Electronic Supplementary Information to

How Long are Ga⇆Ga Double Bonds and Ga–Ga Single Bonds in Dicationic Gallium Dimers?

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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.

All solvents were stored under an atmosphere of argon or nitrogen in sealed vessels. THF, Et_2O, toluene and *n*-pentane were collected from a SPS, degassed and stored over activated molecular sieves. *Ortho*-difluorobenzene (*o*DFB) and fluorobenzene (PhF) were dried over CaH_2 for two days, distilled and degassed prior to use. The water content of the solvents was below 8 ppm, as determined by Carl Fischer titration.

Li[*pf*],[1] Ag[*pf*],[1,2] [Ga(PhF)$_2$][*pf*] and [In(PhF)$_2$][*pf*][3] ([*pf*]$^-$ = [Al(OR^F)$_4$]$^-$, R^F = C(CF$_3$)$_3$)[4] were prepared according to literature protocols. Note that the number of fluorobenzene molecules coordinated to Ga^+ can vary, depending on the vacuum applied when drying the product. Thus, the formula [M(PhF)$_2$][*pf*] (M Ga, In) 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.

Comment on the Absence of Elemental Analysis: Due to the employed perfluorinated alkoxyaluminate anion in the compounds described herein elemental analysis has proven difficult in the past. Even with air-stable crystalline compounds (*e.g.* [NR$_4$][*pf*], R = Et, Bu) the incomplete combustion of perfluorinated alkoxy groups does not lead to correct elemental analysis. The collected analytical data on [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5*o*DFB) are shown herein and imply high bulk purity of the obtained samples. However, the match of the simulated and experimental powder diffractogram of [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([**2**][*pf*]$_2$) is rather poor (section 4) and the NMR spectra reveal that protonated ligand [H–CDP^{Ph}]$^+$ forms reproducibly in various organic solvents (section 5.7). Thus, we cannot exclude that the formation of [**2**][*pf*]$_2$ is accompanied by side products, due to the high reactivity of this compound. The reactivity of this compound and potential decomposition pathways are discussed in detail in section 5.7. Nevertheless, it is likewise conceivable that the isolated crystals are phase pure and that mechanical stress on the crystals prior to powder X-ray analysis resulted in a structural transformation, especially when taking into account the very weak Ga⇆Ga double bond. The amount of protonated ligand increases over time (**Figure S 44**), suggesting that the complex decomposition may only take place in solution.

1.1 Single Crystal X-Ray Diffraction

Crystals were obtained from *ortho*-difluorobenzene at –25 °C (for [**2**][*pf*]$_2$ and [In(CDP^{Ph})][*pf*]) or by layering a concentrated solution of the compounds in *o*DFB with *n*-pentane ([**1**][*pf*]$_2$ · 1.5*o*DFB). Single crystal X-ray diffraction data for these compounds were collected from a shock-cooled single crystal at 100(2) K on a Bruker *D8 VENTURE* dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using 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.[5] Data were collected at 100 K using monochromated Mo K_α radiation (λ = 0.71073 Å).

All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.[6] The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL-2018/3[7] employing shelXle.[8] 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.[9] Graphical representations were prepared using Olex2-1.3.[10]

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[11] CCDC 2220000, 2220001 and 2220002 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.[12]

1.2 Powder Diffraction

The sample was triturated and then sealed with perfluoropolyalkylether oil (*AB128330, abcr* GmbH & Co. KG) in a 0.3 mm thick capillary (*Hilgenberg* GmbH, wall thickness 0.01 mm). The powder diffractogram was measured on a *STOE STADI P* powder diffractogram with a Ge(111) monochromator and a *Dectris MYTHEN 1K* detector at 100 K in the 2θ range 2-40°. Molybdenum Kα_1 radiation (λ = 0.709300 Å) was used. For data acquiring, processing and for spectrum simulation from the single crystal structure the software package *WinXPow* was employed.

1.3 NMR Spectroscopy

^{1}H-, ^{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 spectrometers from *Bruker*. NMR spectra were analyzed using *Bruker TopSpin 3.2.* ^{1}H NMR chemical shifts are given with respect to tetramethylsilane (TMS). All ^{1}H NMR spectra were calibrated using the solvent signal. The chemical shifts of standard solvents were taken from literature[13] and the shift of *o*DFB and PhF were determined experimentally by adding TMS to the aromatic solvent. The most intensive signal of the downfield multiplet of *o*DFB and PhF appears at 6.96 ppm and 6.9 ppm, respectively, when the signal of TMS is at 0.00 ppm (**Figure S 1** and **Figure S 2**).

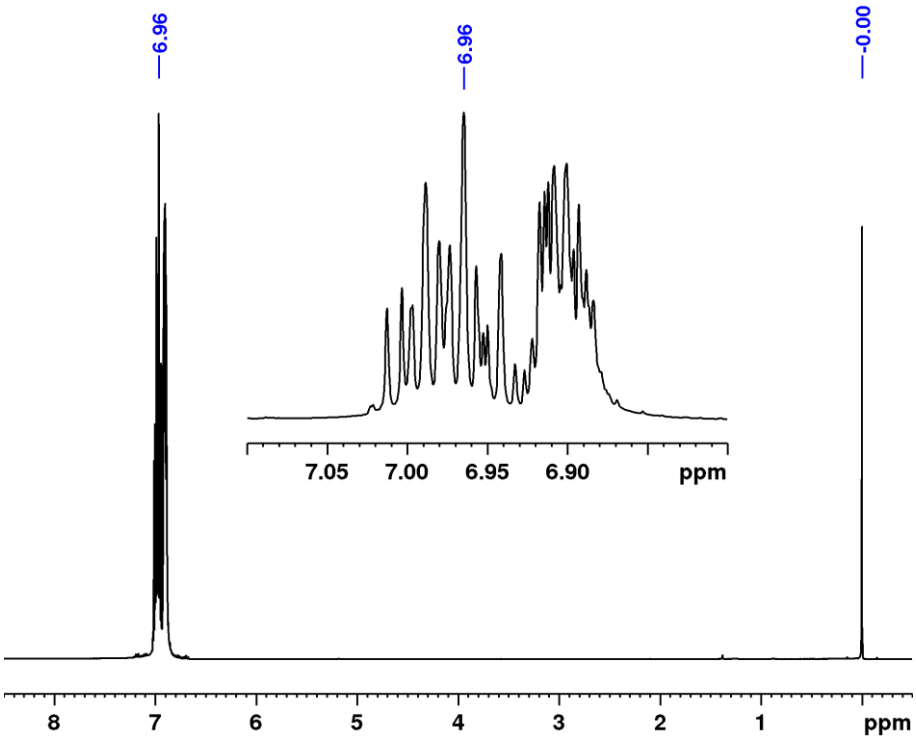


Figure S 1: ^{1}H NMR spectrum (400.17 MHz, *o*DFB, 298 K) of TMS in *o*DFB.

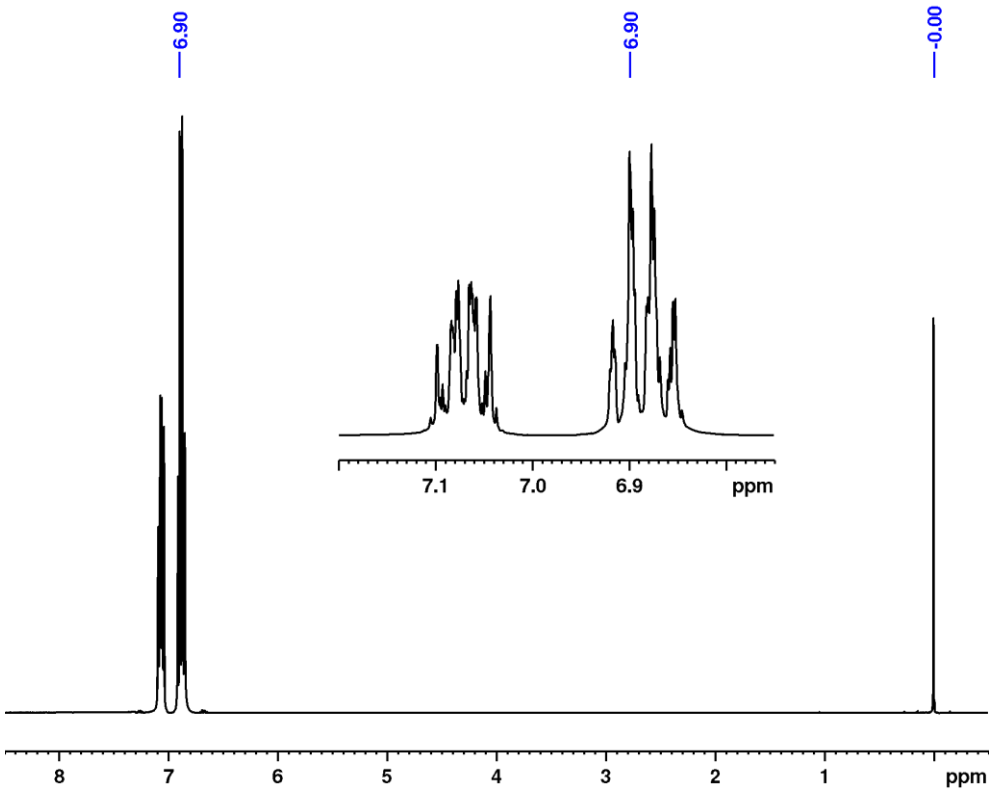


Figure S 2: ^{1}H NMR spectrum (400.17 MHz, PhF, 298 K) of TMS in PhF.

Heteronuclear spectra were calibrated according to the IUPAC χ-table.[14] Unless otherwise stated, the ^{19}F and ^{27}Al NMR spectra show signals at ca. –75 ppm and 35 ppm, respectively, indicating the presence of non-decomposed $[Al(OR^F)_4]^-$ anion. The broad resonance between 50 and 100 ppm in the ^{27}Al NMR spectra is caused by the probe head. For all reaction mixtures presented herein, ^{1}H, ^{13}C, ^{19}F, ^{27}Al, ^{31}P (for [**2**][*pf*]$_2$), ^{71}Ga and 2D correlated spectra, *e.g.* ^{1}H,^{13}C HSQC, ^{1}H,^{13}C HMBC or ^{1}H,^{31}P HMBC (for [**2**][*pf*]$_2$), were recorded.

1.4 IR and Raman 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 employed. 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 %.

Raman spectra were recorded on a Bruker Vertex 70 IR spectrometer equipped with a *Bruker RAM II FT* Raman module at rt in the range of 4000–50 cm^{-1} with a resolution of 4 cm^{-1}. For data processing, the software *OPUS 7.5* (Bruker Optic GmbH) was employed. All spectra were base line corrected (5 cycles). By setting the most intense peak to 100 %, the other Raman 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 %.

1.5 Mass Spectrometry

The mass spectrometric experiments were performed with a Thermo-Fischer LTQ XL linear ion-trap mass spectrometer equipped with an electrospray ionization (ESI) source. Mass spectra were obtained by electrospray ionization from millimolar solutions in oDFB. The solutions were cooled to ca. −30 °C. In order to avoid decomposition, the so-called "pressurized sample infusion" technique described by McIndoe and co-workers was employed.[15] Therefore, the solution was cooled to −30 °C, prior to injection into the ESI source. Instead of PEEK tubing, a very thin and short silica capillary was used. The capillary temperature was adjusted to 60 °C. Nitrogen was used as a sheath, sweep, and auxiliary gas. Data were processed with the *Thermo XCalibur* software.

1.6 Quantum Chemical Calculations

Unless stated otherwise, quantum chemical calculations were performed with *Turbomole* (version 7.2 or 7.5).[16,17] Structures were optimized using density functional theory (DFT),[16] internal coordinates, resolution of identity-approximation (RI),[18,19] D3(BJ)-dispersion correction[20] and a fine integration gridsize (gridsize = m5). Calculations were performed on the RI-BP86[21](D3BJ)/def2-TZVPP[22], RI-BP86(D3BJ)/def2-SVP[18,22] or RI-PBEh-3c(D3BJ)/def2-mSVP[23] level of theory. For species containing indium atoms, an effective core potential (ECP), *i.e*. def2-ECP,[22] was employed. 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.[24] 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 und 10^{-5} a.u., respectively. The coordinates of the herein investigated compounds are listed in section 8.5–8.16.

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

$$H° = E_{SCF} + E_{vrt} + R \cdot T \quad (1)$$

E_{SCF}: electronic SCF energy

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

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

T: temperature in Kelvin (298.15 K)

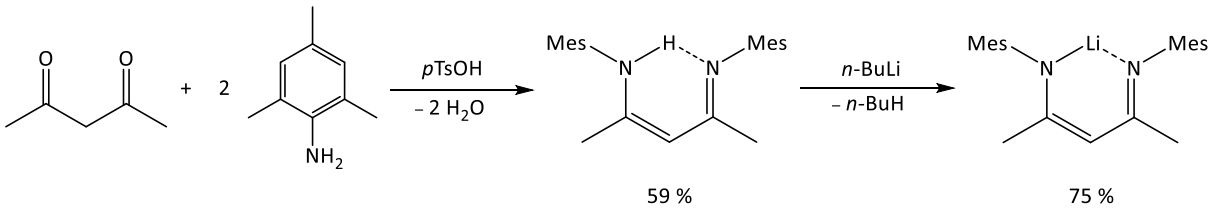
The Gibbs free energy $G°$ follows from the standard enthalpy $H°$ and the standard entropy $S°$:

$$G° = H° - S° \cdot T \quad (2)$$

Solvation effects were incorporated using the conductor like screening model (COSMO)[25] for *o*DFB as the solvent. A dielectric constant of 13.38 D at 298 K was assumed for this solvent.[26] 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.

2 Syntheses

2.1 Lithium β-Diketiminate (LiNacNac^{Mes})

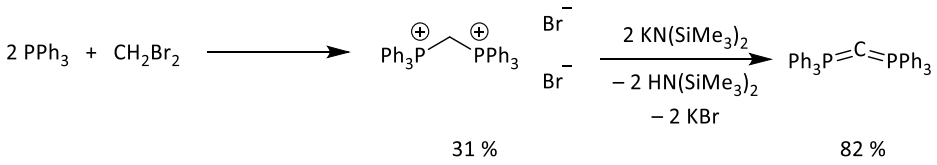


Scheme S 1: Synthesis of LiNacNac^{Mes} *via* HNacNac^{Mes}. Only the enamine form of protonated HNacNac^{Mes} is shown since this is the predominant tautomer in solution.

^{Mes}NacNacLi was synthesized according to literature procedure[27] in two step synthesis. *p*-Toluenesulfonic acid monohydrate (11.4 g, 59.8 mmol, 1.0 eq.) was suspended in toluene (180 mL). Pentane-2,4-dione (6.10 mL, 5.95 g, 59.4 mmol, 1.0 eq.) and 2,4,6-trimethylaniline (17.0 mL, 16.4 g, 121 mmol, 2.0 eq.) were added. The reaction mixture was heated at reflux for 3 h. Water (ca. 2.5 mL) formed in the reaction was removed with a Dean-Stark apparatus. The following purification was carried out in air. The suspension was filtrated, and the solid residue was dried. The crude product was dissolved in dichloromethane (180 mL). The solution was stirred with saturated, aqueous Na_2CO_3 solution (79.0 mL, 7.56 g, 90.0 mmol, 1.5 eq.) for 2 h. The organic phase was separated, dried over $MgSO_4$ and then concentrated to an orange oil under reduced pressure. After adding methanol (100 mL), the solution was stored at −40 °C overnight. The solid was filtrated and washed with cold methanol (100 mL). Removal of the volatiles *in vacuo* (1×10^{-3} mbar) afforded HNacNac^{Mes} (11.6 g, 34.8 mmol, 59 %) as a light-yellow powder.

HNacNac^{Mes} (2,90 g, 8.67 mmol, 1.0 eq.) was suspended in *n*-hexane. A solution of *n*-butyllithium in *n*-hexane (6.0 mL, 1.6 M, 9.6 mmol, 1.1 eq.) was added dropwise at −20 °C. The reaction mixture was slowly warmed to room rt, stirred for 15 h and stored at −40 °C overnight, yielding a yellow solution with a colourless precipitate. The solid was filtrated, washed with *n*-hexane (3×4 mL) and removal of the volatiles *in vacuo* (1×10^{-3} mbar) afforded LiNacNac^{Mes} as a light-yellow powder. The remaining filtrate was concentrated in vacuo to 10 mL and stored at −40 °C again. Filtration and removal of the volatiles *in vacuo* (1×10^{-3} mbar) yielded a second batch of the product (total: 2.21 g, 6.49 mmol, 75 %).

2.2 Hexaphenylcarbodiphosphorane (CDP^{Ph})

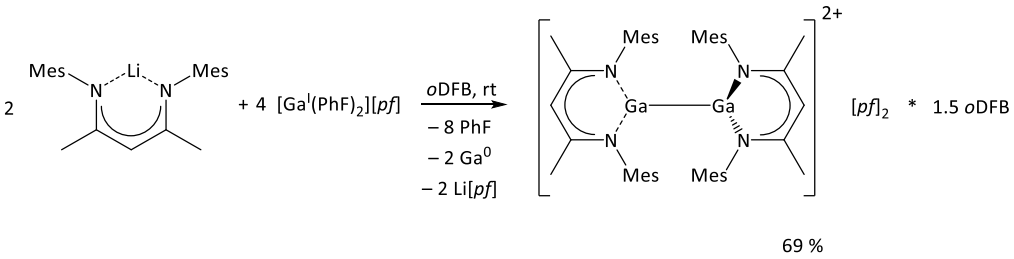


Scheme S 2: Synthesis of CDP^{Ph} *via* the respective *bis*phosphonium bromide.

The *bis*phosphonium bromide was synthesized according to a modified literature procedure.[28] Methylene bromide (2.10 ml, 5.22 g, 30.0 mmol, 1.0 eq.) was added to a stirred solution of triphenylphosphine (15.8 g, 60.4 mmol, 2.0 eq.) in molten triphenylphosphate (13.0 g, 40 mmol) at 90 °C. The mixture was heated for 24 h at 110 °C and then for further 6 h at 150°C. After the reaction mixture was allowed to cool down to 100°C, benzene (200 ml) was added and the yellow suspension was refluxed for additional 1 h at 100 °C. The following purification was carried out in air. The suspension was then filtered, the solid residue was washed with benzene (40 ml) and volatiles were removed *in vacuo*. The product was purified by precipitating it twice from hot methanol (100 ml) by adding EtOAc (900 ml). Drying the obtained solid at 100 °C *in vacuo* for ca. 8 h afforded bisphosphonium salt $[Ph_3P–CH_2–PPh_3]Br_2$ as a hygroscopic white powder (6.51 g, 9.32 mmol, 31 %).

Hexaphenylcarbodiphosphorane was synthesized according to a modified literature procedure.[29] Bisphosphonium salt $[Ph_3P–CH_2–PPh_3]Br_2$ (4.03 g, 5.77 mmol, 1.0 eq.) and KHMDS (2.74 g, 13.7 mmol, 2.4 eq.) were suspended in THF (ca. 60 ml). The reaction solution immediately turned yellow and was stirred for 3 h at rt. The suspension was allowed to cool down to rt, filtered under argon and the solvent removed *in vacuo*. Purification was achieved by washing the crude reaction product with Et_2O (3×8 ml) and pentane (3×20 ml). The residue was filtered and dried *in vacuo* to obtain hexaphenylcarbodiphosphorane $Ph_3P=C=PPh_3$ (2.53 g, 4.71 mmol, 82 %) as a bright yellow, moisture sensitive powder.

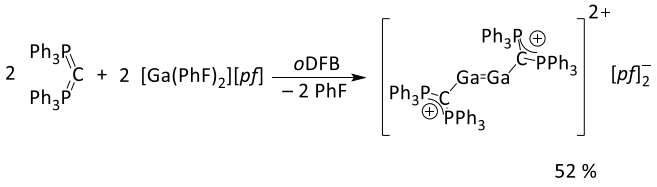
2.3 [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([1][*pf*]$_2$ · 1.5*o*DFB)



Scheme S 3: Synthesis of [**1**][*pf*]$_2$ · 1.5*o*DFB starting from [Ga(PhF)$_x$][*pf*] and LiNacNac^{Mes}.

[Ga(PhF)$_x$][*pf*] (150 mg, 124 µmol (for x = 1.8), 2.0 eq.) and LiNacNac^{Mes} (21.1 mg, 62.0 µmol, 1.0 eq.) were dissolved in *o*DFB (1.1 mL) at rt, yielding a dark solution with a black precipitate. After filtration, a yellow solution was obtained. Layering the solution with *n*-pentane and removal of the volatiles *in vacuo* afforded yellow crystals of [{Ga^{II}(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5oDFB; 62.6 mg, 21.5 µmol, 69 %).

2.4 [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([2][*pf*]$_2$)



Scheme S 4: Synthesis of [**2**][*pf*]$_2$ starting from [Ga(PhF)$_2$][*pf*] and CDP^{Ph}.

In a typical crystallization attempt, [Ga(PhF)$_x$][*pf*] (200 mg, 177 µmol (for x = 1.0), 1.0 eq.) and CDP^{Ph} (104 mg, 194 µmol, 1.1 eq.) were mixed in *o*DFB (1.7 ml) at rt. The solution was concentrated under reduced pressure and then stored at –25°C. After one week, orange-brown crystals were obtained and the solvent was filtered off. Drying the crystals *in vacuo* afforded [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ as a highly air and moisture sensitive brown solid ([**2**][*pf*]$_2$; 146 mg, 46.4 µmol, 52 % (under the simplifying assumption that no [(CDP^{Ph})H][*pf*] is present in the solid)].

2.5 [In(CDP^{Ph})][*pf*]

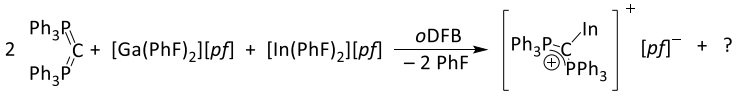


Figure S 3: Synthesis of [In(CDP^{Ph})][*pf*] starting from [In(PhF)$_2$][*pf*], [Ga(PhF)$_2$][*pf*] and CDP^{Ph}.

[In(PhF)$_x$][*pf*] (46.0 mg, 36.0 µmol (x = 2.5), 1.1 eq.), [Ga(PhF)$_x$][*pf*] (38.0 mg, 33.6 µmol (x = 1.0), 1.0 eq.) and CDP^{Ph} (36.0 mg, 67.1 µmol, 2.0 eq.) were dissolved in *o*DFB (0.8 ml) and stirred overnight. A metallic precipitate was observed and light grey crystals were obtained from the brown solution. The yield could not be determined, since most of the crystals were used for the scXRD and Raman measurements. The synthesis could not be reproduced and mixing [In(PhF)$_x$][*pf*] and CDP^{Ph}, even at −40 °C, merely led to precipitation of elemental indium.

3 Crystal Structures

Table S 1: Crystal data and summary of the data collection and refinement for [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5*o*DFB), [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([**2**][*pf*]$_2$) and [In(CDP^{Ph})][*pf*].

CCDC	2220000	2220001	2220002
Empirical formula	$C_{174}H_{128}Al_4F_{150}Ga_4N_8O_{16}$	$C_{106}H_{60}Al_2F_{72}Ga_2O_8P_4$	$C_{53}H_{30}AlF_{36}InO_4P_2$
Formula weight	5823.65	3146.82	1618.51
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	triclinic
Space group (number)	$P\bar{1}$ (2)	$P2_1/c$ (14)	$P\bar{1}$ (2)
a [Å]	18.321(8)	15.9476(12)	11.504(6)
b [Å]	19.089(9)	11.0312(8)	15.151(5)
c [Å]	30.659(14)	33.773(3)	17.514(7)
α [Å]	88.15(2)	90	84.274(8)
β [Å]	87.32(3)	102.211(2)	79.771(12)
γ [Å]	88.370(13)	90	84.889(14)
Volume [Å^3]	10701(9)	5807.0(7)	2981(2)
Z	2	2	2
ρ_{calc} [g/cm^3]	1.807	1.800	1.803
μ [mm^{-1}]	0.706	0.707	0.623
F(000)	5764	3112	1592
Crystal size [mm^3]	0.491×0.386×0.216	0.36×0.28×0.21	0.26×0.22×0.08
Crystal colour	yellow	orange	colourless
Crystal shape	block	block	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.55 to 63.17 (0.68 Å)	2.61 to 61.11 (0.70 Å)	2.71 to 62.11 (0.69 Å)
Index ranges	−26 ≤ h ≤ 26 −28 ≤ k ≤ 28 −45 ≤ l ≤ 45	−22 ≤ h ≤ 22 −15 ≤ k ≤ 15 −48 ≤ l ≤ 48	−16 ≤ h ≤ 16 −21 ≤ k ≤ 21 −25 ≤ l ≤ 25
Reflections collected	347634	348234	168242
Independent reflections	71603 R_{int} = 0.0355 R_{sigma} = 0.0331	17782 R_{int} = 0.0279 R_{sigma} = 0.0097	19043 R_{int} = 0.0562 R_{sigma} = 0.0291
Completeness to θ = 25.242°	100.0 %	100.0 %	99.7 %
Data / Restraints / Parameters	71603/124253/4964	17782/4516/1001	19043/4540/1001
Goodness-of-fit on F^2	1.031	1.042	1.022
Final *R* indexes [I ≥ 2σ(I)]	R_1 = 0.0501 wR_2 = 0.1310	R_1 = 0.0281 wR_2 = 0.0746	R_1 = 0.0442 wR_2 = 0.1296
Final *R* indexes [all data]	R_1 = 0.0714 wR_2 = 0.1461	R_1 = 0.0292 wR_2 = 0.0754	R_1 = 0.0559 wR_2 = 0.1388
Largest peak/hole [eÅ^3]	1.14/-0.67	0.70/-0.41	0.70/-2.47

3.1 [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([1][*pf*]$_2$ · 1.5*o*DFB)

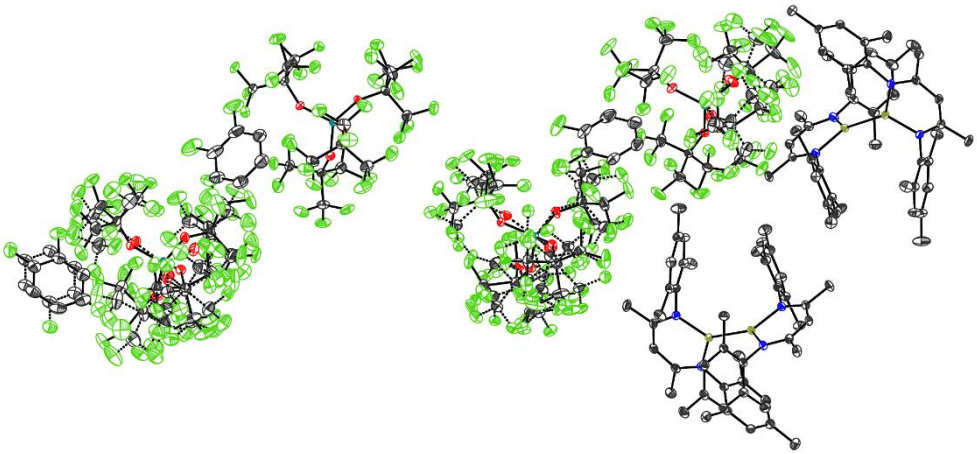


Figure S 4: Molecular structure of [**1**][*pf*]$_2$ · 1.5*o*DFB in the solid state from scXRD. Hydrogen atoms are omitted for clarity, the disorder in the [*pf*]$^-$ anions is shown. Thermal ellipsoids are set at 50 % probability level.

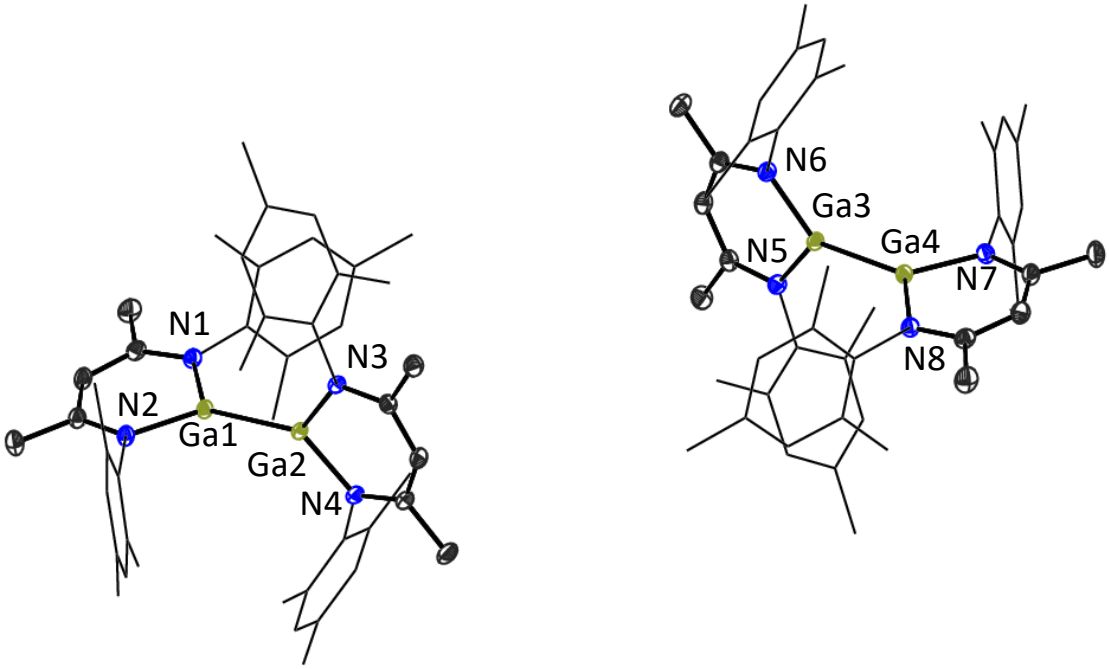


Figure S 5: Molecular structure of the two crystallographically independent **1**$^{2+}$ units in [**1**][*pf*]$_2$ · 1.5*o*DFB. The NacNac–Ga–Ga–NacNac-backbone is highlighted and the mesityl groups are shown as a wireframe model. Hydrogen atoms and anions are omitted for clarity. Thermal ellipsoids are set at 50 % probability level.

Table S 2: Selected bond lengths in [**1**][*pf*]$_2$ · 1.5*o*DFB.

Atom–Atom	Bond Length [pm]
Ga1–N1	184.70(17)
Ga1–N2	184.56(16)
Ga1–Ga2	238.11(9)
Ga2–N3	184.61(18)
Ga2–N4	184.91(17)
Ga3–N5	184.56(18)
Ga3–N6	184.65(17)
Ga3–Ga4	238.32(9)
Ga4–N7	184.65(17)
Ga4–N8	184.80(18)

Table S 3: Selected bond angles in [**1**][*pf*]$_2$ · 1.5*o*DFB.

Atom–Atom–Atom	Angle [°]
N2–Ga1–N1	102.01(7)
N2–Ga1–Ga2	130.68(5)
N1–Ga1–Ga2	127.31(5)
N3–Ga2–N4	102.09(7)
N3–Ga2–Ga1	126.72(5)
N4–Ga2–Ga1	131.19(6)
N5–Ga3–N6	101.87(7)
N5–Ga3–Ga4	125.87(5)
N6–Ga3–Ga4	132.26(5)
N7–Ga4–N8	102.08(7)
N7–Ga4–Ga3	128.28(6)
N8–Ga4–Ga3	129.63(5)

The average angle sum around the Ga atoms is 360.00(7)°; thus, the Ga atoms are coordinated in a trigonal planar fashion by the bidentate [NacNac^{Mes}]$^-$ ligands and the adjacent Ga atom. The dihedral angle between the least-square planes is 83.55(6)° and 85.75(6)°, respectively, for the two independent [(GaNacNac)$_2$] units.

3.2 [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([2][*pf*]$_2$)

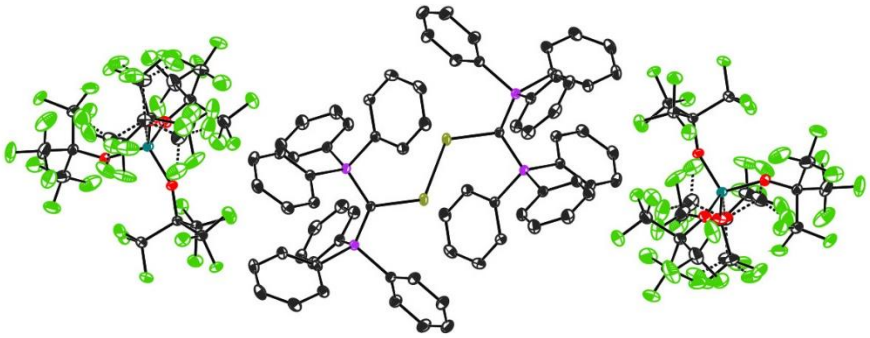


Figure S 6: Molecular structure of [**2**][*pf*]$_2$ in the solid state from scXRD. Hydrogen atoms are omitted for clarity, the disorder in the [*pf*]$^-$ anions is shown. Thermal ellipsoids are set at 50 % probability level.

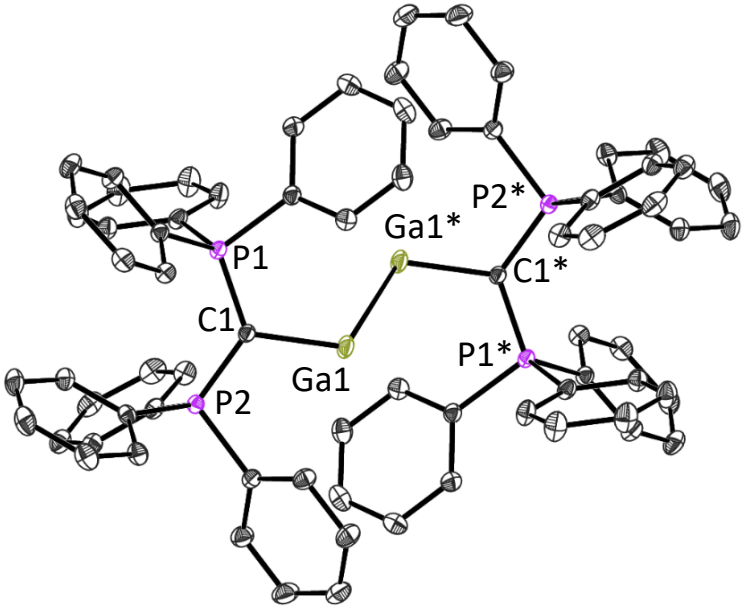


Figure S 7: Molecular structure of **2**$^{2+}$ in the *pf* salt. Hydrogen atoms and anions are omitted for clarity. Thermal ellipsoids are set at 50 % probability level. The asterisks denote symmetry-generated atoms.

Table S 4: Selected bond lengths in [**2**][*pf*]$_2$.

Atom–Atom	Bond Length [pm]
Ga1–Ga1*	269.01(3)
Ga1–C1	200.52(9)
P1–C1	171.27(10)
P2–C1	171.19(10)

Table S 5: Selected bond and dihedral angles in [**2**][*pf*]$_2$.

Atom–Atom–Atom(–Atom)	Angle [°]
C1–Ga1–Ga1*	118.18(3)
P2–C1–P1	125.24(6)
P2–C1–Ga1	114.53(5)
P1–C1–Ga1	116.49(5)
C1–Ga1–Ga1*–C1*	180.00(14)

The P–C^{CDP}–P angle is reduced to 125.24(6)°, compared to 130.1(6)°–180° in free CDP^{Ph}.[30–32] The average C^{CDP}–P distance is approximately 171.2 pm and is thus considerably longer than in free CDP^{Ph} (159.8–164.2 pm),[30,32] reflecting the reduced P–C^{CDP} double bond character in $\mathbf{2}^{2+}$ compared to the free ligand.

3.3 [In(CDP^{Ph})][*pf*]

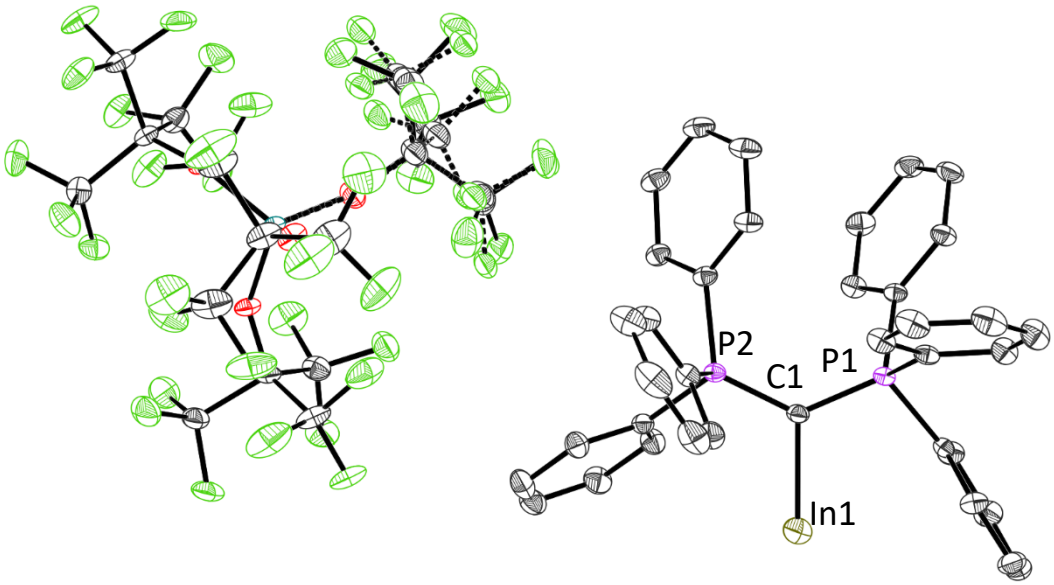


Figure S 8: Molecular structure of [In(CDP^{Ph})]$^{+}$ in the *pf* salt. Hydrogen atoms are omitted for clarity, the disorder in the [*pf*]$^{-}$ anions is shown. Thermal ellipsoids are set at 50 % probability level.

Table S 6: Selected bond lengths in [In(CDP^{Ph})][*pf*].

Atom–Atom	Bond Length [pm]
In1–C1	225.6(2)
P1–C1	169.1(2)
P2–C1	181.5(2)

Table S 7: Selected bond angles in [In(CDP^{Ph})][*pf*].

Atom–Atom–Atom	Angle [°]
P1–C1–P2	129.13(12)
P1–C1–In1	112.17(10)
P2–C1–In1	118.36(10)

The angle sum around C1 (or C^{CDP}) is 359.64(12)°. Thus, the central C^{CDP} atom is coordinated in a trigonal planar fashion.

In principle, it is conceivable the metal atom is a silver instead of an indium cation, since [In(PhF)$_2$][*pf*] is synthesized from Ag[*pf*].[3] In fact, the electron density at the metal center is slightly better described by a silver atom than by an indium atom (R_1 = 0.0381; wR_2 = 0.1103 for M = Ag instead of R_1 = 0.0442; wR_2 = 0.1296 for M = In).

However, a Ag–CDP complex without significant cation-anion or cation-solvent interaction has already been described in literature: The Ag–C^{CDP} bond lengths in [Ag(CDP^{Ph})$_2$]Cl · 1.25(THF) are 211.5(8) pm and 213.4(7) pm, which is considerably shorter than the metal–CDP^{Ph} bond in the herein presented

compound.[33] If only one CDP^{Ph} ligand coordinated to Ag, the Ag–C^{CDP} distance would most likely further decrease in length, in order to diminish the electron deficiency at the In^+ center. In fact, the Ag–C^{CDP} distance in the gas-phase optimized structures of $[(CDP^{Ph})–Ag–(CDP^{Ph})]^+$ (209.0 and 209.4 pm) and $[Ag(CDP^{Ph})]^+$ (207.9 pm; both RI-BP86(D3BJ)/def2-TZVPP, section 8.12 and 8.13) are similar, but the Ag–C^{CDP} bond is indeed shorter in the monocoordinated complex. Thus, it is rather unlikely that the metal atom in the herein presented compound is a silver atom. Quantum chemical calculations confirm that the M–C^{CDP} bond in $[M(CDP^{Ph})]^+$ is longer for M = In (239.7 pm) than for M = Ag (207.9 pm; both RI-BP86(D3BJ)/def2-TZVPP, section 8.11 and 8.12). Since, due to crystal packing effects, the bond lengths in $[\{Ga(CDP^{Ph})\}_2][pf]_2$ ([**2**][*pf*]$_2$) found in the solid state are shorter compared to the calculated bond lengths in its gas phase-optimized structure (section 8.4), it is reasonable to assume that the calculated bond length is in better agreement with the metal being indium instead of silver.

Besides this, the isolated compound could also, in principle, be an In^{III} species, *i.e*. $[H_2In(CDP^{Ph})][pf]$, considering that observing hydrogen atoms in close proximity to the heavy indium atoms by XRD may be difficult. However, the C–In bond length is clearly rather indicative of an indium cation in its lower oxidation state since it is very similar to the bond lengths in other organometallic, monovalent indium species. For example, the covalent C–In bond length of 225.6(2) pm is virtually identical to the C–In bond length in related compounds like monomeric 2,6-$(Tripp)_2C_6H_3$–In^{I} (226.0(7) pm),[34] dimeric $[In\{2,6\text{-}(Dipp)_2C_6H_3\}]_2$ (225.6(2) pm)[35] and in tetrameric $[In\{C(SiMe_3)_3\}]_4$ (225(1) pm).[36] Consequently, the In–C bond lengths even in sterically highly congested organometallic In^{III} species like $X_2In(Mes^*)$ (Mes* = 2,4,6-(tBu)$_3C_6H_3$; X = Cl, Br),[37] $XIn(Mes^*)_2$ (X = Cl, Br),[38] $[Cl_2In(2,6\text{-}Mes_2C_6H_3)]_2$[39] or $BrIn(2,6\text{-}Mes_2C_6H_3)_2$[40] are considerably shorter and range from 210 to 217 pm. Additionally, the experimental Raman spectrum of $[In(CDP^{Ph})][pf]$ compares very well with the simulated spectrum for $[In(CDP^{Ph})]^+$ and the experimental spectrum of NO[*pf*] as can be seen in **Figure S 58**. The spectrum of NO[*pf*] is displayed in order to show the vibrations dedicated to the anion. The absence of the ν(In–H) bands at 1760 cm^{-1} and 1780 cm^{-1} in the experimental Raman spectrum again strongly suggests that no In–H bond is present in the molecule.

Examples of one-coordinated metal atoms in organometallic compounds in a solid state structure are very scarce.[34,41] In this novel compound, the indium atoms barely interact with the $[pf]^-$ anions: the shortest In–F distance is 353.1(3) pm while the sum of the van der Waals radii is 340 pm.[42] On the other hand, the shortest distance between the In atom and a carbon atom of an adjacent phenyl ring is only 302.0(2) pm, which is below the sum of the van der Waals radii (ca. 363 pm[42]) and suggests that the arene moieties donate electron density in the empty 5p orbitals of In^+. The shortest In–In distance exceeds 1000 pm, ruling out any In–In interaction.

4 Powder Diffraction

In **Figure S 9** and **Figure S 10**, the experimental powder diffractograms of [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5*o*DFB) and [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([**2**][*pf*]$_2$) are compared with the respective simulated diffractograms. The diffractogram of [**1**][*pf*]$_2$ · 1.5*o*DFB indicates high purity of the bulk compound, suggesting that the Li[*pf*] or LiNacNac^{Mes} impurity found in the ^{7}Li NMR (**Figure S 21**) is negligible.

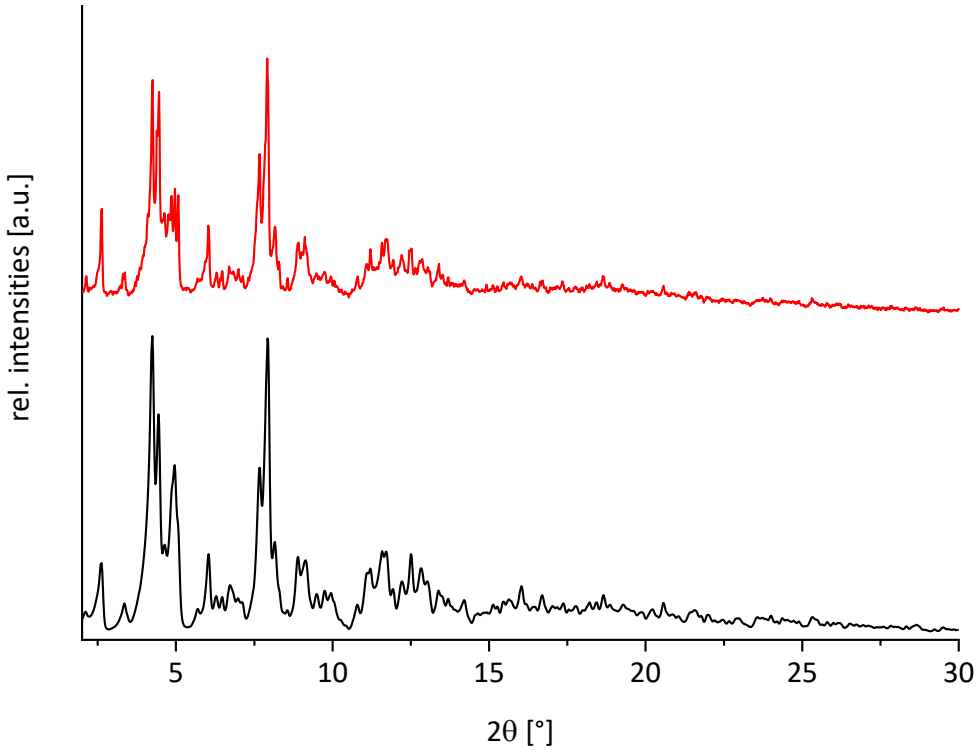


Figure S 9: Comparison of the experimental (red) and simulated (black) powder diffractogram of [**1**][*pf*]$_2$ · 1.5*o*DFB.

By contrast, the experimental diffractogram of [**2**][*pf*]$_2$ does not fit as well to the simulated diffractogram. This is arguably due to the high reactivity and poor stability of this dicationic digallene. It is conceivable that the trituration process and the mechanical stress on the crystals prior to analysis results in a structural transformation, *e.g*. bond dissociation of the weak Ga⇆Ga double bond, leading to a changing powder pattern. Additionally, since the complex is capable of activating C–H bonds (section 5.7), it cannot be ruled out that crystalline side products form during the crystallization process.

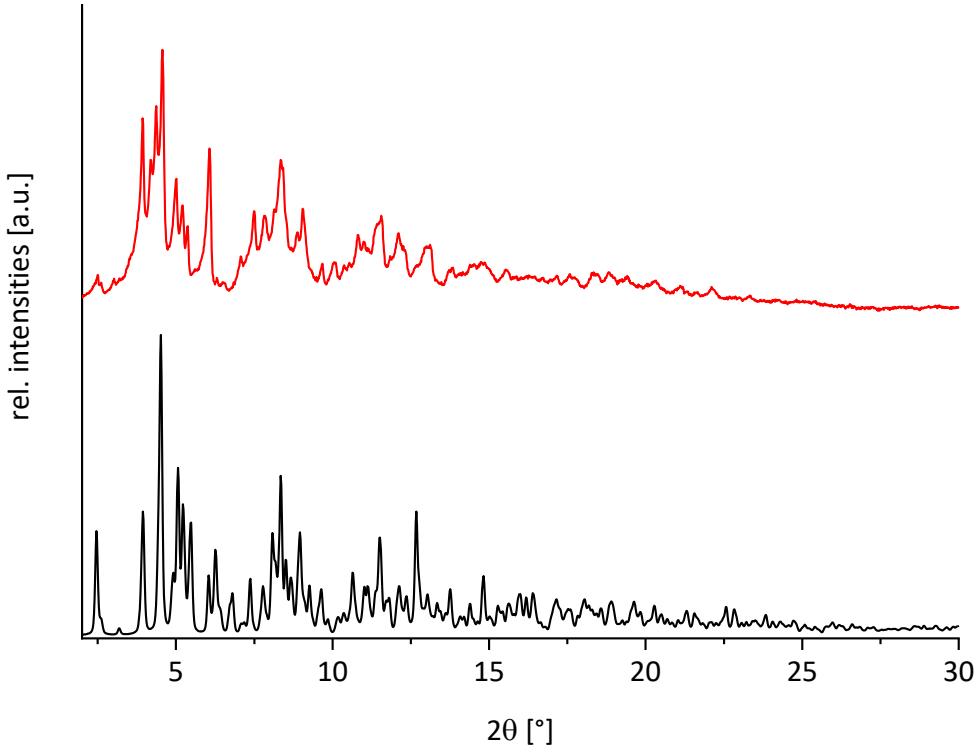
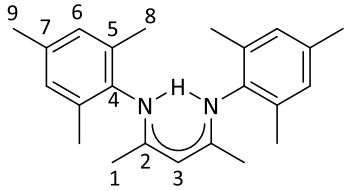


Figure S 10: Comparison of the experimental (red) and simulated (black) powder diffractogram of [**2**][*pf*]$_2$.

5 NMR Spectroscopy

5.1 HNacNac^{Mes}



^{1}H-NMR [300.18 MHz, $CDCl_3$, 298 K]: δ = 12.19 (s, 1 H, N**H**), 6.89 (s, 4 H, C^{6}**H**), 4.89 (s, 1 H, C^{3}**H**), 2.29 (s, 6 H, C^{9}**H**$_3$), 2.16 (s, 12 H, C^{8}**H**$_3$), 1.72 (s, 6 H, C^{1}**H**$_3$) ppm.

^{13}C-NMR [75.48 MHz, $CDCl_3$, 298 K]: δ = 161.0 (2 C, **C**^{2}) 141.3 (2 C, **C**^{7}), 133.6 (4 C, **C**^{5}), 131.8 (2 C, **C**^{4}), 128.5 (4 C, **C**^{6}), 93.5 (1 C, **C**^{3}), 21.0 (4 C, **C**^{8}), 20.4 (2 C, **C**^{9}), 18.4 (2 C, **C**^{1}), ppm.

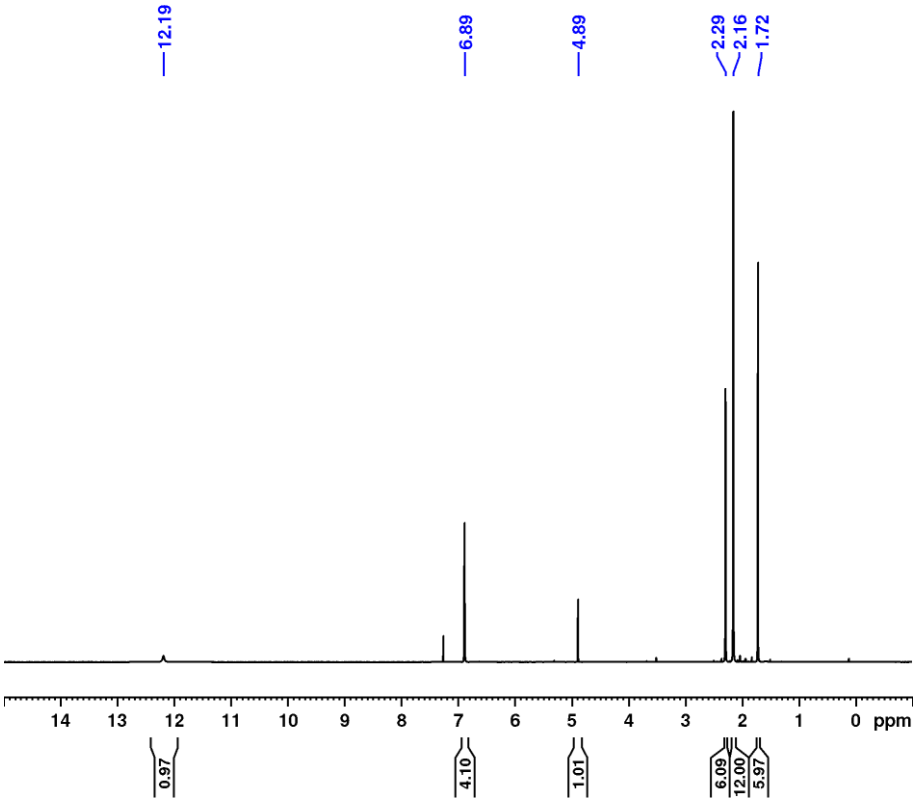


Figure S 11: ^{1}H-NMR spectrum (300.18 MHz, $CDCl_3$, 298 K) of HNacNac^{Mes}.

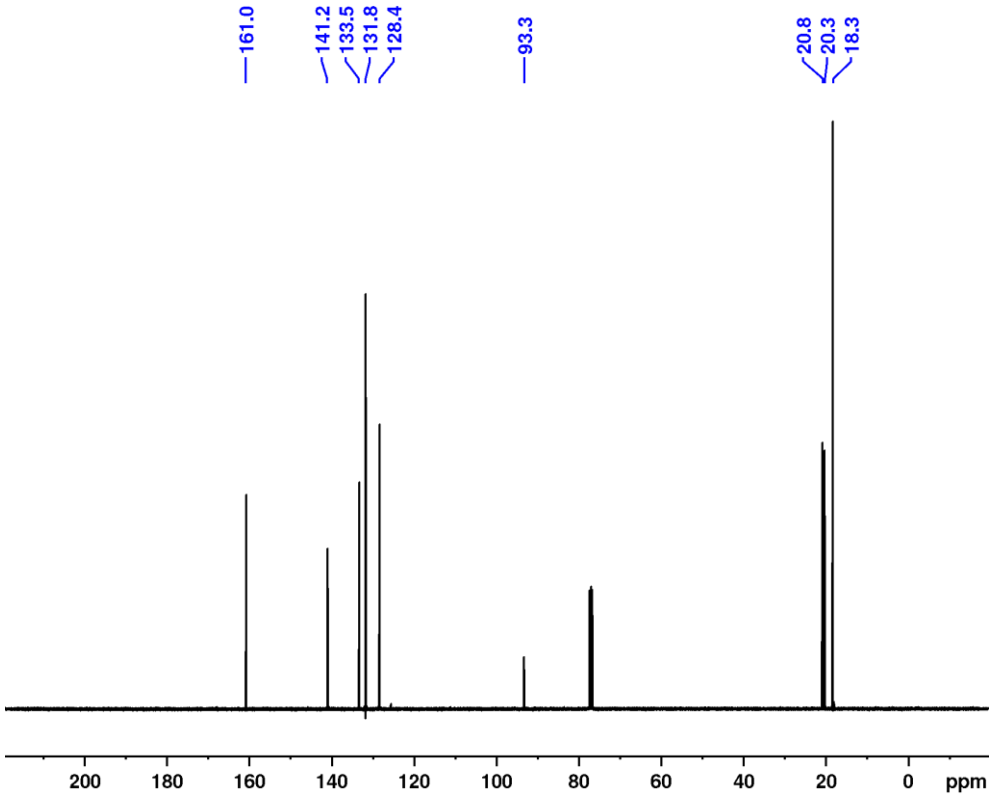


Figure S 12: $^{13}C\{^{1}H\}$-NMR spectrum (100.62 MHz, $CDCl_3$, 298 K) of $HNacNac^{Mes}$.

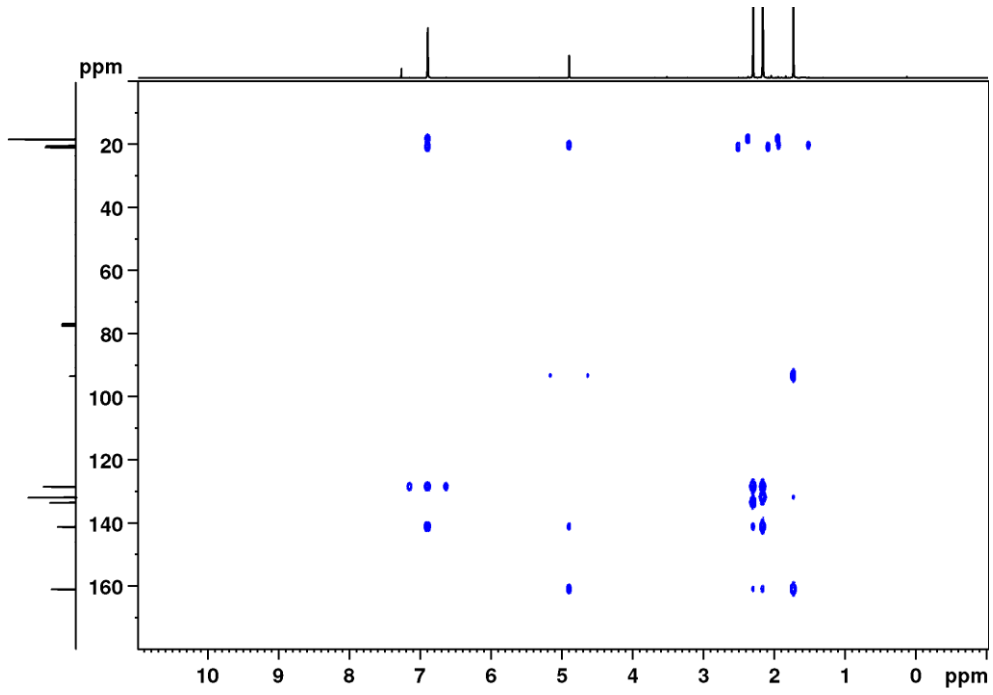
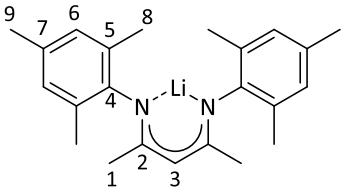


Figure S 13: ^{1}H, ^{13}C HMBC (300.18 MHz, $CDCl_3$, 298 K, optimized for J = 8 Hz) of $HNacNac^{Mes}$.

5.2 LiNacNac^{Mes}



^{1}H-NMR [300.18 MHz, C_6D_6, 298 K]: δ = 6.94 (s, 4 H, C^{6}**H**), 4.79 (s, 1 H, C^{3}**H**), 2.31 (s, 6 H, C^{9}**H**$_3$), 2.04 (s, 12 H, C^{8}**H**$_3$), 1.70 (s, 6 H, C^{1}**H**$_3$) ppm.

^{7}Li-NMR [116.66 MHz, C_6D_6, 298 K]: δ = −0.9 (s, 1 Li, N**Li**) ppm.

^{1}H-NMR [300.18 MHz, *o*DFB, 298 K]: δ = 6.75 (s, 4 H, C^{6}**H**), 4.80 (s, 1 H, C^{3}**H**), 2.18 (s, 6 H, C^{9}**H**$_3$), 2.10 (s, 12 H, C^{8}**H**$_3$), 1.67 (s, 6 H, C^{1}**H**$_3$) ppm.

^{7}Li-NMR [116.66 MHz, *o*DFB, 298 K]: δ = 2.1 (s, 1 Li, N**Li**) ppm.

^{13}C-NMR [75.48 MHz, *o*DFB, 298 K]: δ = 163.4 (2 C, **C**^{2}), 149.4 (2 C, **C**^{4}), 130.6 (2 C, **C**^{7}), 130.2 (4 C, **C**^{5}), 128.3 (4 C, **C**^{6}), 92.5 (1 C, **C**^{3}), 21.9 (2 C, **C**^{1}), 19.8 (2 C, **C**^{9}), 17.7 (4 C, **C**^{8}) ppm.

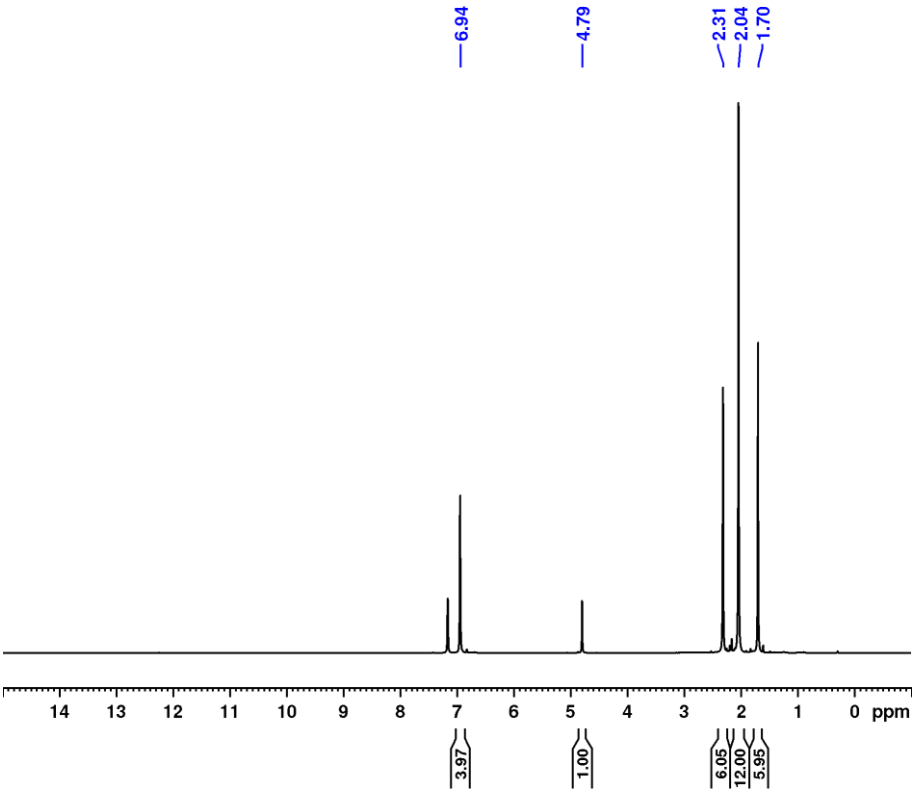


Figure S 14: ^{1}H-NMR spectrum (300.18 MHz, C_6D_6, 298 K) of LiNacNac^{Mes}.

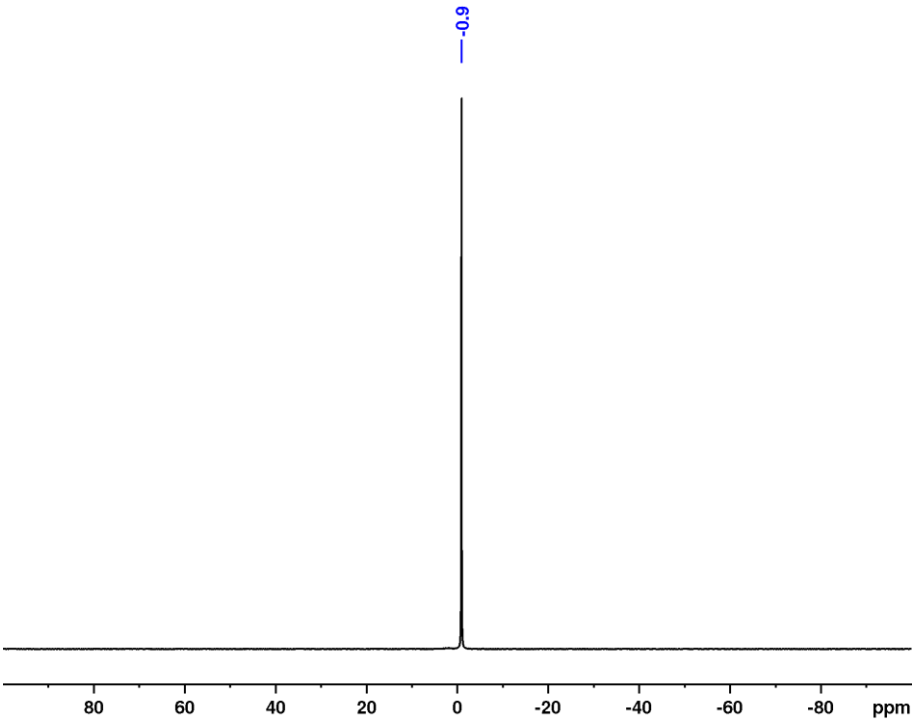


Figure S 15: ^{7}Li-NMR spectrum (116.66 MHz, C_6D_6, 298 K) of LiNacNac^{Mes}.

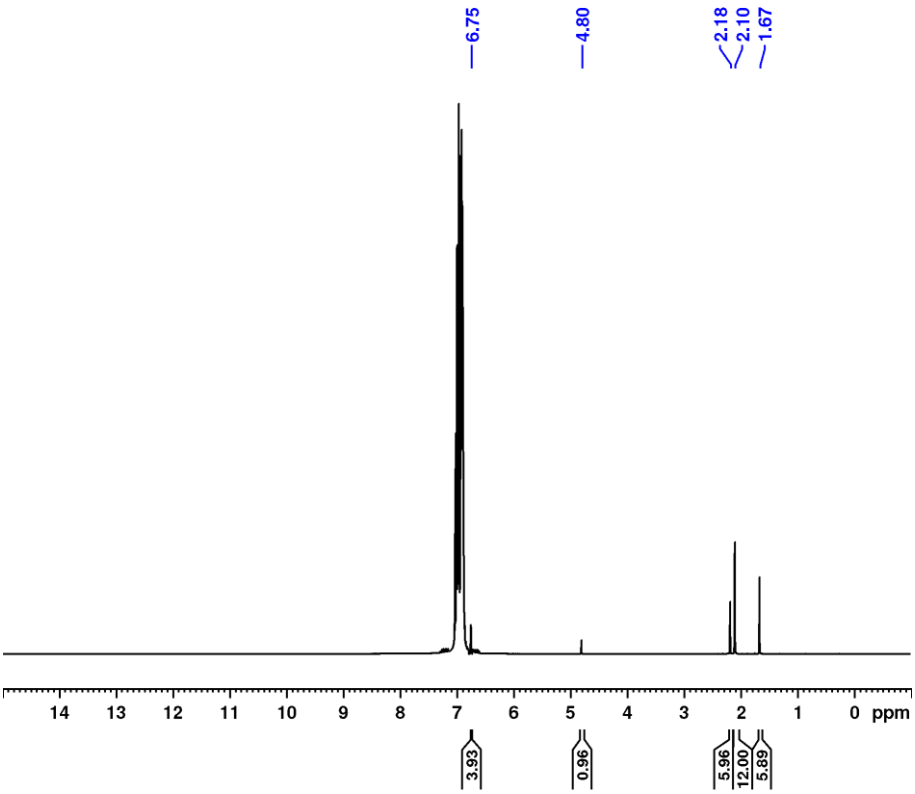


Figure S 16: ^{1}H-NMR spectrum (300.18 MHz, *o*DFB, 298 K) of LiNacNac^{Mes}.

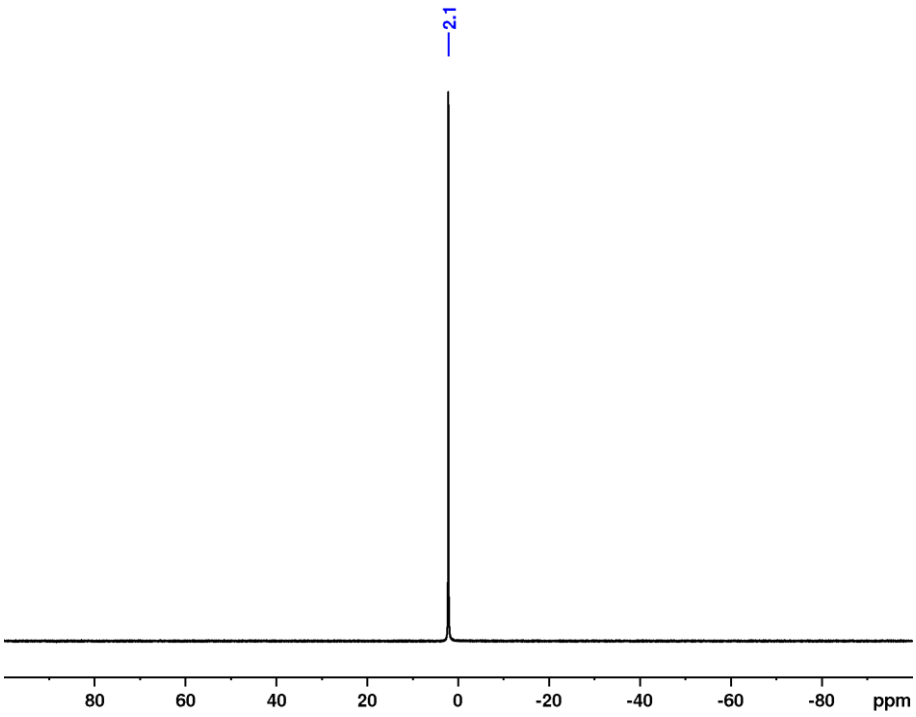


Figure S 17: ^{7}Li-NMR spectrum (116.66 MHz, *o*DFB, 298 K) of LiNacNac^{Mes} (field correction according to ^{1}H-NMR spectrum).

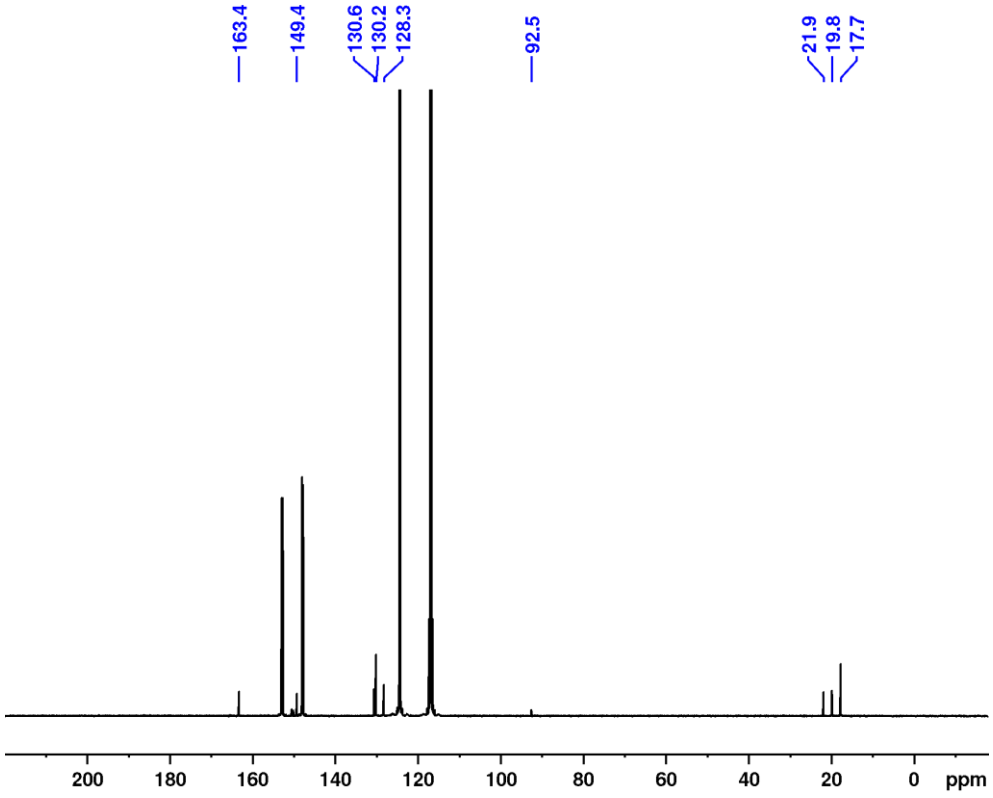


Figure S 18: ^{13}C{^{1}H}-NMR spectrum (50.32 MHz, *o*DFB, 298 K) of LiNacNac^{Mes}.

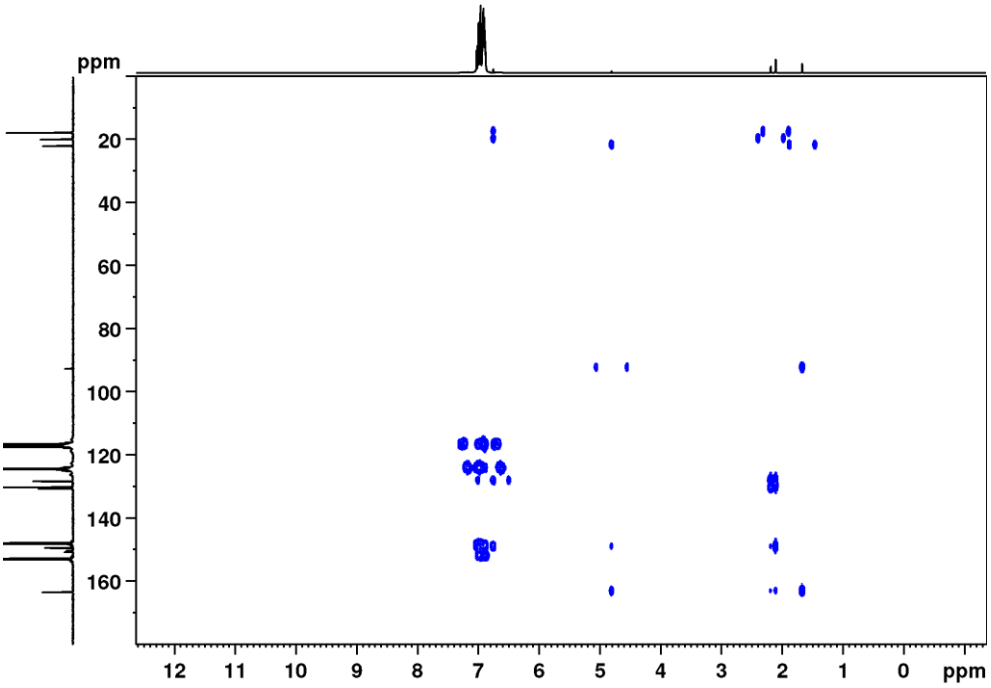
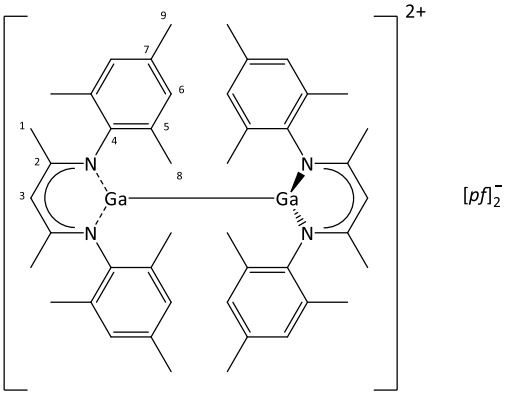


Figure S 19: ^{1}H, ^{13}C HMBC (300.18 MHz, *o*DFB, 298 K, optimized for *J* = 8 Hz) of LiNacNac^{Mes}.

5.3 [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([1][*pf*]$_2$ · 1.5*o*DFB)



^{1}H-NMR [400.17 MHz, *o*DFB, calibrated at *o*$C_6F_2\mathbf{H}_4$ = 6.96 ppm, 298 K]: δ = 7.16 (m, 8 H, C^{6}**H**), 6.30 (s, 2 H, C^{3}**H**), 2.35 (s, 12 H, C^{9}**H**$_3$), 1.98 (s, 12 H, C^{1}**H**$_3$), 1.78 (s, 24 H, C^{8}**H**$_3$), ppm.

^{7}Li-NMR [155.52 MHz, *o*DFB, 298 K]: δ = −0.7 (s, 1 Li, traces of **Li**[*pf*] or **Li**NacNac^{Mes}) ppm.

^{13}C-NMR [75.48 MHz, *o*DFB, 298 K]: δ = 176.6 (4 C, **C**^{2}), 141.4 (4 C, **C**^{7}), 136.1 (4 C, **C**^{4}), 131.6 (8 C, **C**^{5}), 131.1 (8 C, **C**^{6}), 119.7 (12 C, [Al{OC(**C**F$_3$)$_3$}$_4$]$^-$), 106.8 (2 C, **C**^{3}), 79.6 (4 C, [Al{O**C**(CF$_3$)$_3$}$_4$]$^-$), 21.7 (4 C, **C**^{1}), 19.8 (4 C, **C**^{9}), 18.0 (8 C, **C**^{8}), ppm.

^{19}F-NMR [376.54 MHz, *o*$C_6\mathbf{F}_2H_4$ = –139.5 ppm, 298 K]: δ = –75.3 (s, 36 F, [Al{OC(C**F**$_3$)$_3$}$_4$]$^-$) ppm.

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

^{71}Ga-NMR [122.04 MHz, *o*DFB, 298 K]: δ = no signal.

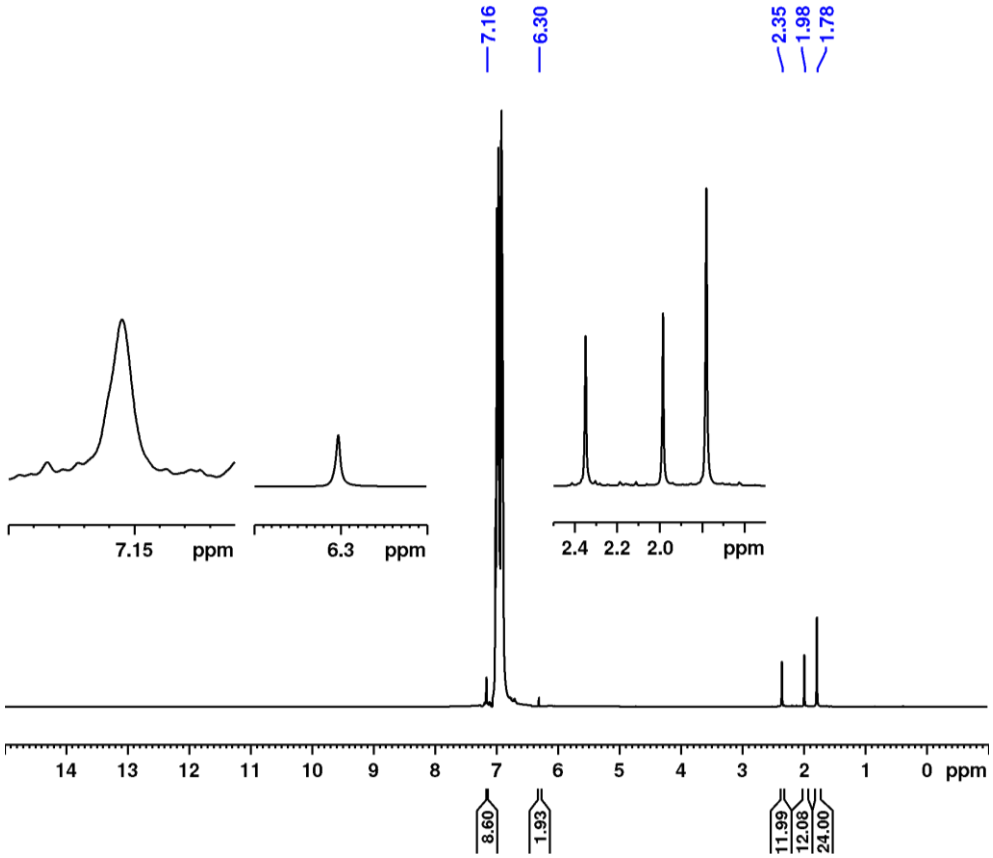


Figure S 20: ^{1}H-NMR spectrum (400.17 MHz, *o*DFB, 298 K) of [**1**][*pf*]$_2$ · 1.5*o*DFB.

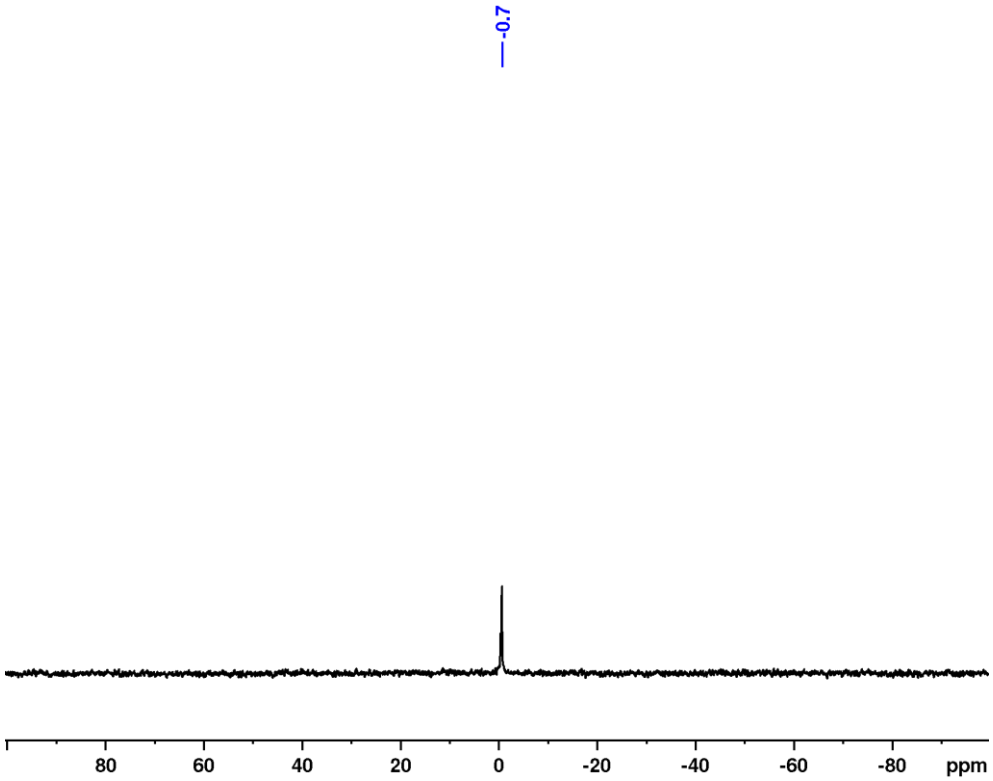


Figure S 21: ^{7}Li-NMR spectrum (155.52 MHz, *o*DFB, 298 K) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

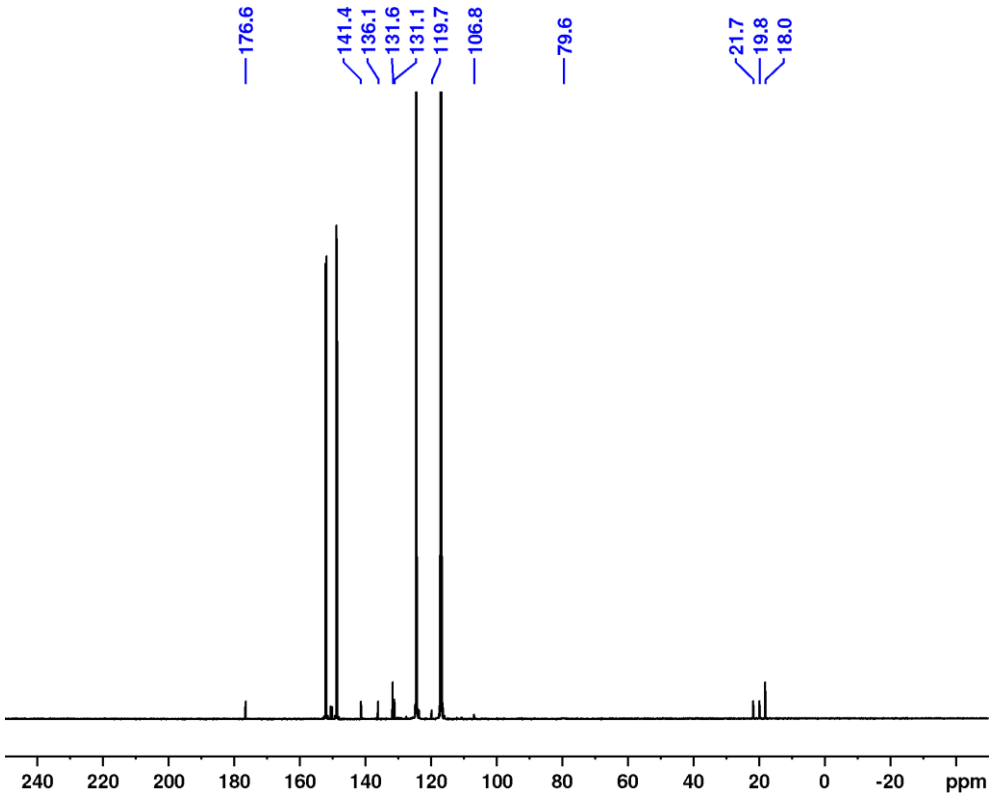


Figure S 22: $^{13}C\{^{1}H\}$-NMR spectrum (75.48 MHz, *o*DFB, 298 K) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

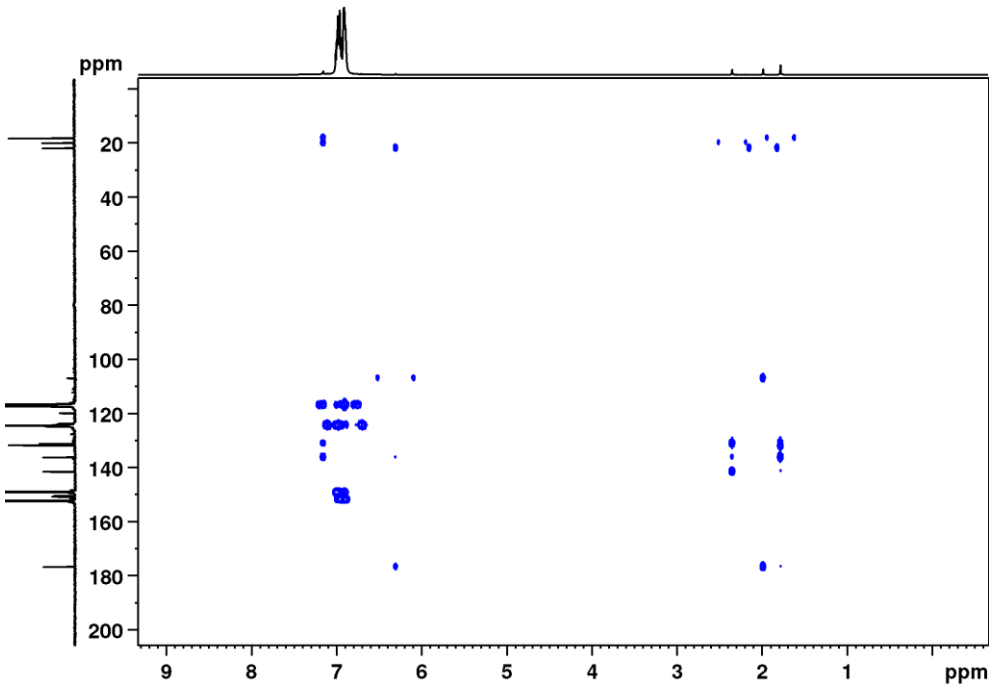


Figure S 23: ^{1}H, ^{13}C HMBC (400.17 MHz, *o*DFB, 298 K, optimized for *J* = 8 Hz) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

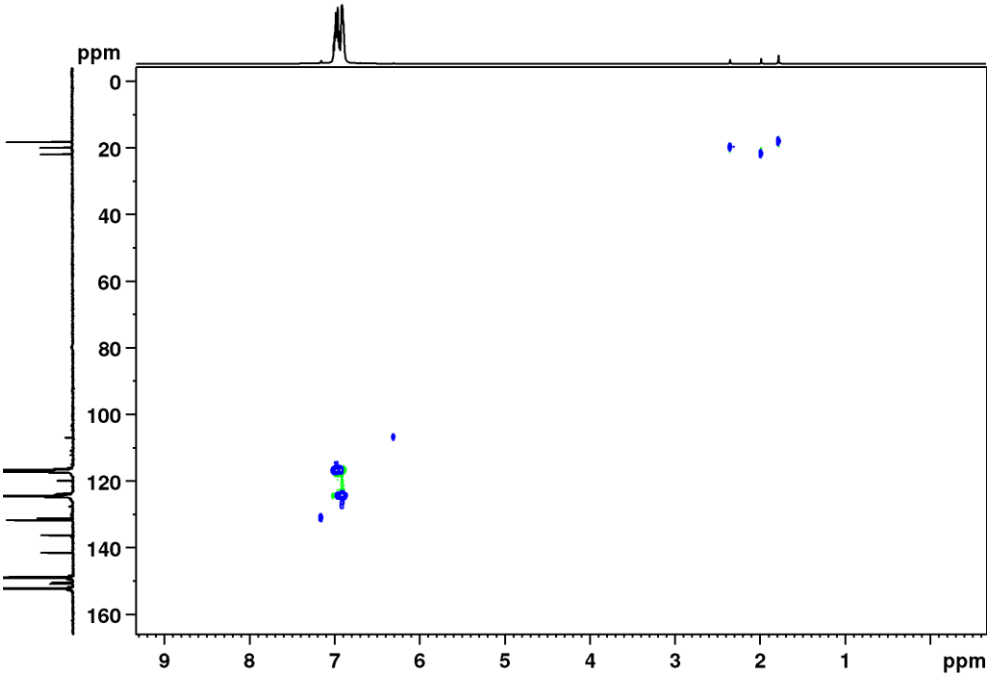


Figure S 24: ^{1}H, ^{13}C HSQC (400.17 MHz, *o*DFB, 298 K, optimized for J = 145 Hz) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

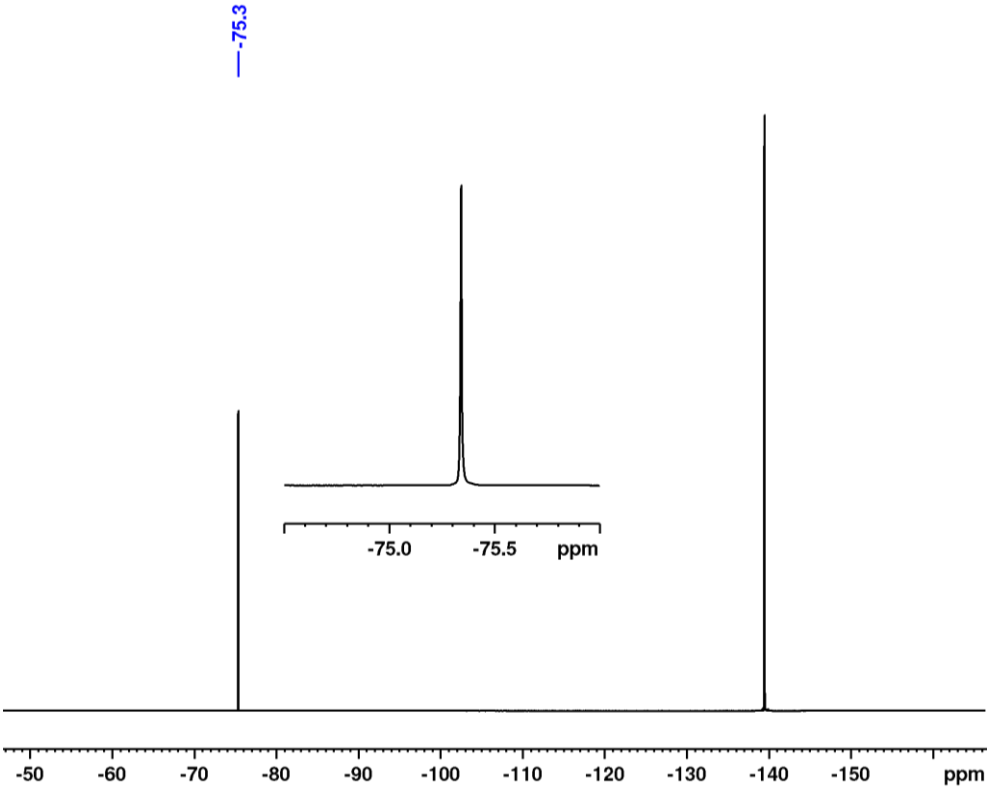


Figure S 25: ^{19}F-NMR spectrum (376.54 MHz, *o*DFB, 298 K) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

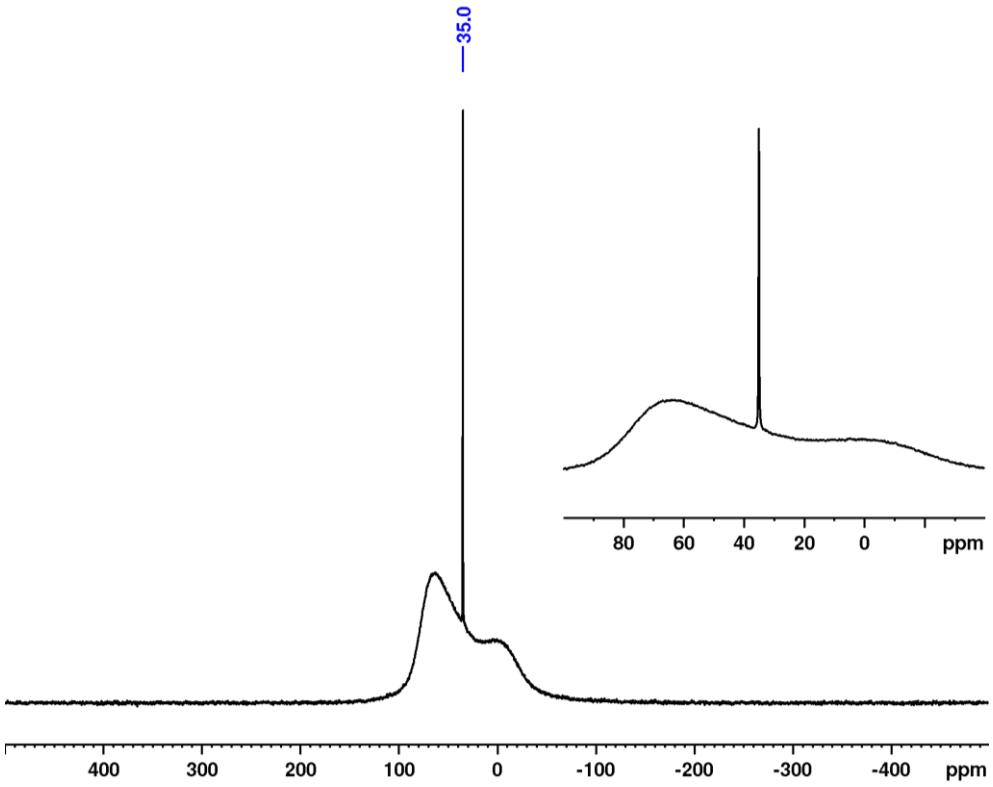


Figure S 26: ^{27}Al-NMR spectrum (104.27 MHz, *o*DFB, 298 K) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB (The broad resonances are caused by the probe head).

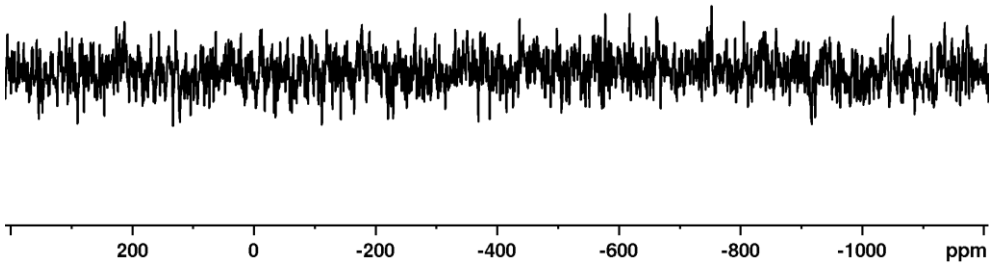


Figure S 27: ^{71}Ga-NMR spectrum (122.04 MHz, *o*DFB, 298 K) of crystalline [**1**][*pf*]$_2$ · 1.5*o*DFB.

5.4 $[Ph_3PCH_2PPh_3]Br_2$

^{1}H-NMR [400.17 MHz, methanol-d_4, calibrated at C**H**D_2OD = 3.31 ppm, 298 K]: δ = 7.85 (m, 18 H, C^2**H** and C^4**H**), 7.60 (m, 12 H, C^3**H**), 4.91 (s, coalescence signal of the solvent **H**O-protons with the acidic $C^{1'}$**H**-protons) ppm.

^{31}P-NMR [161.99 MHz, methanol-d_4, 298 K]: δ = 20.4 (unknown species), 18.7 (s, 2 P, $[H_2C(\mathbf{P}Ph_3)_2]^+$) ppm.

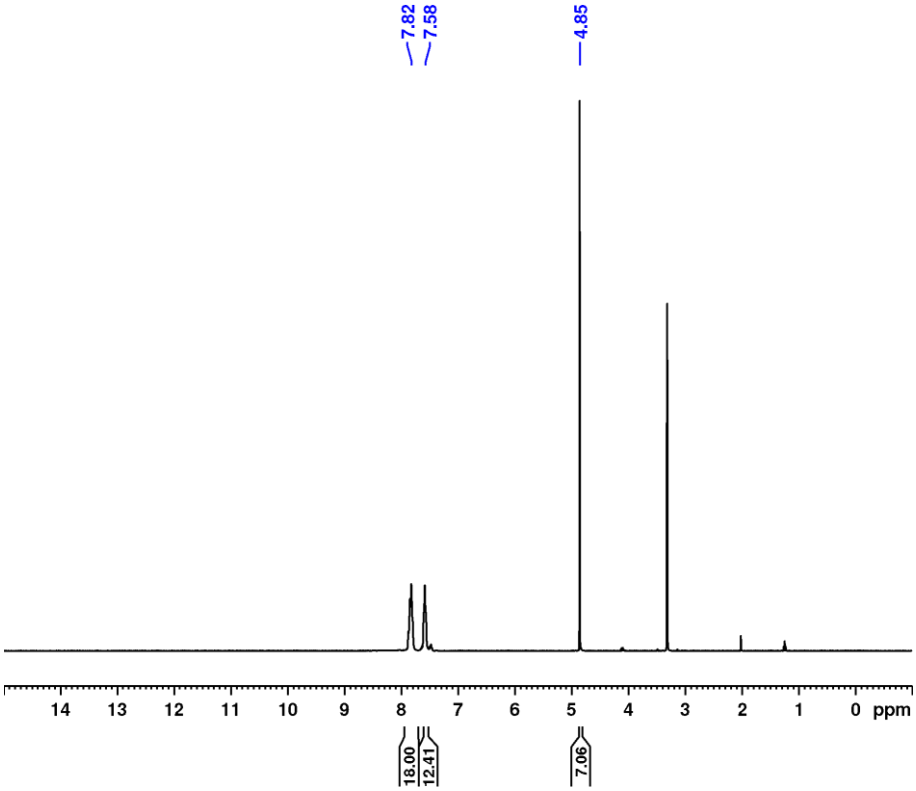


***Figure S 28**: ^{1}H-NMR spectrum (400.17 MHz, CD_3OD, 298 K) of $[Ph_3PCH_2PPh_3]Br_2$.*

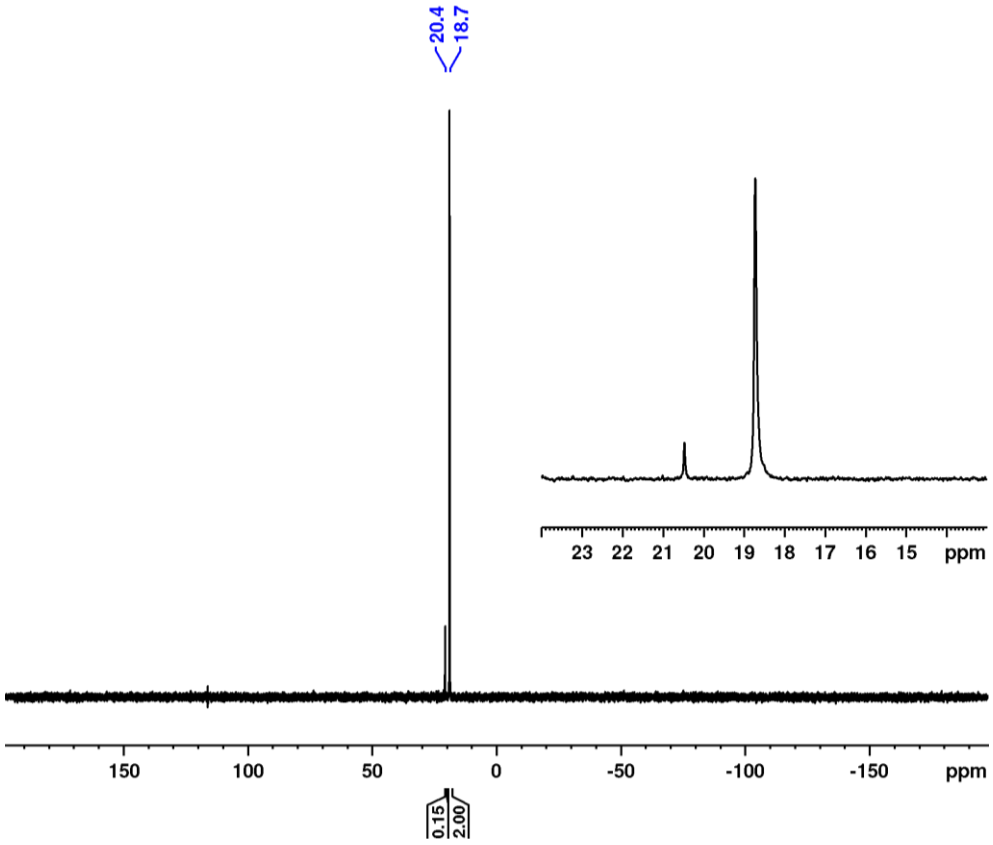


Figure S 29: $^{31}P\{^{1}H\}$-NMR spectrum (161.99 MHz, CD_3OD, 298 K) of $[Ph_3PCH_2PPh_3]Br_2$.

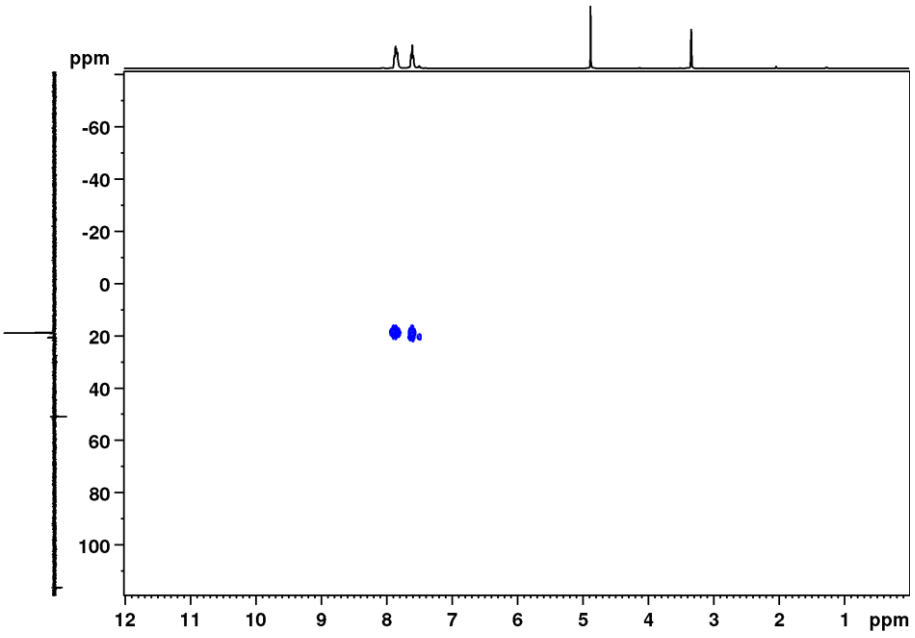
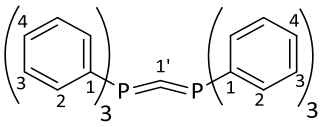


Figure S 30: ^{1}H, ^{31}P HMBC (300.18 MHz, *o*DFB, 298 K, optimized for J = 15 Hz) of $[Ph_3PCH_2PPh_3]Br_2$.

5.5 CDP^{Ph}



^{1}H-NMR [300.18 MHz, *o*DFB, calibrated at *o*C_6F_2**H_4** = 6.96 ppm, 298 K]: δ = 7.76 (m, 12 H, C^{2}**H**), 7.20 (m, 6 H, C^{4}**H**), 7.13 (m, 12 H, C^{3}**H**), 3.65 (m, 4 H, O(C**H_2**CH_2)$_2$), 1.68 (m, 4 H, O(CH_2C**H_2**)$_2$) ppm.

^{13}C-NMR [75.48 MHz, *o*DFB, 298 K]: δ = 137.5 (m, 6 C, **C**^{1}), 132.1 (ps. t, 12 C, **C**^{2}, $^{2}J_{C2,P}$ = 5.3 Hz), 129.0 (ps. t, 6 C, **C**^{4}, $^{4}J_{C4,P}$ = 1.4 Hz), 127.3 (ps. t, 12 C, **C**^{3}, $^{3}J_{C3,P}$ = 5.9 Hz), 12.4 (t, 1 C, **C**$^{1'}$, $^{3}J_{C1',P}$ = 121.0 Hz) ppm.

^{31}P-NMR [121.52 MHz, *o*DFB, 298 K]: δ = –3.9 (s, 2 P, C(**P**Ph_3)$_2$) ppm.

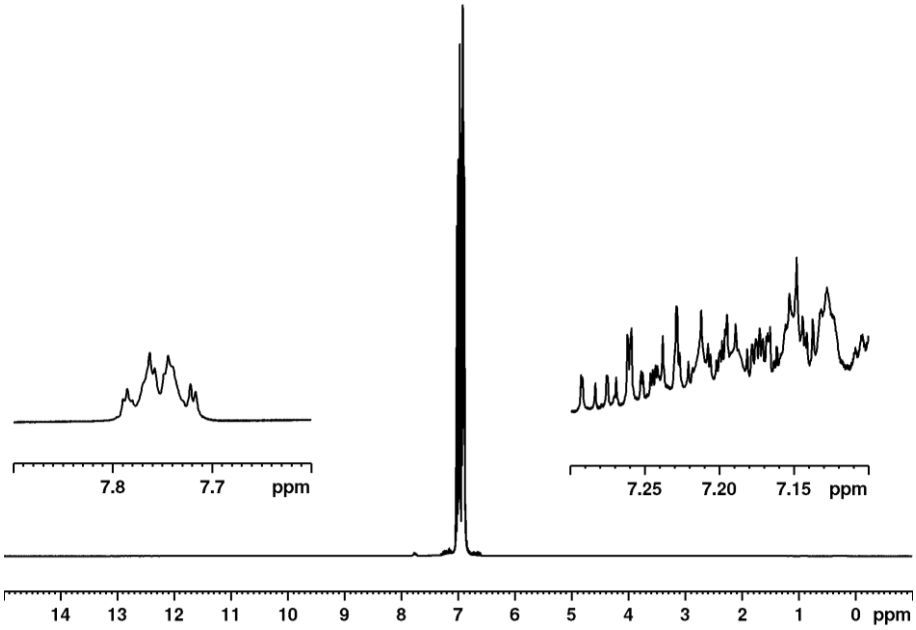


Figure S 31: ^{1}H-NMR spectrum (400.17 MHz, *o*DFB, 298 K) of CDP^{Ph} (in the area between 7.10 and 7.20 ppm the resonances of C^{3}**H** and C^{4}**H** are found but they overlap with the ^{13}C satellites of the solvent).

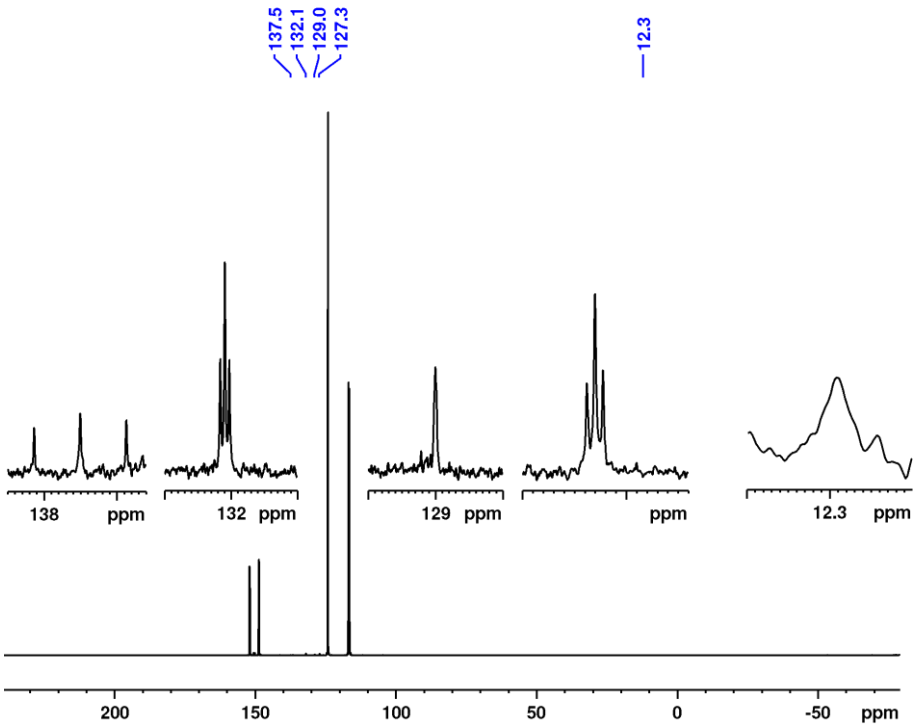


Figure S 32: $^{13}C\{^{1}H\}$-NMR spectrum (75.48 MHz, *o*DFB, 298 K) of CDP^{Ph}.

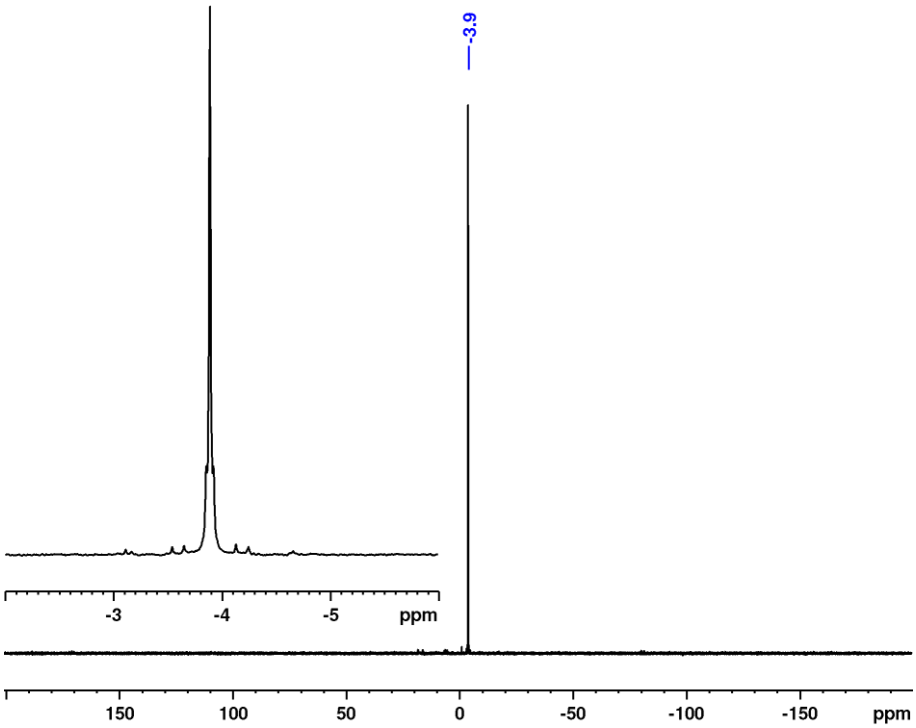


Figure S 33: $^{31}P\{^{1}H\}$-NMR spectrum (121.52 MHz, *o*DFB, 298 K) of CDP^{Ph}.

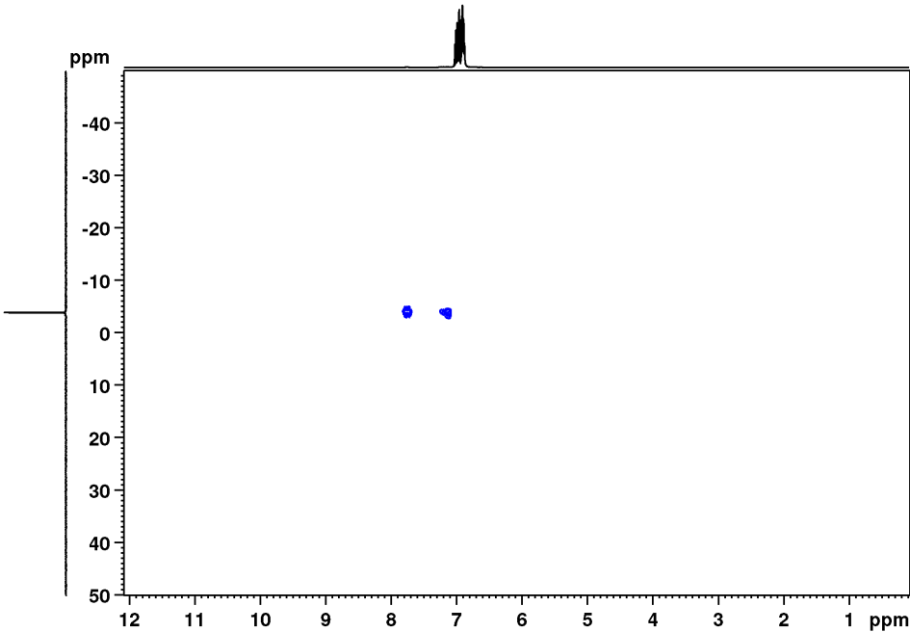
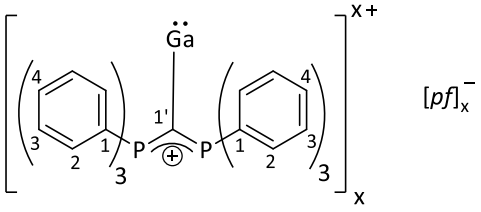


Figure S 34: ^{1}H, ^{31}P HMBC (300.18 MHz, *o*DFB, 298 K, optimized for *J* = 15 Hz) of CDP^{Ph}.

5.6 [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([2][*pf*]$_2$)



^{1}H-NMR [400.17 MHz, *o*DFB, calibrated at *o*$C_6F_2H_4$ = 6.96 ppm, 298 K]: δ = 7.44 (m, 18 H, C^{2}**H** and C^{4}**H**), 7.32 (m, 12 H, C^{3}**H**), small impurity, typically 12-14 %: 1.82 (t, 1 H, [**H**(CDP^{Ph})]$^{+}$, $^{2}J_{H,P}$ = 5.4 Hz) ppm.

^{13}C-NMR [75.48 MHz, *o*DFB, 298 K]: δ = 137.5 (s, 6 C, **C**^{1}), 132.6 (s, 12 C, **C**^{2}H), 128.9 (s, 12 C, **C**^{3}H), 119.8 (12 C, [Al{OC(**C**F_3)$_3$}$_4$]$^{-}$), 79.5 (4 C, [Al{O**C**(CF_3)$_3$}$_4$]$^{-}$), 53.6 (t, 1 C, **C**$^{1'}$H, $^{1}J_{C1',P}$ = 64.5 Hz) ppm.

^{19}F-NMR [376.54 MHz, *o*$C_6F_2H_4$ = –139.5 ppm, 298 K]: δ = –75.3 (s, 36 F, [Al(OC(C**F**$_3$)$_3$)$_4$]$^{-}$) 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 = 16.7 (s, 2 P, [Ga{C(**P**Ph_3)$_2$}]$_x^{x+}$), small impurity, typically 12-14 %: 20.6 ([H{C(**P**Ph_3)$_2$}]$^{+}$) ppm.

^{71}Ga-NMR [122.04 MHz, *o*DFB, 298 K]: no signal

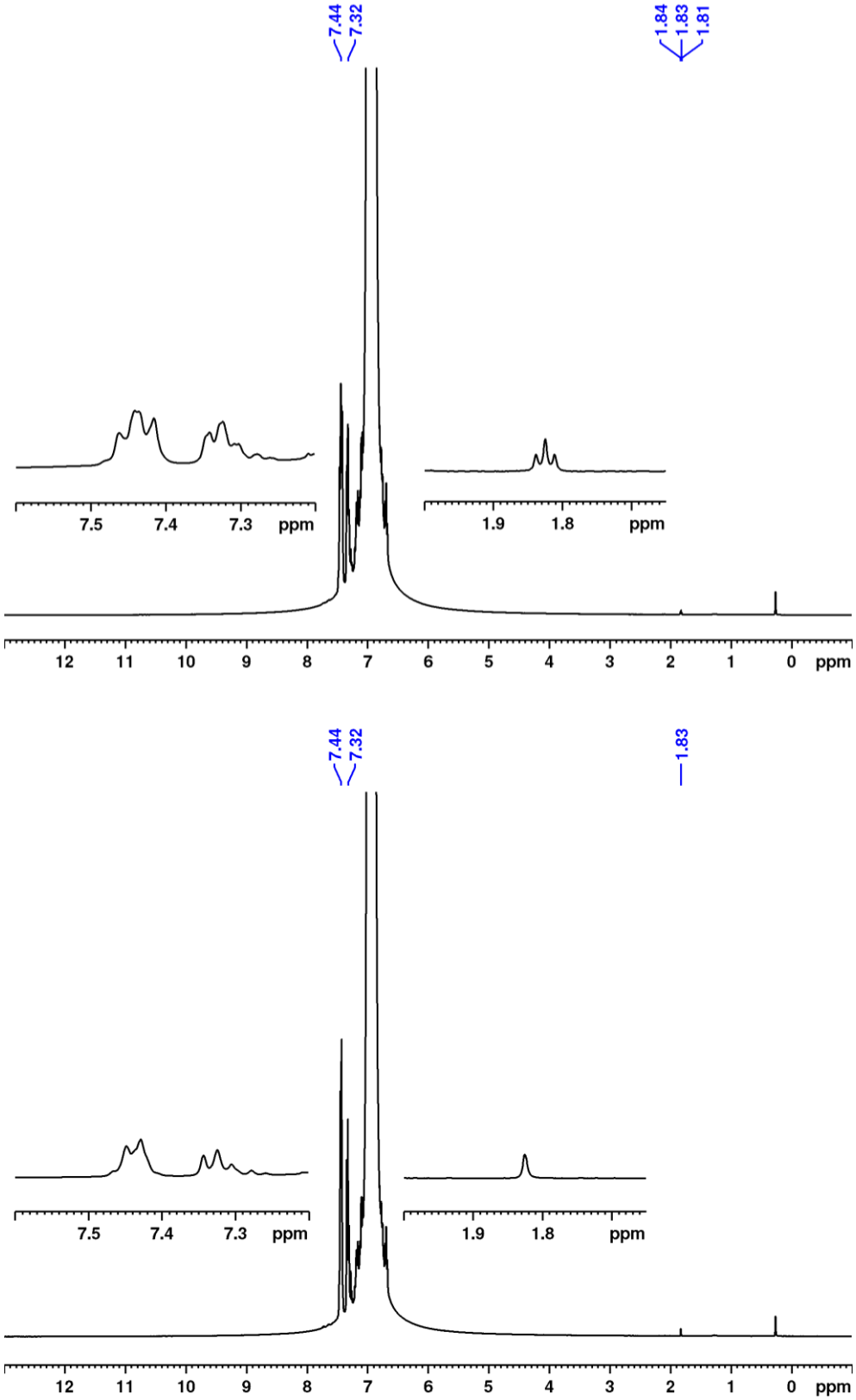


Figure S 35: ^{1}H-NMR (top) and ^{1}H{^{31}P} NMR (bottom) spectra (400.17 MHz, *o*DFB, 298 K) of a [Ga(PhF)$_2$][*pf*]/CDP^{Ph} (1.0 : 1.0) mixture.

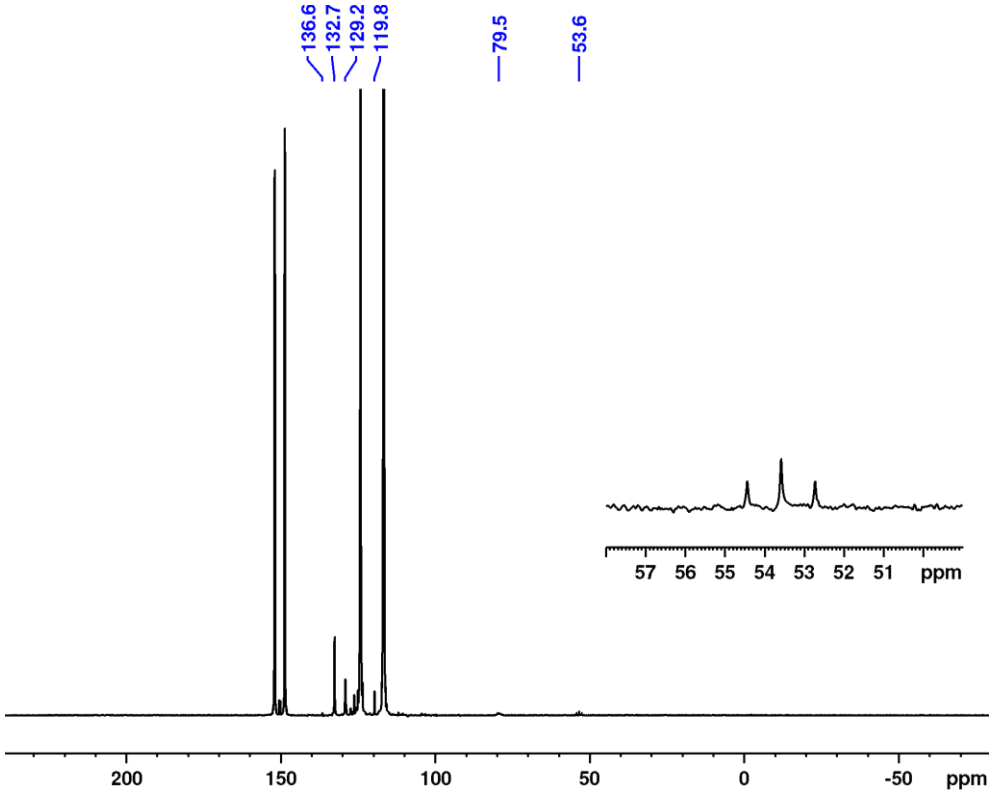


Figure S 36: $^{13}C\{^{1}H\}$-NMR spectrum (75.48 MHz, *o*DFB, 298 K) of crystalline [**2**][*pf*]$_2$.

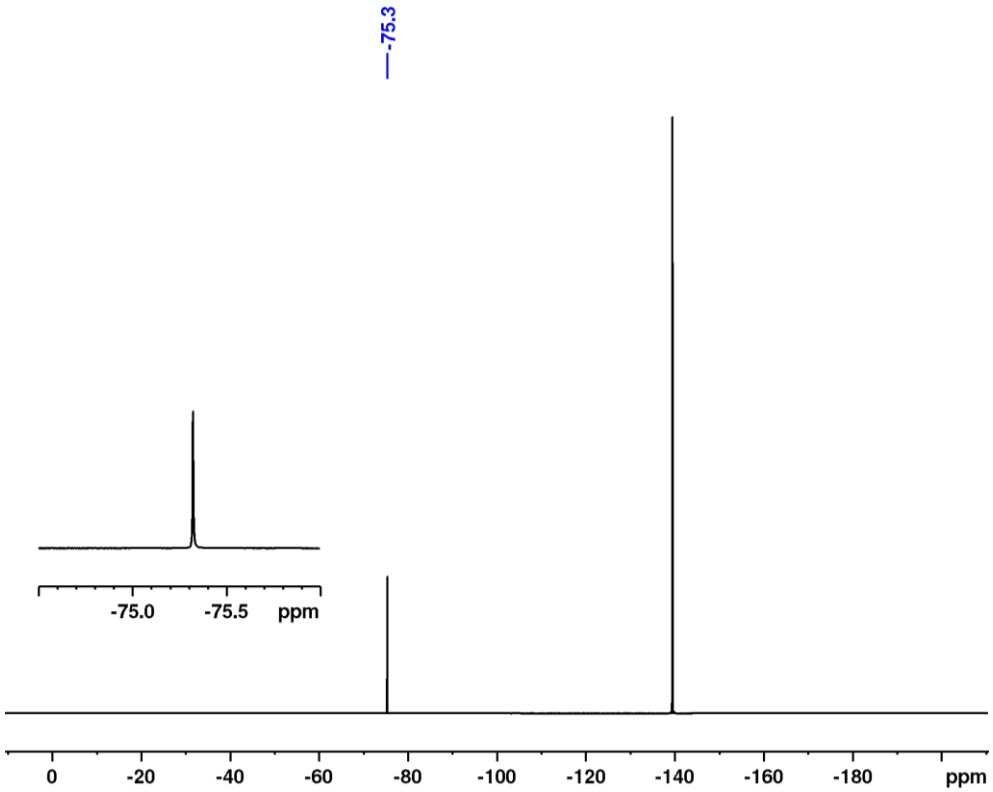


Figure S 37: ^{19}F-NMR spectrum (376.54 MHz, *o*DFB, 298 K) of crystalline [**2**][*pf*]$_2$.

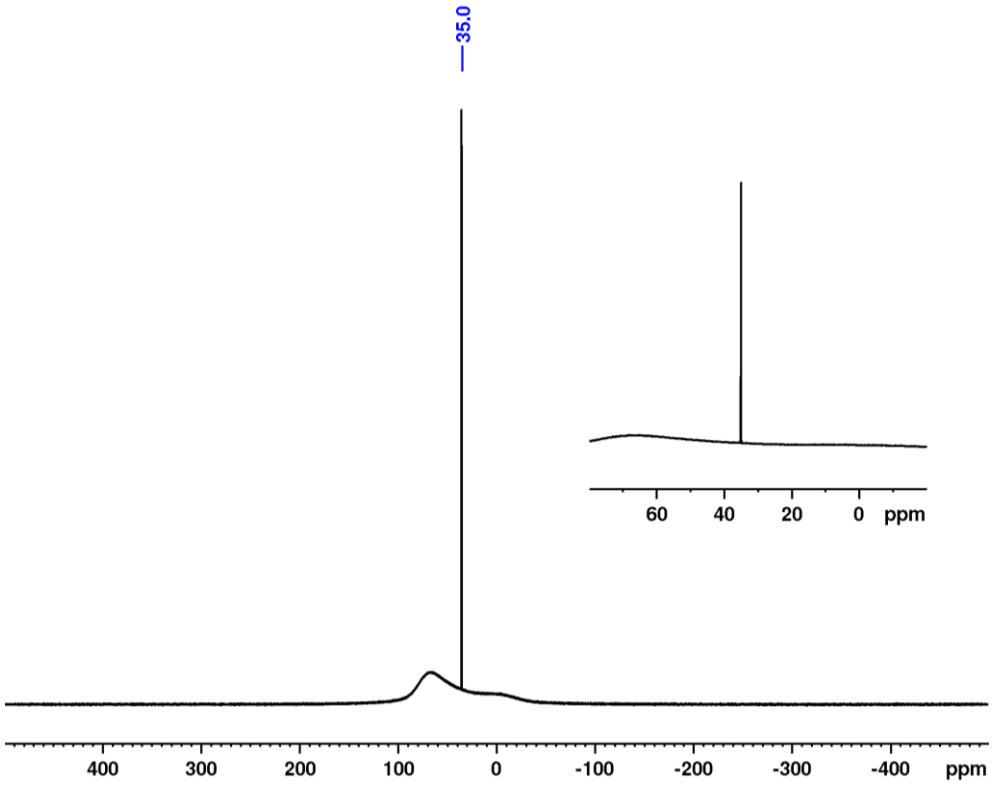


Figure S 38: ^{27}Al-NMR spectrum (104.27 MHz, *o*DFB, 298 K) of crystalline [**2**][*pf*]$_2$.

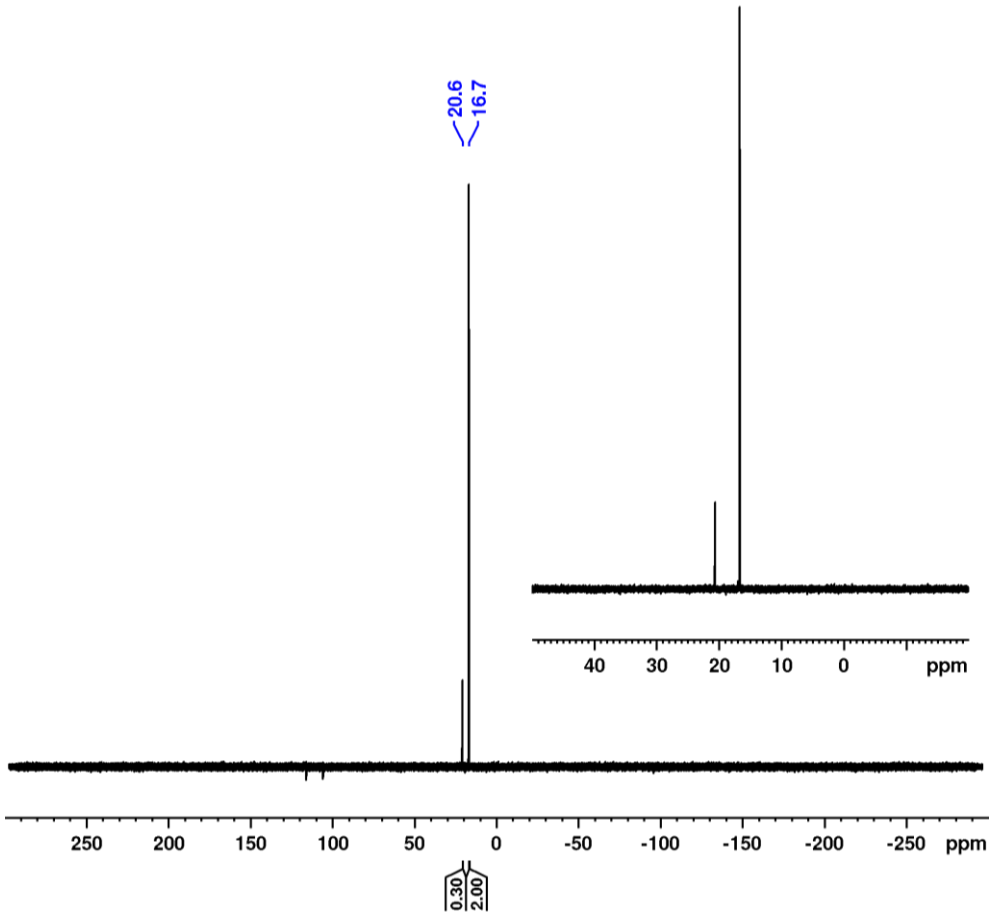


Figure S 39: $^{31}P\{^{1}H\}$-NMR spectrum (161.99 MHz, oDFB, 298 K) of crystalline [**2**][*pf*]$_2$.

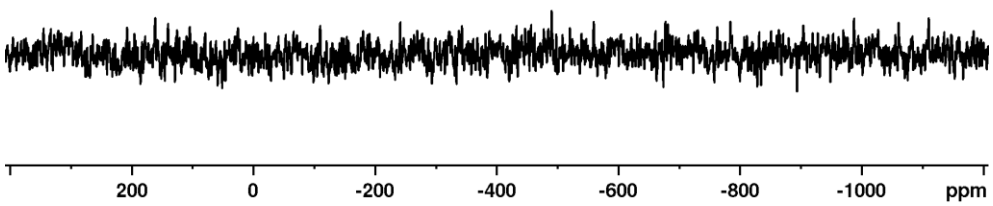


Figure S 40: ^{71}Ga-NMR spectrum (122.04 MHz, *o*DFB, 298 K) of [**2**][*pf*]$_2$.

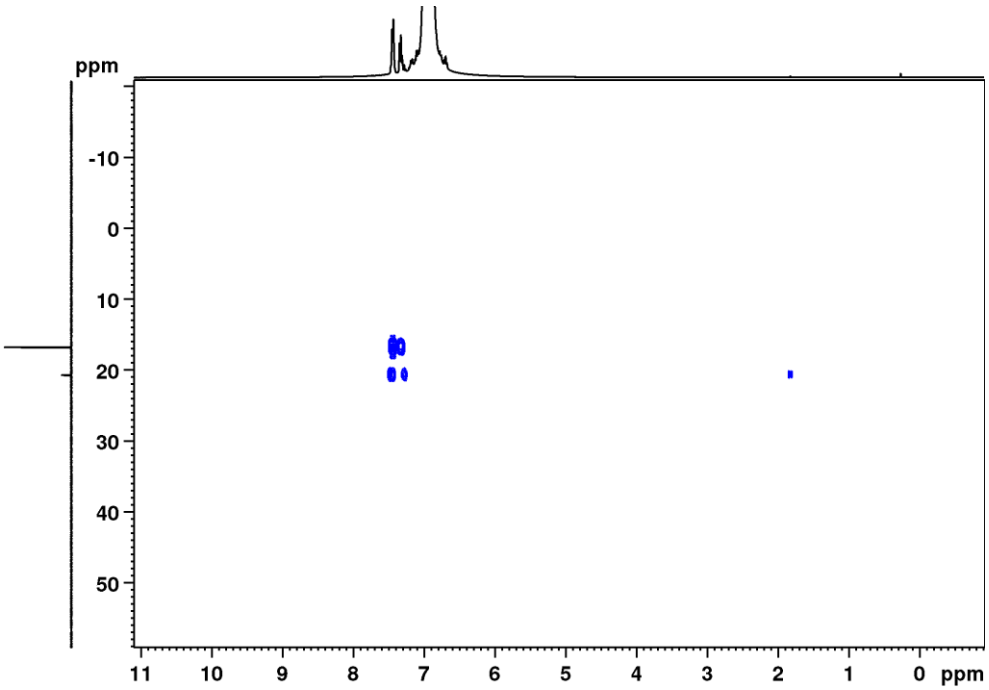


Figure S 41: $^{1}H,^{31}P$-HMBC NMR spectrum (400.17 MHz, *o*DFB, 298 K, optimized for J = 15 Hz) of crystalline [**2**][*pf*]$_2$.

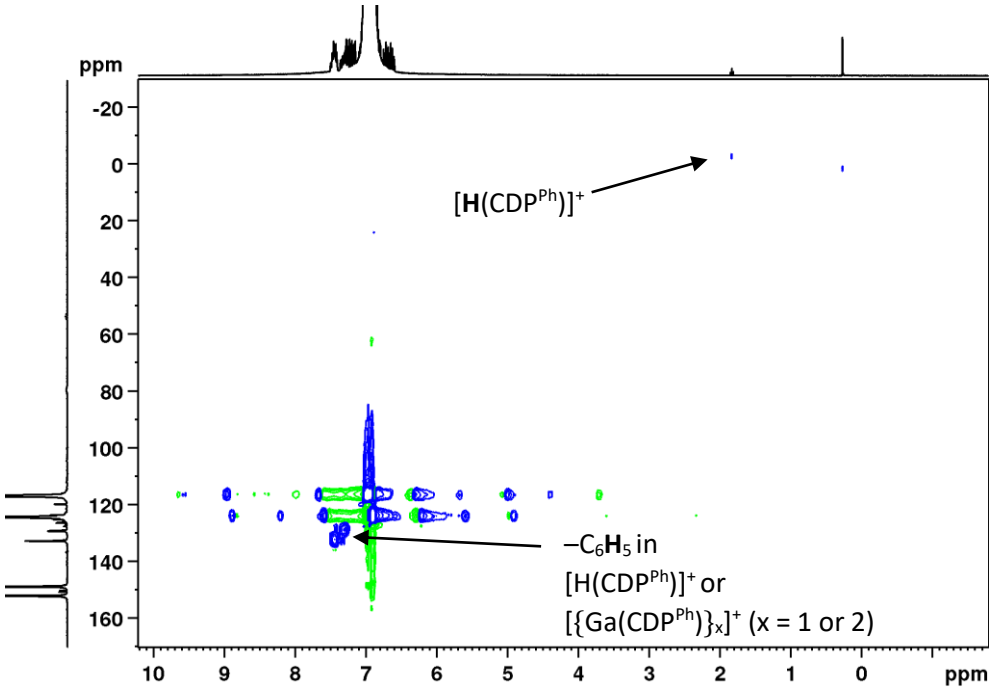


Figure S 42: Edited $^{1}H,^{13}C$-HSQC NMR spectrum (300.18 MHz, *o*DFB, 298 K, optimized for J = 145 Hz) of crystalline [**2**][*pf*]$_2$.

5.7 Formation of $[H(CDP^{Ph})]^+$ in Solution

NMR spectroscopy revealed that, when dissolving crystals of $[\{Ga(CDP^{Ph})\}_2][pf]_2$ ([**2**][*pf*]$_2$) in *o*DFB, ca. 13 % of the CDP^{Ph} ligand is protonated to give $[H(CDP^{Ph})]^+$. Besides this, we also observed the immediate formation of a precipitate. The same applied when mixing $[Ga(PhF)_2][pf]$ and CDP^{Ph} in a 1.0 : 1.0 ratio in a glove box and directly collecting the NMR spectra. Freezing the *o*DFB solution of [**2**][*pf*]$_2$ at −78 °C and thawing the sample in the NMR spectrometer did not have an effect on the concentration of $[H(CDP^{Ph})]^+$ either. Photographs of [**2**][*pf*]$_2$ solutions in *o*DFB, PhF and toluene are shown in **Figure S 43**. The phase boundaries in toluene and PhF indicate the formation of liquid clathrates. It has already been reported that mixing ionic liquids with electron-rich aromatic compounds like benzene or toluene leads to the spontaneous formation of three-dimensional networks of cations, anions and solvent molecules with limited miscibility in the aromatic solvent.[43]

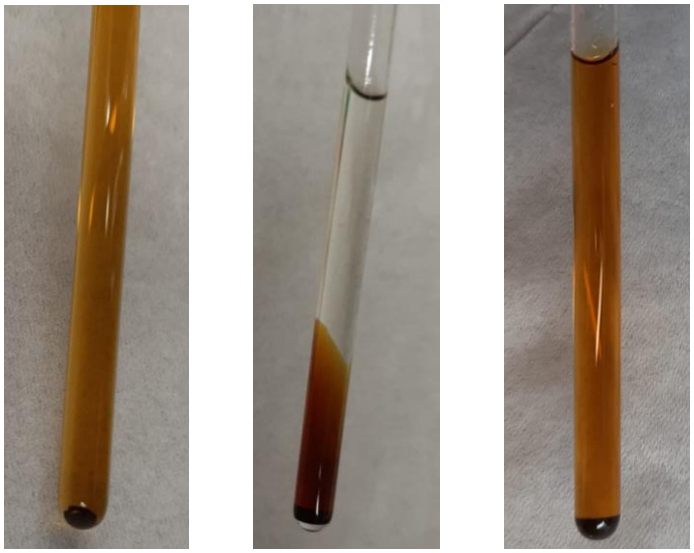


Figure S 43: Photographs of freshly prepared 1.0 : 1.0-mixtures of $[Ga(PhF)_2][pf]$ and CDP^{Ph} in *o*DFB (left), toluene (middle) and in PhF (right).

The amount of protonated ligand is reproducibly formed in flame dried Young-valve NMR tubes, flame sealed NMR tubes, HMDS-treated Youngvalve NMR tubes as well as in PFA tubes. As a consequence, the Si–OH groups of the glass surface are probably not the proton sources. It is noteworthy that the amount of protonated carbodiphosphorane increases slowly over time, as 16 % of protonated ligand were detected after eleven days at rt in *o*DFB (**Figure S 44**). Protonated ligand is formed in various solvents; however, the exact amount of $[H(CDP^{Ph})]^+$ formed is strongly solvent-dependant, as shown in **Table S 8**.

Table S 8: Amount of protonated carbodiphosphorane ligand observed *via* ^{31}P NMR in various solvents. It should be noted that in PhF and toluene, the formation of various phases is observed, which adds uncertainty to the results for these solvents.

Solvent	Amount of $[H(CDP^{Ph})]^+$ (relative to the total concentration of P-containing species in solution)
*o*DFB	11–14 %
PhF	6 %
Toluene	7 %
Diethylether	48 %
Acetonitrile	>97 %

Another conceivable proton-source is water. However, the solvents contained less than 8 ppm H_2O, according to Carl-Fischer titration. Additionally, it is important to note that the amount of $[H(CDP^{Ph})]^+$ in *o*DFB is independent of the $[Ga(PhF)_2][pf]$/CDP^{Ph}-concentration, since it does not significantly increase after dilution of a [**2**][*pf*]$_2$ solution with *o*DFB. This indicates that water or other impurities in the solvents most likely do not account for the formation of $[H(CDP^{Ph})]^+$. It should be noted that NMR spectra of CDP^{Ph} alone showed no signs of the protonation product or significant amounts of other side products in aromatic solvents (**Figure S 31**–**Figure S 33**). As a consequence, the formation of the protonated ligand must be related to the addition of gallium ions. In fact, our experiments show that the presence of the gallium ions alters the reactivity of CDP^{Ph}. This is underlined by the fact that pure CDP^{Ph} is hydrolyzed in the presence of water, giving $Ph_2P(O)CH{=}PPh_3$,[28] while addition of water to a [**2**][*pf*]$_2$ solution resulted in formation of protonated ligand $[H(CDP^{Ph})]^+$. Besides this, we observed complete protonation of the ligand in acetonitrile-solutions of $[Ga(PhF)_2][pf]$/CDP^{Ph} (1.0 : 1.0), whereas CDP^{Ph} showed no signs of protonation in acetonitrile since it is completely insoluble in this solvent. The strongly σ- and π-donating carbodiphosphorane could in part lead to the disproportionation of univalent gallium ions in solution, resulting in the formation of Ga^{III} and of elemental Ga^0, accounting for the precipitate. The thereby generated Ga^{III} ions would be much stronger Lewis acids and increase the reactivity of the superbasic CDP^{Ph}.

While the ^{1}H-signal of $[H(CDP^{Ph})]^+$ in toluene-d_8 is as intensive as in non-deuterated toluene (**Figure S 46** and **Figure S 47**), $[D(CDP^{Ph})]^+$ unambiguously forms in acetonitrile-d_3. It follows from the ^{31}P NMR and the ^{1}H-^{31}P HMBC in acetonitrile-d_3 that $[H(CDP^{Ph})]^+$ is formed. However, the intensity ratio of the $[\mathbf{H}(CDP^{Ph})]^+$ signal and of the aromatic protons is ca. 1 : 620 (instead of 1 : 30; **Figure S 50**), clearly underlining that the majority of the ligand is deuterated instead of protonated. Additionally, the ^{13}C NMR signal of the central C^{CDP} shows (**Figure S 52**) a triplet coupling pattern to ^{31}P (^1J =124.9 Hz) and to ^{2}D (^1J =23.7 Hz). Thus, we were able to show that cationic Gallium-CDP^{Ph} complexes are able to activate C–D and C–H bonds in solution.

As a consequence, we suggest that the species $[H(CDP^{Ph})]^+$ in *o*DFB is generated either by a bond activation of the solvent or, more likely, by an intra- or intermolecular C–H bond activation of the ligand in $\mathbf{2}^{2+}$ (or the monomeric species $[Ga(CDP^{Ph})]^+$) and that the side products of this reaction precipitate, so that they cannot be observed by NMR spectroscopy. As already pointed out, the simultaneous presence of a Lewis acidic Ga^+ ion and of the super basic CDP^{Ph} ligand is pivotal for the protonation of the ligand. Therefore, a frustrated Lewis pair mechanism, involving CDP^{Ph} and a Ga^+-solvent complex, may be operative.[44] Since the amount of protonated ligand is higher in donor-solvents, *i.e*. diethylether and acetonitrile (**Table S 8**) it is reasonable to assume that these solvents coordinate strongly to monomeric $[Ga(CDP^{Ph})]^+$, which increses the reactivity. The fact that the formation of the protonated ligand is less pronounced in toluene, PhF or *o*DFB may indicate that $\mathbf{2}^{2+}$ exists as a dimer in these aromatic solvents.

Interestingly, in *o*DFB, the amount of $[H(CDP^{Ph})]^+$ is virtually identical in the reaction solutions of $[Ga(PhF)_2][pf]$/CDP^{Ph}, in the supernatant solution over $[\mathbf{2}][pf]_2$ crystals and in solutions of dissolved $[\mathbf{2}][pf]_2$ crystals. Therefore, it cannot be ruled out that crystals of $[\mathbf{2}][pf]_2$ are obtained in pure form, but cannot easily be dissolved in a solvent without decomposition. The powder diffraction results (section 4) may suggest that the $[\mathbf{2}][pf]_2$ crystals are not phase pure; however, as already discussed, it is conceivable that trituration of the sample leads to structural changes, especially when taking into account the very weak GaGa double bond.

To conclude, the high basicity of the carbodiphosphorane and its increased reactivity in the presence of Ga^+ or Ga^{3+} probably prevents a clean synthesis of $[\mathbf{2}][pf]_2$ in various solvents and maybe also in the solid state. The exact mechanism of the formation of $[H(CDP^{Ph})]^+$ and the nature of the proton source is not understood yet. Investigations in this direction are hampered by the formation of various phases in solutions (in PhF and toluene) and of a precipitate.

It is well known that carbodiphosphoranes and carbodiphosphorane complexes are highly basic and thus readily protonated, *e.g*. when using halogenated hydrocarbons as solvents.[45] Generally, bond activation with carbodiphosphorane complexes are well known. For example, C–H activations in the *ortho* position of phenyl rings of CDP^{Ph} ligands have been reported for both transition metal complexes and main group adducts with CDP^{Ph} ligands (*e.g*. CDP^{Ph}–Rh,[46,47] CDP^{Ph}–Pt[46–48] and CDP^{Ph}–P complexes).[49]

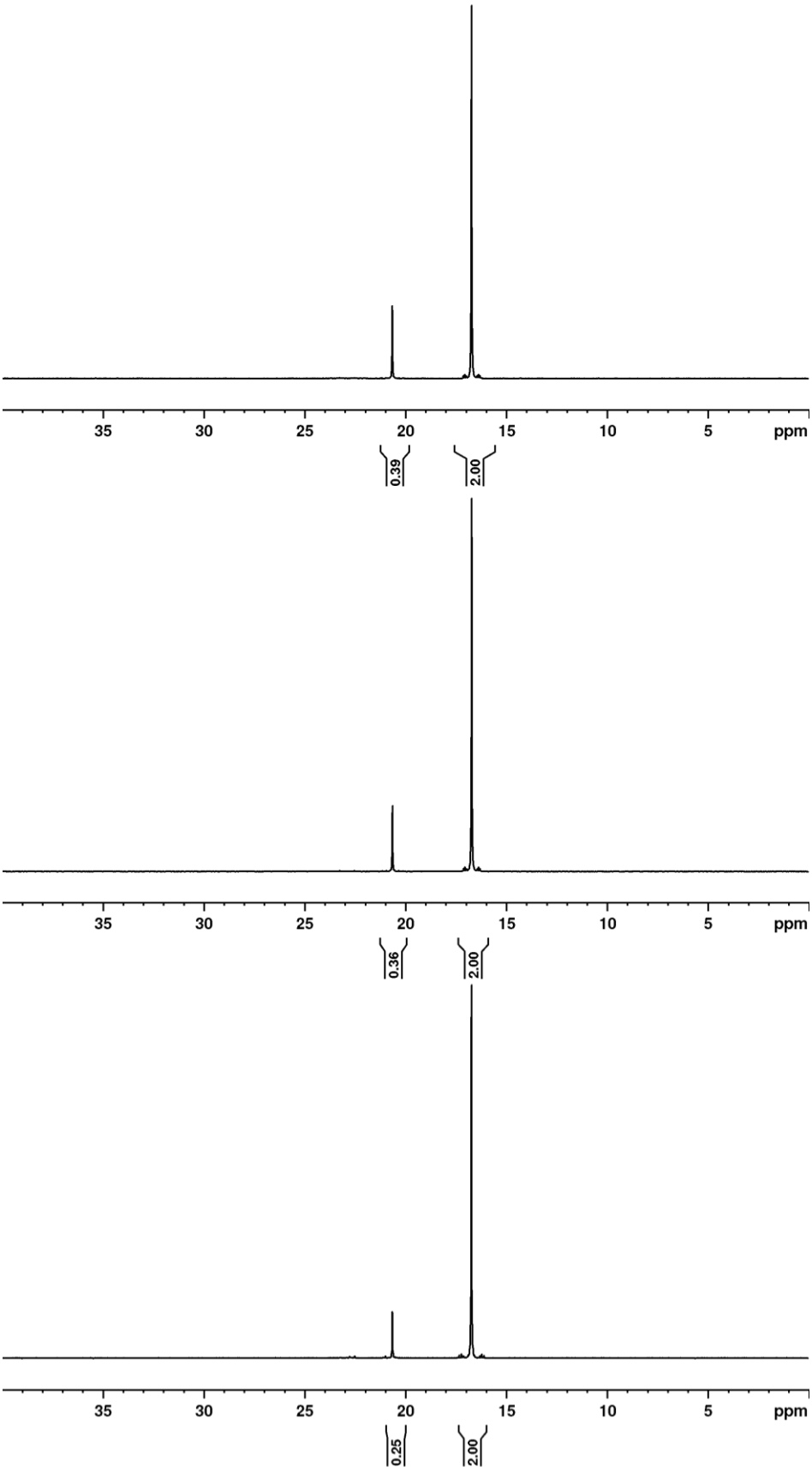


Figure S 44: From bottom to top: $^{31}P\{^{1}H\}$ NMR spectrum (81.01 MHz, *o*DFB, 298 K), $^{31}P\{^{1}H\}$ NMR spectrum (121.52 MHz, *o*DFB, 298 K) and $^{31}P\{^{1}H\}$ NMR spectrum (81.01 MHz, *o*DFB, 298 K) of a mixture of $[Ga(PhF)_2][pf]$ and CDP^{Ph} (1.0 : 1.0) directly after mixing the components, 2 days after mixing the components and 3 months after mixing the components, respectively.

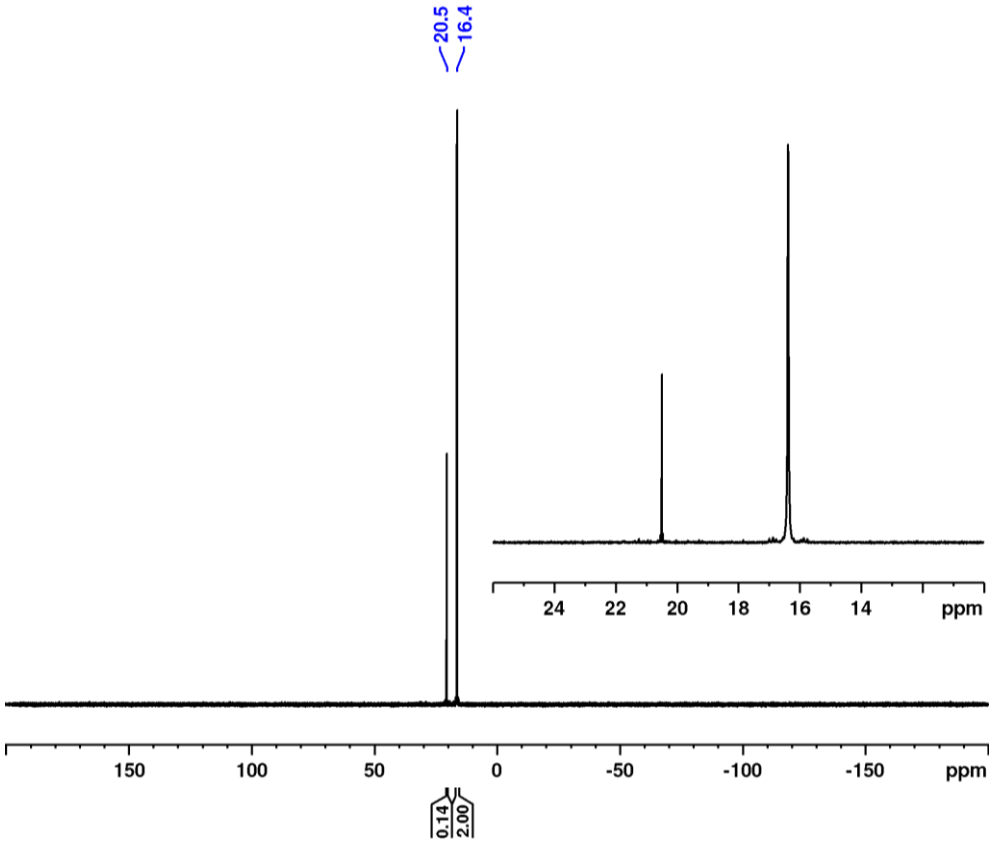


Figure S 45: $^{31}P\{^{1}H\}$-NMR spectrum (81.01 MHz, PhF, 298 K) of a mixture of $[Ga(PhF)_2][pf]$ and CDP^{Ph} (1.0 : 1.0).

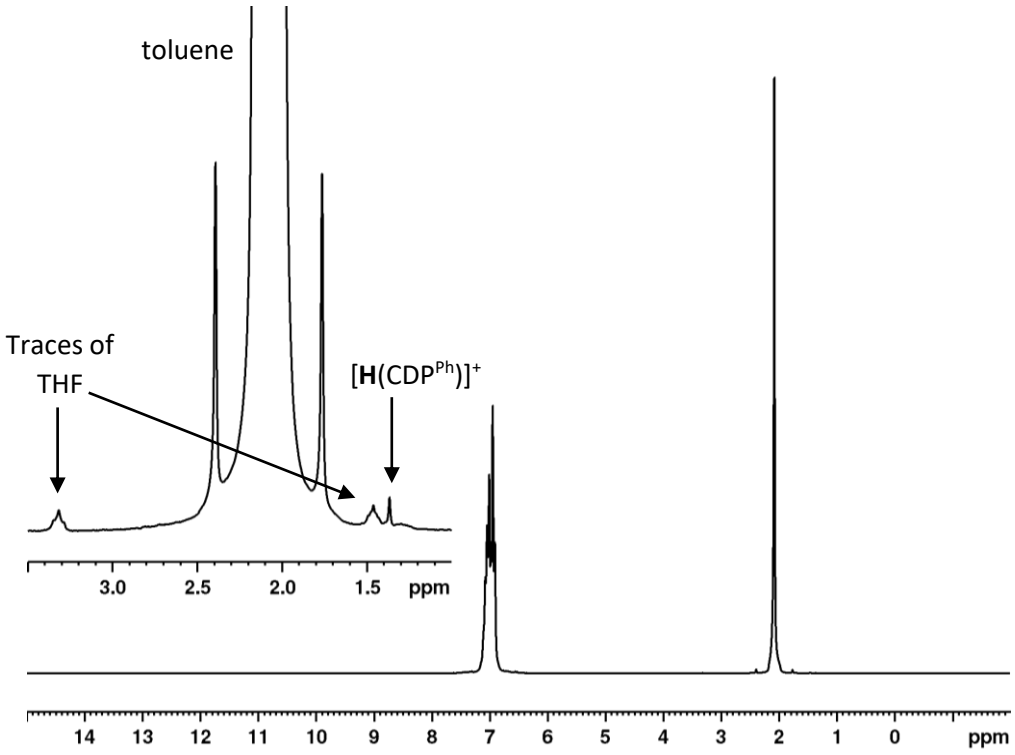


Figure S 46: $^{1}H\{^{31}P\}$-NMR spectrum (200.13 MHz, toluene, 298 K) of a mixture of $[Ga(PhF)_2][pf]$ and CDP^{Ph} (1.0 : 1.0; spectrum).

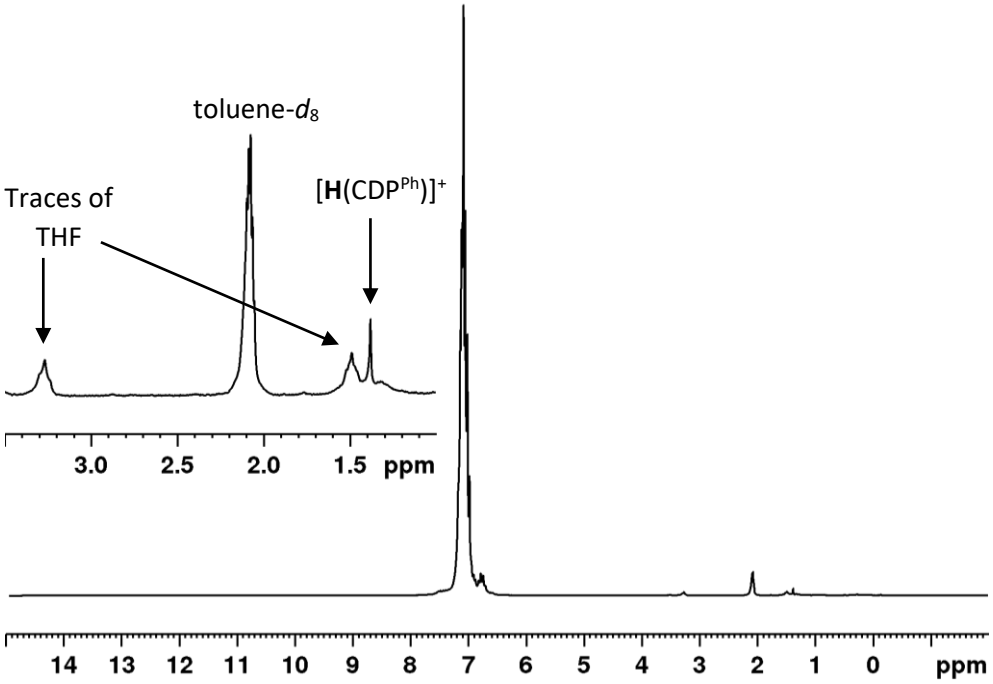


Figure S 47: ^{1}H{^{31}P}-NMR spectrum (200.13 MHz, toluene-d_8, 298 K) of a mixture of [Ga(PhF)$_2$][*pf*] and CDP^{Ph} (1.0 : 1.0).

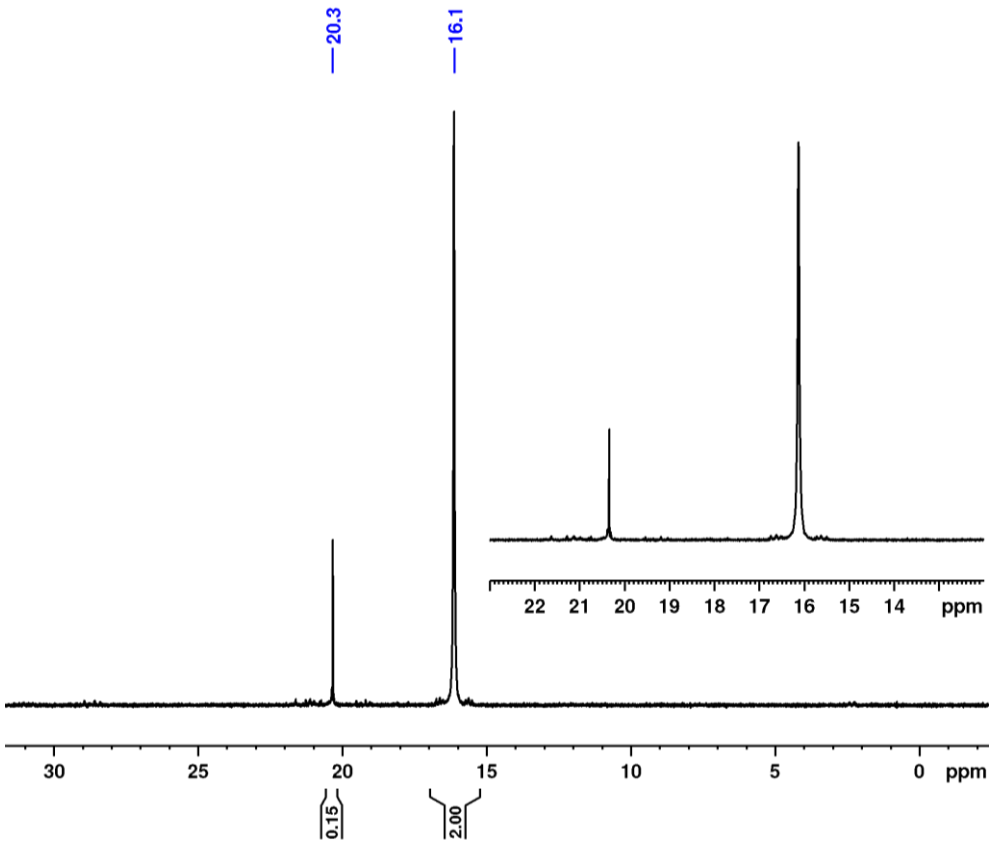


Figure S 48: ^{31}P{^{1}H}-NMR spectrum (81.01 MHz, toluene-d_8, 298 K) of a mixture of [Ga(PhF)$_2$][*pf*] and CDP^{Ph} (1.0 : 1.0).

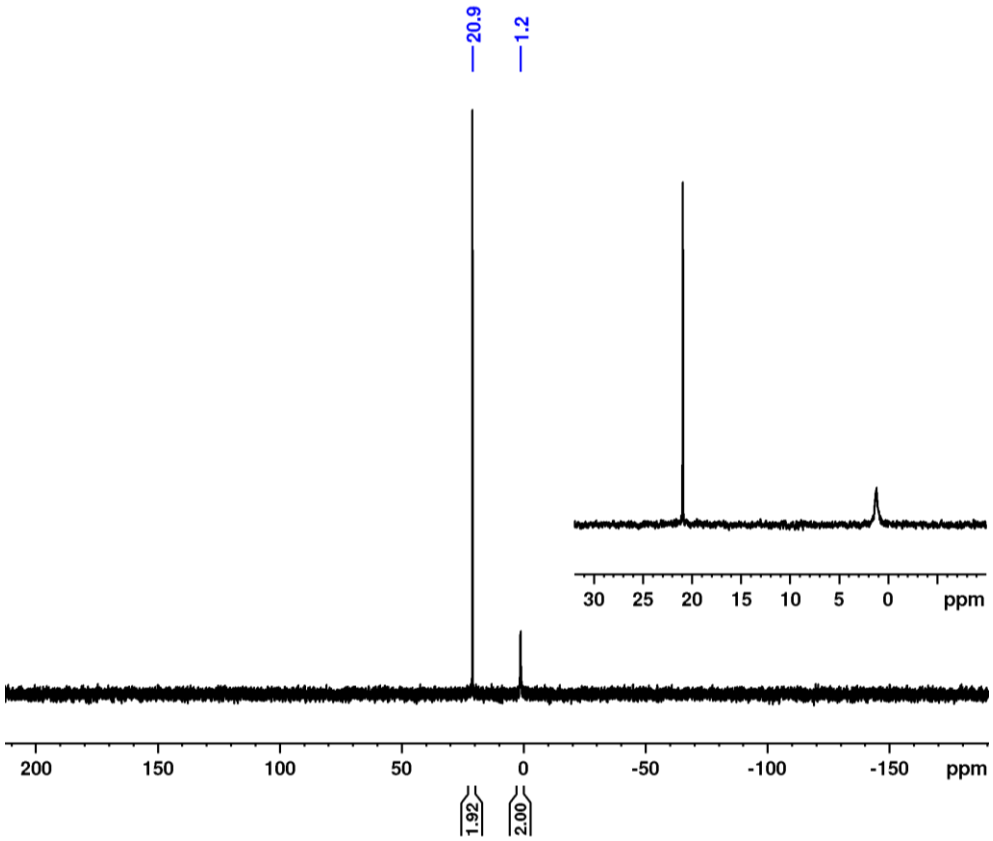


Figure S 49: $^{31}P\{^{1}H\}$-NMR spectrum (121.52 MHz, Et_2O, 298 K) of a $[Ga(PhF)_2][pf]$/CDP^{Ph} (1.0 : 1.0) mixture.

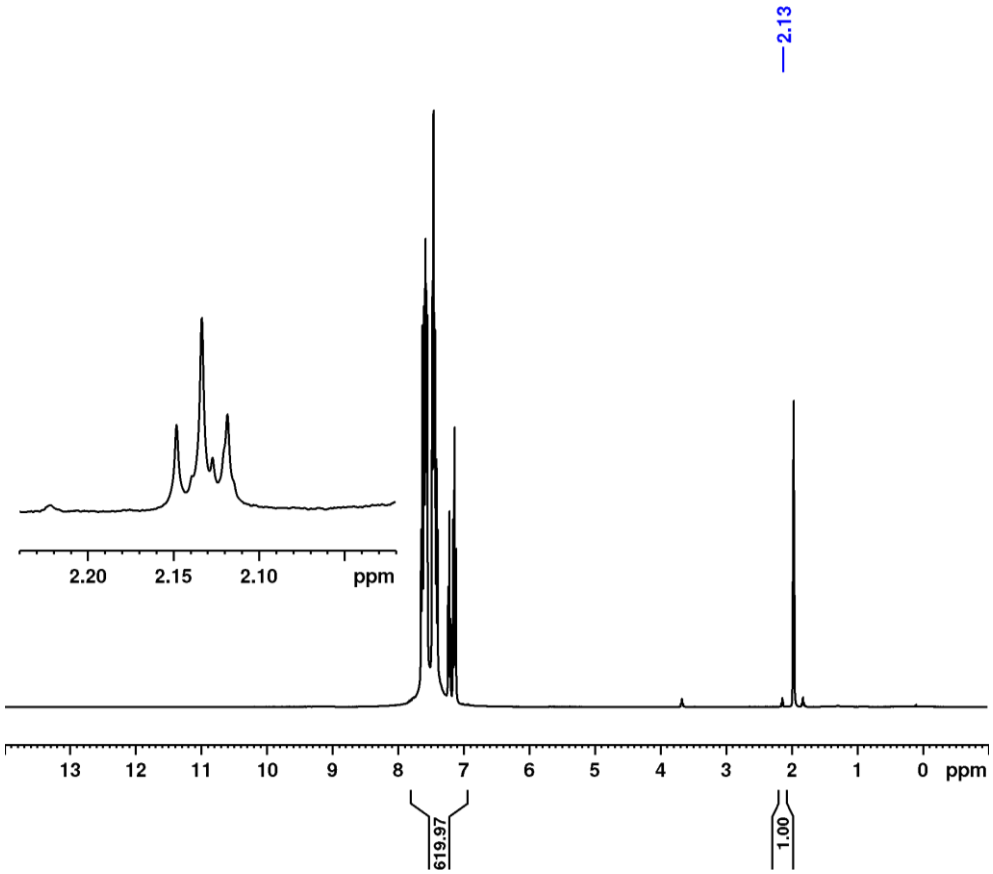


Figure S 50: ^{1}H-NMR spectrum (400.17 MHz, acetonitrile-d_3, 298 K) of a [Ga(PhF)$_2$][*pf*]/CDP^{Ph} (1.0 : 1.0) mixture.

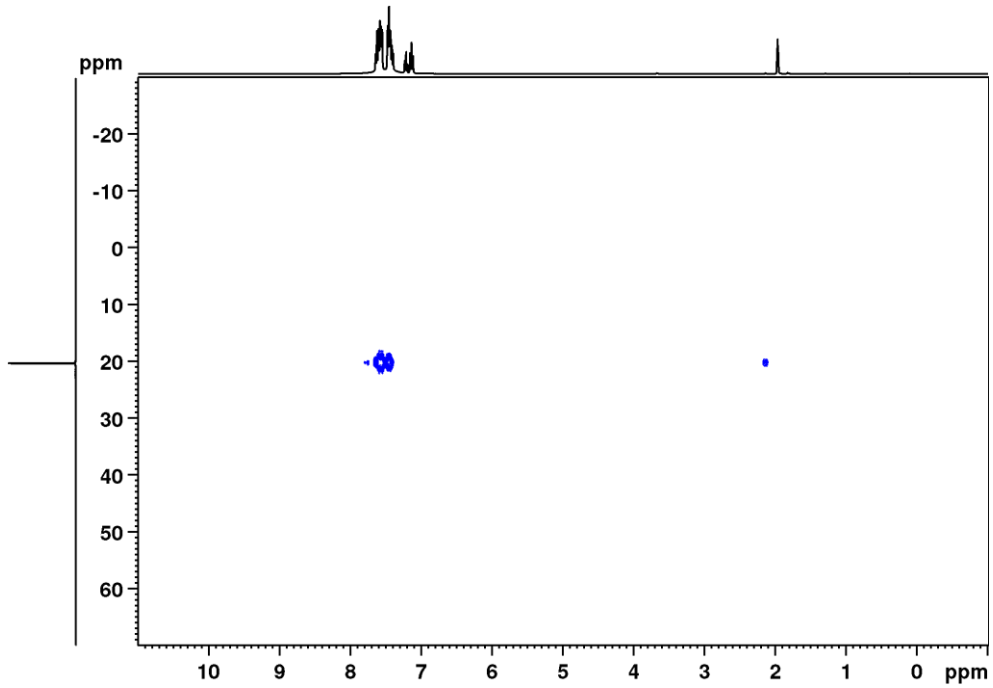


Figure S 51: ^{1}H,^{31}P-HMBC NMR spectrum (400.17 MHz, acetonitrile-d_3, 298 K, optimized for J = 15 Hz) of a [Ga(PhF)$_2$][*pf*]/CDP^{Ph} (1.0 : 1.0) mixture.

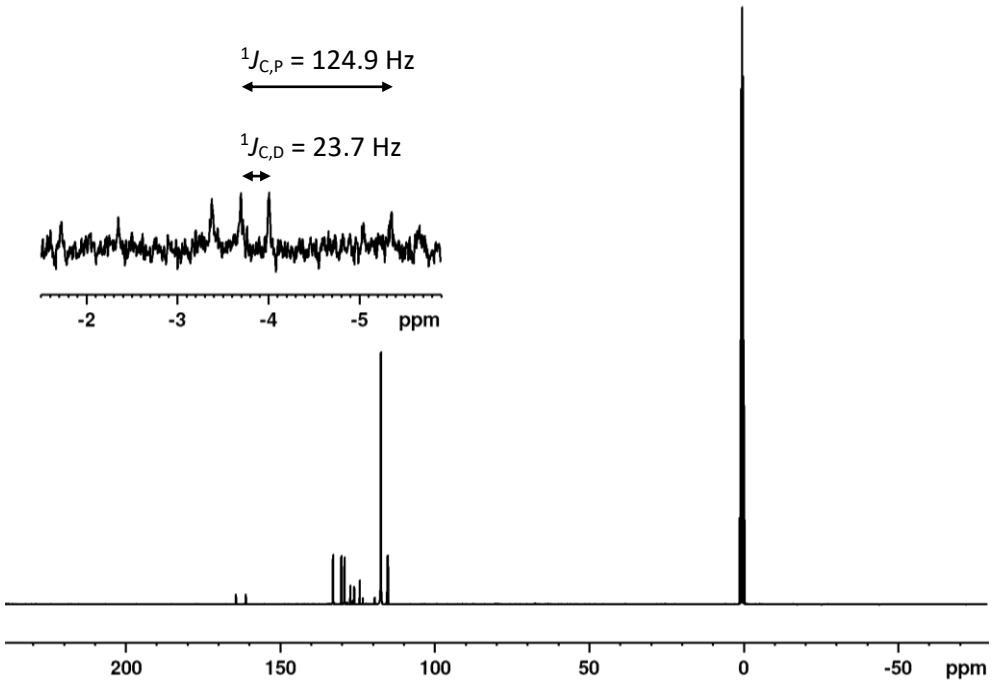


Figure S 52: $^{13}C\{^1H\}$-NMR spectrum (75.48 MHz, acetonitrile-d_3, 298 K) of a [Ga(PhF)$_2$][*pf*]/CDP^{Ph} (1.0 : 1.0) mixture. The enlarged part of the spectrum (top left) shows the coupling pattern of the ^{13}C signal of the central C^{CDP}.

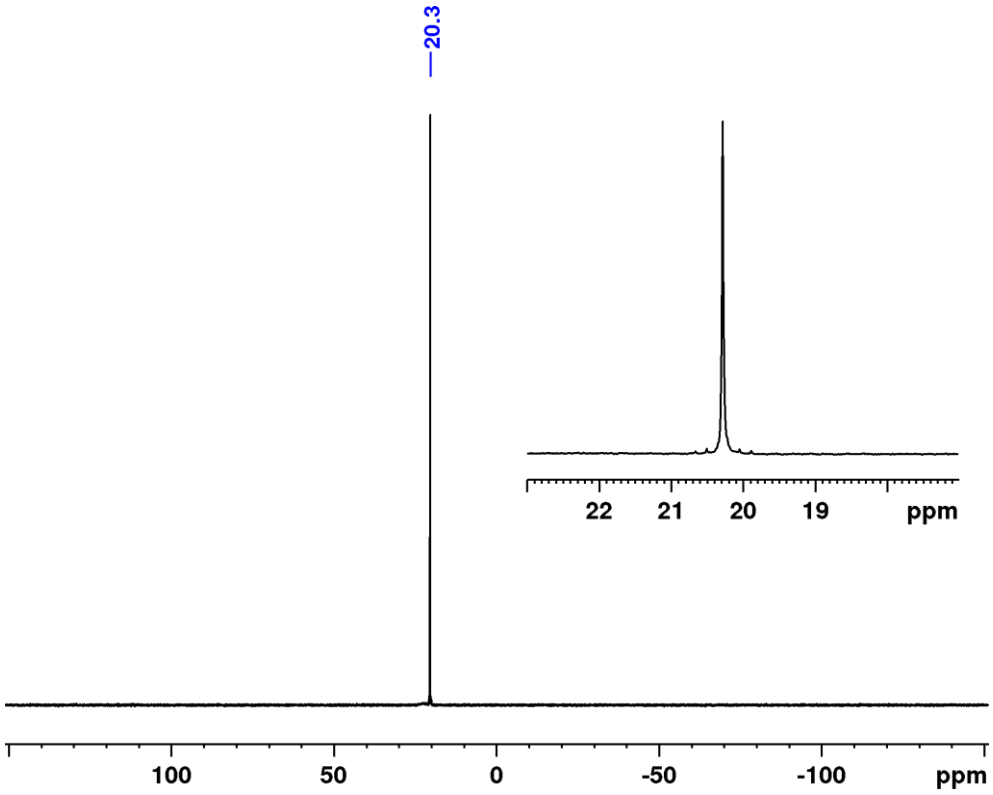


Figure S 53: $^{31}P\{^1H\}$-NMR spectrum (161.99 MHz, acetonitrile-d_3, 298 K) of a [Ga(PhF)$_2$][*pf*]/CDP^{Ph} (1.0 : 1.0) mixture.

5.8 Comparison of NMR shifts and Coupling Constants in CDP^{Ph} and $[\{Ga(CDP^{Ph})\}_x]^{x+}$

The different chemical shifts and coupling constants in **Table S 9** and **Table S 10** clearly confirm that CDP^{Ph} coordinates to Ga^+ in solution.

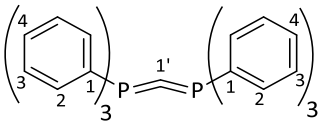


Table S 9: Chemical shifts and coupling constants for CDP^{Ph} in *o*DFB.

Group	δ(^{1}H) [ppm]	δ(^{13}C) [ppm]	δ(^{31}P) [ppm]	$J_{H,P}$	$J_{C,P}$	$J_{P,P}$
1	-	137.5	-	-	$^1J_{\mathbf{C}^1,P}$ = 48.0 Hz	-
2	7.76	132.1	-	$^2J_{C^2\mathbf{H},P}$ = 12.4 Hz	$^2J_{\mathbf{C}^2,P}$ = 5.3 Hz	-
3	7.20	129.0	-	not resolved	$^3J_{\mathbf{C}^3,P}$ = 5.9 Hz	-
4	7.13	127.3	-	not resolved	$^4J_{\mathbf{C}^4,P}$ = 1.4 Hz	-
1′	-	12.4	-	-	$^1J_{\mathbf{C}^{1'},P}$ = 121.0 Hz	-
P	-	-	–3.9	-	-	$^2J_{\mathbf{P},P}$ = 9.0 Hz

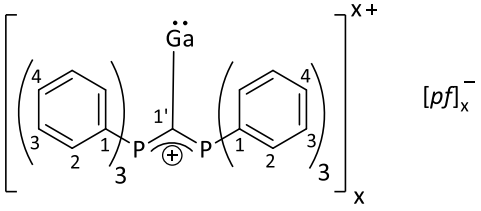


Table S 10: Chemical shifts and coupling constants for $[\{Ga(CDP^{Ph})\}_x][pf]_x$ (x = 1 or 2) in *o*DFB.

Group	δ(^{1}H) [ppm]	δ(^{13}C) [ppm]	δ(^{31}P) [ppm]	$J_{H,P}$	$J_{C,P}$	$J_{P,P}$
1	-	137.5	-	-	$^1J_{\mathbf{C}^1,P}$ = 90.5 Hz	-
2	7.44	132.6	-	not resolved	not resolved	-
3	7.32	128.9	-	not resolved	not resolved	-
4	7.44	not detected	-	not resolved	not resolved	-
1′	-	53.6	-	-	$^1J_{\mathbf{C}^{1'},P}$ = 64.5 Hz	-
P	-	-	16.7	-	-	$^2J_{\mathbf{P},P}$ = 8.9 Hz

5.9 DOSY Measurements

DOSY-NMR spectra with a stimulated echo impulse sequence were measured for solutions of LiNacNac^{Mes}, [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5*o*DFB) and [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([**2**][*pf*]$_2$) in *o*DFB at rt. Calibration of the diffusion coefficients was performed with respect to a solution of D_2O (98.9 %), H_2O (1 %), MeOH (0.1 %) and $GdCl_3$ (0.1 mg).[50] The results are summarized in **Table S 11**.

Table S 11: Diffusion coefficients of different species in an *o*DFB solution at rt. Diffusion coefficients were determined with ^{1}H DOSY NMR experiments (for LiNacNac^{Mes} and **1**$^{2+}$), ^{19}F DOSY NMR experiments (for the [*pf*]$^-$ anion) and ^{31}P DOSY NMR experiments (for the CDP^{Ph} complexes).

Entry	Species	Diffusion Coefficient [10^{-10} m^2 s^{-1}]
1	LiNacNac^{Mes}	6.433±0.003
2	**1**$^{2+}$	4.503±0.002
3	[H(CDP^{Ph})]$^+$	1.004±0.002[a)]
4	[{Ga(CDP^{Ph})}$_x$]$^{x+}$ (x = 1 or 2)	1.084±0.001[a)]
5	[*pf*]$^-$	6.438±0.008[a)]

a) ^{19}F and ^{31}P DOSY NMR measured in the same NMR sample of crystalline [**2**][*pf*] in *o*DFB.

It follows from the diffusion coefficients of LiNacNac^{Mes} and **1**$^{2+}$ (entry 1 and 2 in **Table S 11**) that the intact dimer **1**$^{2+}$ exists in solution, which is in line with quantum chemical calculations (section 8.1).

The dissociation behavior of **2**$^{2+}$ is more ambiguous. On the one hand, the diffusion coefficients obtained for the side product [H(CDP^{Ph})]$^+$ and the putative **2**$^{2+}$ or [Ga(CDP^{Ph})]$^+$ (entry 3 and 4 in **Table S 11**) are very similar, which may suggest that monomeric [Ga(CDP^{Ph})]$^+$ is present in *o*DFB. On the other hand, the diffusion coefficient of the Ga-CDP^{Ph} complex is significantly smaller than the diffusion coefficient of the [*pf*]$^-$ anion (entry 4 and 5 in **Table S 11**). The thermochemical volumes found in the solid state for the [*pf*]$^-$ anion (ca. 720 Å^3, on the basis of the volumes for the alkali metal-*pf* salts)[51] and for **2**$^{2+}$ (ca. 1460 Å^3 as calculated from the latter value and the volume for [**2**][*pf*]$_2$, see **Table S 1**) clearly are in better agreement with the dimer in solution. It cannot be ruled out that the CDP^{Ph} ligands in [H(CDP^{Ph})]$^+$ and [{Ga(CDP^{Ph})}$_x$]$^{x+}$ (x = 1 or 2) undergo ligand exchange or that monomeric [Ga(CDP^{Ph})]$^+$ and dimeric **2**$^{2+}$ are in chemical equilibrium, which stresses the need to be cautious about the interpretation of these diffusion coefficients. Thus, the ^{31}P-DOSY experiments did not allow to clarify whether **2**$^{2+}$ dissociates in solution, while quantum chemical calculations suggest that monomer and dimer are similarly stable in *o*DFB, but that the dimerization is thermodynamically slightly favored (section 8.1).

6 Vibrational Spectroscopy

In **Figure S 54**–**Figure S 58**, the experimental vibrational spectra of [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([**1**][*pf*]$_2$ · 1.5*o*DFB), [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([**2**][*pf*]$_2$) and [In(CDP^{Ph})][*pf*] are compared with the calculated spectra of the cations, calculated spectra of possible cationic side products and the experimental spectra of NO[*pf*]. The spectrum of NO[*pf*] is displayed in order to show the vibrations dedicated to the anion.

6.1 [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([1][*pf*]$_2$ · 1.5*o*DFB)

IR (Diamond-ATR): $\tilde{\nu}$ [cm^{-1}] = 3615 (vw), 3408 (vw), 2931 (vw), 1648 (vw), 1609 (vw), 1546 (vw), 1517 (vw), 1478 (vw), 1442 (vw), 1350 (vw), 1298 (w), 1274 (m), 1240 (m), 1211 (vs), 1171 (w), 1034 (vw), 1026 (vw), 970 (vs), 889 (vw), 857 (vw), 831 (vw), 755 (vw), 726 (vs), 662 (vw), 560 (vw), 536 (w), 443 (w), 415 (vw). **FT-Raman**: $\tilde{\nu}$ [cm^{-1}] = 3034 (vw), 2939 (vw), 2750 (vw), 2124 (vw), 1676 (vw), 1610 (vw), 1478 (vw), 1386 (vw), 1309 (w), 1226 (vw), 1159 (vw), 970 (vw), 797 (w), 745 (w), 646 (w), 575 (m), 528 (m), 412 (m), 363 (m), 321 (s), 285 (s), 215 (s), 138 (s), 104 (vs).

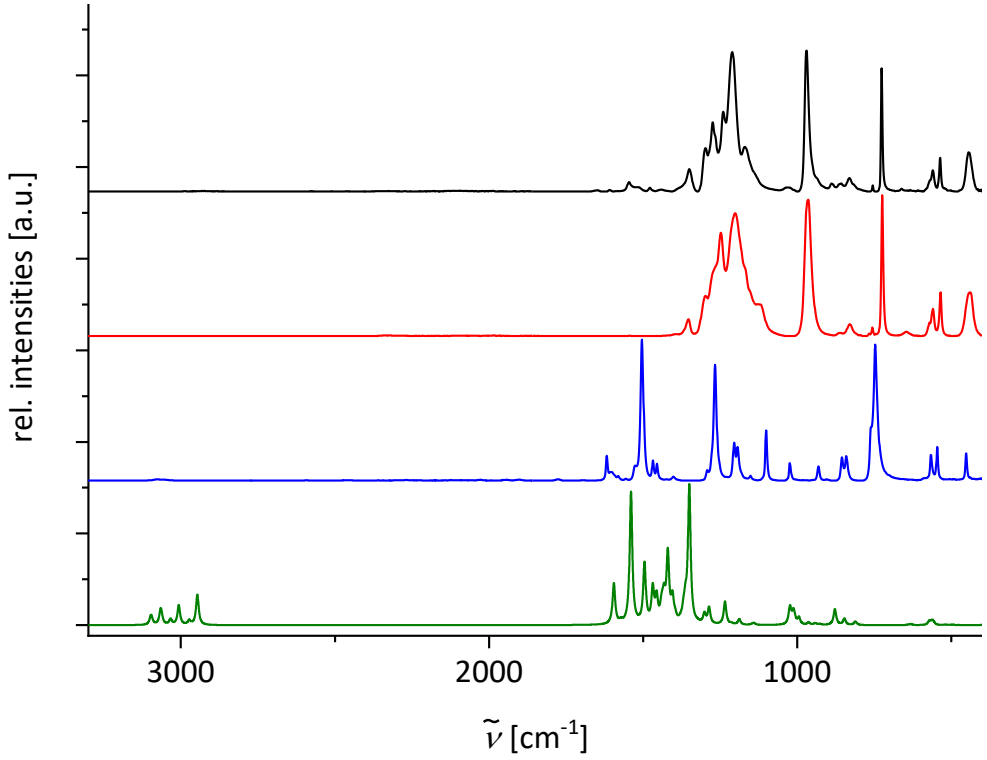


Figure S 54: Comparison of the experimental IR spectra of [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB (black), NO[*pf*] (red) and *o*DFB (blue) with the calculated IR spectra (RI-BP86(D3BJ)/def2-TZVPP) of [{Ga(NacNac^{Mes})}$_2$]$^{2+}$ (green).

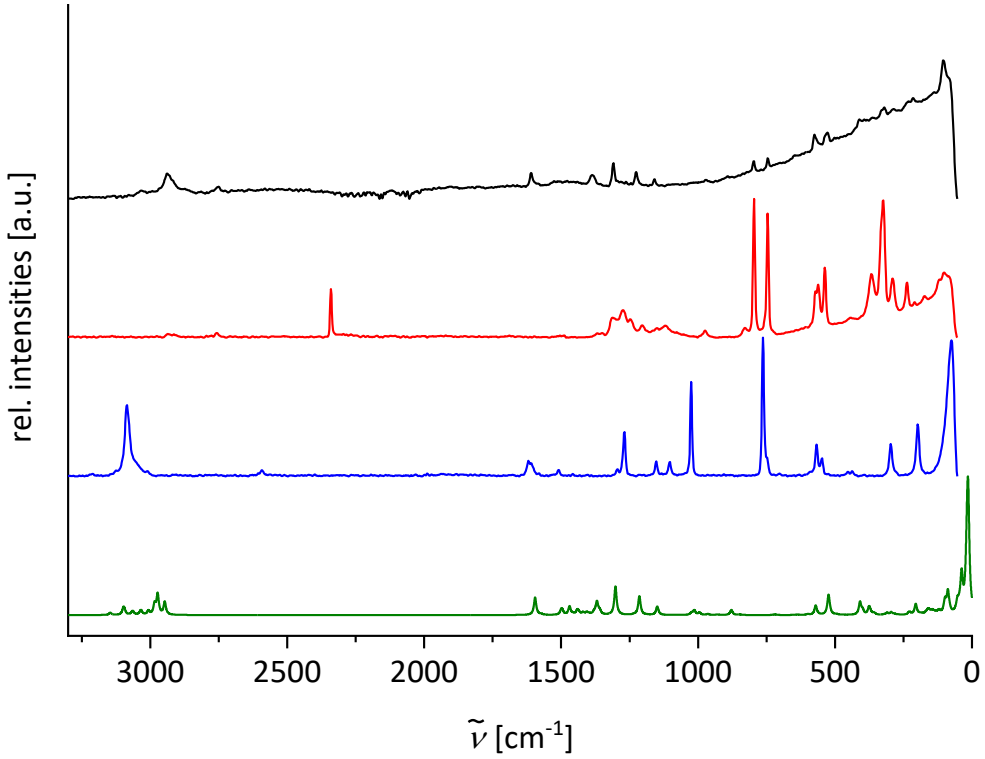


Figure S 55: Comparison of the experimental Raman spectra of [**1**][*pf*]$_2$ · 1.5*o*DFB (black), NO[*pf*] (red) and *o*DFB (blue) with the calculated IR spectra (RI-BP86(D3BJ)/def2-TZVPP) of $\mathbf{1}^{2+}$ (green).

Table S 12: IR and Raman bands with the assignment of the respective vibration modes in [**1**][*pf*]$_2$ · 1.5*o*DFB.

[1][*pf*]$_2$ · 1.5*o*DFB		Assignment
IR	**Raman**	
-	104 (vs)	C–C ([*pf*]$^-$)[a]
-	138 (s)	-
-	215 (s)	C–C, Al–O, O–C ([*pf*]$^-$)[a]
-	285 (s)	C–C ([*pf*]$^-$)[b]
-	321 (s)	C–C, Al–O ([*pf*]$^-$)[b]
-	363 (m)	Al–O, O–C ([*pf*]$^-$)[a]
415 (vw)	412 (m)	Ga–Ga, Ga–N, C–C (mesityl, NacNac)[a]
443 (w)	-	O–C, Al–O, C–F ([*pf*]$^-$)[a]
536 (w)	528 (m)	C–C, C–O ([*pf*]$^-$)[b]
560 (vw)	-	C–C, Al–O ([*pf*]$^-$)[b]
-	575 (m)	C–C, Al–O ([*pf*]$^-$)[b]
-	646 (w)	C–C. C–H (NacNac)[a]
662 (vw)	-	-
726 (vs)	-	C–C, C–O ([*pf*]$^-$)[b]
-	745 (w)	C–H (*o*DFB)[a]
755 (vw)	-	C–C, C–O ([*pf*]$^-$)[b]
-	797 (w)	Al–O, C–C, C–F ([*pf*]$^-$)[a]
831 (vw)	-	Al–O, C–C ([*pf*]$^-$)[b]
857 (vw)	-	C–H (mesityl)[a]
889 (vw)	-	C–H (*o*DFB)[a]

970 (vs)	970 (vw)	C–C, C–F ([*pf*]$^-$)[b]
1026 (vw)	-	C–H, C–C (*o*DFB)[a], C–C (mesityl, NacNac)[a]
1034 (vw)	-	C–C (mesityl, NacNac)[a]
-	1159 (vw)	C–C, C–F ([*pf*]$^-$)[a]
1171 (w)	-	C–C, C–F ([*pf*]$^-$)[a]
1211 (vs)	-	C–H, C–C (mesityl),[a] N–C, N–Ga, C–C, C–F ([*pf*]$^-$)[b]
-	1226 (vw)	C–N, C–H (mesityl, NacNac)[a]
1240 (m)	-	C–H (mesityl),[a] C–C, C–F ([*pf*]$^-$)[b]
1274 (m)	-	C–N, C–C (mesityl),[a] C–C, C–F ([*pf*]$^-$)[b]
1298 (w)	-	C–H (NacNac),[a] C–C (mesityl),[a] C–C, C–F ([*pf*]$^-$)[b]
-	1309 (w)	C–C (mesityl)[a]
1350 (vw)	-	C–H, C–C, C–N (NacNac),[a] C–C, C–F ([*pf*]$^-$)[b]
1442 (vw)	-	C–H (mesityl CH_3 groups)[a]
1478 (vw)	1478 (vw)	C–H, C–C (mesityl)[a]
1517 (vw)	-	C–H, C–C, C–F (*o*DFB)[a]
1546 (vw)	-	C–H, C–C (NacNac)[a]
1609 (vw)	1610 (vw)	C–C (mesityl)[a]
1648 (vw)	-	-
-	1676 (vw)	-
-	2124 (vw)	-
-	2750 (vw)	-
2931 (vw)	2939 (vw)	C–H (mesityl CH_3 groups)[a]
-	3034 (vw)	C–H (mesityl CH_3 groups)[a]
3408 (vw)	-	-
3615 (vw)	-	-

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 8.14). b) Assignments based on literature values.[52–54]

6.2 [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([2][*pf*]$_2$)

IR (Diamond-ATR): $\tilde{\nu}$ [cm^{-1}] = 3070 (vw), 2975 (vw), 1589 (vw), 1483 (vw), 1438 (vw), 1351 (vw), 1297 (w), 1274 (m), 1238 (m), 1211 (vs), 1167 (w), 1102 (w), 1069 (vw), 1026 (vw), 997 (vw), 969 (vs), 832 (vw), 778 (w), 754 (vw), 739 (w), 726 (vs), 691 (m), 678 (w), 618 (vw), 571 (vw), 559 (vw), 536 (vw), 526 (m), 500 (m), 442 (w), 386 (vw). **FT-Raman**: $\tilde{\nu}$ [cm^{-1}] = 3064 (w), 2938 (vw), 1589 (w), 1575 (vw), 1297 (vw), 1188 (vw), 1164 (vw), 1101 (vw), 1030 (w), 1001 (m), 842 (vw), 797 (vw), 746 (vw), 618 (vw), 574 (vw), 322 (vw), 234 (vw), 200 (vw), 173 (vw), 154 (vw), 81 (vs).

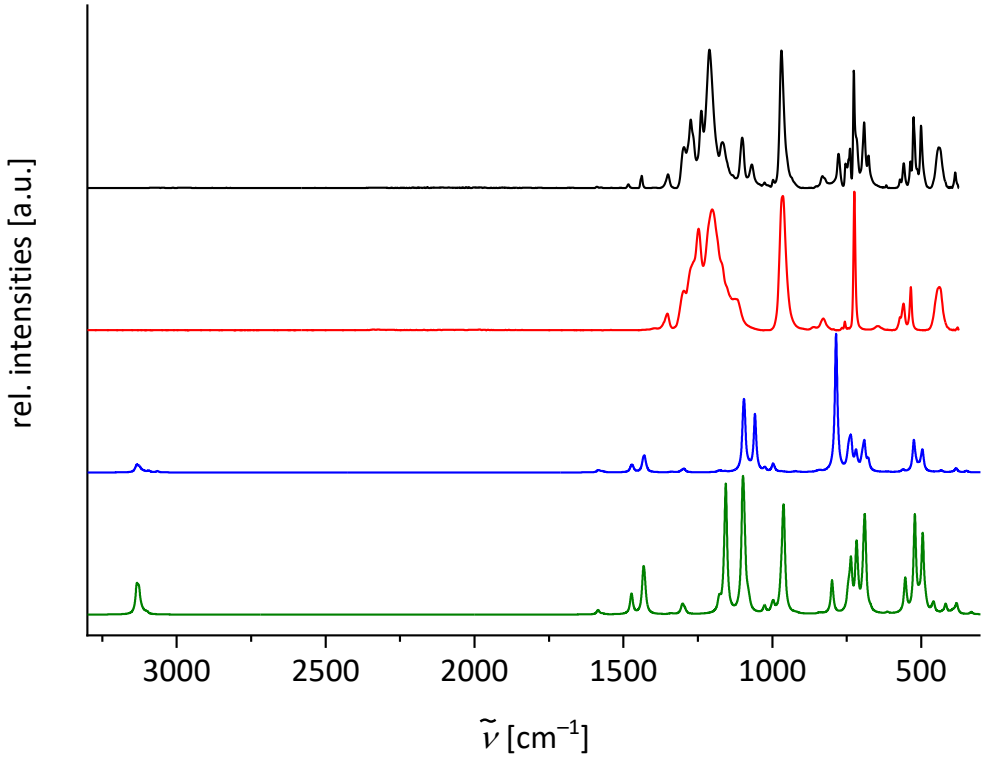


Figure S 56: Comparison of the experimental IR spectra of putative [**2**][*pf*]$_2$ (black) and NO[*pf*] (red) with the calculated IR spectra (RI-BP86(D3BJ)/def2-TZVPP) of **2**$^{2+}$ (blue) and [H(CDP^{Ph})]$^+$ (green).

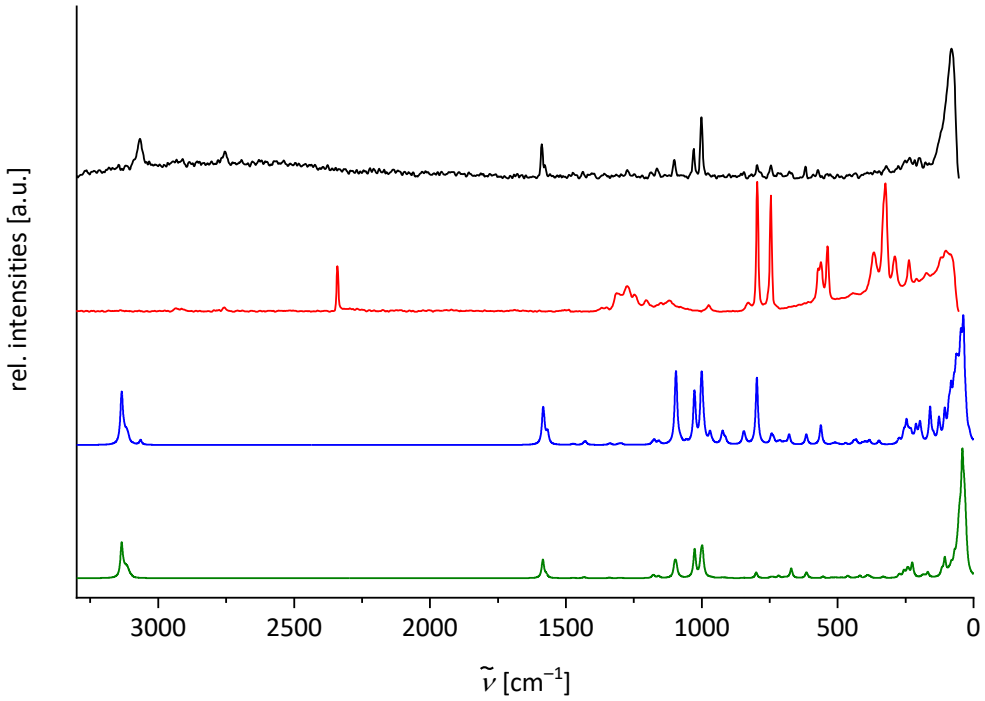


Figure S 57: Comparison of the experimental Raman spectra of putative [**2**][*pf*]$_2$ (black) and NO[*pf*] (red) with the calculated IR spectra (RI-BP86(D3BJ)/def2-TZVPP) of **2**$^{2+}$ (blue) and [H(CDP^{Ph})]$^+$ (green).

Table S 13: IR and Raman bands with the assignment of the respective vibration modes in [**2**][*pf*]$_2$.

[**2**][*pf*]$_2$		**Assignment**
IR	**Raman**	
-	81 (vs)	C–C ([*pf*]$^-$)[a]
-	154 (vw)	Ga–Ga, P–C (CDP)[a]
-	173 (vw)	-
-	200 (vw)	P–C, C–C (CDP)[a]
-	234 (vw)	P–C, C–C (CDP)[a]
-	322 (vw)	C–C, Al–O ([*pf*]$^-$)[b]
386 (vw)	-	C–O ([*pf*]$^-$)[a]
442 (w)	-	C–O, Al–O ([*pf*]$^-$)[a]
500 (m)	-	P–C, C–C, C–H (CDP)[a]
526 (m)	-	P–C, C–C, C–H (CDP)[a]
536 (vw)	-	C–C, C–O ([*pf*]$^-$)[b]
559 (vw)	-	C–C, Al–O ([*pf*]$^-$)[b]
571 (vw)	574 (vw)	C–C, Al–O ([*pf*]$^-$)[b]
618 (vw)	618 (vw)	C–C (CDP)[a]
678 (w)	-	C–Ga, C–C, C–P (CDP)[a]
691 (m)	-	C–C, C–H (CDP)[a]
726 (vs)	-	C–C, C–O ([*pf*]$^-$)[b]
739 (w)	-	C–H (CDP)[a]
-	746 (vw)	C–H (CDP)[a]
754 (vw)	-	C–C, C–O ([*pf*]$^-$)[b]
778 (w)	-	-
-	797 (vw)	C–Ga, C–C, C–P (CDP)[a]
832 (vw)	-	C–C, Al–O ([*pf*]$^-$)[b]

-	842 (vw)	C–H (CDP)[a]
969 (vs)	-	C–C, C–F ([*pf*]$^-$)[b]
997 (vw)	1001 (m)	C–C, C–H (CDP)[a]
1026 (vw)	1030 (w)	C–C, C–H (CDP)[a]
1069 (vw)	-	C–C, C–H (CDP)[a]
1102 (w)	1101 (vw)	C–C, C–H, C–P (CDP)[a]
1167 (w)	1164 (vw)	C–H (CDP)[a]
-	1188 (vw)	C–H (CDP)[a]
1211 (vs)	-	C–C, C–F ([*pf*]$^-$)[b]
1238 (m)	-	C–C, C–F ([*pf*]$^-$)[b]
1274 (m)	-	C–C, C–F ([*pf*]$^-$)[b]
1297 (w)	1297 (vw)	C–C, C–F ([*pf*]$^-$)[b]
1351 (vw)	-	C–C, C–F ([*pf*]$^-$)[b]
1438 (vw)	-	C–C, C–H (CDP)[a]
1483 (vw)	-	C–C, C–H (CDP)[a]
-	1575 (vw)	C–C, C–H (CDP)[a]
1589 (vw)	1589 (w)	C–C, C–H (CDP)[a]
-	2938 (vw)	-
2975 (vw)	-	-
3070 (vw)	3064 (w)	C–H (CDP)[a]

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 8.14). b) Assignments based on literature values.[52–54]

6.3 [In(CDP^{Ph})][*pf*]

FT-Raman: $\tilde{\nu}$ [cm^{-1}] = 3596 (vw), 3538 (vw), 3063 (w), 3046 (vw), 1590 (w), 1576 (vw), 1488 (vw), 1327 (vw), 1309 (vw), 1103 (vw), 1031 (w), 1002 (m), 796 (vw), 767 (vw), 745 (vw), 664 (vw), 618 (vw), 565 (vw), 530 (vw), 320 (vw), 252 (vw), 231 (vw), 204 (vw), 189 (vw), 80 (vs).

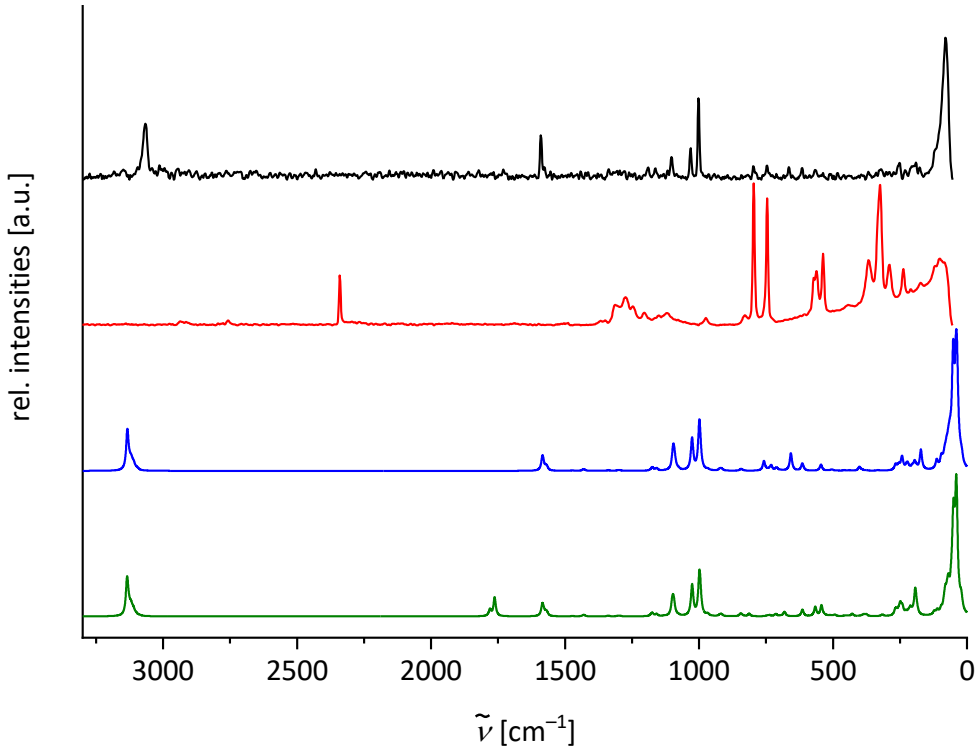


Figure S 58: Comparison of the experimental Raman spectrum of [In(CDP^{Ph})][*pf*] (black), and NO[*pf*] (red) and calculated Raman spectra (RI-BP86(D3BJ)/def2-TZVPP) of [In(CDP^{Ph})]$^+$ (blue) and [H$_2$In(CDP^{Ph})]$^+$ (green).

Table S 14: Raman bands with the assignment of the respective vibration modes in [In(CDP^{Ph})][*pf*].

[In(CDP^{Ph})][*pf*]$_2$ Raman	**Assignment**
80 (vs)	C–C (CDP and [*pf*]$^-$)[a]
189 (vw)	P–C (CDP)[a]
204 (vw)	P–C, C–C (CDP)[a]
231 (vw)	P–C, C–C (CDP)[a]
252 (vw)	P–C, C–C (CDP)[a]
320 (vw)	C–C, Al–O ([*pf*]$^-$)[b]
530 (vw)	P–C, C–C, C–H (CDP)[a]
565 (vw)	C–C, Al–O ([*pf*]$^-$)[b]
618 (vw)	C–C (CDP)[a]
664 (vw)	-
745 (vw)	C–C (CDP)[a]
767 (vw)	C–C, C–F, Al–O, C–O ([*pf*]$^-$)[a]
796 (vw)	C–C, C–P (CDP)[a]
1002 (m)	C–C, C–H (CDP)[a]
1031 (w)	C–C, C–H (CDP)[a]
1103 (vw)	C–C, C–H, C–P (CDP)[a]
1309 (vw)	C–C, C–H, C–P (CDP)[a]
1327 (vw)	C–C, Al–O, C–O ([*pf*]$^-$)[a]
1488 (vw)	C–C, C–H (CDP)[a]
1576 (vw)	C–C, C–H (CDP)[a]
1590 (w)	C–C, C–H (CDP)[a]
3046 (vw)	-
3063 (w)	C–H (CDP)[a]

a) Calculated at RI-BP86(D3BJ)/def2-TZVPP level of theory in the gas phase (section 8.14). b) Assignments based on literature values.[52–54]

7 Mass Spectrometry

In order to investigate Coulomb explosion of $[\{Ga(NacNac^{Mes})\}_2]^{2+}$ (**1**$^{2+}$) and $[\{Ga(CDP^{Ph})\}_2]^{2+}$ (**2**$^{2+}$) in the gas phase, crystals of [**1**][*pf*]$_2$ · 1.5*o*DFB and [**2**][*pf*]$_2$ were dissolved in *o*DFB and analyzed by mass spectrometry (MS). Unfortunately, in both cases, the signal of the protonated ligands, *i.e*. $[H_2NacNac^{Mes}]^+$ and $[H–CDP^{Ph}]^+$ is by far the most intensive signal, and no significant amounts of the dimeric or monomeric Ga complexes are observed (m/z = 402 and 605 for **1**$^{2+}$ and **2**$^{2+}$, respectively). This also the case when cooling the *o*DFB solution to −30 °C or when spraying from a CH_2Cl_2 solution which is cooled to −78 °C. Obviously, **1**$^{2+}$ and **2**$^{2+}$ cannot be analyzed by ESI without protonation of the carbodiphosphorane and β-diketiminate ligands, due to their high basicity.

In **Figure S 59** and **Figure S 60**, the full ESI mass spectra (cation mode) and the isotope patterns of the most intensive signals when spraying from a *o*DFB solution (−30 °C) and a CH_2Cl_2 solution (−78 °C) are shown . The depicted spectra were recorded using the normal scan mode. To confirm the identity of selected ions, the relative signal intensities of the experimental patterns were compared with calculated isotope patterns (black bars).

In the ESI mass spectra of the digallene solutions, $[Ph_3P=CH(POH)Ph_2]^+$ the protonated form of $[Ph_3P=CH(PO)Ph_2]$, is detected (**Figure S 60**), which can attributed to the presence of water during the spraying process. The latter is generated by hydrolysis of CDP^{Ph}.[28] The ESI mass spectra showed more signals at higher m/z values for solutions of [**1**][*pf*]$_2$ · 1.5*o*DFB than for solutions of [**2**][*pf*]$_2$. This may indicate that dinuclear species are only present in the gas phase for the digallane and not for the digallene, again underlining that the Ga–Ga single bond is stronger than the Ga⇆Ga double bond. However, care must be taken since no reasonable elemental composition could be found for these signals.

7.1 [{Ga(NacNac^{Mes})}$_2$][*pf*]$_2$ · 1.5*o*DFB ([1][*pf*]$_2$ · 1.5*o*DFB)

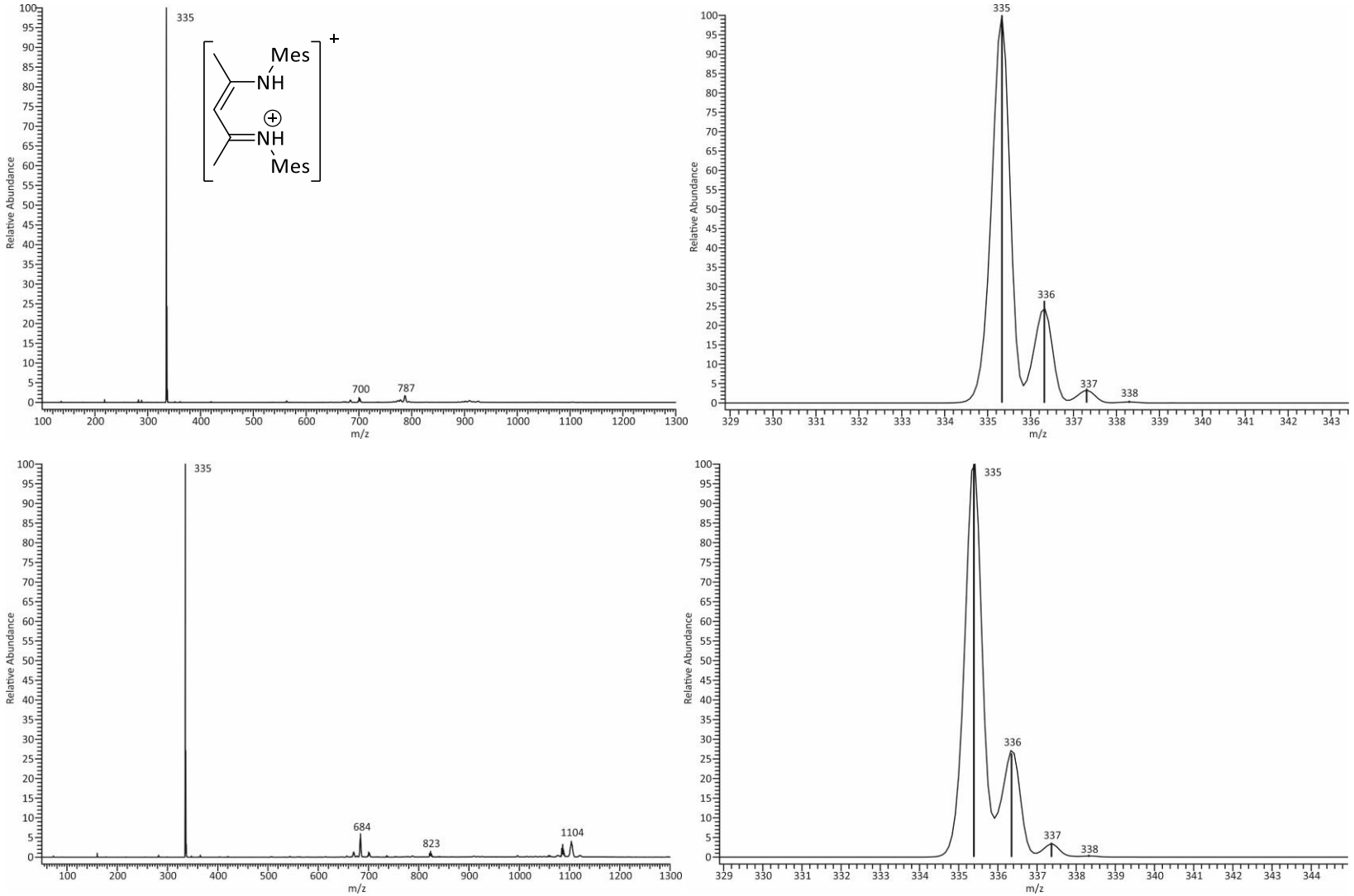


Figure S 59: ESI mass spectra (cation mode) of crystals of [**1**][*pf*]$_2$ · 1.5*o*DFB dissolved in *o*DFB at −30 °C (top left) and in CH_2Cl_2 at –78 °C (bottom left). The signal pattern of the most intensive signal is also shown (top right and bottom right, respectively).

7.2 [{Ga(CDP^{Ph})}$_2$][*pf*]$_2$ ([2][*pf*]$_2$)

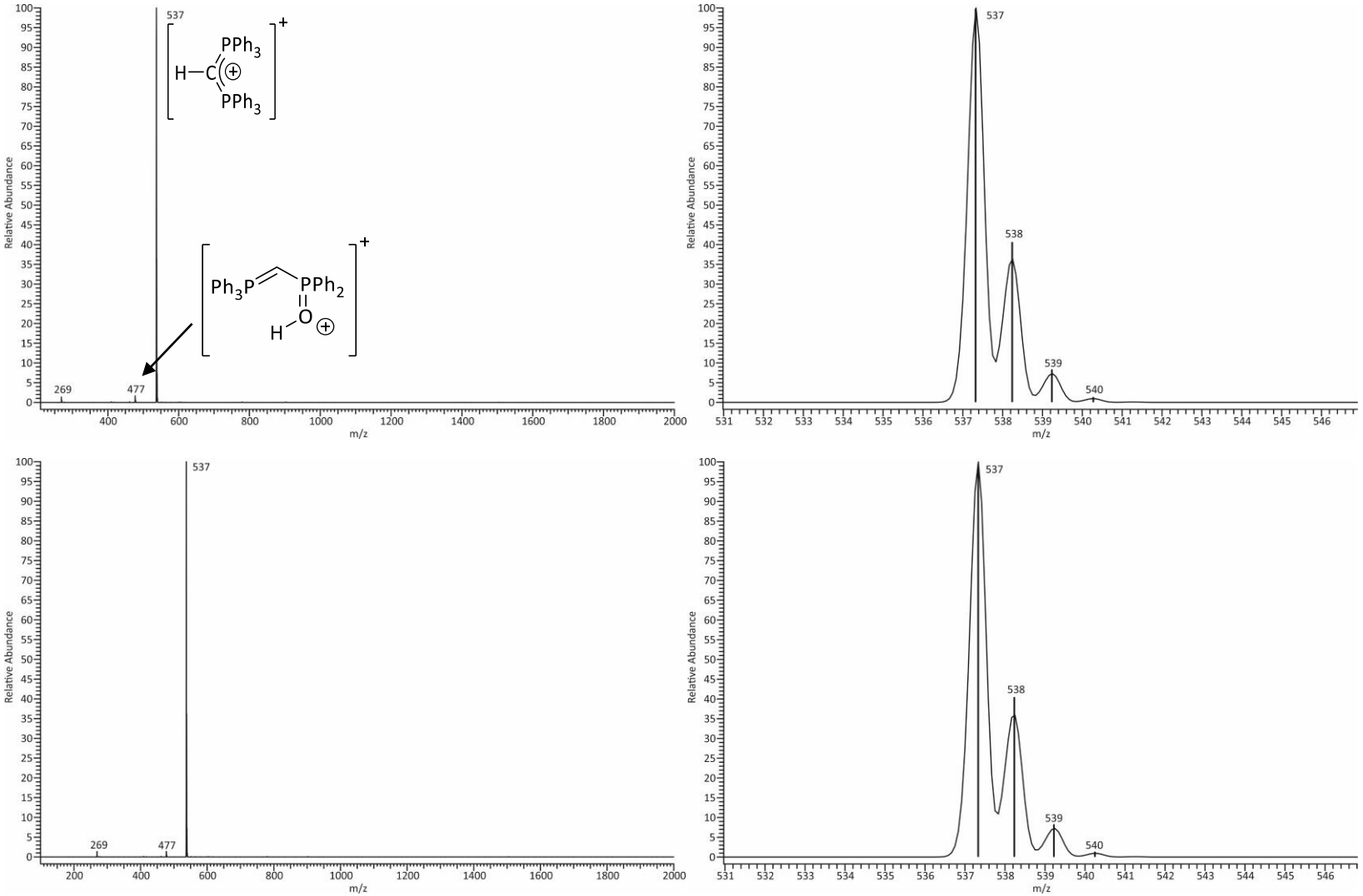


Figure S 60: ESI mass spectra (cation mode) of crystals of [**2**][*pf*]$_2$ dissolved in *o*DFB at −30 °C (top) and in CH_2Cl_2 at –78 °C (bottom). The signal pattern of the most intensive signal is also shown (top right and bottom right, respectively).

8 Quantum Chemical Calculations

8.1 Dissociation of [{Ga(NacNac^{Mes})}$_2$]$^{2+}$ (1^{2+}) and [{Ga(CDP^{Ph})}$_2$]$^{2+}$ (2^{2+})

Quantum chemical calculations (RI-BP86(D3BJ)/def2-TZVPP) suggest that the dissociation of **1**$^{2+}$ into [Ga(NacNac^{Mes})]$^+$ is both endergonic in the gas phase and in an *o*DFB solution, as delineated in **Figure S *61*** (ε = 13.38 D).[26]

Conversely, the twice positively charged **2**$^{2+}$ dimer is predicted to dissociate into the monomers in the gas phase. In this dimer, the weaker Ga⇆Ga bond does not allow to overcome Coulomb explosion. However, in an *o*DFB solution, dimerization of [Ga(CDP^{Ph})]$^+$ to **2**$^{2+}$ is favored by 39 kJ mol^{-1} (RI-BP86(D3BJ)/def2-TZVPP). Since ^{31}P DOSY NMR experiments are inconclusive (section 5.9), it cannot unambiguously be stated whether **2**$^{2+}$ dissociates into monomeric [Ga(CDP^{Ph})]$^+$ in solution.

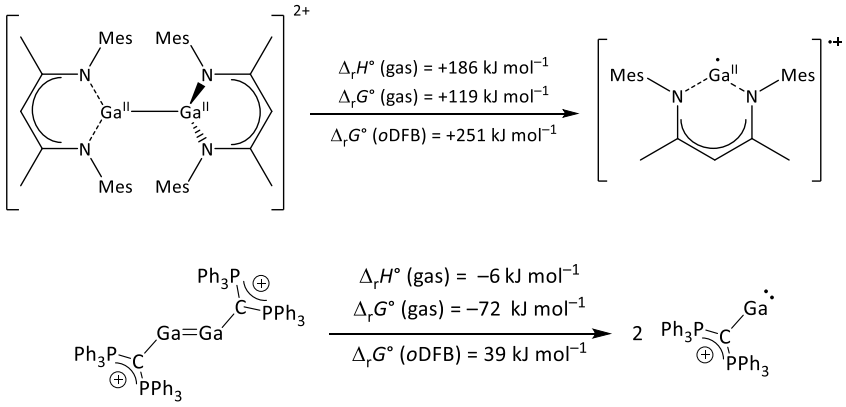


Figure S 61: Dissociation of **1**$^{2+}$ (top) and **2**$^{2+}$ (bottom) and calculated thermodynamics both in the gas phase and in *o*DFB, respectively.

8.2 Molecular orbitals of 1^{2+} and 2^{2+}

In **Figure S 62**, the shape of the Kohn-Sham frontier orbitals of $\mathbf{1}^{2+}$ and $\mathbf{2}^{2+}$ are shown, along with their energy levels.

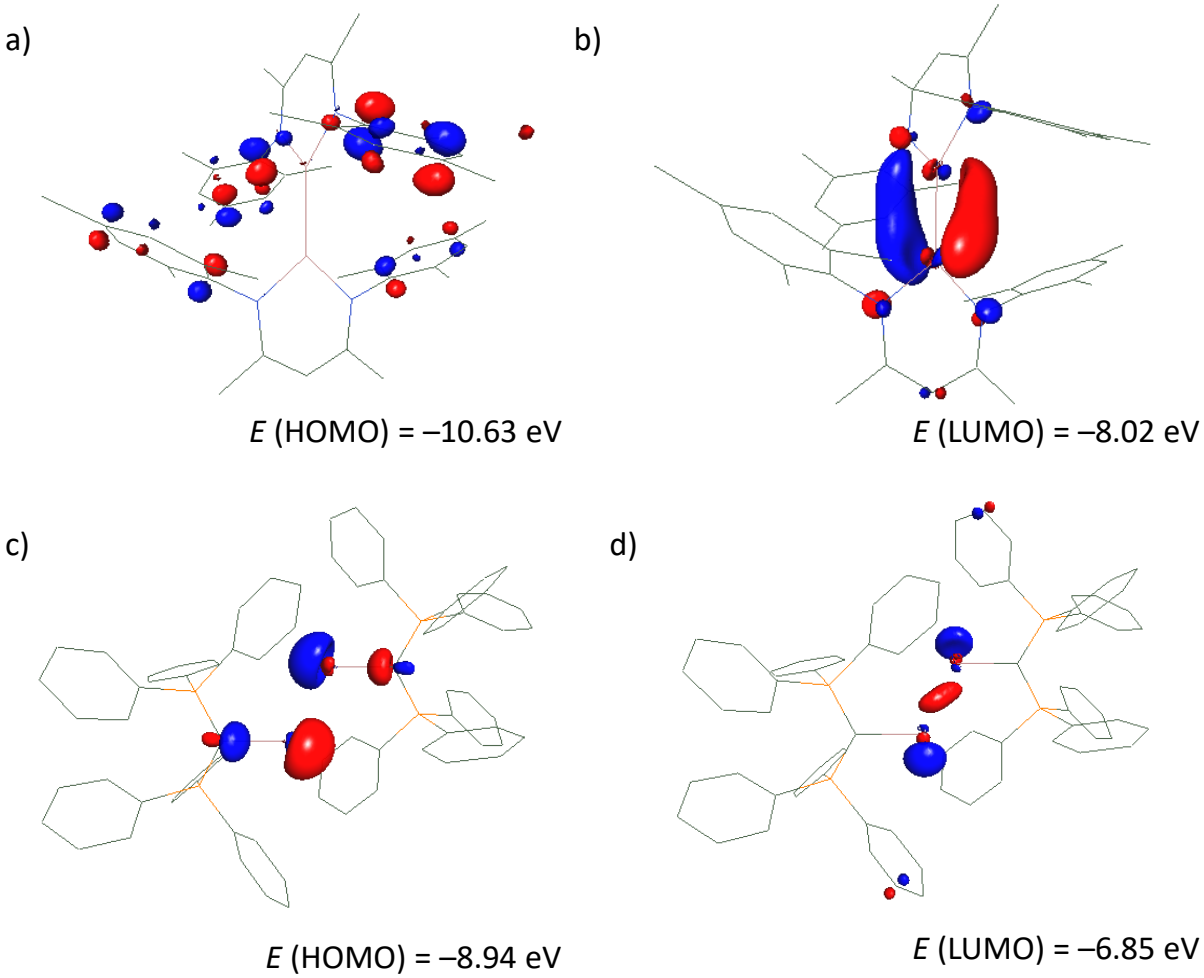


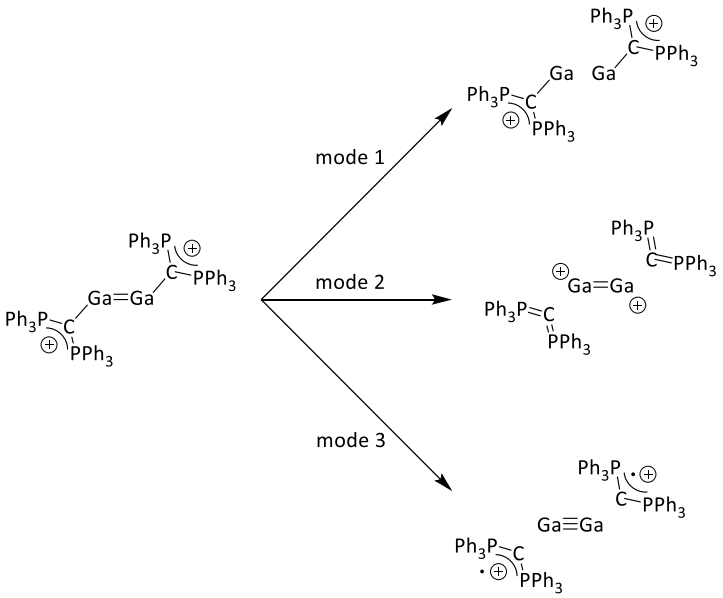
Figure S 62: Kohn-Sham frontier orbitals of $\mathbf{1}^{2+}$ (a) HOMO and b) LUMO) and $\mathbf{2}^{2+}$ (c) HOMO and d) LUMO) as well as their energies (RI-BP86(D3BJ)/def2-TZVPP, *iso* value = 0.065).

The HOMO-LUMO gap is considerably smaller in the dicationic digallene (2.1 eV) than in the dicationic digallane (2.6 eV). This is in good agreement with the reduced stability and increased reactivity of $\mathbf{2}^{2+}$ in solution compared to $\mathbf{1}^{2+}$. Interestingly, the LUMO of both compounds is a GaGa bonding orbital. While it has σ character for $\mathbf{2}^{2+}$, it is a twisted π bond for $\mathbf{1}^{2+}$. The fact that the 10 highest occupied orbitals have no significant Ga–Ga bonding character implies that this bonding interaction is comparatively stable.

8.3 EDA-NOCV Analysis

8.3.1 The Ga–Ga Bond in [{Ga(CDP^{Ph})}$_2$]$^{2+}$ (**2**$^{2+}$)

The bonding situation in [{Ga(CDP^{Ph})}$_2$]$^{2+}$ (**2**$^{2+}$) was analyzed with the EDA-NOCV method.[55] Three different orbital fragmentation modes were investigated, as shown in **Scheme S 5**.



Scheme S 5: Three different orbital fragmentation modes investigated by EDA-NOCV.

An EDA-NOCV analysis was performed for the three different orbital fragmentation modes and for the structure found in the solid state (with optimized position of the hydrogen atoms) as well as for the gas phase-optimized structure, respectively. The orbital interactions for the ΔE_{orb} are summarized in **Table S 15**.

Table S 15: Calculated orbital interactions ΔE_{orb} for the three orbital fragmentation modes depicted in **Scheme S 5**. The interaction energies were calculated for both the gas phase-optimized structure as well as for the structure found in the solid state (values in parentheses; with optimized position of the hydrogen atoms). Energy values are given in kcal mol^{-1}.

	Fragmentation Mode 1	**Fragmentation Mode 2**	**Fragmentation Mode 3**
ΔE_{orb}[a]	−29.9 (−40.4)	−313.2 (−338.3)	−301.8 (−307.2)

a) Values in parentheses refer to the structure found in the solid state.

The EDA-NOCV analysis clearly suggests that the Ga–Ga bond is significantly weaker than the C–Ga bond. In **Table S 16**, the EDA-NOCV results for the weak Ga–Ga interaction are presented.

Table S 16: EDA-NOCV results for the $\mathbf{2}^{2+}$ complex using two $[(CDP^{Ph})Ga]^+$ interacting fragments at the RI-BP86(D3BJ)/def2-TZVPP level. Energy values are given in kcal mol^{-1}. Both the scXRD structure and the gas phase-optimized structure were analyzed.

Energies	Orbital Interaction	$[(CDP^{Ph})Ga]^+ + [Ga(CDP^{Ph})]^+$	
		Solid State Structure	Gas Phase-Optimized Structure
ΔE_{int}		2.9	−1.7
ΔE_{Pauli}		82.5	60.2
ΔE_{disp}[a]		−29.8 (37.4 %)	−36.1 (54.7 %)
ΔE_{elstat}[a]		−9.4 (11.8 %)	4.1
ΔE_{orb}[a]		−40.4 (50.8 %)	−29.9 (45.3 %)
$\Delta E_{orb(1)}$[b]	$(CDP^{Ph})Ga^+$ (HOMO) → $Ga^+(CDP^{Ph})$ (LUMO)	−16.0 (39.6 %) $\lvert\nu_1\rvert$ = 0.50	−8.7 (29.1 %) $\lvert\nu_1\rvert$ = 0.37
$\Delta E_{orb(2)}$[b]	$(CDP^{Ph})Ga^+$ (HOMO) → $Ga^+(CDP^{Ph})$ (LUMO)	−15.0 (37.1 %) $\lvert\nu_2\rvert$ = 0.43	−9.6 (32.1 %) $\lvert\nu_2\rvert$ = 0.36
$\Delta E_{orb(3)}$[b]	$(CDP^{Ph})Ga^+$ (HOMO−1) → $Ga^+(CDP^{Ph})$ (HOMO) (solid state) or $(CDP^{Ph})Ga^+$ (HOMO) → $Ga^+(CDP^{Ph})$ (HOMO−1) (gas phase)	−1.3 (3.2 %) $\lvert\nu_3\rvert$ = 0.11	−1.3 (4.3 %) $\lvert\nu_3\rvert$ = 0.11
$\Delta E_{orb(rest)}$[b]		−9.4 (20.0 %)	−10.3 (34.4 %)

a) Values in parentheses show the contribution to the total attractive interaction. b) Values in parentheses show the contribution to the total orbital interaction ΔE_{orb}. The eigenvalues $\lvert\nu_1\rvert$, $\lvert\nu_2\rvert$ and $\lvert\nu_3\rvert$ give the size of the charge migration in e.

It follows from the breakdown of the attractive interactions between the two $[Ga(CDP^{Ph})]^+$ fragments that the covalent orbital interaction ΔE_{orb} and the dispersion interaction ΔE_{disp} have similar strength and that the electrostatic interaction ΔE_{elstat} is rather negligible. The largest contribution, providing ca. 60–75 %, to the orbital term, comes from the donation of *s*-orbital electron density from one Ga atom into the *p*-orbital of the second Ga atom, which is the typical interaction between heavy elements involved in a non-classical double bond.

The individual orbital interactions are visualized by the associated deformation densities $\Delta\rho$, which are displayed in **Figure S 63** along with the most important fragment orbitals.

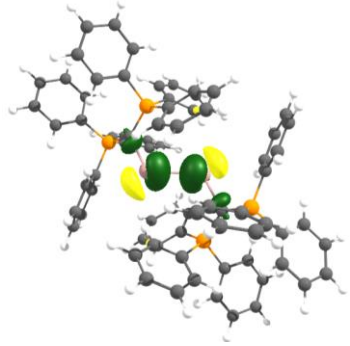
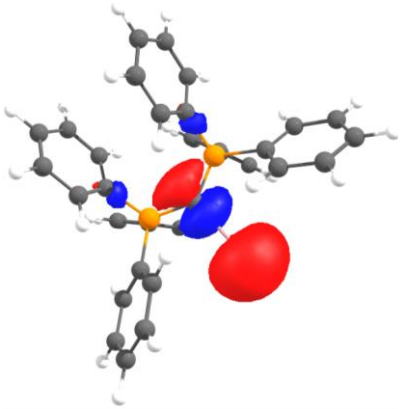
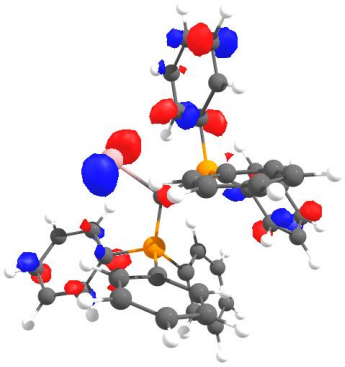
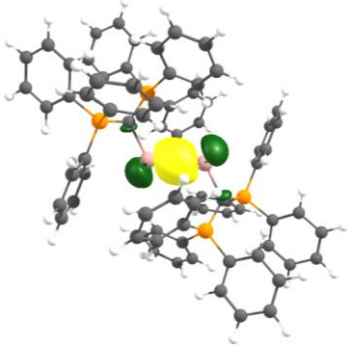
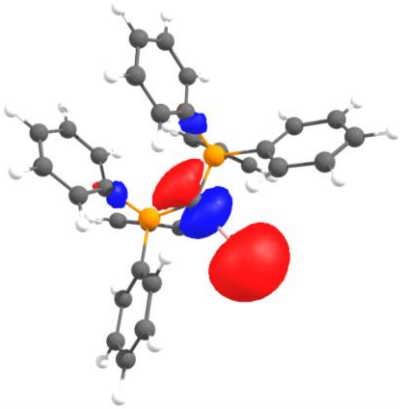
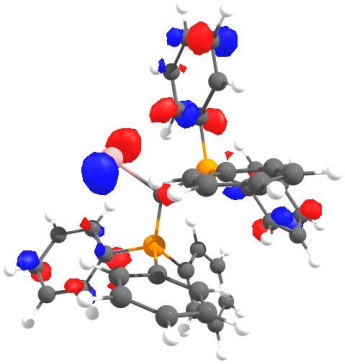
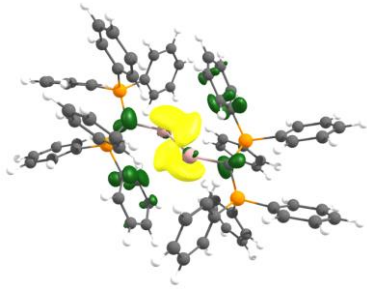
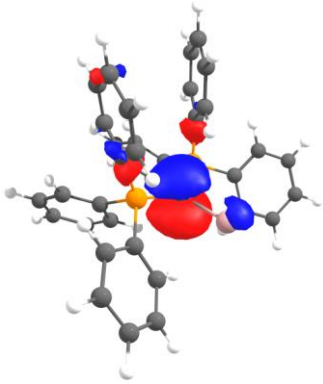
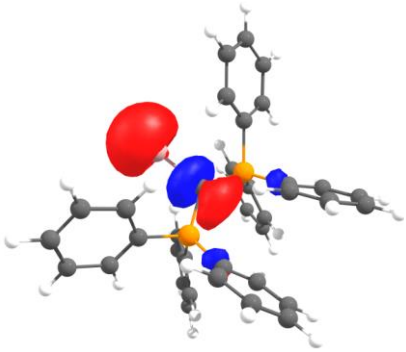
$\Delta\rho$, 2^{2+}	$[(CDP^{Ph})Ga]^+$	$[Ga(CDP^{Ph})]^+$
		
$\Delta\rho_{(1)}$ $\Delta E_{orb(1)}$ = −16.0 kcal/mol; $\lvert\nu_1\rvert$ = 0.50		
		
$\Delta\rho_{(2)}$ $\Delta E_{orb(2)}$ = −15.0 kcal/mol; $\lvert\nu_2\rvert$ = 0.43		
		
$\Delta\rho_{(3)}$ $\Delta E_{orb(3)}$ = −1.3 kcal/mol; $\lvert\nu_3\rvert$ = 0.11		

Figure S 63: Shape of the deformation densities $\Delta\rho_{(1)-(3)}$, corresponding to $\Delta E_{orb(1)-(3)}$, and the fragment orbitals of the two $[(CDP^{Ph})Ga]^+$ moieties at the RI-BP86(D3BJ)/def2-TZVPP level (Isosurface values: 0.002 au for $\Delta\rho_{(1)-(3)}$ (for $\Delta\rho_{(3)}$: 0.0002 au) and 0.05 au for the molecular orbitals). The results for the solid-state structure is shown; note that for the gas phase-optimized structure, the first two deformation densities are virtually identical to the ones shown here, while the shape of $\Delta\rho_{(3)}$ deviates slightly. In the solid-state structure, the HOMO−1 of one $[Ga(CDP^{Ph})]^+$ fragment donates electron density in the HOMO of the other $[Ga(CDP^{Ph})]^+$ fragment, while it is the other way around in the gas phase-optimized structure. The eigenvalues $\lvert\nu_1\rvert$, $\lvert\nu_2\rvert$ and $\lvert\nu_3\rvert$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is green → yellow.

8.3.2 The C–Ga Bond in [Ga(CDP^{Ph})]$^+$

In **Table S 17**, the results for the EDA-NOCV analysis of the CDP^{Ph}/Ga analysis are presented. Obviously, the Ga–CDP^{Ph} bond is likewise stabilized by electrostatic interactions and orbital interactions while dispersion interactions are significantly less important. Interestingly, both the σ (orbital interaction 1) and the π electron pair (orbital interaction 2) at C^{CDP} bind to Ga$^+$. Comparison of $\Delta E_{orb(1)}$ and $\Delta E_{orb(2)}$ reveals that the σ bond is stronger due to better orbital overlap. However, the orbita interaction energy and especially the charge migration associated with the π interaction is still significant.

Table S 17: EDA-NOCV results for the monomeric [Ga(CDP^{Ph})]$^+$ complex using CDP^{Ph} and Ga$^+$ as interacting fragments at the RI-BP86(D3BJ)/def2-TZVPP level. Energy values are given in kcal mol^{-1}. The gas phase-optimized structure of [Ga(CDP^{Ph})]$^+$ was analyzed.

Energies	Orbital Interaction	CDP^{Ph} + Ga$^+$
ΔE_{int}		−110.1
ΔE_{Pauli}		131.3
ΔE_{disp}[a]		−15.3 (6.3 %)
ΔE_{elstat}[a]		−112.1 (46.5 %)
ΔE_{orb}[a]		−113.8 (47.2 %)
$\Delta E_{orb(1)}$[b]	CDP^{Ph} (HOMO−1) → Ga$^+$ (*p*) σ donation	−61.7 (54.2 %) $\lvert\nu_1\rvert$ = 0.76
$\Delta E_{orb(2)}$[b]	CDP^{Ph} (HOMO) → Ga$^+$ (*p*) π donation	−17.6 (15.5 %) $\lvert\nu_2\rvert$ = 0.43
$\Delta E_{orb(3)}$[b]	CDP^{Ph} (HOMO−6) → Ga$^+$ (*p*) σ donation	−8.6 (7.6 %) $\lvert\nu_3\rvert$ = 0.25
$\Delta E_{orb(4)}$[b]	(CDP^{Ph})Ga$^+$ (HOMO−1) → Ga$^+$ (*s*) σ donation	−6.9 (6.1 %) $\lvert\nu_4\rvert$ = 0.24
$\Delta E_{orb(rest)}$[b]		−19.08 (16.8 %)

a) Values in parentheses show the contribution to the total attractive interaction. b) Values in parentheses show the contribution to the total orbital interaction ΔE_{orb}. The eigenvalues $|\nu_1|$, $|\nu_2|$ and $|\nu_3|$ give the size of the charge migration in e.

The individual orbital interactions for the CDP^{Ph} and Ga$^+$ in monomeric [(CDP^{Ph})Ga]$^+$ are visualized by the associated deformation densities Δρ, which are displayed in **Figure S 64** along with the most important fragment orbitals.

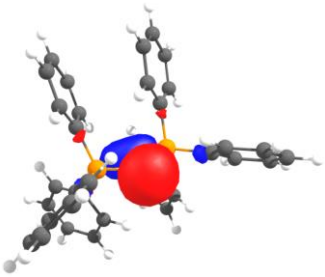
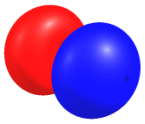
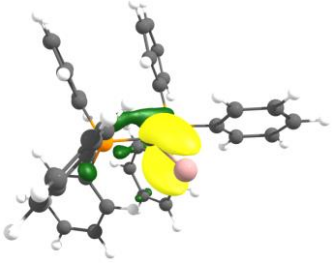
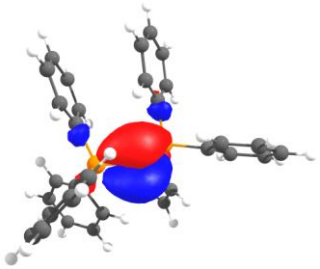
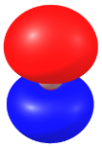
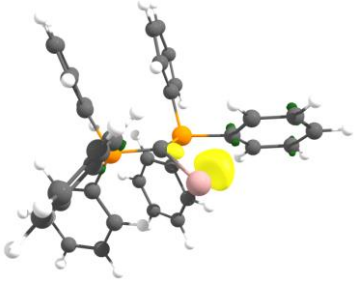
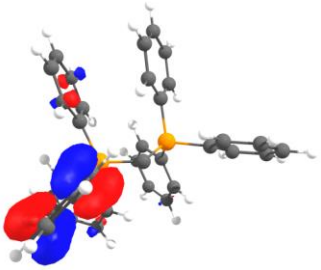
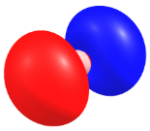
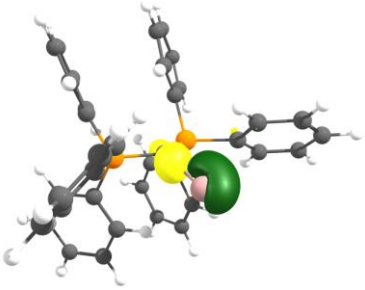
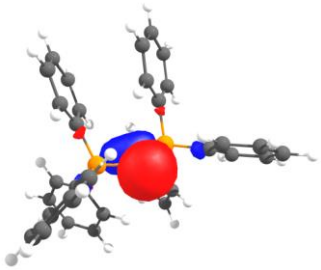
$\Delta\rho$, [(CDP^{Ph})Ga]$^+$	CDP^{Ph}	Ga$^+$
		
$\Delta\rho_{(1)}$ $\Delta E_{orb(1)}$ = −61.7 kcal/mol; $\lvert\nu_1\rvert$ = 0.76		
		
$\Delta\rho_{(2)}$ $\Delta E_{orb(2)}$ = −17.6 kcal/mol; $\lvert\nu_2\rvert$ = 0.43		
		
$\Delta\rho_{(3)}$ $\Delta E_{orb(3)}$ = −8.6 kcal/mol; $\lvert\nu_3\rvert$ = 0.25		
		
$\Delta\rho_{(4)}$ $\Delta E_{orb(4)}$ = −6.9 kcal/mol; $\lvert\nu_4\rvert$ = 0.24		

Figure S 64: Shape of the deformation densities $\Delta\rho_{(1)–(4)}$, corresponding to $\Delta E_{orb(1)–(4)}$, and the fragment orbitals of the CDP^{Ph} moiety and the Ga$^+$cation at the RI-BP86(D3BJ)/def2-TZVPP level (Isosurface values: 0.002 au for $\Delta\rho$ and 0.05 au for the molecular orbitals). The eigenvalues $\lvert\nu_{1\text{-}4}\rvert$ give the size of the charge migration in e. The direction of the charge flow of the deformation densities is green → yellow.

8.4 Structure of $[\{Ga(CDP^{Ph})\}_2]^{2+}$ in the Gas Phase and in the Solid State

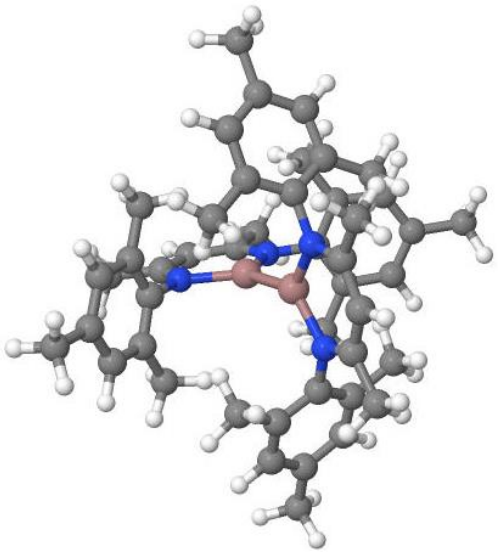
The main structural parameters of the crystal structure and the optimized structure of $\mathbf{2}^{2+}$ are compared in **Table S 18**.

Table S 18: Comparison of structural parameters in the $\mathbf{2}^{2+}$ complex cation for the optimized structures and the molecular structure found by XRD.

Structural Parameter	RI-BP86(D3BJ)/ def2-SVP	RI-BP86(D3BJ)/ def2-TZVPP	RI-PBEh-3c(D3BJ)/ def2-mSVP	Crystal Structure
Ga–Ga [pm]	294.3	297.3	297.3	269.00(3)
C^{CDP}–P [pm]	173.5, 173.3	171.7, 171.6	171.8, 171.4	171.27(10), 171.19(10)
C^{CDP}–Ga [pm]	204.7	205.0	202.1	200.56(11)
Ga–Ga–C^{CDP} [°]	115.3	115.5	118.2	118.18(3)
Angle sum around C^{CDP} [°]	357.3	357.6	359.6	356.3

While the overall structure, *e.g*. the slight pyramidalization around of the C^{CDP} atom and the trans-bent geometry, is well reproduced by DFT calculations, the experimental bond lengths and angles are in poor agreement with quantum chemical calculations. Calculations at the RI-PBEh-3c(D3BJ)/def2-mSVP level of theory predict the C–Ga bond length and the C–Ga–Ga angle very well, but fail to reproduce the Ga–Ga bond length and the pyramidalization about the central carbon atom. The rather poor agreement of the crystal structure with the optimized structures from quantum chemical calculations may be due to the fact that weak interactions are generally difficult to simulate, and that donor-acceptor bonds are often overestimated in gas phase DFT calculations compared to solid state structures.[56] For example, the bond length in a β-diketiminato-indium dimer with "diindene"-character is likewise overestimated by DFT calculations.[57]

8.5 1^{2+}



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

Cartesian coordinates in Ångström:

N	-0.4413626	0.1154015	-1.6557078
C	-0.6423290	-1.1977738	-1.3912982
Ga	-0.2498149	1.3689902	-0.2838043
C	-0.7203144	-1.7094195	-0.0867171
C	-0.7859075	-2.1324526	-2.5541396
C	-0.6174973	-1.0393747	1.1422183
H	-0.8847048	-2.7813575	-0.0180985
N	-0.4123424	0.2961890	1.2371475
C	-0.7381428	-1.8218351	2.4149017
H	-1.6287256	-1.8319731	-3.1917249
H	-0.9433175	-3.1600089	-2.2165707
H	0.1079337	-2.0982276	-3.1921428
H	-0.9023221	-2.8829651	2.2108171
H	-1.5681368	-1.4422747	3.0266027
H	0.1681085	-1.7109503	3.0260763
C	-0.0080348	2.9680474	6.3039963
C	-0.1100953	2.2924098	4.9646349
C	-1.3496878	2.1404139	4.3288230
H	-2.2456162	2.5422369	4.8046158
C	-1.4786504	1.4789360	3.1032897
C	-0.3123407	0.9555827	2.5173441
C	0.9555696	1.1035907	3.1070502
C	2.1902371	0.5621496	2.4383687
C	1.0279967	1.7735805	4.3325910
H	2.0018994	1.8871308	4.8112992
H	-2.3431847	1.9018442	-5.4405912
C	-1.5437244	1.0573275	-3.6347831
C	-1.4380638	1.5618065	-4.9349418
C	-0.3660998	0.6102760	-3.0097040
C	-0.2103730	1.6340193	-5.6068318
C	-0.1335189	2.1395860	-7.0208005
C	0.8907738	0.6835785	-3.6361302
C	0.9399095	1.1969323	-4.9362000
H	1.9048172	1.2500882	-5.4428299

H	2.1219699	-0.5187202	2.2518737
H	3.0762318	0.7392141	3.0569088
H	2.3747275	1.0391246	1.4618944
H	-3.6107463	1.7684309	3.0473435
C	-2.8171699	1.3334207	2.4309695
H	-2.8475593	1.8438535	1.4543754
H	3.0122687	0.3248856	-3.5806844
C	2.1382709	0.2282483	-2.9282152
H	2.3409253	0.8235912	-2.0229809
H	-3.6749269	1.3523395	-3.5765505
C	-2.8694987	0.9973327	-2.9252700
H	-2.8829553	1.6258038	-2.0198053
H	-3.0761098	0.2819481	2.2436878
H	-3.1230497	-0.0224390	-2.6035658
H	2.0742838	-0.8206129	-2.6064584
H	-0.9230223	2.8707909	-7.2321200
H	-0.2596267	1.3099658	-7.7324108
H	0.8376460	2.6030819	-7.2321372
H	-0.7919551	3.7233997	6.4364736
H	0.9677675	3.4494711	6.4406130
H	-0.1243894	2.2330564	7.1144357
H	3.4096286	3.3287774	-3.8263923
H	-3.1496604	4.3395284	-3.8401362
C	2.8297234	3.7440780	-2.9956197
C	-2.4743518	4.5614134	-3.0072900
H	2.7381422	4.8269916	-3.1588341
H	-2.0619232	5.5671918	-3.1686780
H	-1.6280297	3.8587823	-3.0790366
H	1.8119450	3.3272312	-3.0694476
H	5.0829214	2.2820513	-2.5401680
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C	3.4787625	3.4200919	-1.6771014
C	-3.1944309	4.4458208	-1.6909245
C	4.6396876	2.6429529	-1.6107452
C	-4.5352789	4.0529657	-1.6287797
H	3.6624414	6.3339240	-1.5043097
H	-2.4961654	7.2787783	-1.5154427
H	-6.9441417	2.9157391	-1.2303892
H	6.5942423	0.8341433	-1.2021027
Ga	0.1083440	3.7208829	-0.4350886
C	-1.8391774	7.4441618	-0.6504903
C	3.0823348	6.6899510	-0.6418292
C	0.5804861	6.7992476	-0.6286770
C	1.7445374	6.0161230	-0.5892423
C	-0.7647593	6.4006104	-0.5944012
C	2.9352337	3.8873481	-0.4672499
C	-2.5390107	4.7265548	-0.4789154
C	-5.2184384	3.9306773	-0.4113292
C	5.2522553	2.3243364	-0.3912380
C	-6.6725821	3.5496990	-0.3777636
C	6.5252119	1.5249885	-0.3532129
N	1.7193108	4.6644833	-0.5047688
N	-1.1459194	5.1033943	-0.5117463
H	-1.4107456	8.4475769	-0.7153975
H	2.9743102	7.7755118	-0.7088901
H	0.7448612	7.8712534	-0.6962437
H	7.3988026	2.1918753	-0.4048200
H	-7.3058851	4.4481372	-0.4257285

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H    -2.4827551    7.3865300    0.2381297
H     3.6762137    6.4437204    0.2491468
H    -6.9305260    3.0203663    0.5473916
H     6.6124572    0.9477016    0.5750906
C    -4.5182858    4.1996200    0.7725083
C     4.6626774    2.7938468    0.7902223
C    -3.1771565    4.5964606    0.7674006
C     3.5022950    3.5746075    0.7809684
H    -5.0335013    4.1050937    1.7296703
H     5.1238547    2.5514020    1.7489126
C    -2.4389550    4.8721830    2.0495386
C     2.8777511    4.0611886    2.0607955
H     1.8624470    3.6571430    2.2053301
H    -1.5908563    4.1832774    2.1951951
H    -2.0255023    5.8899491    2.0804632
H     2.7869130    5.1560340    2.0891036
H    -3.1023988    4.7546632    2.9126410
H     3.4741959    3.7528645    2.9257180

SCF energy GEOOPT =  -5857.896968119 H
ZPE =   2374. kJ/mol
FREEH energy =  2533.76 kJ/mol
FREEH entropy =   1.43446 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             13.13         0.00983       YES     YES
     8        a             14.37         0.03722       YES     YES
     9        a             16.21         0.03661       YES     YES
    10        a             17.24         0.00413       YES     YES
    11        a             18.64         0.00086       YES     YES
    12        a             20.77         0.00198       YES     YES
    13        a             37.02         0.00006       YES     YES
    14        a             38.68         0.00010       YES     YES
    15        a             42.89         0.25027       YES     YES
    16        a             45.24         0.30895       YES     YES
    17        a             45.96         0.15765       YES     YES
    18        a             48.90         0.19508       YES     YES
    19        a             52.45         0.05032       YES     YES
    20        a             52.66         0.10252       YES     YES
    21        a             53.22         0.03410       YES     YES
    22        a             53.88         0.01451       YES     YES
    23        a             58.44         0.17150       YES     YES
    24        a             59.03         0.19045       YES     YES
    25        a             82.42         0.00247       YES     YES
    26        a             87.71         0.06216       YES     YES
    27        a             88.12         0.03039       YES     YES
    28        a             98.00         0.00066       YES     YES
    29        a             99.56         0.61626       YES     YES
    30        a            101.19         0.79211       YES     YES
    31        a            101.49         0.28934       YES     YES
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32	a	102.51	0.38479	YES	YES
33	a	107.58	0.10791	YES	YES
34	a	119.93	0.03629	YES	YES
35	a	123.24	2.56981	YES	YES
36	a	123.57	3.38676	YES	YES
37	a	124.79	0.91727	YES	YES
38	a	129.28	0.19824	YES	YES
39	a	137.13	1.62963	YES	YES
40	a	137.78	1.60823	YES	YES
41	a	145.01	4.26438	YES	YES
42	a	148.43	0.34226	YES	YES
43	a	150.33	0.14258	YES	YES
44	a	153.45	0.26487	YES	YES
45	a	155.74	0.41074	YES	YES
46	a	156.46	0.13047	YES	YES
47	a	159.95	0.42657	YES	YES
48	a	162.14	0.22612	YES	YES
49	a	169.01	0.34871	YES	YES
50	a	184.35	0.00861	YES	YES
51	a	192.28	6.06946	YES	YES
52	a	192.72	2.21666	YES	YES
53	a	192.98	11.21720	YES	YES
54	a	205.30	0.00289	YES	YES
55	a	207.39	1.94996	YES	YES
56	a	207.78	1.78178	YES	YES
57	a	210.54	1.15003	YES	YES
58	a	210.70	0.95148	YES	YES
59	a	226.14	0.00296	YES	YES
60	a	229.64	0.17304	YES	YES
61	a	229.90	0.19167	YES	YES
62	a	233.07	0.00298	YES	YES
63	a	270.76	0.28546	YES	YES
64	a	270.91	0.51410	YES	YES
65	a	271.07	0.49490	YES	YES
66	a	271.21	0.58393	YES	YES
67	a	283.71	12.71061	YES	YES
68	a	294.67	0.07569	YES	YES
69	a	295.21	0.41552	YES	YES
70	a	309.57	0.98361	YES	YES
71	a	309.93	0.97647	YES	YES
72	a	319.72	0.00005	YES	YES
73	a	353.90	24.24783	YES	YES
74	a	357.69	4.25864	YES	YES
75	a	357.71	4.22751	YES	YES
76	a	369.87	0.01187	YES	YES
77	a	370.38	0.00116	YES	YES
78	a	374.11	0.00316	YES	YES
79	a	376.15	4.95257	YES	YES
80	a	376.23	4.96890	YES	YES
81	a	381.27	4.17184	YES	YES
82	a	381.57	4.13022	YES	YES
83	a	399.23	0.01984	YES	YES
84	a	408.75	0.00005	YES	YES
85	a	476.73	0.34477	YES	YES
86	a	476.76	0.34745	YES	YES
87	a	494.47	0.00244	YES	YES
88	a	494.66	0.00108	YES	YES
89	a	496.72	1.45289	YES	YES

90	a	496.80	1.43753	YES	YES
91	a	502.85	0.00407	YES	YES
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93	a	503.66	0.00964	YES	YES
94	a	503.77	0.00813	YES	YES
95	a	519.62	2.56956	YES	YES
96	a	523.71	0.00003	YES	YES
97	a	528.01	0.00110	YES	YES
98	a	528.34	0.00024	YES	YES
99	a	557.00	3.90198	YES	YES
100	a	557.04	3.89270	YES	YES
101	a	562.22	16.46986	YES	YES
102	a	563.11	0.00158	YES	YES
103	a	570.46	5.94079	YES	YES
104	a	570.50	6.11373	YES	YES
105	a	570.54	1.75784	YES	YES
106	a	571.01	0.75551	YES	YES
107	a	575.02	1.76348	YES	YES
108	a	575.13	1.74712	YES	YES
109	a	598.80	0.00047	YES	YES
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111	a	631.27	2.14839	YES	YES
112	a	631.32	2.31745	YES	YES
113	a	637.89	0.17385	YES	YES
114	a	637.93	0.44782	YES	YES
115	a	642.17	0.64354	YES	YES
116	a	642.39	0.66407	YES	YES
117	a	719.62	0.02953	YES	YES
118	a	720.34	0.17548	YES	YES
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120	a	720.94	0.01862	YES	YES
121	a	811.09	7.69389	YES	YES
122	a	811.31	7.69733	YES	YES
123	a	845.80	3.99447	YES	YES
124	a	845.84	3.88180	YES	YES
125	a	847.40	19.85335	YES	YES
126	a	847.43	0.17504	YES	YES
127	a	871.56	0.57267	YES	YES
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129	a	877.93	68.76695	YES	YES
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131	a	886.13	0.05801	YES	YES
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134	a	887.24	0.13528	YES	YES
135	a	925.24	0.96687	YES	YES
136	a	925.36	1.11906	YES	YES
137	a	925.46	0.51758	YES	YES
138	a	925.47	0.35286	YES	YES
139	a	928.48	1.22069	YES	YES
140	a	930.54	0.00043	YES	YES
141	a	941.52	3.86773	YES	YES
142	a	941.54	3.81472	YES	YES
143	a	963.01	5.13480	YES	YES
144	a	963.04	5.15187	YES	YES
145	a	963.98	0.01228	YES	YES
146	a	964.55	0.00636	YES	YES
147	a	994.26	3.54212	YES	YES

148	a	994.48	12.48490	YES	YES
149	a	994.56	9.75590	YES	YES
150	a	994.77	4.52945	YES	YES
151	a	1005.58	0.02099	YES	YES
152	a	1005.76	0.01961	YES	YES
153	a	1005.80	0.03545	YES	YES
154	a	1005.92	0.00023	YES	YES
155	a	1008.01	7.24066	YES	YES
156	a	1008.07	8.36598	YES	YES
157	a	1012.55	49.19301	YES	YES
158	a	1013.97	0.02037	YES	YES
159	a	1014.79	0.73093	YES	YES
160	a	1014.89	1.62308	YES	YES
161	a	1016.53	0.47008	YES	YES
162	a	1016.77	0.03915	YES	YES
163	a	1020.47	0.08728	YES	YES
164	a	1021.43	0.06208	YES	YES
165	a	1021.52	0.23321	YES	YES
166	a	1021.74	0.06240	YES	YES
167	a	1023.05	1.72132	YES	YES
168	a	1023.09	0.22870	YES	YES
169	a	1023.22	3.37651	YES	YES
170	a	1023.34	14.40212	YES	YES
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172	a	1023.68	14.87318	YES	YES
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174	a	1025.62	0.02149	YES	YES
175	a	1027.26	0.03451	YES	YES
176	a	1027.51	0.03511	YES	YES
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178	a	1028.82	0.00423	YES	YES
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183	a	1188.17	11.82293	YES	YES
184	a	1188.28	11.86710	YES	YES
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190	a	1240.40	0.09269	YES	YES
191	a	1240.63	0.05169	YES	YES
192	a	1240.94	0.00897	YES	YES
193	a	1285.99	5.26581	YES	YES
194	a	1286.10	65.95875	YES	YES
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196	a	1301.01	17.63103	YES	YES
197	a	1301.23	4.93337	YES	YES
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201	a	1322.78	1.57221	YES	YES
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204	a	1350.32	298.65593	YES	YES
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206	a	1359.02	2.05703	YES	YES
207	a	1362.62	39.79768	YES	YES
208	a	1362.87	37.53476	YES	YES
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210	a	1368.99	18.17588	YES	YES
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222	a	1396.06	11.08095	YES	YES
223	a	1396.10	10.87999	YES	YES
224	a	1396.98	0.14711	YES	YES
225	a	1404.46	60.26270	YES	YES
226	a	1405.57	19.96490	YES	YES
227	a	1405.75	21.13420	YES	YES
228	a	1407.33	0.29387	YES	YES
229	a	1417.27	4.19585	YES	YES
230	a	1417.52	1.01613	YES	YES
231	a	1418.18	26.77897	YES	YES
232	a	1418.23	22.09754	YES	YES
233	a	1420.30	247.66913	YES	YES
234	a	1420.59	3.62726	YES	YES
235	a	1431.59	28.04691	YES	YES
236	a	1431.83	28.46738	YES	YES
237	a	1432.27	14.81158	YES	YES
238	a	1432.48	20.35077	YES	YES
239	a	1435.29	0.25687	YES	YES
240	a	1435.77	0.73512	YES	YES
241	a	1436.50	16.60554	YES	YES
242	a	1436.55	15.71113	YES	YES
243	a	1437.38	0.62231	YES	YES
244	a	1437.53	0.56227	YES	YES
245	a	1438.08	0.24772	YES	YES
246	a	1439.54	11.85765	YES	YES
247	a	1439.66	10.83517	YES	YES
248	a	1440.65	0.83538	YES	YES
249	a	1441.36	13.91806	YES	YES
250	a	1441.45	6.82796	YES	YES
251	a	1441.52	6.11585	YES	YES
252	a	1441.59	4.87924	YES	YES
253	a	1455.55	2.30934	YES	YES
254	a	1456.14	31.46319	YES	YES
255	a	1456.23	51.89979	YES	YES
256	a	1456.44	19.90883	YES	YES
257	a	1468.43	46.57304	YES	YES
258	a	1468.44	48.74974	YES	YES
259	a	1469.28	53.17038	YES	YES
260	a	1469.38	2.00352	YES	YES
261	a	1495.57	260.61527	YES	YES
262	a	1499.69	0.00901	YES	YES
263	a	1539.39	288.65622	YES	YES

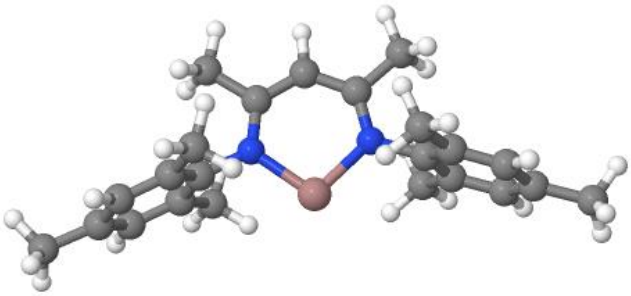
264	a	1539.46	288.70544	YES	YES
265	a	1572.18	5.28449	YES	YES
266	a	1572.21	5.26756	YES	YES
267	a	1572.64	0.01556	YES	YES
268	a	1572.95	0.01827	YES	YES
269	a	1594.91	31.82498	YES	YES
270	a	1594.97	27.07249	YES	YES
271	a	1595.10	64.45992	YES	YES
272	a	1595.16	54.70487	YES	YES
273	a	2945.71	17.09640	YES	YES
274	a	2946.19	28.47532	YES	YES
275	a	2946.29	15.57536	YES	YES
276	a	2946.51	31.63965	YES	YES
277	a	2946.63	14.47065	YES	YES
278	a	2946.96	10.08513	YES	YES
279	a	2947.27	15.39638	YES	YES
280	a	2947.38	0.59867	YES	YES
281	a	2972.98	5.08069	YES	YES
282	a	2972.98	5.88325	YES	YES
283	a	2972.99	5.00807	YES	YES
284	a	2973.00	2.37948	YES	YES
285	a	2984.11	0.09474	YES	YES
286	a	2984.14	0.10292	YES	YES
287	a	2984.31	0.10445	YES	YES
288	a	2984.52	0.10335	YES	YES
289	a	3006.19	1.36259	YES	YES
290	a	3006.39	3.48471	YES	YES
291	a	3006.47	3.23765	YES	YES
292	a	3006.50	4.68748	YES	YES
293	a	3006.76	17.58986	YES	YES
294	a	3006.84	40.22633	YES	YES
295	a	3006.91	13.67634	YES	YES
296	a	3007.13	1.41804	YES	YES
297	a	3033.36	1.62886	YES	YES
298	a	3033.36	5.02341	YES	YES
299	a	3033.37	2.26890	YES	YES
300	a	3033.39	15.27196	YES	YES
301	a	3036.85	0.13541	YES	YES
302	a	3036.90	0.10628	YES	YES
303	a	3037.06	0.20352	YES	YES
304	a	3037.30	0.17513	YES	YES
305	a	3062.30	4.52691	YES	YES
306	a	3062.33	5.29302	YES	YES
307	a	3062.36	6.71800	YES	YES
308	a	3062.37	4.55629	YES	YES
309	a	3064.72	0.08615	YES	YES
310	a	3064.83	0.46556	YES	YES
311	a	3064.89	0.55937	YES	YES
312	a	3065.21	10.81548	YES	YES
313	a	3065.94	1.94352	YES	YES
314	a	3066.07	21.54800	YES	YES
315	a	3066.11	22.06409	YES	YES
316	a	3066.35	0.61825	YES	YES
317	a	3094.17	7.37191	YES	YES
318	a	3094.23	5.96474	YES	YES
319	a	3094.44	0.04307	YES	YES
320	a	3094.50	0.03913	YES	YES
321	a	3097.15	0.48506	YES	YES

322	a	3097.28	10.54623	YES	YES
323	a	3097.31	10.89891	YES	YES
324	a	3097.43	0.63824	YES	YES
325	a	3098.38	1.85094	YES	YES
326	a	3098.43	5.31175	YES	YES
327	a	3098.45	4.18134	YES	YES
328	a	3098.54	0.38599	YES	YES
329	a	3145.96	0.13860	YES	YES
330	a	3146.02	0.12593	YES	YES

$end

COSMO energy + OC correction = -5858.0516036994 H

8.6 [Ga(NacNac^{Mes})]$^{+}$



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

Cartesian coordinates in Ångström:

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H	0.0055929	-4.7906808	1.4819315
C	-3.7305044	0.1507858	1.7143936
C	0.1505600	-3.7302339	1.7136075
H	-3.5613564	-0.1704114	2.7520774
H	-0.1710712	-3.5605540	2.7510518
H	-0.5391683	-3.1543567	1.0745829
H	-3.1542700	-0.5392070	1.0759580
H	-5.2450485	2.2043402	0.7652642
H	2.2044373	-5.2451375	0.7657562
C	-3.3211578	1.5797987	1.4846446
C	1.5796459	-3.3209728	1.4841855
C	-4.2217353	2.5187287	0.9765014
C	2.5187660	-4.2217673	0.9767900
H	-2.8160730	1.5741010	4.3149206
H	1.5743631	-2.8163144	4.3139629
H	4.3616201	-5.6219984	-0.3943174
H	-5.6217790	4.3613984	-0.3951619
Ga	0.0002222	0.0005958	1.0173521
C	1.7499838	-1.7494232	4.5067236
C	-1.7491227	1.7496883	4.5075174
C	0.0002526	-0.0000177	4.1884436
C	-0.9005775	0.9008856	3.6014518
C	0.9010182	-0.9007099	3.6009813
C	-2.0078403	2.0080173	1.7574724
C	2.0077921	-2.0076131	1.7567545
C	3.8459233	-3.8464734	0.7253078
C	-3.8463342	3.8457829	0.7246340

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C     4.8444620   -4.8454172    0.2112269
C    -4.8452369    4.8442806    0.2104014
N    -1.0590074    1.0594903    2.2663965
N     1.0593501   -1.0588668    2.2659186
H     1.5353966   -1.5348841    5.5570811
H    -1.5343841    1.5349034    5.5578067
H     0.0004036   -0.0001359    5.2747666
H    -5.3509441    5.3497395    1.0473570
H     5.3498677   -5.3510681    1.0482476
H     2.8168159   -1.5734600    4.3139439
H    -1.5731897    2.8165784    4.3148985
H     5.6212743   -4.3628805   -0.3942661
H    -4.3626591    5.6210561   -0.3951070
C     4.2218325   -2.5195445    0.9771042
C    -2.5195093    4.2217999    0.9768190
C     3.3213905   -1.5800374    1.4844201
C    -1.5801918    3.3215734    1.4848789
H     5.2454380   -2.2057269    0.7664488
H    -2.2056336    5.2453503    0.7659666
C     3.7313850   -0.1512425    1.7143492
C    -0.1514675    3.7316503    1.7151251
H     0.5390620    3.1558737    1.0768579
H     3.1559666    0.5390282    1.0754982
H     3.5617532    0.1701188    2.7518876
H     0.1694664    3.5625492    2.7529006
H     4.7919426   -0.0067765    1.4828646
H    -0.0068877    4.7920914    1.4831511

SCF energy GEOOPT =  -2928.910685675 H
ZPE =   1181. kJ/mol
FREEH energy =  1259.64 kJ/mol
FREEH entropy =   0.83017 kJ/mol/K

$vibrational spectrum
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#                         cm**(-1)        km/mol          IR     RAMAN
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     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             15.03         0.01319       YES     YES
     8        a             17.00         0.00012       YES     YES
     9        a             32.51         0.01198       YES     YES
    10        a             37.92         0.13491       YES     YES
    11        a             38.07         0.35948       YES     YES
    12        a             41.68         0.00574       YES     YES
    13        a             53.90         0.85453       YES     YES
    14        a             55.68         0.00000       YES     YES
    15        a             87.89         1.20491       YES     YES
    16        a            104.98         0.12984       YES     YES
    17        a            118.85         0.00000       YES     YES
    18        a            130.10         0.46535       YES     YES
    19        a            131.85         0.01355       YES     YES
    20        a            135.98         0.11732       YES     YES
    21        a            136.69         0.18672       YES     YES
    22        a            137.08         1.09312       YES     YES
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23	a	139.85	0.00018	YES	YES
24	a	147.61	0.74079	YES	YES
25	a	151.37	0.00544	YES	YES
26	a	179.96	7.41872	YES	YES
27	a	183.77	1.81629	YES	YES
28	a	206.90	0.98844	YES	YES
29	a	209.82	0.00225	YES	YES
30	a	220.73	0.01276	YES	YES
31	a	220.84	0.00068	YES	YES
32	a	251.84	3.20123	YES	YES
33	a	269.38	0.67504	YES	YES
34	a	269.54	0.00066	YES	YES
35	a	290.26	0.17843	YES	YES
36	a	298.03	6.52160	YES	YES
37	a	324.05	0.01347	YES	YES
38	a	346.08	4.98745	YES	YES
39	a	361.91	2.36479	YES	YES
40	a	370.10	0.00020	YES	YES
41	a	380.98	10.30488	YES	YES
42	a	401.91	0.49169	YES	YES
43	a	470.44	69.18577	YES	YES
44	a	490.30	1.93629	YES	YES
45	a	491.60	0.00007	YES	YES
46	a	494.46	0.93757	YES	YES
47	a	496.99	0.05961	YES	YES
48	a	500.44	0.00001	YES	YES
49	a	525.33	0.00000	YES	YES
50	a	550.58	16.84422	YES	YES
51	a	563.92	8.90897	YES	YES
52	a	569.92	0.05958	YES	YES
53	a	570.09	0.04091	YES	YES
54	a	571.60	1.55996	YES	YES
55	a	594.69	0.00003	YES	YES
56	a	616.81	0.01319	YES	YES
57	a	620.77	30.45469	YES	YES
58	a	640.07	0.22137	YES	YES
59	a	715.91	0.27560	YES	YES
60	a	724.26	47.94845	YES	YES
61	a	795.32	10.60307	YES	YES
62	a	816.12	2.11475	YES	YES
63	a	820.92	65.47330	YES	YES
64	a	852.67	37.87895	YES	YES
65	a	853.31	3.22857	YES	YES
66	a	879.49	0.10534	YES	YES
67	a	879.61	0.19066	YES	YES
68	a	925.27	1.99712	YES	YES
69	a	925.50	0.07927	YES	YES
70	a	927.34	0.01082	YES	YES
71	a	933.38	19.68501	YES	YES
72	a	958.40	13.41381	YES	YES
73	a	959.94	0.07513	YES	YES
74	a	990.39	20.73660	YES	YES
75	a	991.91	0.09300	YES	YES
76	a	1005.40	0.26327	YES	YES
77	a	1005.69	0.00002	YES	YES
78	a	1006.96	8.94786	YES	YES
79	a	1006.98	11.91739	YES	YES
80	a	1014.48	6.06764	YES	YES

81	a	1015.97	0.00004	YES	YES
82	a	1019.13	0.97772	YES	YES
83	a	1019.44	0.03301	YES	YES
84	a	1020.44	1.57610	YES	YES
85	a	1020.68	9.46469	YES	YES
86	a	1021.42	73.36814	YES	YES
87	a	1022.68	3.77680	YES	YES
88	a	1027.52	0.12645	YES	YES
89	a	1028.02	0.00070	YES	YES
90	a	1129.63	114.64825	YES	YES
91	a	1145.66	0.44237	YES	YES
92	a	1180.41	5.91079	YES	YES
93	a	1206.25	1.93498	YES	YES
94	a	1226.24	42.13008	YES	YES
95	a	1240.29	0.00001	YES	YES
96	a	1240.76	0.00013	YES	YES
97	a	1264.72	23.16405	YES	YES
98	a	1290.06	269.74000	YES	YES
99	a	1296.64	0.12589	YES	YES
100	a	1322.75	2.52837	YES	YES
101	a	1323.02	0.84118	YES	YES
102	a	1335.83	4.63070	YES	YES
103	a	1357.26	5.23233	YES	YES
104	a	1357.69	2.02005	YES	YES
105	a	1366.84	0.02341	YES	YES
106	a	1366.84	0.51464	YES	YES
107	a	1366.90	17.24834	YES	YES
108	a	1367.86	9.42013	YES	YES
109	a	1372.61	4.79808	YES	YES
110	a	1374.03	0.09447	YES	YES
111	a	1397.67	0.04953	YES	YES
112	a	1397.89	4.50840	YES	YES
113	a	1402.63	63.15577	YES	YES
114	a	1404.47	12.10456	YES	YES
115	a	1418.06	0.55070	YES	YES
116	a	1418.78	22.56656	YES	YES
117	a	1418.89	106.85453	YES	YES
118	a	1432.60	4.10761	YES	YES
119	a	1433.44	34.22922	YES	YES
120	a	1434.05	0.04495	YES	YES
121	a	1434.60	1.98921	YES	YES
122	a	1436.17	0.00339	YES	YES
123	a	1436.25	9.67132	YES	YES
124	a	1437.30	0.12732	YES	YES
125	a	1440.76	8.47779	YES	YES
126	a	1440.80	16.94764	YES	YES
127	a	1457.38	0.31339	YES	YES
128	a	1457.60	53.30553	YES	YES
129	a	1463.76	0.48034	YES	YES
130	a	1464.52	15.43852	YES	YES
131	a	1498.27	104.29536	YES	YES
132	a	1528.45	36.49513	YES	YES
133	a	1558.63	11.07865	YES	YES
134	a	1559.70	0.02901	YES	YES
135	a	1592.39	557.99405	YES	YES
136	a	1593.05	8.59222	YES	YES
137	a	2941.82	0.01134	YES	YES
138	a	2942.64	11.29819	YES	YES

139	a	2943.64	105.55812	YES	YES
140	a	2944.23	0.22730	YES	YES
141	a	2967.48	1.34724	YES	YES
142	a	2967.50	0.39184	YES	YES
143	a	2985.07	1.18587	YES	YES
144	a	2985.09	1.16246	YES	YES
145	a	3001.20	0.00052	YES	YES
146	a	3001.42	9.29578	YES	YES
147	a	3001.89	14.34030	YES	YES
148	a	3002.28	32.82117	YES	YES
149	a	3028.90	13.80781	YES	YES
150	a	3028.94	14.54889	YES	YES
151	a	3040.19	0.40642	YES	YES
152	a	3040.21	0.69921	YES	YES
153	a	3060.56	5.59000	YES	YES
154	a	3060.57	7.54381	YES	YES
155	a	3064.63	1.94883	YES	YES
156	a	3064.75	16.33744	YES	YES
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158	a	3065.09	4.58529	YES	YES
159	a	3088.85	11.04516	YES	YES
160	a	3089.22	0.23630	YES	YES
161	a	3097.37	6.20297	YES	YES
162	a	3097.40	9.55745	YES	YES
163	a	3098.49	33.77893	YES	YES
164	a	3098.62	1.30730	YES	YES
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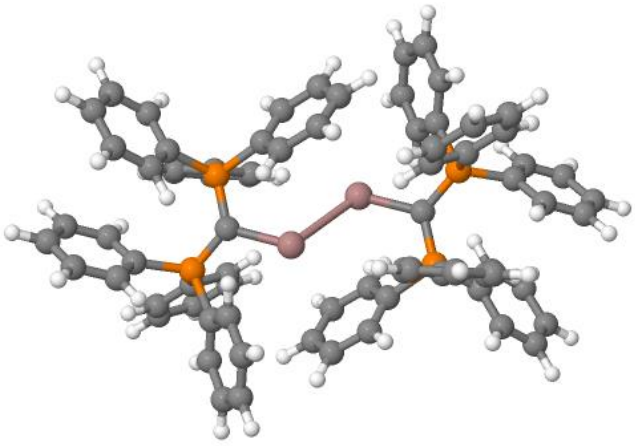
COSMO energy + OC correction = -2928.9628423506 H

8.7 2^{2+} (optimized in the gas phase)



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

Cartesian coordinates in Ångström:

Ga	-1.4822481	-0.0509055	0.0980367
P	-1.7885651	2.1093451	-2.2959706
C	-2.4983425	0.7762944	-1.4783886
P	-3.7568555	-0.1522297	-2.1845218
C	-0.5112288	2.7750740	-1.1831924
C	-0.8192377	2.8750878	0.1867291

H	-1.8295599	2.6547562	0.5335066
C	0.1548861	3.2900281	1.0965034
H	-0.0869485	3.3591413	2.1557127
C	1.4322136	3.6305844	0.6457577
H	2.1959462	3.9379744	1.3579301
C	1.7178383	3.6051186	-0.7222127
H	2.7044657	3.8980748	-1.0765503
C	0.7503463	3.1849060	-1.6358404
H	0.9878944	3.1525357	-2.6973561
C	-0.9778305	1.6404970	-3.8490186
C	-1.6224548	1.8035591	-5.0840617
H	-2.5492748	2.3706671	-5.1439337
C	-1.0756547	1.2473656	-6.2415710
H	-1.5855819	1.3773341	-7.1952307
C	0.1236497	0.5362122	-6.1790937
H	0.5524549	0.1104104	-7.0853601
C	0.7733633	0.3739364	-4.9518305
H	1.7101934	-0.1803322	-4.8993182
C	0.2225302	0.9097163	-3.7903879
H	0.7129457	0.7437662	-2.8290370
C	-2.9096705	3.4925808	-2.6194952
C	-4.0528765	3.6182015	-1.8178971
H	-4.2696939	2.8545834	-1.0727422
C	-4.9115452	4.7009478	-1.9942555
H	-5.8056472	4.7884655	-1.3787580
C	-4.6276235	5.6668566	-2.9632546
H	-5.3022594	6.5103522	-3.1052683
C	-3.4730463	5.5600785	-3.7439823
H	-3.2436652	6.3221453	-4.4877818
C	-2.6080381	4.4797933	-3.5706447
H	-1.7030273	4.4090438	-4.1729456
C	-3.2319471	-1.2023757	-3.5668473
C	-4.1436417	-1.6648893	-4.5299513
H	-5.1902985	-1.3664216	-4.4817148
C	-3.7047156	-2.5024183	-5.5557069
H	-4.4124301	-2.8585169	-6.3032879
C	-2.3603287	-2.8787890	-5.6265599
H	-2.0194495	-3.5255046	-6.4342967
C	-1.4537236	-2.4214741	-4.6667129
H	-0.4033315	-2.7037173	-4.7317505
C	-1.8875649	-1.5884172	-3.6372747
H	-1.1871266	-1.2137572	-2.8925681
C	-5.1810534	0.7860364	-2.7947688
C	-6.2917332	1.0136517	-1.9698731
H	-6.3616506	0.5280012	-0.9971933
C	-7.3155931	1.8588604	-2.3996351
H	-8.1817022	2.0265779	-1.7605384
C	-7.2345944	2.4813199	-3.6475627
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C	-6.1359223	2.2446610	-4.4785600
H	-6.0782240	2.7187738	-5.4574405
C	-5.1142040	1.3972362	-4.0570118
H	-4.2657545	1.1995555	-4.7100406
C	-4.3721121	-1.2741497	-0.8929873
C	-4.7591473	-2.5849283	-1.2043199
H	-4.6675363	-2.9510458	-2.2261000
C	-5.2619643	-3.4215306	-0.2068926
H	-5.5672350	-4.4369296	-0.4571523

C	-5.3760586	-2.9593264	1.1077601
H	-5.7733881	-3.6143644	1.8824513
C	-4.9913461	-1.6548060	1.4255076
H	-5.0904996	-1.2876886	2.4462556
C	-4.4966398	-0.8104437	0.4293705
H	-4.2374323	0.2218180	0.6659179
Ga	1.4822481	0.0509055	-0.0980367
P	1.7885651	-2.1093451	2.2959706
C	2.4983425	-0.7762944	1.4783886
P	3.7568555	0.1522297	2.1845218
C	0.5112288	-2.7750740	1.1831924
C	0.8192377	-2.8750878	-0.1867291
H	1.8295599	-2.6547562	-0.5335066
C	-0.1548861	-3.2900281	-1.0965034
H	0.0869485	-3.3591413	-2.1557127
C	-1.4322136	-3.6305844	-0.6457577
H	-2.1959462	-3.9379744	-1.3579301
C	-1.7178383	-3.6051186	0.7222127
H	-2.7044657	-3.8980748	1.0765503
C	-0.7503463	-3.1849060	1.6358404
H	-0.9878944	-3.1525357	2.6973561
C	0.9778305	-1.6404970	3.8490186
C	1.6224548	-1.8035591	5.0840617
H	2.5492748	-2.3706671	5.1439337
C	1.0756547	-1.2473656	6.2415710
H	1.5855819	-1.3773341	7.1952307
C	-0.1236497	-0.5362122	6.1790937
H	-0.5524549	-0.1104104	7.0853601
C	-0.7733633	-0.3739364	4.9518305
H	-1.7101934	0.1803322	4.8993182
C	-0.2225302	-0.9097163	3.7903879
H	-0.7129457	-0.7437662	2.8290370
C	2.9096705	-3.4925808	2.6194952
C	4.0528765	-3.6182015	1.8178971
H	4.2696939	-2.8545834	1.0727422
C	4.9115452	-4.7009478	1.9942555
H	5.8056472	-4.7884655	1.3787580
C	4.6276235	-5.6668566	2.9632546
H	5.3022594	-6.5103522	3.1052683
C	3.4730463	-5.5600785	3.7439823
H	3.2436652	-6.3221453	4.4877818
C	2.6080381	-4.4797933	3.5706447
H	1.7030273	-4.4090438	4.1729456
C	3.2319471	1.2023757	3.5668473
C	4.1436417	1.6648893	4.5299513
H	5.1902985	1.3664216	4.4817148
C	3.7047156	2.5024183	5.5557069
H	4.4124301	2.8585169	6.3032879
C	2.3603287	2.8787890	5.6265599
H	2.0194495	3.5255046	6.4342967
C	1.4537236	2.4214741	4.6667129
H	0.4033315	2.7037173	4.7317505
C	1.8875649	1.5884172	3.6372747
H	1.1871266	1.2137572	2.8925681
C	5.1810534	-0.7860364	2.7947688
C	6.2917332	-1.0136517	1.9698731
H	6.3616506	-0.5280012	0.9971933
C	7.3155931	-1.8588604	2.3996351

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H     8.1817022   -2.0265779    1.7605384
C     7.2345944   -2.4813199    3.6475627
H     8.0343843   -3.1425143    3.9787267
C     6.1359223   -2.2446610    4.4785600
H     6.0782240   -2.7187738    5.4574405
C     5.1142040   -1.3972362    4.0570118
H     4.2657545   -1.1995555    4.7100406
C     4.3721121    1.2741497    0.8929873
C     4.7591473    2.5849283    1.2043199
H     4.6675363    2.9510458    2.2261000
C     5.2619643    3.4215306    0.2068926
H     5.5672350    4.4369296    0.4571523
C     5.3760586    2.9593264   -1.1077601
H     5.7733881    3.6143644   -1.8824513
C     4.9913461    1.6548060   -1.4255076
H     5.0904996    1.2876886   -2.4462556
C     4.4966398    0.8104437   -0.4293705
H     4.2374323   -0.2218180   -0.6659179

SCF energy GEOOPT =  -8073.093172308 H
ZPE =   2856. kJ/mol
FREEH energy =  3048.96 kJ/mol
FREEH entropy =   1.68039 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             7.37         0.02986       YES     NO
     8        au            13.88         0.17751       YES     NO
     9        ag            15.81         0.00000       NO      YES
    10        au            19.09         0.07407       YES     NO
    11        au            25.56         0.03695       YES     NO
    12        ag            28.10         0.00000       NO      YES
    13        ag            31.72         0.00000       NO      YES
    14        au            36.54         0.02182       YES     NO
    15        ag            36.75         0.00000       NO      YES
    16        ag            39.54         0.00000       NO      YES
    17        au            41.99         0.03150       YES     NO
    18        ag            45.31         0.00000       NO      YES
    19        au            46.32         0.14900       YES     NO
    20        au            47.98         0.11387       YES     NO
    21        ag            48.54         0.00000       NO      YES
    22        ag            52.52         0.00000       NO      YES
    23        au            54.35         0.13317       YES     NO
    24        au            55.89         0.21810       YES     NO
    25        ag            56.46         0.00000       NO      YES
    26        ag            58.51         0.00000       NO      YES
    27        au            62.49         0.02468       YES     NO
    28        ag            63.36         0.00000       NO      YES
    29        ag            65.89         0.00000       NO      YES
    30        au            66.06         0.50459       YES     NO
    31        au            66.29         0.17128       YES     NO
```

32	ag	72.12	0.00000	NO	YES
33	au	72.51	0.16091	YES	NO
34	ag	75.74	0.00000	NO	YES
35	au	78.55	0.63214	YES	NO
36	ag	82.46	0.00000	NO	YES
37	au	84.51	0.36180	YES	NO
38	ag	88.60	0.00000	NO	YES
39	au	90.37	0.05705	YES	NO
40	ag	91.75	0.00000	NO	YES
41	au	95.78	0.14154	YES	NO
42	au	102.00	0.33960	YES	NO
43	ag	105.66	0.00000	NO	YES
44	ag	107.07	0.00000	NO	YES
45	au	112.09	1.01142	YES	NO
46	ag	121.16	0.00000	NO	YES
47	au	125.36	0.35542	YES	NO
48	ag	127.20	0.00000	NO	YES
49	au	132.46	2.93771	YES	NO
50	ag	147.46	0.00000	NO	YES
51	au	150.04	8.50855	YES	NO
52	ag	159.84	0.00000	NO	YES
53	ag	190.24	0.00000	NO	YES
54	au	190.24	0.68480	YES	NO
55	au	196.53	5.94200	YES	NO
56	ag	196.90	0.00000	NO	YES
57	au	201.99	5.80308	YES	NO
58	ag	202.44	0.00000	NO	YES
59	ag	211.99	0.00000	NO	YES
60	au	213.98	28.33492	YES	NO
61	au	221.77	1.92819	YES	NO
62	ag	222.13	0.00000	NO	YES
63	au	229.64	0.50914	YES	NO
64	ag	230.52	0.00000	NO	YES
65	ag	236.80	0.00000	NO	YES
66	au	237.07	5.54100	YES	NO
67	ag	238.91	0.00000	NO	YES
68	au	240.64	7.41471	YES	NO
69	ag	246.52	0.00000	NO	YES
70	au	246.53	7.41447	YES	NO
71	au	254.25	0.73753	YES	NO
72	ag	254.80	0.00000	NO	YES
73	ag	258.30	0.00000	NO	YES
74	au	258.49	0.78959	YES	NO
75	au	272.75	0.84651	YES	NO
76	ag	272.75	0.00000	NO	YES
77	ag	276.82	0.00000	NO	YES
78	au	277.01	3.73519	YES	NO
79	ag	347.96	0.00000	NO	YES
80	au	348.01	12.26368	YES	NO
81	ag	382.21	0.00000	NO	YES
82	au	382.42	25.18018	YES	NO
83	au	384.76	8.76779	YES	NO
84	ag	385.19	0.00000	NO	YES
85	ag	391.66	0.00000	NO	YES
86	au	392.11	1.18984	YES	NO
87	ag	398.36	0.00000	NO	YES
88	au	398.87	1.05162	YES	NO
89	au	399.89	0.97980	YES	NO

90	ag	400.23	0.00000	NO	YES
91	ag	405.10	0.00000	NO	YES
92	au	405.74	0.24385	YES	NO
93	au	408.45	0.25086	YES	NO
94	ag	409.25	0.00000	NO	YES
95	ag	428.93	0.00000	NO	YES
96	au	429.02	0.53613	YES	NO
97	ag	433.02	0.00000	NO	YES
98	au	433.34	14.97277	YES	NO
99	ag	440.83	0.00000	NO	YES
100	au	440.97	0.56773	YES	NO
101	ag	450.94	0.00000	NO	YES
102	au	451.27	3.17721	YES	NO
103	au	470.27	1.61435	YES	NO
104	ag	470.52	0.00000	NO	YES
105	ag	494.00	0.00000	NO	YES
106	au	495.85	157.24199	YES	NO
107	ag	500.26	0.00000	NO	YES
108	au	500.72	35.33910	YES	NO
109	au	508.49	24.15875	YES	NO
110	ag	509.15	0.00000	NO	YES
111	ag	517.05	0.00000	NO	YES
112	au	517.32	32.65251	YES	NO
113	ag	524.38	0.00000	NO	YES
114	au	524.91	248.31892	YES	NO
115	au	561.68	19.36746	YES	NO
116	ag	561.88	0.00000	NO	YES
117	au	612.37	0.92289	YES	NO
118	ag	612.44	0.00000	NO	YES
119	au	613.35	0.09028	YES	NO
120	ag	613.38	0.00000	NO	YES
121	ag	613.74	0.00000	NO	YES
122	au	613.86	0.08043	YES	NO
123	ag	614.35	0.00000	NO	YES
124	au	614.36	0.15856	YES	NO
125	au	615.39	1.39189	YES	NO
126	ag	615.54	0.00000	NO	YES
127	ag	615.83	0.00000	NO	YES
128	au	615.91	0.92267	YES	NO
129	au	677.62	78.57675	YES	NO
130	ag	678.21	0.00000	NO	YES
131	ag	680.85	0.00000	NO	YES
132	au	680.95	3.49786	YES	NO
133	ag	690.17	0.00000	NO	YES
134	au	690.54	165.12984	YES	NO
135	au	691.93	32.43423	YES	NO
136	ag	692.18	0.00000	NO	YES
137	au	695.23	44.48541	YES	NO
138	ag	695.51	0.00000	NO	YES
139	ag	696.71	0.00000	NO	YES
140	au	696.96	26.47631	YES	NO
141	au	699.21	35.73700	YES	NO
142	ag	699.24	0.00000	NO	YES
143	au	702.23	4.52363	YES	NO
144	ag	702.45	0.00000	NO	YES
145	ag	708.81	0.00000	NO	YES
146	au	708.90	1.37570	YES	NO
147	au	711.08	6.56001	YES	NO

148	ag	711.16	0.00000	NO	YES
149	au	716.55	30.82517	YES	NO
150	ag	716.59	0.00000	NO	YES
151	ag	719.48	0.00000	NO	YES
152	au	719.59	119.72412	YES	NO
153	ag	734.88	0.00000	NO	YES
154	au	735.18	140.83170	YES	NO
155	ag	737.44	0.00000	NO	YES
156	au	737.73	86.89234	YES	NO
157	au	740.39	20.51211	YES	NO
158	ag	740.50	0.00000	NO	YES
159	au	742.50	93.81724	YES	NO
160	ag	742.97	0.00000	NO	YES
161	au	744.56	12.00074	YES	NO
162	ag	744.88	0.00000	NO	YES
163	ag	746.60	0.00000	NO	YES
164	au	746.88	56.69228	YES	NO
165	au	786.01	1132.01457	YES	NO
166	ag	797.31	0.00000	NO	YES
167	ag	833.18	0.00000	NO	YES
168	au	833.85	0.70713	YES	NO
169	au	836.54	2.64283	YES	NO
170	ag	837.24	0.00000	NO	YES
171	ag	841.08	0.00000	NO	YES
172	au	841.52	2.09289	YES	NO
173	au	842.26	4.57313	YES	NO
174	ag	842.69	0.00000	NO	YES
175	au	846.43	2.96906	YES	NO
176	ag	846.73	0.00000	NO	YES
177	au	851.29	3.39281	YES	NO
178	ag	851.50	0.00000	NO	YES
179	au	911.35	2.00008	YES	NO
180	ag	911.55	0.00000	NO	YES
181	au	914.01	0.72692	YES	NO
182	ag	914.07	0.00000	NO	YES
183	au	921.93	1.76788	YES	NO
184	ag	921.95	0.00000	NO	YES
185	au	923.19	3.43366	YES	NO
186	ag	923.24	0.00000	NO	YES
187	au	925.43	1.46503	YES	NO
188	ag	925.47	0.00000	NO	YES
189	ag	933.20	0.00000	NO	YES
190	au	933.28	0.42337	YES	NO
191	au	960.59	1.90273	YES	NO
192	ag	960.77	0.00000	NO	YES
193	ag	964.85	0.00000	NO	YES
194	au	965.18	0.17834	YES	NO
195	ag	967.66	0.00000	NO	YES
196	au	967.77	1.49859	YES	NO
197	au	968.47	0.51713	YES	NO
198	ag	968.65	0.00000	NO	YES
199	au	970.22	1.72060	YES	NO
200	ag	970.26	0.00000	NO	YES
201	au	974.87	0.24379	YES	NO
202	ag	975.01	0.00000	NO	YES
203	au	984.24	1.64548	YES	NO
204	ag	984.24	0.00000	NO	YES
205	au	989.38	0.19098	YES	NO

206	ag	989.38	0.00000	NO	YES
207	ag	990.98	0.00000	NO	YES
208	au	990.98	0.26527	YES	NO
209	au	992.20	5.29360	YES	NO
210	ag	992.23	0.00000	NO	YES
211	au	992.53	0.93139	YES	NO
212	ag	992.54	0.00000	NO	YES
213	ag	993.07	0.00000	NO	YES
214	au	993.09	2.21928	YES	NO
215	au	996.64	9.22193	YES	NO
216	ag	996.75	0.00000	NO	YES
217	ag	997.13	0.00000	NO	YES
218	au	997.40	15.05472	YES	NO
219	ag	997.50	0.00000	NO	YES
220	au	997.68	31.58797	YES	NO
221	au	998.48	3.70501	YES	NO
222	ag	998.90	0.00000	NO	YES
223	au	999.21	1.86634	YES	NO
224	ag	999.26	0.00000	NO	YES
225	ag	1001.82	0.00000	NO	YES
226	au	1001.84	1.58252	YES	NO
227	ag	1024.24	0.00000	NO	YES
228	au	1024.41	16.60894	YES	NO
229	ag	1025.51	0.00000	NO	YES
230	au	1025.59	2.79385	YES	NO
231	ag	1026.02	0.00000	NO	YES
232	au	1026.25	1.38329	YES	NO
233	au	1026.47	6.85367	YES	NO
234	ag	1026.74	0.00000	NO	YES
235	au	1027.21	1.74360	YES	NO
236	ag	1027.23	0.00000	NO	YES
237	au	1027.99	1.12554	YES	NO
238	ag	1028.01	0.00000	NO	YES
239	ag	1056.90	0.00000	NO	YES
240	au	1058.35	465.40875	YES	NO
241	au	1073.82	7.33155	YES	NO
242	ag	1073.95	0.00000	NO	YES
243	ag	1075.77	0.00000	NO	YES
244	au	1075.90	1.89249	YES	NO
245	ag	1077.25	0.00000	NO	YES
246	au	1077.33	7.51349	YES	NO
247	au	1078.61	4.06695	YES	NO
248	ag	1078.70	0.00000	NO	YES
249	au	1081.43	0.18900	YES	NO
250	ag	1081.47	0.00000	NO	YES
251	au	1082.69	9.28144	YES	NO
252	ag	1082.72	0.00000	NO	YES
253	au	1092.55	108.49310	YES	NO
254	ag	1092.56	0.00000	NO	YES
255	ag	1093.51	0.00000	NO	YES
256	au	1093.68	11.78013	YES	NO
257	au	1094.43	157.01499	YES	NO
258	ag	1094.49	0.00000	NO	YES
259	ag	1094.81	0.00000	NO	YES
260	au	1094.82	141.42111	YES	NO
261	ag	1097.59	0.00000	NO	YES
262	au	1097.67	135.20653	YES	NO
263	ag	1097.89	0.00000	NO	YES

264	au	1098.02	124.65275	YES	NO
265	ag	1153.43	0.00000	NO	YES
266	au	1153.45	0.79713	YES	NO
267	au	1158.17	0.43994	YES	NO
268	ag	1158.18	0.00000	NO	YES
269	ag	1158.94	0.00000	NO	YES
270	au	1158.96	0.43180	YES	NO
271	au	1159.13	1.42348	YES	NO
272	ag	1159.20	0.00000	NO	YES
273	au	1159.46	1.93736	YES	NO
274	ag	1159.49	0.00000	NO	YES
275	ag	1160.74	0.00000	NO	YES
276	au	1160.76	1.32437	YES	NO
277	au	1173.21	1.92029	YES	NO
278	ag	1173.36	0.00000	NO	YES
279	au	1173.94	2.81223	YES	NO
280	ag	1174.33	0.00000	NO	YES
281	ag	1174.84	0.00000	NO	YES
282	au	1175.40	3.58514	YES	NO
283	ag	1175.84	0.00000	NO	YES
284	au	1176.03	2.92558	YES	NO
285	ag	1179.15	0.00000	NO	YES
286	au	1179.18	2.65071	YES	NO
287	au	1182.60	4.60529	YES	NO
288	ag	1182.77	0.00000	NO	YES
289	au	1289.87	2.24729	YES	NO
290	ag	1289.88	0.00000	NO	YES
291	ag	1295.91	0.00000	NO	YES
292	au	1295.92	6.32165	YES	NO
293	au	1296.55	11.90485	YES	NO
294	ag	1296.57	0.00000	NO	YES
295	ag	1298.63	0.00000	NO	YES
296	au	1298.67	10.79280	YES	NO
297	ag	1304.51	0.00000	NO	YES
298	au	1304.55	2.08441	YES	NO
299	au	1306.12	7.74160	YES	NO
300	ag	1306.15	0.00000	NO	YES
301	au	1335.81	0.86671	YES	NO
302	ag	1335.87	0.00000	NO	YES
303	au	1337.25	2.51852	YES	NO
304	ag	1337.27	0.00000	NO	YES
305	ag	1339.32	0.00000	NO	YES
306	au	1339.39	1.17049	YES	NO
307	au	1339.47	0.20897	YES	NO
308	ag	1339.49	0.00000	NO	YES
309	ag	1340.74	0.00000	NO	YES
310	au	1340.76	0.93821	YES	NO
311	ag	1341.99	0.00000	NO	YES
312	au	1342.00	0.41525	YES	NO
313	au	1423.82	12.61626	YES	NO
314	ag	1423.92	0.00000	NO	YES
315	ag	1428.40	0.00000	NO	YES
316	au	1428.40	28.61287	YES	NO
317	ag	1428.86	0.00000	NO	YES
318	au	1429.02	55.68076	YES	NO
319	ag	1429.41	0.00000	NO	YES
320	au	1429.44	9.25970	YES	NO
321	ag	1433.71	0.00000	NO	YES

322	au	1433.72	12.93917	YES	NO
323	au	1434.07	60.48918	YES	NO
324	ag	1434.17	0.00000	NO	YES
325	ag	1468.08	0.00000	NO	YES
326	au	1468.14	16.21380	YES	NO
327	au	1469.98	13.79948	YES	NO
328	ag	1470.15	0.00000	NO	YES
329	ag	1470.71	0.00000	NO	YES
330	au	1470.86	10.97678	YES	NO
331	ag	1471.24	0.00000	NO	YES
332	au	1471.27	3.81969	YES	NO
333	ag	1474.21	0.00000	NO	YES
334	au	1474.21	18.23805	YES	NO
335	au	1475.07	13.93256	YES	NO
336	ag	1475.10	0.00000	NO	YES
337	au	1563.92	1.68873	YES	NO
338	ag	1564.04	0.00000	NO	YES
339	au	1566.57	0.71855	YES	NO
340	ag	1566.60	0.00000	NO	YES
341	ag	1568.49	0.00000	NO	YES
342	au	1568.49	0.62316	YES	NO
343	ag	1569.27	0.00000	NO	YES
344	au	1569.27	0.74775	YES	NO
345	au	1571.16	1.88663	YES	NO
346	ag	1571.21	0.00000	NO	YES
347	au	1572.03	3.85094	YES	NO
348	ag	1572.12	0.00000	NO	YES
349	au	1579.58	3.94459	YES	NO
350	ag	1579.64	0.00000	NO	YES
351	ag	1580.75	0.00000	NO	YES
352	au	1580.76	1.41647	YES	NO
353	ag	1582.67	0.00000	NO	YES
354	au	1582.67	0.81481	YES	NO
355	au	1583.64	3.91816	YES	NO
356	ag	1583.65	0.00000	NO	YES
357	au	1584.66	3.40910	YES	NO
358	ag	1584.67	0.00000	NO	YES
359	au	1585.20	8.15318	YES	NO
360	ag	1585.21	0.00000	NO	YES
361	au	3064.98	10.28913	YES	NO
362	ag	3065.02	0.00000	NO	YES
363	ag	3091.19	0.00000	NO	YES
364	au	3091.26	4.74259	YES	NO
365	au	3095.62	9.80249	YES	NO
366	ag	3095.68	0.00000	NO	YES
367	au	3104.51	0.56605	YES	NO
368	ag	3104.52	0.00000	NO	YES
369	ag	3107.62	0.00000	NO	YES
370	au	3107.62	1.20586	YES	NO
371	au	3107.94	0.13931	YES	NO
372	ag	3107.94	0.00000	NO	YES
373	au	3109.43	2.32520	YES	NO
374	ag	3109.44	0.00000	NO	YES
375	au	3110.03	1.38778	YES	NO
376	ag	3110.04	0.00000	NO	YES
377	au	3110.91	1.19137	YES	NO
378	ag	3110.92	0.00000	NO	YES
379	ag	3111.97	0.00000	NO	YES

380	au	3111.97	0.91369	YES	NO
381	au	3112.26	0.24167	YES	NO
382	ag	3112.26	0.00000	NO	YES
383	au	3116.14	2.96739	YES	NO
384	ag	3116.16	0.00000	NO	YES
385	ag	3116.62	0.00000	NO	YES
386	au	3116.62	1.65501	YES	NO
387	ag	3117.01	0.00000	NO	YES
388	au	3117.02	1.82119	YES	NO
389	au	3119.02	0.35323	YES	NO
390	ag	3119.03	0.00000	NO	YES
391	ag	3119.26	0.00000	NO	YES
392	au	3119.26	1.86301	YES	NO
393	au	3119.65	0.06302	YES	NO
394	ag	3119.66	0.00000	NO	YES
395	ag	3123.23	0.00000	NO	YES
396	au	3123.23	11.00098	YES	NO
397	au	3124.41	0.82282	YES	NO
398	ag	3124.41	0.00000	NO	YES
399	ag	3125.26	0.00000	NO	YES
400	au	3125.26	4.46880	YES	NO
401	ag	3125.83	0.00000	NO	YES
402	au	3125.84	11.06381	YES	NO
403	au	3126.53	3.90363	YES	NO
404	ag	3126.53	0.00000	NO	YES
405	ag	3127.39	0.00000	NO	YES
406	au	3127.39	9.10859	YES	NO
407	ag	3132.22	0.00000	NO	YES
408	au	3132.23	7.82311	YES	NO
409	ag	3133.18	0.00000	NO	YES
410	au	3133.18	7.65097	YES	NO
411	ag	3133.32	0.00000	NO	YES
412	au	3133.32	6.09943	YES	NO
413	au	3134.41	10.68048	YES	NO
414	ag	3134.41	0.00000	NO	YES
415	ag	3134.92	0.00000	NO	YES
416	au	3134.92	2.13444	YES	NO
417	au	3135.09	18.96669	YES	NO
418	ag	3135.11	0.00000	NO	YES
419	ag	3139.62	0.00000	NO	YES
420	au	3139.62	7.02037	YES	NO

$end

COSMO energy + OC correction = -8073.2358004620 H

Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: ci

Cartesian coordinates in Ångström:

Ga	-1.4662960	-0.0548290	0.1105240
P	-1.7736621	2.1123061	-2.2970011
C	-2.4938638	0.7795676	-1.4504037
P	-3.7691014	-0.1431588	-2.1758734
C	-0.4941656	2.7937583	-1.1777452
C	-0.8065774	2.8889163	0.1990061

H	-1.8257306	2.6621430	0.5479412
C	0.1743014	3.3008875	1.1153801
H	-0.0699071	3.3686014	2.1848101
C	1.4603064	3.6398325	0.6635462
H	2.2329350	3.9436812	1.3836665
C	1.7475055	3.6205795	-0.7123038
H	2.7452608	3.9136529	-1.0675344
C	0.7732635	3.2071667	-1.6341198
H	1.0128329	3.1807206	-2.7061398
C	-0.9540295	1.6092275	-3.8494782
C	-1.6134828	1.7236912	-5.0911040
H	-2.5571105	2.2810787	-5.1658227
C	-1.0645866	1.1320615	-6.2394210
H	-1.5882998	1.2242591	-7.2020273
C	0.1501319	0.4333777	-6.1612585
H	0.5819176	-0.0218369	-7.0646740
C	0.8121317	0.3174583	-4.9266852
H	1.7636683	-0.2311633	-4.8607008
C	0.2597331	0.8878031	-3.7725346
H	0.7599918	0.7506497	-2.8000842
C	-2.9161361	3.4866394	-2.6484756
C	-4.0547201	3.6182988	-1.8280551
H	-4.2459704	2.8698622	-1.0459231
C	-4.9418743	4.6829666	-2.0319355
H	-5.8367330	4.7768866	-1.4000931
C	-4.6898318	5.6230327	-3.0457051
H	-5.3899868	6.4555197	-3.2096868
C	-3.5379129	5.5107297	-3.8430840
H	-3.3319330	6.2581202	-4.6234049
C	-2.6425263	4.4489951	-3.6429682
H	-1.7349048	4.3754959	-4.2599418
C	-3.2345407	-1.1719081	-3.5862277
C	-4.1405220	-1.6043487	-4.5785134
H	-5.1973976	-1.3020979	-4.5363433
C	-3.6853557	-2.4185622	-5.6272314
H	-4.3896457	-2.7542759	-6.4025868
C	-2.3341340	-2.8004335	-5.6889590
H	-1.9804168	-3.4316075	-6.5176103
C	-1.4351736	-2.3735498	-4.6967364
H	-0.3752623	-2.6623776	-4.7534196
C	-1.8834015	-1.5640641	-3.6444394
H	-1.1882258	-1.2105289	-2.8697364
C	-5.2038602	0.8149610	-2.7679445
C	-6.3101315	1.0369014	-1.9229656
H	-6.3750128	0.5315759	-0.9482041
C	-7.3368793	1.9017723	-2.3321620
H	-8.2041269	2.0670128	-1.6760217
C	-7.2621845	2.5478760	-3.5774230
H	-8.0677323	3.2271433	-3.8929405
C	-6.1665674	2.3169404	-4.4267400
H	-6.1121245	2.8135883	-5.4063372
C	-5.1409303	1.4509996	-4.0263305
H	-4.2896167	1.2610831	-4.6945327
C	-4.3815752	-1.2943565	-0.8936642
C	-4.7766018	-2.6036454	-1.2333973
H	-4.6946630	-2.9511147	-2.2737447
C	-5.2749412	-3.4637427	-0.2423166
H	-5.5886685	-4.4827834	-0.5127641

C	-5.3753635	-3.0256102	1.0901295
H	-5.7706055	-3.7021807	1.8624328
C	-4.9812668	-1.7217637	1.4334310
H	-5.0695364	-1.3730873	2.4728541
C	-4.4915100	-0.8524009	0.4449959
H	-4.2232592	0.1836286	0.7023985
Ga	1.4662960	0.0548290	-0.1105240
P	1.7736621	-2.1123061	2.2970011
C	2.4938638	-0.7795676	1.4504037
P	3.7691014	0.1431588	2.1758734
C	0.4941656	-2.7937583	1.1777452
C	0.8065774	-2.8889163	-0.1990061
H	1.8257306	-2.6621430	-0.5479412
C	-0.1743014	-3.3008875	-1.1153801
H	0.0699071	-3.3686014	-2.1848101
C	-1.4603064	-3.6398325	-0.6635462
H	-2.2329350	-3.9436812	-1.3836665
C	-1.7475055	-3.6205795	0.7123038
H	-2.7452608	-3.9136529	1.0675344
C	-0.7732635	-3.2071667	1.6341198
H	-1.0128329	-3.1807206	2.7061398
C	0.9540295	-1.6092275	3.8494782
C	1.6134828	-1.7236912	5.0911040
H	2.5571105	-2.2810787	5.1658227
C	1.0645866	-1.1320615	6.2394210
H	1.5882998	-1.2242591	7.2020273
C	-0.1501319	-0.4333777	6.1612585
H	-0.5819176	0.0218369	7.0646740
C	-0.8121317	-0.3174583	4.9266852
H	-1.7636683	0.2311633	4.8607008
C	-0.2597331	-0.8878031	3.7725346
H	-0.7599918	-0.7506497	2.8000842
C	2.9161361	-3.4866394	2.6484756
C	4.0547201	-3.6182988	1.8280551
H	4.2459704	-2.8698622	1.0459231
C	4.9418743	-4.6829666	2.0319355
H	5.8367330	-4.7768866	1.4000931
C	4.6898318	-5.6230327	3.0457051
H	5.3899868	-6.4555197	3.2096868
C	3.5379129	-5.5107297	3.8430840
H	3.3319330	-6.2581202	4.6234049
C	2.6425263	-4.4489951	3.6429682
H	1.7349048	-4.3754959	4.2599418
C	3.2345407	1.1719081	3.5862277
C	4.1405220	1.6043487	4.5785134
H	5.1973976	1.3020979	4.5363433
C	3.6853557	2.4185622	5.6272314
H	4.3896457	2.7542759	6.4025868
C	2.3341340	2.8004335	5.6889590
H	1.9804168	3.4316075	6.5176103
C	1.4351736	2.3735498	4.6967364
H	0.3752623	2.6623776	4.7534196
C	1.8834015	1.5640641	3.6444394
H	1.1882258	1.2105289	2.8697364
C	5.2038602	-0.8149610	2.7679445
C	6.3101315	-1.0369014	1.9229656
H	6.3750128	-0.5315759	0.9482041
C	7.3368793	-1.9017723	2.3321620

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H     8.2041269   -2.0670128    1.6760217
C     7.2621845   -2.5478760    3.5774230
H     8.0677323   -3.2271433    3.8929405
C     6.1665674   -2.3169404    4.4267400
H     6.1121245   -2.8135883    5.4063372
C     5.1409303   -1.4509996    4.0263305
H     4.2896167   -1.2610831    4.6945327
C     4.3815752    1.2943565    0.8936642
C     4.7766018    2.6036454    1.2333973
H     4.6946630    2.9511147    2.2737447
C     5.2749412    3.4637427    0.2423166
H     5.5886685    4.4827834    0.5127641
C     5.3753635    3.0256102   -1.0901295
H     5.7706055    3.7021807   -1.8624328
C     4.9812668    1.7217637   -1.4334310
H     5.0695364    1.3730873   -2.4728541
C     4.4915100    0.8524009   -0.4449959
H     4.2232592   -0.1836286   -0.7023985

SCF energy GEOOPT =  -8069.059771435 H
ZPE =   2857. kJ/mol
FREEH energy =  3049.39 kJ/mol
FREEH entropy =   1.66775 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             9.14         0.05057       YES     NO
     8        au            15.06         0.16389       YES     NO
     9        ag            17.65         0.00000       NO      YES
    10        au            19.17         0.08858       YES     NO
    11        au            26.57         0.03960       YES     NO
    12        ag            28.93         0.00000       NO      YES
    13        ag            32.52         0.00000       NO      YES
    14        ag            37.40         0.00000       NO      YES
    15        au            37.80         0.02146       YES     NO
    16        ag            40.61         0.00000       NO      YES
    17        au            42.99         0.06456       YES     NO
    18        ag            45.33         0.00000       NO      YES
    19        au            46.60         0.12755       YES     NO
    20        au            48.78         0.16786       YES     NO
    21        ag            48.87         0.00000       NO      YES
    22        ag            53.30         0.00000       NO      YES
    23        au            54.32         0.15813       YES     NO
    24        au            56.58         0.31808       YES     NO
    25        ag            57.50         0.00000       NO      YES
    26        ag            59.53         0.00000       NO      YES
    27        ag            64.27         0.00000       NO      YES
    28        au            65.10         0.03682       YES     NO
    29        au            66.79         0.72460       YES     NO
    30        ag            67.61         0.00000       NO      YES
    31        au            67.84         0.07748       YES     NO
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32	ag	75.35	0.00000	NO	YES
33	au	75.97	0.27222	YES	NO
34	ag	79.21	0.00000	NO	YES
35	au	79.70	0.48515	YES	NO
36	ag	86.11	0.00000	NO	YES
37	au	88.98	0.35763	YES	NO
38	ag	90.97	0.00000	NO	YES
39	au	91.65	0.06309	YES	NO
40	ag	93.89	0.00000	NO	YES
41	au	97.76	0.09526	YES	NO
42	ag	107.28	0.00000	NO	YES
43	au	108.84	0.60799	YES	NO
44	ag	113.28	0.00000	NO	YES
45	au	115.60	0.86768	YES	NO
46	ag	125.68	0.00000	NO	YES
47	au	127.30	0.46590	YES	NO
48	ag	129.40	0.00000	NO	YES
49	au	135.88	2.25796	YES	NO
50	ag	149.85	0.00000	NO	YES
51	au	151.86	9.23687	YES	NO
52	ag	162.48	0.00000	NO	YES
53	ag	191.68	0.00000	NO	YES
54	au	191.73	1.09348	YES	NO
55	au	197.45	6.24895	YES	NO
56	ag	198.57	0.00000	NO	YES
57	ag	203.38	0.00000	NO	YES
58	au	204.18	7.77219	YES	NO
59	ag	213.25	0.00000	NO	YES
60	au	214.47	25.05752	YES	NO
61	au	222.27	2.25714	YES	NO
62	ag	222.61	0.00000	NO	YES
63	au	230.08	0.35211	YES	NO
64	ag	231.18	0.00000	NO	YES
65	ag	237.47	0.00000	NO	YES
66	au	237.80	7.08382	YES	NO
67	ag	239.63	0.00000	NO	YES
68	au	241.09	5.27522	YES	NO
69	ag	246.17	0.00000	NO	YES
70	au	246.18	8.17621	YES	NO
71	au	254.49	1.69811	YES	NO
72	ag	255.06	0.00000	NO	YES
73	ag	257.88	0.00000	NO	YES
74	au	258.33	0.75308	YES	NO
75	ag	273.01	0.00000	NO	YES
76	au	273.05	0.78038	YES	NO
77	ag	276.88	0.00000	NO	YES
78	au	277.04	4.28331	YES	NO
79	au	349.85	15.42203	YES	NO
80	ag	349.89	0.00000	NO	YES
81	ag	382.46	0.00000	NO	YES
82	au	382.67	33.39866	YES	NO
83	au	387.69	2.11115	YES	NO
84	ag	388.28	0.00000	NO	YES
85	ag	394.92	0.00000	NO	YES
86	au	395.41	0.89423	YES	NO
87	ag	402.08	0.00000	NO	YES
88	au	402.71	0.91560	YES	NO
89	au	404.57	1.11545	YES	NO

90	ag	404.90	0.00000	NO	YES
91	ag	409.66	0.00000	NO	YES
92	au	410.35	0.27428	YES	NO
93	au	413.96	0.27705	YES	NO
94	ag	414.84	0.00000	NO	YES
95	ag	431.30	0.00000	NO	YES
96	au	431.59	0.96822	YES	NO
97	ag	434.47	0.00000	NO	YES
98	au	434.73	12.13419	YES	NO
99	ag	442.89	0.00000	NO	YES
100	au	442.92	0.75982	YES	NO
101	ag	453.04	0.00000	NO	YES
102	au	453.44	3.26819	YES	NO
103	au	471.77	2.87933	YES	NO
104	ag	472.23	0.00000	NO	YES
105	ag	493.81	0.00000	NO	YES
106	au	495.74	150.27933	YES	NO
107	ag	500.70	0.00000	NO	YES
108	au	501.09	38.97383	YES	NO
109	au	508.07	19.22663	YES	NO
110	ag	508.74	0.00000	NO	YES
111	ag	516.77	0.00000	NO	YES
112	au	516.90	35.75481	YES	NO
113	ag	524.19	0.00000	NO	YES
114	au	524.66	258.61093	YES	NO
115	au	560.72	13.15976	YES	NO
116	ag	561.02	0.00000	NO	YES
117	au	608.08	0.99120	YES	NO
118	ag	608.15	0.00000	NO	YES
119	au	609.02	0.03779	YES	NO
120	ag	609.05	0.00000	NO	YES
121	ag	609.44	0.00000	NO	YES
122	au	609.54	0.02256	YES	NO
123	au	610.16	0.45992	YES	NO
124	ag	610.20	0.00000	NO	YES
125	au	611.00	0.90524	YES	NO
126	ag	611.10	0.00000	NO	YES
127	ag	611.79	0.00000	NO	YES
128	au	611.87	0.47592	YES	NO
129	au	676.69	39.52162	YES	NO
130	ag	677.04	0.00000	NO	YES
131	ag	678.46	0.00000	NO	YES
132	au	678.55	15.75245	YES	NO
133	ag	693.04	0.00000	NO	YES
134	au	693.11	155.27254	YES	NO
135	ag	693.67	0.00000	NO	YES
136	au	693.72	32.03903	YES	NO
137	au	698.81	41.76570	YES	NO
138	ag	698.90	0.00000	NO	YES
139	ag	701.60	0.00000	NO	YES
140	au	701.78	32.94870	YES	NO
141	ag	703.28	0.00000	NO	YES
142	au	703.42	23.49456	YES	NO
143	au	704.03	4.50518	YES	NO
144	ag	704.89	0.00000	NO	YES
145	ag	706.45	0.00000	NO	YES
146	au	706.94	2.68820	YES	NO
147	au	708.21	8.27715	YES	NO

148	ag	708.34	0.00000	NO	YES
149	ag	713.36	0.00000	NO	YES
150	au	713.45	53.19001	YES	NO
151	ag	716.59	0.00000	NO	YES
152	au	716.78	83.66074	YES	NO
153	ag	735.18	0.00000	NO	YES
154	au	735.63	95.35410	YES	NO
155	ag	738.30	0.00000	NO	YES
156	au	738.67	64.25337	YES	NO
157	au	740.75	23.28039	YES	NO
158	ag	740.99	0.00000	NO	YES
159	au	743.24	74.94239	YES	NO
160	ag	743.90	0.00000	NO	YES
161	au	745.10	6.07379	YES	NO
162	ag	745.33	0.00000	NO	YES
163	ag	746.81	0.00000	NO	YES
164	au	747.12	52.48314	YES	NO
165	au	790.39	1188.95751	YES	NO
166	ag	801.87	0.00000	NO	YES
167	ag	831.41	0.00000	NO	YES
168	au	832.20	1.10435	YES	NO
169	au	833.83	1.23139	YES	NO
170	ag	834.74	0.00000	NO	YES
171	ag	840.77	0.00000	NO	YES
172	au	840.92	2.04995	YES	NO
173	au	841.58	4.35797	YES	NO
174	ag	841.75	0.00000	NO	YES
175	au	845.09	2.50797	YES	NO
176	ag	845.26	0.00000	NO	YES
177	au	849.68	2.94580	YES	NO
178	ag	849.83	0.00000	NO	YES
179	au	908.53	2.46210	YES	NO
180	ag	908.75	0.00000	NO	YES
181	au	912.79	1.17352	YES	NO
182	ag	912.85	0.00000	NO	YES
183	au	919.83	0.75737	YES	NO
184	ag	919.86	0.00000	NO	YES
185	ag	922.66	0.00000	NO	YES
186	au	922.80	3.79223	YES	NO
187	au	923.99	0.96124	YES	NO
188	ag	924.02	0.00000	NO	YES
189	ag	931.01	0.00000	NO	YES
190	au	931.12	0.74779	YES	NO
191	au	961.87	1.98482	YES	NO
192	ag	961.98	0.00000	NO	YES
193	ag	967.11	0.00000	NO	YES
194	au	967.35	0.21645	YES	NO
195	ag	969.35	0.00000	NO	YES
196	au	969.40	1.12351	YES	NO
197	au	971.32	0.93627	YES	NO
198	ag	971.67	0.00000	NO	YES
199	ag	971.73	0.00000	NO	YES
200	au	971.86	1.79507	YES	NO
201	au	975.57	0.87628	YES	NO
202	ag	975.64	0.00000	NO	YES
203	ag	983.93	0.00000	NO	YES
204	au	984.07	41.28743	YES	NO
205	au	984.76	2.30217	YES	NO

206	ag	984.92	0.00000	NO	YES
207	ag	985.29	0.00000	NO	YES
208	au	985.36	8.35639	YES	NO
209	au	986.51	9.99100	YES	NO
210	ag	986.54	0.00000	NO	YES
211	ag	987.64	0.00000	NO	YES
212	au	987.65	1.70869	YES	NO
213	au	989.29	0.79244	YES	NO
214	ag	989.68	0.00000	NO	YES
215	ag	990.84	0.00000	NO	YES
216	au	991.08	1.04495	YES	NO
217	au	997.81	0.26409	YES	NO
218	ag	997.83	0.00000	NO	YES
219	au	999.17	0.13321	YES	NO
220	ag	999.18	0.00000	NO	YES
221	au	999.83	0.46510	YES	NO
222	ag	999.83	0.00000	NO	YES
223	ag	1000.47	0.00000	NO	YES
224	au	1000.49	0.37189	YES	NO
225	au	1001.29	0.29993	YES	NO
226	ag	1001.31	0.00000	NO	YES
227	ag	1021.64	0.00000	NO	YES
228	au	1021.75	10.11658	YES	NO
229	ag	1022.18	0.00000	NO	YES
230	au	1022.24	2.04597	YES	NO
231	ag	1023.10	0.00000	NO	YES
232	au	1023.28	3.58303	YES	NO
233	au	1023.75	11.56002	YES	NO
234	ag	1023.94	0.00000	NO	YES
235	ag	1024.31	0.00000	NO	YES
236	au	1024.34	0.56717	YES	NO
237	au	1025.76	0.99315	YES	NO
238	ag	1025.81	0.00000	NO	YES
239	ag	1044.05	0.00000	NO	YES
240	au	1045.42	497.00665	YES	NO
241	au	1068.23	3.19560	YES	NO
242	ag	1068.38	0.00000	NO	YES
243	ag	1070.22	0.00000	NO	YES
244	au	1070.36	2.03853	YES	NO
245	ag	1071.95	0.00000	NO	YES
246	au	1071.97	8.19454	YES	NO
247	au	1073.33	4.20821	YES	NO
248	ag	1073.39	0.00000	NO	YES
249	au	1076.88	0.05305	YES	NO
250	ag	1076.92	0.00000	NO	YES
251	au	1078.33	10.89570	YES	NO
252	ag	1078.36	0.00000	NO	YES
253	au	1088.57	80.22605	YES	NO
254	ag	1088.71	0.00000	NO	YES
255	ag	1089.94	0.00000	NO	YES
256	au	1090.41	95.78495	YES	NO
257	au	1090.83	85.94336	YES	NO
258	ag	1090.83	0.00000	NO	YES
259	au	1092.25	83.58380	YES	NO
260	ag	1092.69	0.00000	NO	YES
261	ag	1093.79	0.00000	NO	YES
262	au	1093.90	161.54695	YES	NO
263	au	1094.05	97.90957	YES	NO

264	ag	1094.09	0.00000	NO	YES
265	ag	1139.83	0.00000	NO	YES
266	au	1139.87	0.84759	YES	NO
267	au	1144.99	0.48725	YES	NO
268	ag	1145.00	0.00000	NO	YES
269	ag	1145.71	0.00000	NO	YES
270	au	1145.72	0.34447	YES	NO
271	au	1145.89	1.15822	YES	NO
272	ag	1145.97	0.00000	NO	YES
273	au	1146.53	1.60574	YES	NO
274	ag	1146.54	0.00000	NO	YES
275	ag	1147.64	0.00000	NO	YES
276	au	1147.64	1.22055	YES	NO
277	au	1159.00	1.54638	YES	NO
278	ag	1159.12	0.00000	NO	YES
279	au	1159.52	2.56285	YES	NO
280	ag	1160.02	0.00000	NO	YES
281	ag	1160.44	0.00000	NO	YES
282	au	1161.11	3.41895	YES	NO
283	ag	1161.56	0.00000	NO	YES
284	au	1161.71	2.22059	YES	NO
285	ag	1165.74	0.00000	NO	YES
286	au	1165.78	2.62281	YES	NO
287	au	1169.59	4.23707	YES	NO
288	ag	1169.81	0.00000	NO	YES
289	au	1273.96	1.36453	YES	NO
290	ag	1273.97	0.00000	NO	YES
291	ag	1278.40	0.00000	NO	YES
292	au	1278.41	3.81566	YES	NO
293	ag	1279.27	0.00000	NO	YES
294	au	1279.29	11.60460	YES	NO
295	ag	1280.31	0.00000	NO	YES
296	au	1280.34	11.50016	YES	NO
297	au	1287.12	2.90877	YES	NO
298	ag	1287.13	0.00000	NO	YES
299	au	1289.95	5.23518	YES	NO
300	ag	1289.96	0.00000	NO	YES
301	au	1361.29	1.31904	YES	NO
302	ag	1361.34	0.00000	NO	YES
303	ag	1365.08	0.00000	NO	YES
304	au	1365.09	3.40027	YES	NO
305	ag	1365.93	0.00000	NO	YES
306	au	1366.00	2.15318	YES	NO
307	au	1366.45	0.88360	YES	NO
308	ag	1366.48	0.00000	NO	YES
309	ag	1369.21	0.00000	NO	YES
310	au	1369.24	2.42325	YES	NO
311	au	1370.52	0.76712	YES	NO
312	ag	1370.53	0.00000	NO	YES
313	au	1418.62	13.28184	YES	NO
314	ag	1418.77	0.00000	NO	YES
315	ag	1422.74	0.00000	NO	YES
316	au	1422.74	27.40394	YES	NO
317	ag	1423.50	0.00000	NO	YES
318	au	1423.69	67.22299	YES	NO
319	au	1424.26	6.66862	YES	NO
320	ag	1424.27	0.00000	NO	YES
321	ag	1428.56	0.00000	NO	YES

322	au	1428.57	14.53726	YES	NO
323	au	1428.95	60.89851	YES	NO
324	ag	1429.03	0.00000	NO	YES
325	ag	1459.10	0.00000	NO	YES
326	au	1459.15	16.50885	YES	NO
327	au	1461.17	14.15374	YES	NO
328	ag	1461.30	0.00000	NO	YES
329	ag	1461.88	0.00000	NO	YES
330	au	1461.98	12.81167	YES	NO
331	ag	1462.27	0.00000	NO	YES
332	au	1462.30	2.37518	YES	NO
333	ag	1464.98	0.00000	NO	YES
334	au	1464.99	16.08794	YES	NO
335	au	1466.02	14.01671	YES	NO
336	ag	1466.07	0.00000	NO	YES
337	au	1577.88	1.70207	YES	NO
338	ag	1577.98	0.00000	NO	YES
339	au	1580.96	0.68070	YES	NO
340	ag	1580.99	0.00000	NO	YES
341	au	1582.62	0.57585	YES	NO
342	ag	1582.62	0.00000	NO	YES
343	au	1583.77	1.04304	YES	NO
344	ag	1583.77	0.00000	NO	YES
345	au	1586.13	1.99990	YES	NO
346	ag	1586.17	0.00000	NO	YES
347	au	1586.90	4.07331	YES	NO
348	ag	1586.99	0.00000	NO	YES
349	au	1593.24	4.28804	YES	NO
350	ag	1593.30	0.00000	NO	YES
351	ag	1594.48	0.00000	NO	YES
352	au	1594.50	1.14197	YES	NO
353	ag	1596.57	0.00000	NO	YES
354	au	1596.57	0.39181	YES	NO
355	au	1597.57	2.96241	YES	NO
356	ag	1597.58	0.00000	NO	YES
357	ag	1598.41	0.00000	NO	YES
358	au	1598.42	5.06011	YES	NO
359	au	1599.17	6.46770	YES	NO
360	ag	1599.21	0.00000	NO	YES
361	au	3062.05	19.84334	YES	NO
362	ag	3062.12	0.00000	NO	YES
363	ag	3097.91	0.00000	NO	YES
364	au	3097.99	4.22999	YES	NO
365	au	3099.92	8.60013	YES	NO
366	ag	3100.00	0.00000	NO	YES
367	au	3109.33	0.31699	YES	NO
368	ag	3109.34	0.00000	NO	YES
369	ag	3112.27	0.00000	NO	YES
370	au	3112.27	0.28686	YES	NO
371	au	3113.28	0.15626	YES	NO
372	ag	3113.28	0.00000	NO	YES
373	au	3114.60	3.26982	YES	NO
374	ag	3114.61	0.00000	NO	YES
375	ag	3114.68	0.00000	NO	YES
376	au	3114.68	1.12211	YES	NO
377	au	3115.22	1.51137	YES	NO
378	ag	3115.23	0.00000	NO	YES
379	ag	3115.59	0.00000	NO	YES

380	au	3115.59	0.92245	YES	NO
381	ag	3118.82	0.00000	NO	YES
382	au	3118.82	0.14547	YES	NO
383	au	3120.27	3.10405	YES	NO
384	ag	3120.27	0.00000	NO	YES
385	ag	3121.61	0.00000	NO	YES
386	au	3121.61	1.52478	YES	NO
387	ag	3122.19	0.00000	NO	YES
388	au	3122.20	0.62799	YES	NO
389	au	3123.39	0.22633	YES	NO
390	ag	3123.39	0.00000	NO	YES
391	ag	3124.92	0.00000	NO	YES
392	au	3124.93	1.26933	YES	NO
393	au	3125.28	0.57235	YES	NO
394	ag	3125.28	0.00000	NO	YES
395	au	3127.80	6.27998	YES	NO
396	ag	3127.80	0.00000	NO	YES
397	ag	3129.77	0.00000	NO	YES
398	au	3129.77	2.33478	YES	NO
399	au	3129.89	0.52282	YES	NO
400	ag	3129.89	0.00000	NO	YES
401	ag	3130.64	0.00000	NO	YES
402	au	3130.64	5.27321	YES	NO
403	au	3131.74	1.05564	YES	NO
404	ag	3131.74	0.00000	NO	YES
405	ag	3131.92	0.00000	NO	YES
406	au	3131.92	7.04875	YES	NO
407	ag	3137.25	0.00000	NO	YES
408	au	3137.25	5.79453	YES	NO
409	ag	3137.44	0.00000	NO	YES
410	au	3137.44	1.41755	YES	NO
411	ag	3137.53	0.00000	NO	YES
412	au	3137.55	5.71709	YES	NO
413	au	3138.86	6.30869	YES	NO
414	ag	3138.86	0.00000	NO	YES
415	au	3139.23	4.28404	YES	NO
416	ag	3139.24	0.00000	NO	YES
417	au	3139.50	8.36078	YES	NO
418	ag	3139.51	0.00000	NO	YES
419	ag	3144.66	0.00000	NO	YES
420	au	3144.66	4.55334	YES	NO

$end

Method: (RI-)pbeh-3c(D3)/def2-mSVP
Symmetry: ci

Cartesian coordinates in Ångström:

Ga	-1.3611341	0.5790760	0.1465951
P	-1.9288995	2.3856961	-2.3146307
C	-2.4282471	0.9457025	-1.5305661
P	-3.5799610	-0.1595951	-2.1646389
C	-0.4889486	2.9857741	-1.3763530
C	-0.7086390	3.7717241	-0.2407842
H	-1.7147731	4.0586766	0.0396027
C	0.3645333	4.2188019	0.5125272
H	0.1904808	4.8406946	1.3798979

C	1.6596419	3.8834162	0.1445794
H	2.4954924	4.2399130	0.7307984
C	1.8842317	3.1042961	-0.9799666
H	2.8941519	2.8559617	-1.2773705
C	0.8147011	2.6566423	-1.7421092
H	1.0073414	2.0742111	-2.6329242
C	-1.4213668	2.1582657	-4.0399113
C	-1.8059331	3.0203555	-5.0648969
H	-2.4187081	3.8868811	-4.8597822
C	-1.4324619	2.7514278	-6.3728082
H	-1.7367493	3.4230642	-7.1640648
C	-0.6806684	1.6236289	-6.6684383
H	-0.3978453	1.4157138	-7.6915769
C	-0.2998580	0.7586726	-5.6522946
H	0.2749586	-0.1291703	-5.8780317
C	-0.6699098	1.0228173	-4.3444757
H	-0.3860974	0.3326800	-3.5606882
C	-3.0734951	3.7851921	-2.2575972
C	-4.3698877	3.6233327	-1.7881857
H	-4.7066710	2.6544760	-1.4497524
C	-5.2324429	4.7087017	-1.7389921
H	-6.2436909	4.5743896	-1.3801359
C	-4.7967347	5.9600530	-2.1440086
H	-5.4691011	6.8064403	-2.1042539
C	-3.4914507	6.1334803	-2.5883984
H	-3.1448401	7.1134279	-2.8870084
C	-2.6291272	5.0526117	-2.6422453
H	-1.6072929	5.2035417	-2.9709534
C	-2.8877831	-1.4505780	-3.2371361
C	-3.6294539	-2.0005116	-4.2815485
H	-4.6319817	-1.6504773	-4.4904439
C	-3.0823087	-3.0009075	-5.0711037
H	-3.6610463	-3.4187175	-5.8835399
C	-1.7966137	-3.4583543	-4.8235418
H	-1.3693019	-4.2321627	-5.4472473
C	-1.0602300	-2.9218876	-3.7763663
H	-0.0563071	-3.2743637	-3.5796177
C	-1.6043192	-1.9256928	-2.9827741
H	-1.0141624	-1.5089651	-2.1750141
C	-4.9288849	0.5811148	-3.1175593
C	-6.2062925	0.7003071	-2.5751480
H	-6.4379074	0.2769433	-1.6064470
C	-7.1988502	1.3629427	-3.2815469
H	-8.1911170	1.4474313	-2.8596100
C	-6.9232818	1.9060445	-4.5273113
H	-7.6994232	2.4231404	-5.0751380
C	-5.6568499	1.7708060	-5.0793502
H	-5.4444147	2.1760057	-6.0593073
C	-4.6622005	1.1070200	-4.3819572
H	-3.6866522	0.9883878	-4.8355938
C	-4.3590419	-1.0323636	-0.7796360
C	-4.8088365	-2.3421567	-0.9326863
H	-4.6414575	-2.8748632	-1.8599511
C	-5.4784752	-2.9726688	0.1044012
H	-5.8311612	-3.9873824	-0.0221121
C	-5.7004228	-2.3030709	1.3007680
H	-6.2248436	-2.7975173	2.1074323
C	-5.2600613	-0.9966669	1.4565617

H	-5.4451587	-0.4676651	2.3816348
C	-4.5983440	-0.3580969	0.4173371
H	-4.2970831	0.6761970	0.5299401
Ga	1.3611341	-0.5790760	-0.1465951
P	1.9288995	-2.3856961	2.3146307
C	2.4282471	-0.9457025	1.5305661
P	3.5799610	0.1595951	2.1646389
C	0.4889486	-2.9857741	1.3763530
C	0.7086390	-3.7717241	0.2407842
H	1.7147731	-4.0586766	-0.0396027
C	-0.3645333	-4.2188019	-0.5125272
H	-0.1904808	-4.8406946	-1.3798979
C	-1.6596419	-3.8834162	-0.1445794
H	-2.4954924	-4.2399130	-0.7307984
C	-1.8842317	-3.1042961	0.9799666
H	-2.8941519	-2.8559617	1.2773705
C	-0.8147011	-2.6566423	1.7421092
H	-1.0073414	-2.0742111	2.6329242
C	1.4213668	-2.1582657	4.0399113
C	1.8059331	-3.0203555	5.0648969
H	2.4187081	-3.8868811	4.8597822
C	1.4324619	-2.7514278	6.3728082
H	1.7367493	-3.4230642	7.1640648
C	0.6806684	-1.6236289	6.6684383
H	0.3978453	-1.4157138	7.6915769
C	0.2998580	-0.7586726	5.6522946
H	-0.2749586	0.1291703	5.8780317
C	0.6699098	-1.0228173	4.3444757
H	0.3860974	-0.3326800	3.5606882
C	3.0734951	-3.7851921	2.2575972
C	4.3698877	-3.6233327	1.7881857
H	4.7066710	-2.6544760	1.4497524
C	5.2324429	-4.7087017	1.7389921
H	6.2436909	-4.5743896	1.3801359
C	4.7967347	-5.9600530	2.1440086
H	5.4691011	-6.8064403	2.1042539
C	3.4914507	-6.1334803	2.5883984
H	3.1448401	-7.1134279	2.8870084
C	2.6291272	-5.0526117	2.6422453
H	1.6072929	-5.2035417	2.9709534
C	2.8877831	1.4505780	3.2371361
C	3.6294539	2.0005116	4.2815485
H	4.6319817	1.6504773	4.4904439
C	3.0823087	3.0009075	5.0711037
H	3.6610463	3.4187175	5.8835399
C	1.7966137	3.4583543	4.8235418
H	1.3693019	4.2321627	5.4472473
C	1.0602300	2.9218876	3.7763663
H	0.0563071	3.2743637	3.5796177
C	1.6043192	1.9256928	2.9827741
H	1.0141624	1.5089651	2.1750141
C	4.9288849	-0.5811148	3.1175593
C	6.2062925	-0.7003071	2.5751480
H	6.4379074	-0.2769433	1.6064470
C	7.1988502	-1.3629427	3.2815469
H	8.1911170	-1.4474313	2.8596100
C	6.9232818	-1.9060445	4.5273113
H	7.6994232	-2.4231404	5.0751380

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C     5.6568499   -1.7708060    5.0793502
H     5.4444147   -2.1760057    6.0593073
C     4.6622005   -1.1070200    4.3819572
H     3.6866522   -0.9883878    4.8355938
C     4.3590419    1.0323636    0.7796360
C     4.8088365    2.3421567    0.9326863
H     4.6414575    2.8748632    1.8599511
C     5.4784752    2.9726688   -0.1044012
H     5.8311612    3.9873824    0.0221121
C     5.7004228    2.3030709   -1.3007680
H     6.2248436    2.7975173   -2.1074323
C     5.2600613    0.9966669   -1.4565617
H     5.4451587    0.4676651   -2.3816348
C     4.5983440    0.3580969   -0.4173371
H     4.2970831   -0.6761970   -0.5299401

SCF energy GEOOPT =  -8060.881239220 H
ZPE =   3026. kJ/mol
FREEH energy =  3210.72 kJ/mol
FREEH entropy =   1.64482 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             8.93        0.09497       YES     NO
     8        ag            13.50        0.00000       NO      YES
     9        au            13.67        0.16212       YES     NO
    10        au            19.55        0.16875       YES     NO
    11        ag            26.16        0.00000       NO      YES
    12        au            28.18        0.17635       YES     NO
    13        ag            29.00        0.00000       NO      YES
    14        au            29.92        0.43609       YES     NO
    15        ag            32.27        0.00000       NO      YES
    16        au            34.33        0.18099       YES     NO
    17        ag            36.14        0.00000       NO      YES
    18        ag            39.99        0.00000       NO      YES
    19        ag            46.30        0.00000       NO      YES
    20        au            47.79        0.75847       YES     NO
    21        ag            50.85        0.00000       NO      YES
    22        au            51.57        0.24298       YES     NO
    23        ag            54.72        0.00000       NO      YES
    24        au            55.72        0.21024       YES     NO
    25        au            56.89        0.35269       YES     NO
    26        au            61.03        0.13048       YES     NO
    27        ag            61.09        0.00000       NO      YES
    28        ag            63.39        0.00000       NO      YES
    29        au            64.24        0.10644       YES     NO
    30        ag            65.87        0.00000       NO      YES
    31        au            68.56        0.65734       YES     NO
    32        ag            70.90        0.00000       NO      YES
    33        au            71.57        1.05867       YES     NO
    34        au            75.52        0.68314       YES     NO
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35	ag	79.58	0.00000	NO	YES
36	ag	82.80	0.00000	NO	YES
37	au	83.96	0.69010	YES	NO
38	ag	86.95	0.00000	NO	YES
39	au	92.90	0.34516	YES	NO
40	ag	95.78	0.00000	NO	YES
41	au	96.29	0.16943	YES	NO
42	ag	102.21	0.00000	NO	YES
43	au	102.58	0.03868	YES	NO
44	ag	105.92	0.00000	NO	YES
45	au	108.64	0.02041	YES	NO
46	ag	109.16	0.00000	NO	YES
47	au	110.53	0.94849	YES	NO
48	ag	117.62	0.00000	NO	YES
49	au	128.55	3.23248	YES	NO
50	ag	129.60	0.00000	NO	YES
51	au	148.83	11.51437	YES	NO
52	ag	154.60	0.00000	NO	YES
53	ag	205.40	0.00000	NO	YES
54	au	205.75	11.58394	YES	NO
55	au	212.31	15.02783	YES	NO
56	ag	213.88	0.00000	NO	YES
57	au	220.94	13.98659	YES	NO
58	ag	221.78	0.00000	NO	YES
59	au	223.14	4.46353	YES	NO
60	ag	224.77	0.00000	NO	YES
61	au	226.02	1.09986	YES	NO
62	ag	227.96	0.00000	NO	YES
63	ag	238.80	0.00000	NO	YES
64	au	239.30	7.23458	YES	NO
65	au	247.85	2.84371	YES	NO
66	ag	248.05	0.00000	NO	YES
67	ag	261.25	0.00000	NO	YES
68	au	261.75	3.11007	YES	NO
69	au	263.37	4.23628	YES	NO
70	ag	263.92	0.00000	NO	YES
71	au	270.18	1.08690	YES	NO
72	ag	270.65	0.00000	NO	YES
73	au	274.31	1.07735	YES	NO
74	ag	274.42	0.00000	NO	YES
75	au	286.26	2.88290	YES	NO
76	ag	286.84	0.00000	NO	YES
77	ag	287.96	0.00000	NO	YES
78	au	288.28	1.14462	YES	NO
79	au	365.14	6.63827	YES	NO
80	ag	366.80	0.00000	NO	YES
81	ag	408.85	0.00000	NO	YES
82	au	409.31	44.67387	YES	NO
83	au	416.04	0.20313	YES	NO
84	ag	416.24	0.00000	NO	YES
85	ag	418.02	0.00000	NO	YES
86	au	418.48	0.78386	YES	NO
87	au	422.32	0.78696	YES	NO
88	ag	422.55	0.00000	NO	YES
89	au	425.11	0.98986	YES	NO
90	ag	425.51	0.00000	NO	YES
91	au	429.29	0.15741	YES	NO
92	ag	429.75	0.00000	NO	YES

93	ag	432.71	0.00000	NO	YES
94	au	433.17	0.23069	YES	NO
95	au	452.68	0.94300	YES	NO
96	ag	453.10	0.00000	NO	YES
97	au	464.93	8.45939	YES	NO
98	ag	465.21	0.00000	NO	YES
99	au	472.84	12.44413	YES	NO
100	ag	473.24	0.00000	NO	YES
101	ag	477.85	0.00000	NO	YES
102	au	478.47	6.86902	YES	NO
103	ag	490.08	0.00000	NO	YES
104	au	490.96	5.24401	YES	NO
105	au	526.67	93.43142	YES	NO
106	ag	528.79	0.00000	NO	YES
107	ag	532.53	0.00000	NO	YES
108	au	533.99	123.38221	YES	NO
109	au	538.63	92.36731	YES	NO
110	ag	538.70	0.00000	NO	YES
111	ag	548.31	0.00000	NO	YES
112	au	548.70	16.18493	YES	NO
113	ag	556.32	0.00000	NO	YES
114	au	556.73	218.68263	YES	NO
115	au	599.05	5.00124	YES	NO
116	ag	600.07	0.00000	NO	YES
117	ag	641.74	0.00000	NO	YES
118	au	641.85	0.04845	YES	NO
119	au	642.27	0.07973	YES	NO
120	ag	642.42	0.00000	NO	YES
121	ag	642.83	0.00000	NO	YES
122	au	642.84	0.12059	YES	NO
123	au	643.14	0.16889	YES	NO
124	ag	643.18	0.00000	NO	YES
125	au	643.67	0.53594	YES	NO
126	ag	643.76	0.00000	NO	YES
127	ag	644.68	0.00000	NO	YES
128	au	644.83	1.15477	YES	NO
129	au	714.79	86.52791	YES	NO
130	ag	715.42	0.00000	NO	YES
131	au	715.56	3.77530	YES	NO
132	ag	715.87	0.00000	NO	YES
133	au	728.39	82.72398	YES	NO
134	ag	728.94	0.00000	NO	YES
135	ag	731.94	0.00000	NO	YES
136	au	732.39	77.54974	YES	NO
137	au	734.37	95.17094	YES	NO
138	ag	734.63	0.00000	NO	YES
139	ag	734.90	0.00000	NO	YES
140	au	735.20	77.23225	YES	NO
141	au	737.63	32.23128	YES	NO
142	ag	737.70	0.00000	NO	YES
143	au	738.85	11.28743	YES	NO
144	ag	738.95	0.00000	NO	YES
145	au	743.96	0.56469	YES	NO
146	ag	744.54	0.00000	NO	YES
147	au	749.50	8.24436	YES	NO
148	ag	749.84	0.00000	NO	YES
149	au	750.14	42.59344	YES	NO
150	ag	750.23	0.00000	NO	YES

151	ag	754.15	0.00000	NO	YES
152	au	754.21	80.77290	YES	NO
153	ag	789.88	0.00000	NO	YES
154	au	790.53	351.78772	YES	NO
155	au	792.72	73.34809	YES	NO
156	ag	792.82	0.00000	NO	YES
157	ag	794.04	0.00000	NO	YES
158	au	794.05	127.56239	YES	NO
159	au	795.39	109.80507	YES	NO
160	ag	797.78	0.00000	NO	YES
161	au	798.94	134.96372	YES	NO
162	ag	798.99	0.00000	NO	YES
163	ag	800.39	0.00000	NO	YES
164	au	801.12	28.34040	YES	NO
165	au	833.70	1454.98211	YES	NO
166	ag	854.39	0.00000	NO	YES
167	ag	900.13	0.00000	NO	YES
168	au	900.46	0.55191	YES	NO
169	ag	902.17	0.00000	NO	YES
170	au	903.14	9.51777	YES	NO
171	au	904.12	0.40103	YES	NO
172	ag	904.15	0.00000	NO	YES
173	au	906.93	2.42120	YES	NO
174	ag	908.28	0.00000	NO	YES
175	ag	910.43	0.00000	NO	YES
176	au	910.98	1.15776	YES	NO
177	au	912.80	4.39796	YES	NO
178	ag	912.87	0.00000	NO	YES
179	au	986.66	1.34593	YES	NO
180	ag	987.01	0.00000	NO	YES
181	ag	989.61	0.00000	NO	YES
182	au	989.69	2.26827	YES	NO
183	ag	990.69	0.00000	NO	YES
184	au	990.72	0.74761	YES	NO
185	au	993.22	3.70938	YES	NO
186	ag	993.57	0.00000	NO	YES
187	ag	998.05	0.00000	NO	YES
188	au	998.31	0.17070	YES	NO
189	au	998.60	1.09563	YES	NO
190	ag	998.86	0.00000	NO	YES
191	au	1038.44	11.40463	YES	NO
192	ag	1038.80	0.00000	NO	YES
193	ag	1039.39	0.00000	NO	YES
194	au	1039.48	4.77871	YES	NO
195	ag	1039.98	0.00000	NO	YES
196	au	1040.32	16.64691	YES	NO
197	au	1040.45	9.53236	YES	NO
198	ag	1040.55	0.00000	NO	YES
199	ag	1040.98	0.00000	NO	YES
200	au	1041.34	6.00439	YES	NO
201	au	1042.15	5.37780	YES	NO
202	ag	1042.45	0.00000	NO	YES
203	ag	1043.21	0.00000	NO	YES
204	au	1043.27	7.29504	YES	NO
205	ag	1043.65	0.00000	NO	YES
206	au	1043.71	6.47707	YES	NO
207	au	1044.15	2.23609	YES	NO
208	ag	1044.28	0.00000	NO	YES

209	au	1044.84	2.93711	YES	NO
210	ag	1045.61	0.00000	NO	YES
211	ag	1048.06	0.00000	NO	YES
212	au	1048.20	3.81576	YES	NO
213	ag	1048.81	0.00000	NO	YES
214	au	1048.99	0.89372	YES	NO
215	ag	1065.14	0.00000	NO	YES
216	au	1065.20	0.18532	YES	NO
217	au	1067.78	0.36794	YES	NO
218	ag	1067.84	0.00000	NO	YES
219	ag	1069.15	0.00000	NO	YES
220	au	1069.22	0.46396	YES	NO
221	au	1070.56	0.27557	YES	NO
222	ag	1070.59	0.00000	NO	YES
223	au	1070.75	0.50730	YES	NO
224	ag	1070.79	0.00000	NO	YES
225	au	1071.19	0.70678	YES	NO
226	ag	1071.21	0.00000	NO	YES
227	ag	1083.20	0.00000	NO	YES
228	au	1083.31	12.81757	YES	NO
229	au	1084.34	0.93814	YES	NO
230	ag	1084.34	0.00000	NO	YES
231	ag	1084.58	0.00000	NO	YES
232	au	1084.63	1.39759	YES	NO
233	au	1085.29	1.79980	YES	NO
234	ag	1085.32	0.00000	NO	YES
235	ag	1085.62	0.00000	NO	YES
236	au	1085.66	3.56683	YES	NO
237	au	1085.77	0.58383	YES	NO
238	ag	1085.84	0.00000	NO	YES
239	ag	1120.92	0.00000	NO	YES
240	au	1123.40	697.00560	YES	NO
241	ag	1143.09	0.00000	NO	YES
242	au	1143.16	7.51164	YES	NO
243	au	1144.55	8.94456	YES	NO
244	ag	1144.59	0.00000	NO	YES
245	ag	1145.03	0.00000	NO	YES
246	au	1145.50	6.28858	YES	NO
247	au	1146.35	1.24926	YES	NO
248	ag	1146.86	0.00000	NO	YES
249	au	1149.43	2.31581	YES	NO
250	ag	1149.65	0.00000	NO	YES
251	ag	1151.44	0.00000	NO	YES
252	au	1151.61	3.98980	YES	NO
253	au	1162.16	124.50558	YES	NO
254	ag	1162.21	0.00000	NO	YES
255	au	1162.43	136.62713	YES	NO
256	ag	1162.52	0.00000	NO	YES
257	ag	1164.98	0.00000	NO	YES
258	au	1165.64	205.12235	YES	NO
259	au	1165.67	85.69275	YES	NO
260	ag	1165.88	0.00000	NO	YES
261	au	1166.09	180.55044	YES	NO
262	ag	1166.26	0.00000	NO	YES
263	au	1167.11	121.28368	YES	NO
264	ag	1167.18	0.00000	NO	YES
265	au	1220.00	7.43167	YES	NO
266	ag	1220.01	0.00000	NO	YES

267	ag	1220.19	0.00000	NO	YES
268	au	1220.20	0.30036	YES	NO
269	au	1222.28	1.68045	YES	NO
270	ag	1222.32	0.00000	NO	YES
271	au	1222.57	2.08916	YES	NO
272	ag	1222.57	0.00000	NO	YES
273	ag	1222.73	0.00000	NO	YES
274	au	1222.76	0.48688	YES	NO
275	ag	1223.74	0.00000	NO	YES
276	au	1223.74	1.47979	YES	NO
277	ag	1246.77	0.00000	NO	YES
278	au	1246.80	1.74189	YES	NO
279	au	1248.56	4.27700	YES	NO
280	ag	1248.69	0.00000	NO	YES
281	au	1249.99	9.57720	YES	NO
282	ag	1250.00	0.00000	NO	YES
283	ag	1251.32	0.00000	NO	YES
284	au	1251.73	10.22828	YES	NO
285	ag	1254.63	0.00000	NO	YES
286	au	1254.68	4.85413	YES	NO
287	au	1255.98	2.05969	YES	NO
288	ag	1256.21	0.00000	NO	YES
289	au	1365.01	13.29302	YES	NO
290	ag	1365.52	0.00000	NO	YES
291	ag	1365.88	0.00000	NO	YES
292	au	1366.25	3.98601	YES	NO
293	ag	1367.80	0.00000	NO	YES
294	au	1367.88	6.16299	YES	NO
295	au	1368.96	5.91821	YES	NO
296	ag	1368.97	0.00000	NO	YES
297	au	1374.51	3.92735	YES	NO
298	ag	1374.52	0.00000	NO	YES
299	ag	1376.67	0.00000	NO	YES
300	au	1376.67	5.49786	YES	NO
301	au	1403.94	1.81727	YES	NO
302	ag	1403.97	0.00000	NO	YES
303	au	1404.65	4.35407	YES	NO
304	ag	1404.83	0.00000	NO	YES
305	ag	1405.53	0.00000	NO	YES
306	au	1405.55	3.23878	YES	NO
307	ag	1406.34	0.00000	NO	YES
308	au	1406.66	3.11704	YES	NO
309	au	1407.87	4.61016	YES	NO
310	ag	1408.24	0.00000	NO	YES
311	au	1409.69	3.01302	YES	NO
312	ag	1409.70	0.00000	NO	YES
313	ag	1515.81	0.00000	NO	YES
314	au	1515.84	38.22621	YES	NO
315	au	1519.43	63.63072	YES	NO
316	ag	1519.53	0.00000	NO	YES
317	ag	1520.01	0.00000	NO	YES
318	au	1520.03	30.40700	YES	NO
319	ag	1521.06	0.00000	NO	YES
320	au	1521.09	34.06238	YES	NO
321	au	1524.15	57.29652	YES	NO
322	ag	1524.17	0.00000	NO	YES
323	au	1524.82	66.91887	YES	NO
324	ag	1524.82	0.00000	NO	YES

325	au	1569.98	18.43802	YES	NO
326	ag	1570.07	0.00000	NO	YES
327	ag	1570.44	0.00000	NO	YES
328	au	1570.54	24.62268	YES	NO
329	au	1571.54	1.64714	YES	NO
330	ag	1571.55	0.00000	NO	YES
331	ag	1571.73	0.00000	NO	YES
332	au	1571.75	15.39688	YES	NO
333	au	1572.42	22.10725	YES	NO
334	ag	1572.44	0.00000	NO	YES
335	ag	1573.79	0.00000	NO	YES
336	au	1573.80	17.02455	YES	NO
337	au	1689.46	0.61371	YES	NO
338	ag	1689.61	0.00000	NO	YES
339	au	1691.38	0.88232	YES	NO
340	ag	1691.38	0.00000	NO	YES
341	ag	1692.40	0.00000	NO	YES
342	au	1692.43	1.56946	YES	NO
343	au	1692.63	2.16471	YES	NO
344	ag	1692.75	0.00000	NO	YES
345	au	1694.95	3.37371	YES	NO
346	ag	1694.99	0.00000	NO	YES
347	au	1696.49	3.88019	YES	NO
348	ag	1696.52	0.00000	NO	YES
349	au	1706.85	5.31087	YES	NO
350	ag	1706.92	0.00000	NO	YES
351	ag	1707.45	0.00000	NO	YES
352	au	1707.48	3.57438	YES	NO
353	au	1709.44	13.39788	YES	NO
354	ag	1709.45	0.00000	NO	YES
355	ag	1709.84	0.00000	NO	YES
356	au	1709.87	2.28499	YES	NO
357	ag	1710.24	0.00000	NO	YES
358	au	1710.25	22.43896	YES	NO
359	au	1711.24	7.75932	YES	NO
360	ag	1711.24	0.00000	NO	YES
361	au	3252.17	0.04999	YES	NO
362	ag	3252.19	0.00000	NO	YES
363	ag	3256.37	0.00000	NO	YES
364	au	3256.37	2.21911	YES	NO
365	au	3262.25	4.87070	YES	NO
366	ag	3262.27	0.00000	NO	YES
367	au	3265.77	0.60656	YES	NO
368	ag	3265.78	0.00000	NO	YES
369	au	3272.80	0.47150	YES	NO
370	ag	3272.80	0.00000	NO	YES
371	ag	3272.99	0.00000	NO	YES
372	au	3272.99	0.23748	YES	NO
373	au	3273.44	0.64458	YES	NO
374	ag	3273.45	0.00000	NO	YES
375	ag	3273.73	0.00000	NO	YES
376	au	3273.74	1.31599	YES	NO
377	ag	3275.86	0.00000	NO	YES
378	au	3275.86	0.88024	YES	NO
379	ag	3277.98	0.00000	NO	YES
380	au	3277.98	2.03220	YES	NO
381	au	3279.49	0.05963	YES	NO
382	ag	3279.49	0.00000	NO	YES

383	ag	3279.83	0.00000	NO	YES
384	au	3279.84	0.60962	YES	NO
385	au	3280.41	5.05390	YES	NO
386	ag	3280.42	0.00000	NO	YES
387	ag	3281.71	0.00000	NO	YES
388	au	3281.71	0.50695	YES	NO
389	ag	3283.69	0.00000	NO	YES
390	au	3283.69	0.08393	YES	NO
391	au	3285.89	1.70759	YES	NO
392	ag	3285.89	0.00000	NO	YES
393	au	3287.34	5.14264	YES	NO
394	ag	3287.36	0.00000	NO	YES
395	ag	3287.52	0.00000	NO	YES
396	au	3287.54	0.93695	YES	NO
397	ag	3288.94	0.00000	NO	YES
398	au	3288.94	1.75983	YES	NO
399	au	3289.92	1.25441	YES	NO
400	ag	3289.92	0.00000	NO	YES
401	ag	3291.14	0.00000	NO	YES
402	au	3291.14	2.28552	YES	NO
403	au	3293.48	2.22390	YES	NO
404	ag	3293.49	0.00000	NO	YES
405	au	3294.79	0.95425	YES	NO
406	ag	3294.79	0.00000	NO	YES
407	au	3297.55	3.80544	YES	NO
408	ag	3297.56	0.00000	NO	YES
409	au	3297.81	3.56794	YES	NO
410	ag	3297.82	0.00000	NO	YES
411	ag	3298.44	0.00000	NO	YES
412	au	3298.44	2.47980	YES	NO
413	au	3299.42	5.04070	YES	NO
414	ag	3299.42	0.00000	NO	YES
415	au	3300.27	6.42375	YES	NO
416	ag	3300.27	0.00000	NO	YES
417	ag	3300.58	0.00000	NO	YES
418	au	3300.60	5.02248	YES	NO
419	au	3307.00	2.90051	YES	NO
420	ag	3307.00	0.00000	NO	YES

$end

8.8 2^{2+} (positions of non-hydrogen atoms as found in the solid state structure; optimized positions of H atoms)

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

Cartesian coordinates in Ångström:

Ga	-1.3327353	0.1115299	0.1429312
P	-1.6226553	2.2346999	-2.1865088
C	-2.3788453	0.9450399	-1.3510588
P	-3.6286953	-0.0412601	-1.9802088
C	-0.4488053	3.0193499	-1.0476988
C	-0.7329253	3.0762699	0.3241512
H	-1.6760854	2.6798375	0.7029783
C	0.1595147	3.6936899	1.1995412
H	-0.0653114	3.7243971	2.2644678
C	1.3161347	4.2893699	0.7156312

H	2.0080975	4.7727681	1.4040012
C	1.5695047	4.2968699	-0.6519288
H	2.4579083	4.7904054	-1.0419570
C	0.6964647	3.6637899	-1.5329288
H	0.9105413	3.6703627	-2.6000968
C	-0.7102253	1.7436999	-3.6672888
C	-1.3582653	1.6744299	-4.9070988
H	-2.3676856	2.0675470	-5.0173106
C	-0.7164153	1.1095199	-6.0020088
H	-1.2286162	1.0666072	-6.9624003
C	0.5692447	0.5986599	-5.8735988
H	1.0676289	0.1581756	-6.7366957
C	1.2171847	0.6549199	-4.6473188
H	2.2266431	0.2572047	-4.5428533
C	0.5882747	1.2252299	-3.5481288
H	1.0979905	1.2461918	-2.5855140
C	-2.7391053	3.5711299	-2.6634888
C	-3.8787253	3.7829299	-1.8808488
H	-4.0921692	3.1097000	-1.0514258
C	-4.7445553	4.8273599	-2.1799088
H	-5.6369339	4.9796018	-1.5743856
C	-4.4735153	5.6688199	-3.2540188
H	-5.1553888	6.4842070	-3.4933992
C	-3.3309453	5.4754499	-4.0178388
H	-3.1122775	6.1427275	-4.8511578
C	-2.4529853	4.4358699	-3.7247288
H	-1.5548340	4.2997808	-4.3253339
C	-3.1098653	-1.0965001	-3.3599788
C	-4.0070153	-1.5589301	-4.3337388
H	-5.0688028	-1.3290099	-4.2537728
C	-3.5354453	-2.2829101	-5.4243488
H	-4.2339127	-2.6240157	-6.1876190
C	-2.1768453	-2.5616601	-5.5438488
H	-1.8114039	-3.1134239	-6.4096020
C	-1.2910453	-2.1484401	-4.5581988
H	-0.2276790	-2.3669981	-4.6496895
C	-1.7520253	-1.4142001	-3.4685788
H	-1.0500989	-1.0473661	-2.7195389
C	-5.1029753	0.8316399	-2.5634688
C	-6.1826753	1.0488499	-1.7032588
H	-6.1895236	0.6100632	-0.7061557
C	-7.2635253	1.8212499	-2.1280788
H	-8.1083283	1.9812356	-1.4591934
C	-7.2679653	2.3717099	-3.4045388
H	-8.1163136	2.9714043	-3.7331365
C	-6.1995753	2.1551699	-4.2640888
H	-6.2050342	2.5840099	-5.2653897
C	-5.1204253	1.3860699	-3.8498288
H	-4.2878015	1.2103654	-4.5295465
C	-4.1518353	-1.1344501	-0.6291488
C	-4.4940353	-2.4654701	-0.8717688
H	-4.4357093	-2.8674991	-1.8826041
C	-4.9013253	-3.2835501	0.1812212
H	-5.1759508	-4.3186537	-0.0198590
C	-4.9577653	-2.7871401	1.4781412
H	-5.2761837	-3.4333510	2.2956879
C	-4.6259953	-1.4627401	1.7276812
H	-4.6895755	-1.0606929	2.7381673

C	-4.2316853	-0.6339601	0.6786612
H	-4.0186773	0.4185905	0.8677207
Ga	1.3327353	-0.1115299	-0.1429312
P	1.6226553	-2.2346999	2.1865088
C	2.3788453	-0.9450399	1.3510588
P	3.6286953	0.0412601	1.9802088
C	0.4488053	-3.0193499	1.0476988
C	0.7329253	-3.0762699	-0.3241512
H	1.6760854	-2.6798375	-0.7029783
C	-0.1595147	-3.6936899	-1.1995412
H	0.0653114	-3.7243971	-2.2644678
C	-1.3161347	-4.2893699	-0.7156312
H	-2.0080975	-4.7727681	-1.4040012
C	-1.5695047	-4.2968699	0.6519288
H	-2.4579083	-4.7904054	1.0419570
C	-0.6964647	-3.6637899	1.5329288
H	-0.9105413	-3.6703627	2.6000968
C	0.7102253	-1.7436999	3.6672888
C	1.3582653	-1.6744299	4.9070988
H	2.3676856	-2.0675470	5.0173106
C	0.7164153	-1.1095199	6.0020088
H	1.2286162	-1.0666072	6.9624003
C	-0.5692447	-0.5986599	5.8735988
H	-1.0676289	-0.1581756	6.7366957
C	-1.2171847	-0.6549199	4.6473188
H	-2.2266431	-0.2572047	4.5428533
C	-0.5882747	-1.2252299	3.5481288
H	-1.0979905	-1.2461918	2.5855140
C	2.7391053	-3.5711299	2.6634888
C	3.8787253	-3.7829299	1.8808488
H	4.0921692	-3.1097000	1.0514258
C	4.7445553	-4.8273599	2.1799088
H	5.6369339	-4.9796018	1.5743856
C	4.4735153	-5.6688199	3.2540188
H	5.1553888	-6.4842070	3.4933992
C	3.3309453	-5.4754499	4.0178388
H	3.1122775	-6.1427275	4.8511578
C	2.4529853	-4.4358699	3.7247288
H	1.5548340	-4.2997808	4.3253339
C	3.1098653	1.0965001	3.3599788
C	4.0070153	1.5589301	4.3337388
H	5.0688028	1.3290099	4.2537728
C	3.5354453	2.2829101	5.4243488
H	4.2339127	2.6240157	6.1876190
C	2.1768453	2.5616601	5.5438488
H	1.8114039	3.1134239	6.4096020
C	1.2910453	2.1484401	4.5581988
H	0.2276790	2.3669981	4.6496895
C	1.7520253	1.4142001	3.4685788
H	1.0500989	1.0473661	2.7195389
C	5.1029753	-0.8316399	2.5634688
C	6.1826753	-1.0488499	1.7032588
H	6.1895236	-0.6100632	0.7061557
C	7.2635253	-1.8212499	2.1280788
H	8.1083283	-1.9812356	1.4591934
C	7.2679653	-2.3717099	3.4045388
H	8.1163136	-2.9714043	3.7331365
C	6.1995753	-2.1551699	4.2640888

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H      6.2050342   -2.5840099    5.2653897
C      5.1204253   -1.3860699    3.8498288
H      4.2878015   -1.2103654    4.5295465
C      4.1518353    1.1344501    0.6291488
C      4.4940353    2.4654701    0.8717688
H      4.4357093    2.8674991    1.8826041
C      4.9013253    3.2835501   -0.1812212
H      5.1759508    4.3186537    0.0198590
C      4.9577653    2.7871401   -1.4781412
H      5.2761837    3.4333510   -2.2956879
C      4.6259953    1.4627401   -1.7276812
H      4.6895755    1.0606929   -2.7381673
C      4.2316853    0.6339601   -0.6786612
H      4.0186773   -0.4185905   -0.8677207

SCF energy GEOOPT =  -8073.078142926 H
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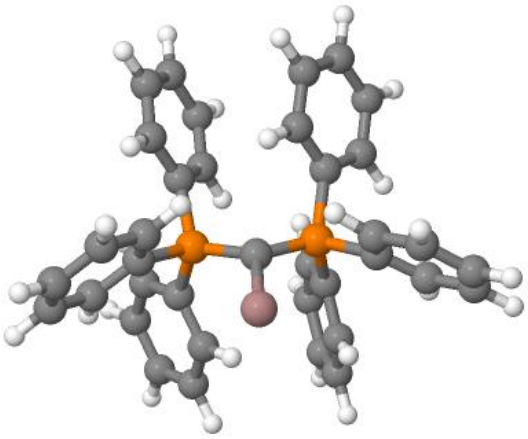
8.9 [Ga(CDP^{Ph})]$^{+}$



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

Cartesian coordinates in Ångström:
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H     -4.3838707    1.2084095    5.7210030
C     -3.6937787    1.3928044    4.8987020
H     -2.7035167    3.0384536    5.8851901
C     -2.7501279    2.4198621    4.9897070
C     -3.7547334    0.6038137    3.7530827
H     -4.4835750   -0.2020465    3.6860685
H     -1.9262755    2.0327870   -0.4928792
C     -1.8596135    2.6457257    3.9378333
C     -2.8732784    0.8371633    2.6849173
H     -1.1114453    3.4339600    4.0145475
P     -3.1006824   -0.0719844    1.1304987
C     -1.9183408    1.8580933    2.7867754
C     -1.2457743    1.1817073   -0.5319677
H     -4.3669122   -2.2716980   -0.2096521
H      0.1517996    2.1608259   -1.8485490
C     -3.9598622   -2.6717642    0.7183064
C     -0.0742149    1.2551152   -1.2872193
C     -1.5450426    0.0139679    0.1970889
C     -3.3057888   -1.8111953    1.6097408
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H    -1.2165672    2.0348104    1.9726165
C    -4.1042340   -4.0225244    1.0280341
H    -4.6205853   -4.6848647    0.3345991
C    -2.7802978   -2.3178694    2.8087660
C     0.8026756    0.1683091   -1.3221540
C    -3.5943265   -4.5219517    2.2291525
C    -0.6575461   -1.0703019    0.1616233
H    -2.2575461   -1.6580095    3.4996285
C    -2.9294402   -3.6707062    3.1157668
C     0.5106605   -0.9902582   -0.5980528
H     1.7139919    0.2236872   -1.9163891
H    -3.7126562   -5.5769987    2.4740314
H    -0.8865129   -1.9791442    0.7160725
H    -2.5239483   -4.0607585    4.0486797
H     1.1922965   -1.8394060   -0.6288341
H    -6.4941486    3.7323115   -3.2889749
C    -6.9680518    2.9709815   -2.6708192
H    -8.8242954    2.9978298   -3.7717316
C    -8.2766660    2.5622794   -2.9368996
C    -6.2673643    2.4125452   -1.6010050
H    -5.2666332    2.7725244   -1.3582894
H    -4.2651142    2.9660249    1.3860070
C    -8.8886542    1.6058860   -2.1226640
C    -6.8670963    1.4229068   -0.8003468
H    -9.9151294    1.2982270   -2.3186674
P    -5.9170771    0.7705409    0.6043219
C    -8.1910186    1.0390848   -1.0550190
C    -5.1420580    3.0038762    2.0305993
H    -6.5213134   -0.4182682    3.2579633
H    -4.5104955    4.7754633    3.0773231
C    -6.7852379   -1.1376874    2.4852261
C    -5.2817784    4.0126755    2.9808625
C    -6.1240382    2.0104296    1.9117322
C    -6.7122855   -0.7737831    1.1333693
H    -8.6779300    0.2977995   -0.4235739
C    -7.2013505   -2.4200882    2.8468044
H    -7.2468613   -2.6953842    3.8997388
C    -7.0614856   -1.7140249    0.1492344
C    -6.4047563    4.0379981    3.8120398
C    -7.5637423   -3.3424989    1.8645111
C    -7.2671678    2.0557312    2.7234984
H    -6.9790607   -1.4543484   -0.9067026
C    -7.5000194   -2.9843142    0.5145452
C    -7.3991449    3.0650794    3.6775834
H    -6.5109848    4.8227705    4.5602861
H    -7.8941803   -4.3407135    2.1488581
H    -8.0533570    1.3099580    2.6115638
H    -7.7819286   -3.7010092   -0.2560853
H    -8.2831497    3.0951496    4.3136222
Ga   -3.9126457    0.3934621   -2.0044267

SCF energy GEOOPT =  -4036.546666519 H
ZPE =   1426. kJ/mol
FREEH energy =  1520.35 kJ/mol
FREEH entropy =   0.94993 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
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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	14.69	0.01374	YES	YES
8	a	26.48	0.10898	YES	YES
9	a	30.82	0.04512	YES	YES
10	a	37.82	0.02867	YES	YES
11	a	38.81	0.05687	YES	YES
12	a	41.29	0.02648	YES	YES
13	a	44.29	0.10315	YES	YES
14	a	48.89	0.07173	YES	YES
15	a	53.30	0.09828	YES	YES
16	a	62.08	0.18585	YES	YES
17	a	65.35	0.00546	YES	YES
18	a	70.60	0.49984	YES	YES
19	a	73.27	0.08187	YES	YES
20	a	82.85	0.31655	YES	YES
21	a	86.40	0.12640	YES	YES
22	a	98.16	0.41758	YES	YES
23	a	109.10	1.32296	YES	YES
24	a	117.46	0.24439	YES	YES
25	a	125.36	2.16516	YES	YES
26	a	142.59	2.22254	YES	YES
27	a	186.43	0.30460	YES	YES
28	a	194.29	5.00370	YES	YES
29	a	195.15	2.63346	YES	YES
30	a	204.57	6.40551	YES	YES
31	a	221.25	0.88636	YES	YES
32	a	228.16	0.35095	YES	YES
33	a	232.92	1.18290	YES	YES
34	a	239.32	5.50095	YES	YES
35	a	243.25	0.91883	YES	YES
36	a	251.89	0.32167	YES	YES
37	a	258.73	0.16254	YES	YES
38	a	270.01	0.32843	YES	YES
39	a	275.57	1.07540	YES	YES
40	a	347.28	5.67538	YES	YES
41	a	380.84	18.87157	YES	YES
42	a	385.02	0.87088	YES	YES
43	a	392.85	0.15507	YES	YES
44	a	396.52	0.19859	YES	YES
45	a	400.59	0.59198	YES	YES
46	a	402.75	0.11872	YES	YES
47	a	406.26	0.04239	YES	YES
48	a	424.09	3.60913	YES	YES
49	a	429.08	2.37971	YES	YES
50	a	443.27	0.95121	YES	YES
51	a	453.33	3.39086	YES	YES
52	a	472.46	0.79241	YES	YES
53	a	496.18	30.51158	YES	YES
54	a	497.32	85.37066	YES	YES
55	a	508.93	21.82243	YES	YES
56	a	516.23	17.50158	YES	YES
57	a	526.03	133.46422	YES	YES

58	a	554.89	24.89149	YES	YES
59	a	612.52	0.08077	YES	YES
60	a	613.35	0.44455	YES	YES
61	a	613.94	0.77318	YES	YES
62	a	614.15	0.50558	YES	YES
63	a	615.11	1.10245	YES	YES
64	a	616.01	0.74802	YES	YES
65	a	671.88	33.77614	YES	YES
66	a	680.71	0.24253	YES	YES
67	a	690.30	109.56060	YES	YES
68	a	693.58	3.47993	YES	YES
69	a	695.06	13.69313	YES	YES
70	a	696.69	14.31132	YES	YES
71	a	698.17	13.85597	YES	YES
72	a	702.05	13.18189	YES	YES
73	a	709.11	3.61357	YES	YES
74	a	711.80	4.32526	YES	YES
75	a	715.32	21.38647	YES	YES
76	a	718.63	50.71467	YES	YES
77	a	734.18	88.44708	YES	YES
78	a	736.37	31.72663	YES	YES
79	a	739.61	7.75154	YES	YES
80	a	741.80	24.92408	YES	YES
81	a	744.14	1.83551	YES	YES
82	a	745.22	14.38676	YES	YES
83	a	775.18	243.71746	YES	YES
84	a	833.40	0.15068	YES	YES
85	a	838.52	1.19316	YES	YES
86	a	839.87	0.95574	YES	YES
87	a	843.14	0.60779	YES	YES
88	a	845.58	0.58916	YES	YES
89	a	847.41	1.95747	YES	YES
90	a	911.11	0.04436	YES	YES
91	a	917.89	0.94228	YES	YES
92	a	920.12	0.60732	YES	YES
93	a	920.60	1.25299	YES	YES
94	a	924.65	0.33359	YES	YES
95	a	928.64	0.31663	YES	YES
96	a	961.43	0.48274	YES	YES
97	a	964.94	0.59474	YES	YES
98	a	966.72	0.42662	YES	YES
99	a	968.34	0.75234	YES	YES
100	a	969.51	1.14877	YES	YES
101	a	971.83	0.51797	YES	YES
102	a	985.74	0.09569	YES	YES
103	a	987.44	0.04978	YES	YES
104	a	988.43	0.03898	YES	YES
105	a	989.54	0.04214	YES	YES
106	a	992.20	2.49003	YES	YES
107	a	994.39	6.32209	YES	YES
108	a	995.54	12.38353	YES	YES
109	a	996.52	2.72010	YES	YES
110	a	997.29	7.33628	YES	YES
111	a	998.04	9.31678	YES	YES
112	a	998.78	1.45088	YES	YES
113	a	1002.35	0.68382	YES	YES
114	a	1024.59	14.12022	YES	YES
115	a	1025.63	1.10976	YES	YES

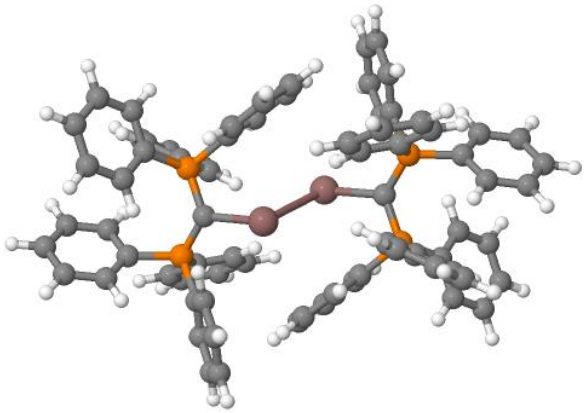
116	a	1025.86	0.48441	YES	YES
117	a	1026.14	1.30590	YES	YES
118	a	1026.92	1.12195	YES	YES
119	a	1027.46	0.26911	YES	YES
120	a	1061.81	319.14056	YES	YES
121	a	1074.61	3.53177	YES	YES
122	a	1076.84	4.26710	YES	YES
123	a	1077.09	4.87014	YES	YES
124	a	1079.01	2.51519	YES	YES
125	a	1081.44	0.50862	YES	YES
126	a	1082.77	2.14943	YES	YES
127	a	1092.47	52.10579	YES	YES
128	a	1093.60	41.78812	YES	YES
129	a	1093.87	59.24879	YES	YES
130	a	1095.60	67.06644	YES	YES
131	a	1097.41	72.27293	YES	YES
132	a	1098.01	78.51407	YES	YES
133	a	1157.40	0.23737	YES	YES
134	a	1157.49	0.46690	YES	YES
135	a	1158.47	0.39383	YES	YES
136	a	1159.01	0.64725	YES	YES
137	a	1159.34	0.19213	YES	YES
138	a	1159.77	0.23095	YES	YES
139	a	1173.71	0.89886	YES	YES
140	a	1174.41	0.61561	YES	YES
141	a	1175.37	3.74838	YES	YES
142	a	1176.18	1.98111	YES	YES
143	a	1178.90	2.40330	YES	YES
144	a	1181.69	0.25181	YES	YES
145	a	1290.09	1.56771	YES	YES
146	a	1294.79	4.73188	YES	YES
147	a	1297.05	3.31437	YES	YES
148	a	1299.02	7.98669	YES	YES
149	a	1304.04	1.29071	YES	YES
150	a	1305.36	4.08995	YES	YES
151	a	1335.98	0.23612	YES	YES
152	a	1338.25	0.54079	YES	YES
153	a	1339.03	0.25745	YES	YES
154	a	1339.42	0.10610	YES	YES
155	a	1340.69	0.30608	YES	YES
156	a	1341.28	0.19972	YES	YES
157	a	1425.82	5.53328	YES	YES
158	a	1427.72	14.01627	YES	YES
159	a	1429.24	17.03144	YES	YES
160	a	1430.76	24.56656	YES	YES
161	a	1433.29	11.87498	YES	YES
162	a	1434.27	14.66782	YES	YES
163	a	1469.48	5.42528	YES	YES
164	a	1470.30	4.77432	YES	YES
165	a	1470.91	5.14864	YES	YES
166	a	1471.70	3.92627	YES	YES
167	a	1474.10	14.70260	YES	YES
168	a	1474.72	3.85746	YES	YES
169	a	1566.85	0.59452	YES	YES
170	a	1567.48	0.09628	YES	YES
171	a	1569.58	0.29375	YES	YES
172	a	1570.51	0.03150	YES	YES
173	a	1572.02	0.36570	YES	YES

174	a	1572.71	0.31280	YES	YES
175	a	1581.41	0.08300	YES	YES
176	a	1581.58	1.52755	YES	YES
177	a	1583.82	0.26093	YES	YES
178	a	1584.39	0.26642	YES	YES
179	a	1585.22	2.40727	YES	YES
180	a	1585.81	0.51960	YES	YES
181	a	3090.81	4.83915	YES	YES
182	a	3094.64	1.68789	YES	YES
183	a	3096.89	2.89319	YES	YES
184	a	3102.83	0.76597	YES	YES
185	a	3105.83	0.28058	YES	YES
186	a	3106.90	0.05388	YES	YES
187	a	3109.62	0.12630	YES	YES
188	a	3110.04	1.43694	YES	YES
189	a	3111.14	0.13664	YES	YES
190	a	3111.90	0.02995	YES	YES
191	a	3112.28	0.13929	YES	YES
192	a	3112.59	0.38680	YES	YES
193	a	3116.52	0.42602	YES	YES
194	a	3117.38	0.92136	YES	YES
195	a	3118.39	1.26263	YES	YES
196	a	3119.28	0.79939	YES	YES
197	a	3120.03	0.91141	YES	YES
198	a	3120.10	0.61286	YES	YES
199	a	3125.02	2.75561	YES	YES
200	a	3125.29	13.40074	YES	YES
201	a	3125.76	2.23021	YES	YES
202	a	3126.56	5.54471	YES	YES
203	a	3127.35	3.31869	YES	YES
204	a	3127.41	5.39217	YES	YES
205	a	3132.63	6.00645	YES	YES
206	a	3133.02	7.83002	YES	YES
207	a	3133.38	8.54069	YES	YES
208	a	3134.02	6.92951	YES	YES
209	a	3134.93	7.63229	YES	YES
210	a	3135.19	5.76313	YES	YES

$end

COSMO energy + OC correction = -4036.5968923039 H

8.10 $[\{In(CDP^{Ph})\}_2]^{2+}$



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

Symmetry: ci

Cartesian coordinates in Ångström:

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P	-3.6610996	-0.1203017	-2.0783595
C	-0.5216604	2.9660805	-1.3170125
C	-0.7685129	3.7225450	-0.1549433
H	-1.7932785	3.9818436	0.1142391
C	0.2971122	4.1863705	0.6183669
H	0.1012867	4.7894405	1.5035125
C	1.6112308	3.8932150	0.2470873
H	2.4409265	4.2556314	0.8512553
C	1.8624739	3.1485432	-0.9065172
H	2.8875693	2.9390088	-1.2085895
C	0.8015624	2.6893924	-1.6914050
H	1.0049965	2.1436351	-2.6109318
C	-1.3944168	1.9671130	-3.9294170
C	-1.8306678	2.6863820	-5.0522894
H	-2.4985153	3.5372877	-4.9316567
C	-1.4323049	2.2923632	-6.3307330
H	-1.7794398	2.8509911	-7.1991407
C	-0.5995947	1.1831730	-6.4982329
H	-0.2976506	0.8755379	-7.4986938
C	-0.1588473	0.4660799	-5.3823034
H	0.4825553	-0.4053244	-5.5074013
C	-0.5544832	0.8541122	-4.1046198
H	-0.2321724	0.2788272	-3.2374734
C	-3.0714555	3.7606625	-2.3293665
C	-4.3747248	3.6620944	-1.8305974
H	-4.7103916	2.7240786	-1.3940471
C	-5.2312452	4.7616917	-1.8945439
H	-6.2483555	4.6775862	-1.5140085
C	-4.7825870	5.9652988	-2.4423022
H	-5.4510209	6.8241341	-2.4920659
C	-3.4704958	6.0764632	-2.9158141
H	-3.1157335	7.0209983	-3.3264523
C	-2.6127085	4.9795302	-2.8582380
H	-1.5862599	5.0736840	-3.2145942
C	-2.8971370	-1.3210940	-3.2106340
C	-3.5113859	-1.7334224	-4.4018340
H	-4.4945479	-1.3519598	-4.6717533
C	-2.8570464	-2.6301549	-5.2494866
H	-3.3336400	-2.9390244	-6.1789702
C	-1.5977987	-3.1280863	-4.9079709
H	-1.0876540	-3.8217195	-5.5755682
C	-0.9951393	-2.7377472	-3.7081754
H	-0.0132324	-3.1237829	-3.4357750
C	-1.6410944	-1.8387033	-2.8646296
H	-1.1582510	-1.5118802	-1.9425765
C	-5.0492315	0.6242065	-2.9766034
C	-6.3118895	0.7326643	-2.3747671
H	-6.5069223	0.2502847	-1.4178391
C	-7.3224719	1.4633022	-3.0018723
H	-8.3025080	1.5413269	-2.5326199
C	-7.0807854	2.0866348	-4.2282377
H	-7.8705482	2.6589173	-4.7132988

C	-5.8296492	1.9644793	-4.8395323
H	-5.6427640	2.4370255	-5.8031288
C	-4.8170628	1.2356777	-4.2200889
H	-3.8452127	1.1459738	-4.7019215
C	-4.3943763	-1.1114926	-0.7436817
C	-4.7637935	-2.4443939	-0.9735869
H	-4.5722137	-2.8998971	-1.9446169
C	-5.3742298	-3.1852918	0.0390927
H	-5.6627451	-4.2194294	-0.1456238
C	-5.6149615	-2.6045077	1.2885998
H	-6.0896868	-3.1871374	2.0771799
C	-5.2591276	-1.2733895	1.5209279
H	-5.4638096	-0.8120973	2.4863230
C	-4.6601883	-0.5244193	0.5051385
H	-4.4355766	0.5317308	0.6618174
In	1.5451500	-0.5760388	-0.6120474
P	1.9599960	-2.3319926	2.2431605
C	2.5568171	-0.9827404	1.3824534
P	3.6610996	0.1203017	2.0783595
C	0.5216604	-2.9660805	1.3170125
C	0.7685129	-3.7225450	0.1549433
H	1.7932785	-3.9818436	-0.1142391
C	-0.2971122	-4.1863705	-0.6183669
H	-0.1012867	-4.7894405	-1.5035125
C	-1.6112308	-3.8932150	-0.2470873
H	-2.4409265	-4.2556314	-0.8512553
C	-1.8624739	-3.1485432	0.9065172
H	-2.8875693	-2.9390088	1.2085895
C	-0.8015624	-2.6893924	1.6914050
H	-1.0049965	-2.1436351	2.6109318
C	1.3944168	-1.9671130	3.9294170
C	1.8306678	-2.6863820	5.0522894
H	2.4985153	-3.5372877	4.9316567
C	1.4323049	-2.2923632	6.3307330
H	1.7794398	-2.8509911	7.1991407
C	0.5995947	-1.1831730	6.4982329
H	0.2976506	-0.8755379	7.4986938
C	0.1588473	-0.4660799	5.3823034
H	-0.4825553	0.4053244	5.5074013
C	0.5544832	-0.8541122	4.1046198
H	0.2321724	-0.2788272	3.2374734
C	3.0714555	-3.7606625	2.3293665
C	4.3747248	-3.6620944	1.8305974
H	4.7103916	-2.7240786	1.3940471
C	5.2312452	-4.7616917	1.8945439
H	6.2483555	-4.6775862	1.5140085
C	4.7825870	-5.9652988	2.4423022
H	5.4510209	-6.8241341	2.4920659
C	3.4704958	-6.0764632	2.9158141
H	3.1157335	-7.0209983	3.3264523
C	2.6127085	-4.9795302	2.8582380
H	1.5862599	-5.0736840	3.2145942
C	2.8971370	1.3210940	3.2106340
C	3.5113859	1.7334224	4.4018340
H	4.4945479	1.3519598	4.6717533
C	2.8570464	2.6301549	5.2494866
H	3.3336400	2.9390244	6.1789702
C	1.5977987	3.1280863	4.9079709

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H     1.0876540    3.8217195    5.5755682
C     0.9951393    2.7377472    3.7081754
H     0.0132324    3.1237829    3.4357750
C     1.6410944    1.8387033    2.8646296
H     1.1582510    1.5118802    1.9425765
C     5.0492315   -0.6242065    2.9766034
C     6.3118895   -0.7326643    2.3747671
H     6.5069223   -0.2502847    1.4178391
C     7.3224719   -1.4633022    3.0018723
H     8.3025080   -1.5413269    2.5326199
C     7.0807854   -2.0866348    4.2282377
H     7.8705482   -2.6589173    4.7132988
C     5.8296492   -1.9644793    4.8395323
H     5.6427640   -2.4370255    5.8031288
C     4.8170628   -1.2356777    4.2200889
H     3.8452127   -1.1459738    4.7019215
C     4.3943763    1.1114926    0.7436817
C     4.7637935    2.4443939    0.9735869
H     4.5722137    2.8998971    1.9446169
C     5.3742298    3.1852918   -0.0390927
H     5.6627451    4.2194294    0.1456238
C     5.6149615    2.6045077   -1.2885998
H     6.0896868    3.1871374   -2.0771799
C     5.2591276    1.2733895   -1.5209279
H     5.4638096    0.8120973   -2.4863230
C     4.6601883    0.5244193   -0.5051385
H     4.4355766   -0.5317308   -0.6618174

SCF energy GEOOPT =  -4603.391736262 H
ZPE =   2854. kJ/mol
FREEH energy =  3048.90 kJ/mol
FREEH entropy =   1.71036 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            12.53         0.01474       YES     NO
     8        au            14.84         0.17098       YES     NO
     9        ag            14.94         0.00000       NO      YES
    10        au            17.71         0.06440       YES     NO
    11        ag            22.34         0.00000       NO      YES
    12        au            24.82         0.07638       YES     NO
    13        ag            24.87         0.00000       NO      YES
    14        au            28.60         0.05426       YES     NO
    15        ag            31.21         0.00000       NO      YES
    16        ag            34.45         0.00000       NO      YES
    17        au            35.06         0.14917       YES     NO
    18        ag            40.16         0.00000       NO      YES
    19        au            40.37         0.12561       YES     NO
    20        ag            43.96         0.00000       NO      YES
    21        au            45.81         0.13191       YES     NO
    22        ag            46.84         0.00000       NO      YES
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23	au	51.04	0.15768	YES	NO
24	ag	52.11	0.00000	NO	YES
25	ag	52.73	0.00000	NO	YES
26	au	54.83	0.26565	YES	NO
27	au	56.13	0.03331	YES	NO
28	ag	60.54	0.00000	NO	YES
29	ag	63.00	0.00000	NO	YES
30	au	63.29	0.27864	YES	NO
31	au	64.92	0.08943	YES	NO
32	au	68.27	0.23673	YES	NO
33	ag	68.78	0.00000	NO	YES
34	ag	78.94	0.00000	NO	YES
35	au	80.54	0.55818	YES	NO
36	ag	81.76	0.00000	NO	YES
37	au	84.13	1.51277	YES	NO
38	ag	85.83	0.00000	NO	YES
39	ag	87.80	0.00000	NO	YES
40	au	87.87	0.31880	YES	NO
41	au	91.59	1.10499	YES	NO
42	ag	92.77	0.00000	NO	YES
43	au	98.77	0.61330	YES	NO
44	ag	101.23	0.00000	NO	YES
45	au	104.25	0.50226	YES	NO
46	ag	106.38	0.00000	NO	YES
47	ag	110.56	0.00000	NO	YES
48	au	112.83	1.95718	YES	NO
49	ag	120.75	0.00000	NO	YES
50	au	122.92	1.32249	YES	NO
51	au	131.58	8.50808	YES	NO
52	ag	134.70	0.00000	NO	YES
53	ag	191.24	0.00000	NO	YES
54	au	191.49	16.40260	YES	NO
55	au	195.90	7.86755	YES	NO
56	ag	196.00	0.00000	NO	YES
57	ag	199.94	0.00000	NO	YES
58	au	200.94	2.33876	YES	NO
59	au	204.13	3.34456	YES	NO
60	ag	204.95	0.00000	NO	YES
61	au	216.35	3.72829	YES	NO
62	ag	218.45	0.00000	NO	YES
63	ag	226.29	0.00000	NO	YES
64	au	228.60	4.29822	YES	NO
65	ag	229.62	0.00000	NO	YES
66	au	230.09	3.69843	YES	NO
67	ag	245.12	0.00000	NO	YES
68	au	245.91	4.45786	YES	NO
69	au	248.11	2.01955	YES	NO
70	ag	248.56	0.00000	NO	YES
71	au	253.70	0.49158	YES	NO
72	ag	254.11	0.00000	NO	YES
73	au	257.46	0.82830	YES	NO
74	ag	257.60	0.00000	NO	YES
75	au	270.75	2.13308	YES	NO
76	ag	271.00	0.00000	NO	YES
77	ag	272.48	0.00000	NO	YES
78	au	272.58	1.56478	YES	NO
79	au	337.00	18.76203	YES	NO
80	ag	337.22	0.00000	NO	YES

81	ag	379.74	0.00000	NO	YES
82	au	380.33	29.62033	YES	NO
83	ag	388.23	0.00000	NO	YES
84	au	388.66	0.52053	YES	NO
85	au	394.45	0.61299	YES	NO
86	ag	394.54	0.00000	NO	YES
87	ag	395.44	0.00000	NO	YES
88	au	395.46	0.06642	YES	NO
89	au	398.95	1.56690	YES	NO
90	ag	399.53	0.00000	NO	YES
91	au	402.57	0.22894	YES	NO
92	ag	403.38	0.00000	NO	YES
93	ag	408.04	0.00000	NO	YES
94	au	408.60	0.55335	YES	NO
95	au	426.52	3.90335	YES	NO
96	ag	426.85	0.00000	NO	YES
97	ag	432.56	0.00000	NO	YES
98	au	433.22	14.44903	YES	NO
99	au	444.59	5.64089	YES	NO
100	ag	444.64	0.00000	NO	YES
101	ag	453.35	0.00000	NO	YES
102	au	454.12	6.79029	YES	NO
103	ag	465.16	0.00000	NO	YES
104	au	465.64	7.06038	YES	NO
105	au	495.15	60.08563	YES	NO
106	ag	496.60	0.00000	NO	YES
107	ag	502.59	0.00000	NO	YES
108	au	504.04	101.77362	YES	NO
109	ag	508.64	0.00000	NO	YES
110	au	508.83	77.86719	YES	NO
111	ag	516.17	0.00000	NO	YES
112	au	516.48	9.10303	YES	NO
113	ag	521.50	0.00000	NO	YES
114	au	521.85	238.71422	YES	NO
115	au	553.51	16.51472	YES	NO
116	ag	554.27	0.00000	NO	YES
117	ag	613.10	0.00000	NO	YES
118	au	613.23	0.29445	YES	NO
119	ag	613.99	0.00000	NO	YES
120	au	613.99	0.39322	YES	NO
121	au	614.21	0.30655	YES	NO
122	ag	614.23	0.00000	NO	YES
123	ag	614.64	0.00000	NO	YES
124	au	614.68	0.84386	YES	NO
125	au	615.09	1.49496	YES	NO
126	ag	615.72	0.00000	NO	YES
127	ag	615.82	0.00000	NO	YES
128	au	616.39	1.24715	YES	NO
129	au	673.21	111.05249	YES	NO
130	ag	673.47	0.00000	NO	YES
131	au	681.57	1.49954	YES	NO
132	ag	681.71	0.00000	NO	YES
133	ag	691.43	0.00000	NO	YES
134	au	692.14	148.20095	YES	NO
135	au	694.38	16.11469	YES	NO
136	ag	694.82	0.00000	NO	YES
137	au	695.38	43.28800	YES	NO
138	ag	695.51	0.00000	NO	YES

139	ag	696.33	0.00000	NO	YES
140	au	696.39	57.18057	YES	NO
141	ag	700.36	0.00000	NO	YES
142	au	700.37	40.87937	YES	NO
143	au	701.60	7.27921	YES	NO
144	ag	701.81	0.00000	NO	YES
145	ag	708.33	0.00000	NO	YES
146	au	708.35	0.79573	YES	NO
147	au	712.36	4.82713	YES	NO
148	ag	712.65	0.00000	NO	YES
149	ag	714.57	0.00000	NO	YES
150	au	714.65	50.97741	YES	NO
151	au	718.36	79.26658	YES	NO
152	ag	718.36	0.00000	NO	YES
153	ag	736.60	0.00000	NO	YES
154	au	738.15	238.75753	YES	NO
155	au	739.57	82.33404	YES	NO
156	ag	740.39	0.00000	NO	YES
157	ag	740.88	0.00000	NO	YES
158	au	741.57	39.89458	YES	NO
159	au	743.20	57.49259	YES	NO
160	ag	745.27	0.00000	NO	YES
161	ag	745.91	0.00000	NO	YES
162	au	746.19	86.72788	YES	NO
163	ag	748.30	0.00000	NO	YES
164	au	748.45	10.63535	YES	NO
165	au	776.29	905.63722	YES	NO
166	ag	783.82	0.00000	NO	YES
167	ag	836.20	0.00000	NO	YES
168	au	837.13	1.21077	YES	NO
169	ag	840.15	0.00000	NO	YES
170	au	840.31	4.24573	YES	NO
171	ag	841.78	0.00000	NO	YES
172	au	842.36	0.83356	YES	NO
173	au	843.54	3.44068	YES	NO
174	ag	845.38	0.00000	NO	YES
175	ag	848.52	0.00000	NO	YES
176	au	849.88	1.15125	YES	NO
177	au	850.84	3.48410	YES	NO
178	ag	850.91	0.00000	NO	YES
179	au	914.35	0.45970	YES	NO
180	ag	915.14	0.00000	NO	YES
181	ag	916.39	0.00000	NO	YES
182	au	917.23	0.27948	YES	NO
183	au	921.55	4.59942	YES	NO
184	ag	921.62	0.00000	NO	YES
185	au	922.05	2.05542	YES	NO
186	ag	922.06	0.00000	NO	YES
187	au	927.16	1.86184	YES	NO
188	ag	927.30	0.00000	NO	YES
189	au	929.80	2.38855	YES	NO
190	ag	929.96	0.00000	NO	YES
191	ag	962.99	0.00000	NO	YES
192	au	963.65	0.35378	YES	NO
193	au	965.83	4.09857	YES	NO
194	ag	966.76	0.00000	NO	YES
195	au	967.86	0.54471	YES	NO
196	ag	968.08	0.00000	NO	YES

197	au	969.61	0.63676	YES	NO
198	ag	970.12	0.00000	NO	YES
199	ag	972.08	0.00000	NO	YES
200	au	972.56	2.08183	YES	NO
201	ag	972.99	0.00000	NO	YES
202	au	973.33	2.54043	YES	NO
203	ag	988.37	0.00000	NO	YES
204	au	988.46	1.36034	YES	NO
205	au	991.53	0.07833	YES	NO
206	ag	991.54	0.00000	NO	YES
207	ag	992.34	0.00000	NO	YES
208	au	992.38	1.11255	YES	NO
209	au	992.67	3.20221	YES	NO
210	ag	992.70	0.00000	NO	YES
211	au	992.87	6.65324	YES	NO
212	ag	992.93	0.00000	NO	YES
213	ag	994.01	0.00000	NO	YES
214	au	994.02	0.78669	YES	NO
215	au	997.58	3.33161	YES	NO
216	ag	997.62	0.00000	NO	YES
217	au	998.05	7.66377	YES	NO
218	ag	998.19	0.00000	NO	YES
219	ag	998.34	0.00000	NO	YES
220	au	998.40	23.13421	YES	NO
221	ag	998.92	0.00000	NO	YES
222	au	999.32	3.01470	YES	NO
223	ag	1000.21	0.00000	NO	YES
224	au	1000.21	12.47265	YES	NO
225	au	1000.76	5.31393	YES	NO
226	ag	1001.12	0.00000	NO	YES
227	ag	1024.07	0.00000	NO	YES
228	au	1024.12	9.22197	YES	NO
229	ag	1024.85	0.00000	NO	YES
230	au	1024.86	2.26871	YES	NO
231	ag	1026.01	0.00000	NO	YES
232	au	1026.10	0.76763	YES	NO
233	ag	1026.53	0.00000	NO	YES
234	au	1026.55	3.02017	YES	NO
235	ag	1027.04	0.00000	NO	YES
236	au	1027.11	2.38612	YES	NO
237	au	1027.91	5.78742	YES	NO
238	ag	1028.04	0.00000	NO	YES
239	ag	1072.71	0.00000	NO	YES
240	au	1073.56	164.45646	YES	NO
241	ag	1074.55	0.00000	NO	YES
242	au	1074.86	65.40474	YES	NO
243	ag	1076.44	0.00000	NO	YES
244	ag	1076.66	0.00000	NO	YES
245	au	1076.71	37.83212	YES	NO
246	au	1077.19	121.01155	YES	NO
247	au	1077.55	7.29252	YES	NO
248	ag	1077.84	0.00000	NO	YES
249	au	1081.44	1.89336	YES	NO
250	ag	1081.67	0.00000	NO	YES
251	ag	1083.21	0.00000	NO	YES
252	au	1083.51	12.87443	YES	NO
253	ag	1092.30	0.00000	NO	YES
254	au	1092.35	100.23512	YES	NO

255	au	1093.84	76.63103	YES	NO
256	ag	1094.09	0.00000	NO	YES
257	ag	1095.78	0.00000	NO	YES
258	au	1095.88	119.47299	YES	NO
259	au	1096.13	138.47923	YES	NO
260	ag	1096.30	0.00000	NO	YES
261	au	1096.96	44.85714	YES	NO
262	ag	1097.07	0.00000	NO	YES
263	ag	1097.53	0.00000	NO	YES
264	au	1099.12	428.78745	YES	NO
265	au	1154.76	4.87540	YES	NO
266	ag	1154.77	0.00000	NO	YES
267	ag	1155.44	0.00000	NO	YES
268	au	1155.54	0.95338	YES	NO
269	ag	1158.70	0.00000	NO	YES
270	au	1158.70	0.71918	YES	NO
271	au	1158.80	1.60486	YES	NO
272	ag	1158.81	0.00000	NO	YES
273	ag	1159.05	0.00000	NO	YES
274	au	1159.05	0.42621	YES	NO
275	ag	1160.22	0.00000	NO	YES
276	au	1160.22	1.31278	YES	NO
277	ag	1173.17	0.00000	NO	YES
278	au	1173.22	1.29592	YES	NO
279	au	1173.89	2.87598	YES	NO
280	ag	1173.92	0.00000	NO	YES
281	ag	1174.79	0.00000	NO	YES
282	au	1174.88	7.18584	YES	NO
283	ag	1176.93	0.00000	NO	YES
284	au	1177.02	6.94823	YES	NO
285	ag	1179.78	0.00000	NO	YES
286	au	1179.88	2.61685	YES	NO
287	ag	1181.56	0.00000	NO	YES
288	au	1181.59	0.76266	YES	NO
289	au	1293.74	13.47534	YES	NO
290	ag	1293.76	0.00000	NO	YES
291	au	1295.82	5.12125	YES	NO
292	ag	1295.85	0.00000	NO	YES
293	au	1295.94	13.50284	YES	NO
294	ag	1295.97	0.00000	NO	YES
295	ag	1296.55	0.00000	NO	YES
296	au	1296.71	7.98851	YES	NO
297	ag	1303.52	0.00000	NO	YES
298	au	1303.54	6.83792	YES	NO
299	ag	1305.19	0.00000	NO	YES
300	au	1305.21	8.64081	YES	NO
301	au	1335.99	2.11849	YES	NO
302	ag	1336.23	0.00000	NO	YES
303	ag	1337.28	0.00000	NO	YES
304	au	1337.39	2.19273	YES	NO
305	ag	1338.00	0.00000	NO	YES
306	au	1338.04	0.77220	YES	NO
307	ag	1338.43	0.00000	NO	YES
308	au	1338.45	0.31228	YES	NO
309	ag	1340.13	0.00000	NO	YES
310	au	1340.38	0.10926	YES	NO
311	au	1340.92	1.15669	YES	NO
312	ag	1341.22	0.00000	NO	YES

313	ag	1423.45	0.00000	NO	YES
314	au	1423.53	20.40569	YES	NO
315	au	1427.36	55.03268	YES	NO
316	ag	1427.42	0.00000	NO	YES
317	ag	1428.18	0.00000	NO	YES
318	au	1428.21	17.80663	YES	NO
319	ag	1429.33	0.00000	NO	YES
320	au	1429.36	18.38010	YES	NO
321	au	1432.33	51.06917	YES	NO
322	ag	1432.36	0.00000	NO	YES
323	au	1432.90	35.63811	YES	NO
324	ag	1432.90	0.00000	NO	YES
325	au	1469.76	12.41793	YES	NO
326	ag	1469.78	0.00000	NO	YES
327	ag	1470.62	0.00000	NO	YES
328	au	1470.65	8.90406	YES	NO
329	au	1471.25	20.79056	YES	NO
330	ag	1471.28	0.00000	NO	YES
331	au	1471.83	5.26480	YES	NO
332	ag	1471.83	0.00000	NO	YES
333	au	1472.52	7.41287	YES	NO
334	ag	1472.53	0.00000	NO	YES
335	ag	1473.72	0.00000	NO	YES
336	au	1473.73	13.71639	YES	NO
337	au	1565.18	0.86545	YES	NO
338	ag	1565.35	0.00000	NO	YES
339	ag	1566.45	0.00000	NO	YES
340	au	1566.46	1.12824	YES	NO
341	ag	1567.96	0.00000	NO	YES
342	au	1567.98	1.30632	YES	NO
343	au	1568.39	2.29166	YES	NO
344	ag	1568.44	0.00000	NO	YES
345	au	1570.39	2.77355	YES	NO
346	ag	1570.42	0.00000	NO	YES
347	au	1571.93	3.56418	YES	NO
348	ag	1571.94	0.00000	NO	YES
349	au	1579.16	2.41851	YES	NO
350	ag	1579.29	0.00000	NO	YES
351	ag	1580.92	0.00000	NO	YES
352	au	1580.93	1.30208	YES	NO
353	ag	1583.00	0.00000	NO	YES
354	au	1583.01	2.46184	YES	NO
355	au	1583.55	6.79810	YES	NO
356	ag	1583.56	0.00000	NO	YES
357	ag	1584.06	0.00000	NO	YES
358	au	1584.06	6.32522	YES	NO
359	ag	1584.34	0.00000	NO	YES
360	au	1584.40	7.21754	YES	NO
361	au	3078.59	4.53779	YES	NO
362	ag	3078.62	0.00000	NO	YES
363	ag	3086.23	0.00000	NO	YES
364	au	3086.25	8.54070	YES	NO
365	ag	3096.02	0.00000	NO	YES
366	au	3096.02	0.62633	YES	NO
367	ag	3097.88	0.00000	NO	YES
368	au	3097.88	3.65549	YES	NO
369	ag	3099.03	0.00000	NO	YES
370	au	3099.03	3.12149	YES	NO

371	ag	3108.07	0.00000	NO	YES
372	au	3108.08	6.98309	YES	NO
373	au	3108.97	0.31808	YES	NO
374	ag	3108.97	0.00000	NO	YES
375	ag	3109.30	0.00000	NO	YES
376	au	3109.30	0.53530	YES	NO
377	au	3112.18	0.38645	YES	NO
378	ag	3112.19	0.00000	NO	YES
379	ag	3113.26	0.00000	NO	YES
380	au	3113.26	0.35948	YES	NO
381	ag	3114.15	0.00000	NO	YES
382	au	3114.15	0.86115	YES	NO
383	ag	3115.52	0.00000	NO	YES
384	au	3115.56	10.05121	YES	NO
385	ag	3116.83	0.00000	NO	YES
386	au	3116.83	7.28931	YES	NO
387	ag	3117.24	0.00000	NO	YES
388	au	3117.25	0.69035	YES	NO
389	au	3119.81	2.56360	YES	NO
390	ag	3119.81	0.00000	NO	YES
391	ag	3121.61	0.00000	NO	YES
392	au	3121.63	2.88031	YES	NO
393	au	3122.42	1.67085	YES	NO
394	ag	3122.43	0.00000	NO	YES
395	ag	3122.50	0.00000	NO	YES
396	au	3122.50	4.31635	YES	NO
397	ag	3125.01	0.00000	NO	YES
398	au	3125.01	3.95493	YES	NO
399	au	3125.11	7.88665	YES	NO
400	ag	3125.11	0.00000	NO	YES
401	ag	3127.00	0.00000	NO	YES
402	au	3127.00	2.44146	YES	NO
403	au	3127.67	2.88906	YES	NO
404	ag	3127.68	0.00000	NO	YES
405	ag	3128.66	0.00000	NO	YES
406	au	3128.66	1.23295	YES	NO
407	au	3131.19	5.11343	YES	NO
408	ag	3131.19	0.00000	NO	YES
409	au	3133.81	7.36819	YES	NO
410	ag	3133.81	0.00000	NO	YES
411	ag	3134.32	0.00000	NO	YES
412	au	3134.32	2.03698	YES	NO
413	ag	3134.36	0.00000	NO	YES
414	au	3134.37	14.12113	YES	NO
415	au	3134.80	16.83055	YES	NO
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417	au	3136.53	11.48316	YES	NO
418	ag	3136.54	0.00000	NO	YES
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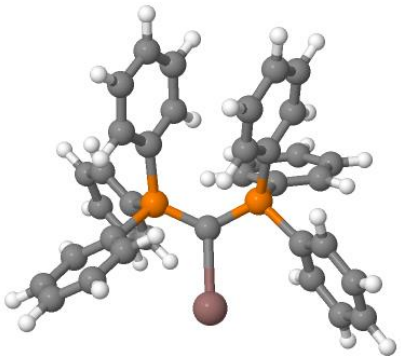
COSMO energy + OC correction = -4603.5331395537 H

8.11 $[In(CDP^{Ph})]^+$



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

Cartesian coordinates in Ångström:

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P	-0.8476099	0.0887604	1.3041749
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C	0.4111226	-1.7576662	-2.1163249
C	0.4443806	1.1835433	1.9729305
C	1.2138007	0.8374059	3.0920398
H	1.0399086	-0.1060582	3.6065923
C	2.2259347	1.6909717	3.5330085
H	2.8256089	1.4139407	4.3994397
C	2.4776629	2.8883880	2.8604900
H	3.2758621	3.5471691	3.2008566
C	1.6424527	-2.2169340	-2.6055840
H	2.5051836	-1.5516655	-2.6214286
C	1.7104054	3.2389816	1.7458631
H	1.9100419	4.1684247	1.2141252
C	0.6979617	2.3910021	1.3036039
H	0.1135398	2.6403701	0.4185767
C	-2.4348488	0.6476187	2.0009321
C	-3.5359656	-0.2287088	1.9556784
H	-3.3938612	-1.2620075	1.6365693
C	-4.8018285	0.2193354	2.3397918
H	-5.6504515	-0.4629165	2.3068974
C	-4.9756513	1.5372721	2.7722016
H	-5.9630497	1.8845411	3.0739539
C	-3.8835616	2.4067684	2.8243737
H	-4.0174228	3.4311712	3.1700628
C	-2.6145000	1.9664343	2.4396384
H	-1.7623020	2.6438256	2.4863592
C	-0.5732142	-1.5334927	2.0783384
C	0.0202881	-2.5690783	1.3461906
H	0.2661703	-2.4218416	0.2966084
C	0.2691005	-3.8025500	1.9498876
H	0.7273321	-4.6039180	1.3713655
C	-0.0790317	-4.0093415	3.2865962
H	0.1107137	-4.9736860	3.7567606
C	-0.6820195	-2.9826247	4.0197572
H	-0.9637559	-3.1456298	5.0594816
C	-0.9305288	-1.7480736	3.4202331
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C     1.7609332   -3.5301504   -3.0648129
H     2.7197448   -3.8882173   -3.4382051
C     0.6538419   -4.3825354   -3.0447646
H     0.7503666   -5.4071922   -3.4023968
C    -0.5765439   -3.9247409   -2.5624425
H    -1.4385745   -4.5907467   -2.5432891
C    -0.6976140   -2.6167241   -2.0959645
H    -1.6423908   -2.2561918   -1.6871719
C    -0.3149998    0.8803892   -3.0279211
C    -0.6840667    2.2327111   -2.8887686
H    -0.6158464    2.7115840   -1.9112219
C    -1.1239421    2.9599297   -3.9950962
H    -1.4024577    4.0068318   -3.8800569
C    -1.2064742    2.3431406   -5.2472398
H    -1.5569626    2.9083864   -6.1100131
C    -0.8402632    1.0037159   -5.3912523
H    -0.9063774    0.5214305   -6.3658043
C    -0.3908469    0.2730619   -4.2881576
H    -0.1080715   -0.7717798   -4.4060364
C     1.8583327    0.5311019   -1.1002597
C     2.5282529   -0.1008269   -0.0387721
H     2.0899835   -0.9722742    0.4476988
C     3.7526776    0.3899131    0.4058552
H     4.2605712   -0.0982491    1.2363736
C     4.3236644    1.5088537   -0.2084087
H     5.2800856    1.8935451    0.1437956
C     3.6726564    2.1272281   -1.2766217
H     4.1225075    2.9901068   -1.7665676
C     2.4416104    1.6424224   -1.7232042
H     1.9384547    2.1291918   -2.5571078

SCF energy GEOOPT =  -2301.699378877 H
ZPE =   1423. kJ/mol
FREEH energy =  1519.44 kJ/mol
FREEH entropy =   0.97133 kJ/mol/K

$vibrational spectrum
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#                         cm**(-1)        km/mol         IR     RAMAN
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     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             18.56         0.03920       YES     YES
     8        a             21.42         0.01731       YES     YES
     9        a             26.29         0.04203       YES     YES
    10        a             35.44         0.08181       YES     YES
    11        a             38.32         0.01874       YES     YES
    12        a             40.88         0.00827       YES     YES
    13        a             42.39         0.01280       YES     YES
    14        a             50.83         0.08666       YES     YES
    15        a             51.46         0.07311       YES     YES
    16        a             53.54         0.00792       YES     YES
    17        a             60.95         0.17747       YES     YES
    18        a             64.96         0.17566       YES     YES
    19        a             68.35         0.02697       YES     YES
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21	a	76.48	0.30548	YES	YES
22	a	82.43	0.94629	YES	YES
23	a	86.24	1.03016	YES	YES
24	a	94.44	6.10893	YES	YES
25	a	97.51	1.76678	YES	YES
26	a	112.85	3.48949	YES	YES
27	a	171.90	8.29964	YES	YES
28	a	188.32	2.36321	YES	YES
29	a	195.43	1.09775	YES	YES
30	a	205.05	1.39726	YES	YES
31	a	217.10	1.84127	YES	YES
32	a	222.01	1.34210	YES	YES
33	a	226.79	0.47474	YES	YES
34	a	241.80	0.25927	YES	YES
35	a	243.81	1.81608	YES	YES
36	a	253.93	1.16007	YES	YES
37	a	258.17	0.03856	YES	YES
38	a	266.25	0.38819	YES	YES
39	a	266.86	1.09981	YES	YES
40	a	332.41	5.41572	YES	YES
41	a	376.06	19.66795	YES	YES
42	a	387.96	0.18884	YES	YES
43	a	389.60	1.26284	YES	YES
44	a	390.91	0.82861	YES	YES
45	a	393.21	0.36211	YES	YES
46	a	398.44	0.01682	YES	YES
47	a	398.81	0.48436	YES	YES
48	a	401.50	5.37588	YES	YES
49	a	439.26	4.92334	YES	YES
50	a	445.09	2.69206	YES	YES
51	a	453.70	8.38395	YES	YES
52	a	459.11	8.29343	YES	YES
53	a	484.50	7.76484	YES	YES
54	a	503.15	108.04960	YES	YES
55	a	507.30	11.56648	YES	YES
56	a	515.11	41.40415	YES	YES
57	a	524.05	82.51825	YES	YES
58	a	544.97	49.97863	YES	YES
59	a	612.88	1.67470	YES	YES
60	a	613.51	0.04970	YES	YES
61	a	613.71	1.24760	YES	YES
62	a	613.81	0.26370	YES	YES
63	a	614.77	1.45499	YES	YES
64	a	615.46	0.32898	YES	YES
65	a	657.17	81.43585	YES	YES
66	a	681.00	1.48294	YES	YES
67	a	690.25	40.75215	YES	YES
68	a	691.60	21.10301	YES	YES
69	a	694.06	34.94507	YES	YES
70	a	696.77	21.05394	YES	YES
71	a	697.81	20.28286	YES	YES
72	a	699.17	10.56983	YES	YES
73	a	709.06	5.11658	YES	YES
74	a	710.56	24.11030	YES	YES
75	a	711.93	10.28593	YES	YES
76	a	713.67	39.93934	YES	YES
77	a	730.77	200.61543	YES	YES

78	a	736.79	28.78207	YES	YES
79	a	741.31	2.25601	YES	YES
80	a	742.87	9.66339	YES	YES
81	a	746.06	12.64768	YES	YES
82	a	746.33	5.81286	YES	YES
83	a	757.70	107.70786	YES	YES
84	a	834.65	0.03150	YES	YES
85	a	837.73	2.46769	YES	YES
86	a	840.83	0.16266	YES	YES
87	a	843.43	0.48965	YES	YES
88	a	844.86	0.45465	YES	YES
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90	a	912.93	0.37485	YES	YES
91	a	916.76	0.56074	YES	YES
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94	a	922.17	0.26990	YES	YES
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97	a	964.55	0.18729	YES	YES
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100	a	968.78	0.95395	YES	YES
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106	a	992.84	0.78380	YES	YES
107	a	993.93	1.10529	YES	YES
108	a	996.09	8.52622	YES	YES
109	a	996.72	6.72340	YES	YES
110	a	997.47	3.13653	YES	YES
111	a	997.61	4.96224	YES	YES
112	a	998.28	2.61780	YES	YES
113	a	999.53	1.67646	YES	YES
114	a	1024.18	4.23577	YES	YES
115	a	1024.80	0.99903	YES	YES
116	a	1025.48	1.56802	YES	YES
117	a	1025.75	1.89914	YES	YES
118	a	1026.27	1.02645	YES	YES
119	a	1027.36	0.40736	YES	YES
120	a	1075.02	1.66449	YES	YES
121	a	1075.52	2.27165	YES	YES
122	a	1075.85	8.12232	YES	YES
123	a	1076.78	0.86083	YES	YES
124	a	1079.65	3.11502	YES	YES
125	a	1082.82	3.46794	YES	YES
126	a	1087.20	17.17883	YES	YES
127	a	1091.16	17.96915	YES	YES
128	a	1093.87	65.01122	YES	YES
129	a	1095.70	33.44435	YES	YES
130	a	1097.16	63.62378	YES	YES
131	a	1098.76	38.51157	YES	YES
132	a	1124.10	599.92258	YES	YES
133	a	1156.80	0.29942	YES	YES
134	a	1157.47	0.40412	YES	YES
135	a	1157.69	0.31195	YES	YES

136	a	1158.54	0.55159	YES	YES
137	a	1158.73	0.25756	YES	YES
138	a	1159.28	0.22687	YES	YES
139	a	1172.58	1.41707	YES	YES
140	a	1174.23	3.04210	YES	YES
141	a	1175.46	1.24066	YES	YES
142	a	1176.05	2.95308	YES	YES
143	a	1177.83	1.81688	YES	YES
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145	a	1294.27	5.93524	YES	YES
146	a	1295.22	2.10422	YES	YES
147	a	1295.97	6.89899	YES	YES
148	a	1296.48	1.98690	YES	YES
149	a	1302.65	6.85333	YES	YES
150	a	1303.48	0.63750	YES	YES
151	a	1336.01	0.43501	YES	YES
152	a	1336.85	0.49336	YES	YES
153	a	1337.25	0.28545	YES	YES
154	a	1338.39	0.44080	YES	YES
155	a	1339.15	0.34181	YES	YES
156	a	1339.95	0.00192	YES	YES
157	a	1426.39	19.52694	YES	YES
158	a	1427.11	12.44448	YES	YES
159	a	1429.17	3.27528	YES	YES
160	a	1429.27	20.07023	YES	YES
161	a	1431.73	18.21378	YES	YES
162	a	1431.83	26.41606	YES	YES
163	a	1469.07	6.25628	YES	YES
164	a	1469.33	1.66542	YES	YES
165	a	1470.41	9.34112	YES	YES
166	a	1471.75	7.49911	YES	YES
167	a	1473.92	2.68684	YES	YES
168	a	1474.94	6.75734	YES	YES
169	a	1566.96	0.17218	YES	YES
170	a	1567.63	0.18361	YES	YES
171	a	1569.44	0.43183	YES	YES
172	a	1570.33	0.21969	YES	YES
173	a	1571.59	1.77325	YES	YES
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175	a	1580.25	0.25693	YES	YES
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189	a	3109.04	0.14643	YES	YES
190	a	3109.53	0.02797	YES	YES
191	a	3111.17	0.67918	YES	YES
192	a	3111.85	0.18531	YES	YES
193	a	3114.96	0.28810	YES	YES

194	a	3116.49	0.13017	YES	YES
195	a	3118.17	1.62229	YES	YES
196	a	3118.31	1.19887	YES	YES
197	a	3119.57	1.44502	YES	YES
198	a	3120.16	7.97406	YES	YES
199	a	3123.11	6.85511	YES	YES
200	a	3124.34	4.13896	YES	YES
201	a	3125.49	0.85592	YES	YES
202	a	3125.82	8.51951	YES	YES
203	a	3127.03	2.81587	YES	YES
204	a	3128.62	2.99826	YES	YES
205	a	3131.77	8.90349	YES	YES
206	a	3132.23	7.12971	YES	YES
207	a	3133.10	11.33862	YES	YES
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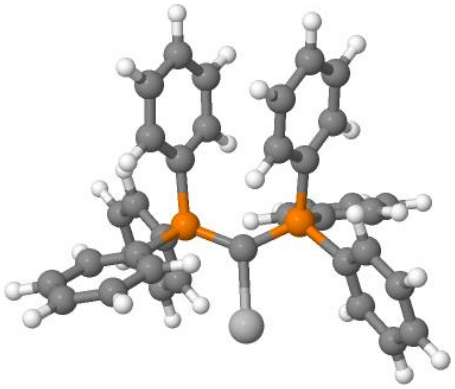
COSMO energy + OC correction = -2301.7484332423 H

8.12 [Ag(CDP^{Ph})]$^{+}$



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

Cartesian coordinates in Ångström:

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C	0.3897352	-1.7849386	-2.1629631
C	0.4682806	1.1753051	1.9440616
C	1.2541067	0.8154395	3.0471397
H	1.0863976	-0.1331504	3.5540618
C	2.2709367	1.6655542	3.4828710
H	2.8827088	1.3805294	4.3381025
C	2.5101357	2.8708630	2.8199157
H	3.3105318	3.5284884	3.1574360
C	1.6511239	-2.2241833	-2.5926854
H	2.5031523	-1.5460648	-2.5655556
C	1.7283046	3.2315353	1.7188400
H	1.9193673	4.1668651	1.1944648
C	0.7087179	2.3892715	1.2811800

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C    -2.4212771    0.7251818    2.0511288
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H    -3.4375665   -1.1709132    1.7696758
C    -4.7803802    0.3597262    2.4871639
H    -5.6453347   -0.3026649    2.5038414
C    -4.9027967    1.6878528    2.9105123
H    -5.8687103    2.0646567    3.2449318
C    -3.7853372    2.5241006    2.9220318
H    -3.8769868    3.5536990    3.2660299
C    -2.5433236    2.0456111    2.4944417
H    -1.6726808    2.7001260    2.5052928
C    -0.6280582   -1.5144312    2.1098441
C    -0.1054053   -2.5683422    1.3504191
H     0.0995643   -2.4223668    0.2911331
C     0.1216205   -3.8124812    1.9406479
H     0.5251390   -4.6287795    1.3425501
C    -0.1796305   -4.0102552    3.2901766
H    -0.0077241   -4.9827978    3.7502565
C    -0.7141549   -2.9647069    4.0499040
H    -0.9604216   -3.1220784    5.0994557
C    -0.9401630   -1.7192892    3.4642327
H    -1.3682247   -0.9094978    4.0555326
C     1.8169439   -3.5340654   -3.0479325
H     2.7998201   -3.8714327   -3.3752487
C     0.7281888   -4.4078627   -3.0818918
H     0.8605866   -5.4298181   -3.4356164
C    -0.5320162   -3.9721971   -2.6596675
H    -1.3826793   -4.6525159   -2.6843681
C    -0.6998452   -2.6673879   -2.2006752
H    -1.6765632   -2.3300605   -1.8477205
C    -0.3682106    0.8540730   -3.0569037
C    -1.0751522    2.0558480   -2.8944359
H    -1.3410639    2.3838795   -1.8891336
C    -1.4347020    2.8093370   -4.0114397
H    -1.9826290    3.7423485   -3.8830528
C    -1.0921809    2.3667538   -5.2928075
H    -1.3779035    2.9532447   -6.1654327
C    -0.3872081    1.1717765   -5.4564143
H    -0.1254708    0.8238272   -6.4549886
C    -0.0217830    0.4148242   -4.3418717
H     0.5202767   -0.5208671   -4.4726962
C     1.7826989    0.5205084   -1.1175213
C     2.4896803   -0.1385625   -0.0983382
H     2.0832670   -1.0408334    0.3588053
C     3.7123294    0.3654145    0.3377954
H     4.2517811   -0.1418603    1.1363136
C     4.2419066    1.5204207   -0.2454624
H     5.1986821    1.9121881    0.0979222
C     3.5497422    2.1680323   -1.2701118
H     3.9665356    3.0619246   -1.7327686
C     2.3194600    1.6734354   -1.7058325
H     1.7772503    2.1826572   -2.5011375

SCF energy GEOOPT =  -2258.508947144 H
ZPE =   1424. kJ/mol
FREEH energy =  1519.77 kJ/mol
FREEH entropy =   0.97176 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	17.65	0.02354	YES	YES
8	a	20.68	0.02458	YES	YES
9	a	26.47	0.08223	YES	YES
10	a	33.42	0.05944	YES	YES
11	a	38.10	0.06857	YES	YES
12	a	42.17	0.09146	YES	YES
13	a	45.86	0.14945	YES	YES
14	a	47.09	0.08183	YES	YES
15	a	52.71	0.05858	YES	YES
16	a	53.73	0.16601	YES	YES
17	a	54.48	0.10762	YES	YES
18	a	55.84	0.98992	YES	YES
19	a	61.58	0.33267	YES	YES
20	a	70.99	0.51208	YES	YES
21	a	75.93	0.24478	YES	YES
22	a	81.00	0.07982	YES	YES
23	a	90.43	0.32766	YES	YES
24	a	97.67	0.05703	YES	YES
25	a	103.60	1.35438	YES	YES
26	a	121.27	0.15743	YES	YES
27	a	184.16	1.74748	YES	YES
28	a	188.26	1.91087	YES	YES
29	a	193.89	2.32881	YES	YES
30	a	211.13	0.88370	YES	YES
31	a	219.03	2.35575	YES	YES
32	a	220.21	0.77622	YES	YES
33	a	225.98	1.00720	YES	YES
34	a	245.03	0.19842	YES	YES
35	a	245.78	1.19393	YES	YES
36	a	254.11	0.69028	YES	YES
37	a	258.65	0.20636	YES	YES
38	a	266.40	1.04007	YES	YES
39	a	269.48	0.79953	YES	YES
40	a	316.78	8.02053	YES	YES
41	a	383.54	26.99789	YES	YES
42	a	386.98	0.34396	YES	YES
43	a	389.38	0.29863	YES	YES
44	a	391.07	0.91266	YES	YES
45	a	393.74	0.15383	YES	YES
46	a	396.88	0.06693	YES	YES
47	a	399.56	0.01517	YES	YES
48	a	427.46	4.52523	YES	YES
49	a	439.62	3.22258	YES	YES
50	a	443.11	1.46327	YES	YES
51	a	448.70	6.51812	YES	YES
52	a	456.76	10.88006	YES	YES
53	a	495.92	84.26406	YES	YES
54	a	500.84	52.00500	YES	YES

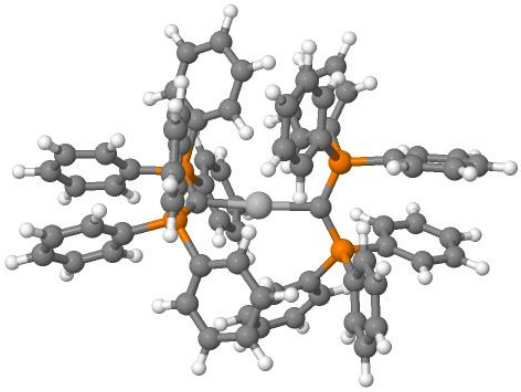
55	a	509.10	28.10911	YES	YES
56	a	509.86	93.30744	YES	YES
57	a	518.54	27.41257	YES	YES
58	a	558.16	3.59644	YES	YES
59	a	612.58	0.24044	YES	YES
60	a	613.53	0.00281	YES	YES
61	a	613.84	0.01991	YES	YES
62	a	614.45	0.04629	YES	YES
63	a	614.73	0.13111	YES	YES
64	a	615.08	0.64807	YES	YES
65	a	677.73	2.93248	YES	YES
66	a	682.27	2.94732	YES	YES
67	a	690.26	60.09042	YES	YES
68	a	691.68	15.90804	YES	YES
69	a	692.10	17.74632	YES	YES
70	a	694.59	24.18531	YES	YES
71	a	695.33	20.47434	YES	YES
72	a	698.82	15.35975	YES	YES
73	a	710.29	26.75798	YES	YES
74	a	710.64	11.63665	YES	YES
75	a	713.49	30.23098	YES	YES
76	a	714.22	14.61487	YES	YES
77	a	735.40	37.22297	YES	YES
78	a	737.54	32.95729	YES	YES
79	a	741.50	17.54505	YES	YES
80	a	742.24	7.28561	YES	YES
81	a	746.07	13.24809	YES	YES
82	a	746.92	9.14125	YES	YES
83	a	791.27	106.25169	YES	YES
84	a	834.93	0.84123	YES	YES
85	a	836.08	0.75848	YES	YES
86	a	838.01	0.03398	YES	YES
87	a	840.46	1.51218	YES	YES
88	a	843.51	0.20570	YES	YES
89	a	846.39	0.13878	YES	YES
90	a	913.71	0.79368	YES	YES
91	a	915.07	1.10869	YES	YES
92	a	916.93	0.39298	YES	YES
93	a	920.72	0.21071	YES	YES
94	a	924.21	0.22130	YES	YES
95	a	925.13	0.23322	YES	YES
96	a	962.46	0.62392	YES	YES
97	a	963.87	0.15215	YES	YES
98	a	965.26	0.01080	YES	YES
99	a	967.81	0.01575	YES	YES
100	a	969.47	0.44680	YES	YES
101	a	971.08	0.26732	YES	YES
102	a	986.44	0.21249	YES	YES
103	a	988.46	0.05913	YES	YES
104	a	989.38	0.18436	YES	YES
105	a	990.66	0.08051	YES	YES
106	a	991.86	0.13202	YES	YES
107	a	992.32	0.05695	YES	YES
108	a	995.89	10.06337	YES	YES
109	a	996.29	5.80857	YES	YES
110	a	997.43	5.09991	YES	YES
111	a	997.61	4.93326	YES	YES
112	a	998.05	0.80604	YES	YES

113	a	999.11	3.19906	YES	YES
114	a	1024.22	2.35087	YES	YES
115	a	1024.85	2.69278	YES	YES
116	a	1025.19	2.24126	YES	YES
117	a	1025.52	1.22858	YES	YES
118	a	1026.48	0.92297	YES	YES
119	a	1027.41	0.91989	YES	YES
120	a	1075.43	2.84639	YES	YES
121	a	1076.28	5.11986	YES	YES
122	a	1077.30	6.83544	YES	YES
123	a	1077.80	0.81339	YES	YES
124	a	1080.81	0.56216	YES	YES
125	a	1082.28	2.24684	YES	YES
126	a	1088.72	14.82805	YES	YES
127	a	1091.76	21.07372	YES	YES
128	a	1094.52	78.94081	YES	YES
129	a	1095.96	10.13005	YES	YES
130	a	1097.72	53.54378	YES	YES
131	a	1100.15	53.18514	YES	YES
132	a	1135.65	668.36026	YES	YES
133	a	1157.34	0.18626	YES	YES
134	a	1157.42	0.71522	YES	YES
135	a	1157.64	0.33138	YES	YES
136	a	1157.84	0.39526	YES	YES
137	a	1158.39	0.33979	YES	YES
138	a	1158.74	0.52355	YES	YES
139	a	1173.64	1.41064	YES	YES
140	a	1175.08	2.50637	YES	YES
141	a	1175.57	4.40819	YES	YES
142	a	1175.99	2.67549	YES	YES
143	a	1177.57	4.80532	YES	YES
144	a	1180.85	3.64045	YES	YES
145	a	1295.38	5.48801	YES	YES
146	a	1295.96	6.02737	YES	YES
147	a	1296.99	2.24660	YES	YES
148	a	1297.78	3.77882	YES	YES
149	a	1302.51	5.84644	YES	YES
150	a	1303.73	0.92155	YES	YES
151	a	1336.73	0.30156	YES	YES
152	a	1337.08	0.11180	YES	YES
153	a	1338.46	0.35040	YES	YES
154	a	1338.91	0.19795	YES	YES
155	a	1339.38	0.07119	YES	YES
156	a	1339.88	0.05583	YES	YES
157	a	1426.81	19.03470	YES	YES
158	a	1428.41	18.16464	YES	YES
159	a	1429.50	6.46655	YES	YES
160	a	1430.35	12.73022	YES	YES
161	a	1431.85	9.82089	YES	YES
162	a	1432.30	36.63173	YES	YES
163	a	1469.77	6.07138	YES	YES
164	a	1470.06	2.79065	YES	YES
165	a	1470.70	8.17214	YES	YES
166	a	1471.83	6.06017	YES	YES
167	a	1473.20	2.91031	YES	YES
168	a	1474.61	6.55326	YES	YES
169	a	1568.52	0.45893	YES	YES
170	a	1568.86	0.15583	YES	YES

171	a	1570.42	0.09801	YES	YES
172	a	1570.71	0.13224	YES	YES
173	a	1571.71	0.62873	YES	YES
174	a	1572.03	1.83946	YES	YES
175	a	1580.27	0.29124	YES	YES
176	a	1582.69	1.36261	YES	YES
177	a	1583.15	0.51541	YES	YES
178	a	1583.37	0.04153	YES	YES
179	a	1584.04	2.87710	YES	YES
180	a	1585.48	1.17345	YES	YES
181	a	3067.92	2.40580	YES	YES
182	a	3087.42	3.70403	YES	YES
183	a	3097.64	0.54262	YES	YES
184	a	3099.79	0.17084	YES	YES
185	a	3101.80	1.38004	YES	YES
186	a	3105.97	0.27140	YES	YES
187	a	3108.08	0.16357	YES	YES
188	a	3109.31	0.20028	YES	YES
189	a	3109.50	0.13063	YES	YES
190	a	3109.56	0.08197	YES	YES
191	a	3110.29	1.38264	YES	YES
192	a	3111.57	0.18174	YES	YES
193	a	3115.19	0.69144	YES	YES
194	a	3116.04	0.63840	YES	YES
195	a	3116.16	0.98807	YES	YES
196	a	3118.35	4.54214	YES	YES
197	a	3118.46	4.40549	YES	YES
198	a	3119.53	1.06425	YES	YES
199	a	3123.02	6.14639	YES	YES
200	a	3123.76	3.98220	YES	YES
201	a	3123.89	5.68620	YES	YES
202	a	3125.04	0.62201	YES	YES
203	a	3126.09	2.35747	YES	YES
204	a	3126.84	6.09753	YES	YES
205	a	3131.78	7.97118	YES	YES
206	a	3132.31	15.09857	YES	YES
207	a	3132.53	9.20161	YES	YES
208	a	3132.73	6.47513	YES	YES
209	a	3132.93	7.22047	YES	YES
210	a	3133.37	10.96002	YES	YES

$end

8.13 [(CDP^{Ph})Ag(CDP^{Ph})]$^{+}$



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

Cartesian coordinates in Ångström:

Ag	-0.0541327	-0.0033249	0.2231782
C	1.2036501	-1.6518445	-0.0405786
P	1.6487411	-2.5471494	1.3019346
C	1.9435047	-4.3075124	0.9691482
C	0.9154280	-5.0325852	0.3422413
H	-0.0104043	-4.5244456	0.0690765
C	1.0884261	-6.3855618	0.0587388
H	0.2844887	-6.9476339	-0.4160269
C	2.2979762	-7.0155746	0.3701615
H	2.4366789	-8.0715545	0.1396189
C	3.3302826	-6.2906679	0.9679064
H	4.2783066	-6.7765948	1.1960695
C	3.1522485	-4.9405602	1.2786620
H	3.9558858	-4.3776967	1.7512589
C	0.3654133	-2.4748175	2.5975625
C	-0.2860696	-3.6203569	3.0705194
H	-0.0155673	-4.6017338	2.6850356
C	-1.2834843	-3.5097802	4.0440961
H	-1.7843793	-4.4073685	4.4060424
C	-1.6326172	-2.2573797	4.5524655
H	-2.4118203	-2.1730095	5.3096925
C	-0.9693043	-1.1129017	4.0983289
H	-1.2194181	-0.1322482	4.5002657
C	0.0301973	-1.2190681	3.1335499
H	0.5580823	-0.3239048	2.8062753
C	3.1416052	-1.9526059	2.1743281
C	3.3093115	-2.1234328	3.5557437
H	2.5349304	-2.6186994	4.1410236
C	4.4606124	-1.6453120	4.1836438
H	4.5841946	-1.7734341	5.2587926
C	5.4532006	-1.0039880	3.4364045
H	6.3506572	-0.6313075	3.9295180
C	5.2910468	-0.8362903	2.0578320
H	6.0615383	-0.3344615	1.4727167
C	4.1340761	-1.3022617	1.4329224
H	3.9822952	-1.1541633	0.3653929
P	1.6761860	-1.8130428	-1.6441636
C	2.2909493	-0.2061771	-2.2865643
C	2.6635091	0.7745152	-1.3561268

H	2.5640945	0.5421744	-0.2962504
C	3.1265608	2.0189105	-1.7806428
H	3.3892305	2.7826436	-1.0486708
C	3.2336618	2.2916173	-3.1458195
H	3.5859901	3.2663607	-3.4806261
C	2.8859831	1.3134021	-4.0804078
H	2.9735976	1.5206239	-5.1466895
C	2.4173872	0.0688633	-3.6545483
H	2.1414152	-0.6794064	-4.3947836
C	0.3041595	-2.2850663	-2.7519440
C	-1.0061905	-2.2532371	-2.2584183
H	-1.1735844	-1.9980363	-1.2104263
C	-2.0808847	-2.5354599	-3.1014003
H	-3.0936304	-2.4967741	-2.7050330
C	-1.8558697	-2.8558213	-4.4408463
H	-2.6966377	-3.0682886	-5.1007044
C	-0.5488658	-2.9214596	-4.9327524
H	-0.3673378	-3.1983822	-5.9709832
C	0.5282869	-2.6446741	-4.0910897
H	1.5454712	-2.7350956	-4.4719300
C	3.0050811	-2.9999787	-1.9954496
C	2.7069198	-4.3458742	-2.2521722
H	1.6706962	-4.6625402	-2.3503566
C	3.7356528	-5.2785488	-2.3738303
H	3.4956523	-6.3236291	-2.5644458
C	5.0671109	-4.8749326	-2.2473656
H	5.8694517	-5.6060769	-2.3417701
C	5.3708639	-3.5312580	-2.0136654
H	6.4090387	-3.2101818	-1.9346022
C	4.3442598	-2.5952416	-1.8924003
H	4.5828999	-1.5434355	-1.7350573
C	-1.3876102	1.5955084	0.4481758
P	-0.6944935	2.9756914	1.0979751
C	-1.8769380	4.1485390	1.8283850
C	-2.9725559	3.6248214	2.5339193
H	-3.0886490	2.5440623	2.6114899
C	-3.9176934	4.4813769	3.0937891
H	-4.7719357	4.0686813	3.6290165
C	-3.7787026	5.8651059	2.9531774
H	-4.5230412	6.5336457	3.3848113
C	-2.6917726	6.3898951	2.2516707
H	-2.5853067	7.4680363	2.1347803
C	-1.7414979	5.5359454	1.6895213
H	-0.9047477	5.9497682	1.1289805
C	0.3427564	3.9649902	-0.0331539
C	1.3679556	4.8045973	0.4294836
H	1.5900527	4.8584795	1.4953478
C	2.1079610	5.5665801	-0.4763291
H	2.9043083	6.2163989	-0.1140339
C	1.8257451	5.4990087	-1.8444661
H	2.4032871	6.0981961	-2.5482079
C	0.8109232	4.6585748	-2.3080564
H	0.5982733	4.5887021	-3.3742975
C	0.0768065	3.8899124	-1.4052053
H	-0.6918036	3.2069854	-1.7639693
C	0.4500714	2.4997534	2.4379621
C	0.0377045	2.4975770	3.7756535
H	-0.9418731	2.8920430	4.0435953

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C     0.8820038    1.9918461    4.7684261
H     0.5532661    1.9912852    5.8073562
C     2.1407292    1.4903224    4.4319176
H     2.7946580    1.0871520    5.2040805
C     2.5665331    1.5090915    3.1006027
H     3.5484936    1.1208047    2.8355271
C     1.7267009    2.0140395    2.1092727
H     2.0581330    2.0367370    1.0727230
P    -2.7561294    1.3665514   -0.4982267
C    -2.4958447    1.3095300   -2.3116669
C    -3.5550547    1.5740473   -3.1945361
H    -4.5232348    1.8889749   -2.8048843
C    -3.3685051    1.4510875   -4.5724851
H    -4.1959192    1.6586630   -5.2506579
C    -2.1232467    1.0702797   -5.0795543
H    -1.9798907    0.9718751   -6.1553487
C    -1.0607392    0.8275392   -4.2064886
H    -0.0844153    0.5383266   -4.5908656
C    -1.2450619    0.9480468   -2.8307649
H    -0.4120396    0.7635331   -2.1486517
C    -4.0833739    2.5845892   -0.2779634
C    -3.8600891    3.9059127   -0.6979657
H    -2.9364938    4.1650599   -1.2163956
C    -4.8115398    4.8900286   -0.4423461
H    -4.6275186    5.9160460   -0.7582017
C    -5.9969082    4.5612970    0.2227800
H    -6.7401978    5.3327876    0.4213671
C    -6.2284313    3.2467996    0.6310219
H    -7.1539824    2.9883561    1.1447842
C    -5.2723594    2.2589217    0.3865079
H    -5.4477467    1.2351591    0.7149109
C    -3.4887390   -0.2626469   -0.1179891
C    -4.4198953   -0.8684180   -0.9731549
H    -4.7203104   -0.3729616   -1.8955748
C    -4.9496718   -2.1200902   -0.6552437
H    -5.6740569   -2.5865464   -1.3227839
C    -4.5423474   -2.7789536    0.5086206
H    -4.9463441   -3.7629840    0.7458631
C    -3.6208523   -2.1741598    1.3670464
H    -3.2966444   -2.6783320    2.2763725
C    -3.1033952   -0.9153925    1.0603388
H    -2.3834523   -0.4323422    1.7206107

SCF energy GEOOPT =  -4370.177913838 H
ZPE =   2850. kJ/mol
FREEH energy =  3038.89 kJ/mol
FREEH entropy =   1.62969 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        -       -
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9	a	21.41	0.03428	YES	YES
10	a	22.58	0.04510	YES	YES
11	a	24.98	0.02265	YES	YES
12	a	27.75	0.09986	YES	YES
13	a	34.35	0.32878	YES	YES
14	a	37.90	0.14942	YES	YES
15	a	39.67	0.05477	YES	YES
16	a	42.12	0.02009	YES	YES
17	a	42.36	0.18340	YES	YES
18	a	44.64	0.07223	YES	YES
19	a	48.69	0.01139	YES	YES
20	a	50.50	0.02204	YES	YES
21	a	52.46	0.06539	YES	YES
22	a	52.62	0.16274	YES	YES
23	a	55.52	0.13122	YES	YES
24	a	58.95	0.03790	YES	YES
25	a	59.50	0.15275	YES	YES
26	a	62.87	0.19841	YES	YES
27	a	65.68	0.04277	YES	YES
28	a	68.11	0.01870	YES	YES
29	a	68.95	0.01610	YES	YES
30	a	72.17	0.11166	YES	YES
31	a	72.74	0.05149	YES	YES
32	a	74.07	0.01707	YES	YES
33	a	79.78	0.08327	YES	YES
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35	a	82.95	0.19127	YES	YES
36	a	84.45	0.09487	YES	YES
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38	a	89.34	0.03269	YES	YES
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63	a	233.39	0.91503	YES	YES
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122	a	616.04	0.32213	YES	YES
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248	a	1085.95	23.89711	YES	YES
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   415        a            3133.59          6.68767       YES     YES
   416        a            3134.25          3.90289       YES     YES
   417        a            3135.08          8.50122       YES     YES
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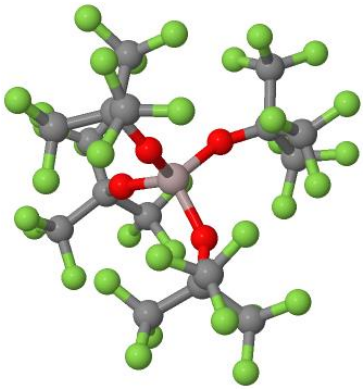
8.14 $[Al(OC(CF_3)_3)_4]^-$



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

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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   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             12.14         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
```

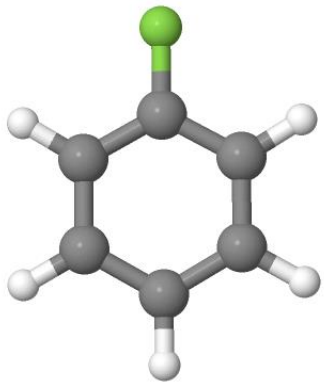
24	a	74.95	0.00725	YES	YES
25	a	76.06	0.04382	YES	YES
26	a	76.33	0.08430	YES	YES
27	a	78.77	0.02043	YES	YES
28	a	79.34	0.03030	YES	YES
29	a	83.51	0.06965	YES	YES
30	a	84.65	0.03538	YES	YES
31	a	86.28	0.00412	YES	YES
32	a	88.48	0.05023	YES	YES
33	a	94.11	0.81131	YES	YES
34	a	95.20	0.63727	YES	YES
35	a	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

8.15 PhF



Method: (RI-)BP86(D3BJ)/def2-TZVPP
Symmetry: c2v

Cartesian coordinates in Ångström:

H	2.1550632	0.0000000	1.2618747
C	1.2092915	0.0000000	0.7205303
C	0.0000000	0.0000000	1.4208330
H	0.0000000	0.0000000	2.5100281

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C    -1.2092915    0.0000000    0.7205303
H    -2.1550632    0.0000000    1.2618747
C    -1.2191887    0.0000000   -0.6766508
H    -2.1478755    0.0000000   -1.2448060
C     0.0000000    0.0000000   -1.3466493
F     0.0000000    0.0000000   -2.7061020
C     1.2191887    0.0000000   -0.6766508
H     2.1478755    0.0000000   -1.2448060

SCF energy GEOOPT =  -331.6471322766 H
ZPE =   235.5 kJ/mol
FREEH energy =   249.35 kJ/mol
FREEH entropy =   0.30410 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        b2           227.78         0.02731       YES     YES
     8        b1           394.37         1.70227       YES     YES
     9        a2           409.06         0.00000       NO      YES
    10        b2           492.59        11.19990       YES     YES
    11        a1           510.47         5.06549       YES     YES
    12        b1           608.44         0.18950       YES     YES
    13        b2           675.13        18.01899       YES     YES
    14        b2           740.97        66.85254       YES     YES
    15        a2           800.87         0.00000       NO      YES
    16        a1           803.96        26.02790       YES     YES
    17        b2           874.72         6.55297       YES     YES
    18        a2           936.73         0.00000       NO      YES
    19        b2           951.26         0.01524       YES     YES
    20        a1           996.74         0.00012       YES     YES
    21        a1          1015.01         3.64079       YES     YES
    22        b1          1063.10         7.70053       YES     YES
    23        a1          1142.79        14.87880       YES     YES
    24        b1          1148.10         0.14934       YES     YES
    25        a1          1212.06        97.62504       YES     YES
    26        b1          1289.26         0.69731       YES     YES
    27        b1          1344.13         0.04402       YES     YES
    28        b1          1446.64         0.91505       YES     YES
    29        a1          1481.31        77.77814       YES     YES
    30        a1          1589.40        44.56221       YES     YES
    31        b1          1598.61         8.72901       YES     YES
    32        a1          3104.24         0.25624       YES     YES
    33        b1          3112.53         8.93415       YES     YES
    34        a1          3125.56        16.17536       YES     YES
    35        b1          3134.09         5.06139       YES     YES
    36        a1          3136.13         0.20040       YES     YES
$end
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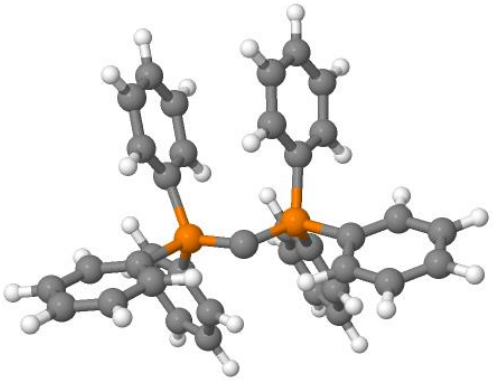
8.16 CDP^{Ph}



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

Cartesian coordinates in Ångström:

C	-0.0000000	0.0000000	-1.2845151
H	1.4378052	2.3163827	3.7284984
C	1.8327294	2.2402925	2.7155876
H	2.8265857	4.1573753	2.7839835
C	2.6092731	3.2732827	2.1848596
C	1.5490605	1.1140035	1.9452835
H	0.9422275	0.3134022	2.3646917
H	1.4841389	0.0067769	-3.3160907
C	3.1015575	3.1698040	0.8811947
C	2.0350825	1.0009197	0.6332260
H	3.7101206	3.9713988	0.4617504
P	1.4188982	-0.3148103	-0.4859529
C	2.8151782	2.0429640	0.1093735
C	2.4995698	-0.2881613	-3.0440149
H	0.0068515	-2.7411490	-0.7910781
H	3.3038250	-0.2436440	-5.0464134
C	0.6264086	-2.8956233	0.0926613
C	3.5140871	-0.4309289	-3.9930705
C	2.7682213	-0.5272809	-1.6928450
C	1.4640444	-1.8526387	0.5148020
H	3.1914939	1.9716417	-0.9113226
C	0.5658910	-4.0856794	0.8137702
H	-0.0994654	-4.8837179	0.4854066
C	2.2509471	-2.0240215	1.6618019
C	4.7969550	-0.8146887	-3.5930449
C	1.3395803	-4.2460201	1.9671049
C	4.0534000	-0.9169036	-1.2930756
H	2.9056488	-1.2209153	1.9993615
C	2.1840879	-3.2161188	2.3874715
C	5.0657918	-1.0590012	-2.2422162
H	5.5888939	-0.9276370	-4.3338486
H	1.2822865	-5.1721117	2.5394370
H	4.2618714	-1.1119341	-0.2405921
H	2.7909131	-3.3382926	3.2851559
H	6.0650235	-1.3633547	-1.9302561
H	-3.3038250	0.2436440	-5.0464134
C	-3.5140871	0.4309289	-3.9930705
H	-5.5888939	0.9276370	-4.3338486
C	-4.7969550	0.8146887	-3.5930449
C	-2.4995698	0.2881613	-3.0440149

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H    -1.4841389   -0.0067769   -3.3160907
H    -0.0068515    2.7411490   -0.7910781
C    -5.0657918    1.0590012   -2.2422162
C    -2.7682213    0.5272809   -1.6928450
H    -6.0650235    1.3633547   -1.9302561
P    -1.4188982    0.3148103   -0.4859529
C    -4.0534000    0.9169036   -1.2930756
C    -0.6264086    2.8956233    0.0926613
H    -0.9422275   -0.3134022    2.3646917
H     0.0994654    4.8837179    0.4854066
C    -1.5490605   -1.1140035    1.9452835
C    -0.5658910    4.0856794    0.8137702
C    -1.4640444    1.8526387    0.5148020
C    -2.0350825   -1.0009197    0.6332260
H    -4.2618714    1.1119341   -0.2405921
C    -1.8327294   -2.2402925    2.7155876
H    -1.4378052   -2.3163827    3.7284984
C    -2.8151782   -2.0429640    0.1093735
C    -1.3395803    4.2460201    1.9671049
C    -2.6092731   -3.2732827    2.1848596
C    -2.2509471    2.0240215    1.6618019
H    -3.1914939   -1.9716417   -0.9113226
C    -3.1015575   -3.1698040    0.8811947
C    -2.1840879    3.2161188    2.3874715
H    -1.2822865    5.1721117    2.5394370
H    -2.8265857   -4.1573753    2.7839835
H    -2.9056488    1.2209153    1.9993615
H    -3.7101206   -3.9713988    0.4617504
H    -2.7909131    3.3382926    3.2851559

SCF energy GEOOPT =  -2111.522037860 H
ZPE =   1417. kJ/mol
FREEH energy =  1507.49 kJ/mol
FREEH entropy =   0.90772 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
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     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             23.03         0.01194       YES     YES
     8        b             28.34         0.25692       YES     YES
     9        a             29.09         0.01488       YES     YES
    10        b             31.38         0.09554       YES     YES
    11        a             32.88         0.00130       YES     YES
    12        a             42.68         0.01457       YES     YES
    13        b             45.18         0.00723       YES     YES
    14        b             51.92         0.33214       YES     YES
    15        a             53.23         0.12158       YES     YES
    16        b             58.29         0.36006       YES     YES
    17        a             66.80         0.17357       YES     YES
    18        a             72.64         0.00238       YES     YES
    19        b             82.57         0.10670       YES     YES
    20        a             89.75         0.08660       YES     YES
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21	b	91.02	0.10866	YES	YES
22	a	107.54	0.04628	YES	YES
23	b	109.36	0.97672	YES	YES
24	a	159.89	1.82641	YES	YES
25	b	177.15	1.25739	YES	YES
26	a	181.70	0.14719	YES	YES
27	b	187.09	4.63233	YES	YES
28	a	218.48	0.03496	YES	YES
29	b	221.88	10.26079	YES	YES
30	a	223.26	0.09264	YES	YES
31	a	235.55	0.02779	YES	YES
32	b	236.35	1.20471	YES	YES
33	b	245.53	0.00735	YES	YES
34	a	251.87	0.00000	YES	YES
35	b	269.53	1.02469	YES	YES
36	a	273.50	0.24055	YES	YES
37	b	322.34	12.01865	YES	YES
38	a	364.50	2.31060	YES	YES
39	b	383.13	0.65425	YES	YES
40	b	384.52	23.06388	YES	YES
41	a	390.07	0.10107	YES	YES
42	b	393.20	0.71241	YES	YES
43	a	394.81	0.15948	YES	YES
44	a	399.54	0.00181	YES	YES
45	b	401.44	0.07449	YES	YES
46	a	433.50	0.08630	YES	YES
47	b	437.51	13.55983	YES	YES
48	a	444.81	7.97506	YES	YES
49	b	461.61	4.92701	YES	YES
50	a	482.55	5.76319	YES	YES
51	b	495.32	144.48181	YES	YES
52	b	510.80	12.54283	YES	YES
53	a	514.38	3.51633	YES	YES
54	b	519.01	174.63754	YES	YES
55	a	528.03	61.85231	YES	YES
56	a	613.55	0.28333	YES	YES
57	b	613.89	0.14165	YES	YES
58	b	614.37	0.26262	YES	YES
59	a	614.85	1.07521	YES	YES
60	b	614.99	0.05465	YES	YES
61	a	617.20	0.00894	YES	YES
62	a	661.95	3.26111	YES	YES
63	b	678.37	0.27812	YES	YES
64	b	686.35	109.52537	YES	YES
65	a	689.66	0.08553	YES	YES
66	b	690.70	55.93183	YES	YES
67	a	691.34	0.26812	YES	YES
68	a	694.96	15.74998	YES	YES
69	b	695.43	19.48974	YES	YES
70	b	702.43	65.36591	YES	YES
71	a	704.71	4.40988	YES	YES
72	b	706.71	11.71424	YES	YES
73	a	709.62	37.27141	YES	YES
74	a	727.40	22.99754	YES	YES
75	b	731.14	9.60023	YES	YES
76	a	734.16	0.40321	YES	YES
77	b	734.49	1.94998	YES	YES
78	a	743.10	1.50185	YES	YES

79	b	743.81	17.75849	YES	YES
80	a	784.16	12.97837	YES	YES
81	b	828.27	0.83973	YES	YES
82	a	834.67	1.96308	YES	YES
83	a	837.44	0.24239	YES	YES
84	b	837.81	0.12771	YES	YES
85	a	840.74	0.11188	YES	YES
86	b	841.48	1.25718	YES	YES
87	b	896.24	1.60122	YES	YES
88	a	904.91	0.60194	YES	YES
89	a	911.32	0.09557	YES	YES
90	b	911.84	0.03457	YES	YES
91	a	914.63	0.83262	YES	YES
92	b	915.30	0.22533	YES	YES
93	b	951.07	0.04065	YES	YES
94	a	956.51	0.13178	YES	YES
95	a	959.20	0.03145	YES	YES
96	b	959.36	0.17863	YES	YES
97	b	962.46	0.09701	YES	YES
98	a	962.65	0.00364	YES	YES
99	b	967.66	0.05125	YES	YES
100	a	969.82	0.31041	YES	YES
101	a	975.69	0.07655	YES	YES
102	b	975.88	0.02479	YES	YES
103	a	976.16	0.15476	YES	YES
104	b	976.62	0.23293	YES	YES
105	b	995.94	0.23198	YES	YES
106	a	996.84	0.14440	YES	YES
107	b	996.85	0.32796	YES	YES
108	b	997.86	1.99701	YES	YES
109	a	998.25	0.31133	YES	YES
110	a	1001.93	0.00817	YES	YES
111	b	1023.27	18.81445	YES	YES
112	a	1024.04	7.41992	YES	YES
113	b	1024.72	0.64479	YES	YES
114	a	1025.13	0.00463	YES	YES
115	b	1025.54	7.00935	YES	YES
116	a	1026.11	1.49115	YES	YES
117	b	1064.74	3.59333	YES	YES
118	a	1066.13	13.93242	YES	YES
119	b	1070.31	6.59064	YES	YES
120	a	1072.36	4.87473	YES	YES
121	b	1073.73	1.86014	YES	YES
122	a	1076.35	2.99050	YES	YES
123	b	1084.04	0.70058	YES	YES
124	a	1086.75	17.39138	YES	YES
125	b	1087.55	70.88827	YES	YES
126	a	1088.13	0.10071	YES	YES
127	b	1094.84	43.59529	YES	YES
128	a	1097.69	34.00721	YES	YES
129	b	1148.91	1.21008	YES	YES
130	a	1149.37	0.01062	YES	YES
131	b	1150.20	0.00001	YES	YES
132	a	1150.27	0.13706	YES	YES
133	b	1150.27	1.18279	YES	YES
134	a	1150.85	0.41489	YES	YES
135	b	1163.91	26.71504	YES	YES
136	a	1165.61	6.42089	YES	YES

137	b	1169.08	26.82390	YES	YES
138	a	1169.65	0.18964	YES	YES
139	b	1171.79	4.18829	YES	YES
140	a	1175.62	0.00018	YES	YES
141	b	1226.48	780.22472	YES	YES
142	b	1289.80	9.65029	YES	YES
143	a	1290.98	2.84290	YES	YES
144	b	1294.47	0.77955	YES	YES
145	a	1294.99	7.40908	YES	YES
146	b	1299.28	0.09790	YES	YES
147	a	1300.54	2.78538	YES	YES
148	b	1334.37	1.10768	YES	YES
149	a	1335.37	0.10619	YES	YES
150	a	1337.71	0.65088	YES	YES
151	b	1337.74	0.61456	YES	YES
152	b	1339.10	0.42082	YES	YES
153	a	1339.61	2.65086	YES	YES
154	b	1424.00	21.35038	YES	YES
155	a	1425.09	2.77886	YES	YES
156	b	1428.94	15.22497	YES	YES
157	a	1429.35	24.59881	YES	YES
158	a	1429.93	3.89885	YES	YES
159	b	1430.01	0.26941	YES	YES
160	a	1467.76	4.29512	YES	YES
161	b	1467.81	6.90588	YES	YES
162	b	1469.16	9.22500	YES	YES
163	a	1469.72	0.80775	YES	YES
164	b	1470.44	17.27181	YES	YES
165	a	1471.50	5.72645	YES	YES
166	b	1566.66	1.54015	YES	YES
167	a	1567.11	0.08947	YES	YES
168	b	1569.72	0.05644	YES	YES
169	a	1570.27	0.00778	YES	YES
170	b	1571.95	0.18733	YES	YES
171	a	1572.42	0.54148	YES	YES
172	b	1582.39	4.99793	YES	YES
173	a	1583.30	0.63168	YES	YES
174	b	1584.10	0.68362	YES	YES
175	a	1584.63	0.45907	YES	YES
176	b	1585.03	0.54955	YES	YES
177	a	1585.65	0.00496	YES	YES
178	b	3084.37	7.63527	YES	YES
179	a	3085.51	2.16178	YES	YES
180	a	3091.97	1.44673	YES	YES
181	b	3091.98	0.06209	YES	YES
182	b	3093.30	1.65842	YES	YES
183	a	3093.36	0.23435	YES	YES
184	b	3093.53	3.66968	YES	YES
185	a	3093.68	2.71289	YES	YES
186	b	3099.58	4.90721	YES	YES
187	a	3099.58	2.72430	YES	YES
188	b	3100.78	1.94687	YES	YES
189	a	3100.93	0.25230	YES	YES
190	b	3101.90	0.49260	YES	YES
191	a	3102.21	0.46799	YES	YES
192	b	3105.81	3.65604	YES	YES
193	a	3105.84	2.31147	YES	YES
194	b	3109.40	2.16655	YES	YES

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   195        a            3109.70        18.09965       YES     YES
   196        b            3110.19         3.40682       YES     YES
   197        a            3110.30        39.52619       YES     YES
   198        a            3113.32        11.65508       YES     YES
   199        b            3113.41        29.34380       YES     YES
   200        b            3117.04        28.08564       YES     YES
   201        a            3117.64         1.61370       YES     YES
   202        b            3120.22        54.10523       YES     YES
   203        a            3120.35        25.83635       YES     YES
   204        b            3121.83        51.69647       YES     YES
   205        a            3121.85         2.15543       YES     YES
   206        b            3124.67         9.81077       YES     YES
   207        a            3124.88        21.38266       YES     YES
$end
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