8187346	43.1902847
H	12.3205402	2.0595969	43.8121982
H	13.9558747	2.5816671	43.4234985
C	10.6465326	3.8073790	42.1193499
H	9.8611597	3.2727227	41.5692122
H	10.7381087	3.3209433	43.1002078
C	10.2872179	5.2856211	42.2810138
H	9.3699056	5.3993074	42.8745244
H	10.1043175	5.7555511	41.3049030
C	11.0520008	7.9971068	42.9776997
H	10.5999569	8.0333605	41.9723233
C	12.2023708	9.0136349	42.9929349
H	12.9234235	8.7580431	42.2051341
H	12.7360794	8.9580571	43.9545520
C	11.6737591	10.4367957	42.7798929
H	12.5063588	11.1519917	42.8396205
H	11.2643147	10.5155940	41.7595166
C	10.5841539	10.7927249	43.7958373
H	11.0205593	10.8179744	44.8083732
H	10.1968939	11.8011343	43.5987066
C	9.4429739	9.7718979	43.7611363
H	8.9397776	9.8137084	42.7813997
H	8.6820865	10.0160631	44.5147245
C	9.9589763	8.3464709	44.0036435
H	10.3735240	8.2834929	45.0208101
H	9.1283045	7.6288343	43.9501033
C	11.8599827	5.6138557	44.7803075
H	12.4284045	4.6761988	44.6310195

C	12.7705454	6.5501448	45.5978905
H	12.2722987	7.5224791	45.7306728
H	13.7057278	6.7435168	45.0468653
C	13.0801590	5.9380387	46.9681714
H	13.6916893	5.0363114	46.8155933
H	13.6865370	6.6429491	47.5535340
C	11.7987116	5.5815342	47.7272660
H	12.0486070	5.1124959	48.6883869
H	11.2404848	6.5021454	47.9654586
C	10.9071500	4.6499432	46.9010080
H	9.9784863	4.4219857	47.4414081
H	11.4264412	3.6899932	46.7435305
C	10.5680325	5.2685122	45.5380374
H	9.9661761	6.1755316	45.6888259
H	9.9489882	4.5717591	44.9544302
P	17.0268566	6.8391386	43.9419502
P	17.5381957	3.7794136	42.8804639
C	16.9417106	8.0242234	42.5320442
H	16.7577530	7.3636016	41.6682040
C	18.1978790	8.8489290	42.2166961
H	19.0681562	8.1948978	42.0641167
H	18.4407042	9.5108257	43.0606721
C	17.9543439	9.6901508	40.9547439
H	18.8451868	10.2948076	40.7381198
H	17.8154190	9.0128420	40.0954276
C	16.7193065	10.5853452	41.1002784
H	16.9003737	11.3288798	41.8937430
H	16.5531401	11.1532943	40.1750743
C	15.4716138	9.7660815	41.4465063
H	15.2169473	9.1050307	40.6027432
H	14.6088892	10.4286649	41.6012415
C	15.6999302	8.9127834	42.6982073
H	15.8328968	9.5700524	43.5722474
H	14.8195945	8.2861292	42.9052708
C	16.8240830	7.6642441	45.5716165
H	15.8090253	8.0971903	45.5305506
C	17.8350226	8.7929817	45.8388972
H	17.7684435	9.5632296	45.0592375
H	18.8575808	8.3841003	45.7993553
C	17.5914556	9.4215163	47.2182365
H	18.3455542	10.1987581	47.4018181
H	16.6128515	9.9295983	47.2125073
C	17.6140866	8.3711036	48.3320137
H	17.4050299	8.8429872	49.3012741
H	18.6255056	7.9385965	48.4075339
C	16.6031859	7.2546185	48.0564853
H	15.5830953	7.6723702	48.0812169
H	16.6456300	6.4867899	48.8409804
C	16.8429731	6.6015647	46.6898167
H	17.8295746	6.1093511	46.7059898
H	16.0981899	5.8191639	46.4881771
C	18.7100596	6.0888522	43.8917627
H	19.4650627	6.8804808	43.8006195
H	18.8803687	5.5894171	44.8546543
C	18.8257183	5.0911509	42.7303954
H	19.8239108	4.6346603	42.7091465
H	18.6773862	5.5904877	41.7633183
C	17.6674272	2.6362293	41.4328456

H	18.2258830	1.7624740	41.8102310
C	16.2520467	2.1808294	41.0398832
H	15.6700000	3.0721673	40.7517613
H	15.7489550	1.7424510	41.9127660
C	16.2836698	1.1889464	39.8752600
H	16.7778817	0.2594034	40.2008064
H	15.2568444	0.9102501	39.5944316
C	17.0307130	1.7765493	38.6748798
H	17.0718925	1.0463909	37.8557888
H	16.4750889	2.6496892	38.2927648
C	18.4464930	2.2088244	39.0702516
H	18.9682735	2.6524479	38.2115038
H	19.0297692	1.3217018	39.3656171
C	18.4312262	3.2144480	40.2303634
H	19.4608745	3.4685144	40.5168013
H	17.9460767	4.1428291	39.8961696
C	17.9530784	2.8253156	44.4029325
H	17.7321296	3.5195677	45.2324111
C	16.9957555	1.6281769	44.5467740
H	15.9574794	1.9836069	44.5318579
H	17.1317406	0.9447307	43.6926906
C	17.2782212	0.8640322	45.8453292
H	17.0382942	1.5150443	46.7015133
H	16.6073009	-0.0036717	45.9124053
C	18.7416545	0.4206847	45.9263254
H	18.9315540	-0.0952385	46.8769307
H	18.9469496	-0.3115753	45.1277724
C	19.6902627	1.6135487	45.7767765
H	20.7371830	1.2817377	45.7951471
H	19.5611639	2.2943174	46.6342985
C	19.4249069	2.3912416	44.4788996
H	19.6656670	1.7505861	43.6144069
H	20.0953654	3.2610844	44.4256711

SCF energy GEOOPT = -7786.509781137 H

ZPE = 3797. kJ/mol

FREEH energy = 3995.14 kJ/mol

FREEH entropy = 1.67563 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		-0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	9.24	0.01557	YES	YES
	8	a	14.04	0.03080	YES	YES
	9	a	21.84	0.02248	YES	YES
	10	a	27.67	0.16634	YES	YES
	11	a	30.72	0.08833	YES	YES
	12	a	33.11	0.04666	YES	YES
	13	a	35.86	0.06009	YES	YES
	14	a	37.05	0.10373	YES	YES
	15	a	39.39	0.02519	YES	YES
	16	a	42.28	0.10669	YES	YES

17	a	44.89	0.39769	YES	YES
18	a	46.01	0.38341	YES	YES
19	a	46.96	0.01385	YES	YES
20	a	52.72	0.14802	YES	YES
21	a	53.37	0.20648	YES	YES
22	a	54.33	0.15677	YES	YES
23	a	55.05	0.23465	YES	YES
24	a	57.71	0.07565	YES	YES
25	a	59.79	0.14960	YES	YES
26	a	63.58	0.20096	YES	YES
27	a	64.99	0.19218	YES	YES
28	a	67.89	0.14474	YES	YES
29	a	69.30	0.25632	YES	YES
30	a	70.25	0.05742	YES	YES
31	a	73.20	0.28569	YES	YES
32	a	76.05	0.27214	YES	YES
33	a	78.54	0.12813	YES	YES
34	a	78.81	0.09322	YES	YES
35	a	85.92	0.23394	YES	YES
36	a	88.40	0.80099	YES	YES
37	a	91.77	0.21903	YES	YES
38	a	101.91	0.48415	YES	YES
39	a	111.54	1.27066	YES	YES
40	a	116.82	0.52846	YES	YES
41	a	121.56	1.12152	YES	YES
42	a	122.47	0.54521	YES	YES
43	a	128.82	0.59950	YES	YES
44	a	133.11	13.87996	YES	YES
45	a	134.56	5.11095	YES	YES
46	a	137.81	1.64007	YES	YES
47	a	145.31	5.65376	YES	YES
48	a	154.87	1.32902	YES	YES
49	a	157.95	0.57647	YES	YES
50	a	160.63	4.49759	YES	YES
51	a	162.20	8.56338	YES	YES
52	a	167.76	8.80044	YES	YES
53	a	173.95	0.45053	YES	YES
54	a	184.24	6.98891	YES	YES
55	a	185.78	8.08973	YES	YES
56	a	189.57	12.70141	YES	YES
57	a	195.97	1.05063	YES	YES
58	a	199.28	5.36061	YES	YES
59	a	208.78	0.28946	YES	YES
60	a	210.98	0.03269	YES	YES
61	a	218.64	0.40917	YES	YES
62	a	220.47	1.57041	YES	YES
63	a	224.69	1.44848	YES	YES
64	a	229.05	0.55385	YES	YES
65	a	230.07	0.24039	YES	YES
66	a	231.68	0.27767	YES	YES
67	a	232.86	1.88275	YES	YES
68	a	233.25	1.68014	YES	YES
69	a	235.02	0.81896	YES	YES
70	a	239.35	0.76055	YES	YES
71	a	239.58	1.70147	YES	YES
72	a	241.75	5.75279	YES	YES
73	a	250.76	0.37811	YES	YES
74	a	253.27	1.05772	YES	YES

75	a	273.10	6.65503	YES	YES
76	a	276.91	1.67477	YES	YES
77	a	283.74	0.15350	YES	YES
78	a	284.64	0.56179	YES	YES
79	a	286.62	2.25824	YES	YES
80	a	306.93	1.09838	YES	YES
81	a	307.90	0.08588	YES	YES
82	a	309.19	0.05069	YES	YES
83	a	310.64	0.46828	YES	YES
84	a	312.83	0.04922	YES	YES
85	a	330.93	0.55180	YES	YES
86	a	332.95	0.48754	YES	YES
87	a	337.05	0.52338	YES	YES
88	a	338.68	0.19807	YES	YES
89	a	339.31	0.58611	YES	YES
90	a	342.45	1.73885	YES	YES
91	a	371.92	0.35346	YES	YES
92	a	377.49	0.72722	YES	YES
93	a	378.91	0.62532	YES	YES
94	a	381.66	0.31478	YES	YES
95	a	387.18	0.95163	YES	YES
96	a	387.41	1.00420	YES	YES
97	a	393.58	0.15983	YES	YES
98	a	405.16	0.19234	YES	YES
99	a	406.04	0.77436	YES	YES
100	a	419.16	1.47759	YES	YES
101	a	420.33	1.53074	YES	YES
102	a	425.84	0.55983	YES	YES
103	a	426.99	0.20211	YES	YES
104	a	430.16	0.07719	YES	YES
105	a	430.26	0.07117	YES	YES
106	a	430.88	0.09349	YES	YES
107	a	431.18	0.13924	YES	YES
108	a	432.65	0.45687	YES	YES
109	a	435.29	0.12582	YES	YES
110	a	444.28	5.50492	YES	YES
111	a	444.64	2.79026	YES	YES
112	a	452.99	2.82139	YES	YES
113	a	464.61	3.88557	YES	YES
114	a	465.42	3.77461	YES	YES
115	a	469.17	3.93706	YES	YES
116	a	487.67	1.93046	YES	YES
117	a	490.91	4.41730	YES	YES
118	a	493.17	1.26075	YES	YES
119	a	494.45	0.62275	YES	YES
120	a	498.09	0.56112	YES	YES
121	a	498.88	0.01750	YES	YES
122	a	501.69	0.24911	YES	YES
123	a	505.86	1.04946	YES	YES
124	a	510.91	5.46908	YES	YES
125	a	511.85	11.36103	YES	YES
126	a	534.22	3.87762	YES	YES
127	a	547.26	4.03587	YES	YES
128	a	550.71	45.96959	YES	YES
129	a	592.24	0.01953	YES	YES
130	a	633.18	15.49844	YES	YES
131	a	636.57	16.26724	YES	YES
132	a	656.62	7.98564	YES	YES

133	a	661.45	12.17719	YES	YES
134	a	692.60	3.87525	YES	YES
135	a	698.44	1.39576	YES	YES
136	a	711.27	5.16079	YES	YES
137	a	716.14	6.47936	YES	YES
138	a	718.40	9.33929	YES	YES
139	a	731.37	4.06743	YES	YES
140	a	740.87	2.04389	YES	YES
141	a	741.86	0.70526	YES	YES
142	a	742.18	12.78774	YES	YES
143	a	742.82	7.19765	YES	YES
144	a	769.31	0.39164	YES	YES
145	a	772.16	0.23581	YES	YES
146	a	772.53	0.05659	YES	YES
147	a	774.10	42.56109	YES	YES
148	a	774.20	8.61989	YES	YES
149	a	774.88	0.39751	YES	YES
150	a	775.10	0.13434	YES	YES
151	a	775.49	0.11917	YES	YES
152	a	779.95	0.03929	YES	YES
153	a	790.62	22.25337	YES	YES
154	a	795.64	20.42728	YES	YES
155	a	806.45	1.73298	YES	YES
156	a	807.47	0.58889	YES	YES
157	a	808.62	1.73390	YES	YES
158	a	809.60	2.82053	YES	YES
159	a	814.82	1.01032	YES	YES
160	a	815.69	2.74621	YES	YES
161	a	817.03	4.54684	YES	YES
162	a	819.00	1.89541	YES	YES
163	a	832.75	2.20322	YES	YES
164	a	834.00	1.23196	YES	YES
165	a	835.47	7.51128	YES	YES
166	a	835.90	3.78878	YES	YES
167	a	838.02	3.05924	YES	YES
168	a	838.92	2.69169	YES	YES
169	a	839.08	4.11694	YES	YES
170	a	840.95	5.89317	YES	YES
171	a	851.85	21.98235	YES	YES
172	a	854.03	10.59386	YES	YES
173	a	871.40	0.05759	YES	YES
174	a	873.90	7.26859	YES	YES
175	a	874.09	0.32752	YES	YES
176	a	875.47	0.39590	YES	YES
177	a	876.84	3.49387	YES	YES
178	a	877.16	7.92906	YES	YES
179	a	877.33	1.92709	YES	YES
180	a	878.08	4.86197	YES	YES
181	a	879.09	1.34760	YES	YES
182	a	879.67	0.20001	YES	YES
183	a	880.82	2.91227	YES	YES
184	a	882.03	1.02722	YES	YES
185	a	882.46	2.56860	YES	YES
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188	a	884.72	2.40099	YES	YES
189	a	887.18	5.93731	YES	YES
190	a	903.76	0.77767	YES	YES

191	a	904.52	1.19707	YES	YES
192	a	905.09	3.97126	YES	YES
193	a	905.59	1.00626	YES	YES
194	a	906.36	3.60810	YES	YES
195	a	907.47	2.35685	YES	YES
196	a	908.04	4.17447	YES	YES
197	a	909.07	0.32415	YES	YES
198	a	936.60	68.36896	YES	YES
199	a	961.09	0.44149	YES	YES
200	a	982.75	7.26946	YES	YES
201	a	984.92	12.45367	YES	YES
202	a	986.18	10.63621	YES	YES
203	a	986.64	2.18273	YES	YES
204	a	990.42	25.62856	YES	YES
205	a	991.39	4.45664	YES	YES
206	a	991.96	26.23018	YES	YES
207	a	992.65	1.51115	YES	YES
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212	a	1015.66	0.69878	YES	YES
213	a	1017.15	0.31017	YES	YES
214	a	1017.55	1.40634	YES	YES
215	a	1018.38	0.18830	YES	YES
216	a	1018.51	0.05476	YES	YES
217	a	1019.32	0.49787	YES	YES
218	a	1031.24	3.24090	YES	YES
219	a	1032.62	4.16107	YES	YES
220	a	1033.06	3.19775	YES	YES
221	a	1033.47	1.18347	YES	YES
222	a	1035.75	0.52067	YES	YES
223	a	1036.95	2.35966	YES	YES
224	a	1039.42	1.52300	YES	YES
225	a	1040.68	1.14660	YES	YES
226	a	1042.29	0.61824	YES	YES
227	a	1056.29	0.20710	YES	YES
228	a	1057.76	3.75477	YES	YES
229	a	1059.86	2.80631	YES	YES
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234	a	1065.36	0.46317	YES	YES
235	a	1068.72	0.03857	YES	YES
236	a	1069.98	0.96008	YES	YES
237	a	1071.17	0.08541	YES	YES
238	a	1071.32	0.22823	YES	YES
239	a	1071.98	0.79709	YES	YES
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241	a	1072.89	0.14127	YES	YES
242	a	1073.57	0.22106	YES	YES
243	a	1075.50	3.82224	YES	YES
244	a	1077.86	15.60667	YES	YES
245	a	1080.35	1.50084	YES	YES
246	a	1093.20	1.13353	YES	YES
247	a	1095.25	0.17439	YES	YES
248	a	1097.17	5.53721	YES	YES

249	a	1099.53	6.44824	YES	YES
250	a	1106.39	7.30056	YES	YES
251	a	1107.58	2.18306	YES	YES
252	a	1108.00	5.57717	YES	YES
253	a	1114.58	9.88900	YES	YES
254	a	1121.83	9.03774	YES	YES
255	a	1128.05	1.62960	YES	YES
256	a	1144.23	1.43763	YES	YES
257	a	1162.70	10.84384	YES	YES
258	a	1163.56	1.20114	YES	YES
259	a	1164.76	12.38511	YES	YES
260	a	1165.59	1.75217	YES	YES
261	a	1166.28	6.69971	YES	YES
262	a	1167.61	6.39939	YES	YES
263	a	1169.63	7.01082	YES	YES
264	a	1171.15	0.91131	YES	YES
265	a	1184.35	3.37712	YES	YES
266	a	1184.83	2.46930	YES	YES
267	a	1185.52	12.34603	YES	YES
268	a	1187.46	4.13929	YES	YES
269	a	1188.17	49.06763	YES	YES
270	a	1194.05	3.30459	YES	YES
271	a	1200.15	9.94630	YES	YES
272	a	1200.93	5.73332	YES	YES
273	a	1205.37	14.67637	YES	YES
274	a	1214.00	1.00700	YES	YES
275	a	1238.42	1.38901	YES	YES
276	a	1240.22	1.50167	YES	YES
277	a	1242.17	0.63881	YES	YES
278	a	1244.21	0.06987	YES	YES
279	a	1246.07	0.23584	YES	YES
280	a	1246.69	0.37160	YES	YES
281	a	1247.65	0.82412	YES	YES
282	a	1248.85	0.67034	YES	YES
283	a	1249.15	0.72375	YES	YES
284	a	1249.61	0.55513	YES	YES
285	a	1251.71	0.71342	YES	YES
286	a	1252.33	0.75313	YES	YES
287	a	1253.40	1.22120	YES	YES
288	a	1255.79	2.73287	YES	YES
289	a	1256.68	1.05722	YES	YES
290	a	1257.77	0.84500	YES	YES
291	a	1258.02	3.98914	YES	YES
292	a	1258.30	3.48267	YES	YES
293	a	1260.05	3.11094	YES	YES
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295	a	1262.25	0.32932	YES	YES
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297	a	1263.17	4.18023	YES	YES
298	a	1264.38	2.17156	YES	YES
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328	a	1325.02	0.62005	YES	YES
329	a	1325.50	0.77662	YES	YES
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335	a	1335.72	0.63345	YES	YES
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337	a	1337.02	0.28519	YES	YES
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341	a	1338.01	0.83155	YES	YES
342	a	1338.14	3.23808	YES	YES
343	a	1338.32	1.41712	YES	YES
344	a	1343.45	1.03538	YES	YES
345	a	1344.21	3.17429	YES	YES
346	a	1344.57	2.56899	YES	YES
347	a	1345.53	2.11278	YES	YES
348	a	1345.98	1.95878	YES	YES
349	a	1347.40	1.38788	YES	YES
350	a	1348.15	1.03737	YES	YES
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355	a	1412.18	19.52449	YES	YES
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357	a	1424.54	0.22894	YES	YES
358	a	1425.27	66.57910	YES	YES
359	a	1426.73	13.41111	YES	YES
360	a	1427.17	3.45751	YES	YES
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362	a	1430.98	5.73757	YES	YES
363	a	1434.09	1.21825	YES	YES
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366	a	1436.45	3.01188	YES	YES
367	a	1436.55	4.83010	YES	YES
368	a	1436.82	5.43684	YES	YES
369	a	1437.46	2.02185	YES	YES
370	a	1437.92	0.89715	YES	YES
371	a	1438.24	4.73980	YES	YES
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373	a	1438.70	5.28901	YES	YES
374	a	1439.13	3.91295	YES	YES
375	a	1439.17	8.69751	YES	YES
376	a	1439.29	0.37649	YES	YES
377	a	1439.55	1.45356	YES	YES
378	a	1440.31	6.48279	YES	YES
379	a	1440.66	10.44441	YES	YES
380	a	1440.89	7.01469	YES	YES
381	a	1441.22	10.41532	YES	YES
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384	a	1444.26	4.71950	YES	YES
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386	a	1445.75	16.20428	YES	YES
387	a	1446.17	11.39947	YES	YES
388	a	1446.34	21.40939	YES	YES
389	a	1448.71	2.32253	YES	YES
390	a	1453.36	1.22355	YES	YES
391	a	1454.67	2.04860	YES	YES
392	a	1454.81	0.82404	YES	YES
393	a	1455.43	1.88260	YES	YES
394	a	1456.48	1.27826	YES	YES
395	a	1457.30	2.92533	YES	YES
396	a	1457.44	1.75436	YES	YES
397	a	1458.04	3.12845	YES	YES
398	a	1561.20	34.17383	YES	YES
399	a	1594.18	68.34051	YES	YES
400	a	2912.30	2.87176	YES	YES
401	a	2934.23	2.92535	YES	YES
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403	a	2937.97	4.86179	YES	YES
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405	a	2940.97	9.54726	YES	YES
406	a	2942.10	8.41945	YES	YES
407	a	2942.91	9.21162	YES	YES
408	a	2943.91	8.00352	YES	YES
409	a	2944.35	12.39605	YES	YES
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413	a	2944.91	13.77158	YES	YES
414	a	2945.05	13.19068	YES	YES
415	a	2945.84	18.82588	YES	YES
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417	a	2949.33	0.64010	YES	YES
418	a	2949.62	8.97836	YES	YES
419	a	2949.92	20.80230	YES	YES
420	a	2950.38	11.77413	YES	YES
421	a	2951.25	7.34070	YES	YES
422	a	2953.29	4.73412	YES	YES

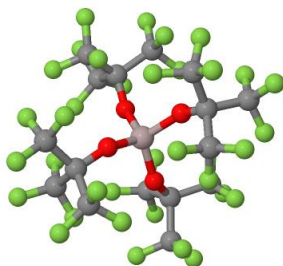
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427	a	2955.09	18.73540	YES	YES
428	a	2955.71	5.77251	YES	YES
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430	a	2957.21	12.51279	YES	YES
431	a	2957.91	12.84252	YES	YES
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441	a	2968.90	27.08825	YES	YES
442	a	2971.15	14.30650	YES	YES
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444	a	2971.73	15.72197	YES	YES
445	a	2973.45	5.48245	YES	YES
446	a	2978.21	10.73567	YES	YES
447	a	2985.30	7.20854	YES	YES
448	a	2986.70	1.52546	YES	YES
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451	a	2990.85	1.75902	YES	YES
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453	a	2993.37	3.50591	YES	YES
454	a	2994.33	44.27883	YES	YES
455	a	2995.00	29.09740	YES	YES
456	a	2996.43	24.36631	YES	YES
457	a	2998.63	23.19345	YES	YES
458	a	3004.04	28.68148	YES	YES
459	a	3008.06	3.15747	YES	YES
460	a	3008.94	21.12357	YES	YES
461	a	3008.99	25.26761	YES	YES
462	a	3010.08	12.31097	YES	YES
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467	a	3011.71	22.03986	YES	YES
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472	a	3014.34	12.11306	YES	YES
473	a	3014.58	27.93758	YES	YES
474	a	3015.51	25.78339	YES	YES
475	a	3015.98	24.98934	YES	YES
476	a	3016.24	35.54905	YES	YES
477	a	3016.43	21.17998	YES	YES
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479	a	3016.67	34.69873	YES	YES
480	a	3016.83	11.18488	YES	YES

481	a	3017.25	26.39423	YES	YES
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483	a	3017.96	17.38459	YES	YES
484	a	3019.07	23.06286	YES	YES
485	a	3019.27	27.03249	YES	YES
486	a	3019.46	12.43774	YES	YES
487	a	3020.00	36.64834	YES	YES
488	a	3022.44	49.66597	YES	YES
489	a	3024.95	2.78208	YES	YES
490	a	3025.18	20.73619	YES	YES
491	a	3027.38	23.34174	YES	YES
492	a	3031.58	0.78983	YES	YES
493	a	3035.62	0.85738	YES	YES
494	a	3039.98	0.30503	YES	YES
495	a	3043.54	0.61801	YES	YES
496	a	3128.92	0.62796	YES	YES
497	a	3140.09	0.03588	YES	YES
498	a	3146.65	0.92999	YES	YES

\$end

Double hybrid single point energy = -7778.632643750329 H
 COSMO energy + OC correction = -7786.6619437140 H (in 3FB)

6.2.59 [pf]⁻



Method: (RI-)BP86 (D3BJ) /def2-TZVPP
 Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.3538979	0.1565687	-0.1776142
O	-0.3651207	-1.4200661	-0.9385292
O	1.3077435	0.4931415	0.2588694
O	-0.9052459	1.4480779	-1.2199807
O	-1.4478824	0.0704481	1.1875528
C	2.4787280	0.0170572	0.7294964
F	2.1732888	-2.3863041	0.6888456
C	2.3003778	-1.3368540	1.5299149
C	-0.6357213	2.3208140	-2.2115072
F	-2.0370396	1.3641571	-3.9357280
C	-2.1495954	0.7597648	2.1105070
F	-3.1767061	0.3060471	4.2896849
C	-1.1056434	-2.4678983	-1.3529385
F	1.7605367	2.1181859	-2.4977573
C	0.5831901	1.8529584	-3.1058013
F	0.6080092	2.4605589	-4.3208766
F	0.5239198	0.5239350	-3.3124793
C	-1.9218542	2.4427852	-3.1258117
F	-1.9009519	3.5466442	-3.9192826
F	-3.0344141	2.5031530	-2.3733626
C	-0.3008540	3.7421243	-1.6010587

F	0.2672368	4.5807011	-2.5087016
F	-1.4215301	4.3470653	-1.1413137
F	0.5473965	3.6210674	-0.5662757
F	4.5447235	-0.9994677	-0.1127905
F	1.1875785	-1.2843179	2.2861813
F	3.3481326	-1.6018011	2.3539075
C	3.4801148	-0.2325445	-0.4706422
F	3.9706807	0.9375918	-0.9436404
F	2.8517575	-0.8487838	-1.4861130
F	2.9621223	2.3361913	1.1759681
C	3.0998280	1.1042342	1.6970569
F	2.4678063	1.0965163	2.8940521
F	4.4235227	0.9032641	1.9345091
F	-3.9163509	0.8314247	0.4759204
C	-3.3354219	1.5674902	1.4394931
F	-4.3013684	1.9151982	2.3330737
F	-2.8849524	2.7075209	0.8718573
F	-3.2036503	-2.9614390	-2.5230925
C	-2.2583411	-2.0049851	-2.3302931
F	-2.8745599	-0.9135603	-1.8369723
F	-1.7598515	-1.6780030	-3.5441855
F	-0.8243920	-4.3731859	-2.8710306
C	-0.1459671	-3.4604235	-2.1256851
F	0.6350325	-4.1466107	-1.2587251
F	0.6687284	-2.7835276	-2.9541291
F	-0.8815806	-3.3036117	0.8952258
C	-1.7533767	-3.2329801	-0.1258270
F	-2.8558728	-2.5905232	0.3183296
F	-2.1252826	-4.5038582	-0.4398313
F	-1.9249878	2.6962223	3.5997257
C	-2.7587589	-0.2803365	3.1361237
F	-1.8482589	-1.2148682	3.4606249
F	-3.8247346	-0.9195965	2.6001132
C	-1.2231397	1.7694483	2.8977182
F	-0.4206947	2.4282507	2.0387580
F	-0.4296921	1.1122640	3.7736550

SCF energy GEOOPT = -4750.100769695 H

ZPE = 556.1 kJ/mol

FREEH energy = 704.29 kJ/mol

FREEH entropy = 1.36309 kJ/mol/K

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
	1		-0.00	0.00000	-	-
	2		-0.00	0.00000	-	-
	3		-0.00	0.00000	-	-
	4		-0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	12.14	0.00088	YES	YES
	8	a	14.29	0.00166	YES	YES
	9	a	15.82	0.00035	YES	YES
	10	a	18.84	0.00147	YES	YES
	11	a	28.46	0.06613	YES	YES
	12	a	28.97	0.02162	YES	YES
	13	a	34.00	0.01822	YES	YES
	14	a	35.78	0.01486	YES	YES
	15	a	36.96	0.08264	YES	YES
	16	a	41.35	0.05066	YES	YES
	17	a	44.17	0.05300	YES	YES

18	a	55.79	0.00469	YES	YES
19	a	58.87	0.00450	YES	YES
20	a	67.30	0.11202	YES	YES
21	a	69.15	0.22878	YES	YES
22	a	71.34	0.16263	YES	YES
23	a	72.82	0.13599	YES	YES
24	a	74.95	0.00725	YES	YES
25	a	76.06	0.04382	YES	YES
26	a	76.33	0.08430	YES	YES
27	a	78.77	0.02043	YES	YES
28	a	79.34	0.03030	YES	YES
29	a	83.51	0.06965	YES	YES
30	a	84.65	0.03538	YES	YES
31	a	86.28	0.00412	YES	YES
32	a	88.48	0.05023	YES	YES
33	a	94.11	0.81131	YES	YES
34	a	95.20	0.63727	YES	YES
35	a	96.36	0.92782	YES	YES
36	a	110.00	0.00732	YES	YES
37	a	154.87	0.06074	YES	YES
38	a	155.27	0.07315	YES	YES
39	a	158.98	0.25295	YES	YES
40	a	159.68	0.01893	YES	YES
41	a	161.32	0.61641	YES	YES
42	a	161.86	0.62425	YES	YES
43	a	163.23	0.06244	YES	YES
44	a	164.35	0.70335	YES	YES
45	a	191.66	3.40987	YES	YES
46	a	193.21	2.74368	YES	YES
47	a	193.47	2.56120	YES	YES
48	a	215.42	0.00775	YES	YES
49	a	257.85	0.66938	YES	YES
50	a	258.32	0.59175	YES	YES
51	a	265.91	3.10218	YES	YES
52	a	267.02	0.01450	YES	YES
53	a	271.45	2.72323	YES	YES
54	a	271.69	2.71180	YES	YES
55	a	274.24	3.01085	YES	YES
56	a	275.82	0.02677	YES	YES
57	a	278.41	0.04230	YES	YES
58	a	278.67	0.03023	YES	YES
59	a	278.98	0.03524	YES	YES
60	a	279.30	0.01240	YES	YES
61	a	296.20	8.44749	YES	YES
62	a	296.83	7.21009	YES	YES
63	a	297.10	7.33376	YES	YES
64	a	302.12	0.00409	YES	YES
65	a	305.81	0.05641	YES	YES
66	a	306.09	0.05818	YES	YES
67	a	310.76	0.22834	YES	YES
68	a	311.77	0.02555	YES	YES
69	a	314.22	1.77185	YES	YES
70	a	314.44	1.78833	YES	YES
71	a	316.43	2.02678	YES	YES
72	a	319.06	0.10187	YES	YES
73	a	336.70	0.74181	YES	YES
74	a	336.89	0.86631	YES	YES
75	a	342.79	2.89438	YES	YES
76	a	349.85	8.37095	YES	YES
77	a	350.15	10.01561	YES	YES
78	a	351.47	2.32253	YES	YES
79	a	366.31	32.74171	YES	YES

80	a	377.70	0.25755	YES	YES
81	a	424.78	51.11989	YES	YES
82	a	435.92	60.82615	YES	YES
83	a	437.33	58.54028	YES	YES
84	a	504.36	0.05727	YES	YES
85	a	508.29	1.29690	YES	YES
86	a	508.46	3.10185	YES	YES
87	a	508.64	1.30362	YES	YES
88	a	509.12	1.07345	YES	YES
89	a	509.52	2.02030	YES	YES
90	a	509.85	4.82870	YES	YES
91	a	509.95	7.94918	YES	YES
92	a	510.17	7.26728	YES	YES
93	a	514.60	2.66144	YES	YES
94	a	515.31	1.94413	YES	YES
95	a	515.38	1.75398	YES	YES
96	a	518.41	0.01329	YES	YES
97	a	533.64	22.23075	YES	YES
98	a	539.02	20.82454	YES	YES
99	a	539.14	20.13014	YES	YES
100	a	543.22	0.15474	YES	YES
101	a	543.34	0.24194	YES	YES
102	a	543.60	0.23582	YES	YES
103	a	543.79	0.36454	YES	YES
104	a	544.63	0.45707	YES	YES
105	a	545.53	3.08530	YES	YES
106	a	547.11	13.52608	YES	YES
107	a	547.51	14.58518	YES	YES
108	a	694.41	1.51306	YES	YES
109	a	694.60	1.28448	YES	YES
110	a	695.16	0.28264	YES	YES
111	a	695.38	0.53084	YES	YES
112	a	696.19	9.41710	YES	YES
113	a	696.95	74.73584	YES	YES
114	a	697.29	73.94284	YES	YES
115	a	697.49	72.54285	YES	YES
116	a	711.64	0.00563	YES	YES
117	a	721.86	2.65177	YES	YES
118	a	723.22	4.59454	YES	YES
119	a	723.37	4.39762	YES	YES
120	a	760.70	0.02067	YES	YES
121	a	796.28	8.50174	YES	YES
122	a	805.97	16.93403	YES	YES
123	a	807.32	16.95684	YES	YES
124	a	924.57	15.70989	YES	YES
125	a	924.78	12.93731	YES	YES
126	a	928.60	4.89130	YES	YES
127	a	929.48	0.81151	YES	YES
128	a	932.47	246.83697	YES	YES
129	a	933.23	115.68420	YES	YES
130	a	935.71	322.19670	YES	YES
131	a	935.92	311.33576	YES	YES
132	a	1054.63	11.82460	YES	YES
133	a	1055.80	11.65854	YES	YES
134	a	1057.35	10.69399	YES	YES
135	a	1064.00	0.10254	YES	YES
136	a	1074.06	1.98165	YES	YES
137	a	1074.54	0.43994	YES	YES
138	a	1076.33	4.14625	YES	YES
139	a	1079.23	4.78011	YES	YES
140	a	1079.35	24.17992	YES	YES
141	a	1083.37	27.41318	YES	YES

142	a	1084.13	17.77077	YES	YES
143	a	1085.24	17.79678	YES	YES
144	a	1140.03	7.05863	YES	YES
145	a	1142.66	6.34285	YES	YES
146	a	1143.57	9.34849	YES	YES
147	a	1148.55	1.80739	YES	YES
148	a	1150.79	8.49246	YES	YES
149	a	1156.06	15.55514	YES	YES
150	a	1157.07	10.46109	YES	YES
151	a	1159.34	95.26427	YES	YES
152	a	1168.07	1279.96386	YES	YES
153	a	1168.29	1311.61166	YES	YES
154	a	1169.47	1193.81607	YES	YES
155	a	1182.24	1.80195	YES	YES
156	a	1183.46	90.36447	YES	YES
157	a	1185.04	31.52730	YES	YES
158	a	1186.04	65.71882	YES	YES
159	a	1187.64	97.98562	YES	YES
160	a	1188.29	166.07991	YES	YES
161	a	1190.44	63.67834	YES	YES
162	a	1200.16	130.54824	YES	YES
163	a	1202.35	122.59652	YES	YES
164	a	1207.59	980.05079	YES	YES
165	a	1209.64	912.69425	YES	YES
166	a	1210.71	750.25926	YES	YES
167	a	1217.14	14.11441	YES	YES
168	a	1295.98	250.06913	YES	YES
169	a	1296.76	276.44271	YES	YES
170	a	1298.92	289.83931	YES	YES
171	a	1324.06	2.10289	YES	YES

\$end

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