Electronic Supporting Information

To

# Soft Interactions with Hard Lewis acids: Generation of Mono- and Dicationic Alkaline-Earth Metal Arene-Complexes by Direct Oxidation.

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## Contents

# S-1 Experimental Details and Characterisation Techniques

All reactions and manipulations were carried out under an inert argon atmosphere, using standard Schlenk-line and glovebox (Box atmosphere kept below 1 ppm $H_2O/O_2$) techniques. Glassware has been stored over-night in an oven set to 180°C and flame dried under vacuum prior to use. $C_6Me_6$ (Alfa Aesar, >99 %) was sublimed under dynamic vacuum prior to use. Ca (ABCR, 99.99 %), Sr (Alfa Aesar, 99.99 %) and Ba ((Alfa Aesar, 99.99 %) were used as received. $I_2$ was sublimed under static vacuum. Pentane was collected from a solvent purification system (SPS) and oxygen removed by purging with Argon. PhF, *o*-DFB, $CD_2Cl_2$, hexane and heptane were refluxed/stirred over $CaH_2$ and distilled. All solvents were stored over activated 3 Å molecular sieves in gas tight ampoules.

**Powder Diffraction.** Powder diffractograms were recorded with the sample sealed with perfluoropolyalkylether oil (AB128330, abcr GmbH & Co. KG) in a 0.3 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) at 100(10) K in the 2θ range 2.0-40.0° with a STOE STADI P powder diffractometer with Mo-$K_{\alpha1}$ radiation (λ = 0.709300 Å) equipped with a Ge-(111) monochromator and Mythen 1K detector. Data acquiring, processing and the calculation of powder diffractograms from single-crystal data were performed using STOE WinXPOW® package. All powder diffractograms were background corrected.

**ATR-IR Spectroscopy.** ATR FT-IR spectra were recorded at ambient temperature on a ZnSe crystal on a FTIR Bruker ALPHA with a QuickSnap Platinum ATR sampling module inside an inert atmosphere glovebox. Spectra were recorded in a range from 4000-500 $cm^{-1}$. The spectra were recorded with either 64 or 128 scans and a resolution of 2 $cm^{-1}$. Data processing was carried out with the software package OPUS 7.5. For all spectra, signal intensity was normalised to one and the relative band intensities were described as follows: ≥ 0.8 = very very strong (vvs), ≥ 0.7 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.5 = medium strong (ms), ≥ 0.4 = medium (m), ≥ 0.3 = medium weak (mw), ≥ 0.2 = weak (w), ≥ 0.1 = very weak (vw), < 0.1 = very very weak (vvw).

**Single crystal X-ray diffraction.** Single crystal X-ray diffraction data were collected using either a Bruker SMART APEXII QUAZAR detector with fixed-Chi D8 Goniometer, INCOATEC Mo microsource or Bruker D8 VENTURE with PHOTONIII detector, fixed-Chi D8 Goniometer and INCOATEC Mo/Cu microsource. Crystals were selected under perfluoropolyether oil, mounted on 0.1 to 0.3 mm diameter CryoLoops and quench-cooled using an Oxford Cryostream 800 open flow $N_2$ cooling device.[1] Data were collected at 100 K using monochromated Cu Kα or Mo Kα radiation (λ = 1.5418/0.71073 Å). Data processing was done with SHELXs/XL and refined by least squares on weighted $F^2$ values for all reflections, disordering of fragments was done with the help of the implemented DSR tool.[2] Graphical representations have been prepared using Olex2-1.2. Finalisation of gathered data was done using final cif tool.[3]

**NMR spectroscopy.** NMR samples were prepared inside an inert atmosphere glovebox in either flame sealable NMR tubes or NMR tubes equipped with a gas-tight J.Young valve. $^{1}$H, $^{13}$C, $^{19}$F, $^{27}$Al, $^{31}$P, $^{115}$In-NMR spectra were acquired either on a Bruker Biospin Avance II+ 400 MHz WB, a Bruker Avance 200 MHz or a Bruker Avance III HD 300 MHz spectrometer. $^{1}$H and $^{13}$C NMR spectra are reported relative to TMS and were calibrated to residual solvent resonances.[4] Data analysis was performed using Bruker TOPSPIN 3.5 software. The broad resonance at δ = 70 ppm observed in $^{27}$Al-NMR spectra corresponds to a background from Al-nuclei in the probe head.

**Quantum Chemical Calculations.** All quantum chemical calculations were carried out with the TURBOMOLE program package using BP86 functionals with def-SV(P) basis sets and D3(BJ) dispersion correction.[5] Vibrational frequencies were calculated using the AOFORCE-module.[6] All calculated structures were checked for consistency in terms of geometric conversion, sensible electron occupations and the absence of imaginary vibrational frequencies. Thermal contributions to the enthalpy and free energy of the systems were calculated with the FREEH application based on the analysis of the vibrations obtained by BP86/def2-def-SV(P)/D3(BJ) calculations. Charge analysis was done by NPA[7], PABOON[8] and AIM[9] analysis on wfn files generated with TURBOMOLE using the program Multiwfn 3.6.[10] Solvation effects were computed using the COSMO module with set dielectricity constants of 8.93 ($CH_2Cl_2$) and 13.38 (1,2-$C_6H_4F_2$).[11]

## S-1.1 Oxidation of Mg with [HMB][Al(OR$^F$)$_4$]

### S-1.1.1 Mg turnings

Magnesium turnings (0.032 g, 1.30 mmol, 6 eq.) were flame heated under reduced pressure and stirred for 12 h under an Argon atmosphere. Ag[Al(OR$^F$)$_4$] (0.116 g, 0.108 mmol) and $C_6Me_6$ (0.035 g, 0.215 mmol, 2 eq.) were dissolved in *o*-DFB (4 ml). Iodine (0.014 g, 0.054 mmol, 0.5 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature, and the supernatant filtered away from formed AgI onto the activated Magnesium turnings and stirred for 5 d at ambient temperature. The deep red colour of the reaction mixture was slightly lightened during this period. Dark red crystals suitable for scXRD experiments were grown by layering of the filtered reaction mixture with n-pentane (8 ml). And revealed the structure of 6,7-difluoro-1,2,3,4-tetramethylanthracenyl tetrafluorotertbutoxyaluminate already described in the literature.[12]

### S-1.1.2 Rieke Magnesium Mg*

Preparation of Rieke Magnesium:

To ensure highest possible activity of employed Magnesium $MgCl_2$ (0.108 g, 1.14 mmol) was suspended in THF (6 ml) and reduced with a solution of Lithium Napthalenide in THF (1 M, 2 ml, 2 mmol, 1.8 eq.). The reaction mixture was stirred for 12 h at ambient temperature during which decolourisation and precipitation of dark grey precipitate was observed. Supernatant solution was filtered, the precipitate washed with THF (3 x 8 ml) and dried under vacuum.

$Ag[Al(OR^F)_4]$ (0.243 g, 0.226 mmol) and $C_6Me_6$ (0.078 g, 0.453 mmol, 2 eq.) were dissolved in *o*-DFB (5 ml). Iodine (0.029 g, 0.113 mmol, 0.5 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered away from formed AgI onto the freshly prepared Rieke Magnesium and stirred for 5 d at ambient temperature. The deep red colour of the reaction mixture was slightly lightened during this period. An aliquot (2 ml) of the reaction mixture was again layered with n-pentane to yield crystals of 6,7-difluoro-1,2,3,4-tetramethylanthracenyl tetrafluorotertbutoxyaluminate described above. The rest of the reaction mixture was spiked with two drops of MeCN with immediate Colour loss upon addition. The reaction mixture was filtered. Crystals suitable for scXRD analysis were grown from concentrated solution at –25°C to reveal hexacoordinate $[Mg(MeCN)_6][Al(OR^F)_2]_2$ **1**.

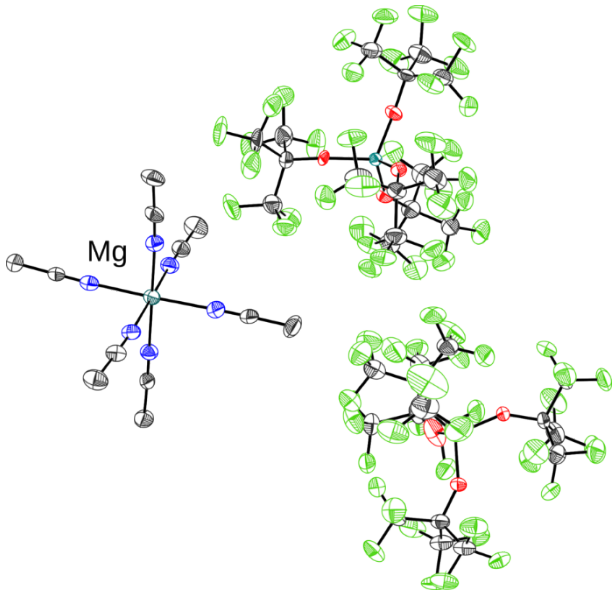


*Figure S- 1 Molecular structure of $[Mg(MeCN)_6][Al(OR^F)_4]_2$. Thermal displacement ellipsoids drawn at 50 % probability. Hydrogen atoms were omitted for clarity.*

## S-1.2 Synthesis of $[Ca(HMB)(oDFB)_2\{f\text{-}al\}][Al(OR^F)_4]$ **2**

$Ag[Al(OR^F)_4]$ (0.226 g, 0.210 mmol) and $C_6Me_6$ (0.034 g, 0.210 mmol, 1 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.027 g, 0.105 mmol, 0.5 eq.) was added under positive argon flow to the stirred

reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered away from formed AgI onto Calcium clippings (0.051 g, 4.21 mmol, 7 eq.) and stirred for 9 d at ambient temperature. The yellow reaction mixture was filtered and layered with n-pentane to yield the title compound as colourless crystals (0.079 g, 0.037 mmol, crystalline yield calculated for **2**: 35 %).

### S-1.3 Synthesis of [HMB][*al-f-al*]

Ag[*al-f-al*] (0.217 g, 0.119 mmol) and $C_6Me_6$ (0.019 g, 0.118 mmol, 0.99 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.015 g, 0.059 mmol, 0.5 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered into an J.Youngs tap NMR tube and NMR spectra collected of the fresh sample and after three and six days. No major change in composition of the sample was detectable. Quantity of [F-(Al(OR$^F$)$_3$] remained at below 2% compared to [$\mu$F-{Al(OR$^F$)$_3$}$_2$].

$^1$H-NMR (200.12 MHz, 1,2-$C_6H_4F_2$, 298 K) δ = 2.19 (br. s, $\omega_{1/2}$ = 118 Hz ) ppm. comp. **1b**-H$^+$ δ = 9.57 (s, 1H, 10-C*H*), 7.94 (m, 1H, 5-C*H*), 7.65 (m, 1H, 8-C*H*), 4.46 (s, 2H, 9-C$H_2$), 2.71 (s, 3H, 14-C$H_3$), 2.45 (s, 3H, 12-C$H_3$), 2.35 (s, 3H, 11-C$H_3$), 2.27 (s, 3H, 13-C$H_3$) ppm. comp. [$C_6Me_7$]$^+$ δ = 2.60 (s, 3H, *p*–C$H_3$), 2.48 (s, 6H, *o*–C$H_3$), 2.12 (s, 6H, *m*–C$H_3$), 1,41 (s, 6H, *ipso*–C$H_3$) ppm. unknown arene δ = 3.71 (s, –C$H_2$) ppm. $^{19}$F-NMR (188.31 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.1 (br. s, F–[Al(OR$^F$)$_3$], >2% compared to [$\mu$F-{Al(OC(C$F_3$)$_3$)$_3$}$_2$]), −75.5 (s, 54 F, [$\mu$F-{Al(OC(C$F_3$)$_3$)$_3$}$_2$]), −76.0 (s), −76.2 (s), −184.5 (br s, 1 F, [$\mu$F-{Al(OC(C$F_3$)$_3$)$_3$}$_2$]) ppm.

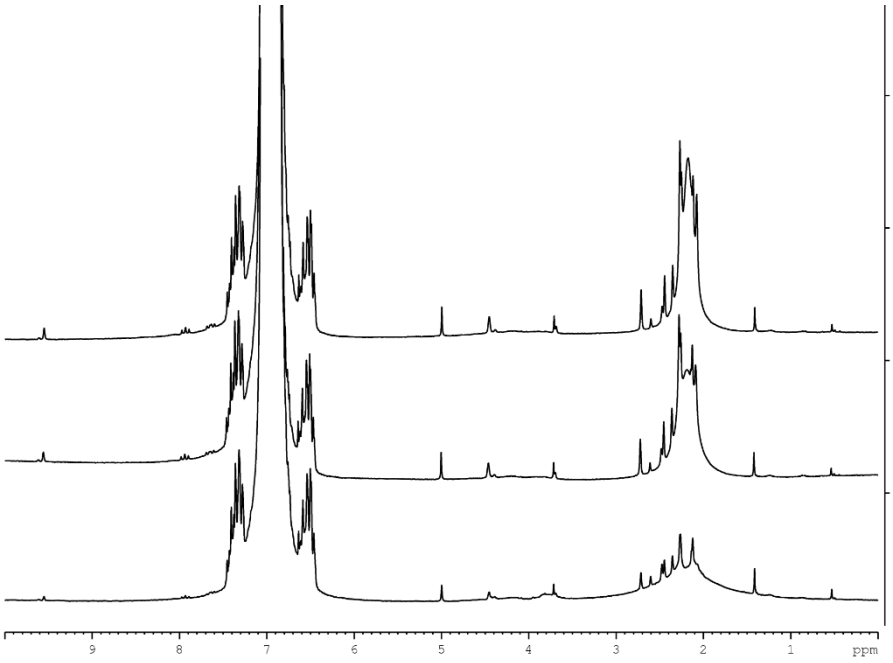


*Figure S- 2: Stacked $^{1}$H-NMR (200.12 MHz, 1,2-$C_6H_4F_2$, 298 K) spectra of freshly prepared solution of [HMB][al-f-al] (bottom trace). Recollected after three (middle trace) and six (top trace) days.*

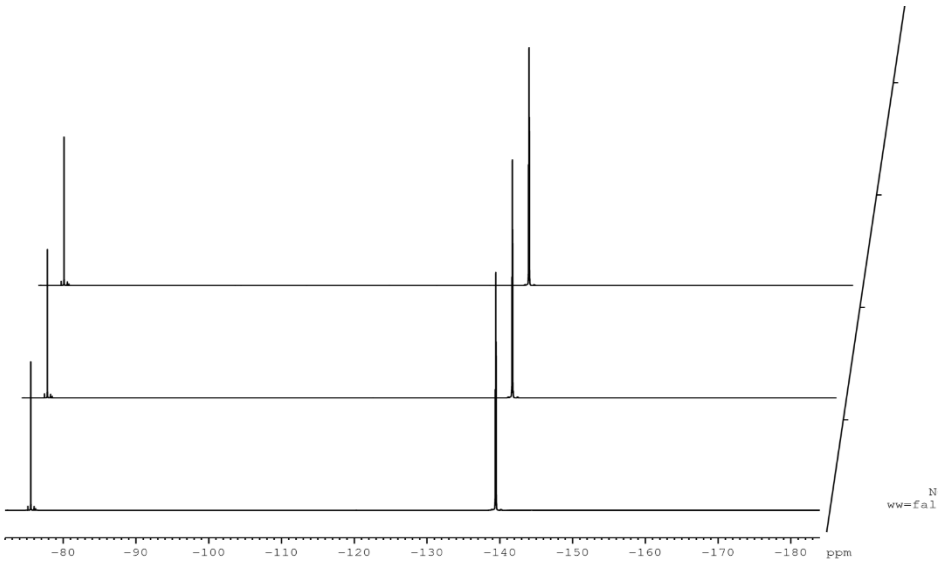


*Figure S- 3 Stacked $^{19}$F-NMR (188.31 MHz, 1,2-$C_6H_4F_2$, 298 K) spectra of freshly prepared solution of [HMB][al-f-al] (bottom trace). Recollected after three (middle trace) and six (top trace) days.*

## S-1.4 Synthesis of [In(HMB)][*al-f-al*]

Ag[*al-f-al*] (0.352 g, 0.193 mmol) and $C_6Me_6$ (0.029 g, 0.1757 mmol, 0.90 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.019 g, 0.0737 mmol, 0.42 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered onto thinly sheeted Indium metal (0.040 g, 0.351 mmol, 2 eq.) and stirred for 12 h at ambient temperature. After 30 min lightening of the dark red color of the

reaction mixture was observed with complete colour change to light yellow after 12 h. The reaction mixture was filtered and layered with n-pentane to yield the title compound in form of yellowish needles (0.220 g, 0.193 mmol, 64% crystalline yield).

$^{1}$H-NMR (300.18 MHz, 1,2-$C_6H_4F_2$, 298 K) δ = 2.45 ( s, 18 H, [In($C_6$($CH_3$)$_6$]$^+$) ppm. $^{13}$C-NMR (100.62 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 15.8 (s, [In($C_6$($CH_3$)$_6$)]$^+$), 137.8 ppm (s, [In($C_6$($CH_3$)$_6$)]$^+$). $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.5 (s, 54 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]), −184.5 (br s, 1 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]) ppm. $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 39.8 ppm (s, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]$^-$). $^{115}$In-NMR (65.77 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −1296.2 ppm (s, [In($C_6Me_6$)]).

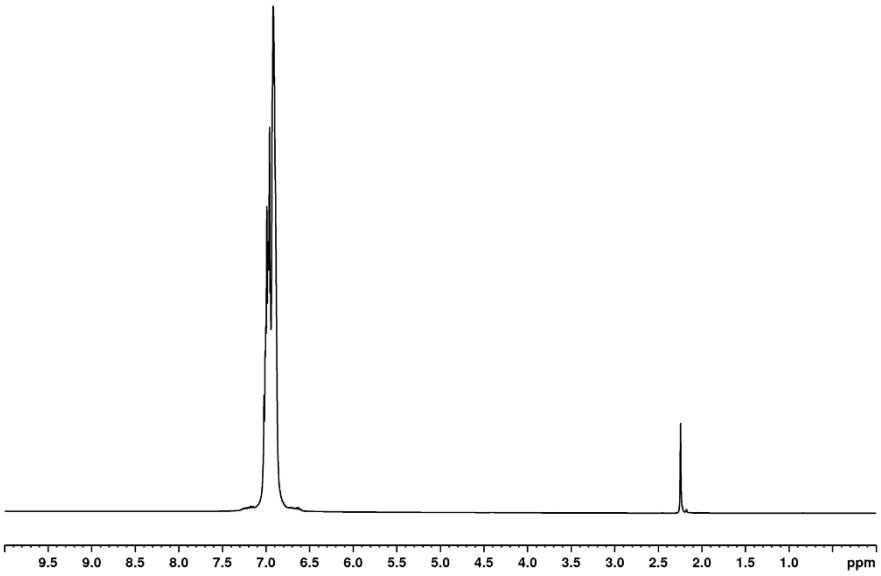


*Figure S- 4 $^{1}$H-NMR (300.18 MHz, 1,2-$C_6F_2H_4$, 298 K) of [In(HMB)][al-f-al].*

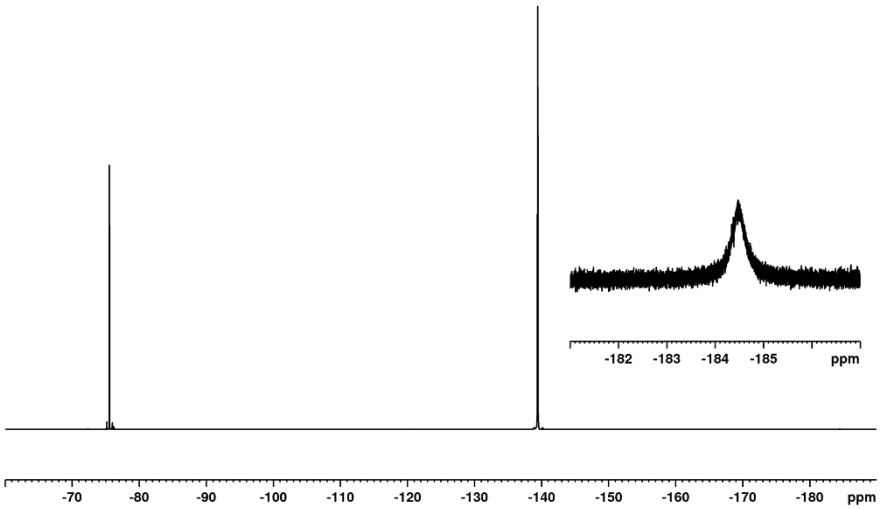


*Figure S- 5 $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) of [In(HMB)][al-f-al].*

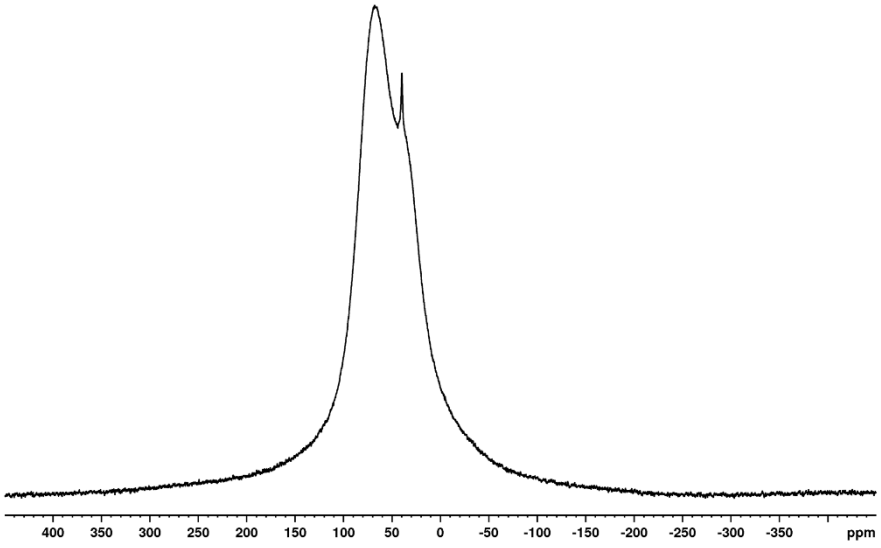


*Figure S- 6 $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) of [In(HMB)][al-f-al].*

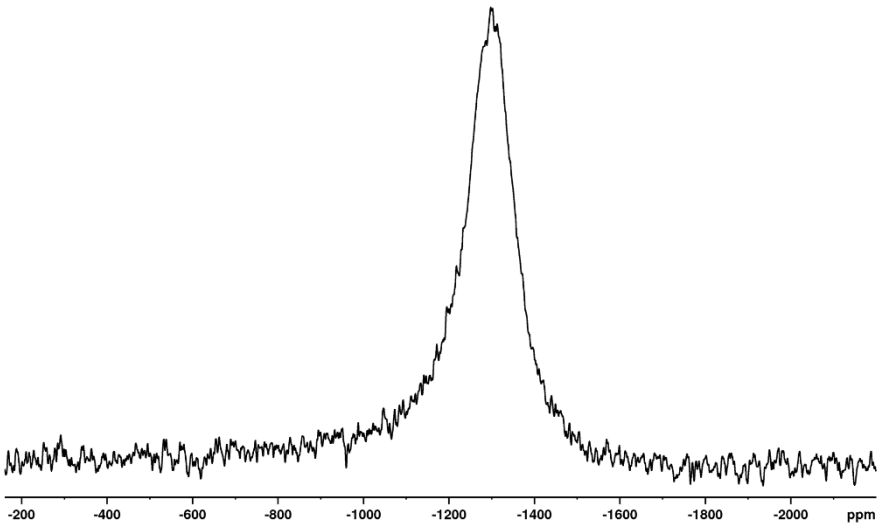


*Figure S- 7 $^{115}$In-NMR (65.77 MHz, 1,2-$C_6F_2H_4$, 298 K) of [In(HMB)][al-f-al].*

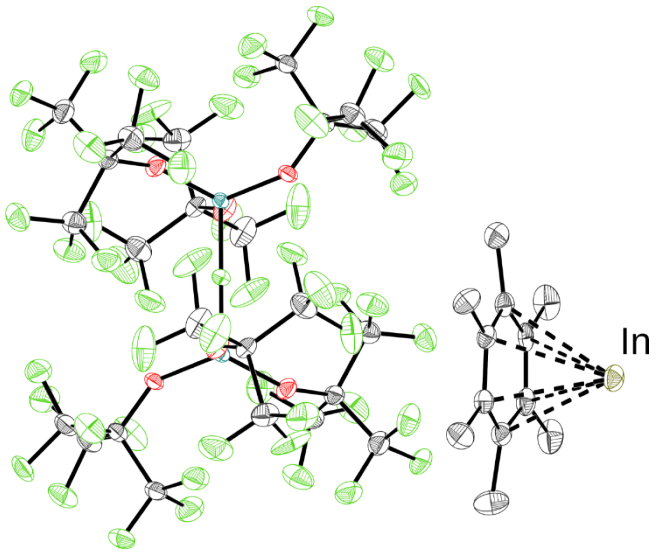


*Figure S- 8 Molecular structure of [In(HMB)][al-f-al]. Thermal displacement ellipsoids drawn at 50 % probability. Hydrogen atoms were omitted for clarity.*

## S-1.5 Synthesis of [Ca(HMB)(oDFB)$_2${*f-al*}][*al-f-al*] **3**

Ca clippings (70 mg, 1.747 mmol) were dissolved in $NH_3$ (4 ml) at −78°C under formation of a deep blue solution and stirred for 1 h at this temperature. $NH_3$ was slowly evaporated by moderate temperature increase with a positive flow of Argon to result in a bronze coloured metal powder. Residual $NH_3$ was removed under reduced pressure at 80°C to yield a dark grey metal powder. To test reactivity of the obtained Ca dust a few grains of the powdered metal were brought in contact with a droplet of water to result in an intense white flame.

Ag[*al-f-al*] (0.309 g, 0.170 mmol) and $C_6Me_6$ (0.027 g, 0.169 mmol, 0.99 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.021 g, 0.084 mmol, 0.49 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered onto the activated Calcium powder and stirred for 10 d at ambient temperature. After 12 h lightening of the dark red color of the reaction mixture was observed but even after 10 d a faint red colour was observable. The reaction mixture was filtered and layered with *n*-pentane to yield the title compound as colourless crystals (0.175 g, 0.066 mmol, 77% crystalline yield).

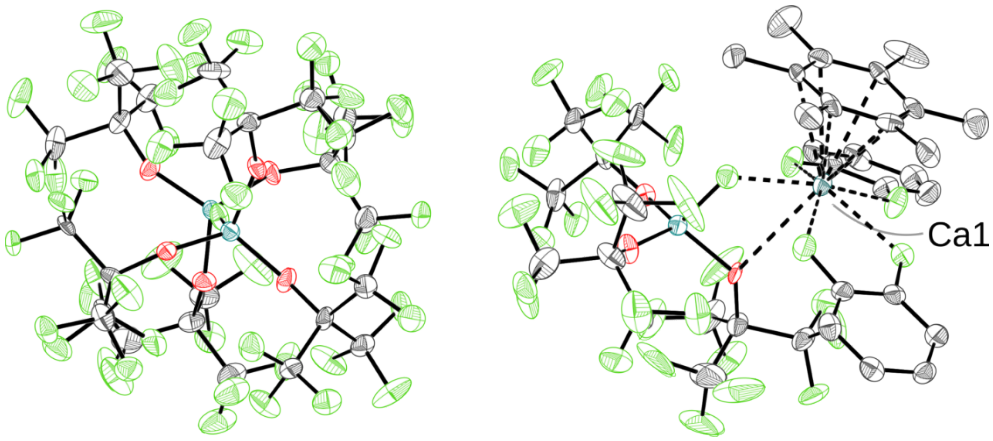


*Figure S- 9 Molecular structure of [Ca(HMB)(oDFB)$_2${f-al}][al-f-al] **3**. Thermal displacement ellipsoids drawn at 50 % probability. Hydrogen atoms were omitted for clarity.*

## S-1.6 Synthesis of [Ca(HMB)(oDFB)$_2${*f-al*}][*al-f-al*] **3** and serendipitous finding of [Ca(HMB)(oDFB)$_4$][al-f-al] **7**

Ag[*al-f-al*] (0.309 g, 0.170 mmol) and $C_6Me_6$ (0.027 g, 0.169 mmol, 0.99 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.021 g, 0.084 mmol, 0.49 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered onto Calcium clippings (0.040 g, 1.004 mmol, 7 eq.) and stirred for 10 d at ambient temperature. After 12 h lightening of the dark red color of the reaction mixture was observed but even after 10 d a faint red colour was observable. The reaction mixture was filtered and layered with *n*-pentane and left to crystallize at −10°C to yield the title compound **3** as colourless needles together with minor product **7** in form of yellowish blocks (0.150 g, 0.056 mmol, 77% crystalline yield calculated with respect to **3**).

$^1$H-NMR (400.17 MHz, 1,2-$C_6H_4F_2$, 298 K) δ = 2.15 ( s, 18 H, ($C_6(CH_3)_6$) ppm. $^{13}$C-NMR (100.62 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 15.6 (s, ($C_6(CH_3)_6$)), 133.3 ppm (s, ($C_6(CH_3)_6$)). $^{19}$F-NMR (376.54 MHz, 1,2-$C_6F_2H_4$,

298 K) δ = −75.5 (s, 54 F, [$\mu$F-{Al(OC(C$F_3$)$_3$)$_3$}$_2$]), -75.9 (s), -76.0 (s, 27 F, [F-Al(O(C(C$F_3$))$_3$]$^-$, ratio [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$] : [F-Al(O(C($CF_3$))$_3$]$^-$; 2.15 : 1), -76.1 (s), −151.5 (s, 1 F, [F-Al(O(C($CF_3$))$_3$]$^-$), −184.5 (br s, 1 F, [$\mu$F-{Al(OC(C$F_3$)$_3$)$_3$}$_2$]) ppm. $^{27}$Al-NMR (104.27 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 39.0 ppm (shoulder, [$\mu$F-{*Al*(OC($CF_3$)$_3$)$_3$}$_2$]$^-$). IR (64 scans, ZnSe ATR, corrected): $\tilde{\nu}$/cm$^{-1}$ (intensity) = 3661 (vvw), 1599 (vvw), 1496 (vvw), 1354 (vw), 1300 (mw), 1242 (vvs), 1212 (vvs), 1176 (ms), 1088 (vvw), 971 (vvs), 861 (vw), 828 (vvw), 753 (vw), 726 (vvs), 637 (vw), 568 (vw).

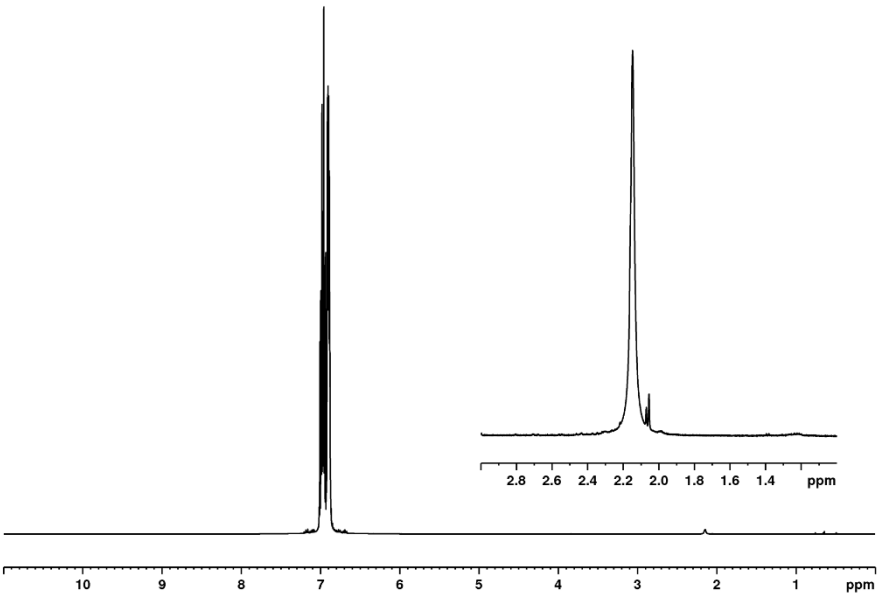


*Figure S- 10 $^1$H-NMR (400.17 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ca(HMB)(oDFB)$_2${f-al}][al-f-al].*

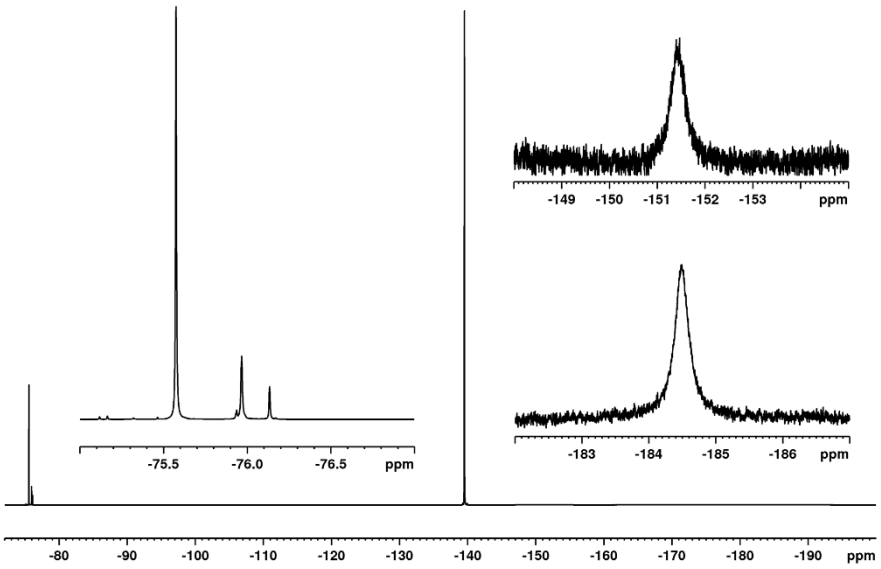


*Figure S- 11 $^{19}$F-NMR (376.54 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ca(HMB)(oDFB)$_2${*f*-al}][*al-f-al*]*

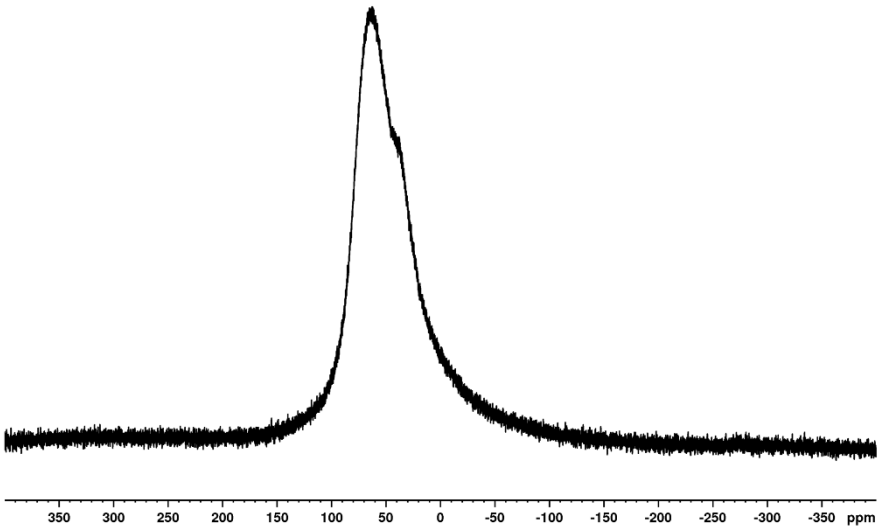


*Figure S- 12 $^{27}$Al-NMR (104.27 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ca(HMB)(oDFB)$_2${*f*-al}][*al-f-al*]*

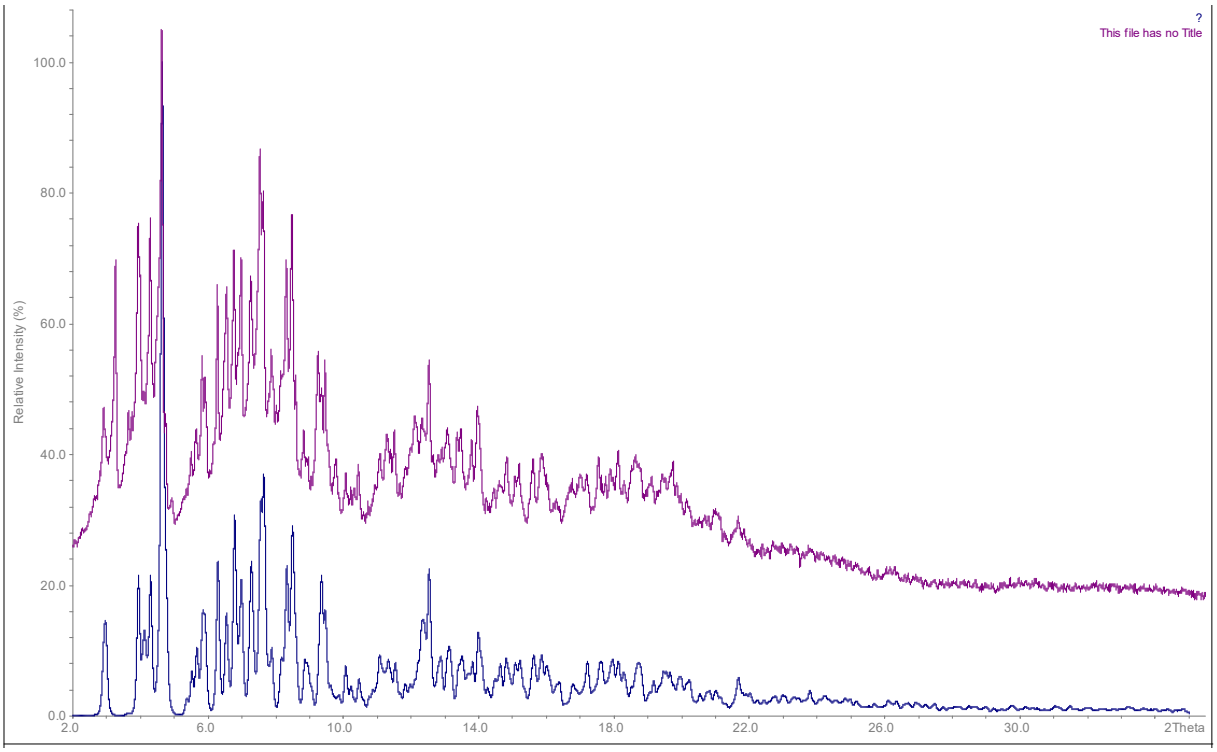


*Figure S- 13 Powder diffractogram of bulk material containing [Ca(HMB)(oDFB)$_2${f-al}][al-f-al] at 100(10) K. (purple trace) simulated diffractogram of the single-crystal X-ray analysis (blue trace), measured at 100(2) K .*

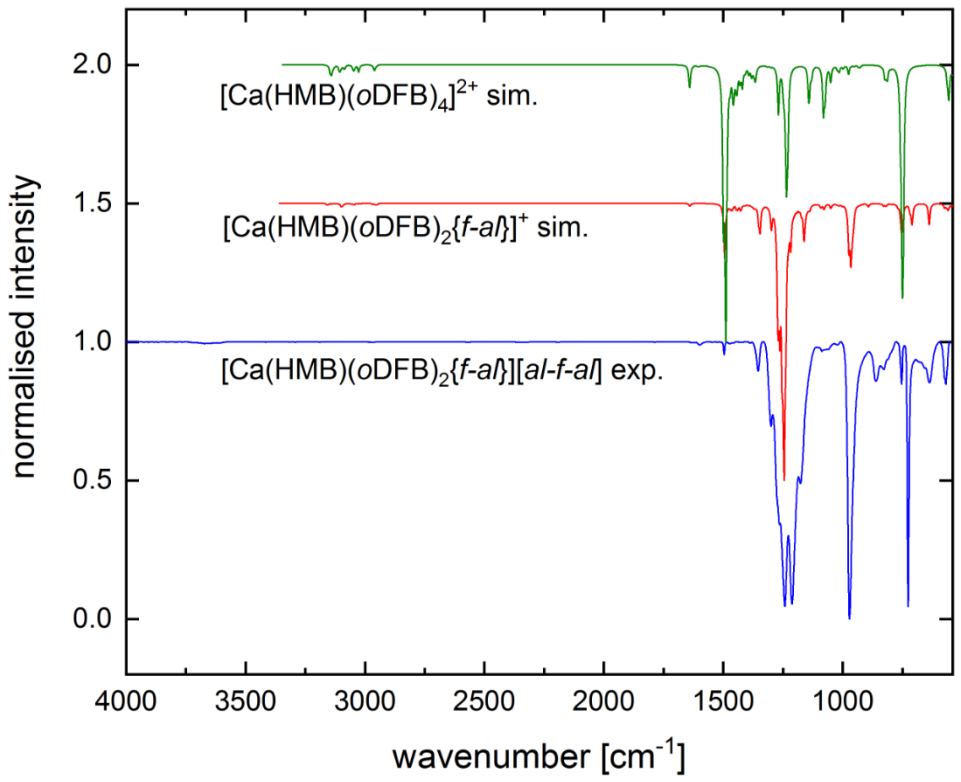


*Figure S- 14 Experimental IR data on bulk material containing [Ca(HMB)(oDFB)$_2${f-al}][al-f-al] **3** (blue). Simulated IR data on [Ca(HMB)(oDFB)$_4$]$^{2+}$ (green) & [Ca(HMB)(oDFB)$_2${f-al}]$^+$ (red) (BP86/def2-def-SV(P)/D3(BJ) ). IR (ZnSe ATR-corrected, 64 scans).*

## S-1.7 Synthesis of [Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4**

Ag[*al-f-al*] (0.430 g, 0.236 mmol) and $C_6Me_6$ (0.038 g, 0.234 mmol, 0.99 eq.) were dissolved in *o*-DFB (4 ml). Iodine (0.030 g, 0.117 mmol, 0.49 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered onto Barium clippings (0.065 g, 0.468 mmol, 2 eq.) and stirred for 10 d at ambient temperature. After 12 h lightening of the dark red color of the reaction mixture was observed but even after 10 d a faint red colour was observable. The reaction mixture was filtered and layered with *n*-pentane and left to crystallize at −10°C to yield the title compound **4** as colourless crystals (0.280 g, 0.117 mmol, 83 % crystalline yield calc. for **4**).

$^1$H-NMR (300.18 MHz, 1,2-$C_6H_4F_2$, 298 K) δ = 2.17 ( s, 18 H, ($C_6(CH_3)_6$) ppm. $^{13}$C-NMR (75.48 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 15.0 (s, ($C_6(CH_3)_6$)), 133.4 ppm (s, ($C_6(CH_3)_6$)). $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.6 (s, 54 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]), -75.8 (s, 27 F, [F-Al(O(C($CF_3$))$_3$]$^-$, ratio [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$] : [F-Al(O(C($CF_3$))$_3$]$^-$; 2.15 : 1), -76.1 (s), −130.3 (br. s, 1 F, [F-Al(O(C($CF_3$))$_3$]$^-$), −184.5 (br. s, 1 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]) ppm. $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 39.7 ppm (br.s , [F-

Al(O(C(C$F_3$))$_3$]$^-$ & [$\mu$F-{*Al*(OC(C$F_3$)$_3$)$_3$}$_2$]$^-$). IR (128 scans, ZnSe ATR, corrected): $\tilde{\nu}$/cm$^{-1}$ (intensity) = 3698 (vvw) 3610 (vvw) 1500 (vw) 1353 (vw) 1299 (mw) 1242 (vvs) 1213 (vvs) 1176 (s) 1093 (vvw) 1062 (vvw) 1021 (vvw) 969 (vvs) 861 (vw) 842 (vw) 796 (vvw) 755 (mw) 725 (vvs) 680 (w) 641 (vw) 564 (vw)

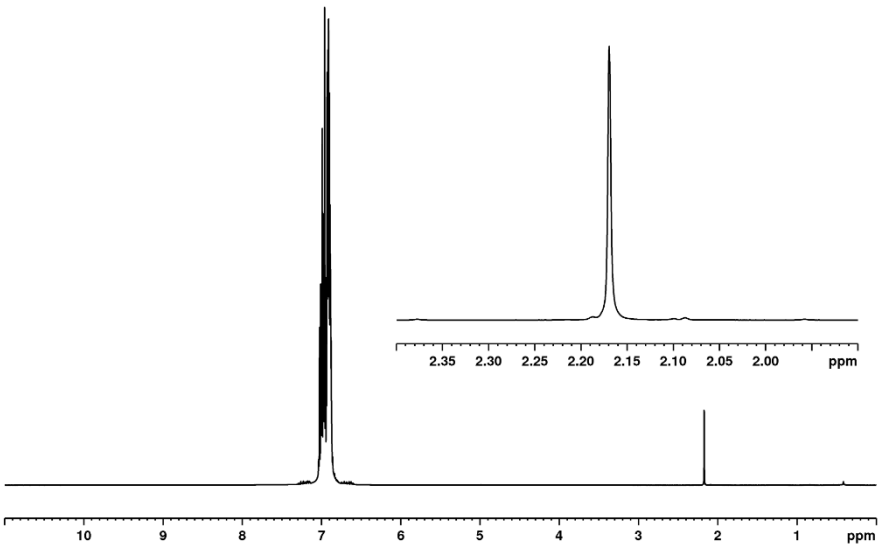


*Figure S- 15 $^1$H-NMR (300.18 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ba(HMB)(oDFB)$_3${*f*-al}][*al*-f-al] **4**.*

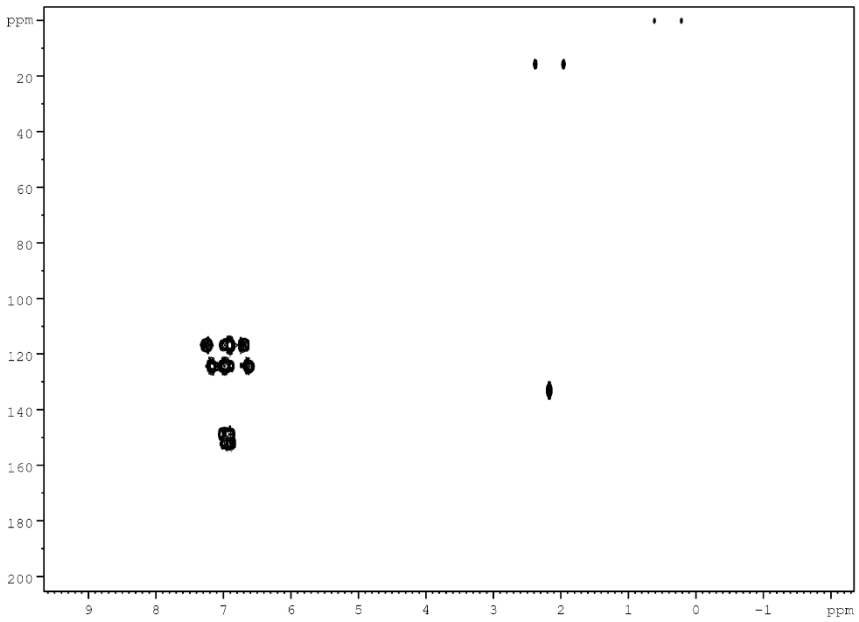


*Figure S- 16 $^{1}H$-$^{13}C$ (hmbc)NMR (75.48 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ba(HMB)(oDFB)$_3${f-al}][al-f-al]* ***4***

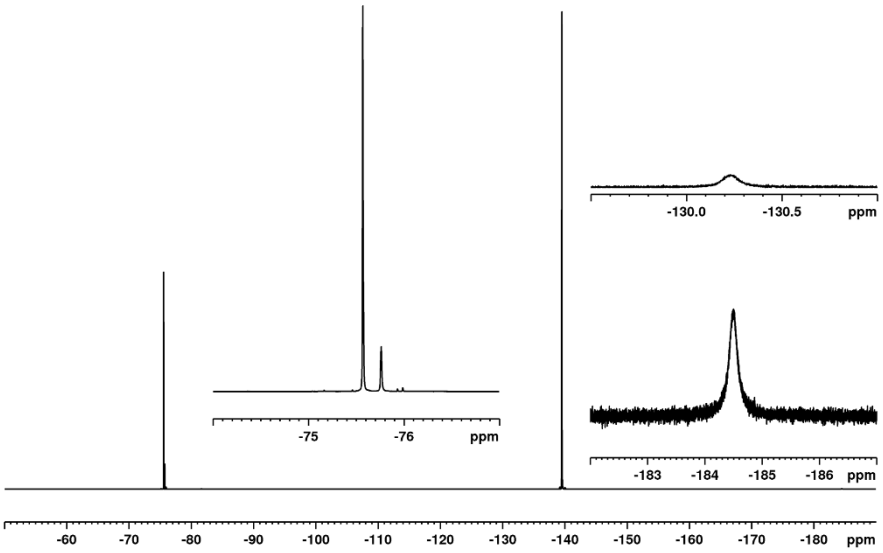


*Figure S- 17 $^{19}F$-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ba(HMB)(oDFB)$_3${f-al}][al-f-al]* ***4***

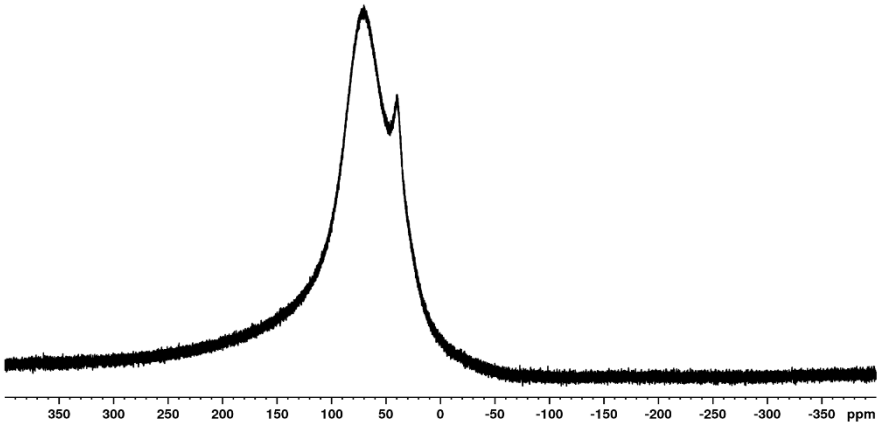


*Figure S- 18 $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4***

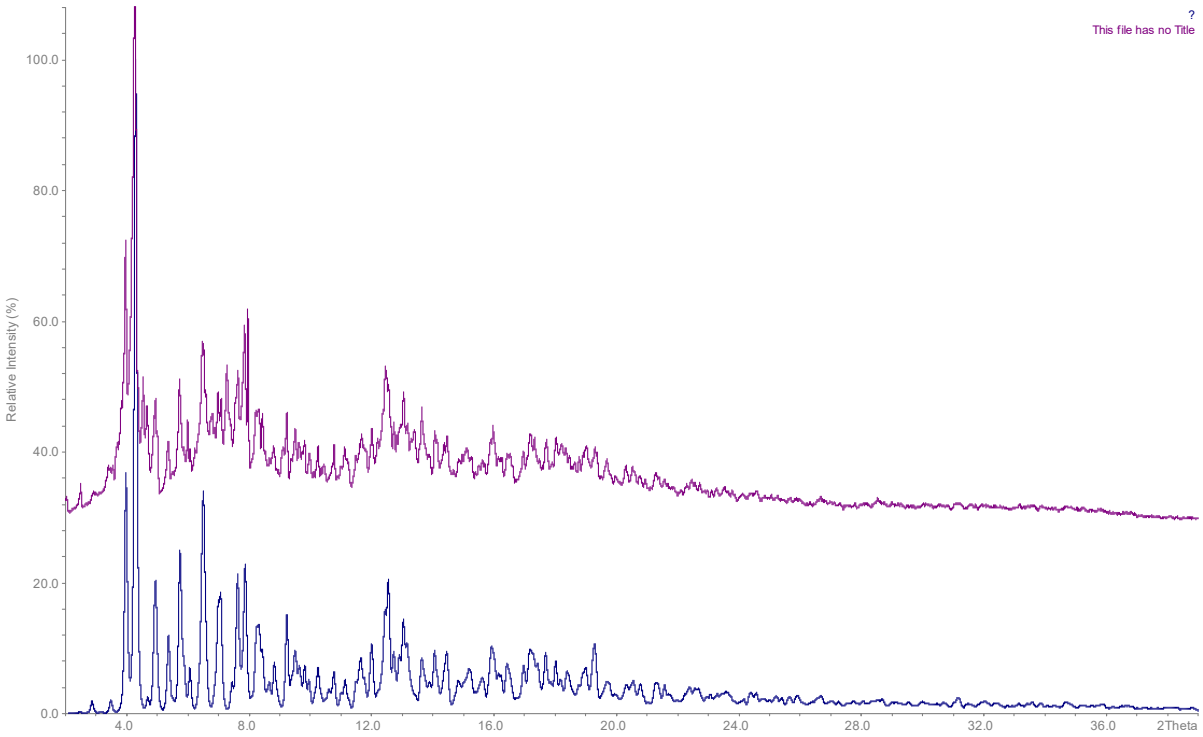


*Figure S- 19 Powder diffractogram of bulk material containing [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** at 100(10) K. (purple trace) simulated diffractogram of the single-crystal X-ray analysis (blue trace), measured at 100(2) K .*

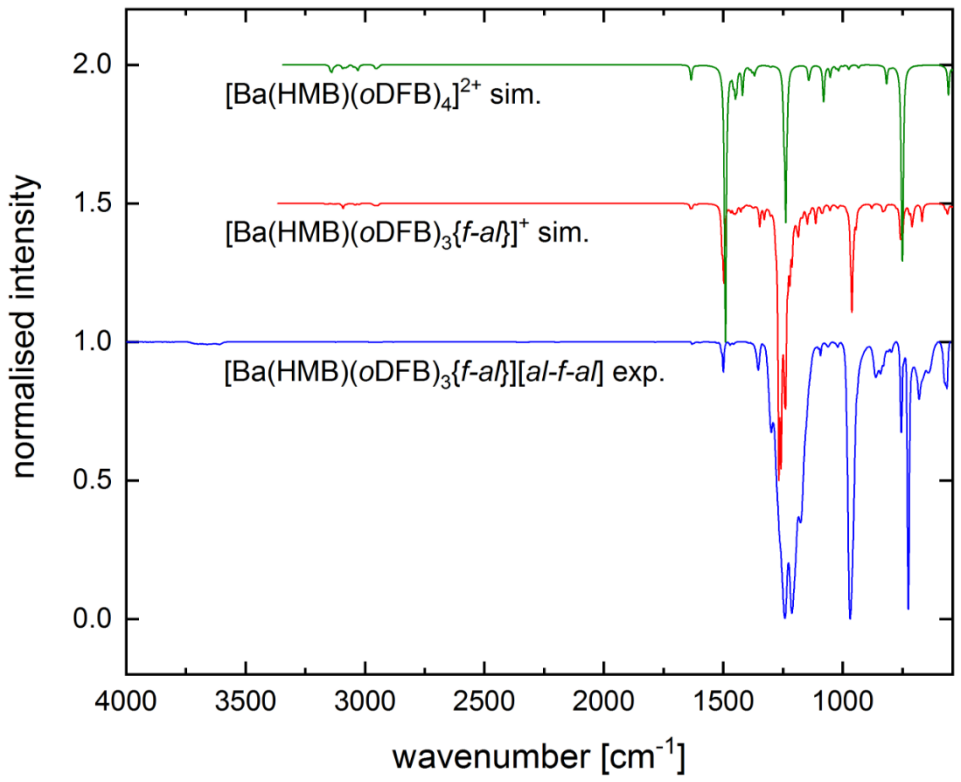


*Figure S- 20 Experimental IR data on bulk material containing [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** (blue). Simulated IR data on [Ba(HMB)(oDFB)$_4$]$^{2+}$ (green) & [Ba(HMB)(oDFB)$_3${f-al}]$^+$ (red) (BP86/def2-def-SV(P)/D3(BJ) ). IR (ZnSe ATR-corrected, 128 scans).*

### S-1.8 Synthesis of [Sr(HMB)(oDFB)$_4$][*al-f-al*] **6** and serendipitous finding of [Sr(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **5**

Ag[*al-f-al*] (0.496 g, 0.272 mmol) and $C_6Me_6$ (0.044 g, 0.270 mmol, 0.99 eq.) were dissolved in *o*-DFB (3 ml). Iodine (0.034 g, 0.135 mmol, 0.49 eq.) was added under positive argon flow to the stirred reaction mixture. Within five minutes the solution developed a dark intensive brown-red colour, accompanied by formation of a yellow precipitate. The reaction mixture was stirred for 2 h at ambient temperature and the supernatant filtered onto Strontium clippings (0.047 g, 0.541 mmol, 2 eq.) and stirred for 8 d at ambient temperature. After 12 h lightening of the dark red color of the reaction mixture was observed. After 4 d only a faint red colour was observable. The reaction mixture was filtered and layered with *n*-pentane and left to crystallize at ambient temperature to yield the title compound **6** as yellowish blocks together with minor product **5** in form of colourless needles (0.374 g, 0.136 mmol, 75 % crystalline yield calculated for **6**).

$^1$H-NMR (300.18 MHz, 1,2-$C_6H_4F_2$, 298 K) δ =2.17 (shoulder), 2.14 ( s, 18 H, ($C_6(CH_3)_6$), 2.09 (s), 2.07 (s) ppm. $^{13}$C-NMR (75.48 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 15.6 (s, ($C_6(CH_3)_6$)), 133.0 ppm (s, ($C_6(CH_3)_6$)). $^{19}$F-NMR

(282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.6 (s, 54 F, [$\mu$F-{Al(OC(C*F*$_3$)$_3$}$_2$]), -75.9 (s), -75.9 (s, 27 F, [F-Al(O(C(C*F*$_3$))$_3$]$^-$, ratio [$\mu$F-{Al(OC(CF$_3$)$_3$}$_3$}$_2$] : [F-Al(O(C(CF$_3$))$_3$]$^-$; 1 : 0.07), −184.5 (br. s, 1 F, [$\mu$F-{Al(OC(C*F*$_3$)$_3$}$_3$}$_2$]) ppm. $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 39.7 ppm (shoulder, [$\mu$F-{*Al*(OC(CF$_3$)$_3$}$_3$}$_2$]$^-$). IR (128 scans, ZnSe ATR, corrected): $\tilde{\nu}$/cm$^{-1}$ (intensity) = 1634 (vvw) 1498 (w) 1473 (vvw) 1354 (vw) 1300 (mw) 1267 (ms) 1240 (vvs) 1212 (vvs) 1176 (ms) 1091 (vvw) 1019 (vvw) 972 (vvs) 863 (vw) 841 (vvw) 828 (vvw) 754 (ms) 726 (vvs) 662 (vw) 634 (vw) 563 (w)

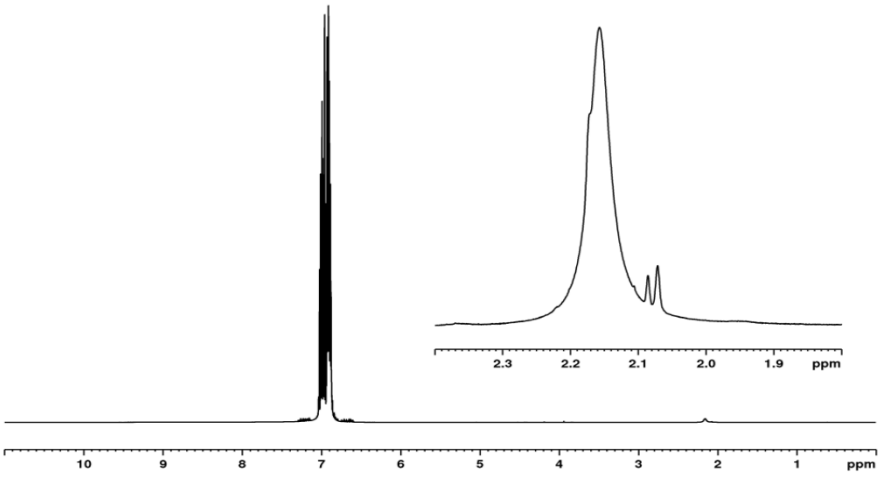


*Figure S- 21: $^1$H-NMR (300.18 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Sr(HMB)(oDFB)$_4$][*al-f-al*]$_2$ **6**.*

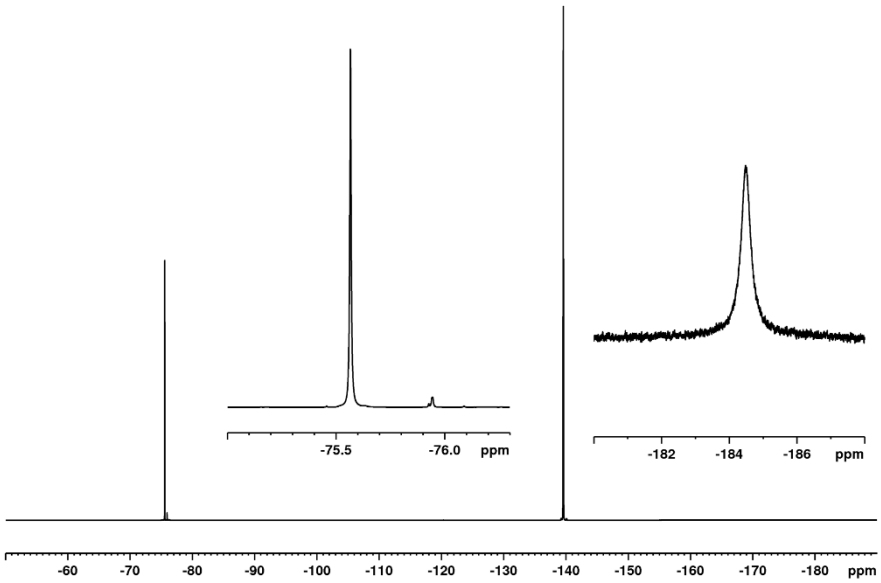


*Figure S- 22 $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Sr(HMB)(oDFB)$_4$][*al-f-al*]$_2$ **6**.*

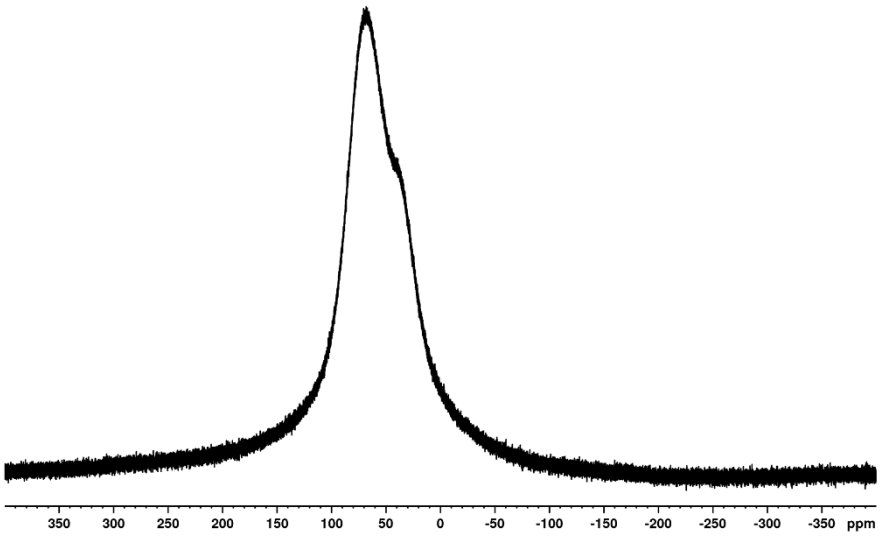


*Figure S- 23 $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) of isolated crystals containing [Sr(HMB)(oDFB)$_4$][al-f-al]$_2$* ***6****.*

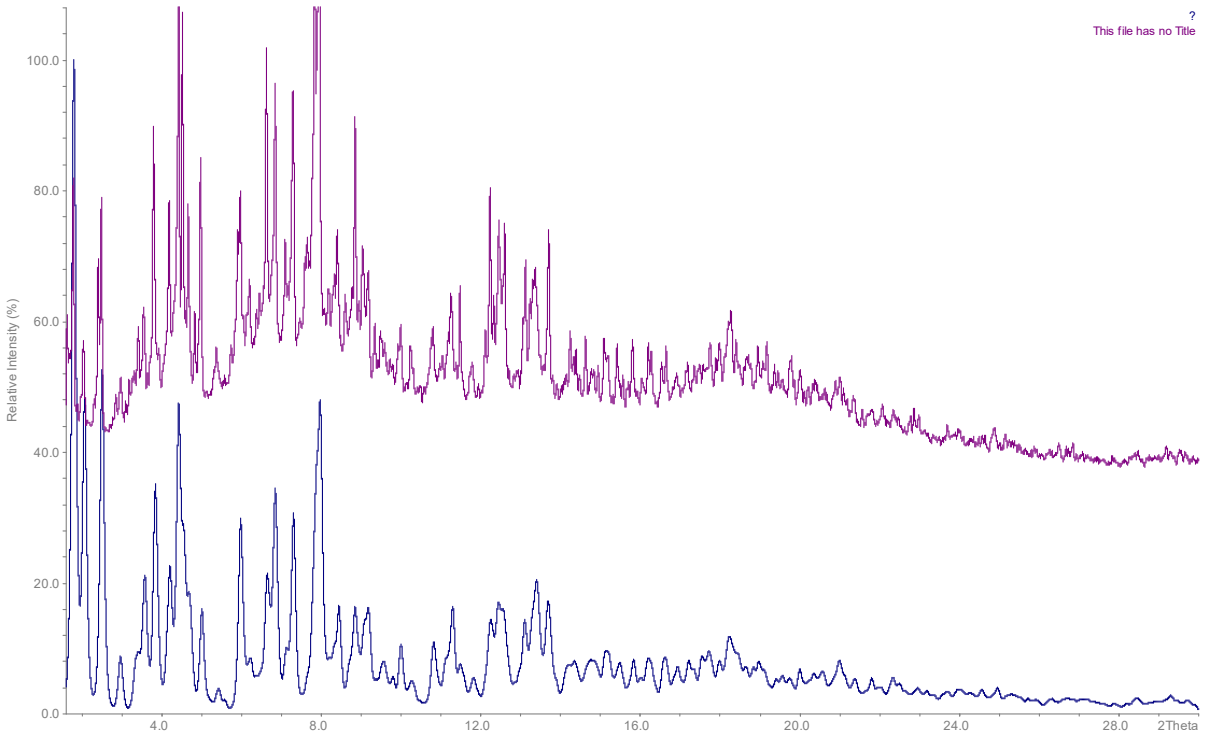


*Figure S- 24 Powder diffractogram of bulk material containing [Sr(HMB)(oDFB)$_4$][al-f-al]$_2$* ***6*** *& [Sr(HMB)(oDFB)$_3${f-al}][al-f-al]* ***5*** *at 100(10) K. (purple trace) simulated diffractogram of the single-crystal X-ray analysis of* ***6*** *(blue trace), measured at 100(2) K . Note that reflex positions are well described by simulation while reflex intensities do not reproduce found experimental pattern, possibly due to heavy disorder oDFB solvent molecules in a solvent channel found in determined single-crystal X-ray analysis of* ***6****.*

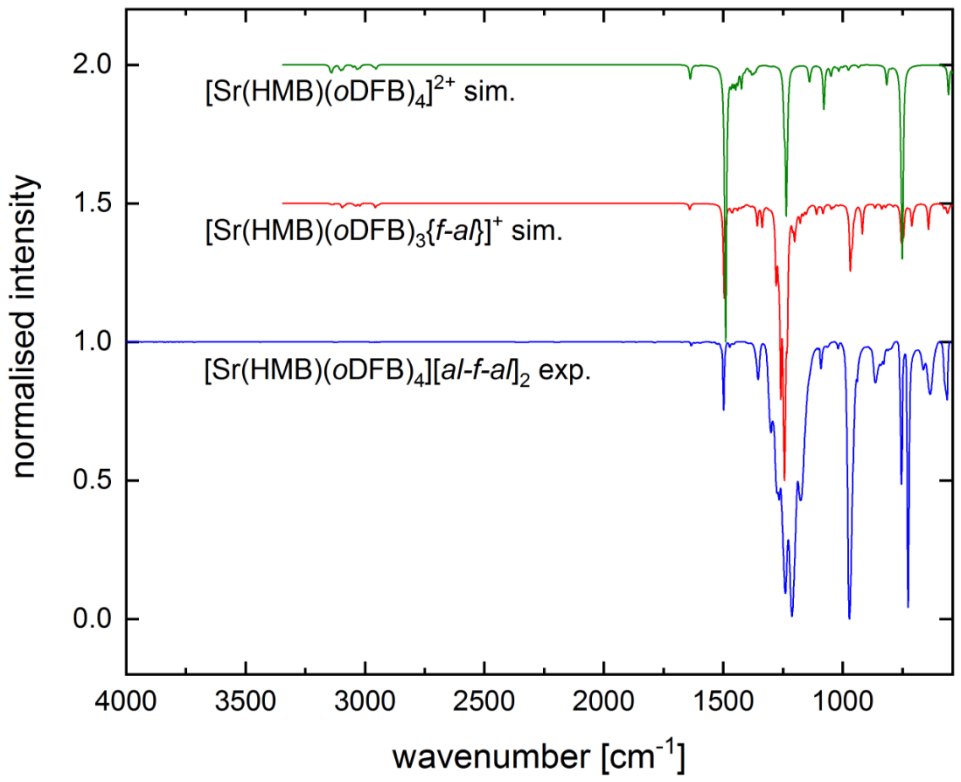


*Figure S- 25 Experimental IR data on bulk material containing [Sr(HMB)(oDFB)$_4$][al-f-al]$_2$ **6** (blue). Simulated IR data on [Sr(HMB)(oDFB)$_4$]$^{2+}$ (green) & [Sr(HMB)(oDFB)$_3${f-al}]$^+$ (red) (BP86/def2-def-SV(P)/D3(BJ) ). IR (ZnSe ATR-corrected, 128 scans).*

## S-1.9 Reaction between [Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4** and TMS-F-Al(OR$^F$)$_3$.

[Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4** (80 mg, 0.028 mmol) and TMS-F-Al(OR$^F$)$_3$ (23 mg, 0.028 mmol, 1.0 eq.) were weighed into an NMR Tube equipped with a J.Young valve and dissolved in *o*DFB (0.8 ml).

Presence of TMS-F-Al(OR$^F$)$_3$ besides [Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4** with no significant change of ratio between [*al-f-al*]$^-$ and Barium coordinated [*f-al*]$^-$. Abstraction of [*f-al*]$^-$ and shift to more dicationic Barium complexes was therefore deemed unsuccessful.

$^1$H-NMR (300.18 MHz, 1,2-$C_6H_4F_2$, 298 K) δ =2.16 ( s, 18 H, ($C_6(CH_3)_6$), 0.59 (s, Si$CH_x$), 0.54 (s, Si$CH_x$) ppm. $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.6 (s, 54 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]), -75.6 (s), -75.8 (s, 27 F, [Ba(HMB)(oDFB)$_3${F-Al(O(C($CF_3$))$_3$}]$^+$, ratio [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$] : [Ba(HMB)(oDFB)$_3${F-Al(O(C($CF_3$))$_3$}]$^+$; 1 : 3.2), −76,0 (s, 27 F, TMS-F-Al(OR$^F$)$_3$), −130.4 (s, 1 F, [Ba(HMB)(oDFB)$_3${*F*-Al(O(C($CF_3$))$_3$}]$^+$), −156.4 (s, 1 F, [*F*-Al(O(C($CF_3$))$_3$]$^-$),−184.5 (br. s, 1 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]) ppm. $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 39.3 ppm (br. s, [F-*Al*(O(C($CF_3$))$_3$]$^-$ & [$\mu$F-{*Al*(OC($CF_3$)$_3$)$_3$}$_2$]$^-$ & TMS-F-Al(OR$^F$)$_3$).

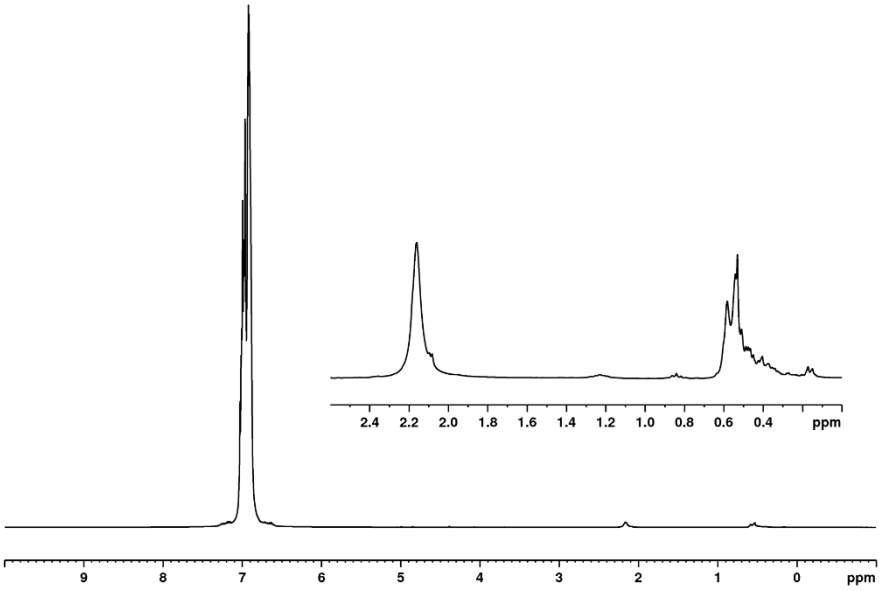


*Figure S- 26 $^{1}$H-NMR (300.18 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and TMS-F-Al(OR$^F$)$_3$.*

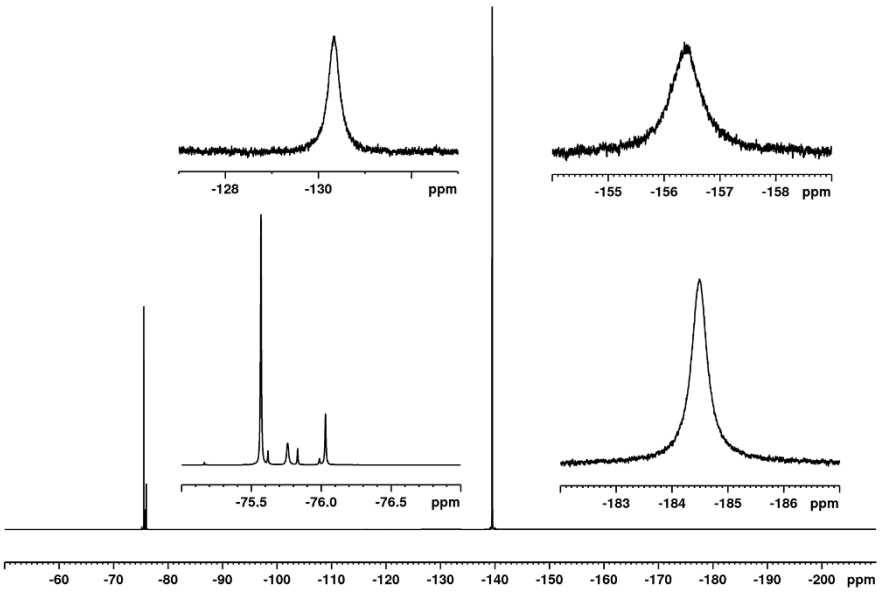


*Figure S- 27 $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and TMS-F-Al(OR$^F$)$_3$.*

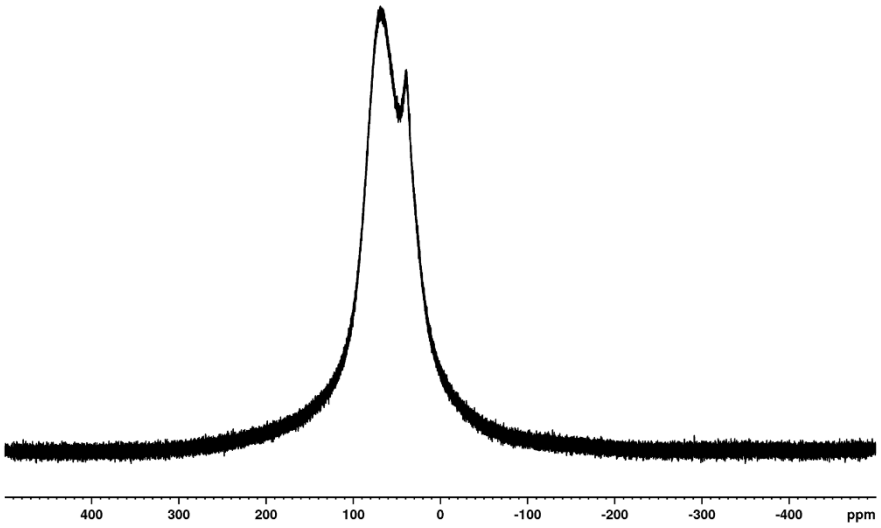


*Figure S- 28 $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and TMS-F-Al(OR$^F$)$_3$.*

## S-1.10 Reaction between [Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4** and $POEt_3$.

[Ba(HMB)(oDFB)$_3${*f-al*}][*al-f-al*] **4** (110 mg, 0.038 mmol) and $POEt_3$ (5 mg, 0.038 mmol, 1.0 eq.) were weighed into an NMR Tube equipped with a J.Young valve and dissolved in *o*DFB (0.8 ml). Sample was collected directly and again after 14 days.

Substantial change in NMR spectra between the two measurements was detected. The fluoride-bridged anion has completely vanished after 14 days. $^1$H-NMR resonance corresponding to HMB has sharpened compared to collected samples of neat **4** suggesting difference in coordination environment. $^{31}$P-NMR resonances have changed in composition and ratio and could not be further determined. Splitting of [*al-f-al*]$^-$ by nucleophilic attack of $POEt_3$ seems likely, as it has been observed before with other σ-Donor ligands, to form respective $POEt_3$ Al(OR$^F$)$_3$ adduct. Similar resonances have been found when reacting TMS-F-Al(OR$^F$)$_3$ with 1 eq. of $POEt_3$ as shown below.

$^1$H-NMR (200.13 MHz, 1,2-$C_6H_4F_2$, 298 K) δ =2.11 ( s, 18 H, ($C_6(CH_3)_6$), 2.02 (m, 3H, -$CH_2CH_3$), 1.24 (m, -$CH_2CH_3$) ppm. $^{19}$F-NMR (188.31 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.6 (s, 54 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]), -75.6 (s), -75.7 (s), -75.8 (s, 27 F, [Ba(HMB)(oDFB)$_3${F-Al(O(C($CF_3$))$_3$}]$^+$), −152.6 (s, 1 F, [*F-*

$Al(O(C(CF_3))_3]^-$),−184.5 (br. s, 1 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]) ppm. $^{31}$P-NMR (81.01 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 85.5 (s), 82.6 (s), 78.2 (s), 64.5 (s) ppm.

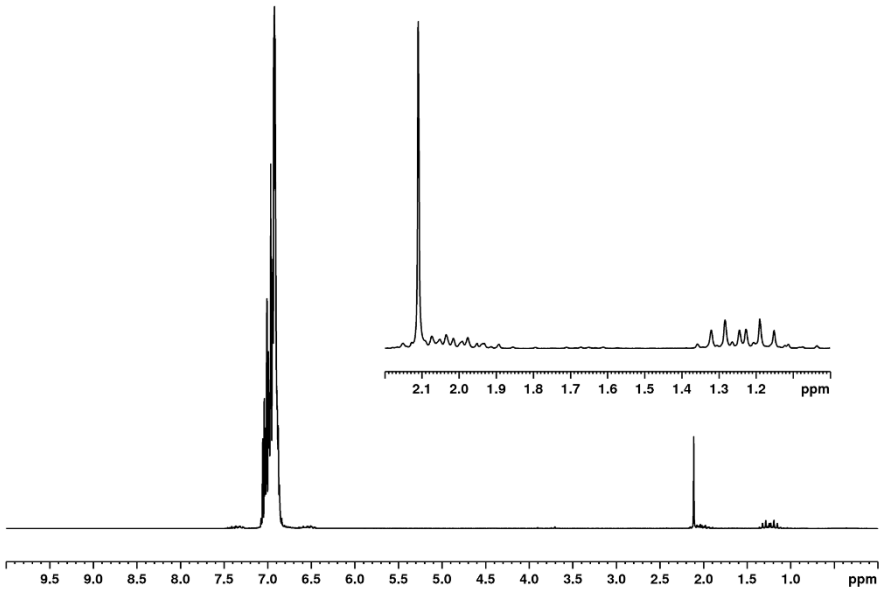


*Figure S- 29 $^1$H-NMR (200.13 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${*f*-al}][*al*-*f*-*al*] **4** and $POEt_3$.*

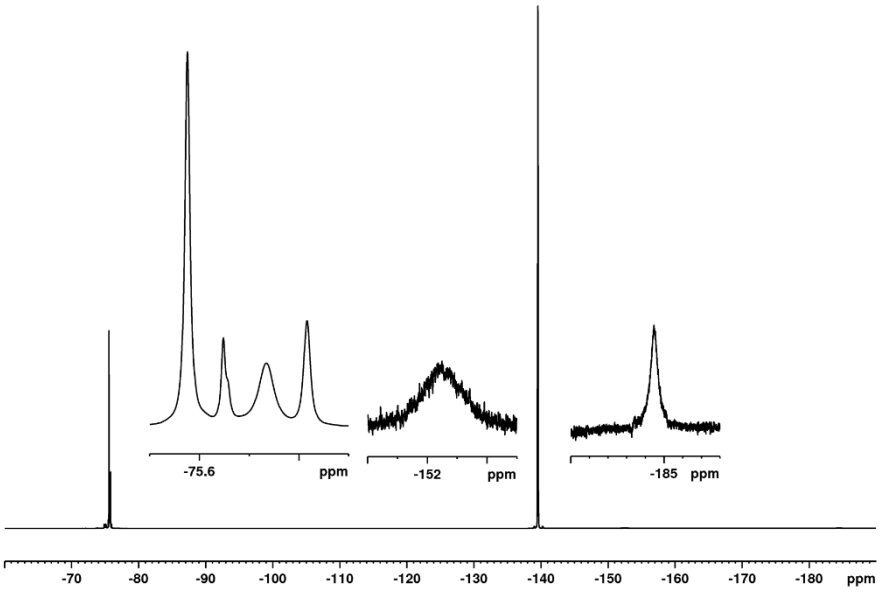


*Figure S- 30 $^1$H-NMR (188.31 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${*f*-al}][*al*-*f*-*al*] **4** and $POEt_3$.*

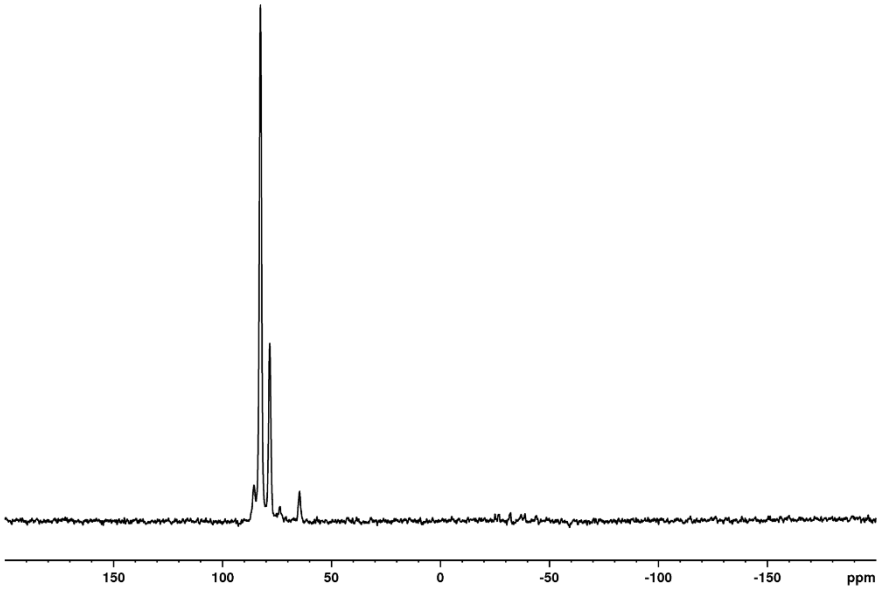


*Figure S- 31 $^{31}$P-NMR (81.01 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$.*

$^1$H-NMR (400.17 MHz, 1,2-$C_6H_4F_2$, 298 K) δ =2.11 ( s, 18 H, ($C_6(CH_3)_6$), 2.02 (m, 3H, -$CH_2CH_3$), 1.22 (m, -$CH_2CH_3$) ppm. $^{19}$F-NMR (376.54 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.7 (s), −75.7 (s), −75.8 (s, 27 F, [F-Al(O(C($CF_3$))$_3$}]$^-$), −135.2 (s, 1 F, [*F*-Al(O(C($CF_3$))$_3$) ppm. $^{31}$P-NMR (161.99 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 85.5 (s), 82.7 (s), 82.5 (s), 78.2 (s) ppm.

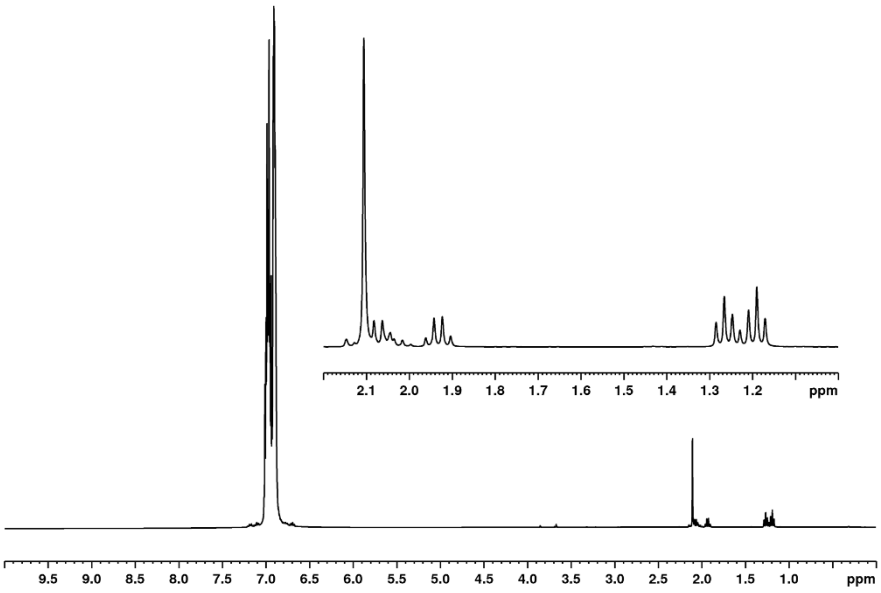


*Figure S- 32 $^1$H-NMR (400.17 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$. Recollected after 14 days.*

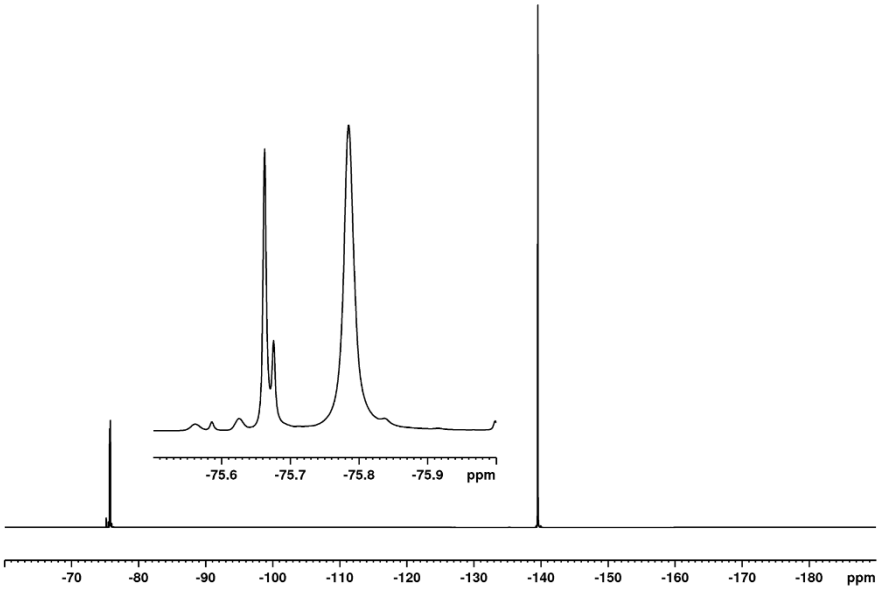


*Figure S- 33 $^{19}$F-NMR (376.54 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$. Recollected after 14 days.*

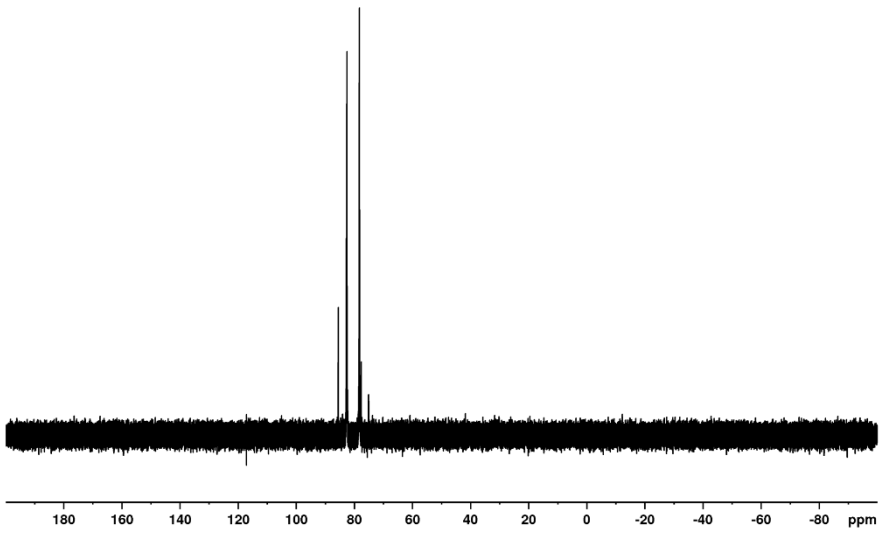


*Figure S- 34 $^{31}$P-NMR (161.99 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$. Recollected after 14 days.*

## S-1.11 Reaction between $POEt_3$ and TMS-F-Al($OR^F$)$_3$.

TMS-F-Al($OR^F$)$_3$ (61 mg, 0.075 mmol) and $POEt_3$ (10 mg, 0.075 mmol, 1.0 eq.) were weighed into an NMR Tube equipped with a J.Young valve and dissolved in *o*DFB (0.8 ml).

$^{1}$H-NMR (300.18 MHz, 1,2-$C_6H_4F_2$, 298 K) δ = 1.94 (m, 3H, -$CH_2CH_3$), 1.19 (m, -$CH_2CH_3$) ppm. 0.17 (d, 9 H, Si($CH_3$)-F-Al($OR^F$)$_3$), 0.1 (s, Si$CH_x$) ppm. $^{19}$F-NMR (282.45 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = −75.6 (s, 27 F, TMS-F-Al(O(C($CF_3$))$_3$), −75.6 (s, 54 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]), −157.7 (dec, 1 F, TMS-*F*-Al(O(C($CF_3$))$_3$), −183.5 (br. s, 1 F, [$\mu$F-{Al(OC($CF_3$)$_3$)$_3$}$_2$]) ppm. $^{27}$Al-NMR (78.22 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 41.3 (br s), 37.6 (TMS-F-Al($OR^F$)$_3$), 1.4 (br. s) ppm. $^{31}$P-NMR (121.52 MHz, 1,2-$C_6F_2H_4$, 298 K) δ = 82.7 (s), 79.63 (s), 78.3 (s), 75.4 (s), 72.4 (s) ppm.

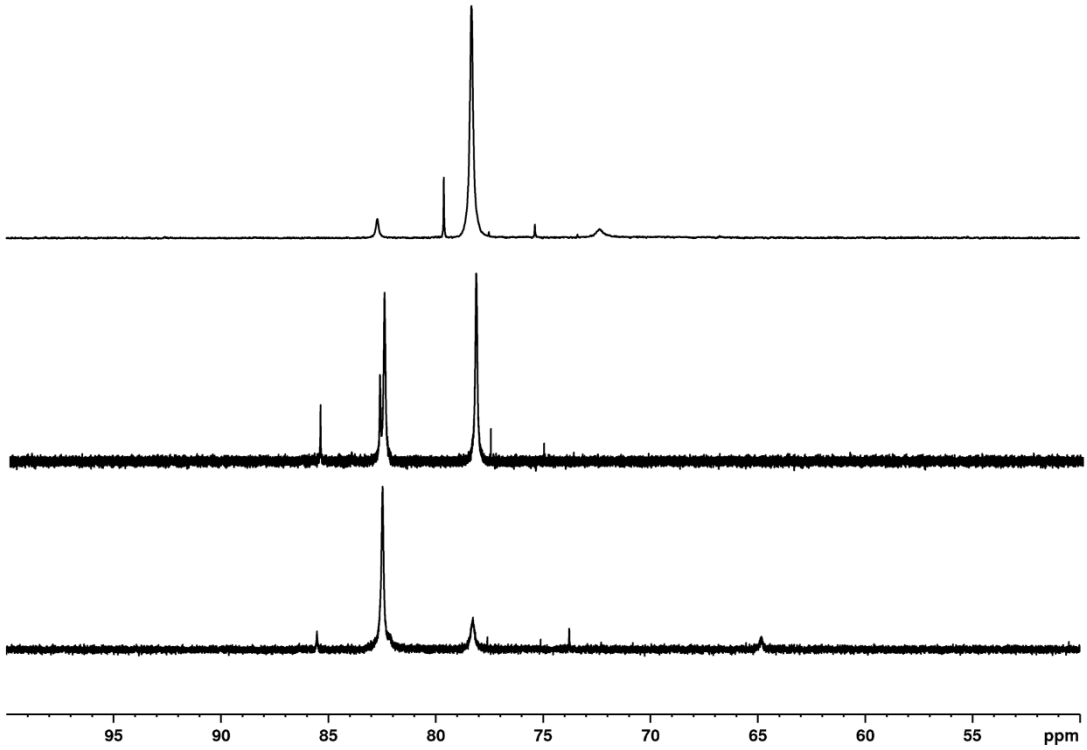


*Figure S- 35 Stacked plot of (bottom trace) $^{31}P\{^1H\}$-NMR (81.01 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$ (middle trace) $^{31}P\{^1H\}$-NMR (161.99 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between [Ba(HMB)(oDFB)$_3${f-al}][al-f-al] **4** and $POEt_3$. Recollected after 14 days.And (top trace) $^{31}P\{^1H\}$-NMR (121.52 MHz, 1,2-$C_6F_2H_4$, 298 K) of reaction between $POEt_3$ and TMS-F-Al($OR^F$)$_3$.*

## S-2 Crystallographic data

| | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Empirical formula | $C_{50}H_{22}Al_2F_{74}MgN_6O_8$ | $C_{52}H_{26}Al_2CaF_{68}O_7$ | $C_{60}H_{26}Al_3CaF_{87}O_9$ | $C_{66}H_{30}Al_3BaF_{89}O_9$ |
| Formula weight | 2319.00 | 2148.77 | 2664.83 | 2876.18 |
| Temperature/K | 100(2) | 100(2) | 100(2) | 100(2) |
| Crystal system | triclinic | monoclinic | monoclinic | monoclinic |
| Space group | $P1$ | $P2_1$ | $P2_1/c$ | *Pc* |
| a/Å | 14.3953(4) | 17.765(6) | 23.4290(15) | 28.173(3) |
| b/Å | 18.2606(5) | 20.654(7) | 18.9075(12) | 16.4313(17) |
| c/Å | 25.8315(7) | 20.031(8) | 22.4874(14) | 20.453(2) |
| α/° | 73.7840(10) | 90 | 90 | 90 |
| β/° | 74.370(2) | 93.018(14) | 118.270(2) | 90.107(4) |
| γ/° | 66.8210(10) | 90 | 90 | 90 |
| Volume/Å$^3$ | 5895.1(3) | 7339(5) | 8773.4(10) | 9467.8(18) |
| Z | 3 | 4 | 4 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.960 | 1.945 | 2.017 | 2.018 |
| μ/mm$^{-1}$ | 0.275 | 0.332 | 0.340 | 0.676 |
| F(000) | 3396 | 4208 | 5200 | 5576 |
| Crystal size/mm$^3$ | 0.25×0.18×0.1 | 0.35×0.27×0.23 | 0.35×0.3×0.28 | 0.3×0.27×0.17 |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073) |
| 2Θ range /° | 1.67 to 52.70 | 2.04 to 52.88 | 1.97 to 55.97 | 1.45 to 54.16 |
| Index ranges | -17 ≤ h ≤ 17, -22 ≤ k ≤ 22, -32 ≤ l ≤ 32 | twinned | -30 ≤ h ≤ 30, -24 ≤ k ≤ 24, -29 ≤ l ≤ 29 | -36 ≤ h ≤ 36; -20 ≤ k ≤ 21; -26 ≤ l ≤ 26 |
| Reflections collected | 110248 | 25915 | 267897 | 241837 |
| Independent reflections | 43456, [$R_{int}$ = 0.0327, $R_{sigma}$ = 0.0506] | 25915 [$R_{int}$ = 0.0615, $R_{sigma}$ = 0.0667] | 21106, [$R_{int}$ = 0.1172, $R_{sigma}$ = 0.0406] | 41457 [$R_{int}$ = 0.0426, $R_{sigma}$ = 0.0340] |
| Data/restraints/parameters | 43456/160301/5086 | 25915/35125/2475 | 21106/30760/2070 | 41457/48470/3041 |
| Goodness-of-fit on F$^2$ | 1.040 | 1.058 | 1.029 | 0.942 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0511, w$R_2$ = 0.1185 | $R_1$ = 0.0863, w$R_2$ = 0.2002 | $R_1$ = 0.0556, w$R_2$ = 0.1526 | $R_1$ = 0.0323, w$R_2$ = 0.0751 |
| Final R indexes [all data] | $R_1$ = 0.0722, w$R_2$ = 0.1294 | $R_1$ = 0.1221, w$R_2$ = 0.2190 | $R_1$ = 0.0769, w$R_2$ = 0.1664 | $R_1$ = 0.0355, w$R_2$ = 0.0768 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.96/-0.53 | 1.21/-0.70 | 0.77/-0.59 | 0.78/-0.45 |
| CCDC ref. | 1969782 | 1969780 | 1969779 | 1969777 |

| | 5 | 6 | 7 | InHMB Al-F-Al |
|---|---|---|---|---|
| Empirical formula | $C_{66}H_{30}Al_3F_{89}O_9Sr$ | $C_{84}H_{34}Al_4F_{118}O_{12}Sr$ | $C_{84}H_{34}Al_4CaF_{118}O_{12}$ | $C_{36}H_{18}Al_2F_{55}InO_6$ |
| Formula weight | 2826.46 | 3672.65 | 3625.11 | 1760.28 |
| Temperature/K | 100(2) | 100(2) | 100(2) | 100(2) |
| Crystal system | triclinic | triclinic | triclinic | triclinic |
| Space group | $P\bar{1}$ | $P\bar{1}$ | $P\bar{1}$ | $P\bar{1}$ |
| a/Å | 13.5412(9) | 13.8661(5) | 13.9542(7) | 10.6319(4) |
| b/Å | 25.3825(17) | 20.2883(8) | 20.3286(11) | 22.3961(8) |
| c/Å | 27.3385(17) | 23.0336(9) | 22.9128(12) | 24.4869(9) |
| α/° | 90.017(2) | 80.0310(10) | 80.085(2) | 79.1440(10) |
| β/° | 90.111(2) | 85.9850(10) | 84.743(2) | 79.6960(10) |
| γ/° | 92.474(2) | 79.9420(10) | 80.239(2) | 77.7590(10) |
| Volume/Å$^3$ | 9387.7(11) | 6278.6(4) | 6296.8(6) | 5537.2(4) |
| Z | 4 | 2 | 2 | 4 |
| $\rho_{calc}$g/cm$^3$ | 2.000 | 1.943 | 1.912 | 2.112 |
| μ/mm$^{-1}$ | 0.833 | 0.687 | 0.307 | 0.689 |
| F(000) | 5504 | 3572 | 3536 | 3408 |
| Crystal size/mm$^3$ | 0.3×0.18×0.14 | 0.29×0.27×0.21 | 0.4×0.35×0.27 | 0.25×0.11×0.07 |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073 Å) | Mo$K_\alpha$ (λ=0.71073 Å) |
| 2Θ range /° | 4.47 to 55.80 | 1.80 to 55.96 | 1.81 to 54.19 | 1.71 to 58.06 |
| Index ranges | -17 ≤ h ≤ 17, -33 ≤ k ≤ 33, -35 ≤ l ≤ 35 | -18 ≤ h ≤ 18, -26 ≤ k ≤ 26, -30 ≤ l ≤ 30 | -17 ≤ h ≤ 17, -26 ≤ k ≤ 26, -29 ≤ l ≤ 29 | -14 ≤ h ≤ 14, -30 ≤ k ≤ 30, -33 ≤ l ≤ 33 |
| Reflections collected | 167981 | 283181 | 221765 | 152697 |
| Independent reflections | 44723 [$R_{int}$ = 0.0624, $R_{sigma}$ = 0.0660] | 30200 [$R_{int}$ = 0.0462, $R_{sigma}$ = 0.0268] | 27716 [$R_{int}$ = 0.0360, $R_{sigma}$ = 0.0221] | 29472 [$R_{int}$ = 0.0536, $R_{sigma}$ = 0.0474] |
| Data/restraints/parameters | 44723/134045/4542 | 30200/44834/2616 | 27716/55435/2874 | 29472/35187/2194 |
| Goodness-of-fit on F$^2$ | 1.026 | 1.008 | 1.031 | 1.049 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0543, w$R_2$ = 0.1357 | $R_1$ = 0.0376, w$R_2$ = 0.0819 | $R_1$ = 0.0519, w$R_2$ = 0.1288 | $R_1$ = 0.0496, w$R_2$ = 0.1162 |
| Final R indexes [all data] | $R_1$ = 0.0746, w$R_2$ = 0.1484 | $R_1$ = 0.0588, w$R_2$ = 0.0907 | $R_1$ = 0.0686, w$R_2$ = 0.1407 | $R_1$ = 0.0780, w$R_2$ = 0.1295 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.82/-0.83 | 0.65/-0.55 | 0.89/-0.48 | 1.22/-0.91 |
| CCDC ref. | 1969784 | 1969783 | 1969778 | 1969781 |

*Table S 1 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for [Mg(MeCN)$_6$][Al(OR$^F$)$_4$]$_2$ **1**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{ij}$ tensor.*

| Atom | *x* | *y* | *z* | $U_{eq}$ |
|---|---|---|---|---|
| Al01 | 0.26289(13) | 0.32665(10) | 0.74561(7) | 0.0198(4) |
| Al02 | 0.59013(14) | -0.03166(11) | 0.39871(7) | 0.0225(4) |
| Al03 | 0.97191(13) | -0.04456(10) | 0.70773(7) | 0.0198(4) |
| Al04 | 0.96147(13) | 0.63078(11) | 0.06903(7) | 0.0216(4) |
| Al05 | 0.63790(13) | 1.27624(10) | 0.05182(7) | 0.0191(4) |
| Al06 | 1.31091(14) | -0.38312(11) | 0.38198(7) | 0.0219(4) |
| O1_1 | 0.6792(3) | 1.3413(2) | -0.00375(16) | 0.0255(9) |
| C1_1 | 0.6532(5) | 1.4086(3) | -0.0433(2) | 0.0269(13) |
| C2_1 | 0.7543(5) | 1.4183(4) | -0.0789(3) | 0.0400(16) |
| F1_1 | 0.7977(3) | 1.3661(3) | -0.11286(17) | 0.0533(11) |
| F2_1 | 0.7396(4) | 1.4931(3) | -0.1101(2) | 0.0618(14) |
| F3_1 | 0.8238(3) | 1.4029(3) | -0.04873(19) | 0.0557(12) |
| C3_1 | 0.5900(6) | 1.4841(4) | -0.0171(3) | 0.0472(18) |
| F4_1 | 0.5181(4) | 1.4711(3) | 0.0236(2) | 0.0669(14) |
| F5_1 | 0.6520(4) | 1.5057(3) | 0.0024(2) | 0.0682(15) |
| F6_1 | 0.5464(4) | 1.5489(3) | -0.0539(2) | 0.0658(14) |
| C4_1 | 0.5909(5) | 1.3993(4) | -0.0797(3) | 0.0367(15) |
| F7_1 | 0.4931(3) | 1.4140(3) | -0.05516(18) | 0.0534(12) |
| F8_1 | 0.5920(3) | 1.4508(3) | -0.12812(16) | 0.0497(11) |
| F9_1 | 0.6281(4) | 1.3254(3) | -0.08975(17) | 0.0503(11) |
| O1_2 | 0.7427(8) | 1.1873(7) | 0.0622(5) | 0.027(3) |
| C1_2 | 0.8231(6) | 1.1319(5) | 0.0375(3) | 0.0258(17) |
| C2_2 | 0.8996(6) | 1.1704(5) | -0.0039(3) | 0.0335(18) |
| F1_2 | 0.9095(11) | 1.2266(5) | 0.0163(6) | 0.0512(19) |
| F2_2 | 0.9942(5) | 1.1163(4) | -0.0148(3) | 0.0419(17) |
| F3_2 | 0.8683(5) | 1.2056(4) | -0.0515(2) | 0.0466(16) |
| C3_2 | 0.7872(6) | 1.0895(5) | 0.0067(3) | 0.0380(19) |
| F4_2 | 0.7430(5) | 1.0382(4) | 0.0418(3) | 0.0571(19) |
| F5_2 | 0.7181(8) | 1.1438(8) | -0.0231(5) | 0.053(2) |
| F6_2 | 0.8640(6) | 1.0446(4) | -0.0267(4) | 0.0433(18) |
| C4_2 | 0.8804(7) | 1.0676(5) | 0.0829(3) | 0.042(2) |
| F7_2 | 0.8139(11) | 1.0468(8) | 0.1254(3) | 0.061(2) |
| F8_2 | 0.9460(6) | 0.9998(5) | 0.0653(4) | 0.055(2) |
| F9_2 | 0.9351(6) | 1.0967(5) | 0.1005(3) | 0.060(2) |
| O1_4 | 0.5944(14) | 1.3143(11) | 0.1112(6) | 0.029(3) |
| C1_4 | 0.6255(7) | 1.3223(6) | 0.1538(5) | 0.030(2) |
| C2_4 | 0.5306(7) | 1.3799(6) | 0.1858(4) | 0.045(2) |
| F1_4 | 0.4668(5) | 1.3403(6) | 0.2158(3) | 0.068(2) |
| F2_4 | 0.5580(17) | 1.4081(11) | 0.2206(5) | 0.053(3) |
| F3_4 | 0.4800(8) | 1.4442(8) | 0.1526(7) | 0.068(3) |
| C3_4 | 0.7118(8) | 1.3596(6) | 0.1342(4) | 0.039(2) |
| F4_4 | 0.7826(10) | 1.3245(7) | 0.0940(4) | 0.053(3) |
| F5_4 | 0.6767(7) | 1.4379(4) | 0.1140(3) | 0.061(2) |
| F6_4 | 0.7625(15) | 1.3474(10) | 0.1741(7) | 0.043(2) |
| C4_4 | 0.6643(8) | 1.2392(6) | 0.1925(3) | 0.036(2) |
| F7_4 | 0.7619(5) | 1.1976(4) | 0.1730(2) | 0.0520(18) |
| F8_4 | 0.6620(13) | 1.2471(12) | 0.2428(6) | 0.052(3) |
| F9_4 | 0.6067(9) | 1.1951(7) | 0.1971(6) | 0.058(3) |
| O1_5 | 0.9282(3) | 0.5908(3) | 0.13731(16) | 0.0284(9) |
| C1_5 | 0.8803(5) | 0.5410(4) | 0.1736(2) | 0.0298(13) |
| C2_5 | 0.9406(5) | 0.4508(4) | 0.1687(2) | 0.0310(13) |
| F1_5 | 1.0414(3) | 0.4352(3) | 0.16008(18) | 0.0456(10) |

| | | | | |
|---|---|---|---|---|
| F2_5 | 0.9172(3) | 0.3990(2) | 0.21414(16) | 0.0455(10) |
| F3_5 | 0.9217(3) | 0.4328(2) | 0.12727(15) | 0.0389(9) |
| C3_5 | 0.7705(5) | 0.5643(4) | 0.1634(3) | 0.0360(15) |
| F4_5 | 0.7105(3) | 0.6350(3) | 0.17849(19) | 0.0525(12) |
| F5_5 | 0.7698(3) | 0.5736(3) | 0.11116(16) | 0.0444(10) |
| F6_5 | 0.7260(3) | 0.5094(2) | 0.19171(18) | 0.0461(10) |
| C4_5 | 0.8769(6) | 0.5505(4) | 0.2322(3) | 0.0433(17) |
| F7_5 | 0.8489(4) | 0.6289(3) | 0.23336(16) | 0.0560(12) |
| F8_5 | 0.8074(4) | 0.5225(3) | 0.26976(16) | 0.0565(12) |
| F9_5 | 0.9675(4) | 0.5124(3) | 0.24723(17) | 0.0544(12) |
| O1_6 | 1.0523(3) | 0.6730(3) | 0.06485(17) | 0.0269(9) |
| C1_6 | 1.1340(5) | 0.6674(4) | 0.0844(2) | 0.0318(14) |
| C2_6 | 1.1692(5) | 0.7391(4) | 0.0498(3) | 0.0420(17) |
| F1_6 | 1.1057(4) | 0.8096(3) | 0.06349(19) | 0.0522(11) |
| F2_6 | 1.2640(3) | 0.7286(3) | 0.0550(2) | 0.0612(13) |
| F3_6 | 1.1732(3) | 0.7457(3) | -0.00371(17) | 0.0492(11) |
| C3_6 | 1.2215(5) | 0.5854(4) | 0.0784(3) | 0.0432(17) |
| F4_6 | 1.1851(3) | 0.5248(2) | 0.09494(19) | 0.0472(10) |
| F5_6 | 1.2694(3) | 0.5849(3) | 0.0265(2) | 0.0543(11) |
| F6_6 | 1.2932(4) | 0.5705(3) | 0.1078(2) | 0.0657(14) |
| C4_6 | 1.1021(6) | 0.6760(5) | 0.1451(3) | 0.0438(17) |
| F7_6 | 1.0987(4) | 0.6055(3) | 0.17828(17) | 0.0565(12) |
| F8_6 | 1.1685(4) | 0.6970(3) | 0.1606(2) | 0.0638(14) |
| F9_6 | 1.0093(4) | 0.7308(3) | 0.15486(18) | 0.0541(11) |
| O1_7 | 0.2482(3) | 0.2594(3) | 0.80579(17) | 0.0350(11) |
| C1_7 | 0.1837(5) | 0.2292(4) | 0.8465(2) | 0.0308(13) |
| C2_7 | 0.2440(5) | 0.1764(4) | 0.8929(3) | 0.0412(16) |
| F1_7 | 0.2549(4) | 0.2217(3) | 0.92167(18) | 0.0590(13) |
| F2_7 | 0.1985(4) | 0.1259(3) | 0.92795(17) | 0.0549(12) |
| F3_7 | 0.3375(3) | 0.1312(3) | 0.87274(18) | 0.0561(12) |
| C3_7 | 0.1451(6) | 0.1771(4) | 0.8256(3) | 0.0462(18) |
| F4_7 | 0.1170(4) | 0.2145(3) | 0.77734(17) | 0.0530(12) |
| F5_7 | 0.2195(4) | 0.1063(3) | 0.8187(2) | 0.0658(14) |
| F6_7 | 0.0651(4) | 0.1608(3) | 0.86019(19) | 0.0636(14) |
| C4_7 | 0.0902(5) | 0.2992(4) | 0.8691(3) | 0.0427(16) |
| F7_7 | 0.0180(3) | 0.3291(3) | 0.83774(18) | 0.0524(11) |
| F8_7 | 0.0474(4) | 0.2736(3) | 0.92017(18) | 0.0664(14) |
| F9_7 | 0.1188(4) | 0.3590(3) | 0.8698(2) | 0.0598(13) |
| O1_8 | 0.2960(5) | 0.2795(3) | 0.6918(2) | 0.0652(18) |
| C1_8 | 0.3639(5) | 0.2288(4) | 0.6584(2) | 0.0388(15) |
| C2_8 | 0.3959(5) | 0.2786(4) | 0.6018(2) | 0.0363(15) |
| F1_8 | 0.3170(3) | 0.3159(3) | 0.57556(16) | 0.0448(10) |
| F2_8 | 0.4717(3) | 0.2320(3) | 0.56964(16) | 0.0480(11) |
| F3_8 | 0.4247(4) | 0.3355(3) | 0.60762(18) | 0.0604(13) |
| C3_8 | 0.4611(6) | 0.1702(5) | 0.6813(3) | 0.0499(19) |
| F4_8 | 0.4384(5) | 0.1430(3) | 0.73518(18) | 0.0684(14) |
| F5_8 | 0.5286(5) | 0.2063(4) | 0.6738(2) | 0.0783(17) |
| F6_8 | 0.5079(3) | 0.1042(3) | 0.65750(19) | 0.0545(11) |
| C4_8 | 0.3047(6) | 0.1781(4) | 0.6514(3) | 0.0497(19) |
| F7_8 | 0.2977(4) | 0.1209(3) | 0.6961(2) | 0.0613(13) |
| F8_8 | 0.3462(4) | 0.1435(3) | 0.6088(2) | 0.0594(13) |
| F9_8 | 0.2075(4) | 0.2239(3) | 0.6442(2) | 0.0703(15) |
| O1_9 | 0.3559(5) | 0.3621(4) | 0.7443(3) | 0.0634(18) |
| C1_9 | 0.4130(5) | 0.3809(4) | 0.7685(3) | 0.0356(15) |
| C2_9 | 0.5003(6) | 0.3972(5) | 0.7219(3) | 0.058(2) |

| | | | | |
|---|---|---|---|---|
| F1_9 | 0.5702(4) | 0.3290(4) | 0.7074(2) | 0.0833(17) |
| F2_9 | 0.5512(4) | 0.4336(4) | 0.7346(3) | 0.091(2) |
| F3_9 | 0.4637(4) | 0.4442(3) | 0.6768(2) | 0.0666(14) |
| C3_9 | 0.3526(8) | 0.4568(6) | 0.7926(4) | 0.075(3) |
| F4_9 | 0.2617(5) | 0.4517(5) | 0.8206(3) | 0.117(3) |
| F5_9 | 0.3368(5) | 0.5239(3) | 0.7530(3) | 0.0821(17) |
| F6_9 | 0.4019(7) | 0.4647(4) | 0.8263(3) | 0.123(3) |
| C4_9 | 0.4601(6) | 0.3086(5) | 0.8126(3) | 0.0466(18) |
| F7_9 | 0.3928(4) | 0.3071(4) | 0.85960(19) | 0.0715(15) |
| F8_9 | 0.5449(3) | 0.3117(3) | 0.8227(2) | 0.0600(13) |
| F9_9 | 0.4887(4) | 0.2384(3) | 0.7975(2) | 0.0657(14) |
| O1_10 | 1.3552(4) | -0.3218(3) | 0.32571(18) | 0.0398(12) |
| C1_10 | 1.4023(5) | -0.3106(4) | 0.2725(2) | 0.0335(14) |
| C2_10 | 1.4420(5) | -0.3880(4) | 0.2483(3) | 0.0377(15) |
| F1_10 | 1.3655(4) | -0.4016(3) | 0.23693(19) | 0.0566(12) |
| F2_10 | 1.5117(3) | -0.3851(3) | 0.20281(16) | 0.0486(11) |
| F3_10 | 1.4837(4) | -0.4525(2) | 0.28465(17) | 0.0510(11) |
| C3_10 | 1.4921(6) | -0.2824(5) | 0.2682(3) | 0.0521(19) |
| F4_10 | 1.4669(4) | -0.2289(3) | 0.2988(2) | 0.0791(18) |
| F5_10 | 1.5723(4) | -0.3458(3) | 0.2849(2) | 0.0649(13) |
| F6_10 | 1.5232(4) | -0.2483(3) | 0.2166(2) | 0.0704(15) |
| C4_10 | 1.3235(7) | -0.2428(5) | 0.2384(3) | 0.064(2) |
| F7_10 | 1.3096(5) | -0.1703(3) | 0.2467(2) | 0.0853(19) |
| F8_10 | 1.3544(5) | -0.2418(4) | 0.18499(19) | 0.093(2) |
| F9_10 | 1.2326(4) | -0.2535(4) | 0.2531(3) | 0.0886(18) |
| O1_11 | 0.1473(7) | 0.4060(4) | 0.7411(3) | 0.0305(19) |
| C1_11 | 0.0883(6) | 0.4691(5) | 0.7080(3) | 0.0340(19) |
| C2_11 | 0.0441(6) | 0.4376(5) | 0.6729(4) | 0.044(2) |
| F1_11 | 0.0164(7) | 0.3752(4) | 0.7027(4) | 0.058(2) |
| F2_11 | -0.0377(6) | 0.4953(4) | 0.6534(3) | 0.059(2) |
| F3_11 | 0.1146(6) | 0.4125(4) | 0.6300(3) | 0.060(2) |
| C3_11 | 0.1516(7) | 0.5206(5) | 0.6697(4) | 0.048(2) |
| F4_11 | 0.1665(6) | 0.5657(5) | 0.6972(4) | 0.068(2) |
| F5_11 | 0.2433(6) | 0.4745(10) | 0.6476(5) | 0.059(2) |
| F6_11 | 0.1057(13) | 0.5720(5) | 0.6287(4) | 0.075(3) |
| C4_11 | -0.0021(6) | 0.5199(5) | 0.7453(3) | 0.043(2) |
| F7_11 | 0.0294(6) | 0.5310(5) | 0.7857(3) | 0.063(2) |
| F8_11 | -0.0508(5) | 0.5941(4) | 0.7185(3) | 0.0624(18) |
| F9_11 | -0.0711(6) | 0.4846(5) | 0.7691(3) | 0.056(2) |
| O1_13 | 1.0521(3) | -0.1398(3) | 0.73363(17) | 0.0300(10) |
| C1_13 | 1.1185(5) | -0.1843(4) | 0.7684(2) | 0.0296(13) |
| C2_13 | 1.0663(6) | -0.1739(4) | 0.8283(3) | 0.0427(16) |
| F1_13 | 1.0646(4) | -0.1053(3) | 0.83748(18) | 0.0566(12) |
| F2_13 | 1.1172(4) | -0.2343(3) | 0.86506(18) | 0.0626(13) |
| F3_13 | 0.9713(3) | -0.1734(3) | 0.83859(18) | 0.0570(12) |
| C3_13 | 1.1518(6) | -0.2748(4) | 0.7645(3) | 0.0494(18) |
| F4_13 | 1.1707(5) | -0.2815(3) | 0.7132(2) | 0.0747(16) |
| F5_13 | 1.0773(4) | -0.3046(3) | 0.7915(2) | 0.0670(14) |
| F6_13 | 1.2355(4) | -0.3202(3) | 0.7858(2) | 0.0709(15) |
| C4_13 | 1.2151(6) | -0.1594(4) | 0.7525(3) | 0.0490(18) |
| F7_13 | 1.2747(4) | -0.1844(4) | 0.7076(2) | 0.0743(15) |
| F8_13 | 1.2714(4) | -0.1895(3) | 0.7919(2) | 0.0728(16) |
| F9_13 | 1.1879(4) | -0.0786(3) | 0.7424(2) | 0.0572(12) |
| O1_14 | 0.8850(4) | -0.0581(3) | 0.68062(19) | 0.0339(11) |
| C1_14 | 0.8234(5) | -0.1000(4) | 0.6844(3) | 0.0401(16) |

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|---|---|---|---|---|
| C2_14 | 0.8870(6) | -0.1928(5) | 0.6899(3) | 0.0522(19) |
| F1_14 | 0.9044(4) | -0.2269(3) | 0.7401(2) | 0.0620(13) |
| F2_14 | 0.8347(4) | -0.2318(3) | 0.6782(3) | 0.0749(16) |
| F3_14 | 0.9752(4) | -0.2057(3) | 0.6555(2) | 0.0632(13) |
| C3_14 | 0.7755(6) | -0.0690(5) | 0.6323(3) | 0.053(2) |
| F4_14 | 0.7445(4) | 0.0117(3) | 0.6191(2) | 0.0627(13) |
| F5_14 | 0.8446(4) | -0.0975(4) | 0.5899(2) | 0.0706(15) |
| F6_14 | 0.6938(4) | -0.0895(4) | 0.6385(2) | 0.0798(18) |
| C4_14 | 0.7364(6) | -0.0871(5) | 0.7351(3) | 0.0498(19) |
| F7_14 | 0.6659(3) | -0.0132(3) | 0.7272(2) | 0.0608(13) |
| F8_14 | 0.6883(4) | -0.1418(3) | 0.7485(2) | 0.0667(14) |
| F9_14 | 0.7741(3) | -0.0947(3) | 0.77911(17) | 0.0540(12) |
| O1_15 | 0.6867(8) | -0.0979(7) | 0.3628(4) | 0.023(2) |
| C1_15 | 0.7318(14) | -0.1141(9) | 0.3116(6) | 0.029(3) |
| C2_15 | 0.8405(15) | -0.1717(11) | 0.3217(8) | 0.036(4) |
| F1_15 | 0.907(3) | -0.133(2) | 0.3081(15) | 0.039(4) |
| F2_15 | 0.8780(10) | -0.2338(7) | 0.2955(5) | 0.047(3) |
| F3_15 | 0.8291(16) | -0.2029(11) | 0.3754(5) | 0.044(4) |
| C3_15 | 0.6801(17) | -0.1628(11) | 0.2955(7) | 0.037(4) |
| F4_15 | 0.5786(17) | -0.1289(19) | 0.3061(15) | 0.038(4) |
| F5_15 | 0.7039(9) | -0.2387(6) | 0.3243(5) | 0.041(2) |
| F6_15 | 0.7077(11) | -0.1652(8) | 0.2423(5) | 0.047(3) |
| C4_15 | 0.7282(10) | -0.0362(8) | 0.2678(5) | 0.033(2) |
| F7_15 | 0.6362(7) | -0.0002(6) | 0.2528(4) | 0.036(2) |
| F8_15 | 0.7994(7) | -0.0504(7) | 0.2228(4) | 0.049(3) |
| F9_15 | 0.7428(7) | 0.0177(5) | 0.2876(4) | 0.0447(14) |
| O1_16 | 1.2183(4) | -0.3249(3) | 0.4259(2) | 0.0465(13) |
| C1_16 | 1.1650(5) | -0.2519(4) | 0.4387(3) | 0.0399(15) |
| C2_16 | 1.2316(6) | -0.1965(5) | 0.4190(4) | 0.057(2) |
| F1_16 | 1.3270(4) | -0.2380(3) | 0.4239(2) | 0.0637(13) |
| F2_16 | 1.1966(4) | -0.1369(4) | 0.4476(3) | 0.0832(18) |
| F3_16 | 1.2304(5) | -0.1606(3) | 0.3652(2) | 0.0718(15) |
| C3_16 | 1.0701(6) | -0.2118(5) | 0.4113(4) | 0.064(2) |
| F4_16 | 0.9977(4) | -0.2472(3) | 0.4407(3) | 0.0776(16) |
| F5_16 | 1.0948(5) | -0.2238(3) | 0.3591(2) | 0.0756(16) |
| F6_16 | 1.0284(4) | -0.1323(3) | 0.4082(3) | 0.0856(19) |
| C4_16 | 1.1326(7) | -0.2614(7) | 0.5020(4) | 0.081(3) |
| F7_16 | 1.0995(5) | -0.3261(5) | 0.5212(2) | 0.102(2) |
| F8_16 | 1.0554(5) | -0.1955(5) | 0.5162(3) | 0.116(3) |
| F9_16 | 1.2123(5) | -0.2720(5) | 0.5236(2) | 0.111(3) |
| O1_17 | 0.4848(10) | 0.0141(8) | 0.3683(6) | 0.027(3) |
| C1_17 | 0.4003(9) | 0.0792(7) | 0.3596(4) | 0.031(3) |
| C2_17 | 0.3560(7) | 0.0703(6) | 0.3149(4) | 0.034(2) |
| F1_17 | 0.4086(9) | 0.0901(9) | 0.2647(5) | 0.075(4) |
| F2_17 | 0.2593(12) | 0.1213(12) | 0.3112(7) | 0.056(4) |
| F3_17 | 0.3565(11) | -0.0022(6) | 0.3204(5) | 0.066(3) |
| C3_17 | 0.3184(8) | 0.0833(9) | 0.4132(4) | 0.058(3) |
| F4_17 | 0.3640(7) | 0.0647(8) | 0.4562(3) | 0.069(3) |
| F5_17 | 0.2794(9) | 0.0227(9) | 0.4223(5) | 0.084(4) |
| F6_17 | 0.2430(7) | 0.1500(9) | 0.4132(5) | 0.097(4) |
| C4_17 | 0.4234(9) | 0.1588(7) | 0.3427(5) | 0.055(3) |
| F7_17 | 0.4340(17) | 0.1811(14) | 0.3862(8) | 0.085(4) |
| F8_17 | 0.3467(9) | 0.2204(5) | 0.3195(6) | 0.095(4) |
| F9_17 | 0.5099(8) | 0.1528(7) | 0.3099(4) | 0.077(3) |
| O1_19 | 1.0385(18) | 0.0111(19) | 0.6573(8) | 0.022(4) |

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|---|---|---|---|---|
| C1_19 | 1.0824(11) | 0.0236(8) | 0.6041(8) | 0.031(3) |
| C2_19 | 1.1593(11) | 0.0664(8) | 0.5998(6) | 0.048(3) |
| F1_19 | 1.1100(8) | 0.1427(5) | 0.6053(4) | 0.066(3) |
| F2_19 | 1.226(2) | 0.0668(18) | 0.5529(8) | 0.075(5) |
| F3_19 | 1.2144(11) | 0.0290(8) | 0.6403(6) | 0.063(4) |
| C3_19 | 1.1401(10) | -0.0569(8) | 0.5828(6) | 0.047(3) |
| F4_19 | 1.0845(9) | -0.1046(8) | 0.6003(6) | 0.061(3) |
| F5_19 | 1.2282(7) | -0.0959(6) | 0.6023(4) | 0.067(3) |
| F6_19 | 1.163(2) | -0.043(2) | 0.5284(7) | 0.065(5) |
| C4_19 | 1.0023(10) | 0.0807(9) | 0.5677(6) | 0.046(3) |
| F7_19 | 0.9517(7) | 0.0402(7) | 0.5580(3) | 0.064(3) |
| F8_19 | 1.047(2) | 0.114(2) | 0.5197(7) | 0.076(5) |
| F9_19 | 0.9340(8) | 0.1395(6) | 0.5934(5) | 0.058(3) |
| O1_20 | 0.9165(3) | 0.0083(3) | 0.76029(17) | 0.0291(10) |
| C1_20 | 0.8704(5) | 0.0822(4) | 0.7739(2) | 0.0356(15) |
| C2_20 | 0.8454(7) | 0.0692(5) | 0.8375(3) | 0.062(2) |
| F1_20 | 0.9301(4) | 0.0494(4) | 0.8578(2) | 0.0782(17) |
| F2_20 | 0.7751(5) | 0.1350(4) | 0.8556(2) | 0.091(2) |
| F3_20 | 0.8060(4) | 0.0100(3) | 0.85813(19) | 0.0759(16) |
| C3_20 | 0.7715(6) | 0.1299(4) | 0.7506(3) | 0.0478(18) |
| F4_20 | 0.7871(4) | 0.1243(3) | 0.69861(17) | 0.0488(11) |
| F5_20 | 0.6963(3) | 0.1002(3) | 0.7792(2) | 0.0643(13) |
| F6_20 | 0.7380(4) | 0.2097(3) | 0.7515(2) | 0.0553(12) |
| C4_20 | 0.9449(6) | 0.1323(5) | 0.7533(3) | 0.0497(18) |
| F7_20 | 0.9433(4) | 0.1672(3) | 0.70055(19) | 0.0577(12) |
| F8_20 | 0.9165(4) | 0.1919(3) | 0.7815(2) | 0.0722(16) |
| F9_20 | 1.0393(3) | 0.0854(3) | 0.7587(2) | 0.0584(13) |
| O1_21 | 0.5981(8) | -0.1198(7) | 0.4457(4) | 0.026(2) |
| C1_21 | 0.5524(11) | -0.1611(8) | 0.4894(6) | 0.030(3) |
| C2_21 | 0.6222(11) | -0.2521(8) | 0.4999(6) | 0.045(3) |
| F1_21 | 0.6179(9) | -0.2898(6) | 0.4639(4) | 0.062(3) |
| F2_21 | 0.5954(10) | -0.2908(7) | 0.5501(4) | 0.054(3) |
| F3_21 | 0.7178(8) | -0.2560(7) | 0.4948(4) | 0.059(3) |
| C3_21 | 0.5255(13) | -0.1262(9) | 0.5406(6) | 0.047(4) |
| F4_21 | 0.4870(8) | -0.0457(6) | 0.5301(4) | 0.0598(18) |
| F5_21 | 0.6126(15) | -0.1465(18) | 0.5602(8) | 0.065(5) |
| F6_21 | 0.4573(10) | -0.1509(8) | 0.5822(4) | 0.065(3) |
| C4_21 | 0.4647(13) | -0.1750(10) | 0.4744(8) | 0.042(4) |
| F7_21 | 0.3750(9) | -0.1291(8) | 0.4956(6) | 0.057(3) |
| F8_21 | 0.4753(10) | -0.2542(7) | 0.4959(4) | 0.055(3) |
| F9_21 | 0.476(3) | -0.162(2) | 0.4205(8) | 0.062(4) |
| O1_22 | 0.6212(17) | 0.0447(14) | 0.4107(9) | 0.030(3) |
| C1_22 | 0.6750(9) | 0.0632(7) | 0.4376(5) | 0.038(3) |
| C2_22 | 0.7849(8) | 0.0019(7) | 0.4373(5) | 0.051(3) |
| F1_22 | 0.8403(10) | 0.0126(10) | 0.3876(4) | 0.087(4) |
| F2_22 | 0.8348(10) | 0.0059(9) | 0.4718(7) | 0.054(4) |
| F3_22 | 0.7885(8) | -0.0735(6) | 0.4466(5) | 0.062(3) |
| C3_22 | 0.6178(10) | 0.0684(8) | 0.4968(5) | 0.060(3) |
| F4_22 | 0.5187(6) | 0.0966(7) | 0.5014(4) | 0.078(3) |
| F5_22 | 0.6463(9) | -0.0115(6) | 0.5266(3) | 0.076(3) |
| F6_22 | 0.6469(8) | 0.1085(6) | 0.5208(4) | 0.073(3) |
| C4_22 | 0.6785(10) | 0.1497(8) | 0.4083(5) | 0.069(4) |
| F7_22 | 0.5837(10) | 0.2062(7) | 0.4246(6) | 0.091(3) |
| F8_22 | 0.7458(9) | 0.1682(6) | 0.4242(5) | 0.093(4) |
| F9_22 | 0.6964(8) | 0.1590(7) | 0.3552(4) | 0.083(3) |

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|---|---|---|---|---|
| O1_23 | 1.4037(5) | -0.4525(5) | 0.4148(3) | 0.089(2) |
| C1_23 | 1.4741(5) | -0.4859(4) | 0.4475(2) | 0.0348(14) |
| C2_23 | 1.4250(8) | -0.4690(5) | 0.5054(3) | 0.068(2) |
| F1_23 | 1.4159(8) | -0.3945(4) | 0.5072(2) | 0.130(3) |
| F2_23 | 1.4800(6) | -0.5196(4) | 0.5425(2) | 0.0886(19) |
| F3_23 | 1.3310(5) | -0.4755(4) | 0.5204(2) | 0.097(2) |
| C3_23 | 1.5105(6) | -0.5791(5) | 0.4495(3) | 0.0496(18) |
| F4_23 | 1.5265(5) | -0.5933(4) | 0.4007(2) | 0.090(2) |
| F5_23 | 1.4428(4) | -0.6115(3) | 0.48203(19) | 0.0707(15) |
| F6_23 | 1.5980(5) | -0.6177(4) | 0.4688(3) | 0.101(2) |
| C4_23 | 1.5639(7) | -0.4564(5) | 0.4233(3) | 0.058(2) |
| F7_23 | 1.6226(4) | -0.4867(3) | 0.3796(2) | 0.0697(15) |
| F8_23 | 1.6238(6) | -0.4749(5) | 0.4586(3) | 0.117(3) |
| F9_23 | 1.5263(6) | -0.3744(3) | 0.4081(2) | 0.096(2) |
| C1_24 | 0.8363(11) | 0.4837(10) | 0.5456(7) | 0.049(3) |
| C2_24 | 0.9124(10) | 0.4162(11) | 0.5661(8) | 0.053(4) |
| C3_24 | 0.8887(11) | 0.3532(11) | 0.6037(9) | 0.055(3) |
| H3_24 | 0.941747 | 0.305966 | 0.617050 | 0.066 |
| C4_24 | 0.7878(12) | 0.3593(10) | 0.6217(9) | 0.057(4) |
| H4_24 | 0.770488 | 0.317216 | 0.648924 | 0.069 |
| C5_24 | 0.7108(12) | 0.4267(12) | 0.6004(10) | 0.066(5) |
| H5_24 | 0.641082 | 0.429626 | 0.611287 | 0.080 |
| C6_24 | 0.7367(12) | 0.4891(10) | 0.5633(7) | 0.062(4) |
| H6_24 | 0.684114 | 0.536640 | 0.549880 | 0.075 |
| F1_24 | 0.8618(15) | 0.5454(9) | 0.5099(6) | 0.075(3) |
| F2_24 | 1.0094(6) | 0.4155(6) | 0.5494(3) | 0.085(3) |
| O1_25 | 1.0046(3) | 0.5529(3) | 0.03398(16) | 0.0265(9) |
| C1_25 | 1.0338(4) | 0.5285(3) | -0.0143(2) | 0.0266(12) |
| C2_25 | 1.0487(5) | 0.5973(4) | -0.0633(2) | 0.0332(14) |
| F1_25 | 0.9590(3) | 0.6500(2) | -0.07607(15) | 0.0385(9) |
| F2_25 | 1.1071(3) | 0.5700(2) | -0.10847(15) | 0.0442(10) |
| F3_25 | 1.0946(3) | 0.6384(2) | -0.04979(16) | 0.0392(9) |
| C3_25 | 1.1374(5) | 0.4562(4) | -0.0135(2) | 0.0285(13) |
| F4_25 | 1.1355(3) | 0.4058(2) | 0.03502(15) | 0.0373(9) |
| F5_25 | 1.2142(3) | 0.4836(2) | -0.02043(17) | 0.0411(9) |
| F6_25 | 1.1595(3) | 0.4133(2) | -0.05214(16) | 0.0418(9) |
| C4_25 | 0.9509(5) | 0.4995(4) | -0.0227(3) | 0.0323(14) |
| F7_25 | 0.9556(3) | 0.4274(2) | 0.00928(16) | 0.0427(10) |
| F8_25 | 0.9638(3) | 0.4928(2) | -0.07448(15) | 0.0395(9) |
| F9_25 | 0.8579(3) | 0.5519(3) | -0.00960(17) | 0.0418(9) |
| C1_26 | 0.1568(6) | 0.0769(6) | 0.2283(4) | 0.046(2) |
| C2_26 | 0.0921(7) | 0.1550(6) | 0.2154(4) | 0.061(3) |
| C3_26 | -0.0123(8) | 0.1734(7) | 0.2271(5) | 0.084(4) |
| H3_26 | -0.056810 | 0.227848 | 0.217997 | 0.101 |
| C4_26 | -0.0516(9) | 0.1128(8) | 0.2519(6) | 0.080(4) |
| H4_26 | -0.123908 | 0.125240 | 0.259258 | 0.096 |
| C5_26 | 0.0092(9) | 0.0366(7) | 0.2661(6) | 0.065(3) |
| H5_26 | -0.019630 | -0.004527 | 0.284471 | 0.078 |
| C6_26 | 0.1156(9) | 0.0173(6) | 0.2540(4) | 0.064(3) |
| H6_26 | 0.159453 | -0.037270 | 0.263508 | 0.076 |
| F1_26 | 0.2567(4) | 0.0600(6) | 0.2160(3) | 0.101(3) |
| F2_26 | 0.1336(8) | 0.2124(6) | 0.1903(4) | 0.119(4) |
| C1_27 | 0.4100(9) | -0.1634(6) | 0.8820(4) | 0.085(3) |
| C2_27 | 0.5018(10) | -0.1924(7) | 0.8996(4) | 0.097(4) |
| C3_27 | 0.5644(13) | -0.1430(10) | 0.8827(6) | 0.142(5) |

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|---|---|---|---|---|
| H3_27 | 0.627526 | -0.160983 | 0.895188 | 0.170 |
| C4_27 | 0.5342(12) | -0.0723(10) | 0.8496(6) | 0.134(5) |
| H4_27 | 0.576799 | -0.039842 | 0.836328 | 0.160 |
| C5_27 | 0.4389(12) | -0.0457(9) | 0.8343(5) | 0.114(4) |
| H5_27 | 0.416431 | 0.007448 | 0.812907 | 0.137 |
| C6_27 | 0.3756(10) | -0.0891(6) | 0.8474(4) | 0.091(3) |
| H6_27 | 0.313138 | -0.070410 | 0.834067 | 0.109 |
| F1_27 | 0.3489(8) | -0.2048(5) | 0.8978(4) | 0.145(4) |
| F2_27 | 0.5396(11) | -0.2617(6) | 0.9311(4) | 0.226(7) |
| O1_28 | 0.862(3) | 0.7057(12) | 0.0379(17) | 0.024(5) |
| C1_28 | 0.8002(12) | 0.7841(11) | 0.0266(6) | 0.028(3) |
| C2_28 | 0.7327(9) | 0.7892(7) | -0.0132(5) | 0.034(3) |
| F1_28 | 0.7871(9) | 0.7894(8) | -0.0643(4) | 0.045(3) |
| F2_28 | 0.6510(7) | 0.8571(6) | -0.0156(5) | 0.044(3) |
| F3_28 | 0.700(3) | 0.7264(15) | 0.0027(11) | 0.051(4) |
| C3_28 | 0.7274(10) | 0.8117(7) | 0.0788(5) | 0.038(3) |
| F4_28 | 0.7793(19) | 0.7862(15) | 0.1207(8) | 0.046(4) |
| F5_28 | 0.653(2) | 0.781(2) | 0.0963(9) | 0.052(4) |
| F6_28 | 0.6844(11) | 0.8930(7) | 0.0726(6) | 0.048(3) |
| C4_28 | 0.8647(11) | 0.8403(8) | -0.0006(6) | 0.029(3) |
| F7_28 | 0.9011(8) | 0.8556(6) | 0.0360(5) | 0.041(2) |
| F8_28 | 0.812(3) | 0.9114(12) | -0.0282(14) | 0.043(5) |
| F9_28 | 0.9458(17) | 0.805(2) | -0.0364(13) | 0.041(4) |
| O1_29 | 0.860(2) | 0.7070(11) | 0.0434(15) | 0.031(6) |
| C1_29 | 0.7988(10) | 0.7860(9) | 0.0374(5) | 0.028(3) |
| C2_29 | 0.6882(8) | 0.7890(7) | 0.0401(5) | 0.040(3) |
| F1_29 | 0.6461(18) | 0.7681(17) | 0.0918(8) | 0.051(4) |
| F2_29 | 0.6281(7) | 0.8636(6) | 0.0195(5) | 0.059(3) |
| F3_29 | 0.689(2) | 0.7389(13) | 0.0118(9) | 0.054(4) |
| C3_29 | 0.8353(9) | 0.8334(7) | -0.0194(4) | 0.035(3) |
| F4_29 | 0.9366(13) | 0.8152(18) | -0.0305(11) | 0.038(3) |
| F5_29 | 0.8097(8) | 0.8154(6) | -0.0594(4) | 0.044(2) |
| F6_29 | 0.791(2) | 0.9137(10) | -0.0227(12) | 0.043(5) |
| C4_29 | 0.8006(9) | 0.8254(7) | 0.0828(5) | 0.040(3) |
| F7_29 | 0.8823(6) | 0.8476(5) | 0.0721(4) | 0.045(2) |
| F8_29 | 0.7169(9) | 0.8913(7) | 0.0893(5) | 0.051(3) |
| F9_29 | 0.8021(16) | 0.7730(12) | 0.1312(6) | 0.045(3) |
| O1_30 | 0.5369(3) | 1.2603(3) | 0.03849(16) | 0.0255(9) |
| C1_30 | 0.4510(4) | 1.2405(4) | 0.0591(2) | 0.0252(12) |
| C2_30 | 0.3705(5) | 1.3000(4) | 0.0965(3) | 0.0337(14) |
| F1_30 | 0.3953(3) | 1.2804(3) | 0.14613(15) | 0.0442(10) |
| F2_30 | 0.2760(3) | 1.2968(3) | 0.10437(17) | 0.0464(10) |
| F3_30 | 0.3674(3) | 1.3750(2) | 0.07467(17) | 0.0455(10) |
| C3_30 | 0.4048(5) | 1.2465(4) | 0.0100(3) | 0.0346(15) |
| F4_30 | 0.4782(3) | 1.2133(3) | -0.03000(16) | 0.0425(10) |
| F5_30 | 0.3582(3) | 1.3230(2) | -0.01190(15) | 0.0386(9) |
| F6_30 | 0.3367(3) | 1.2078(3) | 0.02374(17) | 0.0488(11) |
| C4_30 | 0.4774(5) | 1.1525(4) | 0.0929(3) | 0.0379(15) |
| F7_30 | 0.5215(3) | 1.0980(2) | 0.05989(18) | 0.0466(10) |
| F8_30 | 0.3946(3) | 1.1369(3) | 0.12416(18) | 0.0503(11) |
| F9_30 | 0.5431(3) | 1.1385(3) | 0.12508(17) | 0.0448(10) |
| O1_18 | 1.2607(6) | -0.4339(5) | 0.3578(2) | 0.083(2) |
| C1_18 | 1.2078(6) | -0.4832(4) | 0.3653(3) | 0.0491(18) |
| C2_18 | 1.1492(7) | -0.4551(5) | 0.3171(3) | 0.062(2) |
| F1_18 | 1.2131(4) | -0.4768(3) | 0.2714(2) | 0.0671(14) |

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|---|---|---|---|---|
| F2_18 | 1.0756(4) | -0.4868(4) | 0.3269(2) | 0.0781(16) |
| F3_18 | 1.1040(6) | -0.3754(3) | 0.3057(3) | 0.103(2) |
| C3_18 | 1.1291(7) | -0.4805(5) | 0.4198(3) | 0.057(2) |
| F4_18 | 1.1724(5) | -0.4853(4) | 0.46066(19) | 0.0835(19) |
| F5_18 | 1.0497(5) | -0.4110(3) | 0.4172(3) | 0.0822(17) |
| F6_18 | 1.0917(4) | -0.5407(3) | 0.4344(2) | 0.0600(13) |
| C4_18 | 1.2802(6) | -0.5718(5) | 0.3651(3) | 0.056(2) |
| F7_18 | 1.3131(4) | -0.6050(4) | 0.4127(2) | 0.0874(19) |
| F8_18 | 1.2371(4) | -0.6188(3) | 0.3565(2) | 0.0682(14) |
| F9_18 | 1.3637(4) | -0.5748(4) | 0.3257(2) | 0.0757(15) |
| O1_31 | 1.036(3) | 0.008(3) | 0.6553(11) | 0.032(7) |
| C1_31 | 1.0833(13) | 0.0209(10) | 0.6024(10) | 0.029(4) |
| C2_31 | 1.1011(14) | -0.0494(10) | 0.5743(8) | 0.046(4) |
| F1_31 | 1.0138(10) | -0.0409(10) | 0.5615(4) | 0.067(4) |
| F2_31 | 1.171(3) | -0.051(3) | 0.5284(10) | 0.062(6) |
| F3_31 | 1.1354(13) | -0.1214(9) | 0.6073(8) | 0.058(4) |
| C3_31 | 1.1887(13) | 0.0276(11) | 0.6001(8) | 0.052(4) |
| F4_31 | 1.1817(17) | 0.0701(11) | 0.6356(8) | 0.069(5) |
| F5_31 | 1.2573(8) | -0.0445(10) | 0.6146(5) | 0.073(4) |
| F6_31 | 1.226(3) | 0.060(2) | 0.5499(10) | 0.068(5) |
| C4_31 | 1.0157(14) | 0.1025(11) | 0.5718(9) | 0.059(5) |
| F7_31 | 1.0220(14) | 0.1658(6) | 0.5851(5) | 0.082(5) |
| F8_31 | 1.042(3) | 0.110(3) | 0.5172(9) | 0.066(5) |
| F9_31 | 0.9175(11) | 0.1052(11) | 0.5848(6) | 0.074(4) |
| O1_32 | 0.610(3) | 0.039(3) | 0.4194(16) | 0.039(7) |
| C1_32 | 0.6737(14) | 0.0707(10) | 0.4275(6) | 0.045(4) |
| C2_32 | 0.7250(15) | 0.0174(13) | 0.4774(8) | 0.078(5) |
| F1_32 | 0.7558(15) | -0.0588(11) | 0.4743(9) | 0.080(5) |
| F2_32 | 0.8083(18) | 0.0329(18) | 0.4756(13) | 0.067(6) |
| F3_32 | 0.6494(14) | 0.0355(14) | 0.5228(7) | 0.086(4) |
| C3_32 | 0.6122(15) | 0.1576(12) | 0.4406(8) | 0.081(5) |
| F4_32 | 0.6035(19) | 0.2079(12) | 0.3900(9) | 0.103(6) |
| F5_32 | 0.5242(12) | 0.1589(11) | 0.4736(7) | 0.081(5) |
| F6_32 | 0.6636(14) | 0.1749(14) | 0.4700(10) | 0.129(8) |
| C4_32 | 0.7564(13) | 0.0844(11) | 0.3765(6) | 0.058(4) |
| F7_32 | 0.7157(10) | 0.1101(8) | 0.3324(4) | 0.050(3) |
| F8_32 | 0.7998(10) | 0.1334(8) | 0.3808(6) | 0.062(4) |
| F9_32 | 0.8322(14) | 0.0154(12) | 0.3671(7) | 0.069(5) |
| O1_33 | 0.4658(17) | 0.0108(16) | 0.3844(10) | 0.036(6) |
| C1_33 | 0.3969(14) | 0.0771(11) | 0.3599(6) | 0.038(4) |
| C2_33 | 0.3552(14) | 0.1442(10) | 0.3938(7) | 0.064(5) |
| F1_33 | 0.420(3) | 0.188(2) | 0.3782(13) | 0.083(6) |
| F2_33 | 0.2642(10) | 0.1996(7) | 0.3840(6) | 0.063(4) |
| F3_33 | 0.3498(11) | 0.1173(8) | 0.4471(5) | 0.048(3) |
| C3_33 | 0.3018(13) | 0.0548(11) | 0.3613(8) | 0.068(5) |
| F4_33 | 0.3336(18) | -0.0165(11) | 0.3474(8) | 0.070(5) |
| F5_33 | 0.2468(14) | 0.0535(15) | 0.4133(8) | 0.100(6) |
| F6_33 | 0.246(2) | 0.109(2) | 0.3246(11) | 0.065(7) |
| C4_33 | 0.4428(12) | 0.1094(10) | 0.3003(6) | 0.059(4) |
| F7_33 | 0.4413(16) | 0.0598(12) | 0.2699(8) | 0.077(5) |
| F8_33 | 0.3879(11) | 0.1877(8) | 0.2825(5) | 0.076(5) |
| F9_33 | 0.5382(9) | 0.1054(8) | 0.2977(5) | 0.052(3) |
| C1_34 | 0.850(3) | 0.485(3) | 0.554(2) | 0.054(9) |
| C2_34 | 0.752(3) | 0.482(2) | 0.5681(19) | 0.067(11) |
| C3_34 | 0.735(4) | 0.412(3) | 0.599(3) | 0.052(8) |

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|---|---|---|---|---|
| H3_34 | 0.667799 | 0.409858 | 0.609795 | 0.063 |
| C4_34 | 0.819(4) | 0.345(3) | 0.615(3) | 0.054(10) |
| H4_34 | 0.808712 | 0.296081 | 0.634917 | 0.065 |
| C5_34 | 0.915(4) | 0.350(3) | 0.601(3) | 0.055(3) |
| H5_34 | 0.971879 | 0.304046 | 0.612308 | 0.066 |
| C6_34 | 0.930(3) | 0.420(3) | 0.570(3) | 0.055(9) |
| H6_34 | 0.997468 | 0.422804 | 0.560482 | 0.066 |
| F1_34 | 0.860(5) | 0.554(3) | 0.523(2) | 0.085(10) |
| F2_34 | 0.678(3) | 0.548(2) | 0.5494(15) | 0.125(12) |
| O1_35 | 0.5638(8) | -0.0885(6) | 0.4644(4) | 0.028(2) |
| C1_35 | 0.5486(10) | -0.1578(8) | 0.4953(6) | 0.033(3) |
| C2_35 | 0.6520(11) | -0.2283(8) | 0.4898(5) | 0.045(3) |
| F1_35 | 0.6720(8) | -0.2567(5) | 0.4436(4) | 0.061(3) |
| F2_35 | 0.6556(10) | -0.2929(6) | 0.5314(4) | 0.059(3) |
| F3_35 | 0.7325(7) | -0.2071(6) | 0.4881(4) | 0.057(2) |
| C3_35 | 0.5161(13) | -0.1480(8) | 0.5562(6) | 0.047(3) |
| F4_35 | 0.4460(8) | -0.0760(5) | 0.5608(4) | 0.0598(18) |
| F5_35 | 0.5960(14) | -0.1552(15) | 0.5769(7) | 0.056(4) |
| F6_35 | 0.4750(9) | -0.2034(7) | 0.5867(4) | 0.057(3) |
| C4_35 | 0.4528(13) | -0.1596(11) | 0.4807(8) | 0.054(4) |
| F7_35 | 0.3751(9) | -0.0874(9) | 0.4838(6) | 0.077(4) |
| F8_35 | 0.4131(10) | -0.2160(9) | 0.5123(5) | 0.072(3) |
| F9_35 | 0.469(3) | -0.167(2) | 0.4290(7) | 0.064(4) |
| O1_36 | 0.736(3) | 1.188(3) | 0.060(2) | 0.020(9) |
| C1_36 | 0.820(2) | 1.1289(16) | 0.0406(10) | 0.029(5) |
| C2_36 | 0.826(2) | 1.0466(15) | 0.0804(11) | 0.039(6) |
| F1_36 | 0.810(5) | 1.054(4) | 0.1323(13) | 0.049(6) |
| F2_36 | 0.916(2) | 0.988(2) | 0.070(2) | 0.048(7) |
| F3_36 | 0.753(2) | 1.0214(17) | 0.0760(14) | 0.058(6) |
| C3_36 | 0.813(2) | 1.1263(17) | -0.0175(10) | 0.037(5) |
| F4_36 | 0.829(2) | 1.1901(17) | -0.0536(11) | 0.054(6) |
| F5_36 | 0.718(3) | 1.131(4) | -0.019(2) | 0.048(7) |
| F6_36 | 0.879(3) | 1.059(2) | -0.0349(18) | 0.0433(18) |
| C4_36 | 0.9180(19) | 1.1474(16) | 0.0370(10) | 0.036(5) |
| F7_36 | 0.906(5) | 1.225(2) | 0.014(2) | 0.049(7) |
| F8_36 | 0.999(2) | 1.101(2) | 0.0080(12) | 0.040(6) |
| F9_36 | 0.936(3) | 1.135(2) | 0.0872(11) | 0.054(6) |
| O1_37 | 0.601(4) | 1.316(3) | 0.1098(17) | 0.027(8) |
| C1_37 | 0.6249(16) | 1.3271(12) | 0.1538(11) | 0.026(5) |
| C2_37 | 0.6062(18) | 1.2614(13) | 0.2044(9) | 0.043(5) |
| F1_37 | 0.5064(16) | 1.2792(16) | 0.2256(8) | 0.066(6) |
| F2_37 | 0.650(4) | 1.257(4) | 0.2453(16) | 0.050(6) |
| F3_37 | 0.642(3) | 1.1892(17) | 0.1907(19) | 0.052(6) |
| C3_37 | 0.7399(16) | 1.3185(13) | 0.1403(10) | 0.038(5) |
| F4_37 | 0.764(3) | 1.353(2) | 0.0881(12) | 0.053(6) |
| F5_37 | 0.8009(14) | 1.2413(11) | 0.1467(9) | 0.057(5) |
| F6_37 | 0.764(4) | 1.354(3) | 0.171(2) | 0.040(5) |
| C4_37 | 0.5563(17) | 1.4131(12) | 0.1642(9) | 0.037(5) |
| F7_37 | 0.590(2) | 1.4701(11) | 0.1283(8) | 0.062(6) |
| F8_37 | 0.556(5) | 1.423(3) | 0.2138(13) | 0.045(6) |
| F9_37 | 0.460(2) | 1.430(2) | 0.160(2) | 0.053(6) |
| O1_38 | 0.152(3) | 0.3897(17) | 0.7270(14) | 0.021(7) |
| C1_38 | 0.095(2) | 0.4637(17) | 0.7025(11) | 0.040(6) |
| C2_38 | 0.082(2) | 0.5318(16) | 0.7310(12) | 0.055(7) |
| F1_38 | 0.064(3) | 0.508(3) | 0.7858(12) | 0.062(7) |

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| F2_38 | 0.000(3) | 0.5985(19) | 0.7191(17) | 0.085(9) |
| F3_38 | 0.166(3) | 0.551(3) | 0.718(2) | 0.077(7) |
| C3_38 | 0.148(3) | 0.482(2) | 0.6421(11) | 0.058(7) |
| F4_38 | 0.137(3) | 0.438(2) | 0.6129(13) | 0.067(7) |
| F5_38 | 0.248(3) | 0.466(5) | 0.639(3) | 0.063(8) |
| F6_38 | 0.109(7) | 0.560(2) | 0.619(2) | 0.074(9) |
| C4_38 | -0.013(2) | 0.4630(18) | 0.7039(12) | 0.052(7) |
| F7_38 | -0.004(4) | 0.394(2) | 0.691(2) | 0.062(7) |
| F8_38 | -0.062(3) | 0.523(2) | 0.6675(14) | 0.058(7) |
| F9_38 | -0.070(3) | 0.467(3) | 0.7534(13) | 0.055(7) |
| Mg1_40 | -0.39705(16) | 0.65265(13) | 0.73574(8) | 0.0269(4) |
| N1_40 | -0.5139(4) | 0.6397(4) | 0.8071(2) | 0.0347(13) |
| C1_40 | -0.5745(5) | 0.6283(4) | 0.8438(3) | 0.0326(15) |
| N2_40 | -0.3166(4) | 0.5248(4) | 0.7490(2) | 0.0330(13) |
| C2_40 | -0.6544(6) | 0.6160(5) | 0.8905(3) | 0.050(2) |
| H2A_40 | -0.719951 | 0.634732 | 0.877925 | 0.076 |
| H2B_40 | -0.661051 | 0.647010 | 0.917531 | 0.076 |
| H2C_40 | -0.635940 | 0.558171 | 0.907221 | 0.076 |
| N3_40 | -0.3077(4) | 0.6624(3) | 0.7868(2) | 0.0340(13) |
| C3_40 | -0.2593(5) | 0.6636(4) | 0.8142(3) | 0.0340(15) |
| N4_40 | -0.4709(4) | 0.7828(3) | 0.7190(2) | 0.0317(12) |
| C4_40 | -0.1954(7) | 0.6624(5) | 0.8509(3) | 0.050(2) |
| H4A_40 | -0.125387 | 0.624775 | 0.841922 | 0.075 |
| H4B_40 | -0.224785 | 0.644600 | 0.889068 | 0.075 |
| H4C_40 | -0.193799 | 0.717099 | 0.846097 | 0.075 |
| N5_40 | -0.2822(4) | 0.6646(3) | 0.6635(2) | 0.0331(13) |
| C5_40 | -0.2721(5) | 0.4563(4) | 0.7567(3) | 0.0309(14) |
| N6_40 | -0.4920(4) | 0.6447(3) | 0.6870(2) | 0.0341(13) |
| C7_40 | -0.5072(5) | 0.8512(4) | 0.7064(3) | 0.0318(15) |
| C8_40 | -0.5539(6) | 0.9387(4) | 0.6897(3) | 0.0430(18) |
| H8A_40 | -0.528797 | 0.955221 | 0.650632 | 0.064 |
| H8B_40 | -0.535452 | 0.966108 | 0.711037 | 0.064 |
| H8C_40 | -0.628723 | 0.953705 | 0.696320 | 0.064 |
| C9_40 | -0.2168(5) | 0.6721(4) | 0.6269(3) | 0.0319(15) |
| C10_40 | -0.1354(6) | 0.6826(5) | 0.5823(3) | 0.0467(19) |
| H10A_40 | -0.154290 | 0.739664 | 0.563554 | 0.056 |
| H10B_40 | -0.124302 | 0.648423 | 0.556333 | 0.056 |
| H10C_40 | -0.072181 | 0.666806 | 0.596450 | 0.056 |
| C11_40 | -0.5455(5) | 0.6463(4) | 0.6610(3) | 0.0328(15) |
| C12_40 | -0.6158(7) | 0.6499(5) | 0.6285(3) | 0.051(2) |
| H12A_40 | -0.647360 | 0.706279 | 0.610568 | 0.076 |
| H12B_40 | -0.669435 | 0.629375 | 0.652451 | 0.076 |
| H12C_40 | -0.578008 | 0.616441 | 0.600655 | 0.076 |
| C6_40 | -0.2162(6) | 0.3695(4) | 0.7655(3) | 0.0402(17) |
| H6A_40 | -0.259312 | 0.341211 | 0.792631 | 0.060 |
| H6B_40 | -0.153314 | 0.357921 | 0.778826 | 0.060 |
| H6C_40 | -0.198275 | 0.350846 | 0.730821 | 0.060 |
| Mg1_41 | 0.94771(16) | 0.31199(13) | 0.40635(8) | 0.0287(5) |
| C1_41 | 1.1186(5) | 0.3356(4) | 0.2939(3) | 0.0315(14) |
| N2_41 | 0.8335(4) | 0.3351(3) | 0.3593(2) | 0.0323(12) |
| C2_41 | 1.1956(6) | 0.3453(5) | 0.2457(3) | 0.0450(18) |
| H2A_41 | 1.201912 | 0.310317 | 0.221305 | 0.067 |
| H2B_41 | 1.261854 | 0.329970 | 0.256694 | 0.067 |
| H2C_41 | 1.175147 | 0.402077 | 0.226402 | 0.067 |
| N3_41 | 0.8398(4) | 0.2877(4) | 0.4805(2) | 0.0364(13) |

| | | | | |
|---|---|---|---|---|
| C3_41 | 0.7736(5) | 0.3492(4) | 0.3347(2) | 0.0294(14) |
| N4_41 | 1.0594(4) | 0.2911(3) | 0.4540(2) | 0.0328(12) |
| C4_41 | 0.6967(6) | 0.3678(5) | 0.3012(3) | 0.0436(18) |
| H4A_41 | 0.730934 | 0.363539 | 0.263281 | 0.065 |
| H4B_41 | 0.647990 | 0.423134 | 0.302183 | 0.065 |
| H4C_41 | 0.659760 | 0.329205 | 0.315717 | 0.065 |
| N5_41 | 0.8923(4) | 0.4402(4) | 0.4050(2) | 0.0349(13) |
| C5_41 | 0.7833(5) | 0.2679(5) | 0.5152(3) | 0.0365(16) |
| N6_41 | 0.9997(4) | 0.1867(4) | 0.4019(2) | 0.0353(13) |
| C7_41 | 1.1216(6) | 0.2814(4) | 0.4774(3) | 0.0363(16) |
| C8_41 | 1.2019(7) | 0.2693(5) | 0.5055(3) | 0.051(2) |
| H8A_41 | 1.263429 | 0.224842 | 0.493857 | 0.076 |
| H8B_41 | 1.178892 | 0.255652 | 0.545142 | 0.076 |
| H8C_41 | 1.218148 | 0.319251 | 0.496619 | 0.076 |
| C9_41 | 0.8630(6) | 0.5089(5) | 0.3954(3) | 0.0383(16) |
| C10_41 | 0.8279(7) | 0.5969(5) | 0.3823(4) | 0.055(2) |
| H10A_41 | 0.813828 | 0.615893 | 0.344830 | 0.083 |
| H10B_41 | 0.881165 | 0.615607 | 0.385145 | 0.083 |
| H10C_41 | 0.764953 | 0.618785 | 0.408005 | 0.083 |
| C11_41 | 1.0242(5) | 0.1196(5) | 0.4019(3) | 0.0346(15) |
| C12_41 | 1.0554(7) | 0.0341(5) | 0.4026(4) | 0.054(2) |
| H12A_41 | 1.129683 | 0.012601 | 0.389596 | 0.065 |
| H12B_41 | 1.019388 | 0.026105 | 0.378510 | 0.065 |
| H12C_41 | 1.038297 | 0.005565 | 0.440043 | 0.065 |
| C6_41 | 0.7072(6) | 0.2436(6) | 0.5597(3) | 0.053(2) |
| H6A_41 | 0.647367 | 0.291784 | 0.566996 | 0.080 |
| H6B_41 | 0.737394 | 0.216652 | 0.592798 | 0.080 |
| H6C_41 | 0.685680 | 0.206015 | 0.549017 | 0.080 |
| N1_41 | 1.0575(4) | 0.3284(3) | 0.3322(2) | 0.0315(12) |
| Mg1_42 | 1.31359(16) | 0.95332(13) | 0.05420(8) | 0.0255(4) |
| C1_42 | 1.1647(5) | 1.1429(5) | 0.0597(3) | 0.0327(15) |
| N2_42 | 1.4221(4) | 0.9979(3) | -0.0089(2) | 0.0304(12) |
| C2_42 | 1.0998(6) | 1.2272(5) | 0.0614(4) | 0.050(2) |
| H2A_42 | 1.088464 | 1.256645 | 0.024346 | 0.075 |
| H2B_42 | 1.133596 | 1.252595 | 0.075726 | 0.075 |
| H2C_42 | 1.033584 | 1.228857 | 0.085320 | 0.075 |
| N3_42 | 1.4070(4) | 0.8277(3) | 0.0531(2) | 0.0299(12) |
| C3_42 | 1.4839(5) | 1.0209(4) | -0.0371(3) | 0.0312(14) |
| N4_42 | 1.1989(4) | 0.9170(3) | 0.1177(2) | 0.0285(12) |
| C4_42 | 1.5639(6) | 1.0508(5) | -0.0731(3) | 0.0429(18) |
| H4A_42 | 1.624279 | 1.004776 | -0.083660 | 0.064 |
| H4B_42 | 1.583012 | 1.080599 | -0.053914 | 0.064 |
| H4C_42 | 1.538262 | 1.087057 | -0.106043 | 0.064 |
| N5_42 | 1.2319(4) | 0.9506(3) | -0.0039(2) | 0.0290(12) |
| C5_42 | 1.4497(5) | 0.7587(4) | 0.0597(3) | 0.0304(14) |
| N6_42 | 1.3940(4) | 0.9500(3) | 0.1145(2) | 0.0281(12) |
| C6_42 | 1.5010(7) | 0.6718(5) | 0.0681(3) | 0.0476(19) |
| H6A_42 | 1.456100 | 0.645116 | 0.095158 | 0.057 |
| H6B_42 | 1.564824 | 0.657512 | 0.081357 | 0.057 |
| H6C_42 | 1.517032 | 0.653888 | 0.033294 | 0.057 |
| C7_42 | 1.1296(5) | 0.9046(4) | 0.1472(3) | 0.0281(14) |
| C8_42 | 1.0406(5) | 0.8901(5) | 0.1842(3) | 0.0421(17) |
| H8A_42 | 1.000240 | 0.936853 | 0.201898 | 0.063 |
| H8B_42 | 1.063063 | 0.841306 | 0.212201 | 0.063 |
| H8C_42 | 0.998349 | 0.882246 | 0.163593 | 0.063 |

| | | | | |
|---|---|---|---|---|
| C9_42 | 1.1799(5) | 0.9490(4) | -0.0287(3) | 0.0314(14) |
| C10_42 | 1.1127(6) | 0.9482(5) | -0.0619(3) | 0.0440(18) |
| H10A_42 | 1.098830 | 0.998036 | -0.089959 | 0.066 |
| H10B_42 | 1.047901 | 0.945070 | -0.038362 | 0.066 |
| H10C_42 | 1.146437 | 0.900962 | -0.079598 | 0.066 |
| C11_42 | 1.4401(5) | 0.9461(4) | 0.1448(3) | 0.0301(14) |
| C12_42 | 1.4984(6) | 0.9411(4) | 0.1849(3) | 0.0395(17) |
| H12A_42 | 1.568793 | 0.903543 | 0.176877 | 0.059 |
| H12B_42 | 1.465619 | 0.921331 | 0.221823 | 0.059 |
| H12C_42 | 1.499679 | 0.995069 | 0.182948 | 0.059 |
| N1_42 | 1.2160(4) | 1.0771(3) | 0.0585(2) | 0.0299(12) |
| O1_43 | 0.6853(8) | -0.0620(6) | 0.3423(4) | 0.027(2) |
| C1_43 | 0.7330(12) | -0.1123(8) | 0.3055(5) | 0.025(3) |
| C2_43 | 0.7494(9) | -0.0595(7) | 0.2472(5) | 0.033(2) |
| F1_43 | 0.7854(6) | -0.0039(5) | 0.2484(3) | 0.0447(14) |
| F2_43 | 0.8159(6) | -0.1052(6) | 0.2119(3) | 0.0402(19) |
| F3_43 | 0.6613(7) | -0.0213(6) | 0.2293(4) | 0.039(2) |
| C3_43 | 0.6656(14) | -0.1615(9) | 0.3055(6) | 0.030(3) |
| F4_43 | 0.6704(8) | -0.2219(6) | 0.3492(4) | 0.041(2) |
| F5_43 | 0.5672(13) | -0.1144(16) | 0.3082(13) | 0.033(3) |
| F6_43 | 0.6933(10) | -0.1938(7) | 0.2610(4) | 0.042(2) |
| C4_43 | 0.8425(13) | -0.1666(10) | 0.3146(7) | 0.036(4) |
| F7_43 | 0.8511(13) | -0.2226(9) | 0.3598(5) | 0.040(3) |
| F8_43 | 0.8929(10) | -0.2064(8) | 0.2725(4) | 0.056(3) |
| F9_43 | 0.896(2) | -0.1215(19) | 0.3150(15) | 0.045(5) |
| C1_44 | 0.133(4) | 0.117(4) | 0.224(3) | 0.059(11) |
| C2_44 | 0.032(4) | 0.167(3) | 0.231(3) | 0.067(12) |
| C3_44 | -0.043(4) | 0.133(4) | 0.254(4) | 0.068(13) |
| H3_44 | -0.113148 | 0.167767 | 0.258399 | 0.081 |
| C4_44 | -0.019(5) | 0.051(4) | 0.270(5) | 0.052(12) |
| H4_44 | -0.071483 | 0.028561 | 0.286235 | 0.062 |
| C5_44 | 0.082(6) | 0.001(4) | 0.262(4) | 0.055(11) |
| H5_44 | 0.099045 | -0.056531 | 0.272237 | 0.066 |
| C6_44 | 0.158(4) | 0.034(3) | 0.241(3) | 0.041(10) |
| H6_44 | 0.228022 | -0.000174 | 0.237171 | 0.049 |
| F1_44 | 0.206(5) | 0.149(5) | 0.201(4) | 0.12(3) |
| F2_44 | 0.007(6) | 0.246(3) | 0.215(4) | 0.19(5) |

*Table S 2 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [CaHMB(oDFB)$_2${f-al}][Al(OR$^F$)$_4$]$_2$ **2**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| O1_21 | 0.477(3) | 0.2096(15) | 0.449(3) | 0.037(2) |
| C1_21 | 0.4505(12) | 0.1482(12) | 0.4439(10) | 0.038(5) |
| C2_21 | 0.4404(16) | 0.1295(12) | 0.3692(11) | 0.058(8) |
| F1_21 | 0.5073(18) | 0.1178(19) | 0.3438(15) | 0.067(9) |
| F2_21 | 0.395(2) | 0.0796(17) | 0.3598(18) | 0.102(14) |
| F3_21 | 0.414(3) | 0.1781(19) | 0.3309(18) | 0.094(14) |
| C3_21 | 0.3747(13) | 0.1429(13) | 0.4794(12) | 0.054(7) |
| F4_21 | 0.383(2) | 0.175(2) | 0.5370(17) | 0.073(13) |
| F5_21 | 0.3184(14) | 0.1692(18) | 0.4424(17) | 0.089(10) |
| F6_21 | 0.3557(19) | 0.0826(13) | 0.494(2) | 0.067(11) |
| C4_21 | 0.5096(15) | 0.1017(14) | 0.4788(12) | 0.062(8) |
| F7_21 | 0.5029(18) | 0.1016(18) | 0.5452(11) | 0.082(10) |
| F8_21 | 0.503(3) | 0.0415(14) | 0.456(2) | 0.124(15) |

| | | | | |
|---|---|---|---|---|
| F9_21 | 0.5779(16) | 0.123(2) | 0.466(2) | 0.107(14) |
| C1 | 0.5496(8) | 0.6800(6) | 0.1579(7) | 0.027(3) |
| C2 | 0.4690(8) | 0.6757(6) | 0.1566(7) | 0.029(3) |
| C3 | 0.4362(7) | 0.6364(6) | 0.2039(7) | 0.027(3) |
| C4 | 0.4789(8) | 0.5998(6) | 0.2499(7) | 0.028(3) |
| C5 | 0.5596(7) | 0.6028(6) | 0.2498(6) | 0.025(3) |
| C6 | 0.5934(7) | 0.6443(6) | 0.2050(6) | 0.023(3) |
| C7 | 0.5882(10) | 0.7232(8) | 0.1089(8) | 0.046(4) |
| H7A | 0.625637 | 0.697998 | 0.085827 | 0.069 |
| H7B | 0.613318 | 0.759070 | 0.133194 | 0.069 |
| H7C | 0.550593 | 0.740573 | 0.076106 | 0.069 |
| C8 | 0.4226(10) | 0.7155(8) | 0.1069(9) | 0.047(4) |
| H8A | 0.445714 | 0.714320 | 0.063563 | 0.070 |
| H8B | 0.420464 | 0.760355 | 0.122630 | 0.070 |
| H8C | 0.371469 | 0.697739 | 0.102133 | 0.070 |
| C9 | 0.3504(8) | 0.6398(9) | 0.2067(10) | 0.054(5) |
| H9A | 0.332531 | 0.681969 | 0.189942 | 0.081 |
| H9B | 0.336349 | 0.634344 | 0.253048 | 0.081 |
| H9C | 0.327299 | 0.605318 | 0.178986 | 0.081 |
| C10 | 0.4415(10) | 0.5589(8) | 0.2999(8) | 0.049(4) |
| H10A | 0.393128 | 0.543110 | 0.280508 | 0.073 |
| H10B | 0.432811 | 0.584767 | 0.339831 | 0.073 |
| H10C | 0.473945 | 0.521994 | 0.312318 | 0.073 |
| C11 | 0.6085(10) | 0.5681(8) | 0.3024(7) | 0.046(4) |
| H11A | 0.610731 | 0.521934 | 0.291394 | 0.070 |
| H11B | 0.587080 | 0.573485 | 0.346135 | 0.070 |
| H11C | 0.659457 | 0.586408 | 0.303726 | 0.070 |
| C12 | 0.6782(8) | 0.6563(9) | 0.2097(10) | 0.051(5) |
| H12A | 0.704318 | 0.616477 | 0.224074 | 0.076 |
| H12B | 0.689901 | 0.690771 | 0.242150 | 0.076 |
| H12C | 0.694791 | 0.669256 | 0.165749 | 0.076 |
| C1_19 | 0.0119(9) | 0.6802(6) | 0.6605(6) | 0.031(3) |
| C2_19 | -0.0572(7) | 0.6517(7) | 0.6748(7) | 0.028(3) |
| C3_19 | -0.0571(8) | 0.6020(7) | 0.7233(7) | 0.031(3) |
| C4_19 | 0.0081(8) | 0.5799(7) | 0.7549(6) | 0.029(3) |
| C5_19 | 0.0770(7) | 0.6073(6) | 0.7401(6) | 0.023(3) |
| C6_19 | 0.0790(7) | 0.6582(7) | 0.6927(6) | 0.028(3) |
| C7_19 | 0.0097(12) | 0.7359(7) | 0.6120(8) | 0.053(5) |
| H7A_19 | 0.058155 | 0.738945 | 0.590927 | 0.080 |
| H7B_19 | 0.000300 | 0.776272 | 0.635935 | 0.080 |
| H7C_19 | -0.030680 | 0.728861 | 0.577565 | 0.080 |
| C8_19 | -0.1286(10) | 0.6795(10) | 0.6445(10) | 0.062(5) |
| H8A_19 | -0.129744 | 0.674032 | 0.595867 | 0.093 |
| H8B_19 | -0.131073 | 0.725739 | 0.655293 | 0.093 |
| H8C_19 | -0.171723 | 0.657127 | 0.662440 | 0.093 |
| C9_19 | -0.1324(9) | 0.5758(9) | 0.7458(9) | 0.049(4) |
| H9A_19 | -0.171744 | 0.583239 | 0.710466 | 0.074 |
| H9B_19 | -0.145821 | 0.598132 | 0.786643 | 0.074 |
| H9C_19 | -0.127754 | 0.529262 | 0.754562 | 0.074 |
| C10_19 | 0.0068(11) | 0.5277(8) | 0.8076(9) | 0.056(5) |
| H10A_19 | -0.033931 | 0.536446 | 0.837441 | 0.084 |
| H10B_19 | 0.055157 | 0.527144 | 0.833485 | 0.084 |
| H10C_19 | -0.001617 | 0.485536 | 0.785956 | 0.084 |
| C11_19 | 0.1483(8) | 0.5842(9) | 0.7784(7) | 0.043(4) |
| H11A_19 | 0.191835 | 0.591499 | 0.751342 | 0.064 |

| | | | | |
|---|---|---|---|---|
| H11B_19 | 0.143897 | 0.537838 | 0.788077 | 0.064 |
| H11C_19 | 0.154930 | 0.608263 | 0.820441 | 0.064 |
| C12_19 | 0.1530(9) | 0.6924(9) | 0.6821(9) | 0.052(5) |
| H12A_19 | 0.148027 | 0.718570 | 0.641336 | 0.078 |
| H12B_19 | 0.192916 | 0.660148 | 0.677690 | 0.078 |
| H12C_19 | 0.165780 | 0.720442 | 0.720471 | 0.078 |
| C1_18 | 0.7040(6) | 0.5214(5) | 0.1216(6) | 0.026(3) |
| C2_18 | 0.6812(5) | 0.4746(5) | 0.1652(5) | 0.022(2) |
| C3_18 | 0.7321(6) | 0.4404(6) | 0.2043(6) | 0.026(3) |
| H3_18 | 0.715822 | 0.408495 | 0.234599 | 0.031 |
| C4_18 | 0.8082(6) | 0.4532(6) | 0.1989(6) | 0.029(3) |
| H4_18 | 0.844844 | 0.429303 | 0.224878 | 0.035 |
| C5_18 | 0.8305(7) | 0.5005(6) | 0.1558(7) | 0.033(3) |
| H5_18 | 0.882771 | 0.509114 | 0.152791 | 0.040 |
| C6_18 | 0.7788(6) | 0.5359(6) | 0.1167(6) | 0.029(3) |
| H6_18 | 0.794479 | 0.568956 | 0.087567 | 0.034 |
| F1_18 | 0.6482(4) | 0.5549(4) | 0.0872(3) | 0.0270(16) |
| F2_18 | 0.6042(4) | 0.4656(4) | 0.1678(4) | 0.0299(17) |
| C1_17 | -0.1142(6) | 0.4485(6) | 0.6394(6) | 0.031(3) |
| C2_17 | -0.1470(6) | 0.4932(5) | 0.5971(6) | 0.029(3) |
| C3_17 | -0.2232(7) | 0.4943(7) | 0.5818(7) | 0.044(4) |
| H3_17 | -0.245582 | 0.525324 | 0.551853 | 0.053 |
| C4_17 | -0.2660(8) | 0.4474(8) | 0.6125(8) | 0.049(4) |
| H4_17 | -0.318999 | 0.446323 | 0.603641 | 0.059 |
| C5_17 | -0.2324(8) | 0.4024(8) | 0.6559(8) | 0.053(4) |
| H5_17 | -0.263050 | 0.370968 | 0.675909 | 0.063 |
| C6_17 | -0.1559(7) | 0.4020(7) | 0.6706(7) | 0.039(3) |
| H6_17 | -0.132907 | 0.371350 | 0.700645 | 0.047 |
| F1_17 | -0.0373(4) | 0.4532(3) | 0.6515(4) | 0.0318(18) |
| F2_17 | -0.1012(4) | 0.5394(4) | 0.5706(4) | 0.0327(18) |
| C1_16 | 0.3815(6) | 0.4456(6) | 0.1624(6) | 0.031(3) |
| C2_16 | 0.3429(6) | 0.4873(6) | 0.1210(6) | 0.035(3) |
| C3_16 | 0.2663(7) | 0.4815(7) | 0.1071(7) | 0.047(4) |
| H3_16 | 0.239744 | 0.510825 | 0.077941 | 0.056 |
| C4_16 | 0.2298(8) | 0.4311(8) | 0.1374(8) | 0.054(4) |
| H4_16 | 0.177178 | 0.425145 | 0.128519 | 0.064 |
| C5_16 | 0.2691(7) | 0.3893(8) | 0.1805(9) | 0.054(4) |
| H5_16 | 0.242576 | 0.355972 | 0.201908 | 0.065 |
| C6_16 | 0.3461(7) | 0.3949(7) | 0.1931(8) | 0.045(4) |
| H6_16 | 0.373317 | 0.365374 | 0.221554 | 0.054 |
| F1_16 | 0.4578(4) | 0.4559(4) | 0.1733(4) | 0.0307(17) |
| F2_16 | 0.3845(4) | 0.5367(4) | 0.0944(4) | 0.0318(17) |
| C1_15 | 0.2120(6) | 0.5254(5) | 0.6252(6) | 0.025(2) |
| C2_15 | 0.1868(6) | 0.4737(5) | 0.6615(5) | 0.027(3) |
| C3_15 | 0.2353(6) | 0.4382(6) | 0.7024(6) | 0.028(3) |
| H3_15 | 0.217812 | 0.402728 | 0.727540 | 0.034 |
| C4_15 | 0.3105(6) | 0.4555(7) | 0.7058(7) | 0.036(3) |
| H4_15 | 0.345476 | 0.431466 | 0.733457 | 0.043 |
| C5_15 | 0.3356(7) | 0.5078(6) | 0.6693(7) | 0.035(3) |
| H5_15 | 0.387440 | 0.519161 | 0.672319 | 0.042 |
| C6_15 | 0.2861(6) | 0.5431(7) | 0.6287(7) | 0.037(3) |
| H6_15 | 0.303108 | 0.578956 | 0.603886 | 0.044 |
| F1_15 | 0.1580(4) | 0.5588(4) | 0.5876(4) | 0.0303(17) |
| F2_15 | 0.1104(4) | 0.4623(3) | 0.6576(4) | 0.0286(17) |
| O1_14 | 0.0950(5) | 0.6270(4) | 0.4048(5) | 0.032(2) |

| | | | | |
|---|---|---|---|---|
| C1_14 | 0.1569(6) | 0.6656(5) | 0.3984(5) | 0.029(2) |
| C2_14 | 0.2284(6) | 0.6225(6) | 0.4079(7) | 0.044(3) |
| F1_14 | 0.2352(6) | 0.5847(5) | 0.3537(5) | 0.066(3) |
| F2_14 | 0.2907(4) | 0.6571(5) | 0.4186(5) | 0.061(3) |
| F3_14 | 0.2227(5) | 0.5826(5) | 0.4608(5) | 0.056(3) |
| C3_14 | 0.1586(7) | 0.7195(6) | 0.4525(6) | 0.045(3) |
| F4_14 | 0.0901(5) | 0.7450(5) | 0.4577(5) | 0.051(2) |
| F5_14 | 0.1793(6) | 0.6938(5) | 0.5128(4) | 0.064(3) |
| F6_14 | 0.2062(5) | 0.7672(4) | 0.4396(5) | 0.051(2) |
| C4_14 | 0.1550(6) | 0.6963(6) | 0.3282(6) | 0.041(3) |
| F7_14 | 0.1019(5) | 0.7432(5) | 0.3248(5) | 0.058(3) |
| F8_14 | 0.2207(4) | 0.7222(5) | 0.3142(4) | 0.049(2) |
| F9_14 | 0.1350(6) | 0.6543(5) | 0.2813(4) | 0.057(3) |
| O1_13 | -0.0248(5) | 0.5369(4) | 0.4139(4) | 0.0251(19) |
| C1_13 | -0.0114(6) | 0.4740(5) | 0.4035(5) | 0.028(2) |
| C2_13 | 0.0448(7) | 0.4473(5) | 0.4590(6) | 0.034(3) |
| F1_13 | 0.0217(5) | 0.4621(4) | 0.5204(4) | 0.044(2) |
| F2_13 | 0.0545(6) | 0.3840(4) | 0.4562(5) | 0.056(3) |
| F3_13 | 0.1123(5) | 0.4743(5) | 0.4547(5) | 0.056(3) |
| C3_13 | 0.0224(7) | 0.4633(6) | 0.3344(6) | 0.038(3) |
| F4_13 | -0.0267(5) | 0.4798(5) | 0.2852(4) | 0.050(2) |
| F5_13 | 0.0816(6) | 0.5017(6) | 0.3271(5) | 0.082(4) |
| F6_13 | 0.0434(7) | 0.4032(5) | 0.3234(5) | 0.074(3) |
| C4_13 | -0.0871(7) | 0.4373(5) | 0.4050(6) | 0.036(3) |
| F7_13 | -0.1405(5) | 0.4668(6) | 0.3682(5) | 0.068(3) |
| F8_13 | -0.0832(6) | 0.3775(5) | 0.3811(8) | 0.099(5) |
| F9_13 | -0.1117(7) | 0.4352(7) | 0.4651(5) | 0.086(4) |
| O1_12 | -0.0584(5) | 0.6683(4) | 0.4282(5) | 0.032(2) |
| C1_12 | -0.1157(6) | 0.6897(5) | 0.3877(5) | 0.030(2) |
| C2_12 | -0.1911(6) | 0.6712(6) | 0.4182(6) | 0.039(3) |
| F1_12 | -0.2005(5) | 0.7053(5) | 0.4746(4) | 0.054(2) |
| F2_12 | -0.2509(4) | 0.6818(5) | 0.3775(4) | 0.048(2) |
| F3_12 | -0.1908(5) | 0.6091(4) | 0.4367(4) | 0.050(2) |
| C3_12 | -0.1159(6) | 0.6604(6) | 0.3169(5) | 0.031(3) |
| F4_12 | -0.0450(4) | 0.6552(5) | 0.2984(4) | 0.046(2) |
| F5_12 | -0.1450(5) | 0.6010(4) | 0.3140(4) | 0.043(2) |
| F6_12 | -0.1543(4) | 0.6956(4) | 0.2710(4) | 0.0358(19) |
| C4_12 | -0.1100(6) | 0.7642(5) | 0.3829(6) | 0.038(3) |
| F7_12 | -0.0538(5) | 0.7808(4) | 0.3445(5) | 0.051(2) |
| F8_12 | -0.1723(5) | 0.7928(4) | 0.3576(5) | 0.052(2) |
| F9_12 | -0.0933(6) | 0.7896(4) | 0.4429(5) | 0.056(3) |
| O1_11 | 0.4861(5) | 0.5233(4) | -0.0902(5) | 0.036(2) |
| C1_11 | 0.4858(6) | 0.4583(5) | -0.0819(5) | 0.028(2) |
| C2_11 | 0.5143(7) | 0.4263(6) | -0.1454(6) | 0.038(3) |
| F1_11 | 0.5890(5) | 0.4301(6) | -0.1471(5) | 0.073(3) |
| F2_11 | 0.4967(7) | 0.3622(5) | -0.1482(5) | 0.070(3) |
| F3_11 | 0.4841(5) | 0.4537(4) | -0.2010(4) | 0.043(2) |
| C3_11 | 0.4032(7) | 0.4356(6) | -0.0720(6) | 0.040(3) |
| F4_11 | 0.3712(5) | 0.4756(5) | -0.0290(4) | 0.057(3) |
| F5_11 | 0.3617(5) | 0.4401(5) | -0.1285(4) | 0.050(2) |
| F6_11 | 0.3995(6) | 0.3774(5) | -0.0463(6) | 0.064(3) |
| C4_11 | 0.5366(6) | 0.4373(5) | -0.0204(6) | 0.033(3) |
| F7_11 | 0.5060(5) | 0.4548(4) | 0.0372(4) | 0.0363(18) |
| F8_11 | 0.5489(5) | 0.3737(4) | -0.0172(4) | 0.045(2) |
| F9_11 | 0.6037(4) | 0.4671(4) | -0.0201(5) | 0.046(2) |

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|---|---|---|---|---|
| O1_10 | 0.6064(5) | 0.6139(5) | -0.0676(5) | 0.034(2) |
| C1_10 | 0.6626(6) | 0.6384(5) | -0.1047(5) | 0.030(2) |
| C2_10 | 0.6559(7) | 0.7131(6) | -0.1090(6) | 0.043(3) |
| F1_10 | 0.6027(5) | 0.7298(5) | -0.1551(5) | 0.051(2) |
| F2_10 | 0.7205(5) | 0.7404(5) | -0.1257(6) | 0.070(3) |
| F3_10 | 0.6391(6) | 0.7379(5) | -0.0502(5) | 0.066(3) |
| C3_10 | 0.7379(6) | 0.6194(6) | -0.0676(6) | 0.032(3) |
| F4_10 | 0.7385(4) | 0.5575(4) | -0.0496(4) | 0.0411(19) |
| F5_10 | 0.7506(5) | 0.6535(4) | -0.0120(4) | 0.045(2) |
| F6_10 | 0.7968(4) | 0.6285(5) | -0.1056(4) | 0.056(3) |
| C4_10 | 0.6580(7) | 0.6091(6) | -0.1755(6) | 0.042(3) |
| F7_10 | 0.6842(6) | 0.5483(5) | -0.1747(5) | 0.064(3) |
| F8_10 | 0.6982(5) | 0.6444(6) | -0.2177(4) | 0.064(3) |
| F9_10 | 0.5870(5) | 0.6074(5) | -0.1999(5) | 0.060(3) |
| O1_9 | 0.4571(4) | 0.6592(4) | -0.0900(4) | 0.028(2) |
| C1_9 | 0.3935(6) | 0.6790(5) | -0.1231(5) | 0.027(2) |
| C2_9 | 0.3973(6) | 0.6639(6) | -0.1988(6) | 0.035(3) |
| F1_9 | 0.4467(4) | 0.7033(4) | -0.2264(4) | 0.042(2) |
| F2_9 | 0.3316(4) | 0.6704(5) | -0.2330(4) | 0.048(2) |
| F3_9 | 0.4218(5) | 0.6033(4) | -0.2079(4) | 0.046(2) |
| C3_9 | 0.3228(6) | 0.6463(6) | -0.0958(6) | 0.035(3) |
| F4_9 | 0.3302(5) | 0.6405(5) | -0.0298(4) | 0.055(3) |
| F5_9 | 0.3147(5) | 0.5860(4) | -0.1195(5) | 0.047(2) |
| F6_9 | 0.2591(4) | 0.6778(4) | -0.1112(4) | 0.042(2) |
| C4_9 | 0.3870(6) | 0.7531(5) | -0.1135(6) | 0.035(3) |
| F7_9 | 0.3669(5) | 0.7668(4) | -0.0520(4) | 0.048(2) |
| F8_9 | 0.3355(5) | 0.7803(4) | -0.1564(4) | 0.048(2) |
| F9_9 | 0.4519(4) | 0.7828(4) | -0.1227(5) | 0.048(2) |
| O1_8 | 0.3877(5) | 0.3209(5) | 0.4377(5) | 0.041(3) |
| C1_8 | 0.3329(6) | 0.3651(6) | 0.4387(6) | 0.038(3) |
| C2_8 | 0.3659(8) | 0.4306(6) | 0.4140(7) | 0.060(4) |
| F1_8 | 0.3663(7) | 0.4273(5) | 0.3460(5) | 0.072(3) |
| F2_8 | 0.3249(7) | 0.4805(5) | 0.4305(7) | 0.084(4) |
| F3_8 | 0.4348(5) | 0.4416(5) | 0.4435(5) | 0.060(3) |
| C3_8 | 0.3005(7) | 0.3742(7) | 0.5093(6) | 0.052(3) |
| F4_8 | 0.2956(5) | 0.3160(5) | 0.5384(5) | 0.058(3) |
| F5_8 | 0.3517(7) | 0.4101(6) | 0.5479(6) | 0.081(3) |
| F6_8 | 0.2355(6) | 0.4041(6) | 0.5080(6) | 0.079(4) |
| C4_8 | 0.2662(7) | 0.3445(7) | 0.3906(7) | 0.059(4) |
| F7_8 | 0.2226(6) | 0.3021(6) | 0.4224(7) | 0.089(4) |
| F8_8 | 0.2242(6) | 0.3971(7) | 0.3718(6) | 0.092(4) |
| F9_8 | 0.2916(6) | 0.3184(5) | 0.3354(5) | 0.063(3) |
| O1_7 | 0.479(2) | 0.2118(11) | 0.4499(19) | 0.037(2) |
| C1_7 | 0.4458(10) | 0.1540(9) | 0.4399(8) | 0.032(4) |
| C2_7 | 0.4116(10) | 0.1287(9) | 0.5045(8) | 0.032(4) |
| F1_7 | 0.4642(9) | 0.1089(10) | 0.5486(8) | 0.046(5) |
| F2_7 | 0.3672(17) | 0.0768(12) | 0.4935(13) | 0.075(10) |
| F3_7 | 0.3722(16) | 0.1736(13) | 0.5340(12) | 0.054(7) |
| C3_7 | 0.3802(11) | 0.1586(9) | 0.3859(9) | 0.049(5) |
| F4_7 | 0.4005(15) | 0.1961(11) | 0.3358(11) | 0.054(6) |
| F5_7 | 0.3176(10) | 0.1853(10) | 0.4090(10) | 0.059(5) |
| F6_7 | 0.3593(15) | 0.1011(9) | 0.3616(14) | 0.073(7) |
| C4_7 | 0.5046(11) | 0.1043(8) | 0.4176(11) | 0.050(5) |
| F7_7 | 0.5202(18) | 0.1169(17) | 0.3542(12) | 0.093(10) |
| F8_7 | 0.4800(12) | 0.0436(8) | 0.4223(15) | 0.088(10) |

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|---|---|---|---|---|
| F9_7 | 0.5687(10) | 0.1084(10) | 0.4544(13) | 0.053(5) |
| O1_6 | 0.4689(5) | 0.3013(5) | 0.5583(4) | 0.028(2) |
| C1_6 | 0.5047(6) | 0.3078(5) | 0.6182(5) | 0.025(2) |
| C2_6 | 0.4508(7) | 0.2819(6) | 0.6710(6) | 0.038(3) |
| F1_6 | 0.4434(6) | 0.2183(4) | 0.6663(5) | 0.062(3) |
| F2_6 | 0.4757(5) | 0.2954(5) | 0.7332(4) | 0.054(2) |
| F3_6 | 0.3826(4) | 0.3068(4) | 0.6625(4) | 0.047(2) |
| C3_6 | 0.5245(7) | 0.3794(5) | 0.6344(6) | 0.036(3) |
| F4_6 | 0.5518(4) | 0.4078(4) | 0.5811(4) | 0.0357(18) |
| F5_6 | 0.4663(5) | 0.4122(4) | 0.6542(5) | 0.050(2) |
| F6_6 | 0.5781(5) | 0.3859(5) | 0.6853(4) | 0.049(2) |
| C4_6 | 0.5782(6) | 0.2683(6) | 0.6228(6) | 0.038(3) |
| F7_6 | 0.6323(4) | 0.2968(5) | 0.5903(4) | 0.049(2) |
| F8_6 | 0.6060(6) | 0.2570(6) | 0.6836(5) | 0.068(3) |
| F9_6 | 0.5679(6) | 0.2109(5) | 0.5923(6) | 0.075(3) |
| O1_5 | 0.5492(4) | 0.3292(5) | 0.4463(4) | 0.028(2) |
| C1_5 | 0.6001(6) | 0.3363(5) | 0.3984(5) | 0.029(2) |
| C2_5 | 0.6494(7) | 0.3957(6) | 0.4168(6) | 0.045(3) |
| F1_5 | 0.6986(5) | 0.3823(6) | 0.4685(4) | 0.065(3) |
| F2_5 | 0.6894(6) | 0.4163(5) | 0.3653(5) | 0.066(3) |
| F3_5 | 0.6086(6) | 0.4448(4) | 0.4369(5) | 0.062(3) |
| C3_5 | 0.5590(6) | 0.3479(6) | 0.3289(6) | 0.033(3) |
| F4_5 | 0.5019(4) | 0.3077(4) | 0.3187(4) | 0.0376(19) |
| F5_5 | 0.5319(6) | 0.4082(4) | 0.3238(5) | 0.055(2) |
| F6_5 | 0.6046(5) | 0.3397(5) | 0.2781(4) | 0.048(2) |
| C4_5 | 0.6507(7) | 0.2750(6) | 0.3951(7) | 0.048(3) |
| F7_5 | 0.6152(5) | 0.2277(4) | 0.3612(5) | 0.053(2) |
| F8_5 | 0.7152(5) | 0.2865(6) | 0.3660(6) | 0.072(3) |
| F9_5 | 0.6686(6) | 0.2531(6) | 0.4568(5) | 0.071(3) |
| O1_4 | 0.0943(4) | 0.8274(4) | 0.0667(4) | 0.0259(19) |
| C1_4 | 0.1660(5) | 0.8391(5) | 0.0884(5) | 0.022(2) |
| C2_4 | 0.1911(6) | 0.7953(5) | 0.1482(6) | 0.029(2) |
| F1_4 | 0.2075(4) | 0.7349(3) | 0.1282(4) | 0.0389(19) |
| F2_4 | 0.2504(4) | 0.8160(4) | 0.1850(4) | 0.040(2) |
| F3_4 | 0.1339(4) | 0.7869(4) | 0.1895(4) | 0.042(2) |
| C3_4 | 0.1705(6) | 0.9116(5) | 0.1129(6) | 0.031(3) |
| F4_4 | 0.1339(4) | 0.9500(4) | 0.0693(4) | 0.0386(19) |
| F5_4 | 0.1397(5) | 0.9170(4) | 0.1715(4) | 0.046(2) |
| F6_4 | 0.2422(4) | 0.9312(4) | 0.1207(5) | 0.047(2) |
| C4_4 | 0.2222(6) | 0.8290(6) | 0.0323(6) | 0.032(3) |
| F7_4 | 0.2165(5) | 0.8775(4) | -0.0124(4) | 0.047(2) |
| F8_4 | 0.2932(4) | 0.8243(4) | 0.0563(4) | 0.042(2) |
| F9_4 | 0.2041(4) | 0.7747(4) | -0.0013(4) | 0.043(2) |
| O1_3 | 0.0518(5) | 0.6970(4) | 0.0599(4) | 0.0234(18) |
| C1_3 | 0.0457(6) | 0.6326(5) | 0.0521(5) | 0.027(2) |
| C2_3 | -0.0335(7) | 0.6137(6) | 0.0244(7) | 0.048(3) |
| F1_3 | -0.0835(5) | 0.6206(5) | 0.0733(7) | 0.082(4) |
| F2_3 | -0.0412(5) | 0.5527(4) | 0.0060(5) | 0.060(3) |
| F3_3 | -0.0592(6) | 0.6539(5) | -0.0228(6) | 0.081(4) |
| C3_3 | 0.1048(7) | 0.6082(6) | 0.0033(6) | 0.038(3) |
| F4_3 | 0.1708(5) | 0.6340(5) | 0.0167(6) | 0.065(3) |
| F5_3 | 0.0835(7) | 0.6242(6) | -0.0593(5) | 0.080(4) |
| F6_3 | 0.1125(6) | 0.5439(4) | 0.0043(5) | 0.057(3) |
| C4_3 | 0.0612(7) | 0.5996(6) | 0.1213(6) | 0.040(3) |
| F7_3 | 0.1350(5) | 0.6015(5) | 0.1392(5) | 0.057(2) |

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| F8_3 | 0.0421(6) | 0.5375(4) | 0.1212(5) | 0.058(3) |
| F9_3 | 0.0269(7) | 0.6298(5) | 0.1686(5) | 0.069(3) |
| O1_2 | -0.0587(4) | 0.7980(4) | 0.0499(4) | 0.0236(18) |
| C1_2 | -0.1049(5) | 0.8249(5) | 0.0940(5) | 0.027(2) |
| C2_2 | -0.1166(6) | 0.8976(5) | 0.0775(5) | 0.029(2) |
| F1_2 | -0.1619(4) | 0.9056(4) | 0.0223(4) | 0.0394(19) |
| F2_2 | -0.1494(5) | 0.9294(4) | 0.1268(4) | 0.041(2) |
| F3_2 | -0.0514(4) | 0.9266(4) | 0.0673(4) | 0.0352(18) |
| C3_2 | -0.0715(6) | 0.8189(6) | 0.1674(5) | 0.032(3) |
| F4_2 | -0.0417(5) | 0.7608(4) | 0.1768(4) | 0.043(2) |
| F5_2 | -0.0184(4) | 0.8623(4) | 0.1805(4) | 0.0389(19) |
| F6_2 | -0.1250(5) | 0.8260(4) | 0.2128(4) | 0.047(2) |
| C4_2 | -0.1826(6) | 0.7896(6) | 0.0871(6) | 0.038(3) |
| F7_2 | -0.1779(5) | 0.7311(4) | 0.1149(5) | 0.053(2) |
| F8_2 | -0.2373(4) | 0.8228(5) | 0.1157(5) | 0.056(3) |
| F9_2 | -0.2049(4) | 0.7814(4) | 0.0233(5) | 0.046(2) |
| O1_1 | 0.0331(4) | 0.7719(4) | -0.0559(4) | 0.0213(17) |
| C1_1 | 0.0154(5) | 0.8004(5) | -0.1144(5) | 0.023(2) |
| C2_1 | -0.0596(6) | 0.7728(5) | -0.1459(5) | 0.031(3) |
| F1_1 | -0.0515(5) | 0.7121(4) | -0.1668(5) | 0.051(2) |
| F2_1 | -0.0885(5) | 0.8072(5) | -0.1970(4) | 0.052(2) |
| F3_1 | -0.1118(4) | 0.7710(4) | -0.1000(4) | 0.044(2) |
| C3_1 | 0.0081(6) | 0.8754(5) | -0.1075(5) | 0.027(2) |
| F4_1 | 0.0630(4) | 0.8985(4) | -0.0675(4) | 0.0328(17) |
| F5_1 | -0.0567(4) | 0.8913(4) | -0.0803(4) | 0.0343(18) |
| F6_1 | 0.0088(5) | 0.9062(4) | -0.1663(4) | 0.0372(19) |
| C4_1 | 0.0802(6) | 0.7856(5) | -0.1624(5) | 0.031(3) |
| F7_1 | 0.1416(4) | 0.8194(4) | -0.1447(4) | 0.042(2) |
| F8_1 | 0.0606(5) | 0.7989(4) | -0.2258(4) | 0.044(2) |
| F9_1 | 0.0984(5) | 0.7230(4) | -0.1604(4) | 0.043(2) |
| Ca1 | 0.51794(13) | 0.55035(12) | 0.12317(12) | 0.0207(5) |
| F1 | 0.5079(4) | 0.5939(4) | 0.0240(3) | 0.0280(16) |
| Ca2 | 0.02650(13) | 0.55145(12) | 0.61621(12) | 0.0203(5) |
| Al4 | 0.02991(19) | 0.77371(16) | 0.03038(17) | 0.0176(7) |
| Al1 | 0.51407(19) | 0.59805(17) | -0.06099(18) | 0.0193(7) |
| Al2 | 0.01141(19) | 0.61117(18) | 0.43743(18) | 0.0197(8) |
| Al3 | 0.47093(19) | 0.29039(18) | 0.47271(19) | 0.0210(8) |
| F2 | 0.0269(4) | 0.6061(4) | 0.5225(3) | 0.0265(16) |

*Table S 3 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [CaHMB(oDFB)$_2${f-al}][al-f-al] **3**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| O1_11 | 0.7283(14) | 0.7087(13) | 0.6531(12) | 0.047(5) |
| C1_11 | 0.7224(6) | 0.6622(8) | 0.6963(7) | 0.039(3) |
| C2_11 | 0.7134(8) | 0.5874(8) | 0.6660(8) | 0.043(4) |
| F1_11 | 0.7707(7) | 0.5731(10) | 0.6704(8) | 0.070(3) |
| F2_11 | 0.6942(7) | 0.5392(10) | 0.6945(9) | 0.055(3) |
| F3_11 | 0.6709(8) | 0.5825(10) | 0.6017(7) | 0.084(4) |
| C3_11 | 0.6674(7) | 0.6824(7) | 0.7112(8) | 0.055(3) |
| F4_11 | 0.6792(10) | 0.7465(7) | 0.7401(9) | 0.097(4) |
| F5_11 | 0.6120(6) | 0.6886(8) | 0.6559(8) | 0.071(3) |

| | | | | |
|---|---|---|---|---|
| F6_11 | 0.6602(11) | 0.6381(6) | 0.7525(10) | 0.105(6) |
| C4_11 | 0.7870(8) | 0.6585(9) | 0.7637(8) | 0.079(4) |
| F7_11 | 0.7987(13) | 0.7198(10) | 0.7932(10) | 0.133(6) |
| F8_11 | 0.7857(8) | 0.6061(9) | 0.8015(6) | 0.119(6) |
| F9_11 | 0.8326(6) | 0.6431(10) | 0.7480(8) | 0.105(4) |
| C1_18 | 0.74214(14) | 0.79405(14) | 0.43383(14) | 0.0279(6) |
| C2_18 | 0.79756(13) | 0.75160(14) | 0.45377(13) | 0.0262(5) |
| C3_18 | 0.79074(12) | 0.68006(14) | 0.43589(13) | 0.0240(5) |
| C4_18 | 0.72885(13) | 0.65006(14) | 0.39713(13) | 0.0262(5) |
| C5_18 | 0.67362(13) | 0.69362(17) | 0.37571(14) | 0.0307(6) |
| C6_18 | 0.68029(14) | 0.76479(16) | 0.39479(14) | 0.0319(6) |
| C7_18 | 0.7497(2) | 0.87196(16) | 0.45262(19) | 0.0475(9) |
| H7A_18 | 0.757123 | 0.898920 | 0.419669 | 0.071 |
| H7B_18 | 0.786747 | 0.878161 | 0.497698 | 0.071 |
| H7C_18 | 0.710250 | 0.889045 | 0.452626 | 0.071 |
| C8_18 | 0.86450(16) | 0.7839(2) | 0.49073(17) | 0.0437(8) |
| H8A_18 | 0.891959 | 0.764360 | 0.472756 | 0.066 |
| H8B_18 | 0.883559 | 0.772991 | 0.538985 | 0.066 |
| H8C_18 | 0.861336 | 0.835315 | 0.484399 | 0.066 |
| C9_18 | 0.85067(15) | 0.63528(19) | 0.45562(17) | 0.0409(7) |
| H9A_18 | 0.839015 | 0.585100 | 0.452074 | 0.061 |
| H9B_18 | 0.882866 | 0.646129 | 0.502217 | 0.061 |
| H9C_18 | 0.868904 | 0.645633 | 0.425325 | 0.061 |
| C10_18 | 0.72190(19) | 0.57297(17) | 0.37610(18) | 0.0424(8) |
| H10A_18 | 0.724407 | 0.568721 | 0.333966 | 0.064 |
| H10B_18 | 0.679947 | 0.555037 | 0.369192 | 0.064 |
| H10C_18 | 0.756843 | 0.545350 | 0.411556 | 0.064 |
| C11_18 | 0.60680(15) | 0.6654(3) | 0.32872(17) | 0.0529(10) |
| H11A_18 | 0.590605 | 0.687708 | 0.284307 | 0.079 |
| H11B_18 | 0.577414 | 0.676103 | 0.347245 | 0.079 |
| H11C_18 | 0.609068 | 0.614065 | 0.324135 | 0.079 |
| C12_18 | 0.6209(2) | 0.8114(3) | 0.3703(2) | 0.0665(12) |
| H12A_18 | 0.606848 | 0.825559 | 0.323473 | 0.100 |
| H12B_18 | 0.631399 | 0.853596 | 0.398845 | 0.100 |
| H12C_18 | 0.585962 | 0.785147 | 0.372687 | 0.100 |
| C1_17 | 0.57126(13) | 0.64639(14) | 0.46613(14) | 0.0273(5) |
| C2_17 | 0.59460(13) | 0.58246(15) | 0.45858(15) | 0.0298(6) |
| C3_17 | 0.55533(15) | 0.52459(16) | 0.43230(17) | 0.0370(7) |
| H3_17 | 0.571879 | 0.480726 | 0.426541 | 0.044 |
| C4_17 | 0.49022(15) | 0.53288(18) | 0.41443(16) | 0.0381(7) |
| H4_17 | 0.461548 | 0.493841 | 0.396426 | 0.046 |
| C5_17 | 0.46661(14) | 0.59729(18) | 0.42251(16) | 0.0379(7) |
| H5_17 | 0.421962 | 0.601786 | 0.410056 | 0.045 |
| C6_17 | 0.50732(13) | 0.65549(17) | 0.44861(15) | 0.0322(6) |
| H6_17 | 0.491313 | 0.699854 | 0.454050 | 0.039 |
| F1_17 | 0.61555(8) | 0.70063(8) | 0.49184(9) | 0.0338(4) |
| F2_17 | 0.65995(8) | 0.57949(9) | 0.47833(10) | 0.0361(4) |
| C1_16 | 0.87975(13) | 0.62880(14) | 0.63161(13) | 0.0261(5) |
| C2_16 | 0.85170(12) | 0.56631(14) | 0.60096(13) | 0.0246(5) |
| C3_16 | 0.88350(14) | 0.50299(15) | 0.62158(14) | 0.0297(6) |
| H3_16 | 0.863540 | 0.459806 | 0.600296 | 0.036 |
| C4_16 | 0.94600(14) | 0.50465(16) | 0.67477(15) | 0.0323(6) |
| H4_16 | 0.969440 | 0.461692 | 0.690471 | 0.039 |
| C5_16 | 0.97478(14) | 0.56730(17) | 0.70532(15) | 0.0335(6) |
| H5_16 | 1.017870 | 0.566815 | 0.741466 | 0.040 |

| | | | | |
|---|---|---|---|---|
| C6_16 | 0.94200(13) | 0.63153(16) | 0.68431(14) | 0.0311(6) |
| H6_16 | 0.961611 | 0.674961 | 0.705268 | 0.037 |
| F1_16 | 0.84255(8) | 0.68889(8) | 0.60703(9) | 0.0329(4) |
| F2_16 | 0.78933(8) | 0.57044(8) | 0.54842(8) | 0.0290(3) |
| O1_14 | 0.6427(13) | 0.2214(13) | 0.8066(13) | 0.028(5) |
| C1_14 | 0.6370(7) | 0.1731(8) | 0.7598(7) | 0.036(4) |
| C2_14 | 0.6184(8) | 0.2084(8) | 0.6903(8) | 0.060(3) |
| F1_14 | 0.5538(8) | 0.2206(10) | 0.6648(9) | 0.0541(7) |
| F2_14 | 0.6399(11) | 0.1627(8) | 0.6578(8) | 0.070(5) |
| F3_14 | 0.6570(9) | 0.2639(7) | 0.6989(7) | 0.051(4) |
| C3_14 | 0.7003(8) | 0.1301(9) | 0.7842(9) | 0.053(4) |
| F4_14 | 0.7248(14) | 0.1217(17) | 0.8507(10) | 0.046(5) |
| F5_14 | 0.7431(10) | 0.1683(13) | 0.7737(13) | 0.064(4) |
| F6_14 | 0.6910(16) | 0.0686(10) | 0.7531(16) | 0.041(5) |
| C4_14 | 0.5805(7) | 0.1213(8) | 0.7478(8) | 0.052(4) |
| F7_14 | 0.6019(11) | 0.0741(13) | 0.7962(13) | 0.058(5) |
| F8_14 | 0.5570(8) | 0.0930(11) | 0.6864(9) | 0.069(5) |
| F9_14 | 0.5329(6) | 0.1597(8) | 0.7462(8) | 0.041(3) |
| O1_13 | 0.8494(8) | 0.3298(10) | 0.8528(9) | 0.0324(6) |
| C1_13 | 0.8800(8) | 0.3610(8) | 0.8210(8) | 0.045(4) |
| C2_13 | 0.8470(9) | 0.3372(11) | 0.7465(8) | 0.066(5) |
| F1_13 | 0.7896(11) | 0.3678(17) | 0.7108(14) | 0.074(5) |
| F2_13 | 0.8793(13) | 0.3555(16) | 0.7138(14) | 0.072(4) |
| F3_13 | 0.8333(14) | 0.2692(11) | 0.7403(12) | 0.066(5) |
| C3_13 | 0.9537(8) | 0.3460(10) | 0.8557(9) | 0.052(4) |
| F4_13 | 0.9775(10) | 0.3370(16) | 0.9222(9) | 0.061(4) |
| F5_13 | 0.9668(11) | 0.2871(10) | 0.8317(12) | 0.086(5) |
| F6_13 | 0.9898(13) | 0.3966(14) | 0.8494(15) | 0.064(5) |
| C4_13 | 0.8708(9) | 0.4420(8) | 0.8249(9) | 0.061(4) |
| F7_13 | 0.9091(10) | 0.4638(10) | 0.8868(9) | 0.069(4) |
| F8_13 | 0.8847(14) | 0.4753(14) | 0.7815(12) | 0.078(5) |
| F9_13 | 0.8116(10) | 0.4599(13) | 0.8116(15) | 0.066(5) |
| O1_12 | 0.6621(10) | 0.8460(14) | 0.6241(14) | 0.042(6) |
| C1_12 | 0.6047(8) | 0.8796(8) | 0.5890(7) | 0.033(4) |
| C2_12 | 0.5957(8) | 0.9025(9) | 0.5192(7) | 0.054(4) |
| F1_12 | 0.5849(10) | 0.8499(11) | 0.4782(9) | 0.080(4) |
| F2_12 | 0.5477(10) | 0.9486(10) | 0.4884(8) | 0.088(7) |
| F3_12 | 0.6531(11) | 0.9263(18) | 0.5270(16) | 0.085(5) |
| C3_12 | 0.6050(8) | 0.9494(8) | 0.6265(8) | 0.057(4) |
| F4_12 | 0.6236(11) | 0.9352(10) | 0.6909(8) | 0.062(4) |
| F5_12 | 0.6462(10) | 0.9945(9) | 0.6200(11) | 0.076(4) |
| F6_12 | 0.5445(8) | 0.9742(9) | 0.6017(9) | 0.050(3) |
| C4_12 | 0.5460(7) | 0.8344(8) | 0.5808(9) | 0.055(4) |
| F7_12 | 0.5459(11) | 0.8295(10) | 0.6391(10) | 0.063(4) |
| F8_12 | 0.4915(7) | 0.8620(11) | 0.5323(10) | 0.088(6) |
| F9_12 | 0.5483(8) | 0.7703(7) | 0.5590(9) | 0.054(3) |
| O1_10 | 0.8934(12) | 0.3298(10) | 0.9882(9) | 0.047(4) |
| C1_10 | 0.8955(5) | 0.3708(6) | 1.0387(6) | 0.042(3) |
| C2_10 | 0.9545(6) | 0.4211(6) | 1.0646(6) | 0.065(3) |
| F1_10 | 0.9435(7) | 0.4764(7) | 1.0253(6) | 0.085(3) |
| F2_10 | 0.9688(7) | 0.4463(9) | 1.1255(7) | 0.069(4) |
| F3_10 | 1.0063(9) | 0.3879(13) | 1.0687(12) | 0.077(4) |
| C3_10 | 0.9034(5) | 0.3203(5) | 1.0960(5) | 0.055(2) |
| F4_10 | 0.8632(9) | 0.2665(8) | 1.0742(10) | 0.072(4) |
| F5_10 | 0.9629(4) | 0.2950(6) | 1.1296(5) | 0.074(3) |

| | | | | |
|---|---|---|---|---|
| F6_10 | 0.8896(8) | 0.3528(8) | 1.1404(6) | 0.069(3) |
| C4_10 | 0.8313(5) | 0.4131(5) | 1.0143(5) | 0.055(3) |
| F7_10 | 0.7838(7) | 0.3706(11) | 1.0096(13) | 0.068(3) |
| F8_10 | 0.8376(5) | 0.4653(5) | 1.0561(5) | 0.075(3) |
| F9_10 | 0.8135(8) | 0.4393(10) | 0.9537(7) | 0.070(4) |
| O1_9 | 0.78639(10) | 0.84656(12) | 0.69492(10) | 0.0371(5) |
| C1_9 | 0.84576(13) | 0.87657(16) | 0.72294(14) | 0.0316(6) |
| C2_9 | 0.89789(16) | 0.8215(2) | 0.76711(18) | 0.0489(9) |
| F1_9 | 0.89649(12) | 0.81046(12) | 0.82462(10) | 0.0593(6) |
| F2_9 | 0.95719(10) | 0.84200(16) | 0.78131(14) | 0.0743(8) |
| F3_9 | 0.88533(12) | 0.75981(13) | 0.73487(13) | 0.0688(7) |
| C3_9 | 0.86132(18) | 0.9051(2) | 0.66744(18) | 0.0539(10) |
| F4_9 | 0.80917(13) | 0.93670(16) | 0.61893(11) | 0.0733(8) |
| F5_9 | 0.87670(12) | 0.85301(17) | 0.63884(13) | 0.0791(9) |
| F6_9 | 0.91045(12) | 0.95044(16) | 0.69177(12) | 0.0734(8) |
| C4_9 | 0.84736(16) | 0.93915(17) | 0.76799(17) | 0.0401(7) |
| F7_9 | 0.81767(13) | 0.99596(12) | 0.73114(13) | 0.0657(6) |
| F8_9 | 0.90707(10) | 0.95847(11) | 0.81175(10) | 0.0488(5) |
| F9_9 | 0.81717(11) | 0.92192(12) | 0.80290(11) | 0.0563(6) |
| O1_8 | 0.64963(16) | 0.8334(2) | 0.6105(2) | 0.0274(8) |
| C1_8 | 0.60991(18) | 0.8912(2) | 0.59086(19) | 0.0283(8) |
| C2_8 | 0.5482(2) | 0.8712(2) | 0.5259(2) | 0.0512(11) |
| F1_8 | 0.55898(19) | 0.8684(2) | 0.47395(16) | 0.0824(11) |
| F2_8 | 0.49929(14) | 0.91507(18) | 0.51181(18) | 0.0802(11) |
| F3_8 | 0.52786(13) | 0.80655(17) | 0.52966(18) | 0.0696(10) |
| C3_8 | 0.59062(19) | 0.90741(19) | 0.6467(2) | 0.0419(9) |
| F4_8 | 0.64442(18) | 0.90579(18) | 0.70716(14) | 0.0595(9) |
| F5_8 | 0.55084(18) | 0.85794(15) | 0.64818(19) | 0.0559(8) |
| F6_8 | 0.56230(17) | 0.96913(16) | 0.6388(2) | 0.0607(9) |
| C4_8 | 0.64335(19) | 0.9569(2) | 0.5802(2) | 0.0419(9) |
| F7_8 | 0.68453(13) | 0.98548(13) | 0.63830(16) | 0.0524(7) |
| F8_8 | 0.60076(15) | 1.00587(15) | 0.54291(17) | 0.0694(9) |
| F9_8 | 0.6760(2) | 0.9368(2) | 0.5481(2) | 0.0731(12) |
| O1_7 | 0.7200(5) | 0.7081(4) | 0.6456(4) | 0.0235(11) |
| C1_7 | 0.7078(3) | 0.6642(3) | 0.6874(3) | 0.0301(11) |
| C2_7 | 0.6387(4) | 0.6774(3) | 0.6796(4) | 0.0535(18) |
| F1_7 | 0.6392(4) | 0.7367(2) | 0.7119(4) | 0.089(2) |
| F2_7 | 0.6190(3) | 0.6253(2) | 0.7032(4) | 0.0785(17) |
| F3_7 | 0.5961(2) | 0.6887(2) | 0.6153(3) | 0.0716(14) |
| C3_7 | 0.7077(3) | 0.5877(3) | 0.6633(3) | 0.0327(14) |
| F4_7 | 0.7523(3) | 0.5791(3) | 0.6433(3) | 0.0590(15) |
| F5_7 | 0.6517(2) | 0.5748(3) | 0.6087(2) | 0.0533(11) |
| F6_7 | 0.7181(2) | 0.5392(3) | 0.7097(3) | 0.0409(11) |
| C4_7 | 0.7593(4) | 0.6730(3) | 0.7609(3) | 0.069(2) |
| F7_7 | 0.8160(3) | 0.6470(3) | 0.7722(3) | 0.096(2) |
| F8_7 | 0.7417(4) | 0.6408(3) | 0.8029(2) | 0.106(3) |
| F9_7 | 0.7676(5) | 0.7406(3) | 0.7780(3) | 0.109(3) |
| O1_6 | 0.86436(13) | 0.30380(14) | 0.84474(12) | 0.0324(6) |
| C1_6 | 0.88506(18) | 0.34861(19) | 0.81145(18) | 0.0318(7) |
| C2_6 | 0.89304(19) | 0.3038(2) | 0.75799(19) | 0.0408(8) |
| F1_6 | 0.94737(13) | 0.26601(14) | 0.78670(15) | 0.0551(7) |
| F2_6 | 0.89724(18) | 0.3443(2) | 0.71138(19) | 0.0572(8) |
| F3_6 | 0.84584(17) | 0.25926(17) | 0.72681(16) | 0.0525(8) |
| C3_6 | 0.8341(2) | 0.4078(2) | 0.7750(2) | 0.0474(10) |
| F4_6 | 0.81289(17) | 0.43202(19) | 0.8164(2) | 0.0612(10) |

| | | | | |
|---|---|---|---|---|
| F5_6 | 0.78280(18) | 0.3821(3) | 0.72165(19) | 0.0655(10) |
| F6_6 | 0.85798(18) | 0.46104(17) | 0.75529(18) | 0.0656(10) |
| C4_6 | 0.95015(19) | 0.3830(2) | 0.8607(2) | 0.0423(9) |
| F7_6 | 0.94219(14) | 0.43592(13) | 0.89476(14) | 0.0508(6) |
| F8_6 | 0.9813(2) | 0.4084(2) | 0.8276(2) | 0.0609(10) |
| F9_6 | 0.98911(14) | 0.3370(2) | 0.90585(16) | 0.0538(8) |
| O1_5 | 0.87471(9) | 0.19395(10) | 0.93260(10) | 0.0310(4) |
| C1_5 | 0.91651(11) | 0.13937(13) | 0.95272(13) | 0.0224(5) |
| C2_5 | 0.96937(13) | 0.15057(15) | 1.02704(14) | 0.0295(6) |
| F1_5 | 0.94346(9) | 0.14550(12) | 1.06853(9) | 0.0436(5) |
| F2_5 | 1.01731(8) | 0.10367(9) | 1.04723(9) | 0.0362(4) |
| F3_5 | 0.99547(9) | 0.21420(10) | 1.03487(9) | 0.0404(4) |
| C3_5 | 0.94901(13) | 0.13028(16) | 0.90684(14) | 0.0309(6) |
| F4_5 | 0.90566(9) | 0.13449(11) | 0.84234(8) | 0.0399(4) |
| F5_5 | 0.99200(9) | 0.18266(12) | 0.91947(10) | 0.0461(5) |
| F6_5 | 0.97984(10) | 0.06903(11) | 0.91717(10) | 0.0458(5) |
| C4_5 | 0.87759(13) | 0.07121(15) | 0.94813(15) | 0.0310(6) |
| F7_5 | 0.84254(8) | 0.05058(9) | 0.88475(9) | 0.0367(4) |
| F8_5 | 0.91659(9) | 0.01799(10) | 0.98334(12) | 0.0507(5) |
| F9_5 | 0.83710(9) | 0.08143(11) | 0.97305(9) | 0.0432(4) |
| O1_4 | 0.8972(6) | 0.3403(5) | 0.9781(4) | 0.0293(12) |
| C1_4 | 0.9032(3) | 0.3784(3) | 1.0317(3) | 0.0321(12) |
| C2_4 | 0.8820(3) | 0.4556(3) | 1.0071(2) | 0.0440(12) |
| F1_4 | 0.9269(3) | 0.4899(2) | 0.9994(2) | 0.0565(12) |
| F2_4 | 0.8698(2) | 0.4927(2) | 1.05056(18) | 0.0582(10) |
| F3_4 | 0.8293(3) | 0.4567(4) | 0.9485(3) | 0.0582(16) |
| C3_4 | 0.8593(3) | 0.3484(3) | 1.0603(3) | 0.0451(12) |
| F4_4 | 0.8633(4) | 0.2780(4) | 1.0616(4) | 0.0580(15) |
| F5_4 | 0.7971(3) | 0.3646(6) | 1.0190(5) | 0.0620(17) |
| F6_4 | 0.8749(3) | 0.3728(4) | 1.1212(3) | 0.0576(15) |
| C4_4 | 0.9746(2) | 0.3782(3) | 1.0880(2) | 0.0402(11) |
| F7_4 | 0.9884(2) | 0.3187(2) | 1.1232(2) | 0.0587(11) |
| F8_4 | 0.9879(3) | 0.4311(4) | 1.1315(3) | 0.0490(13) |
| F9_4 | 1.0144(4) | 0.3827(6) | 1.0611(6) | 0.0597(14) |
| O1_3 | 0.65471(19) | 0.22691(19) | 0.79899(18) | 0.0220(8) |
| C1_3 | 0.65453(16) | 0.17539(17) | 0.75658(16) | 0.0233(6) |
| C2_3 | 0.66954(14) | 0.10210(15) | 0.79178(15) | 0.0239(6) |
| F1_3 | 0.61951(16) | 0.07441(19) | 0.7949(2) | 0.0443(7) |
| F2_3 | 0.6887(2) | 0.05479(15) | 0.7613(2) | 0.0342(8) |
| F3_3 | 0.7161(2) | 0.1076(2) | 0.85502(15) | 0.0345(8) |
| C3_3 | 0.7070(2) | 0.19266(17) | 0.73459(18) | 0.0348(8) |
| F4_3 | 0.70562(16) | 0.26038(11) | 0.72017(14) | 0.0484(7) |
| F5_3 | 0.76582(12) | 0.17824(16) | 0.78452(15) | 0.0430(6) |
| F6_3 | 0.69793(15) | 0.15553(12) | 0.68015(11) | 0.0476(6) |
| C4_3 | 0.58640(17) | 0.17396(18) | 0.69448(18) | 0.0401(9) |
| F7_3 | 0.57942(15) | 0.23006(14) | 0.65437(12) | 0.0541(7) |
| F8_3 | 0.57659(14) | 0.11579(13) | 0.65740(13) | 0.0574(8) |
| F9_3 | 0.54111(11) | 0.17713(14) | 0.71248(15) | 0.0526(7) |
| O1_2 | 0.66683(9) | 0.35527(10) | 0.86640(10) | 0.0293(4) |
| C1_2 | 0.62531(12) | 0.40760(13) | 0.83305(14) | 0.0238(5) |
| C2_2 | 0.55782(13) | 0.37811(14) | 0.78188(15) | 0.0303(6) |
| F1_2 | 0.55766(9) | 0.35494(10) | 0.72570(9) | 0.0385(4) |
| F2_2 | 0.51125(9) | 0.42627(10) | 0.76415(12) | 0.0544(6) |
| F3_2 | 0.54200(8) | 0.32341(9) | 0.80771(10) | 0.0360(4) |
| C3_2 | 0.61831(15) | 0.45474(15) | 0.88603(17) | 0.0370(7) |

| | | | | |
|---|---|---|---|---|
| F4_2 | 0.67563(9) | 0.46762(10) | 0.93803(10) | 0.0419(4) |
| F5_2 | 0.58187(11) | 0.42217(11) | 0.90806(12) | 0.0540(6) |
| F6_2 | 0.59075(11) | 0.51670(10) | 0.86053(14) | 0.0611(6) |
| C4_2 | 0.65251(16) | 0.45214(18) | 0.79397(17) | 0.0420(7) |
| F7_2 | 0.70148(10) | 0.49245(11) | 0.83566(11) | 0.0488(5) |
| F8_2 | 0.60755(13) | 0.49460(13) | 0.74869(12) | 0.0721(8) |
| F9_2 | 0.67407(12) | 0.40960(14) | 0.76199(12) | 0.0629(7) |
| O1_1 | 0.70030(10) | 0.22895(11) | 0.94412(10) | 0.0323(4) |
| C1_1 | 0.67284(14) | 0.20441(15) | 0.98133(14) | 0.0302(6) |
| C2_1 | 0.68246(19) | 0.25833(19) | 1.03751(18) | 0.0467(8) |
| F1_1 | 0.74317(12) | 0.25794(14) | 1.08673(11) | 0.0622(6) |
| F2_1 | 0.64367(13) | 0.24306(14) | 1.06417(12) | 0.0640(7) |
| F3_1 | 0.66950(13) | 0.32293(11) | 1.01271(13) | 0.0638(6) |
| C3_1 | 0.59899(16) | 0.19075(17) | 0.93653(17) | 0.0399(7) |
| F4_1 | 0.58756(11) | 0.16069(14) | 0.87907(11) | 0.0611(6) |
| F5_1 | 0.56639(11) | 0.25099(12) | 0.92215(14) | 0.0625(6) |
| F6_1 | 0.57404(10) | 0.14861(10) | 0.96592(11) | 0.0466(5) |
| C4_1 | 0.70703(17) | 0.13411(17) | 1.01442(18) | 0.0418(7) |
| F7_1 | 0.68810(12) | 0.08247(10) | 0.96838(13) | 0.0575(6) |
| F8_1 | 0.69369(12) | 0.11264(13) | 1.06269(12) | 0.0620(6) |
| F9_1 | 0.77062(11) | 0.14051(13) | 1.04089(12) | 0.0593(6) |
| Ca01 | 0.73043(3) | 0.68535(3) | 0.51792(3) | 0.02299(12) |
| Al2 | 0.85818(4) | 0.28142(4) | 0.91532(4) | 0.02037(15) |
| Al3 | 0.72467(4) | 0.79976(4) | 0.63437(4) | 0.01955(15) |
| Al1 | 0.69334(4) | 0.27090(4) | 0.87396(4) | 0.01880(15) |
| F1 | 0.77484(7) | 0.28078(8) | 0.89225(8) | 0.0251(3) |
| F2 | 0.73541(8) | 0.78830(8) | 0.56476(8) | 0.0265(3) |

*Table S 4 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [BaHMB(oDFB)$_3${f-al}][al-f-al] **4**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| C1_25 | 0.2403(3) | 0.3054(5) | 0.6089(4) | 0.0286(17) |
| C2_25 | 0.2334(3) | 0.2426(5) | 0.5650(4) | 0.0270(16) |
| C3_25 | 0.1884(3) | 0.2184(6) | 0.5459(4) | 0.038(2) |
| H3_25 | 0.183707 | 0.174988 | 0.515913 | 0.045 |
| C4_25 | 0.1511(3) | 0.2604(6) | 0.5724(5) | 0.041(2) |
| H4_25 | 0.119621 | 0.246465 | 0.559737 | 0.050 |
| C5_25 | 0.1580(3) | 0.3222(6) | 0.6168(5) | 0.039(2) |
| H5_25 | 0.131310 | 0.349301 | 0.635049 | 0.046 |
| C6_25 | 0.2026(3) | 0.3451(5) | 0.6349(4) | 0.0343(19) |
| H6_25 | 0.207303 | 0.388119 | 0.665259 | 0.041 |
| F1_25 | 0.28663(16) | 0.3233(3) | 0.6247(2) | 0.0341(11) |
| F2_25 | 0.27352(16) | 0.2046(3) | 0.5408(2) | 0.0383(12) |
| C1_24 | 0.4301(3) | 0.4622(5) | 0.7037(4) | 0.0344(18) |
| C2_24 | 0.3877(3) | 0.4467(5) | 0.6741(4) | 0.0322(17) |
| C3_24 | 0.3571(3) | 0.5077(5) | 0.6545(4) | 0.037(2) |
| H3_24 | 0.326864 | 0.495372 | 0.636241 | 0.045 |
| C4_24 | 0.3718(4) | 0.5861(7) | 0.6622(5) | 0.052(3) |
| H4_24 | 0.352447 | 0.629309 | 0.646492 | 0.063 |
| C5_24 | 0.4153(4) | 0.6040(6) | 0.6931(4) | 0.052(3) |
| H5_24 | 0.424390 | 0.659034 | 0.699962 | 0.063 |

| | | | | |
|---|---|---|---|---|
| C6_24 | 0.4450(3) | 0.5415(6) | 0.7137(5) | 0.043(2) |
| H6_24 | 0.474608 | 0.552838 | 0.733988 | 0.052 |
| F1_24 | 0.4581(2) | 0.4003(5) | 0.7230(4) | 0.078(2) |
| F2_24 | 0.37461(17) | 0.3662(3) | 0.6644(2) | 0.0347(11) |
| C1_23 | 0.5010(3) | 0.2384(5) | 0.5306(4) | 0.0261(17) |
| C2_23 | 0.4980(2) | 0.2993(4) | 0.5745(4) | 0.0252(15) |
| C3_23 | 0.5381(3) | 0.3356(5) | 0.5996(4) | 0.0330(17) |
| H3_23 | 0.535888 | 0.379000 | 0.630143 | 0.040 |
| C4_23 | 0.5813(3) | 0.3073(5) | 0.5791(5) | 0.036(2) |
| H4_23 | 0.609406 | 0.330320 | 0.596979 | 0.044 |
| C5_23 | 0.5850(3) | 0.2460(5) | 0.5331(5) | 0.0320(18) |
| H5_23 | 0.615504 | 0.228714 | 0.519038 | 0.038 |
| C6_23 | 0.5448(3) | 0.2095(5) | 0.5072(4) | 0.0332(18) |
| H6_23 | 0.546713 | 0.167297 | 0.475561 | 0.040 |
| F1_23 | 0.45907(15) | 0.2035(3) | 0.5084(2) | 0.0305(10) |
| F2_23 | 0.45362(15) | 0.3224(3) | 0.5946(2) | 0.0331(11) |
| C1_21 | 0.9991(3) | 0.2646(4) | 0.3744(4) | 0.0266(17) |
| C2_21 | 0.9953(3) | 0.2046(5) | 0.3291(4) | 0.0275(17) |
| C3_21 | 1.0345(3) | 0.1657(5) | 0.3032(4) | 0.0295(17) |
| H3_21 | 1.031148 | 0.123797 | 0.271527 | 0.035 |
| C4_21 | 1.0794(3) | 0.1904(5) | 0.3256(4) | 0.0309(18) |
| H4_21 | 1.107139 | 0.164001 | 0.309975 | 0.037 |
| C5_21 | 1.0833(3) | 0.2531(5) | 0.3702(5) | 0.037(2) |
| H5_21 | 1.113965 | 0.270806 | 0.383269 | 0.044 |
| C6_21 | 1.0433(3) | 0.2913(5) | 0.3967(4) | 0.0305(17) |
| H6_21 | 1.046085 | 0.333338 | 0.428348 | 0.037 |
| F1_21 | 0.95829(15) | 0.2986(3) | 0.3976(2) | 0.0279(10) |
| F2_21 | 0.95030(15) | 0.1825(3) | 0.3102(2) | 0.0311(10) |
| C1_20 | 0.9281(3) | 0.0505(5) | 0.2044(4) | 0.0312(17) |
| C2_20 | 0.8843(3) | 0.0614(5) | 0.2321(4) | 0.0285(16) |
| C3_20 | 0.8575(3) | -0.0020(6) | 0.2539(4) | 0.039(2) |
| H3_20 | 0.827461 | 0.007583 | 0.273513 | 0.047 |
| C4_20 | 0.8748(4) | -0.0825(6) | 0.2469(4) | 0.040(2) |
| H4_20 | 0.856588 | -0.128014 | 0.260589 | 0.048 |
| C5_20 | 0.9196(4) | -0.0925(5) | 0.2193(4) | 0.041(2) |
| H5_20 | 0.932223 | -0.145836 | 0.215561 | 0.050 |
| C6_20 | 0.9465(3) | -0.0270(6) | 0.1969(4) | 0.0377(19) |
| H6_20 | 0.976583 | -0.035300 | 0.177007 | 0.045 |
| F1_20 | 0.9524(2) | 0.1156(4) | 0.1828(3) | 0.0524(14) |
| F2_20 | 0.86869(18) | 0.1400(3) | 0.2399(2) | 0.0355(11) |
| C1_19 | 0.7368(3) | 0.1958(5) | 0.3074(4) | 0.0275(16) |
| C2_19 | 0.7308(3) | 0.2517(5) | 0.3558(4) | 0.0281(18) |
| C3_19 | 0.6870(3) | 0.2739(5) | 0.3777(4) | 0.0295(17) |
| H3_19 | 0.683389 | 0.313249 | 0.411284 | 0.035 |
| C4_19 | 0.6481(3) | 0.2367(5) | 0.3489(5) | 0.036(2) |
| H4_19 | 0.617014 | 0.250196 | 0.363340 | 0.043 |
| C5_19 | 0.6541(3) | 0.1795(5) | 0.2989(5) | 0.038(2) |
| H5_19 | 0.627092 | 0.154999 | 0.279138 | 0.046 |
| C6_19 | 0.6986(3) | 0.1589(5) | 0.2784(5) | 0.038(2) |
| H6_19 | 0.703007 | 0.119805 | 0.244771 | 0.046 |
| F1_19 | 0.78288(16) | 0.1793(3) | 0.2886(2) | 0.0366(11) |
| F2_19 | 0.77116(16) | 0.2863(3) | 0.3823(2) | 0.0330(10) |
| O1_18 | 0.82027(18) | 0.3207(3) | 0.5721(3) | 0.0252(11) |
| C1_18 | 0.7765(2) | 0.3485(4) | 0.5855(3) | 0.0269(15) |
| C2_18 | 0.7655(3) | 0.4265(5) | 0.5446(4) | 0.0380(18) |

| | | | | |
|---|---|---|---|---|
| F1_18 | 0.75572(18) | 0.4061(3) | 0.4819(2) | 0.0426(12) |
| F2_18 | 0.72818(19) | 0.4669(3) | 0.5679(3) | 0.0597(15) |
| F3_18 | 0.80283(19) | 0.4751(3) | 0.5434(3) | 0.0461(13) |
| C3_18 | 0.7732(3) | 0.3695(5) | 0.6596(4) | 0.0444(19) |
| F4_18 | 0.7948(2) | 0.3126(4) | 0.6958(2) | 0.0551(14) |
| F5_18 | 0.7945(2) | 0.4399(4) | 0.6723(3) | 0.0578(15) |
| F6_18 | 0.7282(2) | 0.3754(4) | 0.6801(3) | 0.0634(16) |
| C4_18 | 0.7394(3) | 0.2813(5) | 0.5695(4) | 0.0352(17) |
| F7_18 | 0.73964(19) | 0.2231(3) | 0.6156(3) | 0.0491(13) |
| F8_18 | 0.69550(16) | 0.3102(4) | 0.5639(3) | 0.0572(14) |
| F9_18 | 0.75039(17) | 0.2455(3) | 0.5127(2) | 0.0378(11) |
| O1_17 | 0.91911(17) | 0.3073(3) | 0.5535(2) | 0.0236(11) |
| C1_17 | 0.9488(2) | 0.3547(4) | 0.5889(3) | 0.0266(15) |
| C2_17 | 0.9572(3) | 0.4366(4) | 0.5533(4) | 0.0337(17) |
| F1_17 | 0.91619(18) | 0.4665(3) | 0.5314(3) | 0.0415(12) |
| F2_17 | 0.97621(18) | 0.4943(3) | 0.5911(3) | 0.0472(12) |
| F3_17 | 0.98585(19) | 0.4268(3) | 0.5015(2) | 0.0422(12) |
| C3_17 | 0.9966(3) | 0.3091(5) | 0.5971(4) | 0.0403(19) |
| F4_17 | 0.99268(19) | 0.2490(3) | 0.6410(3) | 0.0463(13) |
| F5_17 | 1.00978(17) | 0.2749(3) | 0.5407(3) | 0.0444(13) |
| F6_17 | 1.03169(17) | 0.3581(3) | 0.6163(3) | 0.0538(14) |
| C4_17 | 0.9276(3) | 0.3722(5) | 0.6576(4) | 0.0441(19) |
| F7_17 | 0.9074(2) | 0.3041(3) | 0.6822(2) | 0.0509(14) |
| F8_17 | 0.9608(2) | 0.3959(4) | 0.7008(2) | 0.0634(17) |
| F9_17 | 0.89439(19) | 0.4292(3) | 0.6551(3) | 0.0504(13) |
| O1_16 | 0.86139(18) | 0.2030(3) | 0.4786(2) | 0.0199(10) |
| C1_16 | 0.8673(2) | 0.1220(4) | 0.4924(3) | 0.0208(13) |
| C2_16 | 0.8430(2) | 0.0977(4) | 0.5570(3) | 0.0279(15) |
| F1_16 | 0.79534(16) | 0.0923(3) | 0.5498(3) | 0.0476(14) |
| F2_16 | 0.85788(17) | 0.0252(2) | 0.5795(2) | 0.0373(11) |
| F3_16 | 0.85151(18) | 0.1538(3) | 0.6029(2) | 0.0381(11) |
| C3_16 | 0.9210(2) | 0.1005(4) | 0.4975(4) | 0.0310(15) |
| F4_16 | 0.94502(17) | 0.1399(3) | 0.4509(3) | 0.0438(12) |
| F5_16 | 0.93897(17) | 0.1228(3) | 0.5551(3) | 0.0408(12) |
| F6_16 | 0.92850(18) | 0.0209(3) | 0.4881(3) | 0.0446(12) |
| C4_16 | 0.8447(3) | 0.0747(4) | 0.4349(4) | 0.0356(17) |
| F7_16 | 0.8714(2) | 0.0892(3) | 0.3803(2) | 0.0460(14) |
| F8_16 | 0.8424(2) | -0.0047(3) | 0.4431(3) | 0.0467(12) |
| F9_16 | 0.80101(18) | 0.1028(3) | 0.4217(2) | 0.0454(12) |
| O1_15 | 0.41419(18) | 0.1808(3) | 0.3570(3) | 0.0261(11) |
| C1_15 | 0.4420(3) | 0.1320(4) | 0.3184(3) | 0.0311(16) |
| C2_15 | 0.4169(3) | 0.1161(5) | 0.2530(4) | 0.0414(18) |
| F1_15 | 0.39498(19) | 0.1822(3) | 0.2309(2) | 0.0470(12) |
| F2_15 | 0.4472(2) | 0.0907(4) | 0.2064(3) | 0.0565(15) |
| F3_15 | 0.38374(19) | 0.0575(3) | 0.2593(3) | 0.0571(15) |
| C3_15 | 0.4520(3) | 0.0500(5) | 0.3545(4) | 0.043(2) |
| F4_15 | 0.4832(2) | 0.0619(4) | 0.4033(3) | 0.0596(16) |
| F5_15 | 0.4124(2) | 0.0204(3) | 0.3812(3) | 0.0492(13) |
| F6_15 | 0.4692(2) | -0.0062(3) | 0.3142(3) | 0.0592(15) |
| C4_15 | 0.4891(3) | 0.1776(5) | 0.3068(4) | 0.0388(18) |
| F7_15 | 0.50563(18) | 0.2115(4) | 0.3611(3) | 0.0444(13) |
| F8_15 | 0.52296(18) | 0.1292(4) | 0.2823(3) | 0.0561(15) |
| F9_15 | 0.48213(18) | 0.2375(3) | 0.2632(3) | 0.0460(13) |
| O1_14 | 0.31347(18) | 0.1678(3) | 0.3473(3) | 0.0268(11) |
| C1_14 | 0.2697(2) | 0.1359(4) | 0.3408(3) | 0.0256(14) |

| | | | | |
|---|---|---|---|---|
| C2_14 | 0.2645(3) | 0.0597(4) | 0.3850(4) | 0.0298(15) |
| F1_14 | 0.25894(16) | 0.0812(3) | 0.4469(2) | 0.0344(10) |
| F2_14 | 0.22717(17) | 0.0126(3) | 0.3684(2) | 0.0440(12) |
| F3_14 | 0.30334(17) | 0.0139(3) | 0.3824(3) | 0.0399(12) |
| C3_14 | 0.2614(3) | 0.1118(5) | 0.2679(4) | 0.0425(19) |
| F4_14 | 0.2784(2) | 0.1676(4) | 0.2286(2) | 0.0546(14) |
| F5_14 | 0.2839(2) | 0.0410(3) | 0.2548(2) | 0.0550(14) |
| F6_14 | 0.21585(19) | 0.1001(4) | 0.2536(3) | 0.0572(15) |
| C4_14 | 0.2317(3) | 0.2009(5) | 0.3606(4) | 0.0404(19) |
| F7_14 | 0.2259(2) | 0.2556(3) | 0.3124(3) | 0.0518(14) |
| F8_14 | 0.18959(16) | 0.1670(3) | 0.3731(3) | 0.0538(14) |
| F9_14 | 0.24572(19) | 0.2417(3) | 0.4123(3) | 0.0406(12) |
| O1_13 | 0.35990(18) | 0.2896(3) | 0.4330(3) | 0.0229(10) |
| C1_13 | 0.3636(2) | 0.3702(4) | 0.4137(3) | 0.0228(14) |
| C2_13 | 0.3366(2) | 0.3864(4) | 0.3480(3) | 0.0273(14) |
| F1_13 | 0.29016(17) | 0.3844(3) | 0.3557(3) | 0.0441(13) |
| F2_13 | 0.34851(17) | 0.4571(2) | 0.3221(2) | 0.0346(10) |
| F3_13 | 0.34829(17) | 0.3272(3) | 0.3057(2) | 0.0339(10) |
| C3_13 | 0.4169(3) | 0.3938(4) | 0.4062(4) | 0.0313(15) |
| F4_13 | 0.44144(17) | 0.3638(3) | 0.4565(3) | 0.0449(13) |
| F5_13 | 0.43473(17) | 0.3636(3) | 0.3515(3) | 0.0412(11) |
| F6_13 | 0.42284(18) | 0.4738(3) | 0.4046(3) | 0.0441(12) |
| C4_13 | 0.3398(3) | 0.4207(4) | 0.4688(4) | 0.0358(17) |
| F7_13 | 0.3675(2) | 0.4136(3) | 0.5238(2) | 0.0511(15) |
| F8_13 | 0.3358(2) | 0.4990(3) | 0.4546(3) | 0.0473(13) |
| F9_13 | 0.2980(2) | 0.3917(3) | 0.4848(3) | 0.0534(15) |
| O1_12 | 0.57736(19) | 0.5953(3) | 0.4410(3) | 0.0273(12) |
| C1_12 | 0.5984(2) | 0.5445(4) | 0.3983(3) | 0.0248(14) |
| C2_12 | 0.5628(3) | 0.4773(5) | 0.3778(4) | 0.0401(18) |
| F1_12 | 0.53152(17) | 0.5074(3) | 0.3332(3) | 0.0592(15) |
| F2_12 | 0.5837(2) | 0.4134(3) | 0.3499(3) | 0.0547(15) |
| F3_12 | 0.53863(19) | 0.4506(3) | 0.4289(3) | 0.0525(15) |
| C3_12 | 0.6422(3) | 0.5045(4) | 0.4311(4) | 0.0358(16) |
| F4_12 | 0.66533(16) | 0.5577(3) | 0.4676(2) | 0.0397(11) |
| F5_12 | 0.62890(18) | 0.4419(3) | 0.4701(3) | 0.0482(12) |
| F6_12 | 0.67346(17) | 0.4732(3) | 0.3884(3) | 0.0461(12) |
| C4_12 | 0.6161(3) | 0.5929(4) | 0.3367(3) | 0.0361(16) |
| F7_12 | 0.65489(18) | 0.6346(3) | 0.3507(2) | 0.0420(12) |
| F8_12 | 0.6258(2) | 0.5434(3) | 0.2863(2) | 0.0541(14) |
| F9_12 | 0.5821(2) | 0.6446(3) | 0.3174(3) | 0.0514(13) |
| O1_11 | 0.60875(17) | 0.6666(3) | 0.5641(2) | 0.0230(9) |
| C1_11 | 0.6028(2) | 0.6386(4) | 0.6261(3) | 0.0207(13) |
| C2_11 | 0.5709(2) | 0.6970(4) | 0.6659(3) | 0.0300(15) |
| F1_11 | 0.52451(14) | 0.6839(3) | 0.6492(2) | 0.0395(11) |
| F2_11 | 0.57454(16) | 0.6863(3) | 0.7300(2) | 0.0403(11) |
| F3_11 | 0.58013(17) | 0.7747(3) | 0.6523(2) | 0.0382(11) |
| C3_11 | 0.6532(2) | 0.6356(4) | 0.6590(3) | 0.0272(14) |
| F4_11 | 0.68402(14) | 0.5992(3) | 0.6203(2) | 0.0354(10) |
| F5_11 | 0.66835(16) | 0.7110(3) | 0.6710(2) | 0.0330(10) |
| F6_11 | 0.65304(16) | 0.5947(3) | 0.7154(2) | 0.0388(10) |
| C4_11 | 0.5808(3) | 0.5516(4) | 0.6248(4) | 0.0346(16) |
| F7_11 | 0.61366(18) | 0.4969(3) | 0.6079(3) | 0.0468(13) |
| F8_11 | 0.56398(18) | 0.5300(3) | 0.6840(2) | 0.0444(12) |
| F9_11 | 0.54521(17) | 0.5480(3) | 0.5833(2) | 0.0417(12) |
| O1_10 | 0.52717(16) | 0.7261(3) | 0.4996(3) | 0.0270(11) |

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|---|---|---|---|---|
| C1_10 | 0.4823(3) | 0.7396(4) | 0.4780(4) | 0.0286(16) |
| C2_10 | 0.4595(3) | 0.6617(5) | 0.4502(5) | 0.044(2) |
| F1_10 | 0.46937(19) | 0.5985(3) | 0.4894(3) | 0.0568(15) |
| F2_10 | 0.41241(16) | 0.6662(3) | 0.4422(3) | 0.0505(14) |
| F3_10 | 0.47728(19) | 0.6437(4) | 0.3912(3) | 0.0692(19) |
| C3_10 | 0.4837(3) | 0.8058(6) | 0.4228(4) | 0.054(2) |
| F4_10 | 0.4904(2) | 0.8788(3) | 0.4509(4) | 0.083(2) |
| F5_10 | 0.5192(2) | 0.7884(5) | 0.3824(3) | 0.089(2) |
| F6_10 | 0.4440(2) | 0.8091(4) | 0.3902(3) | 0.0707(19) |
| C4_10 | 0.4524(3) | 0.7694(5) | 0.5365(4) | 0.0346(17) |
| F7_10 | 0.47703(17) | 0.8229(3) | 0.5721(3) | 0.0490(13) |
| F8_10 | 0.41262(17) | 0.8070(3) | 0.5155(3) | 0.0554(15) |
| F9_10 | 0.43983(18) | 0.7082(4) | 0.5754(3) | 0.0555(14) |
| O1_9 | 0.65666(19) | 0.9084(3) | 0.4580(2) | 0.0244(11) |
| C1_9 | 0.6474(2) | 0.9556(4) | 0.5111(3) | 0.0238(14) |
| C2_9 | 0.6694(3) | 1.0408(4) | 0.5004(4) | 0.0313(16) |
| F1_9 | 0.64380(18) | 1.0841(3) | 0.4591(3) | 0.0436(12) |
| F2_9 | 0.6727(2) | 1.0828(3) | 0.5562(3) | 0.0463(13) |
| F3_9 | 0.71272(16) | 1.0350(3) | 0.4759(3) | 0.0439(12) |
| C3_9 | 0.6687(3) | 0.9149(4) | 0.5740(3) | 0.0337(15) |
| F4_9 | 0.66609(18) | 0.8350(3) | 0.5700(2) | 0.0396(10) |
| F5_9 | 0.71405(16) | 0.9335(3) | 0.5820(3) | 0.0462(12) |
| F6_9 | 0.64629(19) | 0.9378(3) | 0.6286(2) | 0.0439(11) |
| C4_9 | 0.5925(2) | 0.9634(4) | 0.5198(4) | 0.0330(15) |
| F7_9 | 0.57439(16) | 0.8939(3) | 0.5419(2) | 0.0425(11) |
| F8_9 | 0.58131(17) | 1.0224(3) | 0.5632(3) | 0.0460(12) |
| F9_9 | 0.57129(16) | 0.9814(3) | 0.4627(3) | 0.0450(12) |
| O1_8 | 0.6506(2) | 0.8218(3) | 0.3399(3) | 0.0318(12) |
| C1_8 | 0.6456(3) | 0.8680(4) | 0.2857(3) | 0.0298(16) |
| C2_8 | 0.6940(3) | 0.9067(4) | 0.2673(3) | 0.0355(16) |
| F1_8 | 0.72401(19) | 0.8509(3) | 0.2417(2) | 0.0473(12) |
| F2_8 | 0.68964(19) | 0.9671(3) | 0.2234(2) | 0.0482(13) |
| F3_8 | 0.71486(18) | 0.9386(3) | 0.3201(2) | 0.0440(12) |
| C3_8 | 0.6091(3) | 0.9368(5) | 0.2954(4) | 0.0438(18) |
| F4_8 | 0.57118(18) | 0.9079(3) | 0.3270(3) | 0.0512(13) |
| F5_8 | 0.62692(19) | 0.9978(3) | 0.3312(3) | 0.0447(12) |
| F6_8 | 0.5930(2) | 0.9680(3) | 0.2389(3) | 0.0579(14) |
| C4_8 | 0.6292(3) | 0.8112(5) | 0.2286(3) | 0.0361(17) |
| F7_8 | 0.58281(19) | 0.7918(4) | 0.2359(3) | 0.0498(13) |
| F8_8 | 0.6346(2) | 0.8467(3) | 0.1705(2) | 0.0510(14) |
| F9_8 | 0.6535(2) | 0.7419(3) | 0.2283(2) | 0.0430(12) |
| O1_7 | 0.71285(18) | 0.7605(3) | 0.4393(3) | 0.0279(12) |
| C1_7 | 0.7604(2) | 0.7471(4) | 0.4411(4) | 0.0275(15) |
| C2_7 | 0.7688(2) | 0.6614(4) | 0.4711(3) | 0.0286(15) |
| F1_7 | 0.75848(16) | 0.6028(3) | 0.4293(2) | 0.0354(11) |
| F2_7 | 0.81376(15) | 0.6509(3) | 0.4908(2) | 0.0407(11) |
| F3_7 | 0.74123(16) | 0.6505(3) | 0.5236(2) | 0.0372(10) |
| C3_7 | 0.7845(2) | 0.8119(4) | 0.4860(4) | 0.0334(16) |
| F4_7 | 0.76895(16) | 0.8853(3) | 0.4712(3) | 0.0446(12) |
| F5_7 | 0.77584(17) | 0.7970(3) | 0.5494(2) | 0.0439(11) |
| F6_7 | 0.83180(16) | 0.8129(3) | 0.4786(3) | 0.0507(14) |
| C4_7 | 0.7825(3) | 0.7488(5) | 0.3725(4) | 0.0370(18) |
| F7_7 | 0.7882(2) | 0.8262(3) | 0.3527(3) | 0.0539(14) |
| F8_7 | 0.82484(16) | 0.7129(3) | 0.3706(3) | 0.0447(12) |
| F9_7 | 0.75328(19) | 0.7117(4) | 0.3302(2) | 0.0477(13) |

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|---|---|---|---|---|
| O1_6 | 0.16005(19) | 0.5956(3) | 0.4597(2) | 0.0259(11) |
| C1_6 | 0.1586(2) | 0.5473(4) | 0.4061(3) | 0.0243(14) |
| C2_6 | 0.1648(3) | 0.4568(5) | 0.4274(4) | 0.0375(18) |
| F1_6 | 0.12485(19) | 0.4280(3) | 0.4538(3) | 0.0456(13) |
| F2_6 | 0.1763(2) | 0.4085(3) | 0.3776(3) | 0.0498(14) |
| F3_6 | 0.19847(18) | 0.4502(3) | 0.4727(3) | 0.0438(12) |
| C3_6 | 0.1995(3) | 0.5698(5) | 0.3578(3) | 0.0334(16) |
| F4_6 | 0.20453(18) | 0.6507(3) | 0.3545(2) | 0.0395(11) |
| F5_6 | 0.24111(15) | 0.5388(3) | 0.3792(2) | 0.0399(11) |
| F6_6 | 0.19176(19) | 0.5423(4) | 0.2974(2) | 0.0518(14) |
| C4_6 | 0.1110(3) | 0.5574(5) | 0.3708(4) | 0.0354(17) |
| F7_6 | 0.10932(19) | 0.6302(3) | 0.3391(2) | 0.0467(12) |
| F8_6 | 0.10130(18) | 0.4988(4) | 0.3274(3) | 0.0523(15) |
| F9_6 | 0.07497(16) | 0.5581(3) | 0.4148(2) | 0.0419(12) |
| O1_5 | 0.21513(17) | 0.7442(3) | 0.4850(3) | 0.0205(11) |
| C1_5 | 0.2619(2) | 0.7545(4) | 0.5018(3) | 0.0213(14) |
| C2_5 | 0.2669(3) | 0.7794(4) | 0.5739(3) | 0.0258(15) |
| F1_5 | 0.26093(16) | 0.7151(3) | 0.6133(2) | 0.0316(10) |
| F2_5 | 0.30966(15) | 0.8116(3) | 0.5885(2) | 0.0339(10) |
| F3_5 | 0.23404(15) | 0.8350(3) | 0.5911(2) | 0.0323(10) |
| C3_5 | 0.2812(2) | 0.8240(5) | 0.4575(4) | 0.0285(16) |
| F4_5 | 0.26882(15) | 0.8135(3) | 0.3949(2) | 0.0333(10) |
| F5_5 | 0.26488(17) | 0.8963(3) | 0.4777(3) | 0.0366(11) |
| F6_5 | 0.32904(14) | 0.8278(3) | 0.4590(2) | 0.0363(11) |
| C4_5 | 0.2904(2) | 0.6753(4) | 0.4902(3) | 0.0291(15) |
| F7_5 | 0.30043(16) | 0.6657(3) | 0.4267(2) | 0.0326(10) |
| F8_5 | 0.33163(15) | 0.6747(3) | 0.5232(2) | 0.0313(10) |
| F9_5 | 0.26518(16) | 0.6109(3) | 0.5099(2) | 0.0321(10) |
| O1_4 | 0.15038(19) | 0.6818(3) | 0.5778(2) | 0.0250(11) |
| C1_4 | 0.1335(2) | 0.6343(4) | 0.6278(3) | 0.0251(15) |
| C2_4 | 0.1711(3) | 0.5761(5) | 0.6536(4) | 0.0410(18) |
| F1_4 | 0.20163(19) | 0.6184(4) | 0.6939(3) | 0.0557(15) |
| F2_4 | 0.15238(17) | 0.5130(3) | 0.6860(2) | 0.0396(11) |
| F3_4 | 0.19648(18) | 0.5441(3) | 0.6040(2) | 0.0456(13) |
| C3_4 | 0.0899(3) | 0.5838(5) | 0.6029(4) | 0.0434(19) |
| F4_4 | 0.06280(19) | 0.6282(4) | 0.5634(3) | 0.0521(14) |
| F5_4 | 0.1060(2) | 0.5161(3) | 0.5712(2) | 0.0509(14) |
| F6_4 | 0.06193(18) | 0.5600(4) | 0.6532(3) | 0.0533(15) |
| C4_4 | 0.1161(3) | 0.6925(5) | 0.6831(4) | 0.0446(19) |
| F7_4 | 0.0745(2) | 0.7265(4) | 0.6667(3) | 0.0628(18) |
| F8_4 | 0.1117(3) | 0.6501(3) | 0.7400(2) | 0.0607(17) |
| F9_4 | 0.1496(3) | 0.7500(3) | 0.6936(3) | 0.0530(16) |
| O1_3 | 0.08591(17) | 0.8241(3) | 0.3462(2) | 0.0194(10) |
| C1_3 | 0.1068(2) | 0.8682(4) | 0.2976(3) | 0.0206(13) |
| C2_3 | 0.1611(2) | 0.8561(4) | 0.2994(4) | 0.0308(15) |
| F1_3 | 0.17684(16) | 0.8596(3) | 0.3615(2) | 0.0398(11) |
| F2_3 | 0.18373(17) | 0.9147(3) | 0.2654(3) | 0.0435(12) |
| F3_3 | 0.17258(17) | 0.7835(3) | 0.2746(3) | 0.0453(12) |
| C3_3 | 0.0858(3) | 0.8391(4) | 0.2308(3) | 0.0280(14) |
| F4_3 | 0.04281(16) | 0.8686(3) | 0.2214(2) | 0.0355(10) |
| F5_3 | 0.0839(2) | 0.7580(3) | 0.2294(2) | 0.0359(11) |
| F6_3 | 0.1135(2) | 0.8622(3) | 0.1815(2) | 0.0448(13) |
| C4_3 | 0.0951(2) | 0.9605(4) | 0.3055(3) | 0.0266(14) |
| F7_3 | 0.05007(15) | 0.9708(3) | 0.3240(2) | 0.0332(10) |
| F8_3 | 0.10176(16) | 1.0025(3) | 0.2501(2) | 0.0333(9) |

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|---|---|---|---|---|
| F9_3 | 0.12289(18) | 0.9939(3) | 0.3523(2) | 0.0353(11) |
| O1_2 | 0.08048(17) | 0.9065(3) | 0.4671(2) | 0.0210(10) |
| C1_2 | 0.0845(2) | 0.9519(4) | 0.5224(3) | 0.0206(13) |
| C2_2 | 0.1353(2) | 0.9437(5) | 0.5515(4) | 0.0318(16) |
| F1_2 | 0.13899(18) | 0.8703(3) | 0.5814(2) | 0.0424(12) |
| F2_2 | 0.14573(18) | 1.0010(3) | 0.5954(2) | 0.0441(12) |
| F3_2 | 0.16801(16) | 0.9469(3) | 0.5055(2) | 0.0392(11) |
| C3_2 | 0.0756(3) | 1.0428(4) | 0.5034(4) | 0.0297(16) |
| F4_2 | 0.03895(17) | 1.0490(3) | 0.4619(2) | 0.0357(11) |
| F5_2 | 0.11284(19) | 1.0761(3) | 0.4761(2) | 0.0418(12) |
| F6_2 | 0.06495(19) | 1.0879(3) | 0.5568(2) | 0.0406(12) |
| C4_2 | 0.0475(3) | 0.9233(5) | 0.5736(3) | 0.0308(15) |
| F7_2 | 0.00434(15) | 0.9526(3) | 0.5579(2) | 0.0356(10) |
| F8_2 | 0.05789(18) | 0.9492(3) | 0.6343(2) | 0.0413(12) |
| F9_2 | 0.04437(18) | 0.8432(3) | 0.5742(2) | 0.0366(10) |
| O1_1 | 0.02676(17) | 0.7569(3) | 0.4421(2) | 0.0197(10) |
| C1_1 | -0.0192(2) | 0.7471(4) | 0.4231(3) | 0.0203(14) |
| C2_1 | -0.0414(3) | 0.6805(4) | 0.4688(4) | 0.0293(16) |
| F1_1 | -0.02533(17) | 0.6064(3) | 0.4519(2) | 0.0341(10) |
| F2_1 | -0.08865(14) | 0.6793(3) | 0.4635(2) | 0.0322(10) |
| F3_1 | -0.02907(16) | 0.6935(3) | 0.5302(2) | 0.0342(10) |
| C3_1 | -0.0476(2) | 0.8273(4) | 0.4298(4) | 0.0272(15) |
| F4_1 | -0.02054(16) | 0.8905(3) | 0.4102(2) | 0.0333(10) |
| F5_1 | -0.05785(17) | 0.8425(3) | 0.4932(2) | 0.0367(11) |
| F6_1 | -0.08792(15) | 0.8296(3) | 0.3968(2) | 0.0336(10) |
| C4_1 | -0.0232(2) | 0.7184(4) | 0.3510(3) | 0.0249(14) |
| F7_1 | -0.01577(17) | 0.7816(3) | 0.3099(2) | 0.0347(10) |
| F8_1 | -0.06579(15) | 0.6870(3) | 0.3361(2) | 0.0326(10) |
| F9_1 | 0.00987(15) | 0.6632(3) | 0.3377(2) | 0.0317(9) |
| Ba1 | 0.86630(2) | 0.26333(2) | 0.34260(2) | 0.01811(8) |
| F4 | 0.12132(16) | 0.7516(3) | 0.4616(2) | 0.0179(7) |
| Ba2 | 0.36912(2) | 0.23927(2) | 0.56958(2) | 0.01915(8) |
| F3 | 0.61844(18) | 0.7504(3) | 0.4527(2) | 0.0202(7) |
| Al3 | 0.66323(8) | 0.81584(13) | 0.42124(10) | 0.0183(4) |
| Al5 | 0.16487(7) | 0.68755(13) | 0.49722(10) | 0.0169(4) |
| Al2 | 0.36136(8) | 0.19219(13) | 0.39619(10) | 0.0184(4) |
| Al1 | 0.86449(8) | 0.29846(13) | 0.51832(10) | 0.0187(4) |
| F1 | 0.85998(15) | 0.3514(2) | 0.44720(19) | 0.0232(9) |
| Al4 | 0.58058(7) | 0.67916(13) | 0.49018(10) | 0.0175(4) |
| Al6 | 0.07631(7) | 0.81518(13) | 0.42830(10) | 0.0159(4) |
| F2 | 0.36066(15) | 0.1431(2) | 0.46989(18) | 0.0224(8) |
| C1 | 0.8278(3) | 0.4275(5) | 0.2810(4) | 0.0272(16) |
| C2 | 0.8286(3) | 0.3737(5) | 0.2274(3) | 0.0224(15) |
| C3 | 0.8724(3) | 0.3462(5) | 0.2018(4) | 0.0275(17) |
| C4 | 0.9153(3) | 0.3710(5) | 0.2328(4) | 0.0280(17) |
| C5 | 0.9145(3) | 0.4255(5) | 0.2851(4) | 0.0250(15) |
| C6 | 0.8709(3) | 0.4519(4) | 0.3106(4) | 0.0302(17) |
| C7 | 0.7814(3) | 0.4621(6) | 0.3080(5) | 0.042(2) |
| H7A | 0.780121 | 0.520746 | 0.299582 | 0.063 |
| H7B | 0.779918 | 0.452252 | 0.355207 | 0.063 |
| H7C | 0.754497 | 0.435346 | 0.286499 | 0.063 |
| C8 | 0.7826(3) | 0.3481(6) | 0.1935(4) | 0.039(2) |
| H8A | 0.772750 | 0.390651 | 0.162684 | 0.058 |
| H8B | 0.757675 | 0.340268 | 0.226307 | 0.058 |
| H8C | 0.787720 | 0.297107 | 0.169752 | 0.058 |

| | | | | |
|---|---|---|---|---|
| C9 | 0.8735(3) | 0.2944(5) | 0.1410(4) | 0.039(2) |
| H9A | 0.851784 | 0.317187 | 0.108296 | 0.058 |
| H9B | 0.863667 | 0.238834 | 0.151825 | 0.058 |
| H9C | 0.905820 | 0.293548 | 0.123320 | 0.058 |
| C10 | 0.9620(3) | 0.3420(7) | 0.2039(4) | 0.043(2) |
| H10A | 0.961098 | 0.282829 | 0.198150 | 0.065 |
| H10B | 0.988117 | 0.356417 | 0.233463 | 0.065 |
| H10C | 0.967021 | 0.368187 | 0.161377 | 0.065 |
| C11 | 0.9594(3) | 0.4594(6) | 0.3143(5) | 0.045(2) |
| H11A | 0.985965 | 0.449775 | 0.284379 | 0.067 |
| H11B | 0.965867 | 0.432525 | 0.356187 | 0.067 |
| H11C | 0.955754 | 0.518072 | 0.321449 | 0.067 |
| C12 | 0.8701(4) | 0.5127(5) | 0.3666(4) | 0.043(2) |
| H12A | 0.858658 | 0.565380 | 0.350469 | 0.064 |
| H12B | 0.902159 | 0.519007 | 0.384404 | 0.064 |
| H12C | 0.848782 | 0.492935 | 0.400940 | 0.064 |
| C1_26 | 0.3385(3) | 0.0767(5) | 0.6377(4) | 0.0306(17) |
| C2_26 | 0.3338(3) | 0.1336(5) | 0.6901(4) | 0.0261(16) |
| C3_26 | 0.3741(3) | 0.1706(5) | 0.7154(4) | 0.0287(17) |
| C4_26 | 0.4195(3) | 0.1505(5) | 0.6908(4) | 0.0352(19) |
| C5_26 | 0.4247(3) | 0.0938(5) | 0.6410(5) | 0.041(2) |
| C6_26 | 0.3831(4) | 0.0557(5) | 0.6147(4) | 0.040(2) |
| C7_26 | 0.2950(4) | 0.0342(6) | 0.6102(5) | 0.058(3) |
| H7A_26 | 0.295776 | 0.036425 | 0.562293 | 0.087 |
| H7B_26 | 0.266297 | 0.061558 | 0.625981 | 0.087 |
| H7C_26 | 0.294778 | -0.022687 | 0.624462 | 0.087 |
| C8_26 | 0.2859(3) | 0.1529(6) | 0.7194(4) | 0.041(2) |
| H8A_26 | 0.282599 | 0.212001 | 0.724200 | 0.062 |
| H8B_26 | 0.283325 | 0.127014 | 0.762407 | 0.062 |
| H8C_26 | 0.260821 | 0.132305 | 0.690631 | 0.062 |
| C9_26 | 0.3678(5) | 0.2305(6) | 0.7726(4) | 0.053(3) |
| H9A_26 | 0.393064 | 0.271519 | 0.771172 | 0.079 |
| H9B_26 | 0.369555 | 0.200778 | 0.814053 | 0.079 |
| H9C_26 | 0.336888 | 0.257324 | 0.768870 | 0.079 |
| C10_26 | 0.4644(3) | 0.1876(8) | 0.7225(5) | 0.061(3) |
| H10A_26 | 0.490691 | 0.185806 | 0.691297 | 0.092 |
| H10B_26 | 0.472831 | 0.156179 | 0.761612 | 0.092 |
| H10C_26 | 0.458066 | 0.244155 | 0.734865 | 0.092 |
| C11_26 | 0.4728(4) | 0.0656(9) | 0.6182(7) | 0.093(5) |
| H11A_26 | 0.469668 | 0.038282 | 0.575814 | 0.140 |
| H11B_26 | 0.486162 | 0.027561 | 0.650234 | 0.140 |
| H11C_26 | 0.493967 | 0.112647 | 0.613728 | 0.140 |
| C12_26 | 0.3885(5) | -0.0091(5) | 0.5623(5) | 0.068(4) |
| H12A_26 | 0.362159 | -0.004752 | 0.531069 | 0.102 |
| H12B_26 | 0.388012 | -0.063099 | 0.582682 | 0.102 |
| H12C_26 | 0.418619 | -0.001338 | 0.539368 | 0.102 |

*Table S 5 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [SrHMB(oDFB)$_3${f-al}][al-f-al] **5**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| Sr1 | 0.42720(3) | 0.28821(2) | 0.28739(2) | 0.02075(8) |
| F2 | 1.000000 | 0.500000 | 0.500000 | 0.0198(6) |
| F4 | 0.000000 | 0.500000 | 0.000000 | 0.0236(2) |
| F3 | -0.0009(6) | 0.0041(3) | 0.0049(2) | 0.0237(2) |

| | | | | |
|---|---|---|---|---|
| F1 | 0.5232(2) | 0.24641(11) | 0.22984(10) | 0.0424(7) |
| F5 | 1.000000 | 0.000000 | 0.500000 | 0.0209(2) |
| Sr2 | -0.59288(3) | 0.78935(2) | 0.21333(2) | 0.02347(8) |
| Al6 | 0.91780(8) | 0.45182(4) | 0.47353(4) | 0.0164(2) |
| Al2 | 0.92369(9) | 0.00159(4) | 0.55244(4) | 0.0209(2) |
| Al3 | 0.07230(9) | 0.04994(5) | -0.02864(4) | 0.0237(2) |
| Al4 | 0.08020(9) | 0.50048(5) | 0.05150(4) | 0.0236(2) |
| Al5 | -0.40646(9) | 0.70892(5) | 0.29711(4) | 0.0213(2) |
| Al1 | 0.60112(10) | 0.20832(5) | 0.19870(4) | 0.0240(2) |
| F6 | -0.4764(2) | 0.75031(11) | 0.26361(10) | 0.0364(6) |
| O1_1 | 0.9857(2) | -0.02514(12) | 0.59970(11) | 0.0308(7) |
| C1_1 | 1.0519(3) | -0.05747(17) | 0.61997(14) | 0.0319(9) |
| C2_1 | 1.1530(3) | -0.04883(18) | 0.59399(16) | 0.0350(10) |
| F1_1 | 1.1503(2) | -0.07288(12) | 0.55045(10) | 0.0408(7) |
| F2_1 | 1.2276(2) | -0.06718(14) | 0.61964(11) | 0.0488(8) |
| F3_1 | 1.1724(2) | 0.00221(12) | 0.58635(11) | 0.0454(7) |
| C3_1 | 1.0625(4) | -0.04304(19) | 0.67517(15) | 0.0385(10) |
| F4_1 | 0.9747(2) | -0.03568(12) | 0.69474(9) | 0.0416(7) |
| F5_1 | 1.1173(2) | 0.00191(12) | 0.68107(10) | 0.0468(7) |
| F6_1 | 1.1049(3) | -0.08095(13) | 0.70059(10) | 0.0497(8) |
| C4_1 | 1.0157(4) | -0.11639(18) | 0.61573(17) | 0.0369(10) |
| F7_1 | 0.9472(3) | -0.12843(12) | 0.64930(11) | 0.0504(8) |
| F8_1 | 1.0890(3) | -0.14862(12) | 0.62128(13) | 0.0560(9) |
| F9_1 | 0.9737(3) | -0.12431(12) | 0.57199(11) | 0.0483(7) |
| O1_2 | 0.8201(2) | -0.03334(12) | 0.53322(11) | 0.0306(7) |
| C1_2 | 0.7268(3) | -0.04946(18) | 0.54510(15) | 0.0336(9) |
| C2_2 | 0.7012(4) | -0.1017(2) | 0.51733(19) | 0.0468(12) |
| F1_2 | 0.6887(3) | -0.09166(15) | 0.47007(12) | 0.0645(10) |
| F2_2 | 0.6179(3) | -0.12584(15) | 0.53408(15) | 0.0703(11) |
| F3_2 | 0.7722(3) | -0.13577(13) | 0.52243(15) | 0.0627(9) |
| C3_2 | 0.7171(4) | -0.0593(3) | 0.60098(18) | 0.0559(14) |
| F4_2 | 0.7661(3) | -0.02221(19) | 0.62580(13) | 0.0774(13) |
| F5_2 | 0.7580(3) | -0.10569(19) | 0.61298(14) | 0.0789(12) |
| F6_2 | 0.6240(2) | -0.06168(19) | 0.61610(13) | 0.0720(12) |
| C4_2 | 0.6534(4) | -0.0072(2) | 0.5302(2) | 0.0534(13) |
| F7_2 | 0.6597(3) | 0.03231(17) | 0.56205(19) | 0.0857(14) |
| F8_2 | 0.5600(2) | -0.0267(2) | 0.53076(16) | 0.0806(13) |
| F9_2 | 0.6717(3) | 0.01010(15) | 0.48558(15) | 0.0678(11) |
| O1_3 | 0.8948(3) | 0.06561(12) | 0.56207(15) | 0.0321(9) |
| C1_3 | 0.9180(4) | 0.11317(17) | 0.58324(17) | 0.0356(11) |
| C2_3 | 0.9694(4) | 0.10653(18) | 0.63425(17) | 0.0369(11) |
| F1_3 | 1.0625(3) | 0.09303(14) | 0.62806(14) | 0.0495(9) |
| F2_3 | 0.9699(3) | 0.15043(12) | 0.66054(12) | 0.0493(9) |
| F3_3 | 0.9231(3) | 0.06854(13) | 0.65968(13) | 0.0422(9) |
| C3_3 | 0.8198(4) | 0.1419(2) | 0.58992(19) | 0.0438(12) |
| F4_3 | 0.7631(3) | 0.13763(16) | 0.54994(14) | 0.0603(11) |
| F5_3 | 0.7670(3) | 0.1198(2) | 0.62555(15) | 0.0576(11) |
| F6_3 | 0.8352(3) | 0.19284(13) | 0.59992(16) | 0.0630(11) |
| C4_3 | 0.9865(5) | 0.14694(19) | 0.54904(19) | 0.0467(13) |
| F7_3 | 0.9368(4) | 0.16440(15) | 0.51083(13) | 0.0597(12) |
| F8_3 | 1.0302(3) | 0.18744(14) | 0.57233(15) | 0.0630(11) |
| F9_3 | 1.0573(3) | 0.11683(15) | 0.53207(14) | 0.0572(10) |
| O1_4 | 0.9161(2) | 0.47205(11) | 0.41401(10) | 0.0244(6) |
| C1_4 | 0.8862(3) | 0.45899(16) | 0.36811(14) | 0.0297(8) |
| C2_4 | 0.7771(3) | 0.43733(16) | 0.36792(14) | 0.0300(9) |

| | | | | |
|---|---|---|---|---|
| F1_4 | 0.7155(2) | 0.47613(11) | 0.37447(10) | 0.0412(6) |
| F2_4 | 0.7504(2) | 0.41261(12) | 0.32639(10) | 0.0459(7) |
| F3_4 | 0.7621(2) | 0.40343(11) | 0.40432(10) | 0.0412(7) |
| C3_4 | 0.9518(4) | 0.4168(2) | 0.34637(18) | 0.0513(13) |
| F4_4 | 1.0457(2) | 0.42559(18) | 0.35874(13) | 0.0712(11) |
| F5_4 | 0.9266(3) | 0.36890(14) | 0.36449(13) | 0.0660(10) |
| F6_4 | 0.9443(3) | 0.41353(19) | 0.29801(12) | 0.0736(12) |
| C4_4 | 0.8946(4) | 0.5099(2) | 0.33642(16) | 0.0465(12) |
| F7_4 | 0.9894(3) | 0.52082(19) | 0.32635(13) | 0.0804(14) |
| F8_4 | 0.8452(2) | 0.50392(14) | 0.29399(10) | 0.0581(9) |
| F9_4 | 0.8585(3) | 0.55032(12) | 0.35931(12) | 0.0568(9) |
| O1_5 | 0.8116(11) | 0.4536(7) | 0.5064(8) | 0.024(3) |
| C1_5 | 0.7392(7) | 0.4784(3) | 0.5308(3) | 0.024(2) |
| C2_5 | 0.7435(5) | 0.5380(3) | 0.5181(3) | 0.0322(16) |
| F1_5 | 0.8184(6) | 0.5623(3) | 0.5405(3) | 0.0437(18) |
| F2_5 | 0.6609(10) | 0.5615(5) | 0.5309(4) | 0.046(3) |
| F3_5 | 0.7528(12) | 0.5462(7) | 0.4703(4) | 0.044(2) |
| C3_5 | 0.6370(5) | 0.4536(3) | 0.5153(3) | 0.0319(16) |
| F4_5 | 0.6389(15) | 0.4008(4) | 0.5146(5) | 0.040(2) |
| F5_5 | 0.6098(5) | 0.4699(3) | 0.4713(2) | 0.0484(16) |
| F6_5 | 0.5657(11) | 0.4654(9) | 0.5457(6) | 0.047(3) |
| C4_5 | 0.7555(6) | 0.4704(3) | 0.5862(3) | 0.0362(18) |
| F7_5 | 0.7231(6) | 0.4227(3) | 0.6010(2) | 0.0444(17) |
| F8_5 | 0.7099(8) | 0.5057(3) | 0.6131(3) | 0.0442(19) |
| F9_5 | 0.8522(9) | 0.4721(7) | 0.5946(7) | 0.049(3) |
| O1_6 | 0.9704(2) | 0.39244(10) | 0.47829(10) | 0.0239(6) |
| C1_6 | 0.9759(3) | 0.34589(14) | 0.50244(14) | 0.0243(8) |
| C2_6 | 1.0379(3) | 0.35362(17) | 0.55002(17) | 0.0356(10) |
| F1_6 | 1.1335(2) | 0.35818(13) | 0.54002(13) | 0.0535(8) |
| F2_6 | 1.0236(2) | 0.31435(11) | 0.58120(11) | 0.0480(7) |
| F3_6 | 1.0115(2) | 0.39786(11) | 0.57240(10) | 0.0463(7) |
| C3_6 | 0.8712(3) | 0.32300(14) | 0.51550(14) | 0.0271(8) |
| F4_6 | 0.80806(19) | 0.33029(10) | 0.47921(10) | 0.0351(6) |
| F5_6 | 0.8360(2) | 0.34695(10) | 0.55454(9) | 0.0342(6) |
| F6_6 | 0.8715(2) | 0.27147(9) | 0.52481(11) | 0.0396(6) |
| C4_6 | 1.0275(4) | 0.30667(17) | 0.46843(17) | 0.0386(10) |
| F7_6 | 0.9644(3) | 0.28748(12) | 0.43432(11) | 0.0514(8) |
| F8_6 | 1.0616(2) | 0.26565(10) | 0.49257(14) | 0.0551(9) |
| F9_6 | 1.1027(2) | 0.33056(10) | 0.44525(12) | 0.0482(8) |
| O1_9 | 0.1190(10) | 0.4383(3) | 0.0621(5) | 0.031(2) |
| C1_9 | 0.1008(6) | 0.3904(4) | 0.0829(3) | 0.0303(19) |
| C2_9 | 0.1241(7) | 0.3919(4) | 0.1387(3) | 0.044(2) |
| F1_9 | 0.2213(4) | 0.3976(3) | 0.1461(2) | 0.0609(16) |
| F2_9 | 0.0879(7) | 0.3487(4) | 0.1623(4) | 0.054(2) |
| F3_9 | 0.0866(5) | 0.4334(2) | 0.15974(17) | 0.0535(16) |
| C3_9 | -0.0062(6) | 0.3700(4) | 0.0747(3) | 0.042(2) |
| F4_9 | -0.0382(4) | 0.3827(2) | 0.0306(2) | 0.0588(18) |
| F5_9 | -0.0662(4) | 0.3934(2) | 0.1063(2) | 0.0581(16) |
| F6_9 | -0.0181(11) | 0.3179(4) | 0.0793(4) | 0.051(2) |
| C4_9 | 0.1724(7) | 0.3525(4) | 0.0576(3) | 0.044(2) |
| F7_9 | 0.1395(6) | 0.3401(2) | 0.0129(2) | 0.0653(18) |
| F8_9 | 0.1843(12) | 0.3087(4) | 0.0835(5) | 0.060(3) |
| F9_9 | 0.2622(4) | 0.3755(2) | 0.0529(3) | 0.0583(16) |
| O1_10 | 0.0205(3) | 0.52583(16) | 0.09925(12) | 0.0450(9) |
| C1_10 | -0.0505(3) | 0.55497(18) | 0.12027(15) | 0.0354(10) |

| | | | | |
|---|---|---|---|---|
| C2_10 | -0.0221(4) | 0.6142(2) | 0.11596(19) | 0.0514(13) |
| F1_10 | 0.0474(3) | 0.62931(16) | 0.14885(14) | 0.0737(12) |
| F2_10 | -0.0986(3) | 0.64458(14) | 0.12346(14) | 0.0681(10) |
| F3_10 | 0.0142(3) | 0.62543(15) | 0.07206(12) | 0.0668(11) |
| C3_10 | -0.1514(4) | 0.54342(19) | 0.09416(18) | 0.0402(10) |
| F4_10 | -0.1647(2) | 0.49213(12) | 0.08646(12) | 0.0496(8) |
| F5_10 | -0.1532(2) | 0.56677(13) | 0.05094(12) | 0.0507(8) |
| F6_10 | -0.2270(2) | 0.55905(14) | 0.11984(13) | 0.0546(8) |
| C4_10 | -0.0564(4) | 0.5385(2) | 0.17455(17) | 0.0443(11) |
| F7_10 | -0.1034(3) | 0.49212(13) | 0.17980(12) | 0.0543(8) |
| F8_10 | -0.1037(3) | 0.57321(14) | 0.20084(11) | 0.0666(11) |
| F9_10 | 0.0342(3) | 0.53513(15) | 0.19367(11) | 0.0571(9) |
| O1_11 | 0.1791(2) | 0.53785(12) | 0.03042(11) | 0.0301(7) |
| C1_11 | 0.2717(3) | 0.55740(17) | 0.04129(15) | 0.0308(9) |
| C2_11 | 0.3496(4) | 0.5188(2) | 0.0237(2) | 0.0492(12) |
| F1_11 | 0.3543(3) | 0.47764(14) | 0.05405(16) | 0.0671(10) |
| F2_11 | 0.4401(2) | 0.54217(18) | 0.02137(15) | 0.0734(11) |
| F3_11 | 0.3280(2) | 0.50064(16) | -0.02105(13) | 0.0613(9) |
| C3_11 | 0.2867(4) | 0.6110(2) | 0.0134(2) | 0.0506(13) |
| F4_11 | 0.2099(3) | 0.64076(12) | 0.02009(13) | 0.0559(8) |
| F5_11 | 0.2968(3) | 0.60064(17) | -0.03438(12) | 0.0679(11) |
| F6_11 | 0.3664(3) | 0.63776(15) | 0.03052(15) | 0.0732(12) |
| C4_11 | 0.2869(4) | 0.5662(2) | 0.09703(17) | 0.0448(11) |
| F7_11 | 0.2429(3) | 0.61045(15) | 0.11095(13) | 0.0658(10) |
| F8_11 | 0.3821(2) | 0.56966(15) | 0.10979(12) | 0.0582(9) |
| F9_11 | 0.2459(3) | 0.52633(14) | 0.12179(11) | 0.0556(9) |
| C1_13 | -0.7587(3) | 0.70897(15) | 0.28921(16) | 0.0289(8) |
| C2_13 | -0.7554(3) | 0.67957(16) | 0.24707(14) | 0.0269(8) |
| C3_13 | -0.8064(3) | 0.63233(19) | 0.24220(16) | 0.0354(10) |
| H3_13 | -0.804065 | 0.612473 | 0.212793 | 0.043 |
| C4_13 | -0.8610(4) | 0.6147(2) | 0.28150(16) | 0.0411(11) |
| H4_13 | -0.897763 | 0.582073 | 0.279413 | 0.049 |
| C5_13 | -0.8632(4) | 0.64379(19) | 0.32400(16) | 0.0415(11) |
| H5_13 | -0.901434 | 0.630719 | 0.350817 | 0.050 |
| C6_13 | -0.8106(4) | 0.69193(18) | 0.32851(16) | 0.0357(10) |
| H6_13 | -0.811398 | 0.711814 | 0.357939 | 0.043 |
| F1_13 | -0.7041(2) | 0.75609(10) | 0.28929(11) | 0.0383(6) |
| F2_13 | -0.69806(19) | 0.70013(10) | 0.20976(10) | 0.0322(5) |
| C1_14 | -0.4463(3) | 0.88857(17) | 0.27672(16) | 0.0333(10) |
| C2_14 | -0.5207(3) | 0.87988(16) | 0.30925(16) | 0.0324(9) |
| C3_14 | -0.5203(4) | 0.9031(2) | 0.35416(19) | 0.0451(12) |
| H3_14 | -0.573844 | 0.897464 | 0.376217 | 0.054 |
| C4_14 | -0.4388(4) | 0.9353(2) | 0.3665(2) | 0.0511(13) |
| H4_14 | -0.435782 | 0.952240 | 0.397431 | 0.061 |
| C5_14 | -0.3629(4) | 0.9426(2) | 0.3342(2) | 0.0538(14) |
| H5_14 | -0.307009 | 0.964271 | 0.343587 | 0.065 |
| C6_14 | -0.3644(3) | 0.91977(18) | 0.2885(2) | 0.0429(11) |
| H6_14 | -0.311284 | 0.925340 | 0.266140 | 0.052 |
| F1_14 | -0.4556(2) | 0.86405(10) | 0.23164(10) | 0.0356(6) |
| F2_14 | -0.5989(2) | 0.84721(11) | 0.29449(11) | 0.0394(6) |
| C1_15 | 0.4778(3) | 0.38491(18) | 0.19383(16) | 0.0325(9) |
| C2_15 | 0.5604(3) | 0.39171(15) | 0.22271(14) | 0.0266(8) |
| C3_15 | 0.6379(3) | 0.42440(16) | 0.20965(18) | 0.0355(9) |
| H3_15 | 0.694627 | 0.429245 | 0.229940 | 0.043 |
| C4_15 | 0.6303(4) | 0.45047(19) | 0.16508(19) | 0.0413(11) |

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|---|---|---|---|---|
| H4_15 | 0.683666 | 0.473103 | 0.154378 | 0.050 |
| C5_15 | 0.5474(4) | 0.4442(2) | 0.1362(2) | 0.0470(12) |
| H5_15 | 0.543365 | 0.463337 | 0.106401 | 0.056 |
| C6_15 | 0.4696(4) | 0.4103(2) | 0.15015(19) | 0.0458(12) |
| H6_15 | 0.412723 | 0.404934 | 0.130056 | 0.055 |
| F1_15 | 0.40455(19) | 0.35044(10) | 0.21015(10) | 0.0363(6) |
| F2_15 | 0.56200(19) | 0.36388(10) | 0.26574(9) | 0.0319(5) |
| C1_16 | 0.2540(3) | 0.18178(16) | 0.25678(15) | 0.0279(9) |
| C2_16 | 0.2355(3) | 0.21658(15) | 0.21965(14) | 0.0258(8) |
| C3_16 | 0.1668(3) | 0.20521(17) | 0.18415(16) | 0.0331(9) |
| H3_16 | 0.154705 | 0.229532 | 0.158651 | 0.040 |
| C4_16 | 0.1154(4) | 0.15694(19) | 0.18668(17) | 0.0379(10) |
| H4_16 | 0.067604 | 0.147640 | 0.162360 | 0.046 |
| C5_16 | 0.1331(4) | 0.12211(19) | 0.22427(16) | 0.0370(10) |
| H5_16 | 0.096150 | 0.089484 | 0.225758 | 0.044 |
| C6_16 | 0.2038(3) | 0.13393(18) | 0.25982(17) | 0.0333(10) |
| H6_16 | 0.216802 | 0.109753 | 0.285309 | 0.040 |
| F1_16 | 0.3237(2) | 0.19694(10) | 0.29089(10) | 0.0366(6) |
| F2_16 | 0.28919(19) | 0.26362(10) | 0.22049(9) | 0.0328(6) |
| C1_17 | 0.6290(3) | 0.25205(15) | 0.36691(15) | 0.0288(8) |
| C2_17 | 0.5654(3) | 0.20951(17) | 0.37121(16) | 0.0327(9) |
| C3_17 | 0.5829(4) | 0.16954(19) | 0.40351(18) | 0.0397(11) |
| H3_17 | 0.537484 | 0.140162 | 0.406817 | 0.048 |
| C4_17 | 0.6682(4) | 0.17338(19) | 0.43096(19) | 0.0403(11) |
| H4_17 | 0.682005 | 0.146367 | 0.453712 | 0.048 |
| C5_17 | 0.7342(4) | 0.21626(18) | 0.42574(18) | 0.0415(11) |
| H5_17 | 0.793561 | 0.217753 | 0.444391 | 0.050 |
| C6_17 | 0.7153(4) | 0.25692(18) | 0.39386(17) | 0.0372(10) |
| H6_17 | 0.759619 | 0.286779 | 0.390642 | 0.045 |
| F1_17 | 0.60366(19) | 0.29114(10) | 0.33399(9) | 0.0333(6) |
| F2_17 | 0.4802(2) | 0.20943(11) | 0.34318(11) | 0.0416(7) |
| O1_18 | -0.4479(3) | 0.71055(17) | 0.35538(11) | 0.0460(9) |
| C1_18 | -0.4324(3) | 0.72367(18) | 0.40267(16) | 0.0382(10) |
| C2_18 | -0.3863(4) | 0.6760(2) | 0.42951(18) | 0.0467(12) |
| F1_18 | -0.4553(3) | 0.63867(14) | 0.44037(14) | 0.0634(9) |
| F2_18 | -0.3438(3) | 0.69041(14) | 0.47201(11) | 0.0560(8) |
| F3_18 | -0.3186(3) | 0.65511(14) | 0.40221(13) | 0.0578(8) |
| C3_18 | -0.3582(5) | 0.7713(2) | 0.4074(2) | 0.0577(14) |
| F4_18 | -0.3768(3) | 0.80604(14) | 0.37187(16) | 0.0780(12) |
| F5_18 | -0.2653(3) | 0.75791(15) | 0.40252(13) | 0.0626(9) |
| F6_18 | -0.3656(4) | 0.79526(16) | 0.44993(16) | 0.0951(16) |
| C4_18 | -0.5321(4) | 0.7354(2) | 0.42548(19) | 0.0569(14) |
| F7_18 | -0.5609(4) | 0.78277(17) | 0.41013(16) | 0.0825(13) |
| F8_18 | -0.5284(3) | 0.73663(17) | 0.47401(12) | 0.0717(11) |
| F9_18 | -0.6018(3) | 0.69986(17) | 0.41154(14) | 0.0656(10) |
| O1_19 | -0.2846(3) | 0.7267(2) | 0.2948(3) | 0.0400(15) |
| C1_19 | -0.2035(4) | 0.7389(2) | 0.26879(19) | 0.0319(12) |
| C2_19 | -0.2135(4) | 0.7128(2) | 0.2175(2) | 0.0435(13) |
| F1_19 | -0.2017(3) | 0.66143(15) | 0.22047(19) | 0.0637(12) |
| F2_19 | -0.1500(3) | 0.73414(18) | 0.18488(15) | 0.0566(11) |
| F3_19 | -0.3057(3) | 0.71964(17) | 0.19967(13) | 0.0501(10) |
| C3_19 | -0.1857(4) | 0.7992(2) | 0.2619(2) | 0.0431(13) |
| F4_19 | -0.1990(3) | 0.82384(16) | 0.30419(15) | 0.0541(10) |
| F5_19 | -0.2515(3) | 0.81733(17) | 0.22972(19) | 0.0571(12) |
| F6_19 | -0.0949(3) | 0.81231(15) | 0.24660(17) | 0.0531(11) |

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|---|---|---|---|---|
| C4_19 | -0.1128(4) | 0.7163(2) | 0.2946(2) | 0.0495(15) |
| F7_19 | -0.0858(3) | 0.74699(18) | 0.33282(18) | 0.0680(14) |
| F8_19 | -0.0360(3) | 0.7131(2) | 0.2664(2) | 0.0742(16) |
| F9_19 | -0.1365(5) | 0.6682(2) | 0.3128(2) | 0.0674(16) |
| O1_20 | -0.4317(4) | 0.65040(14) | 0.26770(17) | 0.0505(12) |
| C1_20 | -0.4617(4) | 0.59901(18) | 0.26960(18) | 0.0287(11) |
| C2_20 | -0.5077(4) | 0.5843(2) | 0.21919(18) | 0.0418(13) |
| F1_20 | -0.5941(5) | 0.6062(3) | 0.21304(19) | 0.0659(13) |
| F2_20 | -0.5227(3) | 0.53238(13) | 0.21321(15) | 0.0503(9) |
| F3_20 | -0.4513(4) | 0.60087(16) | 0.18298(13) | 0.0589(11) |
| C3_20 | -0.3730(4) | 0.5642(2) | 0.27995(18) | 0.0354(11) |
| F4_20 | -0.3173(3) | 0.5846(2) | 0.31543(16) | 0.0589(13) |
| F5_20 | -0.3160(3) | 0.55981(15) | 0.24117(13) | 0.0457(9) |
| F6_20 | -0.4046(3) | 0.51462(18) | 0.2929(2) | 0.0500(12) |
| C4_20 | -0.5406(4) | 0.58971(18) | 0.30995(18) | 0.0316(11) |
| F7_20 | -0.5003(3) | 0.58511(14) | 0.35363(11) | 0.0411(8) |
| F8_20 | -0.5982(3) | 0.54710(14) | 0.30167(15) | 0.0492(10) |
| F9_20 | -0.5988(2) | 0.63096(13) | 0.31180(12) | 0.0386(8) |
| O1_21 | 0.0867(5) | 0.0344(3) | -0.0885(2) | 0.0348(14) |
| C1_21 | 0.0514(5) | 0.0287(3) | -0.1349(3) | 0.0328(16) |
| C2_21 | -0.0617(5) | 0.0189(3) | -0.1394(3) | 0.0508(18) |
| F1_21 | -0.0905(5) | -0.0294(2) | -0.1265(3) | 0.089(2) |
| F2_21 | -0.0978(4) | 0.0273(3) | -0.1811(2) | 0.0676(17) |
| F3_21 | -0.1027(4) | 0.0501(3) | -0.1069(2) | 0.0707(18) |
| C3_21 | 0.0850(6) | 0.0784(3) | -0.1640(3) | 0.056(2) |
| F4_21 | 0.1742(7) | 0.0949(4) | -0.1502(4) | 0.083(2) |
| F5_21 | 0.0256(6) | 0.1181(3) | -0.1544(4) | 0.089(2) |
| F6_21 | 0.0788(7) | 0.0719(4) | -0.2115(2) | 0.080(2) |
| C4_21 | 0.1008(6) | -0.0205(3) | -0.1562(3) | 0.048(2) |
| F7_21 | 0.1954(4) | -0.0073(3) | -0.1636(3) | 0.089(2) |
| F8_21 | 0.0609(12) | -0.0360(7) | -0.1981(4) | 0.070(2) |
| F9_21 | 0.0949(7) | -0.0599(3) | -0.1261(4) | 0.077(2) |
| O1_22 | 0.1861(6) | 0.0485(6) | -0.0048(5) | 0.076(4) |
| C1_22 | 0.2771(7) | 0.0308(3) | 0.0016(3) | 0.041(2) |
| C2_22 | 0.3227(9) | 0.0498(4) | 0.0508(4) | 0.072(3) |
| F1_22 | 0.3345(8) | 0.1023(2) | 0.0517(4) | 0.118(4) |
| F2_22 | 0.4103(8) | 0.0290(7) | 0.0600(7) | 0.090(3) |
| F3_22 | 0.2680(8) | 0.0369(4) | 0.0886(3) | 0.109(3) |
| C3_22 | 0.2810(7) | -0.0294(3) | -0.0007(3) | 0.051(2) |
| F4_22 | 0.2219(6) | -0.0479(2) | -0.0360(2) | 0.0663(18) |
| F5_22 | 0.2530(6) | -0.0505(2) | 0.0411(2) | 0.092(3) |
| F6_22 | 0.3708(9) | -0.0447(7) | -0.0103(6) | 0.087(3) |
| C4_22 | 0.3385(8) | 0.0551(4) | -0.0408(4) | 0.073(3) |
| F7_22 | 0.3194(6) | 0.0289(4) | -0.0818(3) | 0.100(3) |
| F8_22 | 0.4328(8) | 0.0613(7) | -0.0276(7) | 0.128(4) |
| F9_22 | 0.3162(9) | 0.1058(3) | -0.0484(4) | 0.103(3) |
| O1_23 | 0.0089(4) | 0.10501(16) | -0.0153(2) | 0.0379(12) |
| C1_23 | 0.0098(4) | 0.15612(19) | -0.00217(18) | 0.0296(10) |
| C2_23 | 0.0817(5) | 0.1664(2) | 0.0417(2) | 0.0506(14) |
| F1_23 | 0.1752(3) | 0.17269(16) | 0.0264(2) | 0.0660(12) |
| F2_23 | 0.0623(4) | 0.20891(15) | 0.06700(16) | 0.0750(15) |
| F3_23 | 0.0790(4) | 0.12536(17) | 0.07181(14) | 0.0696(13) |
| C3_23 | -0.0964(4) | 0.1689(2) | 0.0140(2) | 0.0434(12) |
| F4_23 | -0.1615(3) | 0.15030(15) | -0.01849(18) | 0.0575(10) |
| F5_23 | -0.1178(3) | 0.14780(16) | 0.05624(16) | 0.0609(12) |

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| F6_23 | -0.1060(3) | 0.22100(13) | 0.01732(18) | 0.0618(12) |
| C4_23 | 0.0431(4) | 0.1913(2) | -0.0454(2) | 0.0460(13) |
| F7_23 | -0.0289(4) | 0.1926(2) | -0.07881(15) | 0.0697(12) |
| F8_23 | 0.0662(4) | 0.24091(14) | -0.03080(18) | 0.0698(13) |
| F9_23 | 0.1208(3) | 0.17146(18) | -0.06718(15) | 0.0590(11) |
| O1_24 | 0.5585(5) | 0.1468(2) | 0.2176(4) | 0.0386(18) |
| C1_24 | 0.5740(5) | 0.0956(3) | 0.2300(2) | 0.0301(14) |
| C2_24 | 0.5770(6) | 0.0612(3) | 0.1830(3) | 0.0486(18) |
| F1_24 | 0.4857(5) | 0.0546(2) | 0.1645(2) | 0.0696(18) |
| F2_24 | 0.6094(9) | 0.0134(3) | 0.1934(6) | 0.075(2) |
| F3_24 | 0.6347(6) | 0.0846(4) | 0.1508(3) | 0.071(2) |
| C3_24 | 0.6748(6) | 0.0914(2) | 0.2577(2) | 0.0426(16) |
| F4_24 | 0.6829(4) | 0.12943(19) | 0.29192(16) | 0.0609(15) |
| F5_24 | 0.7489(3) | 0.09878(18) | 0.22769(19) | 0.0497(12) |
| F6_24 | 0.6825(4) | 0.04532(19) | 0.2802(2) | 0.0740(19) |
| C4_24 | 0.4888(7) | 0.0750(4) | 0.2637(4) | 0.057(2) |
| F7_24 | 0.4999(7) | 0.0982(3) | 0.3081(3) | 0.094(3) |
| F8_24 | 0.4910(11) | 0.0225(3) | 0.2689(6) | 0.068(2) |
| F9_24 | 0.4044(4) | 0.0888(2) | 0.2466(4) | 0.087(2) |
| O1_25 | 0.7218(3) | 0.2180(2) | 0.22062(18) | 0.0271(10) |
| C1_25 | 0.8109(5) | 0.2433(2) | 0.2136(2) | 0.0273(14) |
| C2_25 | 0.8811(5) | 0.2280(3) | 0.2563(2) | 0.0440(16) |
| F1_25 | 0.9116(4) | 0.1790(2) | 0.2482(2) | 0.0577(15) |
| F2_25 | 0.9605(3) | 0.2599(3) | 0.2590(2) | 0.0668(16) |
| F3_25 | 0.8348(4) | 0.2286(3) | 0.29836(15) | 0.0632(16) |
| C3_25 | 0.7984(5) | 0.3039(3) | 0.2143(3) | 0.0452(15) |
| F4_25 | 0.7195(3) | 0.31614(17) | 0.1881(2) | 0.0576(14) |
| F5_25 | 0.7787(5) | 0.3207(2) | 0.2598(2) | 0.0659(16) |
| F6_25 | 0.8747(4) | 0.33179(18) | 0.1984(2) | 0.0636(16) |
| C4_25 | 0.8550(6) | 0.2276(3) | 0.1636(3) | 0.0344(16) |
| F7_25 | 0.8112(3) | 0.2524(2) | 0.12702(16) | 0.0457(11) |
| F8_25 | 0.9518(5) | 0.2415(3) | 0.1616(4) | 0.0459(16) |
| F9_25 | 0.8409(5) | 0.17637(16) | 0.15668(18) | 0.0534(14) |
| O1_26 | 0.5937(6) | 0.2217(4) | 0.1385(3) | 0.0357(14) |
| C1_26 | 0.5391(6) | 0.2248(3) | 0.0978(3) | 0.0303(15) |
| C2_26 | 0.5517(6) | 0.1735(3) | 0.0681(3) | 0.0467(17) |
| F1_26 | 0.6453(5) | 0.1629(3) | 0.0635(3) | 0.0647(18) |
| F2_26 | 0.5145(7) | 0.1787(4) | 0.0230(3) | 0.077(2) |
| F3_26 | 0.5051(5) | 0.1333(2) | 0.0886(3) | 0.0613(16) |
| C3_26 | 0.4286(6) | 0.2293(3) | 0.1098(3) | 0.0377(16) |
| F4_26 | 0.4092(11) | 0.2773(4) | 0.1258(5) | 0.0585(19) |
| F5_26 | 0.4017(5) | 0.1966(3) | 0.1459(3) | 0.0488(19) |
| F6_26 | 0.3676(5) | 0.2195(3) | 0.0722(3) | 0.0546(16) |
| C4_26 | 0.5755(5) | 0.2731(3) | 0.0670(3) | 0.0413(16) |
| F7_26 | 0.5904(6) | 0.3146(2) | 0.0947(3) | 0.0632(17) |
| F8_26 | 0.5117(5) | 0.2846(3) | 0.0321(3) | 0.084(2) |
| F9_26 | 0.6624(5) | 0.2645(3) | 0.0466(3) | 0.062(2) |
| C1_27 | 0.3174(4) | 0.29663(18) | 0.38263(16) | 0.0373(11) |
| C2_27 | 0.2429(4) | 0.3010(2) | 0.34759(17) | 0.0378(11) |
| C3_27 | 0.2437(4) | 0.3441(2) | 0.31558(17) | 0.0381(11) |
| C4_27 | 0.3201(4) | 0.38296(18) | 0.31847(17) | 0.0334(10) |
| C5_27 | 0.3946(3) | 0.37950(16) | 0.35434(15) | 0.0263(8) |
| C6_27 | 0.3938(3) | 0.33584(16) | 0.38647(14) | 0.0269(8) |
| C7_27 | 0.3130(6) | 0.2514(2) | 0.4188(2) | 0.0620(19) |
| H7A_27 | 0.259150 | 0.256294 | 0.442058 | 0.093 |

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|---|---|---|---|---|
| H7B_27 | 0.375847 | 0.250578 | 0.436604 | 0.093 |
| H7C_27 | 0.301215 | 0.218069 | 0.401232 | 0.093 |
| C8_27 | 0.1575(5) | 0.2595(3) | 0.3449(2) | 0.068(2) |
| H8A_27 | 0.097478 | 0.274309 | 0.358116 | 0.101 |
| H8B_27 | 0.174211 | 0.228509 | 0.364043 | 0.101 |
| H8C_27 | 0.146192 | 0.249182 | 0.310705 | 0.101 |
| C9_27 | 0.1605(4) | 0.3505(3) | 0.2788(2) | 0.0637(19) |
| H9A_27 | 0.155515 | 0.387941 | 0.270781 | 0.096 |
| H9B_27 | 0.097955 | 0.336972 | 0.292868 | 0.096 |
| H9C_27 | 0.174525 | 0.330770 | 0.248936 | 0.096 |
| C10_27 | 0.3194(5) | 0.4293(2) | 0.2844(2) | 0.0523(14) |
| H10A_27 | 0.290895 | 0.459235 | 0.301095 | 0.078 |
| H10B_27 | 0.279664 | 0.419978 | 0.255413 | 0.078 |
| H10C_27 | 0.387259 | 0.439004 | 0.274382 | 0.078 |
| C11_27 | 0.4729(4) | 0.42299(18) | 0.36080(19) | 0.0403(11) |
| H11A_27 | 0.484321 | 0.429301 | 0.395765 | 0.060 |
| H11B_27 | 0.450870 | 0.455320 | 0.345400 | 0.060 |
| H11C_27 | 0.534455 | 0.412630 | 0.345437 | 0.060 |
| C12_27 | 0.4744(5) | 0.3346(2) | 0.42499(18) | 0.0465(13) |
| H12A_27 | 0.455536 | 0.355506 | 0.453383 | 0.070 |
| H12B_27 | 0.536444 | 0.349533 | 0.411379 | 0.070 |
| H12C_27 | 0.483408 | 0.298123 | 0.435115 | 0.070 |
| C1_28 | -0.6462(4) | 0.87972(19) | 0.1485(2) | 0.0452(14) |
| C2_28 | -0.6644(4) | 0.8358(2) | 0.11883(17) | 0.0384(11) |
| C3_28 | -0.7413(3) | 0.79796(18) | 0.13079(16) | 0.0319(9) |
| C4_28 | -0.7978(3) | 0.80563(18) | 0.17268(16) | 0.0315(9) |
| C5_28 | -0.7787(3) | 0.84975(19) | 0.20258(17) | 0.0358(10) |
| C6_28 | -0.7019(4) | 0.88662(19) | 0.1906(2) | 0.0425(13) |
| C7_28 | -0.5695(5) | 0.9212(3) | 0.1333(4) | 0.092(3) |
| H7A_28 | -0.577255 | 0.953249 | 0.152638 | 0.137 |
| H7B_28 | -0.577885 | 0.929287 | 0.098481 | 0.137 |
| H7C_28 | -0.503332 | 0.908092 | 0.138709 | 0.137 |
| C8_28 | -0.6092(5) | 0.8294(4) | 0.0722(2) | 0.074(2) |
| H8A_28 | -0.645002 | 0.845586 | 0.045397 | 0.111 |
| H8B_28 | -0.602981 | 0.791721 | 0.065483 | 0.111 |
| H8C_28 | -0.543162 | 0.846481 | 0.075245 | 0.111 |
| C9_28 | -0.7621(5) | 0.7513(2) | 0.0978(2) | 0.0582(16) |
| H9A_28 | -0.832094 | 0.740066 | 0.100328 | 0.087 |
| H9B_28 | -0.721096 | 0.722302 | 0.107755 | 0.087 |
| H9C_28 | -0.746852 | 0.761246 | 0.063960 | 0.087 |
| C10_28 | -0.8837(4) | 0.7678(2) | 0.1850(3) | 0.0571(17) |
| H10A_28 | -0.945951 | 0.785575 | 0.180623 | 0.086 |
| H10B_28 | -0.877945 | 0.756173 | 0.218987 | 0.086 |
| H10C_28 | -0.882893 | 0.737113 | 0.163199 | 0.086 |
| C11_28 | -0.8419(5) | 0.8590(3) | 0.2465(2) | 0.071(2) |
| H11A_28 | -0.866724 | 0.894710 | 0.245029 | 0.106 |
| H11B_28 | -0.802470 | 0.855307 | 0.276303 | 0.106 |
| H11C_28 | -0.897770 | 0.833190 | 0.246870 | 0.106 |
| C12_28 | -0.6828(6) | 0.9352(2) | 0.2219(3) | 0.082(3) |
| H12A_28 | -0.727264 | 0.962666 | 0.211894 | 0.124 |
| H12B_28 | -0.614044 | 0.948103 | 0.217785 | 0.124 |
| H12C_28 | -0.694593 | 0.926225 | 0.256332 | 0.124 |
| O1_29 | 0.5949(10) | 0.1463(4) | 0.2159(8) | 0.044(4) |
| C1_29 | 0.5510(8) | 0.0981(5) | 0.2160(4) | 0.042(3) |
| C2_29 | 0.4581(8) | 0.0971(4) | 0.1821(4) | 0.057(3) |

| | | | | |
|---|---|---|---|---|
| F1_29 | 0.4863(9) | 0.0956(5) | 0.1353(4) | 0.077(3) |
| F2_29 | 0.3972(9) | 0.0570(4) | 0.1920(5) | 0.081(4) |
| F3_29 | 0.4043(7) | 0.1383(4) | 0.1913(4) | 0.057(3) |
| C3_29 | 0.5156(10) | 0.0829(6) | 0.2679(5) | 0.050(3) |
| F4_29 | 0.5915(8) | 0.0922(7) | 0.2987(4) | 0.090(4) |
| F5_29 | 0.4380(9) | 0.1106(5) | 0.2810(5) | 0.062(3) |
| F6_29 | 0.483(2) | 0.0321(6) | 0.2703(12) | 0.078(4) |
| C4_29 | 0.6281(9) | 0.0594(5) | 0.1982(5) | 0.050(3) |
| F7_29 | 0.6967(8) | 0.0512(4) | 0.2319(4) | 0.066(3) |
| F8_29 | 0.5840(19) | 0.0136(7) | 0.1856(12) | 0.085(4) |
| F9_29 | 0.6733(11) | 0.0781(9) | 0.1589(6) | 0.066(4) |
| O1_30 | 0.8076(13) | 0.4526(9) | 0.5023(10) | 0.025(4) |
| C1_30 | 0.7403(8) | 0.4804(4) | 0.5269(4) | 0.025(2) |
| C2_30 | 0.6961(7) | 0.5211(4) | 0.4914(3) | 0.039(2) |
| F1_30 | 0.6303(6) | 0.4985(4) | 0.4609(3) | 0.054(2) |
| F2_30 | 0.6527(14) | 0.5596(7) | 0.5153(6) | 0.053(3) |
| F3_30 | 0.7693(13) | 0.5430(10) | 0.4648(6) | 0.048(3) |
| C3_30 | 0.7877(6) | 0.5091(3) | 0.5710(3) | 0.0335(19) |
| F4_30 | 0.8483(11) | 0.4797(7) | 0.5969(8) | 0.039(2) |
| F5_30 | 0.8413(7) | 0.5509(3) | 0.5571(3) | 0.0375(19) |
| F6_30 | 0.7207(9) | 0.5245(4) | 0.6031(4) | 0.044(2) |
| C4_30 | 0.6564(7) | 0.4402(3) | 0.5436(3) | 0.035(2) |
| F7_30 | 0.6863(7) | 0.4152(4) | 0.5831(3) | 0.050(2) |
| F8_30 | 0.5757(12) | 0.4655(9) | 0.5546(7) | 0.036(3) |
| F9_30 | 0.636(2) | 0.4066(6) | 0.5073(6) | 0.049(3) |
| O1_31 | 0.7011(6) | 0.2424(4) | 0.2192(4) | 0.025(2) |
| C1_31 | 0.8007(9) | 0.2433(4) | 0.2219(4) | 0.035(3) |
| C2_31 | 0.8384(9) | 0.2949(5) | 0.2486(5) | 0.056(3) |
| F1_31 | 0.7895(10) | 0.3354(4) | 0.2306(6) | 0.069(3) |
| F2_31 | 0.9335(7) | 0.3056(5) | 0.2393(6) | 0.080(4) |
| F3_31 | 0.8213(8) | 0.2898(5) | 0.2954(3) | 0.065(3) |
| C3_31 | 0.8333(9) | 0.1939(5) | 0.2508(4) | 0.055(3) |
| F4_31 | 0.8310(10) | 0.1524(4) | 0.2211(5) | 0.084(4) |
| F5_31 | 0.7745(8) | 0.1858(5) | 0.2892(4) | 0.066(3) |
| F6_31 | 0.9262(9) | 0.2036(6) | 0.2659(5) | 0.068(3) |
| C4_31 | 0.8440(11) | 0.2433(6) | 0.1696(5) | 0.052(4) |
| F7_31 | 0.7953(8) | 0.2066(6) | 0.1423(4) | 0.069(4) |
| F8_31 | 0.9387(11) | 0.2303(9) | 0.1696(9) | 0.063(4) |
| F9_31 | 0.8331(11) | 0.2904(6) | 0.1491(6) | 0.094(5) |
| C1_32 | -0.4674(3) | 0.71776(16) | 0.12011(15) | 0.0288(8) |
| C2_32 | -0.4145(3) | 0.76525(16) | 0.11935(16) | 0.0316(9) |
| C3_32 | -0.3366(4) | 0.7734(2) | 0.08868(18) | 0.0443(11) |
| H3_32 | -0.299694 | 0.806056 | 0.088236 | 0.053 |
| C4_32 | -0.3125(4) | 0.7323(2) | 0.0580(2) | 0.0521(14) |
| H4_32 | -0.258433 | 0.736884 | 0.036150 | 0.063 |
| C5_32 | -0.3661(5) | 0.6848(2) | 0.0589(2) | 0.0523(14) |
| H5_32 | -0.348664 | 0.657245 | 0.037497 | 0.063 |
| C6_32 | -0.4450(4) | 0.67699(19) | 0.09059(17) | 0.0398(11) |
| H6_32 | -0.481964 | 0.644341 | 0.091640 | 0.048 |
| F1_32 | -0.5442(2) | 0.71350(11) | 0.15213(10) | 0.0378(6) |
| F2_32 | -0.4424(2) | 0.80314(10) | 0.15170(10) | 0.0367(6) |
| O1_33 | 0.110(2) | 0.4365(6) | 0.0602(10) | 0.048(5) |
| C1_33 | 0.1003(9) | 0.3877(6) | 0.0797(5) | 0.038(3) |
| C2_33 | 0.0004(10) | 0.3616(6) | 0.0631(5) | 0.046(3) |
| F1_33 | 0.0050(7) | 0.3437(3) | 0.0180(3) | 0.055(3) |

| | | | | |
|---|---|---|---|---|
| F2_33 | -0.028(2) | 0.3221(7) | 0.0927(7) | 0.061(4) |
| F3_33 | -0.0685(7) | 0.3981(4) | 0.0650(5) | 0.061(3) |
| C3_33 | 0.1032(11) | 0.3920(6) | 0.1363(5) | 0.058(4) |
| F4_33 | 0.1777(10) | 0.4257(4) | 0.1495(4) | 0.071(3) |
| F5_33 | 0.0204(9) | 0.4091(4) | 0.1536(3) | 0.069(3) |
| F6_33 | 0.1232(14) | 0.3458(6) | 0.1565(8) | 0.067(4) |
| C4_33 | 0.1864(10) | 0.3536(6) | 0.0633(5) | 0.057(4) |
| F7_33 | 0.2700(8) | 0.3662(5) | 0.0872(6) | 0.083(3) |
| F8_33 | 0.168(2) | 0.3024(7) | 0.0731(10) | 0.061(4) |
| F9_33 | 0.2020(10) | 0.3574(4) | 0.0156(4) | 0.071(3) |
| O1_34 | 0.925(4) | 0.0659(8) | 0.5681(18) | 0.043(8) |
| C1_34 | 0.912(2) | 0.1144(8) | 0.5863(10) | 0.046(5) |
| C2_34 | 0.869(2) | 0.1111(12) | 0.6388(10) | 0.048(5) |
| F1_34 | 0.885(4) | 0.0649(14) | 0.6594(16) | 0.047(5) |
| F2_34 | 0.911(4) | 0.1484(15) | 0.6671(13) | 0.052(5) |
| F3_34 | 0.772(2) | 0.117(3) | 0.6393(19) | 0.060(5) |
| C3_34 | 0.842(2) | 0.1453(11) | 0.5532(11) | 0.054(6) |
| F4_34 | 0.889(4) | 0.162(2) | 0.5134(14) | 0.065(5) |
| F5_34 | 0.764(3) | 0.1151(17) | 0.5394(18) | 0.063(5) |
| F6_34 | 0.809(4) | 0.1873(14) | 0.5763(17) | 0.065(5) |
| C4_34 | 1.016(2) | 0.1433(11) | 0.5886(11) | 0.057(6) |
| F7_34 | 1.063(3) | 0.1424(19) | 0.5460(13) | 0.064(5) |
| F8_34 | 1.008(3) | 0.1932(11) | 0.6018(18) | 0.067(5) |
| F9_34 | 1.071(3) | 0.1193(18) | 0.6217(16) | 0.062(5) |
| O1_36 | -0.449(2) | 0.6462(5) | 0.2971(9) | 0.053(6) |
| C1_36 | -0.4484(13) | 0.5989(7) | 0.2739(6) | 0.044(4) |
| C2_36 | -0.3843(16) | 0.6023(8) | 0.2270(7) | 0.073(7) |
| F1_36 | -0.4041(18) | 0.6458(8) | 0.2027(8) | 0.066(7) |
| F2_36 | -0.407(3) | 0.5640(9) | 0.1949(8) | 0.100(10) |
| F3_36 | -0.2893(15) | 0.6040(12) | 0.2397(12) | 0.097(9) |
| C3_36 | -0.4063(16) | 0.5587(8) | 0.3104(7) | 0.054(5) |
| F4_36 | -0.4774(19) | 0.5443(9) | 0.3415(9) | 0.070(6) |
| F5_36 | -0.3291(19) | 0.5789(14) | 0.3350(10) | 0.069(5) |
| F6_36 | -0.373(3) | 0.5175(10) | 0.2864(12) | 0.056(5) |
| C4_36 | -0.5557(14) | 0.5811(8) | 0.2603(8) | 0.065(6) |
| F7_36 | -0.6157(16) | 0.5912(11) | 0.2976(9) | 0.071(7) |
| F8_36 | -0.566(2) | 0.5294(9) | 0.2533(15) | 0.101(10) |
| F9_36 | -0.586(3) | 0.6080(18) | 0.2221(12) | 0.078(5) |
| O1_37 | -0.2946(13) | 0.7421(11) | 0.2910(11) | 0.040(6) |
| C1_37 | -0.2034(13) | 0.7450(7) | 0.2711(6) | 0.049(5) |
| C2_37 | -0.2122(13) | 0.7589(7) | 0.2161(6) | 0.050(4) |
| F1_37 | -0.247(2) | 0.7167(8) | 0.1918(8) | 0.065(3) |
| F2_37 | -0.1261(15) | 0.7732(13) | 0.1961(10) | 0.096(9) |
| F3_37 | -0.2707(17) | 0.7980(8) | 0.2078(9) | 0.067(4) |
| C3_37 | -0.1326(16) | 0.7848(8) | 0.2988(8) | 0.099(8) |
| F4_37 | -0.162(3) | 0.7877(12) | 0.3454(7) | 0.129(11) |
| F5_37 | -0.134(3) | 0.8330(9) | 0.2813(13) | 0.129(13) |
| F6_37 | -0.0409(16) | 0.7666(15) | 0.2978(14) | 0.157(13) |
| C4_37 | -0.1524(18) | 0.6912(8) | 0.2744(8) | 0.083(6) |
| F7_37 | -0.121(3) | 0.6837(12) | 0.3197(9) | 0.071(5) |
| F8_37 | -0.076(2) | 0.6905(14) | 0.2447(10) | 0.103(9) |
| F9_37 | -0.209(3) | 0.6506(10) | 0.2607(14) | 0.130(10) |
| O1_38 | 0.1824(9) | 0.0486(8) | 0.0041(4) | 0.027(3) |
| C1_38 | 0.2791(11) | 0.0364(5) | 0.0027(5) | 0.042(3) |
| C2_38 | 0.3200(11) | 0.0369(6) | 0.0566(5) | 0.056(3) |

| | | | | |
|---|---|---|---|---|
| F1_38 | 0.2927(10) | 0.0812(5) | 0.0783(5) | 0.072(3) |
| F2_38 | 0.4184(11) | 0.0349(12) | 0.0564(12) | 0.073(4) |
| F3_38 | 0.2776(8) | -0.0029(5) | 0.0809(4) | 0.068(3) |
| C3_38 | 0.2872(11) | -0.0195(5) | -0.0186(5) | 0.057(4) |
| F4_38 | 0.2840(11) | -0.0206(6) | -0.0668(4) | 0.098(5) |
| F5_38 | 0.2072(9) | -0.0483(4) | -0.0044(6) | 0.075(3) |
| F6_38 | 0.3648(16) | -0.0431(13) | -0.0009(11) | 0.082(4) |
| C4_38 | 0.3464(10) | 0.0754(5) | -0.0271(5) | 0.066(4) |
| F7_38 | 0.3052(15) | 0.0871(7) | -0.0698(5) | 0.087(4) |
| F8_38 | 0.4315(13) | 0.0539(12) | -0.0388(11) | 0.111(5) |
| F9_38 | 0.3601(9) | 0.1209(4) | -0.0066(5) | 0.094(4) |
| O1_12 | 0.0425(15) | 0.0403(8) | -0.0881(5) | 0.069(5) |
| C1_12 | 0.0545(10) | 0.0340(5) | -0.1365(5) | 0.048(3) |
| C2_12 | 0.1439(11) | 0.0638(6) | -0.1611(6) | 0.072(3) |
| F1_12 | 0.1611(17) | 0.1098(7) | -0.1397(10) | 0.082(4) |
| F2_12 | 0.1262(15) | 0.0675(10) | -0.2086(6) | 0.100(5) |
| F3_12 | 0.2270(10) | 0.0401(6) | -0.1607(8) | 0.121(6) |
| C3_12 | 0.0628(11) | -0.0248(5) | -0.1492(6) | 0.053(4) |
| F4_12 | -0.0163(13) | -0.0504(5) | -0.1320(6) | 0.105(6) |
| F5_12 | 0.1420(13) | -0.0468(7) | -0.1309(7) | 0.076(4) |
| F6_12 | 0.069(3) | -0.0319(15) | -0.1974(6) | 0.069(4) |
| C4_12 | -0.0375(11) | 0.0589(6) | -0.1596(6) | 0.088(4) |
| F7_12 | -0.1226(11) | 0.0553(7) | -0.1371(7) | 0.106(4) |
| F8_12 | -0.0578(12) | 0.0364(7) | -0.2035(6) | 0.096(4) |
| F9_12 | -0.0175(14) | 0.1106(5) | -0.1547(10) | 0.101(4) |
| O1_35 | 0.601(3) | 0.218(2) | 0.1374(6) | 0.0357(14) |
| C1_35 | 0.538(2) | 0.2284(10) | 0.1003(8) | 0.036(3) |
| C2_35 | 0.592(2) | 0.2197(13) | 0.0511(9) | 0.046(5) |
| F1_35 | 0.644(4) | 0.2631(18) | 0.039(2) | 0.060(5) |
| F2_35 | 0.530(4) | 0.209(2) | 0.0143(12) | 0.074(5) |
| F3_35 | 0.652(4) | 0.1804(19) | 0.0542(19) | 0.058(4) |
| C3_35 | 0.445(2) | 0.1908(11) | 0.1043(13) | 0.047(4) |
| F4_35 | 0.414(5) | 0.188(2) | 0.1504(16) | 0.049(5) |
| F5_35 | 0.467(3) | 0.1427(11) | 0.090(2) | 0.058(5) |
| F6_35 | 0.370(3) | 0.206(2) | 0.078(2) | 0.052(4) |
| C4_35 | 0.509(2) | 0.2867(10) | 0.1040(11) | 0.052(5) |
| F7_35 | 0.437(3) | 0.2935(17) | 0.1359(17) | 0.059(4) |
| F8_35 | 0.481(4) | 0.3045(16) | 0.0606(14) | 0.081(11) |
| F9_35 | 0.588(3) | 0.3159(14) | 0.1181(19) | 0.054(4) |
| O1_39 | 0.5682(13) | 0.2136(8) | 0.1360(6) | 0.0357(14) |
| C1_39 | 0.5406(9) | 0.2418(5) | 0.0962(4) | 0.033(3) |
| C2_39 | 0.4268(9) | 0.2496(6) | 0.0980(5) | 0.042(3) |
| F1_39 | 0.3801(8) | 0.2047(4) | 0.1113(5) | 0.049(2) |
| F2_39 | 0.3910(8) | 0.2669(4) | 0.0559(3) | 0.051(3) |
| F3_39 | 0.409(2) | 0.2842(9) | 0.1331(9) | 0.055(3) |
| C3_39 | 0.5963(10) | 0.2967(5) | 0.0969(5) | 0.051(3) |
| F4_39 | 0.6875(7) | 0.2934(4) | 0.0795(4) | 0.052(2) |
| F5_39 | 0.6032(9) | 0.3153(4) | 0.1424(4) | 0.049(2) |
| F6_39 | 0.5498(9) | 0.3320(4) | 0.0711(4) | 0.052(2) |
| C4_39 | 0.5685(10) | 0.2126(5) | 0.0483(4) | 0.043(3) |
| F7_39 | 0.6591(9) | 0.1964(5) | 0.0511(5) | 0.055(3) |
| F8_39 | 0.5648(10) | 0.2457(5) | 0.0104(3) | 0.057(3) |
| F9_39 | 0.5093(13) | 0.1707(6) | 0.0424(6) | 0.065(3) |
| O1_40 | 0.032(3) | 0.1038(10) | -0.0082(16) | 0.045(7) |
| C1_40 | 0.0223(14) | 0.1555(9) | 0.0004(7) | 0.043(4) |

| | | | | |
|---|---|---|---|---|
| C2_40 | -0.0626(17) | 0.1652(9) | 0.0368(9) | 0.053(5) |
| F1_40 | -0.1491(17) | 0.1542(11) | 0.0153(12) | 0.054(4) |
| F2_40 | -0.059(3) | 0.2144(10) | 0.0533(14) | 0.091(11) |
| F3_40 | -0.056(3) | 0.1341(15) | 0.0755(11) | 0.090(10) |
| C3_40 | 0.1195(16) | 0.1792(10) | 0.0234(9) | 0.064(4) |
| F4_40 | 0.1952(17) | 0.1640(12) | -0.0029(13) | 0.064(5) |
| F5_40 | 0.129(3) | 0.1641(15) | 0.0694(9) | 0.109(11) |
| F6_40 | 0.122(3) | 0.2313(9) | 0.0235(16) | 0.103(11) |
| C4_40 | 0.0036(19) | 0.1856(10) | -0.0479(8) | 0.061(4) |
| F7_40 | 0.085(2) | 0.1891(13) | -0.0745(10) | 0.059(4) |
| F8_40 | -0.022(3) | 0.2343(10) | -0.0366(14) | 0.102(11) |
| F9_40 | -0.068(2) | 0.1617(14) | -0.0741(11) | 0.072(5) |

*Table S 6 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [SrHMB(oDFB)$_4$][al-f-al]$_2$ **6**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| O1_19 | 0.3015(13) | 0.0574(15) | 0.9827(12) | 0.025(5) |
| C1_19 | 0.2274(10) | 0.0276(6) | 1.0108(5) | 0.025(3) |
| C2_19 | 0.1335(6) | 0.0671(6) | 0.9804(4) | 0.038(2) |
| F1_19 | 0.1268(11) | 0.0501(7) | 0.9280(5) | 0.058(3) |
| F2_19 | 0.0552(6) | 0.0511(6) | 1.0152(5) | 0.056(2) |
| F3_19 | 0.128(3) | 0.1336(8) | 0.9748(15) | 0.046(4) |
| C3_19 | 0.2204(7) | 0.0349(5) | 1.0770(4) | 0.033(2) |
| F4_19 | 0.3077(12) | 0.0240(13) | 1.1000(12) | 0.040(4) |
| F5_19 | 0.1717(12) | 0.0950(6) | 1.0848(6) | 0.053(3) |
| F6_19 | 0.1660(11) | -0.0079(7) | 1.1083(9) | 0.047(3) |
| C4_19 | 0.2463(9) | -0.0488(6) | 1.0050(5) | 0.053(3) |
| F7_19 | 0.3112(11) | -0.0822(7) | 1.0444(5) | 0.063(3) |
| F8_19 | 0.1686(9) | -0.0781(7) | 1.0153(7) | 0.068(3) |
| F9_19 | 0.2897(12) | -0.0578(10) | 0.9525(7) | 0.052(4) |
| O1_18 | 0.1025(13) | 0.6915(9) | 0.2011(3) | 0.030(2) |
| C1_18 | 0.1326(6) | 0.7165(4) | 0.1455(4) | 0.0319(19) |
| C2_18 | 0.1022(4) | 0.6694(3) | 0.1062(2) | 0.0413(12) |
| F1_18 | 0.0065(2) | 0.6857(2) | 0.09658(14) | 0.0523(10) |
| F2_18 | 0.1475(7) | 0.6765(6) | 0.0525(3) | 0.0561(17) |
| F3_18 | 0.1220(7) | 0.6069(4) | 0.1359(4) | 0.065(2) |
| C3_18 | 0.2466(4) | 0.7095(3) | 0.1428(2) | 0.0508(14) |
| F4_18 | 0.2710(11) | 0.7391(7) | 0.1876(6) | 0.079(3) |
| F5_18 | 0.2868(3) | 0.6447(3) | 0.1486(2) | 0.0620(13) |
| F6_18 | 0.2786(6) | 0.7437(3) | 0.0931(3) | 0.0580(16) |
| C4_18 | 0.0836(5) | 0.7905(3) | 0.1240(2) | 0.0449(13) |
| F7_18 | 0.1276(4) | 0.8339(2) | 0.14672(18) | 0.0686(13) |
| F8_18 | 0.0941(9) | 0.8050(7) | 0.0651(4) | 0.057(3) |
| F9_18 | -0.0112(6) | 0.8015(5) | 0.1390(4) | 0.0515(16) |
| O1_17 | 0.43293(11) | 0.12486(7) | 1.03138(6) | 0.0286(3) |
| C1_17 | 0.43820(14) | 0.18793(10) | 1.04171(9) | 0.0246(4) |
| C2_17 | 0.51225(17) | 0.22217(12) | 0.99758(11) | 0.0354(5) |
| F1_17 | 0.47242(11) | 0.24724(7) | 0.94600(6) | 0.0441(3) |
| F2_17 | 0.54163(12) | 0.27312(8) | 1.01755(7) | 0.0524(4) |
| F3_17 | 0.59107(11) | 0.17753(8) | 0.98869(7) | 0.0532(4) |
| C3_17 | 0.47308(15) | 0.18064(11) | 1.10548(10) | 0.0287(4) |
| F4_17 | 0.42710(9) | 0.13758(6) | 1.14263(5) | 0.0314(3) |
| F5_17 | 0.56857(9) | 0.15611(8) | 1.10808(6) | 0.0419(3) |
| F6_17 | 0.45782(11) | 0.23949(7) | 1.12559(6) | 0.0451(4) |

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|---|---|---|---|---|
| C4_17 | 0.33613(17) | 0.23369(12) | 1.03619(11) | 0.0349(5) |
| F7_17 | 0.27753(10) | 0.21782(8) | 1.08335(7) | 0.0474(4) |
| F8_17 | 0.34095(12) | 0.29930(7) | 1.03165(7) | 0.0531(4) |
| F9_17 | 0.29271(11) | 0.22488(8) | 0.98905(7) | 0.0468(4) |
| O1_16 | 0.3060(3) | 0.0480(4) | 0.9829(3) | 0.0233(10) |
| C1_16 | 0.2291(3) | 0.02422(19) | 1.01383(16) | 0.0219(8) |
| C2_16 | 0.1869(2) | -0.02092(16) | 0.97765(13) | 0.0385(7) |
| F1_16 | 0.1350(3) | 0.01759(15) | 0.93376(12) | 0.0501(7) |
| F2_16 | 0.1261(2) | -0.05782(16) | 1.01056(15) | 0.0564(8) |
| F3_16 | 0.2559(3) | -0.0613(3) | 0.95378(17) | 0.0487(8) |
| C3_16 | 0.26231(18) | -0.01818(13) | 1.07410(11) | 0.0255(6) |
| F4_16 | 0.3246(3) | 0.0129(3) | 1.0965(3) | 0.0301(7) |
| F5_16 | 0.3094(2) | -0.07900(16) | 1.06755(11) | 0.0412(6) |
| F6_16 | 0.1889(2) | -0.02592(16) | 1.11369(18) | 0.0365(7) |
| C4_16 | 0.14893(19) | 0.08490(15) | 1.02540(13) | 0.0325(7) |
| F7_16 | 0.1771(2) | 0.11457(13) | 1.06772(13) | 0.0397(7) |
| F8_16 | 0.06224(14) | 0.06707(13) | 1.04257(11) | 0.0493(6) |
| F9_16 | 0.1365(6) | 0.13160(19) | 0.9771(3) | 0.0428(10) |
| O1_15 | 0.45200(10) | 0.10985(7) | 0.91158(6) | 0.0234(3) |
| C1_15 | 0.43558(14) | 0.11826(10) | 0.85314(8) | 0.0221(4) |
| C2_15 | 0.34250(16) | 0.17223(11) | 0.83809(9) | 0.0298(5) |
| F1_15 | 0.36084(10) | 0.23459(6) | 0.83782(6) | 0.0406(3) |
| F2_15 | 0.30929(10) | 0.17028(7) | 0.78544(6) | 0.0386(3) |
| F3_15 | 0.27063(9) | 0.16211(7) | 0.87814(6) | 0.0387(3) |
| C3_15 | 0.42185(16) | 0.04991(11) | 0.83578(9) | 0.0282(4) |
| F4_15 | 0.48568(10) | -0.00066(6) | 0.86262(6) | 0.0386(3) |
| F5_15 | 0.33239(10) | 0.03615(7) | 0.85212(6) | 0.0365(3) |
| F6_15 | 0.43374(11) | 0.04998(7) | 0.77776(6) | 0.0397(3) |
| C4_15 | 0.52593(16) | 0.14378(11) | 0.81841(9) | 0.0294(5) |
| F7_15 | 0.60039(9) | 0.09243(7) | 0.81608(6) | 0.0382(3) |
| F8_15 | 0.50550(10) | 0.17114(7) | 0.76256(6) | 0.0402(3) |
| F9_15 | 0.55717(10) | 0.18922(7) | 0.84340(6) | 0.0360(3) |
| O1_14 | 0.30178(11) | 0.03841(9) | 0.51444(10) | 0.0273(4) |
| C1_14 | 0.21374(19) | 0.01961(14) | 0.51190(12) | 0.0186(5) |
| C2_14 | 0.2229(3) | -0.03762(18) | 0.47470(17) | 0.0321(8) |
| F1_14 | 0.2317(3) | -0.01280(17) | 0.41761(14) | 0.0454(8) |
| F2_14 | 0.1468(2) | -0.07080(16) | 0.48347(15) | 0.0420(7) |
| F3_14 | 0.3030(2) | -0.08287(16) | 0.48825(16) | 0.0484(7) |
| C3_14 | 0.1761(2) | -0.00535(15) | 0.57586(12) | 0.0283(6) |
| F4_14 | 0.19184(18) | 0.03563(10) | 0.61182(8) | 0.0446(5) |
| F5_14 | 0.22384(13) | -0.06725(8) | 0.59631(7) | 0.0381(4) |
| F6_14 | 0.08121(12) | -0.00852(9) | 0.57911(7) | 0.0452(5) |
| C4_14 | 0.1385(2) | 0.08136(16) | 0.48392(15) | 0.0277(7) |
| F7_14 | 0.10825(13) | 0.12392(9) | 0.52151(9) | 0.0409(5) |
| F8_14 | 0.06003(12) | 0.06214(9) | 0.46588(10) | 0.0459(5) |
| F9_14 | 0.17961(11) | 0.11589(7) | 0.43694(7) | 0.0347(4) |
| O1_13 | 0.43482(10) | 0.11344(6) | 0.54590(6) | 0.0226(3) |
| C1_13 | 0.41136(14) | 0.17277(9) | 0.56730(9) | 0.0206(4) |
| C2_13 | 0.47718(16) | 0.22385(11) | 0.53561(11) | 0.0315(5) |
| F1_13 | 0.44609(10) | 0.24984(6) | 0.48155(6) | 0.0384(3) |
| F2_13 | 0.47789(11) | 0.27519(7) | 0.56453(7) | 0.0453(4) |
| F3_13 | 0.56920(9) | 0.19260(7) | 0.53073(7) | 0.0460(4) |
| C3_13 | 0.42880(17) | 0.15805(11) | 0.63408(10) | 0.0313(5) |
| F4_13 | 0.39168(11) | 0.10340(7) | 0.65990(6) | 0.0413(3) |
| F5_13 | 0.52526(11) | 0.14473(8) | 0.64330(7) | 0.0457(4) |

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|---|---|---|---|---|
| F6_13 | 0.38792(11) | 0.20947(7) | 0.66107(6) | 0.0397(3) |
| C4_13 | 0.30189(15) | 0.20468(10) | 0.55747(10) | 0.0275(4) |
| F7_13 | 0.24290(9) | 0.17162(7) | 0.59597(6) | 0.0374(3) |
| F8_13 | 0.28296(9) | 0.26997(6) | 0.56258(6) | 0.0348(3) |
| F9_13 | 0.27852(9) | 0.19937(7) | 0.50333(6) | 0.0344(3) |
| O1_12 | 0.4134(2) | 0.1154(2) | 0.42501(12) | 0.0272(7) |
| C1_12 | 0.4426(2) | 0.12566(16) | 0.36800(15) | 0.0189(7) |
| C2_12 | 0.3523(3) | 0.1613(2) | 0.33167(18) | 0.0264(8) |
| F1_12 | 0.2917(4) | 0.1174(3) | 0.33013(19) | 0.0381(9) |
| F2_12 | 0.3774(2) | 0.18660(15) | 0.27650(11) | 0.0399(6) |
| F3_12 | 0.3020(3) | 0.21152(19) | 0.35699(12) | 0.0324(6) |
| C3_12 | 0.5223(2) | 0.17267(16) | 0.35915(14) | 0.0296(7) |
| F4_12 | 0.58525(13) | 0.15455(9) | 0.40206(11) | 0.0426(6) |
| F5_12 | 0.4815(4) | 0.23736(18) | 0.35982(19) | 0.0374(8) |
| F6_12 | 0.57341(15) | 0.17015(10) | 0.30799(11) | 0.0458(6) |
| C4_12 | 0.4859(2) | 0.05733(17) | 0.34736(14) | 0.0246(6) |
| F7_12 | 0.57593(12) | 0.03448(9) | 0.36814(10) | 0.0320(4) |
| F8_12 | 0.49351(19) | 0.06216(11) | 0.28902(9) | 0.0395(5) |
| F9_12 | 0.4316(3) | 0.0106(2) | 0.36910(18) | 0.0318(8) |
| O1_11 | 0.30932(10) | 0.51218(8) | 0.37276(6) | 0.0309(3) |
| C1_11 | 0.27544(14) | 0.49100(10) | 0.42797(9) | 0.0231(4) |
| C2_11 | 0.30491(16) | 0.53618(12) | 0.46954(11) | 0.0333(5) |
| F1_11 | 0.39979(9) | 0.52033(7) | 0.48041(7) | 0.0437(3) |
| F2_11 | 0.25422(11) | 0.53012(8) | 0.52146(6) | 0.0479(4) |
| F3_11 | 0.28806(10) | 0.60113(7) | 0.44544(7) | 0.0459(4) |
| C3_11 | 0.16213(15) | 0.49676(11) | 0.42999(9) | 0.0261(4) |
| F4_11 | 0.13496(9) | 0.47428(7) | 0.38384(6) | 0.0347(3) |
| F5_11 | 0.11945(9) | 0.56124(6) | 0.42674(6) | 0.0342(3) |
| F6_11 | 0.12693(10) | 0.46175(7) | 0.47858(6) | 0.0398(3) |
| C4_11 | 0.32264(17) | 0.41606(11) | 0.44934(11) | 0.0342(5) |
| F7_11 | 0.27978(11) | 0.37387(7) | 0.42548(7) | 0.0486(4) |
| F8_11 | 0.31563(12) | 0.39929(7) | 0.50749(6) | 0.0497(4) |
| F9_11 | 0.41694(10) | 0.40592(7) | 0.43274(7) | 0.0435(3) |
| O1_10 | 0.26816(10) | 0.48303(7) | 0.25808(7) | 0.0276(3) |
| C1_10 | 0.29433(14) | 0.42693(10) | 0.23243(9) | 0.0239(4) |
| C2_10 | 0.2824(2) | 0.44645(12) | 0.16518(11) | 0.0432(6) |
| F1_10 | 0.18794(13) | 0.46244(8) | 0.15245(7) | 0.0554(4) |
| F2_10 | 0.32350(16) | 0.39607(9) | 0.13669(7) | 0.0684(5) |
| F3_10 | 0.32439(14) | 0.50009(8) | 0.14417(7) | 0.0609(5) |
| C3_10 | 0.40142(16) | 0.39220(11) | 0.24532(11) | 0.0339(5) |
| F4_10 | 0.42077(10) | 0.39390(8) | 0.30061(7) | 0.0461(4) |
| F5_10 | 0.46499(10) | 0.42506(7) | 0.21051(8) | 0.0508(4) |
| F6_10 | 0.41950(10) | 0.32790(7) | 0.23728(7) | 0.0455(4) |
| C4_10 | 0.22422(16) | 0.37600(11) | 0.25872(11) | 0.0327(5) |
| F7_10 | 0.24712(11) | 0.34793(7) | 0.31302(7) | 0.0471(4) |
| F8_10 | 0.22715(11) | 0.32623(7) | 0.22732(8) | 0.0502(4) |
| F9_10 | 0.13184(9) | 0.40762(7) | 0.26060(8) | 0.0466(4) |
| O1_9 | 0.4110(3) | 0.5611(3) | 0.2699(3) | 0.0228(9) |
| C1_9 | 0.4946(3) | 0.58524(18) | 0.27654(16) | 0.0233(8) |
| C2_9 | 0.5401(3) | 0.6044(2) | 0.21372(18) | 0.0307(9) |
| F1_9 | 0.49209(16) | 0.66257(11) | 0.18600(11) | 0.0401(5) |
| F2_9 | 0.63430(16) | 0.61098(14) | 0.21458(13) | 0.0458(6) |
| F3_9 | 0.5360(2) | 0.55700(15) | 0.18100(14) | 0.0404(6) |
| C3_9 | 0.5673(3) | 0.5291(2) | 0.31330(18) | 0.0308(9) |
| F4_9 | 0.52246(12) | 0.49871(12) | 0.36060(8) | 0.0372(5) |

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| F5_9 | 0.60559(17) | 0.48114(10) | 0.28164(9) | 0.0454(5) |
| F6_9 | 0.64107(16) | 0.55347(13) | 0.33127(13) | 0.0491(6) |
| C4_9 | 0.4728(3) | 0.6484(2) | 0.30711(19) | 0.0359(9) |
| F7_9 | 0.45658(19) | 0.63032(11) | 0.36538(9) | 0.0492(6) |
| F8_9 | 0.5459(3) | 0.68416(19) | 0.29942(18) | 0.0530(9) |
| F9_9 | 0.39307(16) | 0.68910(11) | 0.28666(12) | 0.0508(6) |
| O1_8 | 0.0980(13) | 0.7033(9) | 0.2028(4) | 0.035(3) |
| C1_8 | 0.1322(6) | 0.7230(4) | 0.1471(4) | 0.0264(18) |
| C2_8 | 0.0451(4) | 0.7719(3) | 0.1166(2) | 0.0311(11) |
| F1_8 | -0.0200(2) | 0.7376(2) | 0.10245(14) | 0.0510(11) |
| F2_8 | 0.0724(9) | 0.8113(7) | 0.0674(4) | 0.0413(17) |
| F3_8 | 0.0008(7) | 0.8124(6) | 0.1530(4) | 0.054(2) |
| C3_8 | 0.2196(4) | 0.7619(3) | 0.1494(2) | 0.0455(14) |
| F4_8 | 0.2827(11) | 0.7233(7) | 0.1889(6) | 0.071(3) |
| F5_8 | 0.1880(4) | 0.8217(3) | 0.1639(2) | 0.0692(14) |
| F6_8 | 0.2672(6) | 0.7726(3) | 0.0974(3) | 0.0539(15) |
| C4_8 | 0.1666(5) | 0.6644(3) | 0.1126(3) | 0.0556(16) |
| F7_8 | 0.2544(4) | 0.6324(3) | 0.1266(3) | 0.098(2) |
| F8_8 | 0.1745(8) | 0.6836(7) | 0.0556(4) | 0.071(2) |
| F9_8 | 0.1034(7) | 0.6184(4) | 0.1197(4) | 0.062(2) |
| O1_7 | 0.01167(9) | 0.64430(7) | 0.31030(6) | 0.0193(3) |
| C1_7 | -0.07898(12) | 0.62864(9) | 0.30738(8) | 0.0176(4) |
| C2_7 | -0.07481(14) | 0.57368(10) | 0.26778(9) | 0.0252(4) |
| F1_7 | -0.07108(10) | 0.60045(7) | 0.21079(5) | 0.0347(3) |
| F2_7 | -0.15277(9) | 0.54177(6) | 0.27717(6) | 0.0343(3) |
| F3_7 | 0.00463(9) | 0.52679(6) | 0.27778(6) | 0.0365(3) |
| C3_7 | -0.11488(13) | 0.60118(10) | 0.37102(9) | 0.0210(4) |
| F4_7 | -0.09320(8) | 0.63755(6) | 0.40927(5) | 0.0264(3) |
| F5_7 | -0.07077(9) | 0.53704(6) | 0.38796(5) | 0.0278(3) |
| F6_7 | -0.21115(8) | 0.60131(6) | 0.37530(6) | 0.0305(3) |
| C4_7 | -0.15204(13) | 0.69307(10) | 0.28200(9) | 0.0224(4) |
| F7_7 | -0.17389(9) | 0.73467(6) | 0.32150(6) | 0.0303(3) |
| F8_7 | -0.23525(8) | 0.67760(6) | 0.26685(6) | 0.0326(3) |
| F9_7 | -0.11227(8) | 0.72731(6) | 0.23460(5) | 0.0290(3) |
| O1_6 | 0.15067(10) | 0.73196(7) | 0.31059(7) | 0.0314(3) |
| C1_6 | 0.12907(14) | 0.78421(9) | 0.34131(9) | 0.0228(4) |
| C2_6 | 0.22731(15) | 0.80827(10) | 0.34920(10) | 0.0268(4) |
| F1_6 | 0.28164(9) | 0.76252(7) | 0.38767(6) | 0.0365(3) |
| F2_6 | 0.21267(9) | 0.86724(6) | 0.36919(6) | 0.0346(3) |
| F3_6 | 0.27903(9) | 0.81593(6) | 0.29875(6) | 0.0317(3) |
| C3_6 | 0.05784(15) | 0.84368(10) | 0.30718(10) | 0.0275(4) |
| F4_6 | -0.01311(9) | 0.81956(7) | 0.28543(6) | 0.0379(3) |
| F5_6 | 0.10377(10) | 0.87739(6) | 0.26189(6) | 0.0364(3) |
| F6_6 | 0.01561(10) | 0.88837(6) | 0.34119(6) | 0.0358(3) |
| C4_6 | 0.08062(15) | 0.76139(10) | 0.40261(10) | 0.0285(5) |
| F7_6 | -0.01374(9) | 0.75887(6) | 0.39858(6) | 0.0333(3) |
| F8_6 | 0.08693(10) | 0.80314(7) | 0.44087(6) | 0.0363(3) |
| F9_6 | 0.12413(10) | 0.69986(7) | 0.42611(7) | 0.0444(4) |
| C1 | 0.89870(16) | 0.37912(11) | 0.14900(10) | 0.0289(5) |
| C2 | 0.96402(15) | 0.33384(11) | 0.11936(9) | 0.0272(4) |
| C3 | 0.93010(15) | 0.28184(11) | 0.09768(9) | 0.0263(4) |
| C4 | 0.83022(16) | 0.27406(11) | 0.10601(10) | 0.0290(5) |
| C5 | 0.76508(15) | 0.31892(12) | 0.13673(10) | 0.0313(5) |
| C6 | 0.79908(15) | 0.37157(11) | 0.15830(10) | 0.0300(5) |
| C7 | 0.93412(19) | 0.43811(13) | 0.16797(12) | 0.0419(6) |

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|---|---|---|---|---|
| H7A | 0.957656 | 0.467070 | 0.133204 | 0.063 |
| H7B | 0.987695 | 0.420973 | 0.195014 | 0.063 |
| H7C | 0.880003 | 0.464559 | 0.187991 | 0.063 |
| C8 | 1.06987(17) | 0.34290(13) | 0.10869(12) | 0.0376(5) |
| H8A | 1.110196 | 0.299510 | 0.103199 | 0.056 |
| H8B | 1.091983 | 0.358458 | 0.142701 | 0.056 |
| H8C | 1.076188 | 0.376633 | 0.073230 | 0.056 |
| C9 | 1.00066(17) | 0.23774(13) | 0.06164(10) | 0.0357(5) |
| H9A | 0.967585 | 0.203135 | 0.050503 | 0.054 |
| H9B | 1.057213 | 0.215612 | 0.085077 | 0.054 |
| H9C | 1.022934 | 0.265892 | 0.025959 | 0.054 |
| C10 | 0.79065(18) | 0.22088(13) | 0.08032(11) | 0.0392(6) |
| H10A | 0.749337 | 0.242980 | 0.047315 | 0.059 |
| H10B | 0.751620 | 0.195951 | 0.110776 | 0.059 |
| H10C | 0.845368 | 0.189245 | 0.066225 | 0.059 |
| C11 | 0.65801(17) | 0.31147(16) | 0.14435(13) | 0.0486(7) |
| H11A | 0.628227 | 0.322374 | 0.105773 | 0.073 |
| H11B | 0.623992 | 0.342539 | 0.170178 | 0.073 |
| H11C | 0.652471 | 0.264674 | 0.162035 | 0.073 |
| C12 | 0.72902(19) | 0.42240(13) | 0.18721(13) | 0.0448(6) |
| H12A | 0.716326 | 0.465292 | 0.159734 | 0.067 |
| H12B | 0.757620 | 0.429945 | 0.222743 | 0.067 |
| H12C | 0.667335 | 0.405178 | 0.198066 | 0.067 |
| C1_4 | 0.71978(14) | 0.28425(10) | 0.34149(9) | 0.0239(4) |
| C2_4 | 0.78990(14) | 0.24023(10) | 0.37439(9) | 0.0232(4) |
| C3_4 | 0.79201(15) | 0.23651(10) | 0.43406(9) | 0.0263(4) |
| H3_4 | 0.840605 | 0.205725 | 0.456562 | 0.032 |
| C4_4 | 0.71993(15) | 0.27975(11) | 0.46038(10) | 0.0296(5) |
| H4_4 | 0.719001 | 0.278745 | 0.501804 | 0.036 |
| C5_4 | 0.64966(15) | 0.32416(11) | 0.42722(10) | 0.0311(5) |
| H5_4 | 0.601344 | 0.353511 | 0.446120 | 0.037 |
| C6_4 | 0.64846(15) | 0.32661(11) | 0.36672(10) | 0.0279(4) |
| H6_4 | 0.599714 | 0.356696 | 0.343798 | 0.033 |
| F1_4 | 0.72670(9) | 0.28440(7) | 0.28133(5) | 0.0319(3) |
| F2_4 | 0.86141(9) | 0.20177(6) | 0.34418(5) | 0.0302(3) |
| C1_3 | 0.94134(15) | 0.34191(10) | 0.34142(9) | 0.0262(4) |
| C2_3 | 1.02163(15) | 0.29240(11) | 0.35039(9) | 0.0283(5) |
| C3_3 | 1.07361(16) | 0.28159(11) | 0.40047(10) | 0.0311(5) |
| H3_3 | 1.129665 | 0.247167 | 0.406362 | 0.037 |
| C4_3 | 1.04101(16) | 0.32300(11) | 0.44225(10) | 0.0303(5) |
| H4_3 | 1.074854 | 0.316755 | 0.477767 | 0.036 |
| C5_3 | 0.95976(16) | 0.37331(11) | 0.43281(10) | 0.0301(5) |
| H5_3 | 0.939067 | 0.401417 | 0.461836 | 0.036 |
| C6_3 | 0.90810(16) | 0.38343(10) | 0.38191(10) | 0.0274(4) |
| H6_3 | 0.852019 | 0.417721 | 0.375384 | 0.033 |
| F1_3 | 0.89262(10) | 0.34734(7) | 0.28987(6) | 0.0362(3) |
| F2_3 | 1.04703(10) | 0.25397(7) | 0.30614(6) | 0.0417(3) |
| C1_2 | 1.13280(14) | 0.13640(10) | 0.22571(9) | 0.0237(4) |
| C2_2 | 1.08576(14) | 0.09796(10) | 0.26994(9) | 0.0237(4) |
| C3_2 | 1.12673(16) | 0.03350(11) | 0.29360(10) | 0.0295(5) |
| H3_2 | 1.093777 | 0.007129 | 0.324238 | 0.035 |
| C4_2 | 1.21879(17) | 0.00811(11) | 0.27093(11) | 0.0330(5) |
| H4_2 | 1.249532 | -0.036530 | 0.286291 | 0.040 |
| C5_2 | 1.26595(16) | 0.04683(12) | 0.22653(10) | 0.0329(5) |
| H5_2 | 1.328791 | 0.028540 | 0.211730 | 0.039 |

| | | | | |
|---|---|---|---|---|
| C6_2 | 1.22282(15) | 0.11228(12) | 0.20310(10) | 0.0300(5) |
| H6_2 | 1.254975 | 0.139178 | 0.172447 | 0.036 |
| F1_2 | 1.08523(8) | 0.20094(6) | 0.20417(5) | 0.0286(3) |
| F2_2 | 0.99459(8) | 0.12680(6) | 0.28931(5) | 0.0293(3) |
| C1_1 | 0.89589(15) | 0.07936(11) | 0.19527(9) | 0.0262(4) |
| C2_1 | 0.81486(15) | 0.09002(11) | 0.23179(10) | 0.0297(5) |
| C3_1 | 0.76679(17) | 0.03807(12) | 0.25744(10) | 0.0351(5) |
| H3_1 | 0.710621 | 0.045688 | 0.283003 | 0.042 |
| C4_1 | 0.80362(17) | -0.02613(12) | 0.24451(10) | 0.0357(5) |
| H4_1 | 0.772326 | -0.063378 | 0.261659 | 0.043 |
| C5_1 | 0.88483(17) | -0.03664(12) | 0.20722(10) | 0.0326(5) |
| H5_1 | 0.908405 | -0.080942 | 0.198701 | 0.039 |
| C6_1 | 0.93282(16) | 0.01673(11) | 0.18183(10) | 0.0293(5) |
| H6_1 | 0.989030 | 0.009819 | 0.156171 | 0.035 |
| F1_1 | 0.93993(9) | 0.13507(6) | 0.17322(6) | 0.0313(3) |
| F2_1 | 0.78455(9) | 0.15540(7) | 0.24266(6) | 0.0396(3) |
| Sr1 | 0.90281(2) | 0.24471(2) | 0.23005(2) | 0.02543(5) |
| Al1 | 0.40601(4) | 0.07156(3) | 0.49322(3) | 0.01613(11) |
| Al2 | 0.11078(4) | 0.67525(3) | 0.27561(2) | 0.01517(11) |
| Al4 | 0.41576(4) | 0.07581(3) | 0.98097(2) | 0.01731(11) |
| Al3 | 0.30455(4) | 0.53643(3) | 0.29884(3) | 0.01636(11) |
| F3 | 0.500000 | 0.000000 | 1.000000 | 0.0204(3) |
| F2 | 0.20843(7) | 0.60625(5) | 0.28660(5) | 0.0196(2) |
| F1 | 0.500000 | 0.000000 | 0.500000 | 0.0174(3) |
| O1_22 | 0.4016(14) | 0.5713(16) | 0.2667(12) | 0.028(5) |
| C1_22 | 0.4895(11) | 0.5906(7) | 0.2699(6) | 0.027(3) |
| C2_22 | 0.5586(10) | 0.5361(7) | 0.3092(6) | 0.033(3) |
| F1_22 | 0.5346(6) | 0.5352(6) | 0.3666(4) | 0.046(2) |
| F2_22 | 0.6532(6) | 0.5425(6) | 0.3005(5) | 0.044(2) |
| F3_22 | 0.5534(7) | 0.4742(4) | 0.2987(5) | 0.046(2) |
| C3_22 | 0.5377(11) | 0.6053(8) | 0.2072(6) | 0.035(4) |
| F4_22 | 0.4721(7) | 0.6398(5) | 0.1697(5) | 0.043(2) |
| F5_22 | 0.5740(10) | 0.5472(7) | 0.1889(8) | 0.057(3) |
| F6_22 | 0.6094(9) | 0.6414(6) | 0.2058(7) | 0.059(3) |
| C4_22 | 0.4693(12) | 0.6565(8) | 0.2982(7) | 0.045(4) |
| F7_22 | 0.4304(9) | 0.7084(4) | 0.2586(5) | 0.059(3) |
| F8_22 | 0.5530(13) | 0.6667(9) | 0.3173(9) | 0.060(4) |
| F9_22 | 0.4023(8) | 0.6476(5) | 0.3421(5) | 0.052(2) |
| O1_23 | 0.2987(6) | 0.0518(6) | 0.4783(5) | 0.020(2) |
| C1_23 | 0.2161(9) | 0.0256(7) | 0.4980(6) | 0.023(3) |
| C2_23 | 0.1231(10) | 0.0780(8) | 0.4808(7) | 0.033(4) |
| F1_23 | 0.1339(10) | 0.1386(6) | 0.4911(7) | 0.055(3) |
| F2_23 | 0.0443(7) | 0.0595(6) | 0.5107(6) | 0.048(3) |
| F3_23 | 0.1102(9) | 0.0872(7) | 0.4231(5) | 0.063(4) |
| C3_23 | 0.2186(15) | -0.0381(9) | 0.4691(9) | 0.031(4) |
| F4_23 | 0.2797(17) | -0.0900(12) | 0.4968(13) | 0.061(5) |
| F5_23 | 0.250(2) | -0.0263(13) | 0.4133(9) | 0.046(4) |
| F6_23 | 0.1313(14) | -0.0555(11) | 0.4691(10) | 0.038(4) |
| C4_23 | 0.2153(11) | 0.0054(8) | 0.5656(6) | 0.047(4) |
| F7_23 | 0.3046(9) | -0.0199(8) | 0.5842(6) | 0.080(5) |
| F8_23 | 0.1597(11) | -0.0420(7) | 0.5859(5) | 0.050(3) |
| F9_23 | 0.1804(14) | 0.0608(8) | 0.5907(7) | 0.064(4) |
| O1_5 | 0.4468(10) | 0.1114(9) | 0.4215(5) | 0.023(3) |
| C1_5 | 0.4460(10) | 0.1270(7) | 0.3607(6) | 0.025(3) |
| C2_5 | 0.4699(10) | 0.0624(8) | 0.3309(6) | 0.032(3) |

| | | | | |
|---|---|---|---|---|
| F1_5 | 0.4175(17) | 0.0156(12) | 0.3566(11) | 0.042(4) |
| F2_5 | 0.4480(10) | 0.0720(6) | 0.2749(5) | 0.046(3) |
| F3_5 | 0.5651(7) | 0.0380(5) | 0.3349(6) | 0.045(3) |
| C3_5 | 0.5210(9) | 0.1746(8) | 0.3344(6) | 0.037(3) |
| F4_5 | 0.488(2) | 0.2370(9) | 0.3453(11) | 0.041(4) |
| F5_5 | 0.6056(6) | 0.1539(5) | 0.3601(6) | 0.047(3) |
| F6_5 | 0.5378(9) | 0.1798(6) | 0.2762(5) | 0.053(3) |
| C4_5 | 0.3424(12) | 0.1652(9) | 0.3417(7) | 0.023(3) |
| F7_5 | 0.3073(15) | 0.2092(10) | 0.3771(6) | 0.033(3) |
| F8_5 | 0.3396(10) | 0.1979(8) | 0.2862(5) | 0.036(3) |
| F9_5 | 0.2817(18) | 0.1203(13) | 0.3457(10) | 0.037(4) |

*Table S 7 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [CaHMB(oDFB)$_4$][al-f-al]$_2$ **7**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| Ca1 | -0.11359(4) | 0.23605(3) | 0.22817(3) | 0.02805(12) |
| Al1 | 0.89483(5) | 0.32319(3) | 0.72588(3) | 0.01628(14) |
| Al2 | 0.41515(5) | 0.07338(3) | 0.97836(3) | 0.01689(14) |
| Al3 | 0.41122(5) | 0.07276(3) | 0.48497(3) | 0.01771(14) |
| Al4 | 0.70391(5) | 0.46135(3) | 0.70564(3) | 0.01900(15) |
| F1 | 0.500000 | 0.000000 | 0.500000 | 0.0199(4) |
| F2 | 0.500000 | 0.000000 | 1.000000 | 0.0213(4) |
| F3 | 0.80126(9) | 0.39359(7) | 0.71669(6) | 0.0222(3) |
| O1_3 | 0.73739(17) | 0.51584(10) | 0.74589(12) | 0.0471(6) |
| C1_3 | 0.71855(19) | 0.57157(13) | 0.77178(13) | 0.0304(6) |
| C2_3 | 0.6124(2) | 0.60786(15) | 0.76567(16) | 0.0407(7) |
| F1_3 | 0.55197(14) | 0.57392(11) | 0.80266(12) | 0.0636(6) |
| F2_3 | 0.59999(14) | 0.67104(9) | 0.77660(10) | 0.0538(5) |
| F3_3 | 0.58577(14) | 0.61007(11) | 0.71095(10) | 0.0581(6) |
| C3_3 | 0.7883(2) | 0.62185(16) | 0.74083(16) | 0.0432(7) |
| F4_3 | 0.87786(14) | 0.58957(11) | 0.73258(12) | 0.0682(7) |
| F5_3 | 0.75822(16) | 0.65247(11) | 0.68856(10) | 0.0612(6) |
| F6_3 | 0.79491(16) | 0.66931(10) | 0.77270(11) | 0.0631(6) |
| C4_3 | 0.7402(3) | 0.55186(16) | 0.83816(15) | 0.0464(8) |
| F7_3 | 0.83523(16) | 0.53438(10) | 0.84445(11) | 0.0608(6) |
| F8_3 | 0.7075(2) | 0.60222(13) | 0.86844(10) | 0.0794(8) |
| F9_3 | 0.69811(19) | 0.49917(12) | 0.86286(11) | 0.0714(7) |
| O1_4 | 0.99706(11) | 0.35220(9) | 0.69303(8) | 0.0223(3) |
| C1_4 | 1.08615(16) | 0.36871(12) | 0.69746(11) | 0.0211(5) |
| C2_4 | 1.15789(18) | 0.30547(13) | 0.72299(12) | 0.0274(5) |
| F1_4 | 1.18358(13) | 0.26431(8) | 0.68261(8) | 0.0401(4) |
| F2_4 | 1.23938(11) | 0.32118(9) | 0.73854(9) | 0.0424(4) |
| F3_4 | 1.11689(12) | 0.27036(9) | 0.76982(8) | 0.0390(4) |
| C3_4 | 1.0786(2) | 0.42351(14) | 0.73762(13) | 0.0331(6) |
| F4_4 | 1.00001(14) | 0.46901(10) | 0.72793(10) | 0.0530(5) |
| F5_4 | 1.07209(15) | 0.39587(11) | 0.79512(8) | 0.0498(5) |
| F6_4 | 1.15548(13) | 0.45524(10) | 0.73036(10) | 0.0492(5) |
| C4_4 | 1.12551(18) | 0.39705(13) | 0.63390(12) | 0.0277(5) |
| F7_4 | 1.08059(13) | 0.46051(9) | 0.61711(8) | 0.0439(4) |
| F8_4 | 1.22049(12) | 0.39946(9) | 0.63074(8) | 0.0414(4) |
| F9_4 | 1.10846(13) | 0.36083(9) | 0.59470(7) | 0.0380(4) |

| | | | | |
|---|---|---|---|---|
| O1_5 | 0.8999(9) | 0.3005(7) | 0.7998(3) | 0.037(2) |
| C1_5 | 0.8664(5) | 0.2742(3) | 0.8549(3) | 0.0302(15) |
| C2_5 | 0.7822(4) | 0.2340(3) | 0.8524(2) | 0.0445(12) |
| F1_5 | 0.8163(4) | 0.1737(2) | 0.83971(19) | 0.0648(12) |
| F2_5 | 0.7314(5) | 0.2251(3) | 0.9044(2) | 0.0664(14) |
| F3_5 | 0.7218(7) | 0.2702(4) | 0.8102(4) | 0.0676(19) |
| C3_5 | 0.8294(4) | 0.3341(2) | 0.8885(3) | 0.0515(14) |
| F4_5 | 0.8889(8) | 0.3803(3) | 0.8791(4) | 0.0639(18) |
| F5_5 | 0.7411(4) | 0.3642(3) | 0.8713(4) | 0.0826(19) |
| F6_5 | 0.8206(6) | 0.3146(5) | 0.9467(3) | 0.0745(19) |
| C4_5 | 0.9533(4) | 0.2277(3) | 0.8860(2) | 0.0383(11) |
| F7_5 | 1.0156(2) | 0.2641(2) | 0.90079(13) | 0.0516(9) |
| F8_5 | 0.9269(7) | 0.1903(7) | 0.9367(3) | 0.0527(18) |
| F9_5 | 1.0009(5) | 0.1864(5) | 0.8509(4) | 0.0578(18) |
| O1_6 | 0.6050(4) | 0.4265(4) | 0.7330(4) | 0.061(2) |
| C1_6 | 0.5161(5) | 0.4088(3) | 0.7321(3) | 0.0347(15) |
| C2_6 | 0.4673(5) | 0.3978(4) | 0.7955(3) | 0.0472(18) |
| F1_6 | 0.4335(3) | 0.45585(18) | 0.8153(2) | 0.0633(11) |
| F2_6 | 0.3921(4) | 0.3642(3) | 0.7984(4) | 0.0676(16) |
| F3_6 | 0.5285(2) | 0.3629(2) | 0.83421(17) | 0.0553(10) |
| C3_6 | 0.5343(6) | 0.3427(4) | 0.7065(3) | 0.0564(18) |
| F4_6 | 0.6025(3) | 0.34854(17) | 0.6614(2) | 0.0728(13) |
| F5_6 | 0.5677(3) | 0.29120(16) | 0.7466(2) | 0.0720(12) |
| F6_6 | 0.4534(6) | 0.3306(5) | 0.6870(3) | 0.086(2) |
| C4_6 | 0.4509(5) | 0.4655(3) | 0.6924(3) | 0.0430(17) |
| F7_6 | 0.4763(3) | 0.4638(2) | 0.63595(17) | 0.0571(10) |
| F8_6 | 0.3570(3) | 0.4611(3) | 0.7023(3) | 0.0594(13) |
| F9_6 | 0.4597(3) | 0.52609(16) | 0.7028(2) | 0.0599(11) |
| O1_7 | 0.69791(16) | 0.48733(13) | 0.63225(10) | 0.0497(6) |
| C1_7 | 0.7312(2) | 0.50726(13) | 0.57591(12) | 0.0306(6) |
| C2_7 | 0.6862(3) | 0.58187(15) | 0.55518(16) | 0.0463(8) |
| F1_7 | 0.73166(19) | 0.62335(10) | 0.57731(13) | 0.0735(7) |
| F2_7 | 0.69113(19) | 0.59810(12) | 0.49655(10) | 0.0711(7) |
| F3_7 | 0.59395(16) | 0.59345(10) | 0.57419(11) | 0.0616(6) |
| C3_7 | 0.6978(2) | 0.46251(17) | 0.53614(17) | 0.0474(8) |
| F4_7 | 0.71255(17) | 0.39844(10) | 0.56110(15) | 0.0801(8) |
| F5_7 | 0.60327(14) | 0.47914(11) | 0.52751(11) | 0.0589(6) |
| F6_7 | 0.74578(18) | 0.46760(15) | 0.48279(11) | 0.0756(7) |
| C4_7 | 0.8443(2) | 0.49977(15) | 0.57068(14) | 0.0378(6) |
| F7_7 | 0.88396(13) | 0.43523(9) | 0.57419(10) | 0.0509(5) |
| F8_7 | 0.87881(16) | 0.53358(12) | 0.52119(9) | 0.0592(6) |
| F9_7 | 0.87412(14) | 0.52211(11) | 0.61618(10) | 0.0541(5) |
| O1_8 | 0.85320(13) | 0.27049(9) | 0.68722(9) | 0.0327(4) |
| C1_8 | 0.87562(18) | 0.21649(12) | 0.65826(12) | 0.0257(5) |
| C2_8 | 0.9452(2) | 0.15880(13) | 0.69366(13) | 0.0326(6) |
| F1_8 | 0.89755(15) | 0.12611(9) | 0.73974(8) | 0.0452(4) |
| F2_8 | 0.98938(14) | 0.11315(8) | 0.66086(8) | 0.0422(4) |
| F3_8 | 1.01379(13) | 0.18457(9) | 0.71544(8) | 0.0421(4) |
| C3_8 | 0.9254(2) | 0.23718(13) | 0.59597(13) | 0.0330(6) |
| F4_8 | 0.88128(14) | 0.29669(9) | 0.57003(9) | 0.0491(5) |
| F5_8 | 1.01816(12) | 0.24264(9) | 0.60015(8) | 0.0404(4) |
| F6_8 | 0.92372(14) | 0.19256(9) | 0.55975(8) | 0.0420(4) |
| C4_8 | 0.7783(2) | 0.19118(14) | 0.65161(14) | 0.0341(6) |
| F7_8 | 0.72755(13) | 0.23270(10) | 0.61006(9) | 0.0463(4) |
| F8_8 | 0.79533(14) | 0.12935(9) | 0.63606(9) | 0.0450(4) |

| | | | | |
|---|---|---|---|---|
| F9_8 | 0.72396(13) | 0.18726(10) | 0.70176(9) | 0.0447(4) |
| O1_9 | 0.42638(15) | 0.12567(9) | 1.02716(8) | 0.0313(4) |
| C1_9 | 0.43237(18) | 0.18873(12) | 1.03680(11) | 0.0254(5) |
| C2_9 | 0.46058(19) | 0.18289(13) | 1.10179(12) | 0.0290(5) |
| F1_9 | 0.55388(12) | 0.15721(9) | 1.10736(8) | 0.0403(4) |
| F2_9 | 0.44528(14) | 0.24258(9) | 1.12058(8) | 0.0447(4) |
| F3_9 | 0.40922(12) | 0.14217(8) | 1.13857(7) | 0.0335(4) |
| C3_9 | 0.3335(2) | 0.23583(15) | 1.02819(14) | 0.0381(7) |
| F4_9 | 0.29401(15) | 0.22576(11) | 0.98032(9) | 0.0523(5) |
| F5_9 | 0.27018(13) | 0.22326(11) | 1.07463(9) | 0.0514(5) |
| F6_9 | 0.34170(16) | 0.30102(9) | 1.02207(10) | 0.0550(5) |
| C4_9 | 0.5120(2) | 0.21988(15) | 0.99378(14) | 0.0380(7) |
| F7_9 | 0.47866(16) | 0.24298(9) | 0.94031(8) | 0.0506(5) |
| F8_9 | 0.54122(15) | 0.27074(10) | 1.01309(9) | 0.0519(5) |
| F9_9 | 0.58919(15) | 0.17334(11) | 0.98777(10) | 0.0580(6) |
| O1_10 | 0.45503(13) | 0.10302(9) | 0.90761(7) | 0.0240(4) |
| C1_10 | 0.43917(17) | 0.11048(12) | 0.84910(10) | 0.0223(5) |
| C2_10 | 0.4222(2) | 0.04235(13) | 0.83274(12) | 0.0295(6) |
| F1_10 | 0.33199(13) | 0.03033(9) | 0.85122(7) | 0.0388(4) |
| F2_10 | 0.43244(14) | 0.04109(9) | 0.77473(7) | 0.0391(4) |
| F3_10 | 0.48388(14) | -0.00852(8) | 0.85946(9) | 0.0454(4) |
| C3_10 | 0.5314(2) | 0.13283(14) | 0.81226(11) | 0.0308(6) |
| F4_10 | 0.56534(13) | 0.17767(9) | 0.83647(7) | 0.0398(4) |
| F5_10 | 0.60282(12) | 0.08006(10) | 0.81056(8) | 0.0427(4) |
| F6_10 | 0.51271(13) | 0.15878(9) | 0.75634(7) | 0.0375(4) |
| C4_10 | 0.3495(2) | 0.16567(13) | 0.83391(12) | 0.0296(6) |
| F7_10 | 0.37176(14) | 0.22685(8) | 0.83318(8) | 0.0421(4) |
| F8_10 | 0.31651(12) | 0.16392(9) | 0.78153(7) | 0.0372(4) |
| F9_10 | 0.27698(12) | 0.15760(9) | 0.87484(8) | 0.0410(4) |
| O1_11 | 0.3067(2) | 0.0445(3) | 0.9815(2) | 0.0236(9) |
| C1_11 | 0.2288(2) | 0.02297(16) | 1.01416(14) | 0.0211(6) |
| C2_11 | 0.1498(2) | 0.08450(16) | 1.02440(14) | 0.0321(7) |
| F1_11 | 0.17616(17) | 0.11592(12) | 1.06594(11) | 0.0423(6) |
| F2_11 | 0.06292(16) | 0.06743(14) | 1.04247(12) | 0.0482(7) |
| F3_11 | 0.1406(4) | 0.12922(16) | 0.9744(2) | 0.0471(10) |
| C3_11 | 0.1867(3) | -0.02402(18) | 0.97997(14) | 0.0377(8) |
| F4_11 | 0.2545(2) | -0.06563(15) | 0.95704(13) | 0.0519(7) |
| F5_11 | 0.13663(18) | 0.01336(15) | 0.93505(10) | 0.0523(7) |
| F6_11 | 0.1237(2) | -0.05862(15) | 1.01496(13) | 0.0549(8) |
| C4_11 | 0.2596(2) | -0.01659(14) | 1.07525(13) | 0.0246(6) |
| F7_11 | 0.30674(18) | -0.07782(11) | 1.07058(10) | 0.0399(5) |
| F8_11 | 0.1860(2) | -0.02275(16) | 1.11596(14) | 0.0358(7) |
| F9_11 | 0.3216(2) | 0.0166(2) | 1.0966(2) | 0.0338(7) |
| O1_1 | 0.4284(3) | 0.11352(18) | 0.54112(16) | 0.0241(8) |
| C1_1 | 0.4142(2) | 0.17437(15) | 0.56071(13) | 0.0211(6) |
| C2_1 | 0.3055(2) | 0.20727(15) | 0.55830(14) | 0.0304(6) |
| F1_1 | 0.2511(2) | 0.17625(19) | 0.6011(2) | 0.0444(8) |
| F2_1 | 0.29248(16) | 0.27248(9) | 0.56319(9) | 0.0385(5) |
| F3_1 | 0.27291(16) | 0.20198(11) | 0.50669(10) | 0.0447(5) |
| C3_1 | 0.4787(2) | 0.22283(16) | 0.52184(15) | 0.0342(7) |
| F4_1 | 0.56613(16) | 0.18899(11) | 0.50984(14) | 0.0561(7) |
| F5_1 | 0.43863(18) | 0.24912(9) | 0.47087(9) | 0.0462(5) |
| F6_1 | 0.49072(16) | 0.27348(10) | 0.54892(11) | 0.0481(6) |
| C4_1 | 0.4432(2) | 0.16068(15) | 0.62555(14) | 0.0328(7) |
| F7_1 | 0.54035(18) | 0.14698(13) | 0.62723(12) | 0.0515(6) |

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| F8_1 | 0.40993(18) | 0.21359(9) | 0.65338(8) | 0.0437(6) |
| F9_1 | 0.40611(19) | 0.10788(10) | 0.65627(8) | 0.0447(6) |
| O1_2 | 0.44944(18) | 0.11417(12) | 0.41629(10) | 0.0253(5) |
| C1_2 | 0.4373(2) | 0.12879(16) | 0.35731(14) | 0.0225(7) |
| C2_2 | 0.3304(3) | 0.16323(17) | 0.34480(15) | 0.0277(7) |
| F1_2 | 0.27049(15) | 0.11757(12) | 0.35284(10) | 0.0322(5) |
| F2_2 | 0.32284(17) | 0.19624(10) | 0.28961(9) | 0.0376(5) |
| F3_2 | 0.2991(3) | 0.20724(17) | 0.38193(13) | 0.0407(8) |
| C3_2 | 0.5083(3) | 0.17847(17) | 0.32850(16) | 0.0357(7) |
| F4_2 | 0.59656(15) | 0.15873(12) | 0.34862(11) | 0.0459(6) |
| F5_2 | 0.47633(18) | 0.24039(10) | 0.34110(11) | 0.0454(6) |
| F6_2 | 0.51937(17) | 0.18308(12) | 0.26925(9) | 0.0499(6) |
| C4_2 | 0.4602(2) | 0.06349(19) | 0.32842(16) | 0.0303(7) |
| F7_2 | 0.55590(15) | 0.04131(12) | 0.32615(11) | 0.0409(5) |
| F8_2 | 0.43176(17) | 0.07249(11) | 0.27367(9) | 0.0425(5) |
| F9_2 | 0.4185(2) | 0.01412(15) | 0.36260(12) | 0.0368(6) |
| O1_12 | 0.3043(6) | 0.0457(7) | 0.4818(6) | 0.0208(18) |
| C1_12 | 0.2298(5) | 0.0128(4) | 0.5059(3) | 0.0210(14) |
| C2_12 | 0.2104(5) | -0.0340(4) | 0.4631(3) | 0.0263(14) |
| F1_12 | 0.1628(3) | 0.0010(2) | 0.41805(16) | 0.0504(10) |
| F2_12 | 0.1569(7) | -0.0806(5) | 0.4906(5) | 0.0412(13) |
| F3_12 | 0.2943(3) | -0.0659(2) | 0.4423(2) | 0.0481(10) |
| C3_12 | 0.2583(6) | -0.0319(4) | 0.5661(3) | 0.0589(19) |
| F4_12 | 0.2986(5) | 0.0044(4) | 0.5982(2) | 0.082(2) |
| F5_12 | 0.3198(3) | -0.0866(2) | 0.5568(2) | 0.0841(16) |
| F6_12 | 0.1745(8) | -0.0462(6) | 0.5982(7) | 0.081(2) |
| C4_12 | 0.1374(5) | 0.0643(3) | 0.5144(4) | 0.0516(18) |
| F7_12 | 0.1441(4) | 0.0927(3) | 0.5630(3) | 0.0816(18) |
| F8_12 | 0.0575(7) | 0.0351(5) | 0.5244(6) | 0.068(2) |
| F9_12 | 0.1268(3) | 0.1130(2) | 0.4668(3) | 0.0640(13) |
| C1_13 | 0.04153(19) | 0.27189(13) | 0.36563(12) | 0.0290(5) |
| C2_13 | -0.03355(19) | 0.31733(13) | 0.34046(11) | 0.0274(5) |
| C3_13 | -0.0801(2) | 0.37067(13) | 0.36625(13) | 0.0311(6) |
| H3_13 | -0.131653 | 0.401678 | 0.347864 | 0.037 |
| C4_13 | -0.0494(2) | 0.37798(14) | 0.42047(13) | 0.0340(6) |
| H4_13 | -0.080394 | 0.414325 | 0.439967 | 0.041 |
| C5_13 | 0.0263(2) | 0.33244(14) | 0.44606(12) | 0.0331(6) |
| H5_13 | 0.046995 | 0.338026 | 0.483029 | 0.040 |
| C6_13 | 0.0721(2) | 0.27926(14) | 0.41898(13) | 0.0324(6) |
| H6_13 | 0.124070 | 0.248170 | 0.436874 | 0.039 |
| F1_13 | 0.08230(14) | 0.22078(10) | 0.33675(9) | 0.0509(5) |
| F2_13 | -0.06291(13) | 0.30699(9) | 0.28675(7) | 0.0386(4) |
| C1_14 | -0.21555(19) | 0.23901(13) | 0.38252(13) | 0.0290(5) |
| C2_14 | -0.27814(19) | 0.28044(13) | 0.34456(12) | 0.0277(5) |
| C3_14 | -0.3499(2) | 0.32840(14) | 0.36348(14) | 0.0348(6) |
| H3_14 | -0.393734 | 0.356505 | 0.336835 | 0.042 |
| C4_14 | -0.3559(2) | 0.33413(16) | 0.42294(14) | 0.0409(7) |
| H4_14 | -0.404444 | 0.367031 | 0.437692 | 0.049 |
| C5_14 | -0.2921(2) | 0.29255(17) | 0.46120(14) | 0.0427(7) |
| H5_14 | -0.297170 | 0.297366 | 0.501932 | 0.051 |
| C6_14 | -0.2211(2) | 0.24418(15) | 0.44116(14) | 0.0387(7) |
| H6_14 | -0.177462 | 0.215363 | 0.467480 | 0.046 |
| F1_14 | -0.14605(13) | 0.19483(9) | 0.35747(10) | 0.0489(5) |
| F2_14 | -0.26526(13) | 0.27233(9) | 0.28543(7) | 0.0405(4) |
| C1_15 | 0.06483(19) | 0.10528(14) | 0.27103(12) | 0.0278(5) |

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| C2_15 | 0.11224(18) | 0.14704(13) | 0.22907(11) | 0.0257(5) |
| C3_15 | 0.20287(19) | 0.12642(15) | 0.20456(12) | 0.0312(6) |
| H3_15 | 0.234920 | 0.155877 | 0.175436 | 0.037 |
| C4_15 | 0.2461(2) | 0.06078(15) | 0.22396(14) | 0.0378(7) |
| H4_15 | 0.309262 | 0.044704 | 0.207994 | 0.045 |
| C5_15 | 0.1990(2) | 0.01850(15) | 0.26592(15) | 0.0421(7) |
| H5_15 | 0.230048 | -0.026473 | 0.278289 | 0.050 |
| C6_15 | 0.1067(2) | 0.04035(15) | 0.29067(14) | 0.0387(7) |
| H6_15 | 0.074223 | 0.011368 | 0.319972 | 0.046 |
| F1_15 | -0.02722(11) | 0.13150(9) | 0.29054(7) | 0.0353(4) |
| F2_15 | 0.06230(11) | 0.21099(8) | 0.21096(7) | 0.0320(3) |
| C1_16 | -0.18498(18) | 0.08428(14) | 0.23336(12) | 0.0292(6) |
| C2_16 | -0.10442(18) | 0.07676(13) | 0.19498(11) | 0.0245(5) |
| C3_16 | -0.06398(19) | 0.01529(14) | 0.17989(12) | 0.0292(6) |
| H3_16 | -0.008329 | 0.010608 | 0.152870 | 0.035 |
| C4_16 | -0.1081(2) | -0.03994(14) | 0.20588(13) | 0.0345(6) |
| H4_16 | -0.082215 | -0.083411 | 0.196373 | 0.041 |
| C5_16 | -0.1887(2) | -0.03284(15) | 0.24527(13) | 0.0366(6) |
| H5_16 | -0.217110 | -0.071494 | 0.262685 | 0.044 |
| C6_16 | -0.2288(2) | 0.02984(16) | 0.25974(13) | 0.0370(6) |
| H6_16 | -0.284260 | 0.035071 | 0.286808 | 0.044 |
| F1_16 | -0.21872(12) | 0.14866(9) | 0.24555(8) | 0.0398(4) |
| F2_16 | -0.06524(11) | 0.13467(8) | 0.17291(7) | 0.0306(3) |
| C1 | -0.24718(19) | 0.30744(15) | 0.14587(13) | 0.0329(6) |
| C2 | -0.1814(2) | 0.26651(14) | 0.11167(12) | 0.0297(6) |
| C3 | -0.0834(2) | 0.27675(14) | 0.10137(12) | 0.0282(5) |
| C4 | -0.0514(2) | 0.32844(14) | 0.12524(12) | 0.0294(6) |
| C5 | -0.1162(2) | 0.36944(14) | 0.15831(13) | 0.0332(6) |
| C6 | -0.2146(2) | 0.36007(14) | 0.16851(13) | 0.0342(6) |
| C7 | -0.3526(2) | 0.29708(19) | 0.15605(17) | 0.0474(8) |
| H7A | -0.386869 | 0.316332 | 0.120020 | 0.071 |
| H7B | -0.383476 | 0.319600 | 0.189074 | 0.071 |
| H7C | -0.355852 | 0.248592 | 0.165634 | 0.071 |
| C8 | -0.2195(2) | 0.21486(17) | 0.08339(15) | 0.0423(7) |
| H8A | -0.263463 | 0.238203 | 0.052742 | 0.063 |
| H8B | -0.254912 | 0.186358 | 0.113776 | 0.063 |
| H8C | -0.164706 | 0.186602 | 0.065325 | 0.063 |
| C9 | -0.0112(2) | 0.23570(17) | 0.06331(14) | 0.0396(7) |
| H9A | 0.007897 | 0.265007 | 0.026998 | 0.059 |
| H9B | -0.041165 | 0.199411 | 0.052857 | 0.059 |
| H9C | 0.046584 | 0.216030 | 0.085335 | 0.059 |
| C10 | 0.0533(2) | 0.34121(17) | 0.11114(15) | 0.0417(7) |
| H10A | 0.088420 | 0.308018 | 0.087280 | 0.063 |
| H10B | 0.085313 | 0.336954 | 0.148226 | 0.063 |
| H10C | 0.053491 | 0.386888 | 0.088844 | 0.063 |
| C11 | -0.0821(3) | 0.42745(17) | 0.18062(17) | 0.0485(8) |
| H11A | -0.014279 | 0.413930 | 0.191251 | 0.073 |
| H11B | -0.123324 | 0.438611 | 0.215633 | 0.073 |
| H11C | -0.086631 | 0.467120 | 0.149327 | 0.073 |
| C12 | -0.2840(3) | 0.40909(18) | 0.20050(18) | 0.0540(9) |
| H12A | -0.282146 | 0.455249 | 0.179712 | 0.081 |
| H12B | -0.264945 | 0.405285 | 0.241207 | 0.081 |
| H12C | -0.350241 | 0.398654 | 0.201429 | 0.081 |
| O1_18 | 0.2972(13) | 0.0560(15) | 0.4809(13) | 0.023(4) |
| C1_18 | 0.2215(10) | 0.0227(7) | 0.5048(6) | 0.023(3) |

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| C2_18 | 0.1245(11) | 0.0724(7) | 0.4940(6) | 0.050(3) |
| F1_18 | 0.1032(7) | 0.0766(6) | 0.4382(4) | 0.072(3) |
| F2_18 | 0.0503(16) | 0.0500(13) | 0.5279(12) | 0.069(4) |
| F3_18 | 0.1376(10) | 0.1315(6) | 0.5054(6) | 0.074(3) |
| C3_18 | 0.2344(10) | -0.0025(7) | 0.5713(6) | 0.047(3) |
| F4_18 | 0.3289(8) | -0.0221(8) | 0.5807(6) | 0.074(4) |
| F5_18 | 0.2095(12) | 0.0481(7) | 0.6007(6) | 0.084(3) |
| F6_18 | 0.1943(17) | -0.0571(11) | 0.5962(14) | 0.073(4) |
| C4_18 | 0.2224(11) | -0.0350(8) | 0.4695(6) | 0.035(3) |
| F7_18 | 0.2990(10) | -0.0825(6) | 0.4798(6) | 0.060(3) |
| F8_18 | 0.1414(11) | -0.0616(8) | 0.4784(9) | 0.063(3) |
| F9_18 | 0.2280(11) | -0.0134(6) | 0.4118(4) | 0.051(3) |
| O1_19 | 0.9044(16) | 0.2935(13) | 0.7995(5) | 0.037(4) |
| C1_19 | 0.8712(7) | 0.2793(5) | 0.8574(5) | 0.033(3) |
| C2_19 | 0.9003(6) | 0.3282(5) | 0.8956(4) | 0.043(2) |
| F1_19 | 0.9951(4) | 0.3125(4) | 0.9044(3) | 0.0517(16) |
| F2_19 | 0.8527(9) | 0.3239(8) | 0.9488(5) | 0.059(3) |
| F3_19 | 0.8824(14) | 0.3899(7) | 0.8643(9) | 0.066(3) |
| C3_19 | 0.7579(6) | 0.2847(6) | 0.8615(4) | 0.061(2) |
| F4_19 | 0.7351(13) | 0.2505(8) | 0.8199(7) | 0.074(3) |
| F5_19 | 0.7195(8) | 0.3494(6) | 0.8543(6) | 0.074(3) |
| F6_19 | 0.7249(10) | 0.2535(5) | 0.9132(4) | 0.072(3) |
| C4_19 | 0.9187(8) | 0.2058(4) | 0.8802(4) | 0.050(2) |
| F7_19 | 0.8772(8) | 0.1605(4) | 0.8598(3) | 0.072(2) |
| F8_19 | 0.9013(15) | 0.1934(12) | 0.9391(6) | 0.058(4) |
| F9_19 | 1.0129(9) | 0.1956(8) | 0.8645(6) | 0.052(3) |
| O1_22 | 0.432(3) | 0.1209(16) | 0.5338(14) | 0.030(6) |
| C1_22 | 0.4194(11) | 0.1656(8) | 0.5723(7) | 0.028(4) |
| C2_22 | 0.5201(11) | 0.1657(9) | 0.5956(8) | 0.047(4) |
| F1_22 | 0.5890(12) | 0.1640(12) | 0.5522(10) | 0.068(6) |
| F2_22 | 0.5210(14) | 0.2181(11) | 0.6219(12) | 0.088(8) |
| F3_22 | 0.5400(18) | 0.1104(11) | 0.6359(10) | 0.070(5) |
| C3_22 | 0.3458(14) | 0.1449(10) | 0.6241(8) | 0.058(5) |
| F4_22 | 0.2550(16) | 0.1619(19) | 0.6076(16) | 0.048(5) |
| F5_22 | 0.361(2) | 0.0785(10) | 0.6396(12) | 0.096(9) |
| F6_22 | 0.3523(15) | 0.1735(14) | 0.6706(8) | 0.077(7) |
| C4_22 | 0.3798(12) | 0.2365(8) | 0.5388(7) | 0.043(4) |
| F7_22 | 0.3105(14) | 0.2340(12) | 0.5041(9) | 0.064(4) |
| F8_22 | 0.3455(16) | 0.2772(9) | 0.5783(9) | 0.053(4) |
| F9_22 | 0.4522(14) | 0.2621(10) | 0.5051(10) | 0.055(3) |
| O1_23 | 0.5999(8) | 0.4353(7) | 0.7397(6) | 0.019(2) |
| C1_23 | 0.5190(9) | 0.4112(6) | 0.7288(5) | 0.029(3) |
| C2_23 | 0.4459(10) | 0.4675(7) | 0.6943(6) | 0.044(3) |
| F1_23 | 0.4159(8) | 0.5152(4) | 0.7275(5) | 0.079(3) |
| F2_23 | 0.3688(8) | 0.4449(6) | 0.6798(6) | 0.061(3) |
| F3_23 | 0.4882(5) | 0.4996(5) | 0.6463(4) | 0.066(3) |
| C3_23 | 0.5268(11) | 0.3492(7) | 0.6981(6) | 0.052(3) |
| F4_23 | 0.6027(8) | 0.3037(5) | 0.7147(5) | 0.085(3) |
| F5_23 | 0.5348(8) | 0.3627(6) | 0.6389(3) | 0.094(3) |
| F6_23 | 0.4481(13) | 0.3182(10) | 0.7108(7) | 0.077(3) |
| C4_23 | 0.4741(10) | 0.3905(6) | 0.7934(6) | 0.042(3) |
| F7_23 | 0.5189(5) | 0.3308(4) | 0.8181(4) | 0.053(2) |
| F8_23 | 0.3797(8) | 0.3905(6) | 0.7962(8) | 0.061(3) |
| F9_23 | 0.4879(9) | 0.4363(6) | 0.8253(5) | 0.081(3) |
| O1_25 | 0.3061(7) | 0.0376(7) | 0.5147(7) | 0.036(3) |

| | | | | |
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| C1_25 | 0.2168(9) | 0.0193(7) | 0.5133(6) | 0.029(3) |
| C2_25 | 0.1748(11) | -0.0063(9) | 0.5768(6) | 0.068(3) |
| F1_25 | 0.2274(15) | -0.0625(10) | 0.6011(11) | 0.081(4) |
| F2_25 | 0.0854(9) | -0.0205(8) | 0.5772(7) | 0.085(4) |
| F3_25 | 0.1743(19) | 0.0391(12) | 0.6113(9) | 0.099(5) |
| C3_25 | 0.1432(10) | 0.0808(8) | 0.4876(7) | 0.055(3) |
| F4_25 | 0.1763(10) | 0.1113(6) | 0.4362(7) | 0.070(3) |
| F5_25 | 0.1169(17) | 0.1223(11) | 0.5271(10) | 0.076(4) |
| F6_25 | 0.0603(9) | 0.0620(10) | 0.4780(11) | 0.100(6) |
| C4_25 | 0.2314(14) | -0.0417(9) | 0.4800(7) | 0.043(4) |
| F7_25 | 0.2617(13) | -0.0271(10) | 0.4231(7) | 0.051(3) |
| F8_25 | 0.159(2) | -0.0770(19) | 0.4883(18) | 0.055(4) |
| F9_25 | 0.3020(18) | -0.0879(10) | 0.5058(9) | 0.081(5) |
| O1_26 | 0.3035(15) | 0.0524(19) | 0.9793(15) | 0.024(6) |
| C1_26 | 0.2277(12) | 0.0250(8) | 1.0086(8) | 0.036(4) |
| C2_26 | 0.2238(14) | 0.0284(9) | 1.0762(7) | 0.044(4) |
| F1_26 | 0.3106(18) | 0.0076(19) | 1.0975(16) | 0.045(5) |
| F2_26 | 0.1646(18) | -0.0132(14) | 1.1056(12) | 0.048(5) |
| F3_26 | 0.1856(18) | 0.0887(10) | 1.0873(9) | 0.067(4) |
| C3_26 | 0.1348(11) | 0.0690(9) | 0.9827(7) | 0.042(4) |
| F4_26 | 0.1256(15) | 0.0594(13) | 0.9278(7) | 0.066(4) |
| F5_26 | 0.133(3) | 0.1345(10) | 0.9813(18) | 0.036(4) |
| F6_26 | 0.0589(11) | 0.0500(12) | 1.0184(8) | 0.052(4) |
| C4_26 | 0.2407(14) | -0.0500(8) | 1.0010(8) | 0.059(4) |
| F7_26 | 0.2989(16) | -0.0608(12) | 0.9534(9) | 0.055(4) |
| F8_26 | 0.1617(15) | -0.0785(12) | 1.0057(13) | 0.071(5) |
| F9_26 | 0.2921(17) | -0.0870(10) | 1.0449(9) | 0.072(4) |
| O1_27 | 0.4062(13) | 0.1081(11) | 0.4184(6) | 0.046(5) |
| C1_27 | 0.4430(10) | 0.1289(8) | 0.3646(7) | 0.031(4) |
| C2_27 | 0.5237(11) | 0.1727(8) | 0.3641(8) | 0.053(4) |
| F1_27 | 0.4847(16) | 0.2334(8) | 0.3768(11) | 0.077(4) |
| F2_27 | 0.5741(13) | 0.1751(9) | 0.3119(7) | 0.059(3) |
| F3_27 | 0.5822(10) | 0.1456(10) | 0.4066(7) | 0.070(5) |
| C3_27 | 0.4855(13) | 0.0653(9) | 0.3358(8) | 0.046(4) |
| F4_27 | 0.4201(18) | 0.0238(13) | 0.3430(11) | 0.053(4) |
| F5_27 | 0.5695(10) | 0.0393(8) | 0.3596(8) | 0.047(3) |
| F6_27 | 0.4935(14) | 0.0836(10) | 0.2775(6) | 0.065(4) |
| C4_27 | 0.3526(12) | 0.1683(10) | 0.3326(7) | 0.041(4) |
| F7_27 | 0.2914(14) | 0.1263(11) | 0.3275(9) | 0.059(4) |
| F8_27 | 0.3794(15) | 0.1968(10) | 0.2795(7) | 0.069(4) |
| F9_27 | 0.307(2) | 0.2146(13) | 0.3638(10) | 0.049(4) |

*Table S 8 Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for [InHMB][al-f-al]. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.*

| **Atom** | ***x*** | ***y*** | ***z*** | $U_{eq}$ |
|---|---|---|---|---|
| C1_18 | -0.6951(3) | 0.21183(16) | 0.25691(13) | 0.0216(7) |
| C2_18 | -0.7232(3) | 0.15905(15) | 0.24101(13) | 0.0229(7) |
| C3_18 | -0.8418(3) | 0.16227(15) | 0.22171(13) | 0.0228(7) |
| C4_18 | -0.9351(3) | 0.21760(15) | 0.21947(13) | 0.0194(6) |
| C5_18 | -0.9090(3) | 0.26912(15) | 0.23765(13) | 0.0191(6) |
| C6_18 | -0.7887(3) | 0.26718(15) | 0.25494(13) | 0.0203(6) |
| C7_18 | -0.5679(4) | 0.2073(2) | 0.27815(17) | 0.0395(10) |
| H7A_18 | -0.496143 | 0.203255 | 0.246986 | 0.059 |
| H7B_18 | -0.555179 | 0.170989 | 0.307383 | 0.059 |

| | | | | |
|---|---|---|---|---|
| H7C_18 | -0.569760 | 0.244673 | 0.293839 | 0.059 |
| C8_18 | -0.6286(4) | 0.09820(18) | 0.24791(18) | 0.0404(10) |
| H8A_18 | -0.648754 | 0.070106 | 0.225831 | 0.061 |
| H8B_18 | -0.636218 | 0.079640 | 0.287654 | 0.061 |
| H8C_18 | -0.539732 | 0.105449 | 0.234699 | 0.061 |
| C9_18 | -0.8680(5) | 0.10543(18) | 0.20519(18) | 0.0408(10) |
| H9A_18 | -0.958512 | 0.112462 | 0.198476 | 0.061 |
| H9B_18 | -0.852963 | 0.070439 | 0.235486 | 0.061 |
| H9C_18 | -0.809656 | 0.096228 | 0.170810 | 0.061 |
| C10_18 | -1.0639(4) | 0.22247(18) | 0.19972(16) | 0.0318(8) |
| H10A_18 | -1.080130 | 0.260192 | 0.172294 | 0.048 |
| H10B_18 | -1.133484 | 0.224040 | 0.231900 | 0.048 |
| H10C_18 | -1.061757 | 0.186348 | 0.182136 | 0.048 |
| C11_18 | -1.0139(4) | 0.32661(17) | 0.24027(17) | 0.0318(8) |
| H11A_18 | -1.031735 | 0.345018 | 0.202198 | 0.048 |
| H11B_18 | -0.984351 | 0.356561 | 0.257164 | 0.048 |
| H11C_18 | -1.093490 | 0.315369 | 0.263157 | 0.048 |
| C12_18 | -0.7627(4) | 0.32349(18) | 0.27350(16) | 0.0329(8) |
| H12A_18 | -0.668651 | 0.320686 | 0.271115 | 0.049 |
| H12B_18 | -0.804090 | 0.325482 | 0.312387 | 0.049 |
| H12C_18 | -0.798388 | 0.360827 | 0.249033 | 0.049 |
| C1_17 | 0.6743(3) | 0.79235(15) | 0.23435(14) | 0.0216(6) |
| C2_17 | 0.7820(3) | 0.74423(16) | 0.24087(14) | 0.0233(7) |
| C3_17 | 0.8871(3) | 0.75331(17) | 0.26431(14) | 0.0260(7) |
| C4_17 | 0.8801(3) | 0.80880(17) | 0.28495(14) | 0.0268(7) |
| C5_17 | 0.7748(3) | 0.85797(16) | 0.27606(13) | 0.0243(7) |
| C6_17 | 0.6734(3) | 0.85001(15) | 0.24933(14) | 0.0235(7) |
| C7_17 | 0.5613(4) | 0.78384(18) | 0.20823(16) | 0.0324(8) |
| H7A_17 | 0.569481 | 0.803295 | 0.168727 | 0.049 |
| H7B_17 | 0.479234 | 0.803155 | 0.228516 | 0.049 |
| H7C_17 | 0.562152 | 0.739585 | 0.210608 | 0.049 |
| C8_17 | 0.7860(4) | 0.68388(17) | 0.22102(17) | 0.0349(9) |
| H8A_17 | 0.807588 | 0.689074 | 0.179993 | 0.052 |
| H8B_17 | 0.700740 | 0.671586 | 0.232248 | 0.052 |
| H8C_17 | 0.852131 | 0.651807 | 0.237942 | 0.052 |
| C9_17 | 1.0075(4) | 0.7036(2) | 0.2647(2) | 0.0457(11) |
| H9A_17 | 1.038266 | 0.694148 | 0.226571 | 0.069 |
| H9B_17 | 0.986974 | 0.666235 | 0.289766 | 0.069 |
| H9C_17 | 1.075491 | 0.718137 | 0.278093 | 0.069 |
| C10_17 | 0.9864(4) | 0.8165(2) | 0.31508(18) | 0.0436(11) |
| H10A_17 | 1.044294 | 0.841372 | 0.289323 | 0.065 |
| H10B_17 | 1.036277 | 0.775806 | 0.328007 | 0.065 |
| H10C_17 | 0.947475 | 0.837495 | 0.347463 | 0.065 |
| C11_17 | 0.7733(4) | 0.91943(19) | 0.29330(18) | 0.0401(10) |
| H11A_17 | 0.806879 | 0.947376 | 0.260717 | 0.060 |
| H11B_17 | 0.828118 | 0.913219 | 0.322833 | 0.060 |
| H11C_17 | 0.683958 | 0.937580 | 0.307531 | 0.060 |
| C12_17 | 0.5675(4) | 0.90334(18) | 0.23274(17) | 0.0362(9) |
| H12A_17 | 0.564629 | 0.907675 | 0.192378 | 0.054 |
| H12B_17 | 0.585374 | 0.941517 | 0.241233 | 0.054 |
| H12C_17 | 0.483577 | 0.895527 | 0.253812 | 0.054 |
| O1_16 | 0.9914(19) | 0.8754(9) | 0.0030(9) | 0.019(3) |
| C1_16 | 0.9115(10) | 0.8336(5) | 0.0230(4) | 0.024(2) |
| C2_16 | 0.9443(7) | 0.7970(3) | 0.0809(3) | 0.0298(17) |
| F1_16 | 1.0701(10) | 0.7819(8) | 0.0817(5) | 0.034(3) |

| | | | | |
|---|---|---|---|---|
| F2_16 | 0.8924(19) | 0.7462(7) | 0.0941(6) | 0.040(3) |
| F3_16 | 0.8996(9) | 0.8312(4) | 0.1206(3) | 0.049(2) |
| C3_16 | 0.7668(7) | 0.8669(4) | 0.0303(4) | 0.045(2) |
| F4_16 | 0.7261(13) | 0.8827(7) | -0.0187(5) | 0.086(4) |
| F5_16 | 0.761(2) | 0.9171(6) | 0.0540(8) | 0.088(5) |
| F6_16 | 0.6887(12) | 0.8323(7) | 0.0641(6) | 0.058(4) |
| C4_16 | 0.9332(9) | 0.7883(4) | -0.0201(3) | 0.043(2) |
| F7_16 | 0.934(2) | 0.8186(12) | -0.0724(5) | 0.0538(9) |
| F8_16 | 0.8371(8) | 0.7553(4) | -0.0102(3) | 0.054(2) |
| F9_16 | 1.0470(10) | 0.7506(5) | -0.0183(4) | 0.063(3) |
| O1_15 | 1.522(2) | 0.4480(8) | 0.1109(10) | 0.026(5) |
| C1_15 | 1.6161(12) | 0.3977(6) | 0.1219(5) | 0.020(3) |
| C2_15 | 1.7467(10) | 0.4197(5) | 0.1198(4) | 0.030(2) |
| F1_15 | 1.764(2) | 0.4636(9) | 0.0762(8) | 0.042(6) |
| F2_15 | 1.8480(18) | 0.3734(8) | 0.1133(11) | 0.035(4) |
| F3_15 | 1.7495(11) | 0.4397(5) | 0.1668(4) | 0.048(3) |
| C3_15 | 1.5771(9) | 0.3608(5) | 0.1806(4) | 0.031(2) |
| F4_15 | 1.4863(19) | 0.3286(11) | 0.1787(9) | 0.047(4) |
| F5_15 | 1.526(2) | 0.3985(9) | 0.2180(8) | 0.042(4) |
| F6_15 | 1.6764(11) | 0.3210(5) | 0.1994(6) | 0.052(4) |
| C4_15 | 1.6337(9) | 0.3550(4) | 0.0763(4) | 0.029(2) |
| F7_15 | 1.5155(15) | 0.3514(11) | 0.0672(10) | 0.053(6) |
| F8_15 | 1.7007(10) | 0.2992(4) | 0.0917(5) | 0.045(2) |
| F9_15 | 1.6959(10) | 0.3805(6) | 0.0285(4) | 0.038(2) |
| O1_14 | 0.431(2) | 0.4423(7) | 0.4212(12) | 0.016(3) |
| C1_14 | 0.4114(11) | 0.3832(7) | 0.4399(5) | 0.020(3) |
| C2_14 | 0.3048(10) | 0.3847(4) | 0.4920(4) | 0.026(2) |
| F1_14 | 0.3566(12) | 0.3892(5) | 0.5362(4) | 0.047(3) |
| F2_14 | 0.2533(17) | 0.3332(6) | 0.5045(8) | 0.034(3) |
| F3_14 | 0.2095(11) | 0.4332(6) | 0.4851(8) | 0.026(3) |
| C3_14 | 0.3623(10) | 0.3608(5) | 0.3924(4) | 0.027(2) |
| F4_14 | 0.4344(19) | 0.3727(11) | 0.3434(7) | 0.032(3) |
| F5_14 | 0.2411(8) | 0.3904(4) | 0.3885(4) | 0.040(2) |
| F6_14 | 0.357(3) | 0.3016(7) | 0.4037(15) | 0.046(5) |
| C4_14 | 0.5352(10) | 0.3381(4) | 0.4567(4) | 0.026(2) |
| F7_14 | 0.6134(9) | 0.3204(4) | 0.4114(4) | 0.043(2) |
| F8_14 | 0.511(2) | 0.2876(7) | 0.4918(8) | 0.034(3) |
| F9_14 | 0.6008(13) | 0.3656(6) | 0.4824(7) | 0.023(2) |
| O1_13 | -0.2049(2) | 0.08662(11) | 0.53975(9) | 0.0212(5) |
| C1_13 | -0.2590(3) | 0.08561(13) | 0.59433(12) | 0.0176(6) |
| C2_13 | -0.3795(3) | 0.05418(15) | 0.60400(14) | 0.0255(7) |
| F1_13 | -0.47991(19) | 0.09284(10) | 0.58278(10) | 0.0348(5) |
| F2_13 | -0.4191(2) | 0.03678(10) | 0.65843(9) | 0.0362(5) |
| F3_13 | -0.3542(2) | 0.00463(10) | 0.57917(10) | 0.0351(5) |
| C3_13 | -0.1604(3) | 0.04898(14) | 0.63386(13) | 0.0227(6) |
| F4_13 | -0.04327(19) | 0.06359(10) | 0.61521(9) | 0.0305(5) |
| F5_13 | -0.1474(2) | -0.01182(9) | 0.63481(9) | 0.0298(5) |
| F6_13 | -0.1953(2) | 0.06015(10) | 0.68664(8) | 0.0331(5) |
| C4_13 | -0.3007(3) | 0.15329(15) | 0.60638(14) | 0.0246(7) |
| F7_13 | -0.1982(2) | 0.17610(9) | 0.61115(9) | 0.0332(5) |
| F8_13 | -0.3847(2) | 0.15698(10) | 0.65437(9) | 0.0359(5) |
| F9_13 | -0.3594(2) | 0.18967(9) | 0.56543(9) | 0.0302(5) |
| O1_12 | -0.1214(2) | 0.08928(10) | 0.42325(9) | 0.0195(4) |
| C1_12 | -0.2229(3) | 0.10207(14) | 0.39328(13) | 0.0205(6) |
| C2_12 | -0.3168(3) | 0.05633(18) | 0.41638(16) | 0.0342(8) |

| | | | | |
|---|---|---|---|---|
| F1_12 | -0.3959(2) | 0.07237(14) | 0.46220(10) | 0.0526(7) |
| F2_12 | -0.3932(2) | 0.05407(13) | 0.37854(11) | 0.0486(6) |
| F3_12 | -0.2521(3) | -0.00020(11) | 0.43030(12) | 0.0521(7) |
| C3_12 | -0.1657(3) | 0.09474(15) | 0.33161(14) | 0.0256(7) |
| F4_12 | -0.0616(2) | 0.12077(11) | 0.31546(9) | 0.0349(5) |
| F5_12 | -0.1286(2) | 0.03542(10) | 0.32574(9) | 0.0354(5) |
| F6_12 | -0.2509(2) | 0.12072(10) | 0.29618(9) | 0.0358(5) |
| C4_12 | -0.2963(4) | 0.16941(17) | 0.39526(16) | 0.0342(8) |
| F7_12 | -0.2295(3) | 0.20963(10) | 0.36196(11) | 0.0492(7) |
| F8_12 | -0.4136(2) | 0.17931(12) | 0.37936(11) | 0.0508(7) |
| F9_12 | -0.3130(3) | 0.18242(12) | 0.44710(10) | 0.0491(7) |
| O1_11 | 0.0485(2) | 0.11484(11) | 0.49052(10) | 0.0265(5) |
| C1_11 | 0.1063(3) | 0.16509(14) | 0.47243(13) | 0.0197(6) |
| C2_11 | 0.1440(4) | 0.17387(15) | 0.40784(14) | 0.0270(7) |
| F1_11 | 0.0400(2) | 0.19987(10) | 0.38244(9) | 0.0364(5) |
| F2_11 | 0.2328(2) | 0.20996(11) | 0.39025(9) | 0.0394(5) |
| F3_11 | 0.1921(2) | 0.12002(10) | 0.39024(9) | 0.0404(6) |
| C3_11 | 0.2313(3) | 0.15306(15) | 0.50073(15) | 0.0249(7) |
| F4_11 | 0.2066(2) | 0.13180(10) | 0.55526(9) | 0.0317(5) |
| F5_11 | 0.3225(2) | 0.11074(10) | 0.47776(10) | 0.0381(5) |
| F6_11 | 0.2805(2) | 0.20402(10) | 0.49596(10) | 0.0369(5) |
| C4_11 | 0.0148(3) | 0.22446(16) | 0.48942(15) | 0.0299(7) |
| F7_11 | 0.0126(2) | 0.22707(11) | 0.54402(9) | 0.0419(6) |
| F8_11 | 0.0501(2) | 0.27567(9) | 0.45982(10) | 0.0401(5) |
| F9_11 | -0.1062(2) | 0.22416(12) | 0.48231(11) | 0.0431(6) |
| O1_10 | 0.4481(11) | 0.4375(4) | 0.4213(5) | 0.029(2) |
| C1_10 | 0.4093(5) | 0.3821(3) | 0.4394(2) | 0.0169(13) |
| C2_10 | 0.4815(5) | 0.3456(2) | 0.4880(2) | 0.0339(12) |
| F1_10 | 0.4290(6) | 0.3679(2) | 0.53595(17) | 0.0557(14) |
| F2_10 | 0.4745(9) | 0.2852(3) | 0.4966(4) | 0.048(2) |
| F3_10 | 0.6054(7) | 0.3510(4) | 0.4774(4) | 0.081(3) |
| C3_10 | 0.4427(6) | 0.3461(2) | 0.3888(2) | 0.0328(12) |
| F4_10 | 0.4081(10) | 0.3839(5) | 0.3431(3) | 0.050(2) |
| F5_10 | 0.5703(5) | 0.32506(19) | 0.3793(2) | 0.0614(14) |
| F6_10 | 0.3849(11) | 0.2980(3) | 0.3979(6) | 0.041(2) |
| C4_10 | 0.2620(5) | 0.3915(2) | 0.4602(2) | 0.0357(13) |
| F7_10 | 0.1943(4) | 0.4056(3) | 0.4170(2) | 0.0662(15) |
| F8_10 | 0.2250(8) | 0.3424(3) | 0.4930(4) | 0.049(2) |
| F9_10 | 0.2291(8) | 0.4383(3) | 0.4899(4) | 0.077(3) |
| O1_9 | 0.4253(3) | 0.56788(11) | 0.40234(13) | 0.0420(7) |
| C1_9 | 0.3294(3) | 0.60159(14) | 0.37401(14) | 0.0226(6) |
| C2_9 | 0.2020(4) | 0.61746(18) | 0.41540(15) | 0.0347(8) |
| F1_9 | 0.2104(3) | 0.66006(11) | 0.44503(10) | 0.0437(6) |
| F2_9 | 0.1004(2) | 0.63929(13) | 0.38811(11) | 0.0491(6) |
| F3_9 | 0.1805(3) | 0.56750(13) | 0.45059(11) | 0.0673(9) |
| C3_9 | 0.3025(3) | 0.56669(15) | 0.32942(14) | 0.0249(7) |
| F4_9 | 0.4125(2) | 0.53500(10) | 0.30604(10) | 0.0378(5) |
| F5_9 | 0.2257(2) | 0.52604(10) | 0.35245(10) | 0.0374(5) |
| F6_9 | 0.2465(2) | 0.60463(10) | 0.28841(9) | 0.0387(5) |
| C4_9 | 0.3754(3) | 0.66209(16) | 0.34456(17) | 0.0332(8) |
| F7_9 | 0.4688(3) | 0.65086(12) | 0.30179(13) | 0.0615(8) |
| F8_9 | 0.2813(2) | 0.70528(10) | 0.32418(10) | 0.0417(6) |
| F9_9 | 0.4242(3) | 0.68722(11) | 0.37894(12) | 0.0505(7) |
| O1_8 | 0.6732(2) | 0.49273(13) | 0.40687(11) | 0.0347(6) |
| C1_8 | 0.7789(3) | 0.48571(15) | 0.36668(13) | 0.0228(7) |

| | | | | |
|---|---|---|---|---|
| C2_8 | 0.8535(4) | 0.53960(19) | 0.36264(16) | 0.0362(9) |
| F1_8 | 0.9165(2) | 0.53114(14) | 0.40632(11) | 0.0546(7) |
| F2_8 | 0.9406(2) | 0.54366(13) | 0.31620(11) | 0.0510(7) |
| F3_8 | 0.7721(3) | 0.59322(12) | 0.36255(13) | 0.0593(8) |
| C3_8 | 0.7395(3) | 0.48658(16) | 0.30830(14) | 0.0253(7) |
| F4_8 | 0.6470(2) | 0.45317(10) | 0.31358(9) | 0.0328(5) |
| F5_8 | 0.6908(2) | 0.54372(11) | 0.28579(10) | 0.0430(6) |
| F6_8 | 0.8391(2) | 0.46354(11) | 0.27214(8) | 0.0335(5) |
| C4_8 | 0.8679(4) | 0.42304(19) | 0.38382(16) | 0.0385(9) |
| F7_8 | 0.8185(3) | 0.37629(11) | 0.37450(11) | 0.0496(6) |
| F8_8 | 0.9876(2) | 0.41972(13) | 0.35469(11) | 0.0513(7) |
| F9_8 | 0.8807(3) | 0.41406(14) | 0.43729(10) | 0.0601(8) |
| O1_7 | 1.2896(2) | 0.53056(10) | 0.08304(9) | 0.0207(5) |
| C1_7 | 1.1769(3) | 0.51191(15) | 0.10844(14) | 0.0234(7) |
| C2_7 | 1.1573(4) | 0.51248(17) | 0.17243(16) | 0.0339(8) |
| F1_7 | 1.1193(3) | 0.56966(12) | 0.18410(11) | 0.0536(7) |
| F2_7 | 1.0671(2) | 0.47963(12) | 0.20019(10) | 0.0443(6) |
| F3_7 | 1.2670(2) | 0.48852(12) | 0.19322(9) | 0.0402(5) |
| C3_7 | 1.1782(4) | 0.44535(19) | 0.09768(18) | 0.0405(9) |
| F4_7 | 1.2386(3) | 0.43750(13) | 0.04642(12) | 0.0597(8) |
| F5_7 | 1.2455(2) | 0.40301(10) | 0.13336(12) | 0.0465(6) |
| F6_7 | 1.0617(3) | 0.43149(14) | 0.10395(13) | 0.0594(8) |
| C4_7 | 1.0631(4) | 0.5571(2) | 0.08278(19) | 0.0473(11) |
| F7_7 | 1.0572(3) | 0.54584(16) | 0.03122(12) | 0.0656(9) |
| F8_7 | 0.9483(2) | 0.55102(15) | 0.11400(13) | 0.0684(9) |
| F9_7 | 1.0770(2) | 0.61434(12) | 0.07680(13) | 0.0605(8) |
| O1_6 | 1.5112(9) | 0.4452(4) | 0.1097(5) | 0.0166(16) |
| C1_6 | 1.6093(6) | 0.3997(3) | 0.1254(2) | 0.0173(13) |
| C2_6 | 1.6248(5) | 0.4015(2) | 0.1870(2) | 0.0290(11) |
| F1_6 | 1.6927(5) | 0.4443(2) | 0.18845(19) | 0.0467(11) |
| F2_6 | 1.6863(5) | 0.3471(2) | 0.2110(2) | 0.0461(13) |
| F3_6 | 1.5089(9) | 0.4141(4) | 0.2177(3) | 0.0348(16) |
| C3_6 | 1.5734(5) | 0.3371(2) | 0.1220(2) | 0.0284(11) |
| F4_6 | 1.5227(6) | 0.3404(4) | 0.0753(4) | 0.0351(14) |
| F5_6 | 1.4822(9) | 0.3226(5) | 0.1652(4) | 0.0370(16) |
| F6_6 | 1.6746(4) | 0.29104(17) | 0.1231(2) | 0.0451(11) |
| C4_6 | 1.7399(4) | 0.4060(2) | 0.0856(2) | 0.0233(10) |
| F7_6 | 1.7385(5) | 0.3892(3) | 0.03699(18) | 0.0341(10) |
| F8_6 | 1.8427(8) | 0.3710(5) | 0.1079(5) | 0.040(2) |
| F9_6 | 1.7543(10) | 0.4648(3) | 0.0768(4) | 0.035(2) |
| O1_5 | 1.5246(2) | 0.57635(10) | 0.06599(9) | 0.0201(5) |
| C1_5 | 1.5231(3) | 0.62483(14) | 0.09225(13) | 0.0219(6) |
| C2_5 | 1.6353(4) | 0.65790(16) | 0.06108(14) | 0.0295(8) |
| F1_5 | 1.6063(2) | 0.69029(10) | 0.01162(9) | 0.0384(5) |
| F2_5 | 1.6596(3) | 0.69710(11) | 0.09104(10) | 0.0471(6) |
| F3_5 | 1.7438(2) | 0.61792(11) | 0.04985(10) | 0.0368(5) |
| C3_5 | 1.5456(4) | 0.60129(18) | 0.15414(15) | 0.0359(9) |
| F4_5 | 1.4742(2) | 0.55732(11) | 0.17657(9) | 0.0406(6) |
| F5_5 | 1.6688(3) | 0.57632(13) | 0.15763(10) | 0.0497(7) |
| F6_5 | 1.5093(3) | 0.64614(13) | 0.18556(10) | 0.0597(8) |
| C4_5 | 1.3908(4) | 0.67131(17) | 0.08990(19) | 0.0407(9) |
| F7_5 | 1.2994(2) | 0.65085(12) | 0.12956(12) | 0.0516(7) |
| F8_5 | 1.4010(3) | 0.72680(11) | 0.09818(14) | 0.0650(8) |
| F9_5 | 1.3528(2) | 0.67730(11) | 0.04037(12) | 0.0502(6) |
| O1_4 | 0.9877(17) | 0.8793(8) | -0.0002(8) | 0.023(3) |

| | | | | |
|---|---|---|---|---|
| C1_4 | 0.9064(8) | 0.8389(4) | 0.0227(3) | 0.0170(18) |
| C2_4 | 0.8401(6) | 0.8307(3) | -0.0261(3) | 0.0313(15) |
| F1_4 | 0.7520(9) | 0.8808(4) | -0.0399(3) | 0.049(2) |
| F2_4 | 0.7762(6) | 0.7834(3) | -0.0135(3) | 0.0457(16) |
| F3_4 | 0.9267(18) | 0.8219(10) | -0.0716(5) | 0.0538(9) |
| C3_4 | 0.9822(6) | 0.7752(3) | 0.0478(3) | 0.0307(14) |
| F4_4 | 1.0670(10) | 0.7826(6) | 0.0777(5) | 0.048(3) |
| F5_4 | 1.0501(8) | 0.7445(4) | 0.0070(3) | 0.0482(18) |
| F6_4 | 0.9042(15) | 0.7393(5) | 0.0787(5) | 0.042(3) |
| C4_4 | 0.8007(6) | 0.8655(3) | 0.0687(3) | 0.0326(15) |
| F7_4 | 0.8456(7) | 0.8568(3) | 0.1168(3) | 0.0479(17) |
| F8_4 | 0.6973(12) | 0.8386(7) | 0.0776(5) | 0.056(3) |
| F9_4 | 0.7609(13) | 0.9260(4) | 0.0530(4) | 0.045(2) |
| O1_3 | 1.1374(2) | 0.90952(10) | 0.07397(9) | 0.0224(5) |
| C1_3 | 1.1649(3) | 0.92617(14) | 0.12020(13) | 0.0204(6) |
| C2_3 | 1.2905(3) | 0.95406(17) | 0.10620(16) | 0.0300(8) |
| F1_3 | 1.3967(2) | 0.90941(11) | 0.10287(10) | 0.0408(6) |
| F2_3 | 1.3021(2) | 0.98600(11) | 0.14501(11) | 0.0419(6) |
| F3_3 | 1.2941(2) | 0.99078(11) | 0.05740(10) | 0.0430(6) |
| C3_3 | 1.0487(3) | 0.97511(16) | 0.14240(15) | 0.0272(7) |
| F4_3 | 0.9367(2) | 0.96005(10) | 0.13946(10) | 0.0377(5) |
| F5_3 | 1.0522(2) | 1.03066(9) | 0.11060(10) | 0.0357(5) |
| F6_3 | 1.0495(2) | 0.98107(10) | 0.19538(9) | 0.0356(5) |
| C4_3 | 1.1827(4) | 0.86820(16) | 0.16537(14) | 0.0286(7) |
| F7_3 | 1.0677(2) | 0.85167(11) | 0.18609(9) | 0.0395(5) |
| F8_3 | 1.2345(2) | 0.87791(11) | 0.20809(9) | 0.0363(5) |
| F9_3 | 1.2587(2) | 0.82069(10) | 0.14373(10) | 0.0411(6) |
| O1_2 | 1.2146(2) | 0.92935(10) | -0.04574(9) | 0.0180(4) |
| C1_2 | 1.3211(3) | 0.89394(13) | -0.07162(13) | 0.0189(6) |
| C2_2 | 1.2835(3) | 0.87218(16) | -0.12182(15) | 0.0290(7) |
| F1_2 | 1.2062(2) | 0.83035(11) | -0.10356(10) | 0.0382(5) |
| F2_2 | 1.3869(2) | 0.84542(10) | -0.15457(9) | 0.0333(5) |
| F3_2 | 1.2196(2) | 0.91849(11) | -0.15400(10) | 0.0451(6) |
| C3_2 | 1.4289(3) | 0.93298(15) | -0.09216(15) | 0.0283(7) |
| F4_2 | 1.4443(2) | 0.96295(11) | -0.05343(11) | 0.0447(6) |
| F5_2 | 1.4016(2) | 0.97431(11) | -0.13749(11) | 0.0459(6) |
| F6_2 | 1.54373(19) | 0.89784(10) | -0.10790(10) | 0.0365(5) |
| C4_2 | 1.3727(3) | 0.83591(15) | -0.03010(14) | 0.0252(7) |
| F7_2 | 1.4381(2) | 0.85086(11) | 0.00557(10) | 0.0405(5) |
| F8_2 | 1.4518(2) | 0.79162(10) | -0.05537(9) | 0.0371(5) |
| F9_2 | 1.2738(2) | 0.81241(10) | 0.00111(10) | 0.0373(5) |
| In2 | -0.72141(2) | 0.25018(2) | 0.13883(2) | 0.02404(6) |
| In1 | 0.67612(3) | 0.75890(2) | 0.35535(2) | 0.02949(7) |
| Al1 | 1.09060(8) | 0.92373(4) | 0.00922(4) | 0.01320(17) |
| Al4 | -0.07524(8) | 0.07869(4) | 0.48822(4) | 0.01300(17) |
| Al3 | 0.51090(8) | 0.49836(4) | 0.42765(4) | 0.01241(17) |
| Al2 | 1.45512(8) | 0.51334(4) | 0.07023(4) | 0.01245(17) |
| F1 | 1.000000 | 1.000000 | 0.000000 | 0.0171(5) |
| F4 | 0.000000 | 0.000000 | 0.500000 | 0.0190(5) |
| F2 | 1.500000 | 0.500000 | 0.000000 | 0.0153(5) |
| F3 | 0.500000 | 0.500000 | 0.500000 | 0.0181(5) |

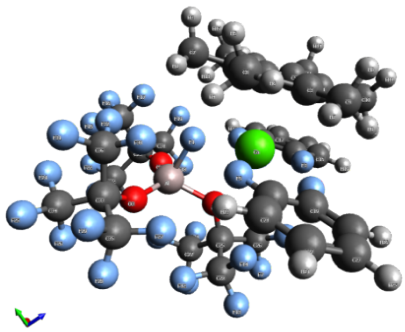
# S-3 Quantum chemical calculations

*Table S 9* SCF energy, FreeH energy and FreeH entropy of presented compounds. (*BP86/def2-def-SV(P)/D3(BJ) )*

| Compound | SCF /*Hartree* | FreeH energy [kJ/mol] | FreeH entropy [kJ/mol K] | COSMO DFB/*Hartee* ε = 8.93 | COSMO DCM/*Hartree* ε = 13.38 |
|---|---|---|---|---|---|
| [Ca(HMB)oDFB$_2${*f-al*}]$^+$ **2$^+$** | -5725.166289288 | 1765.47 | 1.74063 | -5725.2197376847 | -5725.2164611434 |
| [Sr(HMB)oDFB$_3${*f-al*}]$^+$ **5$^+$** | -5508.784111417 | 2001.96 | 1.92245 | -5508.8442714488 | -5508.8403896611 |
| [Ba(HMB)oDFB$_3${*f-al*}]$^+$ **4$^+$** | -5503.583757382 | 2003.98 | 1.93475 | -5503.6338738050 | -5503.6308525042 |
| [Ca(HMB)oDFB$_4$]$^{2+}$ **7$^{2+}$** | -2866.854410856 | 1683.52 | 1.19609 | -2867.0185296993 | -2867.0090879921 |
| [Sr(HMB)oDFB$_4$]$^{2+}$ **6$^{2+}$** | -2220.038458915 | 1682.68 | 1.22634 | -2220.2007673224 | -2220.1913875602 |
| [Ba(HMB)oDFB$_4$]$^{2+}$ | -2214.821898745 | 1681.97 | 1.25849 | -2214.9838152870 | -2214.9744720839 |
| F-Ca(HMB)oDFB$_2${*f-al*} | -5825.169460385 | 1772.60 | 1.80006 | | -5825.1856053590 |
| F-Sr(HMB)oDFB$_2${*f-al*} | -5178.347256196 | 1771.97 | 1.81809 | | -5178.3646423792 |
| Ba(HMB)oDFB$_2${*f-al*} | -5173.123266665 | 1771.81 | 1.81006 | | -5173.1419648063 |
| [F-Ca(HMB)oDFB$_3$]$^+$ | -2536.510662890 | 1454.51 | 1.05702 | | -2536.5608022626 |
| [F-Sr(HMB)oDFB$_3$]$^+$ | -2320.133267672 | 1692.09 | 1.23892 | | -2320.1848629439 |
| [F-Ba(HMB)oDFB$_3$]$^+$ | -2314.911646911 | 1691.56 | 1.26804 | | -2314.9633109872 |
| H-Ca(HMB)oDFB$_2${*f-al*} | -5725.883417646 | 1777.17 | 1.78788 | | -5725.9033928264 |
| H-Sr(HMB)oDFB$_2${*f-al*} | -5079.061452805 | 1775.75 | 1.79115 | | -5079.0834714081 |
| H-Ba(HMB)oDFB$_2${*f-al*} | -5073.838370815 | 1775.20 | 1.78700 | | -5073.8660490436 |
| [H-Ca(HMB)oDFB$_4$]$^+$ | -2867.673876950 | 1698.19 | 1.22031 | | -2867.7262895978 |
| [H-Sr(HMB)oDFB$_4$]$^+$ | -2220.848284775 | 1696.56 | 1.22036 | | -2220.9034685658 |

| Compound | SCF /*Hartree* | FreeH energy [kJ/mol] | FreeH entropy [kJ/mol K] | COSMO DFB/*Hartee* ε = 8.93 | COSMO DCM/*Hartree* ε = 13.38 |
|---|---|---|---|---|---|
| $[H\text{-}Ba(HMB)oDFB_4]^+$ | -2215.628495887 | 1695.26 | 1.25254 | | -2215.6861118948 |
| $TMS^+$ | -408.8229362860 | 297.92 | 0.35871 | | -408.8998081732 |
| TMSF | -508.9440076315 | 310.97 | 0.35438 | | -508.9476831331 |
| TMSH | -409.7051205360 | 322.40 | 0.33278 | | -409.7067280146 |
| $B(C_6F_5)_3$ | -2206.833841130 | 471.80 | 0.80761 | | -2206.8384767034 |
| $[F\text{-}B(C_6F_5)_3]^-$ | -2306.761000073 | 477.95 | 0.83999 | | -2306.8094516177 |
| $[H\text{-}B(C_6F_5)_3]^-$ | -2207.533999697 | 492.76 | 0.83117 | | -2207.5805375446 |
| $SbF_5$ | -504.3473889830 | 47.25 | 0.35306 | | -504.3541263397 |
| $[SbF_6]^-$ | -604.2900640637 | 55.65 | 0.37270 | | -604.3603604560 |
| $Al(OR^F)_3$ | -3619.007051245 | 541.05 | 1.05312 | | -3619.0099881445 |
| $[F\text{-}Al(OR^F)_3]^-$ | -3718.966875203 | 549.76 | 1.12120 | -3719.0165703535 | -3719.0135782148 |
| $[H\text{-}Al(OR^F)_3]^-$ | -3619.706895153 | 558.45 | 1.09480 | | -3619.7534163216 |
| *o*DFB·$AlOR^F_3$ | -4049.460707085 | 781.47 | 1.23993 | -4049.4662816509 | |
| $[\mu F\text{-}(AlOR^F_3)_2]^-$ | -7338.057560602 | 1100.10 | 1.97932 | | -7338.0944456007 |
| $[Sr(HMB)_2]^{2+}$ | -966.0017307724 | 1451.06 | 0.88925 | -966.2035236 | |
| $[Sr(oDFB)_8]^2$ | -3474.008175471 | 1913.62 | 1.56152 | -3474.160776 | |
| $[Ga(HMB)]^+$ | -2392.531049289 | 726.50 | 0.54884 | | |
| $[In(HMB)]^+$ | -469.5634901721 | 726.13 | 0.53802 | | |
| $[Tl(HMB)]^+$ | -469.6645925246 | 725.92 | 0.54987 | | |
| $F^-$ | -99.689938761 | | | | -99.8190863141 |
| $H^-$ | -0.48829116996 | | | | -0.6576594152 |

[Ca(HMB)oDFB$_2${*f-al*}]$^+$ **2**$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| Ca | -0.15826 | -0.38921 | 0.95701 |
| F | -0.08599 | 1.10611 | -0.60962 |
| Al | 0.22695 | 0.33512 | -2.17273 |
| C | -0.20863 | 2.30274 | 2.02075 |
| C | -1.43141 | 1.73904 | 2.49045 |
| C | -1.39652 | 0.64285 | 3.40091 |
| C | -0.14271 | 0.14863 | 3.87820 |
| C | 1.07999 | 0.74570 | 3.44619 |
| C | 1.04243 | 1.81349 | 2.49745 |
| C | -0.23128 | 3.48285 | 1.08001 |
| H | -1.15438 | 3.52202 | 0.47560 |
| H | 0.61554 | 3.46545 | 0.37007 |
| H | -0.16600 | 4.43423 | 1.65875 |
| C | -2.73175 | 2.37808 | 2.05459 |
| H | -2.84247 | 2.37575 | 0.95062 |
| H | -2.75849 | 3.44287 | 2.37494 |
| H | -3.62288 | 1.88754 | 2.48594 |
| C | -2.66871 | 0.06029 | 3.98048 |
| H | -3.54960 | 0.20623 | 3.32895 |
| H | -2.90153 | 0.54490 | 4.95722 |
| H | -2.58321 | -1.02517 | 4.17802 |
| C | -0.16449 | -0.96250 | 4.90765 |
| H | -0.63917 | -1.88473 | 4.50584 |
| H | -0.75707 | -0.66126 | 5.79895 |
| H | 0.84140 | -1.23966 | 5.26860 |
| C | 2.39737 | 0.33267 | 4.07246 |
| H | 2.41148 | -0.72355 | 4.39779 |
| H | 2.59557 | 0.95512 | 4.97567 |
| H | 3.25884 | 0.46706 | 3.39322 |
| C | 2.30021 | 2.50094 | 2.01239 |
| H | 3.21732 | 2.12917 | 2.50262 |
| H | 2.24599 | 3.59367 | 2.20792 |
| H | 2.43301 | 2.38198 | 0.91550 |
| C | 3.12042 | -1.22878 | 1.25176 |
| C | 2.51290 | -2.19059 | 2.05965 |
| C | 3.26036 | -3.10032 | 2.79744 |
| H | 2.75412 | -3.85253 | 3.42084 |
| C | 4.66355 | -3.01650 | 2.70988 |
| H | 5.28126 | -3.72495 | 3.28268 |
| C | 5.27611 | -2.04469 | 1.89896 |

| | | | |
|---|---|---|---|
| H | 6.37384 | -1.99276 | 1.83742 |
| C | 4.50371 | -1.13327 | 1.15371 |
| H | 4.95092 | -0.36737 | 0.50518 |
| F | 2.29014 | -0.37086 | 0.57448 |
| F | 1.13457 | -2.18886 | 2.10609 |
| C | -3.12363 | -1.97231 | 1.51003 |
| C | -3.49920 | -0.90652 | 0.69215 |
| C | -4.83099 | -0.67075 | 0.37117 |
| H | -5.09219 | 0.16678 | -0.29123 |
| C | -5.79522 | -1.54700 | 0.90507 |
| H | -6.85756 | -1.38635 | 0.66589 |
| C | -5.41591 | -2.62340 | 1.72695 |
| H | -6.18136 | -3.30318 | 2.13136 |
| C | -4.06138 | -2.84968 | 2.04037 |
| H | -3.73817 | -3.68520 | 2.67918 |
| F | -1.77651 | -2.10079 | 1.78369 |
| F | -2.49238 | -0.10473 | 0.22147 |
| O | 0.05774 | -1.30616 | -1.34092 |
| C | 0.01970 | -2.55588 | -1.94595 |
| C | 0.62964 | -3.60963 | -0.96544 |
| F | -0.18459 | -3.75999 | 0.11065 |
| F | 0.80641 | -4.80214 | -1.53803 |
| F | 1.81977 | -3.17741 | -0.50064 |
| C | 0.86134 | -2.54567 | -3.27631 |
| F | 0.59824 | -1.36908 | -3.91856 |
| F | 2.17444 | -2.58546 | -3.03019 |
| F | 0.53753 | -3.54959 | -4.09227 |
| C | -1.47361 | -2.93809 | -2.27800 |
| F | -1.90857 | -2.25141 | -3.34289 |
| F | -1.61945 | -4.24908 | -2.51821 |
| F | -2.26158 | -2.61603 | -1.22614 |
| O | 1.91067 | 0.62344 | -2.42268 |
| C | 2.91868 | 1.32555 | -3.00276 |
| C | 2.71933 | 2.86887 | -2.76675 |
| F | 1.74131 | 3.34110 | -3.55981 |
| F | 3.83827 | 3.57192 | -2.99329 |
| F | 2.33428 | 3.08842 | -1.48481 |
| C | 4.26070 | 0.85501 | -2.33215 |
| F | 4.27521 | -0.48193 | -2.20140 |
| F | 4.36721 | 1.37427 | -1.07639 |
| F | 5.34235 | 1.23347 | -3.02597 |
| C | 2.96674 | 1.02692 | -4.54943 |
| F | 3.43802 | -0.21655 | -4.76798 |
| F | 3.74458 | 1.90129 | -5.20778 |
| F | 1.72278 | 1.08920 | -5.05841 |
| O | -1.06075 | 0.72719 | -3.24427 |
| C | -2.05416 | 1.57506 | -3.62283 |
| C | -1.75801 | 2.07067 | -5.09054 |
| F | -0.77444 | 2.99245 | -5.07234 |
| F | -2.84772 | 2.62126 | -5.65681 |
| F | -1.35168 | 1.04222 | -5.84427 |
| C | -3.41864 | 0.79152 | -3.58941 |
| F | -3.50013 | 0.06919 | -2.44421 |
| F | -3.50657 | -0.06666 | -4.61458 |
| F | -4.47903 | 1.61950 | -3.62803 |

| | | | |
|---|---|---|---|
| C | -2.14140 | 2.81500 | -2.65877 |
| F | -2.72624 | 2.45869 | -1.48096 |
| F | -2.84444 | 3.82943 | -3.17472 |
| F | -0.90294 | 3.25533 | -2.36231 |

Vibrational analysis

| 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 | 7.66 | 0.13703 | YES | YES |
| 8 | a | 15.13 | 0.17788 | YES | YES |
| 9 | a | 18.43 | 0.03700 | YES | YES |
| 10 | a | 21.97 | 0.21452 | YES | YES |
| 11 | a | 23.20 | 0.09402 | YES | YES |
| 12 | a | 23.55 | 0.33919 | YES | YES |
| 13 | a | 25.85 | 0.06372 | YES | YES |
| 14 | a | 28.00 | 0.38951 | YES | YES |
| 15 | a | 32.30 | 0.08813 | YES | YES |
| 16 | a | 34.58 | 0.79821 | YES | YES |
| 17 | a | 37.39 | 1.08051 | YES | YES |
| 18 | a | 37.89 | 0.48235 | YES | YES |
| 19 | a | 42.28 | 1.27638 | YES | YES |
| 20 | a | 42.86 | 0.35035 | YES | YES |
| 21 | a | 43.44 | 1.01251 | YES | YES |
| 22 | a | 50.55 | 0.56859 | YES | YES |
| 23 | a | 53.16 | 0.58566 | YES | YES |
| 24 | a | 55.31 | 0.22967 | YES | YES |
| 25 | a | 60.73 | 1.98049 | YES | YES |
| 26 | a | 64.72 | 0.44120 | YES | YES |
| 27 | a | 65.62 | 0.21695 | YES | YES |
| 28 | a | 65.92 | 0.64580 | YES | YES |
| 29 | a | 68.35 | 0.02043 | YES | YES |
| 30 | a | 70.11 | 0.19009 | YES | YES |
| 31 | a | 73.11 | 1.51668 | YES | YES |
| 32 | a | 75.45 | 0.17252 | YES | YES |
| 33 | a | 77.53 | 0.20696 | YES | YES |
| 34 | a | 80.79 | 0.67779 | YES | YES |
| 35 | a | 81.34 | 0.47664 | YES | YES |
| 36 | a | 83.59 | 0.24733 | YES | YES |
| 37 | a | 84.74 | 0.21490 | YES | YES |
| 38 | a | 86.91 | 0.74406 | YES | YES |
| 39 | a | 89.18 | 1.60811 | YES | YES |
| 40 | a | 94.44 | 0.41201 | YES | YES |
| 41 | a | 98.94 | 2.03735 | YES | YES |
| 42 | a | 100.17 | 1.14634 | YES | YES |
| 43 | a | 102.92 | 0.85536 | YES | YES |
| 44 | a | 105.09 | 0.81307 | YES | YES |
| 45 | a | 107.17 | 2.96786 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 113.22 | 0.85505 | YES | YES |
| 47 | a | 121.39 | 0.86808 | YES | YES |
| 48 | a | 134.86 | 18.99054 | YES | YES |
| 49 | a | 136.95 | 0.91134 | YES | YES |
| 50 | a | 140.23 | 25.62029 | YES | YES |
| 51 | a | 148.93 | 11.32136 | YES | YES |
| 52 | a | 151.49 | 1.14699 | YES | YES |
| 53 | a | 156.00 | 12.30671 | YES | YES |
| 54 | a | 158.45 | 1.79417 | YES | YES |
| 55 | a | 158.67 | 0.30025 | YES | YES |
| 56 | a | 162.75 | 0.19939 | YES | YES |
| 57 | a | 165.24 | 11.14885 | YES | YES |
| 58 | a | 170.79 | 4.02230 | YES | YES |
| 59 | a | 172.54 | 2.54507 | YES | YES |
| 60 | a | 175.14 | 1.67837 | YES | YES |
| 61 | a | 181.27 | 0.48440 | YES | YES |
| 62 | a | 183.86 | 3.77749 | YES | YES |
| 63 | a | 188.29 | 1.04714 | YES | YES |
| 64 | a | 198.35 | 0.46693 | YES | YES |
| 65 | a | 199.20 | 11.72236 | YES | YES |
| 66 | a | 207.59 | 1.95680 | YES | YES |
| 67 | a | 211.13 | 9.37855 | YES | YES |
| 68 | a | 211.73 | 7.06656 | YES | YES |
| 69 | a | 214.17 | 39.06239 | YES | YES |
| 70 | a | 248.21 | 25.35693 | YES | YES |
| 71 | a | 257.12 | 2.39584 | YES | YES |
| 72 | a | 267.57 | 1.62658 | YES | YES |
| 73 | a | 275.78 | 3.60236 | YES | YES |
| 74 | a | 278.77 | 3.38832 | YES | YES |
| 75 | a | 283.17 | 5.82252 | YES | YES |
| 76 | a | 283.92 | 1.05056 | YES | YES |
| 77 | a | 284.24 | 0.14994 | YES | YES |
| 78 | a | 284.83 | 0.05186 | YES | YES |
| 79 | a | 288.64 | 4.39858 | YES | YES |
| 80 | a | 298.18 | 1.12569 | YES | YES |
| 81 | a | 298.70 | 0.47496 | YES | YES |
| 82 | a | 302.61 | 0.54028 | YES | YES |
| 83 | a | 308.85 | 3.95163 | YES | YES |
| 84 | a | 309.68 | 4.13745 | YES | YES |
| 85 | a | 314.12 | 13.62550 | YES | YES |
| 86 | a | 315.74 | 0.42579 | YES | YES |
| 87 | a | 317.04 | 1.94895 | YES | YES |
| 88 | a | 318.29 | 5.51057 | YES | YES |
| 89 | a | 319.59 | 2.18250 | YES | YES |
| 90 | a | 320.94 | 2.66263 | YES | YES |
| 91 | a | 322.94 | 2.08597 | YES | YES |
| 92 | a | 326.48 | 0.36706 | YES | YES |
| 93 | a | 330.88 | 1.09845 | YES | YES |
| 94 | a | 331.61 | 0.60402 | YES | YES |
| 95 | a | 347.57 | 0.07961 | YES | YES |
| 96 | a | 350.45 | 0.42570 | YES | YES |
| 97 | a | 355.00 | 15.46826 | YES | YES |
| 98 | a | 357.34 | 3.67024 | YES | YES |
| 99 | a | 368.32 | 17.02699 | YES | YES |
| 100 | a | 373.96 | 1.27628 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 101 | a | 377.75 | 7.17515 | YES | YES |
| 102 | a | 382.44 | 3.26018 | YES | YES |
| 103 | a | 393.11 | 44.71204 | YES | YES |
| 104 | a | 404.31 | 0.06037 | YES | YES |
| 105 | a | 424.35 | 5.99952 | YES | YES |
| 106 | a | 425.82 | 39.17458 | YES | YES |
| 107 | a | 436.18 | 0.05811 | YES | YES |
| 108 | a | 437.86 | 0.19366 | YES | YES |
| 109 | a | 438.76 | 5.87319 | YES | YES |
| 110 | a | 443.41 | 0.22404 | YES | YES |
| 111 | a | 444.96 | 1.56664 | YES | YES |
| 112 | a | 448.43 | 4.10686 | YES | YES |
| 113 | a | 448.90 | 53.99785 | YES | YES |
| 114 | a | 462.08 | 0.00983 | YES | YES |
| 115 | a | 484.27 | 26.43802 | YES | YES |
| 116 | a | 516.96 | 6.31692 | YES | YES |
| 117 | a | 517.94 | 0.38905 | YES | YES |
| 118 | a | 518.63 | 6.17296 | YES | YES |
| 119 | a | 519.15 | 7.81393 | YES | YES |
| 120 | a | 519.98 | 1.28227 | YES | YES |
| 121 | a | 520.92 | 3.07729 | YES | YES |
| 122 | a | 523.74 | 0.76741 | YES | YES |
| 123 | a | 524.62 | 3.35397 | YES | YES |
| 124 | a | 526.00 | 2.75805 | YES | YES |
| 125 | a | 527.98 | 3.11913 | YES | YES |
| 126 | a | 540.48 | 2.56739 | YES | YES |
| 127 | a | 540.60 | 0.13729 | YES | YES |
| 128 | a | 541.40 | 0.40289 | YES | YES |
| 129 | a | 542.12 | 4.54489 | YES | YES |
| 130 | a | 545.64 | 14.27867 | YES | YES |
| 131 | a | 552.14 | 1.86673 | YES | YES |
| 132 | a | 553.39 | 0.82098 | YES | YES |
| 133 | a | 554.10 | 0.01967 | YES | YES |
| 134 | a | 554.44 | 0.77807 | YES | YES |
| 135 | a | 555.08 | 0.77258 | YES | YES |
| 136 | a | 557.37 | 0.80539 | YES | YES |
| 137 | a | 558.24 | 33.55101 | YES | YES |
| 138 | a | 558.99 | 10.04928 | YES | YES |
| 139 | a | 561.02 | 0.33980 | YES | YES |
| 140 | a | 565.41 | 19.61616 | YES | YES |
| 141 | a | 569.03 | 0.09469 | YES | YES |
| 142 | a | 573.31 | 30.59723 | YES | YES |
| 143 | a | 577.74 | 0.14624 | YES | YES |
| 144 | a | 580.64 | 0.18521 | YES | YES |
| 145 | a | 636.31 | 162.70744 | YES | YES |
| 146 | a | 678.86 | 0.10975 | YES | YES |
| 147 | a | 680.09 | 0.29161 | YES | YES |
| 148 | a | 689.53 | 0.25399 | YES | YES |
| 149 | a | 706.36 | 5.62499 | YES | YES |
| 150 | a | 706.65 | 14.15923 | YES | YES |
| 151 | a | 708.37 | 32.55714 | YES | YES |
| 152 | a | 708.80 | 19.35273 | YES | YES |
| 153 | a | 709.92 | 45.76022 | YES | YES |
| 154 | a | 710.65 | 53.76454 | YES | YES |
| 155 | a | 718.09 | 49.91287 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 156 | a | 735.93 | 2.23452 | YES | YES |
| 157 | a | 740.25 | 0.51768 | YES | YES |
| 158 | a | 747.49 | 62.86708 | YES | YES |
| 159 | a | 750.45 | 73.84094 | YES | YES |
| 160 | a | 753.74 | 149.72648 | YES | YES |
| 161 | a | 756.93 | 25.10139 | YES | YES |
| 162 | a | 769.02 | 20.94318 | YES | YES |
| 163 | a | 789.63 | 0.77726 | YES | YES |
| 164 | a | 797.80 | 3.90199 | YES | YES |
| 165 | a | 817.13 | 0.69873 | YES | YES |
| 166 | a | 818.58 | 19.55916 | YES | YES |
| 167 | a | 828.46 | 17.90131 | YES | YES |
| 168 | a | 839.51 | 1.00120 | YES | YES |
| 169 | a | 844.52 | 0.53837 | YES | YES |
| 170 | a | 892.57 | 22.63008 | YES | YES |
| 171 | a | 929.35 | 4.03026 | YES | YES |
| 172 | a | 933.91 | 2.38491 | YES | YES |
| 173 | a | 950.31 | 0.11717 | YES | YES |
| 174 | a | 953.30 | 53.54245 | YES | YES |
| 175 | a | 956.24 | 78.45358 | YES | YES |
| 176 | a | 958.64 | 3.66369 | YES | YES |
| 177 | a | 960.80 | 144.40096 | YES | YES |
| 178 | a | 965.55 | 135.37296 | YES | YES |
| 179 | a | 966.28 | 230.99310 | YES | YES |
| 180 | a | 973.66 | 12.87771 | YES | YES |
| 181 | a | 973.98 | 292.38480 | YES | YES |
| 182 | a | 977.50 | 1.87535 | YES | YES |
| 183 | a | 978.95 | 0.42719 | YES | YES |
| 184 | a | 979.70 | 11.80462 | YES | YES |
| 185 | a | 1001.52 | 6.29136 | YES | YES |
| 186 | a | 1002.70 | 3.01109 | YES | YES |
| 187 | a | 1015.29 | 5.90938 | YES | YES |
| 188 | a | 1016.90 | 5.21537 | YES | YES |
| 189 | a | 1020.89 | 1.47076 | YES | YES |
| 190 | a | 1025.31 | 2.16975 | YES | YES |
| 191 | a | 1031.45 | 0.09802 | YES | YES |
| 192 | a | 1048.44 | 19.97241 | YES | YES |
| 193 | a | 1050.33 | 13.76248 | YES | YES |
| 194 | a | 1072.46 | 0.21678 | YES | YES |
| 195 | a | 1075.16 | 7.63996 | YES | YES |
| 196 | a | 1076.95 | 10.09819 | YES | YES |
| 197 | a | 1078.48 | 25.26699 | YES | YES |
| 198 | a | 1081.86 | 0.12095 | YES | YES |
| 199 | a | 1088.79 | 4.03158 | YES | YES |
| 200 | a | 1089.39 | 6.37295 | YES | YES |
| 201 | a | 1092.50 | 20.12850 | YES | YES |
| 202 | a | 1135.66 | 11.36635 | YES | YES |
| 203 | a | 1138.53 | 12.22213 | YES | YES |
| 204 | a | 1139.07 | 0.45830 | YES | YES |
| 205 | a | 1139.39 | 16.83741 | YES | YES |
| 206 | a | 1143.75 | 15.30857 | YES | YES |
| 207 | a | 1149.61 | 18.95163 | YES | YES |
| 208 | a | 1156.25 | 42.46397 | YES | YES |
| 209 | a | 1161.18 | 204.74168 | YES | YES |
| 210 | a | 1163.52 | 68.65489 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 211 | a | 1172.08 | 47.54859 | YES | YES |
| 212 | a | 1174.64 | 12.70814 | YES | YES |
| 213 | a | 1182.17 | 0.93604 | YES | YES |
| 214 | a | 1182.98 | 20.86467 | YES | YES |
| 215 | a | 1192.22 | 23.20875 | YES | YES |
| 216 | a | 1195.58 | 3.89172 | YES | YES |
| 217 | a | 1201.57 | 17.68985 | YES | YES |
| 218 | a | 1205.11 | 14.64140 | YES | YES |
| 219 | a | 1207.97 | 13.69563 | YES | YES |
| 220 | a | 1217.64 | 265.60674 | YES | YES |
| 221 | a | 1225.95 | 100.30260 | YES | YES |
| 222 | a | 1229.58 | 44.07193 | YES | YES |
| 223 | a | 1237.25 | 368.26526 | YES | YES |
| 224 | a | 1238.88 | 372.82479 | YES | YES |
| 225 | a | 1244.53 | 849.04253 | YES | YES |
| 226 | a | 1244.94 | 652.41478 | YES | YES |
| 227 | a | 1247.39 | 32.34826 | YES | YES |
| 228 | a | 1248.45 | 236.71630 | YES | YES |
| 229 | a | 1248.75 | 243.32543 | YES | YES |
| 230 | a | 1250.55 | 3.30028 | YES | YES |
| 231 | a | 1253.76 | 830.98723 | YES | YES |
| 232 | a | 1262.79 | 682.12853 | YES | YES |
| 233 | a | 1269.57 | 515.40215 | YES | YES |
| 234 | a | 1272.70 | 405.49245 | YES | YES |
| 235 | a | 1298.21 | 141.58845 | YES | YES |
| 236 | a | 1298.58 | 14.61625 | YES | YES |
| 237 | a | 1312.63 | 0.35474 | YES | YES |
| 238 | a | 1345.75 | 190.98273 | YES | YES |
| 239 | a | 1352.01 | 109.26279 | YES | YES |
| 240 | a | 1357.02 | 0.10923 | YES | YES |
| 241 | a | 1359.59 | 1.36153 | YES | YES |
| 242 | a | 1364.69 | 2.22787 | YES | YES |
| 243 | a | 1366.12 | 14.85740 | YES | YES |
| 244 | a | 1371.31 | 10.55075 | YES | YES |
| 245 | a | 1374.32 | 12.74298 | YES | YES |
| 246 | a | 1382.42 | 7.22613 | YES | YES |
| 247 | a | 1382.56 | 0.93927 | YES | YES |
| 248 | a | 1386.38 | 1.30471 | YES | YES |
| 249 | a | 1393.19 | 7.99507 | YES | YES |
| 250 | a | 1408.82 | 8.52154 | YES | YES |
| 251 | a | 1412.09 | 6.98427 | YES | YES |
| 252 | a | 1415.39 | 0.29118 | YES | YES |
| 253 | a | 1425.02 | 24.81076 | YES | YES |
| 254 | a | 1426.29 | 5.45127 | YES | YES |
| 255 | a | 1430.43 | 25.17025 | YES | YES |
| 256 | a | 1440.22 | 28.87050 | YES | YES |
| 257 | a | 1444.69 | 26.77556 | YES | YES |
| 258 | a | 1446.93 | 2.30203 | YES | YES |
| 259 | a | 1455.87 | 3.68342 | YES | YES |
| 260 | a | 1459.27 | 1.17993 | YES | YES |
| 261 | a | 1459.51 | 12.90842 | YES | YES |
| 262 | a | 1464.34 | 34.94974 | YES | YES |
| 263 | a | 1471.10 | 23.47228 | YES | YES |
| 264 | a | 1493.13 | 365.91984 | YES | YES |
| 265 | a | 1495.59 | 80.12346 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 266 | a | 1553.25 | 0.99626 | YES | YES |
| 267 | a | 1558.79 | 0.24307 | YES | YES |
| 268 | a | 1609.93 | 0.02106 | YES | YES |
| 269 | a | 1611.12 | 0.34879 | YES | YES |
| 270 | a | 1639.41 | 12.68492 | YES | YES |
| 271 | a | 1640.75 | 9.75004 | YES | YES |
| 272 | a | 2948.33 | 4.30438 | YES | YES |
| 273 | a | 2951.47 | 5.88852 | YES | YES |
| 274 | a | 2955.18 | 2.57428 | YES | YES |
| 275 | a | 2956.27 | 5.83149 | YES | YES |
| 276 | a | 2966.84 | 2.91108 | YES | YES |
| 277 | a | 2967.52 | 4.05479 | YES | YES |
| 278 | a | 3020.50 | 4.69875 | YES | YES |
| 279 | a | 3035.32 | 2.06458 | YES | YES |
| 280 | a | 3042.24 | 0.83548 | YES | YES |
| 281 | a | 3046.42 | 9.81784 | YES | YES |
| 282 | a | 3055.49 | 6.32314 | YES | YES |
| 283 | a | 3070.23 | 0.90541 | YES | YES |
| 284 | a | 3086.13 | 2.81634 | YES | YES |
| 285 | a | 3089.14 | 2.68155 | YES | YES |
| 286 | a | 3095.52 | 13.33028 | YES | YES |
| 287 | a | 3098.92 | 17.52223 | YES | YES |
| 288 | a | 3101.87 | 4.98804 | YES | YES |
| 289 | a | 3113.26 | 0.62548 | YES | YES |
| 290 | a | 3124.81 | 1.02058 | YES | YES |
| 291 | a | 3124.91 | 0.77974 | YES | YES |
| 292 | a | 3134.68 | 1.30588 | YES | YES |
| 293 | a | 3134.78 | 1.54004 | YES | YES |
| 294 | a | 3141.84 | 1.42535 | YES | YES |
| 295 | a | 3141.93 | 1.74762 | YES | YES |
| 296 | a | 3152.80 | 3.96260 | YES | YES |
| 297 | a | 3158.68 | 12.46511 | YES | YES |

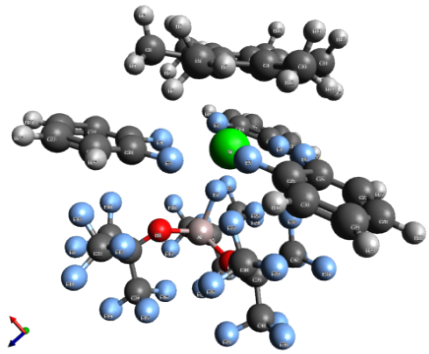
Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 ca | 1.76875 | 1.3150 | 1.617964 |
| 2 f | -0.74113 | -0.3250 | -0.849804 |
| 3 al | 1.95774 | 0.3391 | 2.550191 |
| 4 c | -0.04934 | 0.0572 | -0.050827 |
| 5 c | -0.07149 | 0.0435 | -0.067007 |
| 6 c | -0.09110 | 0.0309 | -0.083345 |
| 7 c | -0.07383 | 0.0555 | -0.069548 |
| 8 c | -0.07714 | 0.0464 | -0.067622 |
| 9 c | -0.06085 | 0.0453 | -0.063950 |
| 10 c | -0.65892 | -0.1894 | -0.042770 |
| 11 h | 0.25150 | 0.0579 | 0.072521 |
| 12 h | 0.24726 | 0.0503 | 0.048267 |
| 13 h | 0.24030 | 0.0469 | 0.058628 |
| 14 c | -0.65951 | -0.2031 | -0.050879 |
| 15 h | 0.24789 | 0.0664 | 0.068441 |
| 16 h | 0.25311 | 0.0502 | 0.057343 |
| 17 h | 0.23126 | 0.0374 | 0.036762 |
| 18 c | -0.65815 | -0.1862 | -0.048275 |
| 19 h | 0.23348 | 0.0452 | 0.039347 |

| | | | | |
|---|---|---|---|---|
| 20 | h | 0.25587 | 0.0546 | 0.059562 |
| 21 | h | 0.23333 | 0.0310 | 0.034890 |
| 22 | c | -0.65223 | -0.1892 | -0.043037 |
| 23 | h | 0.23486 | 0.0458 | 0.036202 |
| 24 | h | 0.24881 | 0.0454 | 0.053873 |
| 25 | h | 0.23466 | 0.0407 | 0.043452 |
| 26 | c | -0.65529 | -0.2041 | -0.048703 |
| 27 | h | 0.22997 | 0.0455 | 0.033663 |
| 28 | h | 0.25757 | 0.0552 | 0.061035 |
| 29 | h | 0.23434 | 0.0503 | 0.040274 |
| 30 | c | -0.66006 | -0.2023 | -0.052042 |
| 31 | h | 0.23236 | 0.0385 | 0.038608 |
| 32 | h | 0.25039 | 0.0476 | 0.055607 |
| 33 | h | 0.25340 | 0.0742 | 0.075872 |
| 34 | c | 0.33740 | 0.2132 | 0.448659 |
| 35 | c | 0.33093 | 0.2020 | 0.432928 |
| 36 | c | -0.26740 | -0.0135 | -0.005245 |
| 37 | h | 0.26019 | 0.0233 | 0.110071 |
| 38 | c | -0.20214 | 0.0206 | -0.015979 |
| 39 | h | 0.25127 | 0.0280 | 0.097364 |
| 40 | c | -0.20065 | 0.0200 | -0.015377 |
| 41 | h | 0.25207 | 0.0290 | 0.098428 |
| 42 | c | -0.25733 | -0.0169 | -0.003208 |
| 43 | h | 0.26483 | 0.0389 | 0.141115 |
| 44 | f | -0.35537 | -0.1674 | -0.620061 |
| 45 | f | -0.37185 | -0.2145 | -0.623541 |
| 46 | c | 0.33345 | 0.2058 | 0.429407 |
| 47 | c | 0.33570 | 0.2076 | 0.452588 |
| 48 | c | -0.25645 | -0.0097 | 0.002195 |
| 49 | h | 0.26729 | 0.0341 | 0.130307 |
| 50 | c | -0.20100 | 0.0168 | -0.016876 |
| 51 | h | 0.25213 | 0.0296 | 0.100428 |
| 52 | c | -0.20183 | 0.0197 | -0.014377 |
| 53 | h | 0.25136 | 0.0283 | 0.096848 |
| 54 | c | -0.26439 | -0.0133 | -0.002533 |
| 55 | h | 0.26013 | 0.0234 | 0.110815 |
| 56 | f | -0.37252 | -0.2182 | -0.621660 |
| 57 | f | -0.35641 | -0.1734 | -0.617932 |
| 58 | o | -1.00243 | -0.2812 | -1.296803 |
| 59 | c | 0.01681 | -0.0593 | 0.647655 |
| 60 | c | 1.10588 | 0.5320 | 1.657085 |
| 61 | f | -0.35465 | -0.1905 | -0.583633 |
| 62 | f | -0.32613 | -0.1513 | -0.575835 |
| 63 | f | -0.34416 | -0.1702 | -0.592013 |
| 64 | c | 1.10574 | 0.5333 | 1.671072 |
| 65 | f | -0.33022 | -0.1302 | -0.589225 |
| 66 | f | -0.32499 | -0.1504 | -0.574133 |
| 67 | f | -0.32333 | -0.1495 | -0.574150 |
| 68 | c | 1.10936 | 0.5311 | 1.676975 |
| 69 | f | -0.32855 | -0.1527 | -0.576360 |
| 70 | f | -0.33447 | -0.1646 | -0.575613 |
| 71 | f | -0.35394 | -0.1835 | -0.596166 |
| 72 | o | -0.96053 | -0.1873 | -1.342393 |
| 73 | c | 0.03310 | -0.0709 | 0.726689 |
| 74 | c | 1.10435 | 0.5268 | 1.654168 |

| | | | | |
|---|---|---|---|---|
| 75 | f | -0.33664 | -0.1658 | -0.578497 |
| 76 | f | -0.33606 | -0.1661 | -0.578898 |
| 77 | f | -0.35443 | -0.1817 | -0.589788 |
| 78 | c | 1.10848 | 0.5356 | 1.650442 |
| 79 | f | -0.34075 | -0.1678 | -0.585391 |
| 80 | f | -0.36283 | -0.1996 | -0.588777 |
| 81 | f | -0.33608 | -0.1643 | -0.579527 |
| 82 | c | 1.10556 | 0.5311 | 1.674132 |
| 83 | f | -0.34525 | -0.1821 | -0.580092 |
| 84 | f | -0.33909 | -0.1713 | -0.579300 |
| 85 | f | -0.33713 | -0.1578 | -0.581471 |
| 86 | o | -0.95954 | -0.1917 | -1.341619 |
| 87 | c | 0.03438 | -0.0626 | 0.723809 |
| 88 | c | 1.11050 | 0.5378 | 1.688011 |
| 89 | f | -0.34510 | -0.1816 | -0.579589 |
| 90 | f | -0.34433 | -0.1799 | -0.580080 |
| 91 | f | -0.33405 | -0.1614 | -0.578241 |
| 92 | c | 1.10764 | 0.5377 | 1.659635 |
| 93 | f | -0.35823 | -0.1924 | -0.593020 |
| 94 | f | -0.33555 | -0.1661 | -0.578963 |
| 95 | f | -0.34436 | -0.1780 | -0.581210 |
| 96 | c | 1.10030 | 0.5231 | 1.638822 |
| 97 | f | -0.36085 | -0.1967 | -0.590835 |
| 98 | f | -0.33145 | -0.1577 | -0.579027 |
| 99 | f | -0.33419 | -0.1522 | -0.586904 |

[Sr(HMB)oDFB$_3${f-al}]$^+$ 5$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 3.23188 | 0.18850 | -2.61633 |
| C | 3.40702 | -1.15901 | -2.18250 |
| C | 2.59557 | -2.20552 | -2.71271 |
| C | 1.60935 | -1.90079 | -3.69471 |
| C | 1.43642 | -0.55420 | -4.13410 |
| C | 2.23232 | 0.49688 | -3.58861 |
| C | 4.19005 | 1.23531 | -2.08444 |
| H | 5.23971 | 0.96550 | -2.33427 |
| H | 4.13363 | 1.32017 | -0.97760 |
| H | 4.00865 | 2.24275 | -2.49891 |
| C | 4.56804 | -1.50341 | -1.27276 |
| H | 4.38598 | -2.40706 | -0.66106 |
| H | 4.82906 | -0.68342 | -0.57779 |
| H | 5.47878 | -1.70685 | -1.88466 |
| C | 2.88601 | -3.62950 | -2.28439 |

| | | | |
|---|---|---|---|
| H | 2.20947 | -4.36837 | -2.74976 |
| H | 2.80284 | -3.75455 | -1.18301 |
| H | 3.92419 | -3.91811 | -2.56106 |
| C | 0.80759 | -2.98729 | -4.38124 |
| H | 1.28371 | -3.26622 | -5.35009 |
| H | -0.22363 | -2.66250 | -4.62251 |
| H | 0.72812 | -3.91461 | -3.78472 |
| C | 0.45393 | -0.28266 | -5.25627 |
| H | 0.65480 | -0.94751 | -6.12407 |
| H | 0.50046 | 0.75623 | -5.62857 |
| H | -0.59623 | -0.47510 | -4.94337 |
| C | 2.06812 | 1.90233 | -4.13532 |
| H | 2.52921 | 1.98679 | -5.14590 |
| H | 2.54218 | 2.67193 | -3.50061 |
| H | 1.00322 | 2.19007 | -4.24293 |
| C | -0.53500 | 2.89979 | -2.06626 |
| C | 0.68478 | 3.17037 | -1.44497 |
| C | 1.15967 | 4.47237 | -1.32646 |
| H | 2.12091 | 4.65868 | -0.82461 |
| C | 0.36796 | 5.51503 | -1.83979 |
| H | 0.71889 | 6.55395 | -1.74597 |
| C | -0.86900 | 5.24271 | -2.44915 |
| H | -1.48749 | 6.06783 | -2.83388 |
| C | -1.33472 | 3.92053 | -2.56884 |
| H | -2.30007 | 3.67878 | -3.03784 |
| F | -0.91054 | 1.58046 | -2.18730 |
| F | 1.40953 | 2.10693 | -0.97516 |
| C | 2.51723 | -2.04699 | 1.37150 |
| C | 2.96670 | -0.73461 | 1.51062 |
| C | 4.10320 | -0.43915 | 2.25583 |
| H | 4.42665 | 0.60623 | 2.36762 |
| C | 4.79807 | -1.50791 | 2.84991 |
| H | 5.69811 | -1.29800 | 3.44767 |
| C | 4.34938 | -2.83172 | 2.69773 |
| H | 4.89820 | -3.65743 | 3.17568 |
| C | 3.18892 | -3.11505 | 1.95517 |
| H | 2.80062 | -4.13768 | 1.83847 |
| F | 1.39226 | -2.25090 | 0.60320 |
| F | 2.27522 | 0.24309 | 0.84539 |
| C | -1.43234 | -3.38818 | -1.95976 |
| C | -2.10982 | -2.36413 | -2.62353 |
| C | -3.35298 | -2.57268 | -3.20975 |
| H | -3.87182 | -1.74013 | -3.70735 |
| C | -3.90770 | -3.86352 | -3.12962 |
| H | -4.89260 | -4.05483 | -3.58212 |
| C | -3.22057 | -4.90084 | -2.47499 |
| H | -3.66706 | -5.90523 | -2.41687 |
| C | -1.96822 | -4.66917 | -1.87662 |
| H | -1.41952 | -5.45867 | -1.34145 |
| F | -0.23413 | -3.07389 | -1.37590 |
| F | -1.49876 | -1.13177 | -2.66663 |
| Sr | 0.32927 | -0.37982 | -0.90352 |
| F | -0.55438 | 0.97472 | 0.72603 |
| Al | -1.34051 | 0.98646 | 2.31484 |
| O | -0.19325 | -0.05364 | 3.16888 |

| | | | |
|---|---|---|---|
| C | 0.02672 | -0.32010 | 4.49339 |
| C | 0.91239 | 0.81925 | 5.12591 |
| F | 1.48439 | 0.43318 | 6.28205 |
| F | 0.17274 | 1.91601 | 5.36481 |
| F | 1.89042 | 1.16473 | 4.26149 |
| C | 0.78585 | -1.69245 | 4.61011 |
| F | 0.63637 | -2.25671 | 5.81941 |
| F | 2.11251 | -1.52698 | 4.39848 |
| F | 0.33733 | -2.55657 | 3.67731 |
| C | -1.33609 | -0.43313 | 5.27120 |
| F | -1.19324 | -0.32544 | 6.59805 |
| F | -1.94117 | -1.60387 | 4.99406 |
| F | -2.16048 | 0.55643 | 4.84924 |
| O | -1.38259 | 2.62169 | 2.88111 |
| C | -2.04290 | 3.80519 | 2.76782 |
| C | -1.22141 | 4.87959 | 3.57473 |
| F | -1.40266 | 4.71666 | 4.89592 |
| F | 0.09031 | 4.74316 | 3.31575 |
| F | -1.58925 | 6.13563 | 3.24545 |
| C | -3.50098 | 3.69426 | 3.35404 |
| F | -3.48488 | 3.01970 | 4.51078 |
| F | -4.04987 | 4.90479 | 3.56640 |
| F | -4.29557 | 3.01836 | 2.49288 |
| C | -2.12025 | 4.23242 | 1.25806 |
| F | -0.90637 | 4.63869 | 0.82216 |
| F | -3.00023 | 5.21560 | 1.02119 |
| F | -2.47131 | 3.16546 | 0.49430 |
| O | -2.91273 | 0.26525 | 2.05208 |
| C | -3.64138 | -0.66461 | 1.40607 |
| C | -2.80859 | -1.97708 | 1.17649 |
| F | -2.54030 | -2.60432 | 2.31559 |
| F | -1.56551 | -1.64461 | 0.62479 |
| F | -3.37508 | -2.83748 | 0.31939 |
| C | -4.90260 | -1.02168 | 2.29328 |
| F | -4.52144 | -1.21633 | 3.55982 |
| F | -5.51213 | -2.14380 | 1.84874 |
| F | -5.79075 | -0.01694 | 2.26295 |
| C | -4.11926 | -0.09353 | 0.01884 |
| F | -3.04223 | 0.00133 | -0.83251 |
| F | -4.61473 | 1.13219 | 0.15261 |
| F | -5.02868 | -0.87569 | -0.59019 |

Vibrational analysis

| 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 | 6.67 | 0.03474 | YES | YES |
| 8 | a | 13.11 | 0.09867 | YES | YES |
| 9 | a | 15.02 | 0.86536 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 10 | a | 17.23 | 1.43987 | YES | YES |
| 11 | a | 20.52 | 0.47365 | YES | YES |
| 12 | a | 21.90 | 0.22622 | YES | YES |
| 13 | a | 22.91 | 0.21744 | YES | YES |
| 14 | a | 26.51 | 0.47708 | YES | YES |
| 15 | a | 27.40 | 0.14217 | YES | YES |
| 16 | a | 29.04 | 0.46756 | YES | YES |
| 17 | a | 31.86 | 0.73170 | YES | YES |
| 18 | a | 34.43 | 0.35990 | YES | YES |
| 19 | a | 35.41 | 0.27704 | YES | YES |
| 20 | a | 37.65 | 0.31128 | YES | YES |
| 21 | a | 39.58 | 1.05700 | YES | YES |
| 22 | a | 45.11 | 1.62281 | YES | YES |
| 23 | a | 47.44 | 1.52467 | YES | YES |
| 24 | a | 52.07 | 0.33321 | YES | YES |
| 25 | a | 55.85 | 1.63776 | YES | YES |
| 26 | a | 56.95 | 0.27693 | YES | YES |
| 27 | a | 58.41 | 0.48558 | YES | YES |
| 28 | a | 61.00 | 0.26376 | YES | YES |
| 29 | a | 61.84 | 0.03727 | YES | YES |
| 30 | a | 64.30 | 0.14284 | YES | YES |
| 31 | a | 66.22 | 0.20746 | YES | YES |
| 32 | a | 66.38 | 0.73952 | YES | YES |
| 33 | a | 70.33 | 0.47028 | YES | YES |
| 34 | a | 71.73 | 0.37116 | YES | YES |
| 35 | a | 73.29 | 0.88492 | YES | YES |
| 36 | a | 75.78 | 2.01476 | YES | YES |
| 37 | a | 78.82 | 0.24550 | YES | YES |
| 38 | a | 79.81 | 1.08432 | YES | YES |
| 39 | a | 81.30 | 0.62184 | YES | YES |
| 40 | a | 82.55 | 0.37778 | YES | YES |
| 41 | a | 85.13 | 1.99479 | YES | YES |
| 42 | a | 85.98 | 0.90116 | YES | YES |
| 43 | a | 87.71 | 0.58836 | YES | YES |
| 44 | a | 90.30 | 0.15930 | YES | YES |
| 45 | a | 90.62 | 0.91344 | YES | YES |
| 46 | a | 94.32 | 0.26246 | YES | YES |
| 47 | a | 94.59 | 6.69183 | YES | YES |
| 48 | a | 96.65 | 0.23549 | YES | YES |
| 49 | a | 97.77 | 1.92832 | YES | YES |
| 50 | a | 102.03 | 4.30832 | YES | YES |
| 51 | a | 106.11 | 3.05553 | YES | YES |
| 52 | a | 112.44 | 30.45705 | YES | YES |
| 53 | a | 127.52 | 0.29774 | YES | YES |
| 54 | a | 129.36 | 0.93579 | YES | YES |
| 55 | a | 138.40 | 10.01118 | YES | YES |
| 56 | a | 139.60 | 8.35255 | YES | YES |
| 57 | a | 150.42 | 2.82912 | YES | YES |
| 58 | a | 152.49 | 20.55437 | YES | YES |
| 59 | a | 154.51 | 0.97608 | YES | YES |
| 60 | a | 155.42 | 0.30809 | YES | YES |
| 61 | a | 157.19 | 0.26060 | YES | YES |
| 62 | a | 160.61 | 3.21196 | YES | YES |
| 63 | a | 161.99 | 3.17898 | YES | YES |
| 64 | a | 164.71 | 0.83992 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 65 | a | 165.82 | 0.71592 | YES | YES |
| 66 | a | 168.07 | 1.68171 | YES | YES |
| 67 | a | 172.59 | 0.07013 | YES | YES |
| 68 | a | 175.71 | 3.19140 | YES | YES |
| 69 | a | 182.43 | 2.52843 | YES | YES |
| 70 | a | 190.58 | 4.83947 | YES | YES |
| 71 | a | 193.24 | 5.40003 | YES | YES |
| 72 | a | 200.87 | 1.20692 | YES | YES |
| 73 | a | 201.67 | 0.92685 | YES | YES |
| 74 | a | 205.22 | 2.35381 | YES | YES |
| 75 | a | 208.83 | 1.09526 | YES | YES |
| 76 | a | 214.05 | 0.82602 | YES | YES |
| 77 | a | 229.85 | 10.04305 | YES | YES |
| 78 | a | 245.78 | 16.10522 | YES | YES |
| 79 | a | 263.22 | 3.19492 | YES | YES |
| 80 | a | 268.66 | 9.63079 | YES | YES |
| 81 | a | 276.90 | 1.61032 | YES | YES |
| 82 | a | 281.72 | 0.03298 | YES | YES |
| 83 | a | 282.45 | 2.93735 | YES | YES |
| 84 | a | 283.25 | 6.09176 | YES | YES |
| 85 | a | 286.51 | 0.14940 | YES | YES |
| 86 | a | 287.35 | 1.19725 | YES | YES |
| 87 | a | 290.81 | 0.07773 | YES | YES |
| 88 | a | 293.32 | 0.76885 | YES | YES |
| 89 | a | 296.21 | 0.77292 | YES | YES |
| 90 | a | 298.40 | 1.72606 | YES | YES |
| 91 | a | 304.22 | 5.60272 | YES | YES |
| 92 | a | 307.04 | 6.03489 | YES | YES |
| 93 | a | 307.44 | 6.03127 | YES | YES |
| 94 | a | 308.99 | 3.36393 | YES | YES |
| 95 | a | 309.16 | 2.68813 | YES | YES |
| 96 | a | 310.27 | 4.35365 | YES | YES |
| 97 | a | 313.58 | 1.01262 | YES | YES |
| 98 | a | 315.11 | 7.92775 | YES | YES |
| 99 | a | 320.12 | 1.90337 | YES | YES |
| 100 | a | 322.62 | 1.16995 | YES | YES |
| 101 | a | 325.45 | 3.22694 | YES | YES |
| 102 | a | 328.83 | 0.78742 | YES | YES |
| 103 | a | 330.37 | 0.47240 | YES | YES |
| 104 | a | 334.52 | 3.49635 | YES | YES |
| 105 | a | 343.84 | 0.12585 | YES | YES |
| 106 | a | 348.65 | 0.71135 | YES | YES |
| 107 | a | 358.40 | 2.23523 | YES | YES |
| 108 | a | 358.83 | 3.91132 | YES | YES |
| 109 | a | 360.37 | 2.02459 | YES | YES |
| 110 | a | 369.08 | 14.06632 | YES | YES |
| 111 | a | 379.65 | 0.66028 | YES | YES |
| 112 | a | 387.00 | 52.70123 | YES | YES |
| 113 | a | 401.74 | 0.01522 | YES | YES |
| 114 | a | 414.14 | 4.06943 | YES | YES |
| 115 | a | 415.18 | 0.02903 | YES | YES |
| 116 | a | 434.40 | 0.08509 | YES | YES |
| 117 | a | 437.17 | 0.17434 | YES | YES |
| 118 | a | 438.69 | 0.13123 | YES | YES |
| 119 | a | 440.32 | 2.73668 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 120 | a | 440.66 | 0.05512 | YES | YES |
| 121 | a | 441.65 | 1.36139 | YES | YES |
| 122 | a | 443.56 | 2.99641 | YES | YES |
| 123 | a | 446.24 | 0.19118 | YES | YES |
| 124 | a | 449.56 | 44.63614 | YES | YES |
| 125 | a | 451.86 | 0.10352 | YES | YES |
| 126 | a | 465.57 | 24.96508 | YES | YES |
| 127 | a | 508.58 | 5.66956 | YES | YES |
| 128 | a | 517.93 | 2.88155 | YES | YES |
| 129 | a | 518.71 | 2.21339 | YES | YES |
| 130 | a | 519.55 | 2.98318 | YES | YES |
| 131 | a | 519.68 | 4.69758 | YES | YES |
| 132 | a | 520.78 | 6.48738 | YES | YES |
| 133 | a | 521.36 | 1.16837 | YES | YES |
| 134 | a | 523.74 | 2.37177 | YES | YES |
| 135 | a | 525.82 | 0.67511 | YES | YES |
| 136 | a | 527.16 | 0.57376 | YES | YES |
| 137 | a | 537.14 | 0.59600 | YES | YES |
| 138 | a | 537.49 | 1.29116 | YES | YES |
| 139 | a | 537.74 | 1.40923 | YES | YES |
| 140 | a | 540.03 | 2.21831 | YES | YES |
| 141 | a | 541.32 | 3.97096 | YES | YES |
| 142 | a | 542.36 | 3.54236 | YES | YES |
| 143 | a | 550.02 | 0.67372 | YES | YES |
| 144 | a | 551.27 | 0.96824 | YES | YES |
| 145 | a | 552.77 | 2.78713 | YES | YES |
| 146 | a | 553.55 | 6.38179 | YES | YES |
| 147 | a | 554.91 | 1.11784 | YES | YES |
| 148 | a | 555.12 | 1.75737 | YES | YES |
| 149 | a | 555.27 | 0.29881 | YES | YES |
| 150 | a | 558.83 | 21.91362 | YES | YES |
| 151 | a | 559.68 | 24.28678 | YES | YES |
| 152 | a | 560.42 | 1.67184 | YES | YES |
| 153 | a | 560.97 | 1.76262 | YES | YES |
| 154 | a | 563.52 | 31.52126 | YES | YES |
| 155 | a | 575.43 | 0.01230 | YES | YES |
| 156 | a | 575.78 | 32.44596 | YES | YES |
| 157 | a | 579.71 | 0.21206 | YES | YES |
| 158 | a | 582.37 | 0.19540 | YES | YES |
| 159 | a | 640.42 | 188.40366 | YES | YES |
| 160 | a | 671.45 | 0.05744 | YES | YES |
| 161 | a | 672.88 | 0.06768 | YES | YES |
| 162 | a | 674.40 | 0.15279 | YES | YES |
| 163 | a | 699.89 | 23.07182 | YES | YES |
| 164 | a | 706.68 | 19.96077 | YES | YES |
| 165 | a | 707.56 | 15.30044 | YES | YES |
| 166 | a | 708.39 | 0.06519 | YES | YES |
| 167 | a | 709.33 | 15.14853 | YES | YES |
| 168 | a | 710.44 | 47.05203 | YES | YES |
| 169 | a | 710.78 | 75.18240 | YES | YES |
| 170 | a | 724.49 | 11.76431 | YES | YES |
| 171 | a | 734.83 | 1.41365 | YES | YES |
| 172 | a | 739.49 | 1.60078 | YES | YES |
| 173 | a | 743.34 | 25.16955 | YES | YES |
| 174 | a | 744.10 | 84.82083 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 175 | a | 746.34 | 114.44558 | YES | YES |
| 176 | a | 753.66 | 128.73226 | YES | YES |
| 177 | a | 754.77 | 122.03614 | YES | YES |
| 178 | a | 759.38 | 6.21044 | YES | YES |
| 179 | a | 788.25 | 1.31830 | YES | YES |
| 180 | a | 788.40 | 15.06429 | YES | YES |
| 181 | a | 796.74 | 3.90143 | YES | YES |
| 182 | a | 817.37 | 0.38604 | YES | YES |
| 183 | a | 819.99 | 11.45732 | YES | YES |
| 184 | a | 820.45 | 12.27321 | YES | YES |
| 185 | a | 833.89 | 1.09675 | YES | YES |
| 186 | a | 836.09 | 31.51843 | YES | YES |
| 187 | a | 836.44 | 3.39277 | YES | YES |
| 188 | a | 837.19 | 0.25171 | YES | YES |
| 189 | a | 864.45 | 29.80628 | YES | YES |
| 190 | a | 917.28 | 214.36326 | YES | YES |
| 191 | a | 925.59 | 3.98956 | YES | YES |
| 192 | a | 926.84 | 6.31241 | YES | YES |
| 193 | a | 927.90 | 3.82643 | YES | YES |
| 194 | a | 948.19 | 0.22506 | YES | YES |
| 195 | a | 950.16 | 47.76813 | YES | YES |
| 196 | a | 958.75 | 117.20000 | YES | YES |
| 197 | a | 958.83 | 0.56017 | YES | YES |
| 198 | a | 960.44 | 114.62215 | YES | YES |
| 199 | a | 966.81 | 227.63893 | YES | YES |
| 200 | a | 967.53 | 7.16162 | YES | YES |
| 201 | a | 968.76 | 235.76866 | YES | YES |
| 202 | a | 972.67 | 1.01966 | YES | YES |
| 203 | a | 972.82 | 0.21260 | YES | YES |
| 204 | a | 975.37 | 0.01665 | YES | YES |
| 205 | a | 979.27 | 10.33850 | YES | YES |
| 206 | a | 999.29 | 2.47219 | YES | YES |
| 207 | a | 1003.74 | 2.02931 | YES | YES |
| 208 | a | 1017.63 | 4.20302 | YES | YES |
| 209 | a | 1017.87 | 3.18086 | YES | YES |
| 210 | a | 1018.63 | 2.81439 | YES | YES |
| 211 | a | 1024.95 | 0.58546 | YES | YES |
| 212 | a | 1025.86 | 0.71527 | YES | YES |
| 213 | a | 1028.94 | 1.67202 | YES | YES |
| 214 | a | 1037.04 | 20.06380 | YES | YES |
| 215 | a | 1045.90 | 19.74599 | YES | YES |
| 216 | a | 1048.22 | 15.89461 | YES | YES |
| 217 | a | 1071.32 | 1.85756 | YES | YES |
| 218 | a | 1073.61 | 1.03329 | YES | YES |
| 219 | a | 1078.76 | 0.72810 | YES | YES |
| 220 | a | 1080.42 | 0.43467 | YES | YES |
| 221 | a | 1081.64 | 35.84693 | YES | YES |
| 222 | a | 1082.74 | 31.52030 | YES | YES |
| 223 | a | 1092.65 | 7.94319 | YES | YES |
| 224 | a | 1096.51 | 5.41071 | YES | YES |
| 225 | a | 1109.11 | 71.88798 | YES | YES |
| 226 | a | 1138.11 | 2.58451 | YES | YES |
| 227 | a | 1138.80 | 1.76146 | YES | YES |
| 228 | a | 1139.10 | 1.09430 | YES | YES |
| 229 | a | 1139.47 | 1.54271 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 230 | a | 1145.27 | 5.79926 | YES | YES |
| 231 | a | 1147.54 | 2.80745 | YES | YES |
| 232 | a | 1149.88 | 23.99013 | YES | YES |
| 233 | a | 1153.93 | 39.37067 | YES | YES |
| 234 | a | 1161.07 | 14.62949 | YES | YES |
| 235 | a | 1165.20 | 43.66206 | YES | YES |
| 236 | a | 1168.07 | 9.68261 | YES | YES |
| 237 | a | 1177.28 | 101.60907 | YES | YES |
| 238 | a | 1182.46 | 13.82420 | YES | YES |
| 239 | a | 1186.86 | 17.24454 | YES | YES |
| 240 | a | 1193.30 | 41.15820 | YES | YES |
| 241 | a | 1195.54 | 30.90161 | YES | YES |
| 242 | a | 1200.40 | 85.93301 | YES | YES |
| 243 | a | 1201.25 | 108.33273 | YES | YES |
| 244 | a | 1209.04 | 98.42468 | YES | YES |
| 245 | a | 1217.97 | 13.49533 | YES | YES |
| 246 | a | 1230.89 | 434.52086 | YES | YES |
| 247 | a | 1233.00 | 345.50035 | YES | YES |
| 248 | a | 1239.07 | 393.05910 | YES | YES |
| 249 | a | 1240.52 | 244.80164 | YES | YES |
| 250 | a | 1243.11 | 562.07069 | YES | YES |
| 251 | a | 1244.14 | 686.51650 | YES | YES |
| 252 | a | 1245.79 | 4.50767 | YES | YES |
| 253 | a | 1246.21 | 115.38109 | YES | YES |
| 254 | a | 1247.88 | 256.54832 | YES | YES |
| 255 | a | 1248.55 | 122.32605 | YES | YES |
| 256 | a | 1249.59 | 16.48999 | YES | YES |
| 257 | a | 1250.59 | 201.86110 | YES | YES |
| 258 | a | 1258.92 | 1129.46542 | YES | YES |
| 259 | a | 1264.76 | 133.83925 | YES | YES |
| 260 | a | 1269.67 | 219.94936 | YES | YES |
| 261 | a | 1278.43 | 465.06492 | YES | YES |
| 262 | a | 1302.00 | 1.95106 | YES | YES |
| 263 | a | 1307.91 | 1.38593 | YES | YES |
| 264 | a | 1308.55 | 12.82914 | YES | YES |
| 265 | a | 1336.86 | 157.25406 | YES | YES |
| 266 | a | 1356.51 | 0.91472 | YES | YES |
| 267 | a | 1357.45 | 146.72527 | YES | YES |
| 268 | a | 1358.39 | 1.13829 | YES | YES |
| 269 | a | 1363.06 | 1.34494 | YES | YES |
| 270 | a | 1364.27 | 2.95653 | YES | YES |
| 271 | a | 1369.86 | 0.25718 | YES | YES |
| 272 | a | 1373.95 | 5.64846 | YES | YES |
| 273 | a | 1382.91 | 3.87737 | YES | YES |
| 274 | a | 1383.47 | 2.87861 | YES | YES |
| 275 | a | 1384.69 | 2.86483 | YES | YES |
| 276 | a | 1389.64 | 8.27716 | YES | YES |
| 277 | a | 1393.45 | 1.26647 | YES | YES |
| 278 | a | 1411.43 | 2.31262 | YES | YES |
| 279 | a | 1414.79 | 11.91450 | YES | YES |
| 280 | a | 1416.58 | 1.60949 | YES | YES |
| 281 | a | 1420.99 | 0.60454 | YES | YES |
| 282 | a | 1423.96 | 17.55833 | YES | YES |
| 283 | a | 1430.16 | 17.78264 | YES | YES |
| 284 | a | 1440.16 | 36.44064 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 285 | a | 1445.35 | 4.67661 | YES | YES |
| 286 | a | 1449.15 | 11.32468 | YES | YES |
| 287 | a | 1452.48 | 5.82982 | YES | YES |
| 288 | a | 1459.34 | 4.27608 | YES | YES |
| 289 | a | 1459.73 | 9.23692 | YES | YES |
| 290 | a | 1460.40 | 4.35542 | YES | YES |
| 291 | a | 1462.07 | 33.21741 | YES | YES |
| 292 | a | 1467.70 | 25.75391 | YES | YES |
| 293 | a | 1495.69 | 347.11164 | YES | YES |
| 294 | a | 1496.06 | 341.40960 | YES | YES |
| 295 | a | 1499.54 | 10.43645 | YES | YES |
| 296 | a | 1555.14 | 0.55946 | YES | YES |
| 297 | a | 1560.52 | 0.16572 | YES | YES |
| 298 | a | 1611.47 | 0.21829 | YES | YES |
| 299 | a | 1613.45 | 0.49713 | YES | YES |
| 300 | a | 1613.76 | 0.29345 | YES | YES |
| 301 | a | 1639.36 | 18.90861 | YES | YES |
| 302 | a | 1639.90 | 15.89386 | YES | YES |
| 303 | a | 1641.59 | 11.30208 | YES | YES |
| 304 | a | 2941.29 | 6.32369 | YES | YES |
| 305 | a | 2948.19 | 7.93591 | YES | YES |
| 306 | a | 2954.87 | 4.65290 | YES | YES |
| 307 | a | 2956.11 | 11.71293 | YES | YES |
| 308 | a | 2957.40 | 9.71942 | YES | YES |
| 309 | a | 2958.10 | 5.39713 | YES | YES |
| 310 | a | 3020.61 | 5.81144 | YES | YES |
| 311 | a | 3021.73 | 6.96118 | YES | YES |
| 312 | a | 3022.88 | 6.30487 | YES | YES |
| 313 | a | 3037.06 | 5.90915 | YES | YES |
| 314 | a | 3038.30 | 12.29075 | YES | YES |
| 315 | a | 3045.23 | 7.97711 | YES | YES |
| 316 | a | 3082.96 | 4.18334 | YES | YES |
| 317 | a | 3086.49 | 3.11523 | YES | YES |
| 318 | a | 3087.71 | 7.10344 | YES | YES |
| 319 | a | 3093.67 | 11.94021 | YES | YES |
| 320 | a | 3095.82 | 16.34375 | YES | YES |
| 321 | a | 3098.27 | 5.09895 | YES | YES |
| 322 | a | 3123.54 | 0.68321 | YES | YES |
| 323 | a | 3123.89 | 0.66284 | YES | YES |
| 324 | a | 3124.41 | 0.69178 | YES | YES |
| 325 | a | 3133.15 | 2.74836 | YES | YES |
| 326 | a | 3133.59 | 3.00507 | YES | YES |
| 327 | a | 3133.70 | 1.90126 | YES | YES |
| 328 | a | 3139.50 | 1.20701 | YES | YES |
| 329 | a | 3140.04 | 1.60513 | YES | YES |
| 330 | a | 3140.57 | 1.77976 | YES | YES |
| 331 | a | 3144.34 | 0.52432 | YES | YES |
| 332 | a | 3144.94 | 1.15491 | YES | YES |
| 333 | a | 3145.29 | 1.21574 | YES | YES |

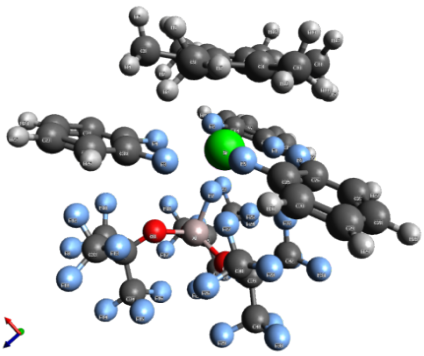
Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 c | -0.05345 | 0.0819 | -0.049199 |
| 2 c | -0.06217 | 0.0531 | -0.065430 |
| 3 c | -0.05609 | 0.0545 | -0.051810 |
| 4 c | -0.06112 | 0.0466 | -0.051782 |

| | | | | |
|---|---|---|---|---|
| 5 | c | -0.05288 | 0.0523 | -0.055702 |
| 6 | c | -0.06800 | 0.0575 | -0.058091 |
| 7 | c | -0.65150 | -0.1732 | -0.036533 |
| 8 | h | 0.24574 | 0.0398 | 0.047921 |
| 9 | h | 0.23516 | 0.0590 | 0.036768 |
| 10 | h | 0.23183 | 0.0402 | 0.039284 |
| 11 | c | -0.66320 | -0.1820 | -0.054848 |
| 12 | h | 0.23475 | 0.0406 | 0.036139 |
| 13 | h | 0.23489 | 0.0428 | 0.035337 |
| 14 | h | 0.25240 | 0.0481 | 0.052366 |
| 15 | c | -0.64967 | -0.1947 | -0.039341 |
| 16 | h | 0.23237 | 0.0346 | 0.039326 |
| 17 | h | 0.22987 | 0.0441 | 0.031021 |
| 18 | h | 0.24663 | 0.0407 | 0.049837 |
| 19 | c | -0.65816 | -0.1985 | -0.045608 |
| 20 | h | 0.25301 | 0.0477 | 0.054920 |
| 21 | h | 0.23156 | 0.0347 | 0.031698 |
| 22 | h | 0.23033 | 0.0396 | 0.034925 |
| 23 | c | -0.65682 | -0.1998 | -0.049053 |
| 24 | h | 0.24507 | 0.0393 | 0.047922 |
| 25 | h | 0.23820 | 0.0376 | 0.045250 |
| 26 | h | 0.23506 | 0.0464 | 0.038189 |
| 27 | c | -0.65825 | -0.1956 | -0.042766 |
| 28 | h | 0.25261 | 0.0471 | 0.053828 |
| 29 | h | 0.23107 | 0.0469 | 0.036309 |
| 30 | h | 0.23257 | 0.0483 | 0.031523 |
| 31 | c | 0.33649 | 0.2192 | 0.440499 |
| 32 | c | 0.34061 | 0.2227 | 0.458537 |
| 33 | c | -0.26006 | -0.0103 | 0.006949 |
| 34 | h | 0.25850 | 0.0197 | 0.106348 |
| 35 | c | -0.19859 | 0.0237 | -0.003926 |
| 36 | h | 0.24952 | 0.0228 | 0.093556 |
| 37 | c | -0.20458 | 0.0174 | -0.010855 |
| 38 | h | 0.24950 | 0.0233 | 0.093075 |
| 39 | c | -0.26221 | -0.0109 | 0.001293 |
| 40 | h | 0.25952 | 0.0199 | 0.109843 |
| 41 | f | -0.37265 | -0.2109 | -0.617630 |
| 42 | f | -0.36073 | -0.1867 | -0.625334 |
| 43 | c | 0.33390 | 0.2118 | 0.437359 |
| 44 | c | 0.34327 | 0.2283 | 0.463777 |
| 45 | c | -0.25906 | -0.0045 | 0.008511 |
| 46 | h | 0.26183 | 0.0227 | 0.113353 |
| 47 | c | -0.19996 | 0.0221 | -0.007723 |
| 48 | h | 0.24998 | 0.0233 | 0.093817 |
| 49 | c | -0.20191 | 0.0209 | -0.007714 |
| 50 | h | 0.24942 | 0.0227 | 0.092357 |
| 51 | c | -0.26713 | -0.0105 | 0.005190 |
| 52 | h | 0.25944 | 0.0193 | 0.106717 |
| 53 | f | -0.37347 | -0.2087 | -0.619504 |
| 54 | f | -0.35803 | -0.1786 | -0.615669 |
| 55 | c | 0.33327 | 0.2092 | 0.455660 |
| 56 | c | 0.32663 | 0.2060 | 0.431876 |
| 57 | c | -0.25931 | -0.0082 | 0.003177 |
| 58 | h | 0.26124 | 0.0231 | 0.113983 |
| 59 | c | -0.20102 | 0.0190 | -0.011552 |

| | | | | |
|---|---|---|---|---|
| 60 | h | 0.25101 | 0.0255 | 0.096602 |
| 61 | c | -0.19987 | 0.0206 | -0.011411 |
| 62 | h | 0.25066 | 0.0250 | 0.095590 |
| 63 | c | -0.26130 | -0.0134 | 0.000861 |
| 64 | h | 0.25924 | 0.0210 | 0.109288 |
| 65 | f | -0.35711 | -0.2008 | -0.621561 |
| 66 | f | -0.37008 | -0.2168 | -0.622712 |
| 67 | sr | 1.78466 | 1.3735 | 1.722213 |
| 68 | f | -0.75621 | -0.4189 | -0.854902 |
| 69 | al | 1.97231 | 0.4103 | 2.549710 |
| 70 | o | -0.94369 | -0.2355 | -1.309403 |
| 71 | c | 0.02446 | -0.0641 | 0.708254 |
| 72 | c | 1.10382 | 0.5316 | 1.661816 |
| 73 | f | -0.34447 | -0.1811 | -0.581491 |
| 74 | f | -0.33628 | -0.1660 | -0.580358 |
| 75 | f | -0.35028 | -0.1829 | -0.589636 |
| 76 | c | 1.10819 | 0.5340 | 1.650708 |
| 77 | f | -0.34018 | -0.1729 | -0.581153 |
| 78 | f | -0.35774 | -0.1947 | -0.607783 |
| 79 | f | -0.34756 | -0.1700 | -0.590177 |
| 80 | c | 1.09913 | 0.5262 | 1.654210 |
| 81 | f | -0.33394 | -0.1655 | -0.579914 |
| 82 | f | -0.34256 | -0.1787 | -0.580612 |
| 83 | f | -0.33258 | -0.1442 | -0.587311 |
| 84 | o | -0.94928 | -0.2090 | -1.328616 |
| 85 | c | 0.03116 | -0.0719 | 0.729000 |
| 86 | c | 1.11173 | 0.5408 | 1.677894 |
| 87 | f | -0.34099 | -0.1767 | -0.580422 |
| 88 | f | -0.34416 | -0.1776 | -0.583570 |
| 89 | f | -0.35074 | -0.1909 | -0.583614 |
| 90 | c | 1.10295 | 0.5297 | 1.667885 |
| 91 | f | -0.33471 | -0.1641 | -0.580621 |
| 92 | f | -0.34404 | -0.1810 | -0.581013 |
| 93 | f | -0.34871 | -0.1884 | -0.583148 |
| 94 | c | 1.09872 | 0.5251 | 1.626915 |
| 95 | f | -0.35390 | -0.1840 | -0.604631 |
| 96 | f | -0.33746 | -0.1677 | -0.582952 |
| 97 | f | -0.34757 | -0.1488 | -0.596063 |
| 98 | o | -0.93784 | -0.2438 | -1.325049 |
| 99 | c | 0.03848 | -0.0707 | 0.776800 |
| 100 | c | 1.09939 | 0.5307 | 1.597786 |
| 101 | f | -0.31468 | -0.1234 | -0.576940 |
| 102 | f | -0.41014 | -0.2076 | -0.611539 |
| 103 | f | -0.33380 | -0.1539 | -0.595854 |
| 104 | c | 1.11288 | 0.5376 | 1.690297 |
| 105 | f | -0.33268 | -0.1610 | -0.577810 |
| 106 | f | -0.35278 | -0.1959 | -0.582040 |
| 107 | f | -0.33725 | -0.1731 | -0.577686 |
| 108 | c | 1.10160 | 0.5243 | 1.635620 |
| 109 | f | -0.38011 | -0.1979 | -0.597603 |
| 110 | f | -0.31949 | -0.1354 | -0.577092 |
| 111 | f | -0.34242 | -0.1746 | -0.585136 |

[Ba(HMB)oDFB$_3${*f-al*}]$^+$ **4**$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| Ba | -0.1446259 | -0.2829654 | -0.8479521 |
| Al | -0.3072122 | 0.4617063 | 2.6490765 |
| F | -0.2901718 | 1.3268284 | 1.1296704 |
| C | 3.6524589 | -0.0602381 | -0.4180623 |
| C | 3.5519852 | -1.0221502 | -1.4249013 |
| C | 4.6762756 | -1.5611293 | -2.0418469 |
| H | 4.5550039 | -2.3231933 | -2.8266439 |
| C | 5.9371936 | -1.0957985 | -1.6254189 |
| H | 6.8453303 | -1.5042633 | -2.0945484 |
| C | 6.0425363 | -0.1169548 | -0.6207194 |
| H | 7.0342788 | 0.2405922 | -0.3040640 |
| C | 4.8949192 | 0.4125097 | -0.0023013 |
| H | 4.9523384 | 1.1664628 | 0.7940627 |
| F | 2.4857149 | 0.3975894 | 0.1248370 |
| F | 2.2882231 | -1.3987533 | -1.8021027 |
| C | 1.7616527 | -3.3997821 | -4.0630052 |
| C | 0.9130153 | -3.5462543 | -2.9570416 |
| C | 1.0110749 | -4.6431887 | -2.1034031 |
| H | 0.3317025 | -4.7261503 | -1.2437252 |
| C | 1.9902292 | -5.6173322 | -2.3683129 |
| H | 2.0779327 | -6.4897349 | -1.7028851 |
| C | 2.8470022 | -5.4797563 | -3.4734286 |
| H | 3.6096458 | -6.2462580 | -3.6805470 |
| C | 2.7353231 | -4.3674733 | -4.3265995 |
| H | 3.3877079 | -4.2383172 | -5.2041180 |
| F | 1.6420337 | -2.3103658 | -4.8461363 |
| F | -0.0072972 | -2.5572821 | -2.7090927 |
| C | -3.8148614 | -1.0278578 | -1.7083558 |
| C | -3.9281068 | -0.0914132 | -0.6777732 |
| C | -5.1709668 | 0.3362872 | -0.2191241 |
| H | -5.2264218 | 1.0663992 | 0.6002194 |
| C | -6.3185796 | -0.2039094 | -0.8277721 |
| H | -7.3124926 | 0.1170701 | -0.4803114 |
| C | -6.2066547 | -1.1470601 | -1.8650343 |
| H | -7.1125915 | -1.5636220 | -2.3313740 |
| C | -4.9429917 | -1.5694960 | -2.3184153 |
| H | -4.8268606 | -2.3042702 | -3.1293557 |
| F | -2.5512135 | -1.3806287 | -2.1073079 |
| F | -2.7688808 | 0.3888330 | -0.1378567 |
| O | -1.5014784 | 1.0112646 | 3.7624733 |
| C | -2.7061288 | 1.6060763 | 3.9656706 |
| C | -2.8831132 | 2.8472928 | 3.0143405 |
| F | -3.1849303 | 2.4247049 | 1.7501115 |

| | | | |
|---|---|---|---|
| F | -3.8608213 | 3.6728952 | 3.4093376 |
| F | -1.7368921 | 3.5395070 | 2.9284834 |
| C | -2.7650160 | 2.0829458 | 5.4665136 |
| F | -2.2818880 | 1.1279307 | 6.2688183 |
| F | -2.0165312 | 3.1904060 | 5.6281155 |
| F | -4.0293459 | 2.3656689 | 5.8389579 |
| C | -3.8564830 | 0.5672726 | 3.6904355 |
| F | -3.9709729 | -0.3089106 | 4.6972321 |
| F | -5.0527726 | 1.1600306 | 3.4986182 |
| F | -3.5631945 | -0.1380902 | 2.5691853 |
| O | 1.3161616 | 0.3212012 | 3.2525982 |
| C | 2.2454959 | 1.0175486 | 3.9659836 |
| C | 2.5039734 | 2.4158521 | 3.2934628 |
| F | 1.3230882 | 2.9748349 | 2.9455691 |
| F | 3.1628241 | 3.2690164 | 4.0848484 |
| F | 3.2173495 | 2.2744838 | 2.1436026 |
| C | 3.5687376 | 0.1683186 | 3.9673872 |
| F | 3.4727603 | -0.8632174 | 4.8210155 |
| F | 3.7891674 | -0.3443397 | 2.7360434 |
| F | 4.6410841 | 0.9090057 | 4.3058722 |
| C | 1.7605043 | 1.2386078 | 5.4513426 |
| F | 1.1994456 | 0.1154645 | 5.9201001 |
| F | 2.7757295 | 1.5879485 | 6.2611277 |
| F | 0.8300705 | 2.2161079 | 5.4915361 |
| O | -0.6463906 | -1.1036970 | 1.7775507 |
| C | -0.6128800 | -2.4372666 | 2.0993497 |
| C | -1.0019503 | -2.7029857 | 3.6024382 |
| F | -2.3308734 | -2.6366725 | 3.7724967 |
| F | -0.5778141 | -3.9119107 | 4.0037727 |
| F | -0.4328504 | -1.7593843 | 4.3741484 |
| C | 0.8420568 | -2.9886060 | 1.8284247 |
| F | 1.3194500 | -2.4035584 | 0.6722117 |
| F | 1.6811201 | -2.6603922 | 2.8059490 |
| F | 0.8800500 | -4.3139654 | 1.6351894 |
| C | -1.6386201 | -3.1541794 | 1.1560856 |
| F | -1.1754302 | -3.0266796 | -0.1459598 |
| F | -1.7869950 | -4.4529957 | 1.4057008 |
| F | -2.8302286 | -2.5541971 | 1.1810536 |
| C | -1.3027617 | 2.5649828 | -2.1458086 |
| C | -1.3260908 | 1.6646842 | -3.2504719 |
| C | -0.1016662 | 1.1885955 | -3.8082446 |
| C | 1.1499277 | 1.5669342 | -3.2366269 |
| C | 1.1712436 | 2.4711990 | -2.1315506 |
| C | -0.0531323 | 2.9497583 | -1.5783643 |
| C | -2.5682594 | 3.1911745 | -1.6004644 |
| H | -2.5209060 | 4.2981121 | -1.7000563 |
| H | -2.7079684 | 2.9746622 | -0.5212257 |
| H | -3.4787491 | 2.8581934 | -2.1312400 |
| C | -2.6279963 | 1.2532474 | -3.9074971 |
| H | -2.8666303 | 1.9208427 | -4.7679614 |
| H | -3.4900846 | 1.2998348 | -3.2156042 |
| H | -2.5821140 | 0.2206382 | -4.3049355 |
| C | -0.1615256 | 0.3393496 | -5.0625847 |
| H | -0.8433266 | 0.7974061 | -5.8103355 |
| H | -0.5435968 | -0.6872126 | -4.8643222 |

| | | | |
|---|---|---|---|
| H | 0.8240649 | 0.2273987 | -5.5481545 |
| C | 2.4352399 | 1.0472646 | -3.8519537 |
| H | 2.3437018 | -0.0102442 | -4.1681190 |
| H | 3.2917796 | 1.1051129 | -3.1548215 |
| H | 2.7135512 | 1.6375224 | -4.7552386 |
| C | 2.4629253 | 3.0203443 | -1.5630050 |
| H | 3.3650664 | 2.6146662 | -2.0555059 |
| H | 2.5556217 | 2.8258735 | -0.4740904 |
| H | 2.4922567 | 4.1257243 | -1.6872458 |
| C | -0.0138887 | 3.9334278 | -0.4320635 |
| H | 0.1422952 | 4.9701448 | -0.8131137 |
| H | 0.8087810 | 3.7166048 | 0.2754954 |
| H | -0.9468756 | 3.9317412 | 0.1595876 |

Vibrational analysis

| 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 | 7.98 | 0.16081 | YES | YES |
| 8 | a | 13.70 | 0.23451 | YES | YES |
| 9 | a | 17.57 | 0.52876 | YES | YES |
| 10 | a | 19.72 | 0.59733 | YES | YES |
| 11 | a | 24.05 | 0.35150 | YES | YES |
| 12 | a | 24.53 | 0.20212 | YES | YES |
| 13 | a | 25.91 | 0.55458 | YES | YES |
| 14 | a | 27.28 | 0.01394 | YES | YES |
| 15 | a | 29.08 | 0.40142 | YES | YES |
| 16 | a | 30.10 | 0.11051 | YES | YES |
| 17 | a | 33.35 | 0.37580 | YES | YES |
| 18 | a | 35.18 | 0.09275 | YES | YES |
| 19 | a | 38.43 | 1.18254 | YES | YES |
| 20 | a | 38.54 | 0.09482 | YES | YES |
| 21 | a | 39.79 | 0.64181 | YES | YES |
| 22 | a | 40.25 | 0.77619 | YES | YES |
| 23 | a | 44.39 | 0.10748 | YES | YES |
| 24 | a | 46.24 | 0.52972 | YES | YES |
| 25 | a | 46.93 | 1.24565 | YES | YES |
| 26 | a | 48.78 | 0.38575 | YES | YES |
| 27 | a | 52.46 | 0.60795 | YES | YES |
| 28 | a | 55.29 | 0.20487 | YES | YES |
| 29 | a | 58.81 | 0.22981 | YES | YES |
| 30 | a | 59.83 | 0.53268 | YES | YES |
| 31 | a | 62.27 | 0.16538 | YES | YES |
| 32 | a | 62.89 | 0.15862 | YES | YES |
| 33 | a | 65.67 | 0.61911 | YES | YES |
| 34 | a | 68.71 | 0.14413 | YES | YES |
| 35 | a | 70.61 | 1.56108 | YES | YES |
| 36 | a | 72.60 | 0.07665 | YES | YES |
| 37 | a | 74.78 | 0.59302 | YES | YES |
| 38 | a | 76.48 | 0.67323 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 39 | a | 77.70 | 0.43170 | YES | YES |
| 40 | a | 78.21 | 2.12683 | YES | YES |
| 41 | a | 82.56 | 0.47750 | YES | YES |
| 42 | a | 83.14 | 0.54543 | YES | YES |
| 43 | a | 85.10 | 0.50645 | YES | YES |
| 44 | a | 87.00 | 0.68725 | YES | YES |
| 45 | a | 87.22 | 0.32983 | YES | YES |
| 46 | a | 88.46 | 1.59340 | YES | YES |
| 47 | a | 91.12 | 3.44184 | YES | YES |
| 48 | a | 95.41 | 1.72715 | YES | YES |
| 49 | a | 97.22 | 0.99066 | YES | YES |
| 50 | a | 99.66 | 6.25103 | YES | YES |
| 51 | a | 101.85 | 2.30776 | YES | YES |
| 52 | a | 103.25 | 11.39594 | YES | YES |
| 53 | a | 106.46 | 1.42224 | YES | YES |
| 54 | a | 109.86 | 10.15685 | YES | YES |
| 55 | a | 122.28 | 0.92798 | YES | YES |
| 56 | a | 123.94 | 14.02748 | YES | YES |
| 57 | a | 129.27 | 2.99714 | YES | YES |
| 58 | a | 140.17 | 2.44260 | YES | YES |
| 59 | a | 144.61 | 1.45180 | YES | YES |
| 60 | a | 154.34 | 0.49489 | YES | YES |
| 61 | a | 157.92 | 0.07215 | YES | YES |
| 62 | a | 161.53 | 1.09687 | YES | YES |
| 63 | a | 162.46 | 2.09094 | YES | YES |
| 64 | a | 162.62 | 2.18386 | YES | YES |
| 65 | a | 171.00 | 0.39906 | YES | YES |
| 66 | a | 172.09 | 1.58318 | YES | YES |
| 67 | a | 172.83 | 0.53493 | YES | YES |
| 68 | a | 177.39 | 2.24539 | YES | YES |
| 69 | a | 185.86 | 2.20245 | YES | YES |
| 70 | a | 188.46 | 0.33928 | YES | YES |
| 71 | a | 195.67 | 10.70344 | YES | YES |
| 72 | a | 196.24 | 2.04689 | YES | YES |
| 73 | a | 197.04 | 0.71623 | YES | YES |
| 74 | a | 199.43 | 0.80991 | YES | YES |
| 75 | a | 206.50 | 0.55286 | YES | YES |
| 76 | a | 213.78 | 4.32133 | YES | YES |
| 77 | a | 239.22 | 19.06585 | YES | YES |
| 78 | a | 246.59 | 2.80343 | YES | YES |
| 79 | a | 269.67 | 1.69418 | YES | YES |
| 80 | a | 274.75 | 4.99867 | YES | YES |
| 81 | a | 275.61 | 3.03319 | YES | YES |
| 82 | a | 278.73 | 7.18770 | YES | YES |
| 83 | a | 281.78 | 0.65413 | YES | YES |
| 84 | a | 284.45 | 0.53485 | YES | YES |
| 85 | a | 285.60 | 2.02906 | YES | YES |
| 86 | a | 285.75 | 0.40117 | YES | YES |
| 87 | a | 287.70 | 2.79136 | YES | YES |
| 88 | a | 289.81 | 0.23762 | YES | YES |
| 89 | a | 290.18 | 0.52389 | YES | YES |
| 90 | a | 294.34 | 0.44293 | YES | YES |
| 91 | a | 295.37 | 2.79229 | YES | YES |
| 92 | a | 297.01 | 5.23358 | YES | YES |
| 93 | a | 304.62 | 6.19552 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 94 | a | 307.69 | 6.77923 | YES | YES |
| 95 | a | 308.95 | 4.96981 | YES | YES |
| 96 | a | 312.85 | 3.74123 | YES | YES |
| 97 | a | 315.56 | 2.50225 | YES | YES |
| 98 | a | 319.40 | 2.48630 | YES | YES |
| 99 | a | 320.93 | 2.36961 | YES | YES |
| 100 | a | 321.79 | 0.79280 | YES | YES |
| 101 | a | 325.93 | 2.82203 | YES | YES |
| 102 | a | 327.92 | 1.86727 | YES | YES |
| 103 | a | 329.90 | 0.20281 | YES | YES |
| 104 | a | 332.53 | 0.36913 | YES | YES |
| 105 | a | 349.97 | 0.60952 | YES | YES |
| 106 | a | 350.72 | 0.32443 | YES | YES |
| 107 | a | 360.21 | 6.37601 | YES | YES |
| 108 | a | 362.37 | 5.22603 | YES | YES |
| 109 | a | 364.81 | 0.72206 | YES | YES |
| 110 | a | 370.94 | 32.72850 | YES | YES |
| 111 | a | 379.00 | 1.80196 | YES | YES |
| 112 | a | 388.97 | 51.87348 | YES | YES |
| 113 | a | 403.35 | 0.05012 | YES | YES |
| 114 | a | 413.89 | 0.68765 | YES | YES |
| 115 | a | 418.29 | 0.17819 | YES | YES |
| 116 | a | 431.78 | 0.22863 | YES | YES |
| 117 | a | 436.27 | 0.05847 | YES | YES |
| 118 | a | 437.24 | 0.02337 | YES | YES |
| 119 | a | 439.90 | 0.11113 | YES | YES |
| 120 | a | 445.06 | 0.08564 | YES | YES |
| 121 | a | 445.85 | 1.96044 | YES | YES |
| 122 | a | 446.90 | 1.87413 | YES | YES |
| 123 | a | 452.47 | 0.65975 | YES | YES |
| 124 | a | 453.11 | 2.26107 | YES | YES |
| 125 | a | 455.34 | 45.69043 | YES | YES |
| 126 | a | 469.42 | 37.62080 | YES | YES |
| 127 | a | 513.02 | 6.96915 | YES | YES |
| 128 | a | 516.11 | 3.40105 | YES | YES |
| 129 | a | 518.35 | 0.42936 | YES | YES |
| 130 | a | 519.02 | 6.35386 | YES | YES |
| 131 | a | 520.51 | 3.04234 | YES | YES |
| 132 | a | 520.96 | 3.13994 | YES | YES |
| 133 | a | 521.58 | 3.12666 | YES | YES |
| 134 | a | 524.03 | 0.27207 | YES | YES |
| 135 | a | 525.01 | 2.24089 | YES | YES |
| 136 | a | 527.65 | 1.10328 | YES | YES |
| 137 | a | 535.74 | 5.63817 | YES | YES |
| 138 | a | 539.88 | 4.32423 | YES | YES |
| 139 | a | 540.54 | 0.51821 | YES | YES |
| 140 | a | 541.30 | 0.02484 | YES | YES |
| 141 | a | 542.10 | 2.73616 | YES | YES |
| 142 | a | 543.66 | 11.86969 | YES | YES |
| 143 | a | 546.84 | 0.12549 | YES | YES |
| 144 | a | 550.68 | 1.07656 | YES | YES |
| 145 | a | 553.43 | 1.02997 | YES | YES |
| 146 | a | 553.96 | 0.75004 | YES | YES |
| 147 | a | 554.08 | 0.88847 | YES | YES |
| 148 | a | 554.76 | 1.07523 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 149 | a | 555.40 | 0.44382 | YES | YES |
| 150 | a | 559.94 | 29.21003 | YES | YES |
| 151 | a | 560.41 | 10.25634 | YES | YES |
| 152 | a | 562.35 | 19.19537 | YES | YES |
| 153 | a | 562.93 | 7.72190 | YES | YES |
| 154 | a | 566.81 | 0.08811 | YES | YES |
| 155 | a | 570.28 | 24.22465 | YES | YES |
| 156 | a | 571.01 | 2.42628 | YES | YES |
| 157 | a | 577.00 | 0.45893 | YES | YES |
| 158 | a | 582.96 | 0.63333 | YES | YES |
| 159 | a | 667.40 | 112.36785 | YES | YES |
| 160 | a | 675.83 | 0.10346 | YES | YES |
| 161 | a | 678.13 | 0.27494 | YES | YES |
| 162 | a | 679.33 | 0.14609 | YES | YES |
| 163 | a | 698.46 | 0.04248 | YES | YES |
| 164 | a | 702.33 | 23.72319 | YES | YES |
| 165 | a | 706.25 | 19.91263 | YES | YES |
| 166 | a | 707.31 | 27.59576 | YES | YES |
| 167 | a | 709.39 | 30.18237 | YES | YES |
| 168 | a | 710.00 | 12.37207 | YES | YES |
| 169 | a | 710.57 | 62.86415 | YES | YES |
| 170 | a | 721.11 | 46.69657 | YES | YES |
| 171 | a | 737.91 | 8.74651 | YES | YES |
| 172 | a | 739.70 | 2.29673 | YES | YES |
| 173 | a | 748.39 | 55.76971 | YES | YES |
| 174 | a | 749.56 | 51.43576 | YES | YES |
| 175 | a | 749.75 | 76.97152 | YES | YES |
| 176 | a | 754.03 | 69.96373 | YES | YES |
| 177 | a | 758.14 | 138.24838 | YES | YES |
| 178 | a | 760.66 | 27.24561 | YES | YES |
| 179 | a | 776.05 | 13.38567 | YES | YES |
| 180 | a | 793.41 | 0.33061 | YES | YES |
| 181 | a | 800.81 | 2.86633 | YES | YES |
| 182 | a | 822.54 | 2.52288 | YES | YES |
| 183 | a | 822.73 | 26.27104 | YES | YES |
| 184 | a | 827.75 | 18.53600 | YES | YES |
| 185 | a | 832.56 | 38.45613 | YES | YES |
| 186 | a | 838.08 | 0.96972 | YES | YES |
| 187 | a | 844.03 | 0.39351 | YES | YES |
| 188 | a | 845.67 | 0.94576 | YES | YES |
| 189 | a | 878.33 | 28.23883 | YES | YES |
| 190 | a | 924.91 | 8.64627 | YES | YES |
| 191 | a | 932.61 | 2.12208 | YES | YES |
| 192 | a | 933.98 | 3.54249 | YES | YES |
| 193 | a | 943.64 | 111.30273 | YES | YES |
| 194 | a | 952.66 | 46.97699 | YES | YES |
| 195 | a | 954.86 | 64.80556 | YES | YES |
| 196 | a | 955.62 | 0.69615 | YES | YES |
| 197 | a | 959.86 | 211.48661 | YES | YES |
| 198 | a | 961.36 | 413.67021 | YES | YES |
| 199 | a | 964.40 | 1.94523 | YES | YES |
| 200 | a | 967.10 | 176.16813 | YES | YES |
| 201 | a | 969.63 | 0.36357 | YES | YES |
| 202 | a | 975.49 | 3.58434 | YES | YES |
| 203 | a | 976.85 | 0.91266 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 204 | a | 977.02 | 1.26137 | YES | YES |
| 205 | a | 982.40 | 12.69309 | YES | YES |
| 206 | a | 1003.32 | 3.48134 | YES | YES |
| 207 | a | 1007.23 | 0.84616 | YES | YES |
| 208 | a | 1019.65 | 14.66506 | YES | YES |
| 209 | a | 1019.76 | 3.15066 | YES | YES |
| 210 | a | 1023.32 | 6.82037 | YES | YES |
| 211 | a | 1027.93 | 2.25712 | YES | YES |
| 212 | a | 1028.72 | 2.41544 | YES | YES |
| 213 | a | 1032.71 | 1.39208 | YES | YES |
| 214 | a | 1051.17 | 11.19762 | YES | YES |
| 215 | a | 1053.51 | 17.01179 | YES | YES |
| 216 | a | 1053.84 | 14.38381 | YES | YES |
| 217 | a | 1074.50 | 0.04284 | YES | YES |
| 218 | a | 1075.18 | 0.48762 | YES | YES |
| 219 | a | 1081.51 | 10.82801 | YES | YES |
| 220 | a | 1083.52 | 20.53434 | YES | YES |
| 221 | a | 1084.62 | 9.13006 | YES | YES |
| 222 | a | 1087.50 | 6.14450 | YES | YES |
| 223 | a | 1088.31 | 18.97816 | YES | YES |
| 224 | a | 1090.53 | 15.75031 | YES | YES |
| 225 | a | 1112.75 | 117.62575 | YES | YES |
| 226 | a | 1136.16 | 29.10389 | YES | YES |
| 227 | a | 1137.41 | 2.39221 | YES | YES |
| 228 | a | 1138.69 | 0.92705 | YES | YES |
| 229 | a | 1139.73 | 8.42759 | YES | YES |
| 230 | a | 1147.49 | 101.55791 | YES | YES |
| 231 | a | 1153.73 | 19.41109 | YES | YES |
| 232 | a | 1154.63 | 8.00661 | YES | YES |
| 233 | a | 1166.65 | 27.45516 | YES | YES |
| 234 | a | 1168.19 | 14.49273 | YES | YES |
| 235 | a | 1171.77 | 27.61013 | YES | YES |
| 236 | a | 1175.54 | 8.90697 | YES | YES |
| 237 | a | 1180.11 | 25.75455 | YES | YES |
| 238 | a | 1185.08 | 124.88723 | YES | YES |
| 239 | a | 1188.63 | 37.03798 | YES | YES |
| 240 | a | 1191.04 | 46.79252 | YES | YES |
| 241 | a | 1196.65 | 34.77675 | YES | YES |
| 242 | a | 1202.67 | 38.43262 | YES | YES |
| 243 | a | 1209.23 | 22.36709 | YES | YES |
| 244 | a | 1211.71 | 248.83546 | YES | YES |
| 245 | a | 1213.74 | 7.40026 | YES | YES |
| 246 | a | 1220.85 | 329.27529 | YES | YES |
| 247 | a | 1228.84 | 240.56655 | YES | YES |
| 248 | a | 1237.70 | 812.06546 | YES | YES |
| 249 | a | 1242.48 | 573.08461 | YES | YES |
| 250 | a | 1242.72 | 64.45501 | YES | YES |
| 251 | a | 1246.68 | 218.35657 | YES | YES |
| 252 | a | 1247.45 | 25.54038 | YES | YES |
| 253 | a | 1249.75 | 4.49994 | YES | YES |
| 254 | a | 1250.82 | 84.67159 | YES | YES |
| 255 | a | 1251.47 | 141.26071 | YES | YES |
| 256 | a | 1256.85 | 891.41356 | YES | YES |
| 257 | a | 1259.23 | 485.21167 | YES | YES |
| 258 | a | 1264.34 | 142.39117 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 259 | a | 1267.19 | 1063.74324 | YES | YES |
| 260 | a | 1267.94 | 338.89604 | YES | YES |
| 261 | a | 1280.29 | 107.02854 | YES | YES |
| 262 | a | 1300.84 | 5.85606 | YES | YES |
| 263 | a | 1302.55 | 28.17576 | YES | YES |
| 264 | a | 1313.12 | 1.07768 | YES | YES |
| 265 | a | 1328.26 | 79.17698 | YES | YES |
| 266 | a | 1347.01 | 133.94919 | YES | YES |
| 267 | a | 1358.93 | 0.24608 | YES | YES |
| 268 | a | 1364.41 | 0.06174 | YES | YES |
| 269 | a | 1364.85 | 3.14539 | YES | YES |
| 270 | a | 1370.14 | 4.47039 | YES | YES |
| 271 | a | 1373.24 | 9.87681 | YES | YES |
| 272 | a | 1376.38 | 0.53779 | YES | YES |
| 273 | a | 1377.85 | 7.54958 | YES | YES |
| 274 | a | 1381.27 | 2.89365 | YES | YES |
| 275 | a | 1381.91 | 1.97414 | YES | YES |
| 276 | a | 1387.86 | 0.80473 | YES | YES |
| 277 | a | 1393.64 | 7.83164 | YES | YES |
| 278 | a | 1408.75 | 2.67108 | YES | YES |
| 279 | a | 1414.35 | 3.37846 | YES | YES |
| 280 | a | 1416.48 | 13.46148 | YES | YES |
| 281 | a | 1426.47 | 38.20601 | YES | YES |
| 282 | a | 1428.00 | 4.03916 | YES | YES |
| 283 | a | 1433.38 | 3.25371 | YES | YES |
| 284 | a | 1443.33 | 32.78781 | YES | YES |
| 285 | a | 1447.18 | 7.46997 | YES | YES |
| 286 | a | 1450.07 | 32.56507 | YES | YES |
| 287 | a | 1455.26 | 16.76276 | YES | YES |
| 288 | a | 1456.44 | 14.28681 | YES | YES |
| 289 | a | 1458.86 | 5.56405 | YES | YES |
| 290 | a | 1459.10 | 10.23896 | YES | YES |
| 291 | a | 1467.85 | 36.51015 | YES | YES |
| 292 | a | 1475.05 | 13.67213 | YES | YES |
| 293 | a | 1497.43 | 456.48471 | YES | YES |
| 294 | a | 1498.90 | 3.99795 | YES | YES |
| 295 | a | 1504.88 | 214.52756 | YES | YES |
| 296 | a | 1554.87 | 0.02123 | YES | YES |
| 297 | a | 1560.01 | 0.08045 | YES | YES |
| 298 | a | 1611.49 | 5.86270 | YES | YES |
| 299 | a | 1611.69 | 0.34284 | YES | YES |
| 300 | a | 1612.96 | 0.37850 | YES | YES |
| 301 | a | 1630.20 | 21.08955 | YES | YES |
| 302 | a | 1635.84 | 17.34681 | YES | YES |
| 303 | a | 1637.95 | 11.19956 | YES | YES |
| 304 | a | 2944.83 | 6.54795 | YES | YES |
| 305 | a | 2948.30 | 7.34160 | YES | YES |
| 306 | a | 2953.01 | 5.30466 | YES | YES |
| 307 | a | 2956.62 | 5.94944 | YES | YES |
| 308 | a | 2960.62 | 6.03125 | YES | YES |
| 309 | a | 2965.42 | 5.49124 | YES | YES |
| 310 | a | 3024.60 | 7.30358 | YES | YES |
| 311 | a | 3030.26 | 1.81421 | YES | YES |
| 312 | a | 3040.13 | 3.57152 | YES | YES |
| 313 | a | 3041.15 | 5.25830 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 314 | a | 3043.80 | 2.65265 | YES | YES |
| 315 | a | 3055.95 | 2.38455 | YES | YES |
| 316 | a | 3078.09 | 3.55768 | YES | YES |
| 317 | a | 3080.70 | 2.27313 | YES | YES |
| 318 | a | 3091.02 | 19.29973 | YES | YES |
| 319 | a | 3091.95 | 11.09775 | YES | YES |
| 320 | a | 3098.93 | 3.96566 | YES | YES |
| 321 | a | 3101.20 | 0.91836 | YES | YES |
| 322 | a | 3119.11 | 1.09233 | YES | YES |
| 323 | a | 3121.45 | 1.25136 | YES | YES |
| 324 | a | 3122.81 | 0.95561 | YES | YES |
| 325 | a | 3128.80 | 1.85759 | YES | YES |
| 326 | a | 3130.08 | 0.56003 | YES | YES |
| 327 | a | 3132.99 | 1.91704 | YES | YES |
| 328 | a | 3136.63 | 0.42078 | YES | YES |
| 329 | a | 3138.30 | 1.04541 | YES | YES |
| 330 | a | 3140.25 | 0.56821 | YES | YES |
| 331 | a | 3154.01 | 0.75073 | YES | YES |
| 332 | a | 3156.54 | 4.38266 | YES | YES |
| 333 | a | 3164.58 | 5.35101 | YES | YES |

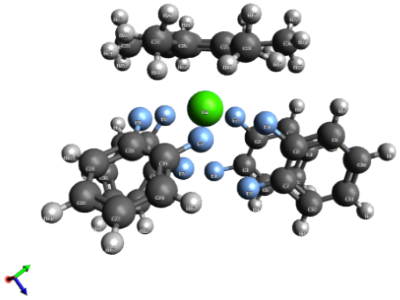
Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 ba | 1.78931 | 0.8230 | 1.696827 |
| 2 al | 1.96132 | 0.3813 | 2.543947 |
| 3 f | -0.73378 | -0.3486 | -0.863149 |
| 4 c | 0.34008 | 0.2171 | 0.461406 |
| 5 c | 0.33334 | 0.2124 | 0.435416 |
| 6 c | -0.26650 | -0.0247 | -0.009359 |
| 7 h | 0.25390 | 0.0177 | 0.103787 |
| 8 c | -0.20635 | 0.0131 | -0.018238 |
| 9 h | 0.24733 | 0.0184 | 0.089127 |
| 10 c | -0.20534 | 0.0117 | -0.018081 |
| 11 h | 0.24909 | 0.0210 | 0.092349 |
| 12 c | -0.25788 | -0.0187 | 0.000510 |
| 13 h | 0.26573 | 0.0319 | 0.133700 |
| 14 f | -0.34841 | -0.1672 | -0.616567 |
| 15 f | -0.36623 | -0.2041 | -0.633231 |
| 16 c | 0.35534 | 0.2417 | 0.520072 |
| 17 c | 0.33574 | 0.2158 | 0.444084 |
| 18 c | -0.27252 | -0.0435 | -0.014148 |
| 19 h | 0.24930 | 0.0268 | 0.105019 |
| 20 c | -0.21306 | 0.0097 | -0.021135 |
| 21 h | 0.24566 | 0.0161 | 0.085178 |
| 22 c | -0.21127 | 0.0101 | -0.023157 |
| 23 h | 0.24607 | 0.0164 | 0.086280 |
| 24 c | -0.28268 | -0.0496 | -0.028908 |
| 25 h | 0.25450 | 0.0181 | 0.099894 |
| 26 f | -0.31761 | -0.1698 | -0.601178 |
| 27 f | -0.36759 | -0.2143 | -0.619334 |
| 28 c | 0.33313 | 0.2096 | 0.442390 |
| 29 c | 0.33638 | 0.2123 | 0.455922 |
| 30 c | -0.25964 | -0.0202 | -0.003498 |
| 31 h | 0.26303 | 0.0296 | 0.129367 |
| 32 c | -0.20507 | 0.0116 | -0.017536 |
| 33 h | 0.24923 | 0.0214 | 0.092834 |

| | | | | |
|---|---|---|---|---|
| 34 | c | -0.20612 | 0.0127 | -0.018405 |
| 35 | h | 0.24833 | 0.0201 | 0.091613 |
| 36 | c | -0.26731 | -0.0218 | -0.009414 |
| 37 | h | 0.25696 | 0.0175 | 0.105779 |
| 38 | f | -0.36003 | -0.1926 | -0.618487 |
| 39 | f | -0.35403 | -0.1383 | -0.619601 |
| 40 | o | -0.95479 | -0.2215 | -1.339479 |
| 41 | c | 0.03366 | -0.0702 | 0.728281 |
| 42 | c | 1.10086 | 0.5168 | 1.639064 |
| 43 | f | -0.36474 | -0.1963 | -0.592913 |
| 44 | f | -0.33419 | -0.1656 | -0.580029 |
| 45 | f | -0.33213 | -0.1543 | -0.583072 |
| 46 | c | 1.11269 | 0.5352 | 1.691166 |
| 47 | f | -0.33367 | -0.1655 | -0.578589 |
| 48 | f | -0.34361 | -0.1842 | -0.579244 |
| 49 | f | -0.34740 | -0.1892 | -0.580760 |
| 50 | c | 1.10230 | 0.5249 | 1.648206 |
| 51 | f | -0.33452 | -0.1675 | -0.579147 |
| 52 | f | -0.34719 | -0.1846 | -0.583808 |
| 53 | f | -0.35258 | -0.1685 | -0.593932 |
| 54 | o | -0.95359 | -0.2054 | -1.325519 |
| 55 | c | 0.02873 | -0.0726 | 0.718881 |
| 56 | c | 1.10240 | 0.5218 | 1.634449 |
| 57 | f | -0.33572 | -0.1506 | -0.586071 |
| 58 | f | -0.33171 | -0.1608 | -0.579662 |
| 59 | f | -0.36294 | -0.1994 | -0.592606 |
| 60 | c | 1.11122 | 0.5350 | 1.665521 |
| 61 | f | -0.33898 | -0.1753 | -0.579334 |
| 62 | f | -0.35432 | -0.1843 | -0.593445 |
| 63 | f | -0.34574 | -0.1846 | -0.582440 |
| 64 | c | 1.10397 | 0.5275 | 1.675483 |
| 65 | f | -0.33458 | -0.1665 | -0.579846 |
| 66 | f | -0.34136 | -0.1801 | -0.579652 |
| 67 | f | -0.34309 | -0.1825 | -0.581306 |
| 68 | o | -0.98551 | -0.2780 | -1.304572 |
| 69 | c | 0.01945 | -0.0356 | 0.694817 |
| 70 | c | 1.10916 | 0.5388 | 1.689650 |
| 71 | f | -0.33285 | -0.1638 | -0.575291 |
| 72 | f | -0.33538 | -0.1716 | -0.575632 |
| 73 | f | -0.32014 | -0.1233 | -0.579706 |
| 74 | c | 1.10654 | 0.5446 | 1.641383 |
| 75 | f | -0.39006 | -0.1884 | -0.597821 |
| 76 | f | -0.31487 | -0.1174 | -0.574952 |
| 77 | f | -0.33301 | -0.1579 | -0.580607 |
| 78 | c | 1.10458 | 0.5370 | 1.633880 |
| 79 | f | -0.39433 | -0.2133 | -0.595607 |
| 80 | f | -0.32233 | -0.1424 | -0.577927 |
| 81 | f | -0.32381 | -0.1148 | -0.580725 |
| 82 | c | -0.05644 | 0.1445 | -0.054375 |
| 83 | c | -0.07384 | 0.1141 | -0.069587 |
| 84 | c | -0.06629 | 0.1168 | -0.066220 |
| 85 | c | -0.07933 | 0.1006 | -0.069898 |
| 86 | c | -0.06408 | 0.1147 | -0.062676 |
| 87 | c | -0.04353 | 0.1264 | -0.046637 |
| 88 | c | -0.66141 | -0.1860 | -0.050878 |

| | | | | |
|---|---|---|---|---|
| 89 | h | 0.24949 | 0.0428 | 0.050669 |
| 90 | h | 0.24601 | 0.0754 | 0.067909 |
| 91 | h | 0.23052 | 0.0368 | 0.033953 |
| 92 | c | -0.65865 | -0.1759 | -0.047398 |
| 93 | h | 0.25156 | 0.0480 | 0.054284 |
| 94 | h | 0.22975 | 0.0475 | 0.032674 |
| 95 | h | 0.23505 | 0.0349 | 0.037162 |
| 96 | c | -0.65796 | -0.1870 | -0.044948 |
| 97 | h | 0.24347 | 0.0381 | 0.045505 |
| 98 | h | 0.23715 | 0.0574 | 0.040497 |
| 99 | h | 0.24145 | 0.0389 | 0.050662 |
| 100 | c | -0.66256 | -0.2064 | -0.052182 |
| 101 | h | 0.23693 | 0.0541 | 0.049890 |
| 102 | h | 0.22768 | 0.0442 | 0.031269 |
| 103 | h | 0.25127 | 0.0457 | 0.052857 |
| 104 | c | -0.65915 | -0.1896 | -0.050362 |
| 105 | h | 0.23092 | 0.0365 | 0.034558 |
| 106 | h | 0.24115 | 0.0560 | 0.056585 |
| 107 | h | 0.25021 | 0.0412 | 0.052385 |
| 108 | c | -0.65673 | -0.1771 | -0.042730 |
| 109 | h | 0.24413 | 0.0420 | 0.044657 |
| 110 | h | 0.24261 | 0.0482 | 0.056594 |
| 111 | h | 0.24187 | 0.0482 | 0.056623 |

[Ca(HMB)oDFB$_4$]$^{2+}$ **7**$^{2+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| Ca | -0.13925 | -0.02584 | -0.38951 |
| C | 2.35461 | 1.18525 | 2.72790 |
| C | 1.48154 | 2.02993 | 2.03529 |
| C | 0.97760 | 3.20663 | 2.57684 |
| H | 0.29559 | 3.83938 | 1.98969 |
| C | 1.36558 | 3.54493 | 3.88508 |
| H | 0.98597 | 4.47241 | 4.33946 |
| C | 2.23871 | 2.70767 | 4.60244 |
| H | 2.54498 | 2.98021 | 5.62413 |
| C | 2.73783 | 1.52467 | 4.02901 |
| H | 3.42935 | 0.86206 | 4.57217 |
| F | 2.78790 | 0.05825 | 2.13316 |
| F | 1.08538 | 1.63738 | 0.75411 |
| C | -1.02976 | 0.57665 | 3.07852 |
| C | -1.87656 | 1.37921 | 2.31410 |
| C | -2.62870 | 2.40490 | 2.87396 |
| H | -3.29456 | 3.01720 | 2.24745 |
| C | -2.50454 | 2.61452 | 4.26169 |

| | | | |
|---|---|---|---|
| H | -3.09033 | 3.41526 | 4.73856 |
| C | -1.65076 | 1.80991 | 5.03736 |
| H | -1.56793 | 1.98491 | 6.12094 |
| C | -0.90014 | 0.77408 | 4.44973 |
| H | -0.22368 | 0.13486 | 5.03624 |
| F | -0.31563 | -0.37615 | 2.40639 |
| F | -1.90292 | 1.11996 | 0.95272 |
| C | 2.15302 | -2.47489 | 0.52681 |
| C | 2.83736 | -1.71872 | -0.42398 |
| C | 4.08586 | -2.09435 | -0.90277 |
| H | 4.60651 | -1.47603 | -1.64949 |
| C | 4.64672 | -3.28098 | -0.38982 |
| H | 5.63669 | -3.60435 | -0.74617 |
| C | 3.95855 | -4.04811 | 0.56703 |
| H | 4.41138 | -4.97178 | 0.95878 |
| C | 2.69264 | -3.64921 | 1.03974 |
| H | 2.13762 | -4.22981 | 1.79203 |
| F | 0.92489 | -2.00237 | 0.92754 |
| F | 2.19933 | -0.57470 | -0.88010 |
| C | -1.94041 | -2.90441 | -0.25309 |
| C | -0.90470 | -3.31811 | -1.09204 |
| C | -0.77311 | -4.64769 | -1.47700 |
| H | 0.05064 | -4.95232 | -2.14016 |
| C | -1.72573 | -5.56558 | -0.99243 |
| H | -1.64787 | -6.62420 | -1.28393 |
| C | -2.76967 | -5.14506 | -0.14896 |
| H | -3.50709 | -5.87453 | 0.21943 |
| C | -2.88857 | -3.79473 | 0.23570 |
| H | -3.69509 | -3.44195 | 0.89619 |
| F | -1.97520 | -1.55587 | 0.07407 |
| F | -0.02765 | -2.34767 | -1.52320 |
| C | -2.02775 | 1.02004 | -2.16764 |
| C | -1.32912 | 0.04286 | -2.94558 |
| C | 0.06982 | 0.19207 | -3.19819 |
| C | 0.75064 | 1.35446 | -2.71953 |
| C | 0.04213 | 2.34869 | -1.98381 |
| C | -1.35229 | 2.19762 | -1.72835 |
| C | -3.50272 | 0.82409 | -1.89123 |
| H | -4.12067 | 1.28336 | -2.69696 |
| H | -3.81575 | 1.28464 | -0.93496 |
| H | -3.78019 | -0.24619 | -1.84474 |
| C | -2.13112 | -1.09318 | -3.54434 |
| H | -2.99618 | -0.68774 | -4.11192 |
| H | -2.55590 | -1.77621 | -2.77587 |
| H | -1.54624 | -1.71023 | -4.24844 |
| C | 0.84112 | -0.83059 | -4.00545 |
| H | 1.04386 | -0.44954 | -5.03176 |
| H | 0.30406 | -1.78920 | -4.11093 |
| H | 1.82280 | -1.05840 | -3.54333 |
| C | 2.20366 | 1.60853 | -3.05392 |
| H | 2.64734 | 0.82113 | -3.68806 |
| H | 2.83253 | 1.70219 | -2.14205 |
| H | 2.30384 | 2.56824 | -3.60671 |
| C | 0.75868 | 3.61022 | -1.56410 |
| H | 1.81410 | 3.42377 | -1.28585 |

| | | | |
|---|---|---|---|
| H | 0.26888 | 4.11665 | -0.71138 |
| H | 0.77336 | 4.33974 | -2.40721 |
| C | -2.09762 | 3.33820 | -1.07209 |
| H | -1.97885 | 4.26283 | -1.67841 |
| H | -1.70685 | 3.57203 | -0.05798 |
| H | -3.18198 | 3.14912 | -0.98080 |

Vibrational analysis

| 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 | 10.65 | 1.35236 | YES | YES |
| 8 | a | 15.48 | 0.12709 | YES | YES |
| 9 | a | 16.89 | 0.16342 | YES | YES |
| 10 | a | 19.43 | 0.61751 | YES | YES |
| 11 | a | 29.03 | 1.85030 | YES | YES |
| 12 | a | 32.10 | 1.15689 | YES | YES |
| 13 | a | 35.58 | 0.62228 | YES | YES |
| 14 | a | 37.51 | 1.02905 | YES | YES |
| 15 | a | 43.74 | 0.90199 | YES | YES |
| 16 | a | 50.61 | 0.28932 | YES | YES |
| 17 | a | 54.02 | 0.90872 | YES | YES |
| 18 | a | 58.06 | 0.24434 | YES | YES |
| 19 | a | 61.92 | 0.08986 | YES | YES |
| 20 | a | 63.75 | 0.47496 | YES | YES |
| 21 | a | 69.45 | 0.75560 | YES | YES |
| 22 | a | 71.32 | 0.29441 | YES | YES |
| 23 | a | 79.47 | 0.43573 | YES | YES |
| 24 | a | 84.16 | 0.10826 | YES | YES |
| 25 | a | 85.60 | 1.09671 | YES | YES |
| 26 | a | 92.92 | 1.09496 | YES | YES |
| 27 | a | 96.45 | 3.68983 | YES | YES |
| 28 | a | 99.24 | 1.55207 | YES | YES |
| 29 | a | 102.86 | 0.92391 | YES | YES |
| 30 | a | 111.04 | 1.24561 | YES | YES |
| 31 | a | 115.11 | 3.64436 | YES | YES |
| 32 | a | 116.34 | 1.44472 | YES | YES |
| 33 | a | 122.84 | 0.09879 | YES | YES |
| 34 | a | 132.17 | 0.84132 | YES | YES |
| 35 | a | 134.74 | 1.66972 | YES | YES |
| 36 | a | 159.99 | 1.12662 | YES | YES |
| 37 | a | 170.03 | 1.70624 | YES | YES |
| 38 | a | 181.87 | 35.85961 | YES | YES |
| 39 | a | 189.58 | 37.83398 | YES | YES |
| 40 | a | 194.11 | 3.22649 | YES | YES |
| 41 | a | 195.98 | 11.10351 | YES | YES |
| 42 | a | 202.64 | 4.14458 | YES | YES |
| 43 | a | 203.51 | 8.20232 | YES | YES |
| 44 | a | 209.67 | 7.38488 | YES | YES |
| 45 | a | 222.36 | 1.48813 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 46 | a | 231.57 | 47.85143 | YES | YES |
| 47 | a | 265.15 | 58.27036 | YES | YES |
| 48 | a | 279.64 | 1.54628 | YES | YES |
| 49 | a | 286.25 | 1.51463 | YES | YES |
| 50 | a | 289.62 | 0.95311 | YES | YES |
| 51 | a | 291.26 | 2.31992 | YES | YES |
| 52 | a | 299.81 | 0.22543 | YES | YES |
| 53 | a | 310.88 | 7.79232 | YES | YES |
| 54 | a | 312.78 | 5.97548 | YES | YES |
| 55 | a | 320.15 | 3.61325 | YES | YES |
| 56 | a | 332.69 | 0.91203 | YES | YES |
| 57 | a | 346.44 | 0.52053 | YES | YES |
| 58 | a | 378.73 | 1.97708 | YES | YES |
| 59 | a | 388.42 | 1.79586 | YES | YES |
| 60 | a | 397.15 | 0.01668 | YES | YES |
| 61 | a | 408.74 | 0.01715 | YES | YES |
| 62 | a | 430.92 | 1.02297 | YES | YES |
| 63 | a | 434.65 | 0.42284 | YES | YES |
| 64 | a | 435.34 | 2.13000 | YES | YES |
| 65 | a | 437.02 | 1.25354 | YES | YES |
| 66 | a | 437.63 | 2.55999 | YES | YES |
| 67 | a | 438.38 | 0.52895 | YES | YES |
| 68 | a | 440.14 | 4.15050 | YES | YES |
| 69 | a | 440.57 | 0.96279 | YES | YES |
| 70 | a | 441.99 | 0.19478 | YES | YES |
| 71 | a | 445.90 | 1.48475 | YES | YES |
| 72 | a | 447.67 | 0.00671 | YES | YES |
| 73 | a | 531.96 | 2.67521 | YES | YES |
| 74 | a | 533.79 | 0.30314 | YES | YES |
| 75 | a | 534.58 | 3.90554 | YES | YES |
| 76 | a | 536.47 | 0.30500 | YES | YES |
| 77 | a | 539.11 | 1.41176 | YES | YES |
| 78 | a | 539.20 | 6.24785 | YES | YES |
| 79 | a | 540.28 | 1.47411 | YES | YES |
| 80 | a | 542.76 | 6.64776 | YES | YES |
| 81 | a | 551.53 | 3.49009 | YES | YES |
| 82 | a | 554.79 | 34.32765 | YES | YES |
| 83 | a | 555.66 | 18.71400 | YES | YES |
| 84 | a | 557.62 | 12.21956 | YES | YES |
| 85 | a | 562.08 | 21.70183 | YES | YES |
| 86 | a | 563.81 | 0.56238 | YES | YES |
| 87 | a | 571.57 | 0.77456 | YES | YES |
| 88 | a | 575.58 | 0.69528 | YES | YES |
| 89 | a | 581.65 | 0.56724 | YES | YES |
| 90 | a | 668.67 | 0.08061 | YES | YES |
| 91 | a | 673.06 | 0.14030 | YES | YES |
| 92 | a | 673.28 | 0.17694 | YES | YES |
| 93 | a | 675.06 | 0.00421 | YES | YES |
| 94 | a | 685.33 | 0.16084 | YES | YES |
| 95 | a | 744.17 | 57.12358 | YES | YES |
| 96 | a | 745.50 | 110.58587 | YES | YES |
| 97 | a | 747.20 | 52.81872 | YES | YES |
| 98 | a | 749.34 | 126.06024 | YES | YES |
| 99 | a | 749.73 | 78.62067 | YES | YES |
| 100 | a | 750.44 | 31.07005 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 101 | a | 751.17 | 114.00948 | YES | YES |
| 102 | a | 757.61 | 88.22783 | YES | YES |
| 103 | a | 792.34 | 1.36310 | YES | YES |
| 104 | a | 799.05 | 2.77655 | YES | YES |
| 105 | a | 811.98 | 3.94141 | YES | YES |
| 106 | a | 812.82 | 17.75426 | YES | YES |
| 107 | a | 817.63 | 12.99228 | YES | YES |
| 108 | a | 823.54 | 20.84866 | YES | YES |
| 109 | a | 834.07 | 1.93765 | YES | YES |
| 110 | a | 839.40 | 0.31952 | YES | YES |
| 111 | a | 840.45 | 0.07506 | YES | YES |
| 112 | a | 842.41 | 0.04721 | YES | YES |
| 113 | a | 928.00 | 3.46983 | YES | YES |
| 114 | a | 931.29 | 0.74652 | YES | YES |
| 115 | a | 933.21 | 1.77922 | YES | YES |
| 116 | a | 935.37 | 1.31542 | YES | YES |
| 117 | a | 952.58 | 2.53743 | YES | YES |
| 118 | a | 959.51 | 0.43971 | YES | YES |
| 119 | a | 974.68 | 4.62951 | YES | YES |
| 120 | a | 975.11 | 13.29653 | YES | YES |
| 121 | a | 978.89 | 0.07757 | YES | YES |
| 122 | a | 981.97 | 0.07424 | YES | YES |
| 123 | a | 983.63 | 0.00151 | YES | YES |
| 124 | a | 985.75 | 0.00558 | YES | YES |
| 125 | a | 997.78 | 4.05972 | YES | YES |
| 126 | a | 999.85 | 2.15784 | YES | YES |
| 127 | a | 1014.13 | 4.72076 | YES | YES |
| 128 | a | 1014.39 | 4.04759 | YES | YES |
| 129 | a | 1014.63 | 2.43682 | YES | YES |
| 130 | a | 1017.72 | 1.07099 | YES | YES |
| 131 | a | 1020.55 | 4.63773 | YES | YES |
| 132 | a | 1023.58 | 1.41500 | YES | YES |
| 133 | a | 1024.78 | 1.78114 | YES | YES |
| 134 | a | 1049.46 | 23.20415 | YES | YES |
| 135 | a | 1051.78 | 9.80174 | YES | YES |
| 136 | a | 1071.98 | 22.36087 | YES | YES |
| 137 | a | 1073.94 | 31.64945 | YES | YES |
| 138 | a | 1074.82 | 1.29712 | YES | YES |
| 139 | a | 1075.37 | 6.86877 | YES | YES |
| 140 | a | 1078.13 | 4.16075 | YES | YES |
| 141 | a | 1080.64 | 81.86619 | YES | YES |
| 142 | a | 1081.83 | 3.75802 | YES | YES |
| 143 | a | 1129.39 | 12.79001 | YES | YES |
| 144 | a | 1130.84 | 3.22341 | YES | YES |
| 145 | a | 1132.98 | 5.29240 | YES | YES |
| 146 | a | 1139.43 | 37.40321 | YES | YES |
| 147 | a | 1141.54 | 4.89007 | YES | YES |
| 148 | a | 1141.76 | 6.61063 | YES | YES |
| 149 | a | 1142.04 | 2.48635 | YES | YES |
| 150 | a | 1142.82 | 31.62976 | YES | YES |
| 151 | a | 1229.29 | 114.60143 | YES | YES |
| 152 | a | 1233.76 | 83.38439 | YES | YES |
| 153 | a | 1235.85 | 135.89557 | YES | YES |
| 154 | a | 1240.24 | 33.18213 | YES | YES |
| 155 | a | 1244.53 | 1.84655 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 156 | a | 1245.45 | 22.15345 | YES | YES |
| 157 | a | 1248.74 | 23.36913 | YES | YES |
| 158 | a | 1253.44 | 0.37078 | YES | YES |
| 159 | a | 1268.80 | 92.71148 | YES | YES |
| 160 | a | 1299.49 | 1.98404 | YES | YES |
| 161 | a | 1314.37 | 1.70099 | YES | YES |
| 162 | a | 1357.83 | 1.17151 | YES | YES |
| 163 | a | 1358.63 | 0.09708 | YES | YES |
| 164 | a | 1363.72 | 7.45336 | YES | YES |
| 165 | a | 1365.01 | 8.90402 | YES | YES |
| 166 | a | 1366.92 | 14.21290 | YES | YES |
| 167 | a | 1372.32 | 9.71300 | YES | YES |
| 168 | a | 1378.31 | 2.65466 | YES | YES |
| 169 | a | 1380.49 | 6.77151 | YES | YES |
| 170 | a | 1381.61 | 7.62533 | YES | YES |
| 171 | a | 1383.04 | 3.47937 | YES | YES |
| 172 | a | 1384.58 | 1.17848 | YES | YES |
| 173 | a | 1393.09 | 13.98144 | YES | YES |
| 174 | a | 1405.14 | 1.11178 | YES | YES |
| 175 | a | 1408.43 | 8.52185 | YES | YES |
| 176 | a | 1413.26 | 0.70203 | YES | YES |
| 177 | a | 1419.61 | 37.74451 | YES | YES |
| 178 | a | 1426.90 | 6.04755 | YES | YES |
| 179 | a | 1430.38 | 21.34769 | YES | YES |
| 180 | a | 1440.65 | 18.94156 | YES | YES |
| 181 | a | 1443.13 | 22.11441 | YES | YES |
| 182 | a | 1446.82 | 19.45151 | YES | YES |
| 183 | a | 1453.96 | 6.23177 | YES | YES |
| 184 | a | 1454.95 | 13.81359 | YES | YES |
| 185 | a | 1457.10 | 4.78712 | YES | YES |
| 186 | a | 1457.55 | 6.96433 | YES | YES |
| 187 | a | 1458.32 | 12.33536 | YES | YES |
| 188 | a | 1459.01 | 26.74924 | YES | YES |
| 189 | a | 1471.12 | 21.67680 | YES | YES |
| 190 | a | 1487.14 | 198.00993 | YES | YES |
| 191 | a | 1488.98 | 280.32457 | YES | YES |
| 192 | a | 1491.64 | 94.92735 | YES | YES |
| 193 | a | 1499.07 | 267.68861 | YES | YES |
| 194 | a | 1551.52 | 0.14879 | YES | YES |
| 195 | a | 1555.19 | 0.73691 | YES | YES |
| 196 | a | 1600.74 | 1.56113 | YES | YES |
| 197 | a | 1602.91 | 0.05626 | YES | YES |
| 198 | a | 1604.23 | 0.14135 | YES | YES |
| 199 | a | 1605.92 | 1.57282 | YES | YES |
| 200 | a | 1639.38 | 14.45151 | YES | YES |
| 201 | a | 1639.85 | 9.50571 | YES | YES |
| 202 | a | 1641.39 | 15.78210 | YES | YES |
| 203 | a | 1642.54 | 8.36946 | YES | YES |
| 204 | a | 2953.19 | 1.31910 | YES | YES |
| 205 | a | 2957.32 | 1.58551 | YES | YES |
| 206 | a | 2959.96 | 5.42647 | YES | YES |
| 207 | a | 2960.10 | 2.29341 | YES | YES |
| 208 | a | 2961.87 | 1.79696 | YES | YES |
| 209 | a | 2964.56 | 1.43881 | YES | YES |
| 210 | a | 3025.89 | 8.62428 | YES | YES |

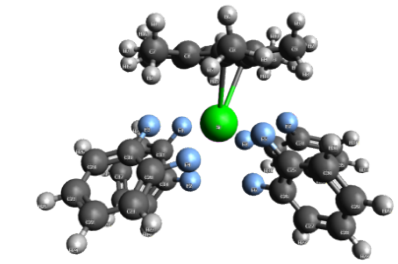
| | | | | | |
|---|---|---|---|---|---|
| 211 | a | 3026.56 | 3.01688 | YES | YES |
| 212 | a | 3027.56 | 2.49235 | YES | YES |
| 213 | a | 3043.38 | 3.78378 | YES | YES |
| 214 | a | 3047.29 | 7.22196 | YES | YES |
| 215 | a | 3051.01 | 4.10124 | YES | YES |
| 216 | a | 3084.06 | 3.18194 | YES | YES |
| 217 | a | 3087.33 | 6.11865 | YES | YES |
| 218 | a | 3096.82 | 1.38678 | YES | YES |
| 219 | a | 3100.45 | 3.78553 | YES | YES |
| 220 | a | 3105.08 | 6.96389 | YES | YES |
| 221 | a | 3107.67 | 6.14823 | YES | YES |
| 222 | a | 3124.34 | 0.31330 | YES | YES |
| 223 | a | 3126.02 | 0.23512 | YES | YES |
| 224 | a | 3127.26 | 0.47843 | YES | YES |
| 225 | a | 3127.96 | 0.66487 | YES | YES |
| 226 | a | 3131.03 | 1.49114 | YES | YES |
| 227 | a | 3134.39 | 0.61141 | YES | YES |
| 228 | a | 3134.59 | 0.77577 | YES | YES |
| 229 | a | 3135.04 | 0.66170 | YES | YES |
| 230 | a | 3136.44 | 1.99262 | YES | YES |
| 231 | a | 3139.77 | 4.93211 | YES | YES |
| 232 | a | 3140.08 | 5.80637 | YES | YES |
| 233 | a | 3140.41 | 3.46476 | YES | YES |
| 234 | a | 3143.54 | 1.72314 | YES | YES |
| 235 | a | 3145.25 | 3.40125 | YES | YES |
| 236 | a | 3145.49 | 3.41520 | YES | YES |
| 237 | a | 3145.65 | 4.20903 | YES | YES |

Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 ca | 1.74686 | 1.2838 | 1.620658 |
| 2 c | 0.35847 | 0.2532 | 0.529534 |
| 3 c | 0.30950 | 0.1792 | 0.362785 |
| 4 c | -0.27324 | -0.0260 | -0.004200 |
| 5 h | 0.25330 | 0.0182 | 0.094704 |
| 6 c | -0.20412 | 0.0225 | -0.013727 |
| 7 h | 0.25543 | 0.0260 | 0.102718 |
| 8 c | -0.19626 | 0.0239 | -0.016420 |
| 9 h | 0.25727 | 0.0289 | 0.107133 |
| 10 c | -0.26526 | -0.0355 | -0.018215 |
| 11 h | 0.26530 | 0.0303 | 0.121427 |
| 12 f | -0.31570 | -0.1727 | -0.600277 |
| 13 f | -0.40295 | -0.2553 | -0.644329 |
| 14 c | 0.33292 | 0.2066 | 0.451311 |
| 15 c | 0.32352 | 0.1906 | 0.392948 |
| 16 c | -0.26878 | -0.0241 | -0.008867 |
| 17 h | 0.26244 | 0.0226 | 0.114627 |
| 18 c | -0.19760 | 0.0177 | -0.015048 |
| 19 h | 0.25861 | 0.0320 | 0.110968 |
| 20 c | -0.19330 | 0.0247 | -0.013250 |
| 21 h | 0.25809 | 0.0304 | 0.110218 |
| 22 c | -0.26000 | -0.0114 | -0.001059 |
| 23 h | 0.26555 | 0.0255 | 0.119944 |
| 24 f | -0.34871 | -0.1781 | -0.614238 |
| 25 f | -0.37956 | -0.2336 | -0.634618 |
| 26 c | 0.32938 | 0.2012 | 0.439018 |

| | | | | |
|---|---|---|---|---|
| 27 | c | 0.32915 | 0.1968 | 0.407290 |
| 28 | c | -0.26154 | -0.0204 | -0.000903 |
| 29 | h | 0.26442 | 0.0250 | 0.119397 |
| 30 | c | -0.19294 | 0.0201 | -0.010444 |
| 31 | h | 0.25971 | 0.0339 | 0.114062 |
| 32 | c | -0.19347 | 0.0200 | -0.011685 |
| 33 | h | 0.25906 | 0.0329 | 0.112551 |
| 34 | c | -0.26072 | -0.0196 | -0.004077 |
| 35 | h | 0.26492 | 0.0253 | 0.121205 |
| 36 | f | -0.36450 | -0.2020 | -0.617969 |
| 37 | f | -0.38146 | -0.2389 | -0.631756 |
| 38 | c | 0.32376 | 0.1942 | 0.398599 |
| 39 | c | 0.32185 | 0.1932 | 0.424673 |
| 40 | c | -0.26004 | -0.0179 | -0.003327 |
| 41 | h | 0.26625 | 0.0270 | 0.123254 |
| 42 | c | -0.19036 | 0.0233 | -0.010303 |
| 43 | h | 0.26079 | 0.0348 | 0.116075 |
| 44 | c | -0.19080 | 0.0232 | -0.009264 |
| 45 | h | 0.26129 | 0.0357 | 0.117629 |
| 46 | c | -0.25769 | -0.0144 | -0.000197 |
| 47 | h | 0.26786 | 0.0278 | 0.126517 |
| 48 | f | -0.38166 | -0.2366 | -0.623078 |
| 49 | f | -0.36437 | -0.2155 | -0.635704 |
| 50 | c | -0.08953 | 0.1198 | -0.088930 |
| 51 | c | -0.07946 | 0.1549 | -0.076535 |
| 52 | c | -0.08107 | 0.1186 | -0.075528 |
| 53 | c | -0.06902 | 0.1036 | -0.073578 |
| 54 | c | -0.06903 | 0.0887 | -0.072562 |
| 55 | c | -0.06586 | 0.1236 | -0.064423 |
| 56 | c | -0.66075 | -0.1957 | -0.050978 |
| 57 | h | 0.26459 | 0.0627 | 0.077267 |
| 58 | h | 0.23982 | 0.0424 | 0.049994 |
| 59 | h | 0.24020 | 0.0362 | 0.047282 |
| 60 | c | -0.65484 | -0.2011 | -0.047158 |
| 61 | h | 0.26237 | 0.0549 | 0.073095 |
| 62 | h | 0.23140 | 0.0445 | 0.033056 |
| 63 | h | 0.24510 | 0.0463 | 0.059584 |
| 64 | c | -0.65673 | -0.2017 | -0.043380 |
| 65 | h | 0.26395 | 0.0610 | 0.076216 |
| 66 | h | 0.23803 | 0.0406 | 0.051839 |
| 67 | h | 0.23680 | 0.0407 | 0.042978 |
| 68 | c | -0.65976 | -0.1963 | -0.049554 |
| 69 | h | 0.24449 | 0.0422 | 0.056566 |
| 70 | h | 0.24280 | 0.0469 | 0.048056 |
| 71 | h | 0.26057 | 0.0546 | 0.071980 |
| 72 | c | -0.65992 | -0.1915 | -0.047865 |
| 73 | h | 0.24459 | 0.0397 | 0.053022 |
| 74 | h | 0.23496 | 0.0346 | 0.039429 |
| 75 | h | 0.26504 | 0.0627 | 0.076720 |
| 76 | c | -0.65576 | -0.1985 | -0.042785 |
| 77 | h | 0.26239 | 0.0561 | 0.073677 |
| 78 | h | 0.22949 | 0.0366 | 0.029709 |
| 79 | h | 0.24449 | 0.0442 | 0.056517 |

$[Sr(HMB)oDFB_4]^{2+}$ **6**$^{2+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 2.3920369 | 0.9669280 | -1.8637739 |
| C | 2.7655147 | -0.3650225 | -1.5077175 |
| C | 2.0254978 | -1.4825438 | -1.9966540 |
| C | 0.8543397 | -1.2595167 | -2.7804331 |
| C | 0.4851826 | 0.0711501 | -3.1468802 |
| C | 1.2432417 | 1.1899445 | -2.6837802 |
| C | 3.2919007 | 2.0969157 | -1.4103119 |
| H | 4.3356458 | 1.9129811 | -1.7455208 |
| H | 3.3338650 | 2.1878642 | -0.3018853 |
| H | 2.9924022 | 3.0803253 | -1.8125709 |
| C | 4.0117831 | -0.5813960 | -0.6777720 |
| H | 4.0423836 | -1.5801891 | -0.2056698 |
| H | 4.1136460 | 0.1727203 | 0.1291639 |
| H | 4.9233743 | -0.4896762 | -1.3129497 |
| C | 2.5468806 | -2.8787446 | -1.7308280 |
| H | 1.9996482 | -3.6530926 | -2.2975318 |
| H | 2.4973460 | -3.1531791 | -0.6544282 |
| H | 3.6132800 | -2.9520050 | -2.0334202 |
| C | 0.0158437 | -2.4081762 | -3.2998244 |
| H | 0.2811085 | -2.6450247 | -4.3559578 |
| H | -1.0661777 | -2.1641942 | -3.2949698 |
| H | 0.1492426 | -3.3366737 | -2.7155969 |
| C | -0.6827828 | 0.2578498 | -4.0930096 |
| H | -0.5932804 | -0.4295075 | -4.9605544 |
| H | -0.7438414 | 1.2831770 | -4.4991395 |
| H | -1.6606651 | 0.0329322 | -3.6097916 |
| C | 0.8427227 | 2.5858708 | -3.1142220 |
| H | 1.1807529 | 2.7875318 | -4.1560752 |
| H | 1.2776405 | 3.3716783 | -2.4715398 |
| H | -0.2562100 | 2.7223799 | -3.0945118 |
| C | -2.4144727 | 2.5189850 | -0.4966605 |
| C | -2.3635683 | 2.3725980 | 0.8912097 |
| C | -2.9658390 | 3.2925084 | 1.7428817 |
| H | -2.9036375 | 3.1559850 | 2.8330715 |
| C | -3.6415959 | 4.3814831 | 1.1600808 |
| H | -4.1327861 | 5.1208360 | 1.8110360 |
| C | -3.6966447 | 4.5285401 | -0.2376508 |
| H | -4.2320027 | 5.3822598 | -0.6807419 |
| C | -3.0754205 | 3.5918088 | -1.0864887 |
| H | -3.1074665 | 3.6870057 | -2.1825244 |
| F | -1.7593932 | 1.5722608 | -1.2554343 |
| F | -1.6611601 | 1.2924853 | 1.3839261 |

| | | | |
|---|---|---|---|
| C | 0.6890766 | 3.2907993 | 1.1870104 |
| C | 1.1207201 | 2.4920390 | 2.2468266 |
| C | 1.3244765 | 3.0227078 | 3.5163602 |
| H | 1.6670196 | 2.3759890 | 4.3383670 |
| C | 1.0815984 | 4.3984302 | 3.6969627 |
| H | 1.2406092 | 4.8452954 | 4.6903424 |
| C | 0.6426829 | 5.2009620 | 2.6281123 |
| H | 0.4579881 | 6.2744877 | 2.7864212 |
| C | 0.4375119 | 4.6485028 | 1.3494211 |
| H | 0.0887616 | 5.2518519 | 0.4978184 |
| F | 0.4972271 | 2.6613600 | -0.0251046 |
| F | 1.3177875 | 1.1526288 | 1.9791034 |
| C | 1.2261999 | -2.3326955 | 2.3765324 |
| C | -0.1096761 | -2.1595923 | 2.7454642 |
| C | -0.7098070 | -2.9745109 | 3.6999193 |
| H | -1.7657352 | -2.8203600 | 3.9690414 |
| C | 0.0766598 | -3.9795295 | 4.2950811 |
| H | -0.3729869 | -4.6335348 | 5.0578195 |
| C | 1.4234458 | -4.1501662 | 3.9279196 |
| H | 2.0286600 | -4.9369649 | 4.4037072 |
| C | 2.0150041 | -3.3222219 | 2.9541852 |
| H | 3.0667882 | -3.4376639 | 2.6511170 |
| F | 1.7275937 | -1.4979295 | 1.3985445 |
| F | -0.8185118 | -1.1626698 | 2.1088465 |
| C | -1.4666916 | -3.2595464 | -0.0961459 |
| C | -2.5456416 | -2.4113734 | -0.3490617 |
| C | -3.8572857 | -2.8706200 | -0.2974700 |
| H | -4.6932152 | -2.1846825 | -0.5024362 |
| C | -4.0630818 | -4.2272257 | 0.0208782 |
| H | -5.0911835 | -4.6181114 | 0.0642230 |
| C | -2.9754643 | -5.0803513 | 0.2812871 |
| H | -3.1533413 | -6.1381351 | 0.5284262 |
| C | -1.6531084 | -4.5992018 | 0.2269248 |
| H | -0.7845239 | -5.2444831 | 0.4271806 |
| F | -0.2070352 | -2.7056237 | -0.1700977 |
| F | -2.2512721 | -1.0938301 | -0.6444203 |
| Sr | 0.1304151 | -0.0120931 | -0.1536558 |

Vibrational analysis

| 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 | 7.56 | 0.03078 | YES | YES |
| 8 | a | 12.65 | 0.21775 | YES | YES |
| 9 | a | 14.38 | 0.05365 | YES | YES |
| 10 | a | 18.08 | 0.12805 | YES | YES |
| 11 | a | 22.20 | 0.39970 | YES | YES |
| 12 | a | 28.42 | 0.46838 | YES | YES |
| 13 | a | 30.43 | 0.93369 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 14 | a | 38.73 | 0.22282 | YES | YES |
| 15 | a | 43.45 | 0.18332 | YES | YES |
| 16 | a | 44.86 | 0.20863 | YES | YES |
| 17 | a | 46.77 | 0.06447 | YES | YES |
| 18 | a | 57.78 | 0.24628 | YES | YES |
| 19 | a | 59.10 | 0.26270 | YES | YES |
| 20 | a | 66.69 | 1.09037 | YES | YES |
| 21 | a | 72.66 | 0.40402 | YES | YES |
| 22 | a | 75.92 | 0.12488 | YES | YES |
| 23 | a | 76.50 | 1.36944 | YES | YES |
| 24 | a | 78.34 | 1.79690 | YES | YES |
| 25 | a | 79.81 | 0.03613 | YES | YES |
| 26 | a | 83.74 | 0.36680 | YES | YES |
| 27 | a | 86.11 | 3.58860 | YES | YES |
| 28 | a | 91.56 | 0.79691 | YES | YES |
| 29 | a | 94.13 | 1.73468 | YES | YES |
| 30 | a | 99.12 | 3.32697 | YES | YES |
| 31 | a | 102.29 | 1.98906 | YES | YES |
| 32 | a | 119.39 | 3.30746 | YES | YES |
| 33 | a | 122.19 | 2.79581 | YES | YES |
| 34 | a | 126.97 | 0.19981 | YES | YES |
| 35 | a | 133.39 | 0.94624 | YES | YES |
| 36 | a | 140.52 | 16.85117 | YES | YES |
| 37 | a | 146.82 | 14.40462 | YES | YES |
| 38 | a | 153.15 | 29.87893 | YES | YES |
| 39 | a | 157.16 | 6.41038 | YES | YES |
| 40 | a | 165.81 | 10.06073 | YES | YES |
| 41 | a | 168.77 | 1.09013 | YES | YES |
| 42 | a | 189.63 | 6.17033 | YES | YES |
| 43 | a | 203.15 | 0.09284 | YES | YES |
| 44 | a | 203.47 | 0.20053 | YES | YES |
| 45 | a | 207.87 | 0.34204 | YES | YES |
| 46 | a | 211.12 | 0.16546 | YES | YES |
| 47 | a | 253.74 | 36.24847 | YES | YES |
| 48 | a | 285.85 | 0.94768 | YES | YES |
| 49 | a | 287.81 | 0.84517 | YES | YES |
| 50 | a | 290.23 | 0.94313 | YES | YES |
| 51 | a | 290.66 | 0.63336 | YES | YES |
| 52 | a | 305.34 | 5.36116 | YES | YES |
| 53 | a | 306.63 | 0.32110 | YES | YES |
| 54 | a | 310.17 | 11.39157 | YES | YES |
| 55 | a | 313.05 | 2.49792 | YES | YES |
| 56 | a | 330.35 | 0.40843 | YES | YES |
| 57 | a | 350.43 | 0.54487 | YES | YES |
| 58 | a | 370.93 | 1.07701 | YES | YES |
| 59 | a | 387.02 | 1.57636 | YES | YES |
| 60 | a | 392.69 | 0.11470 | YES | YES |
| 61 | a | 411.27 | 0.01033 | YES | YES |
| 62 | a | 431.85 | 0.03012 | YES | YES |
| 63 | a | 433.48 | 0.03053 | YES | YES |
| 64 | a | 434.55 | 0.07863 | YES | YES |
| 65 | a | 435.19 | 0.05362 | YES | YES |
| 66 | a | 438.32 | 2.67426 | YES | YES |
| 67 | a | 438.90 | 0.25994 | YES | YES |
| 68 | a | 439.25 | 2.06380 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 69 | a | 440.21 | 2.76304 | YES | YES |
| 70 | a | 441.29 | 2.35114 | YES | YES |
| 71 | a | 442.92 | 0.01684 | YES | YES |
| 72 | a | 445.30 | 0.01696 | YES | YES |
| 73 | a | 533.65 | 1.94886 | YES | YES |
| 74 | a | 533.83 | 1.13180 | YES | YES |
| 75 | a | 534.92 | 0.53501 | YES | YES |
| 76 | a | 535.49 | 0.56357 | YES | YES |
| 77 | a | 538.73 | 7.72007 | YES | YES |
| 78 | a | 539.60 | 2.58810 | YES | YES |
| 79 | a | 540.02 | 6.31161 | YES | YES |
| 80 | a | 541.14 | 0.94897 | YES | YES |
| 81 | a | 549.94 | 2.95614 | YES | YES |
| 82 | a | 556.18 | 9.79828 | YES | YES |
| 83 | a | 556.40 | 46.54349 | YES | YES |
| 84 | a | 556.77 | 13.14464 | YES | YES |
| 85 | a | 558.48 | 13.99935 | YES | YES |
| 86 | a | 564.75 | 0.17981 | YES | YES |
| 87 | a | 572.92 | 0.57276 | YES | YES |
| 88 | a | 579.12 | 0.64828 | YES | YES |
| 89 | a | 580.31 | 0.62286 | YES | YES |
| 90 | a | 666.05 | 0.03016 | YES | YES |
| 91 | a | 667.09 | 0.05645 | YES | YES |
| 92 | a | 669.17 | 0.02693 | YES | YES |
| 93 | a | 669.18 | 0.01886 | YES | YES |
| 94 | a | 699.28 | 0.25944 | YES | YES |
| 95 | a | 747.02 | 51.26555 | YES | YES |
| 96 | a | 747.71 | 67.56720 | YES | YES |
| 97 | a | 749.46 | 89.76369 | YES | YES |
| 98 | a | 750.17 | 81.44684 | YES | YES |
| 99 | a | 750.60 | 162.97659 | YES | YES |
| 100 | a | 751.44 | 14.66166 | YES | YES |
| 101 | a | 751.99 | 106.15246 | YES | YES |
| 102 | a | 756.03 | 82.71623 | YES | YES |
| 103 | a | 789.45 | 1.15022 | YES | YES |
| 104 | a | 798.80 | 4.07376 | YES | YES |
| 105 | a | 812.56 | 2.41763 | YES | YES |
| 106 | a | 814.05 | 2.30789 | YES | YES |
| 107 | a | 815.13 | 26.60994 | YES | YES |
| 108 | a | 815.88 | 23.12351 | YES | YES |
| 109 | a | 839.70 | 0.00664 | YES | YES |
| 110 | a | 839.76 | 0.04979 | YES | YES |
| 111 | a | 840.16 | 0.02926 | YES | YES |
| 112 | a | 842.12 | 0.06866 | YES | YES |
| 113 | a | 933.52 | 2.29221 | YES | YES |
| 114 | a | 933.86 | 1.82409 | YES | YES |
| 115 | a | 933.95 | 1.44620 | YES | YES |
| 116 | a | 935.54 | 1.68784 | YES | YES |
| 117 | a | 950.20 | 0.28920 | YES | YES |
| 118 | a | 962.03 | 0.26452 | YES | YES |
| 119 | a | 970.99 | 3.51328 | YES | YES |
| 120 | a | 976.08 | 12.73348 | YES | YES |
| 121 | a | 983.25 | 0.03004 | YES | YES |
| 122 | a | 983.55 | 0.00810 | YES | YES |
| 123 | a | 984.07 | 0.00232 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 124 | a | 984.88 | 0.00245 | YES | YES |
| 125 | a | 999.51 | 3.73274 | YES | YES |
| 126 | a | 1001.54 | 1.39826 | YES | YES |
| 127 | a | 1015.54 | 3.32178 | YES | YES |
| 128 | a | 1015.74 | 3.99303 | YES | YES |
| 129 | a | 1016.67 | 5.33415 | YES | YES |
| 130 | a | 1016.78 | 2.99845 | YES | YES |
| 131 | a | 1024.30 | 0.92094 | YES | YES |
| 132 | a | 1025.08 | 1.47625 | YES | YES |
| 133 | a | 1028.71 | 2.20939 | YES | YES |
| 134 | a | 1047.75 | 22.25398 | YES | YES |
| 135 | a | 1051.78 | 11.08929 | YES | YES |
| 136 | a | 1072.68 | 0.27735 | YES | YES |
| 137 | a | 1073.06 | 2.08554 | YES | YES |
| 138 | a | 1074.92 | 7.45983 | YES | YES |
| 139 | a | 1077.19 | 9.52728 | YES | YES |
| 140 | a | 1078.18 | 56.76015 | YES | YES |
| 141 | a | 1079.06 | 48.49878 | YES | YES |
| 142 | a | 1080.39 | 5.27881 | YES | YES |
| 143 | a | 1131.66 | 5.89962 | YES | YES |
| 144 | a | 1134.16 | 0.66245 | YES | YES |
| 145 | a | 1137.30 | 17.01364 | YES | YES |
| 146 | a | 1139.22 | 20.41788 | YES | YES |
| 147 | a | 1141.33 | 4.75378 | YES | YES |
| 148 | a | 1141.60 | 2.76111 | YES | YES |
| 149 | a | 1141.68 | 1.86999 | YES | YES |
| 150 | a | 1141.82 | 3.13989 | YES | YES |
| 151 | a | 1229.78 | 0.40029 | YES | YES |
| 152 | a | 1231.53 | 110.74249 | YES | YES |
| 153 | a | 1236.23 | 349.69422 | YES | YES |
| 154 | a | 1244.24 | 88.25237 | YES | YES |
| 155 | a | 1245.13 | 1.94579 | YES | YES |
| 156 | a | 1245.39 | 1.67834 | YES | YES |
| 157 | a | 1245.64 | 18.49839 | YES | YES |
| 158 | a | 1245.75 | 18.91515 | YES | YES |
| 159 | a | 1252.36 | 0.58614 | YES | YES |
| 160 | a | 1299.85 | 2.50547 | YES | YES |
| 161 | a | 1309.80 | 1.25284 | YES | YES |
| 162 | a | 1357.35 | 0.64737 | YES | YES |
| 163 | a | 1358.99 | 2.12050 | YES | YES |
| 164 | a | 1363.82 | 4.98903 | YES | YES |
| 165 | a | 1365.17 | 8.40656 | YES | YES |
| 166 | a | 1371.45 | 9.21180 | YES | YES |
| 167 | a | 1374.06 | 8.64339 | YES | YES |
| 168 | a | 1379.69 | 3.60026 | YES | YES |
| 169 | a | 1379.89 | 2.58483 | YES | YES |
| 170 | a | 1380.76 | 10.14908 | YES | YES |
| 171 | a | 1380.99 | 2.81522 | YES | YES |
| 172 | a | 1384.46 | 1.06751 | YES | YES |
| 173 | a | 1390.54 | 10.70311 | YES | YES |
| 174 | a | 1403.01 | 1.12506 | YES | YES |
| 175 | a | 1409.36 | 8.10850 | YES | YES |
| 176 | a | 1413.05 | 4.73448 | YES | YES |
| 177 | a | 1422.25 | 6.67894 | YES | YES |
| 178 | a | 1423.46 | 50.42002 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 179 | a | 1428.48 | 3.80253 | YES | YES |
| 180 | a | 1438.54 | 35.79240 | YES | YES |
| 181 | a | 1443.25 | 4.85057 | YES | YES |
| 182 | a | 1448.03 | 44.15152 | YES | YES |
| 183 | a | 1452.73 | 4.38115 | YES | YES |
| 184 | a | 1456.97 | 8.07051 | YES | YES |
| 185 | a | 1457.18 | 12.90318 | YES | YES |
| 186 | a | 1457.59 | 7.44582 | YES | YES |
| 187 | a | 1457.83 | 4.92936 | YES | YES |
| 188 | a | 1465.91 | 27.34644 | YES | YES |
| 189 | a | 1469.04 | 11.17882 | YES | YES |
| 190 | a | 1488.49 | 30.67183 | YES | YES |
| 191 | a | 1489.00 | 467.33246 | YES | YES |
| 192 | a | 1489.20 | 186.23866 | YES | YES |
| 193 | a | 1493.42 | 178.81147 | YES | YES |
| 194 | a | 1549.75 | 0.04994 | YES | YES |
| 195 | a | 1555.80 | 0.14412 | YES | YES |
| 196 | a | 1604.73 | 0.47723 | YES | YES |
| 197 | a | 1605.15 | 0.11317 | YES | YES |
| 198 | a | 1606.05 | 0.07703 | YES | YES |
| 199 | a | 1606.87 | 1.25536 | YES | YES |
| 200 | a | 1636.40 | 16.96656 | YES | YES |
| 201 | a | 1636.80 | 6.34876 | YES | YES |
| 202 | a | 1639.01 | 13.36226 | YES | YES |
| 203 | a | 1639.24 | 6.15725 | YES | YES |
| 204 | a | 2950.76 | 2.69507 | YES | YES |
| 205 | a | 2953.49 | 4.61513 | YES | YES |
| 206 | a | 2954.68 | 4.61232 | YES | YES |
| 207 | a | 2955.42 | 0.69430 | YES | YES |
| 208 | a | 2962.33 | 1.40765 | YES | YES |
| 209 | a | 2964.11 | 3.83960 | YES | YES |
| 210 | a | 3020.21 | 5.78411 | YES | YES |
| 211 | a | 3027.05 | 5.54754 | YES | YES |
| 212 | a | 3031.66 | 4.94509 | YES | YES |
| 213 | a | 3034.51 | 4.19419 | YES | YES |
| 214 | a | 3034.82 | 2.18799 | YES | YES |
| 215 | a | 3049.45 | 5.82821 | YES | YES |
| 216 | a | 3087.24 | 1.34494 | YES | YES |
| 217 | a | 3091.42 | 7.64362 | YES | YES |
| 218 | a | 3093.61 | 2.83394 | YES | YES |
| 219 | a | 3099.29 | 6.40249 | YES | YES |
| 220 | a | 3100.54 | 4.59021 | YES | YES |
| 221 | a | 3105.48 | 7.57685 | YES | YES |
| 222 | a | 3126.16 | 0.49374 | YES | YES |
| 223 | a | 3126.27 | 0.58519 | YES | YES |
| 224 | a | 3126.65 | 0.47764 | YES | YES |
| 225 | a | 3127.06 | 0.54269 | YES | YES |
| 226 | a | 3133.30 | 1.25164 | YES | YES |
| 227 | a | 3133.46 | 1.01606 | YES | YES |
| 228 | a | 3134.06 | 0.83954 | YES | YES |
| 229 | a | 3134.22 | 0.95629 | YES | YES |
| 230 | a | 3138.61 | 4.23127 | YES | YES |
| 231 | a | 3138.79 | 4.65762 | YES | YES |
| 232 | a | 3139.27 | 3.54652 | YES | YES |
| 233 | a | 3139.40 | 4.08994 | YES | YES |

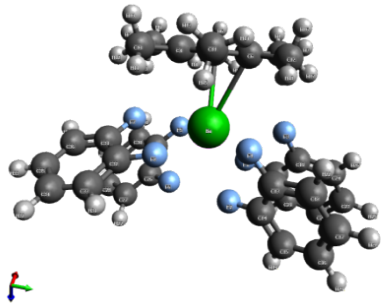
| | | | | | |
|---|---|---|---|---|---|
| 234 | a | 3144.42 | 3.43858 | YES | YES |
| 235 | a | 3144.48 | 2.97735 | YES | YES |
| 236 | a | 3144.74 | 2.95571 | YES | YES |
| 237 | a | 3145.08 | 3.20501 | YES | YES |

Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 c | -0.07623 | 0.0638 | -0.075347 |
| 2 c | -0.08006 | 0.0321 | -0.084491 |
| 3 c | -0.06491 | 0.0577 | -0.062545 |
| 4 c | -0.08235 | 0.0552 | -0.081059 |
| 5 c | -0.06896 | 0.0621 | -0.074434 |
| 6 c | -0.07503 | 0.0328 | -0.068855 |
| 7 c | -0.65486 | -0.1797 | -0.044644 |
| 8 h | 0.25970 | 0.0560 | 0.070665 |
| 9 h | 0.23309 | 0.0546 | 0.032754 |
| 10 h | 0.24258 | 0.0484 | 0.056184 |
| 11 c | -0.66281 | -0.1769 | -0.050208 |
| 12 h | 0.24140 | 0.0389 | 0.048839 |
| 13 h | 0.24085 | 0.0481 | 0.040877 |
| 14 h | 0.26280 | 0.0631 | 0.074018 |
| 15 c | -0.65685 | -0.1969 | -0.043617 |
| 16 h | 0.24314 | 0.0495 | 0.055385 |
| 17 h | 0.23653 | 0.0510 | 0.040417 |
| 18 h | 0.25840 | 0.0518 | 0.068796 |
| 19 c | -0.66443 | -0.1732 | -0.049519 |
| 20 h | 0.26506 | 0.0659 | 0.076266 |
| 21 h | 0.23821 | 0.0566 | 0.037694 |
| 22 h | 0.23778 | 0.0526 | 0.047783 |
| 23 c | -0.65980 | -0.1849 | -0.050051 |
| 24 h | 0.25651 | 0.0549 | 0.067086 |
| 25 h | 0.24638 | 0.0445 | 0.057877 |
| 26 h | 0.24088 | 0.0644 | 0.041720 |
| 27 c | -0.65782 | -0.2013 | -0.042291 |
| 28 h | 0.26288 | 0.0588 | 0.073782 |
| 29 h | 0.23713 | 0.0476 | 0.047909 |
| 30 h | 0.23513 | 0.0446 | 0.040455 |
| 31 c | 0.33143 | 0.2090 | 0.428372 |
| 32 c | 0.32141 | 0.2032 | 0.419579 |
| 33 c | -0.25951 | -0.0158 | -0.002869 |
| 34 h | 0.26540 | 0.0278 | 0.120133 |
| 35 c | -0.19728 | 0.0188 | -0.013885 |
| 36 h | 0.25830 | 0.0323 | 0.110348 |
| 37 c | -0.19589 | 0.0202 | -0.014985 |
| 38 h | 0.25917 | 0.0338 | 0.112801 |
| 39 c | -0.26318 | -0.0240 | -0.006421 |
| 40 h | 0.26426 | 0.0273 | 0.118092 |
| 41 f | -0.36901 | -0.2200 | -0.624493 |
| 42 f | -0.37004 | -0.2133 | -0.619080 |
| 43 c | 0.31645 | 0.1969 | 0.413318 |
| 44 c | 0.33089 | 0.2182 | 0.423031 |
| 45 c | -0.25884 | -0.0158 | -0.003490 |
| 46 h | 0.26623 | 0.0290 | 0.123412 |
| 47 c | -0.19398 | 0.0221 | -0.012877 |
| 48 h | 0.25960 | 0.0345 | 0.113777 |

| | | | | |
|---|---|---|---|---|
| 49 | c | -0.19518 | 0.0207 | -0.012802 |
| 50 | h | 0.25849 | 0.0327 | 0.111128 |
| 51 | c | -0.26117 | -0.0161 | -0.003013 |
| 52 | h | 0.26439 | 0.0258 | 0.118488 |
| 53 | f | -0.36929 | -0.2169 | -0.637684 |
| 54 | f | -0.37072 | -0.2009 | -0.615580 |
| 55 | c | 0.33094 | 0.2062 | 0.424922 |
| 56 | c | 0.32264 | 0.2024 | 0.422519 |
| 57 | c | -0.26022 | -0.0179 | -0.004512 |
| 58 | h | 0.26512 | 0.0276 | 0.120310 |
| 59 | c | -0.19692 | 0.0186 | -0.014123 |
| 60 | h | 0.25843 | 0.0327 | 0.111269 |
| 61 | c | -0.19524 | 0.0208 | -0.013892 |
| 62 | h | 0.25910 | 0.0337 | 0.113005 |
| 63 | c | -0.26296 | -0.0238 | -0.006145 |
| 64 | h | 0.26406 | 0.0270 | 0.118305 |
| 65 | f | -0.37162 | -0.2251 | -0.624829 |
| 66 | f | -0.36907 | -0.2134 | -0.617572 |
| 67 | c | 0.31797 | 0.1984 | 0.417551 |
| 68 | c | 0.33074 | 0.2148 | 0.416710 |
| 69 | c | -0.25818 | -0.0162 | -0.002764 |
| 70 | h | 0.26610 | 0.0283 | 0.124004 |
| 71 | c | -0.19296 | 0.0235 | -0.011092 |
| 72 | h | 0.25978 | 0.0347 | 0.114085 |
| 73 | c | -0.19402 | 0.0216 | -0.012397 |
| 74 | h | 0.25891 | 0.0333 | 0.112731 |
| 75 | c | -0.26117 | -0.0174 | -0.004625 |
| 76 | h | 0.26428 | 0.0260 | 0.119077 |
| 77 | f | -0.36790 | -0.2113 | -0.637504 |
| 78 | f | -0.37539 | -0.2080 | -0.618792 |
| 79 | sr | 1.78126 | 1.4120 | 1.657010 |

[Ba(HMB)oDFB$_4$]$^{2+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 2.4889610 | 0.9128569 | -2.0735830 |
| C | 2.8472608 | -0.4095713 | -1.6772551 |
| C | 2.0834884 | -1.5296352 | -2.1213680 |
| C | 0.8980848 | -1.3154139 | -2.8849600 |
| C | 0.5298287 | 0.0095741 | -3.2705847 |
| C | 1.3057863 | 1.1286155 | -2.8425264 |
| C | 3.4157515 | 2.0548158 | -1.7108161 |
| H | 4.4700239 | 1.7794412 | -1.9236673 |
| H | 3.3699207 | 2.3224517 | -0.6303949 |

| | | | |
|---|---|---|---|
| H | 3.2010425 | 2.9733735 | -2.2866976 |
| C | 4.0792855 | -0.6246459 | -0.8242575 |
| H | 4.0197732 | -1.5544520 | -0.2263087 |
| H | 4.2516352 | 0.2144935 | -0.1198149 |
| H | 4.9946694 | -0.7029038 | -1.4562376 |
| C | 2.5840457 | -2.9255460 | -1.8137203 |
| H | 2.1006472 | -3.6941769 | -2.4442611 |
| H | 2.4189462 | -3.2148029 | -0.7513384 |
| H | 3.6756192 | -2.9964284 | -2.0014903 |
| C | 0.0293549 | -2.4736633 | -3.3293470 |
| H | 0.2620039 | -2.7695196 | -4.3784318 |
| H | -1.0487438 | -2.2123178 | -3.3062642 |
| H | 0.1657172 | -3.3727797 | -2.7007433 |
| C | -0.6686069 | 0.2031897 | -4.1777600 |
| H | -0.7212647 | -0.5979081 | -4.9425385 |
| H | -0.6277922 | 1.1638364 | -4.7242596 |
| H | -1.6356885 | 0.1805607 | -3.6223556 |
| C | 0.8827952 | 2.5314337 | -3.2293249 |
| H | 1.2950444 | 2.8157960 | -4.2247629 |
| H | 1.2320674 | 3.2869172 | -2.5007566 |
| H | -0.2188420 | 2.6257033 | -3.2928811 |
| C | -2.3150852 | 2.8017150 | -0.3161867 |
| C | -2.3524207 | 2.5248882 | 1.0538315 |
| C | -2.8446335 | 3.4511456 | 1.9679057 |
| H | -2.8603802 | 3.2070561 | 3.0406394 |
| C | -3.3051446 | 4.6849296 | 1.4730858 |
| H | -3.7033025 | 5.4320938 | 2.1764451 |
| C | -3.2654787 | 4.9661290 | 0.0956750 |
| H | -3.6346205 | 5.9326960 | -0.2802583 |
| C | -2.7646546 | 4.0193210 | -0.8184396 |
| H | -2.7308133 | 4.2150623 | -1.9010321 |
| F | -1.7878318 | 1.8348638 | -1.1460879 |
| F | -1.8499075 | 1.3119561 | 1.4690590 |
| C | 0.6443236 | 3.4967930 | 1.1784550 |
| C | 0.8284129 | 2.7555377 | 2.3487372 |
| C | 0.7092330 | 3.3483966 | 3.6021821 |
| H | 0.8612758 | 2.7476682 | 4.5118651 |
| C | 0.4027324 | 4.7218577 | 3.6550225 |
| H | 0.3109132 | 5.2138645 | 4.6354904 |
| C | 0.2236249 | 5.4662282 | 2.4752081 |
| H | -0.0100050 | 6.5403231 | 2.5319167 |
| C | 0.3435887 | 4.8540920 | 1.2139793 |
| H | 0.2020948 | 5.4116466 | 0.2761983 |
| F | 0.7393570 | 2.8147305 | -0.0167861 |
| F | 1.1081108 | 1.4138567 | 2.2095673 |
| C | 1.2029331 | -2.4940951 | 2.4663385 |
| C | -0.1456877 | -2.3423497 | 2.8013626 |
| C | -0.7879242 | -3.2473011 | 3.6411729 |
| H | -1.8520965 | -3.1075328 | 3.8844333 |
| C | -0.0368386 | -4.3211773 | 4.1549022 |
| H | -0.5223118 | -5.0450531 | 4.8271951 |
| C | 1.3209967 | -4.4713583 | 3.8213009 |
| H | 1.9003469 | -5.3119883 | 4.2329584 |
| C | 1.9568275 | -3.5523355 | 2.9645334 |
| H | 3.0187289 | -3.6484478 | 2.6913479 |

| | | | |
|---|---|---|---|
| F | 1.7566183 | -1.5711504 | 1.6022676 |
| F | -0.8278835 | -1.2820574 | 2.2467060 |
| C | -1.4041350 | -3.3955272 | -0.0400373 |
| C | -2.5213442 | -2.5975442 | -0.2980674 |
| C | -3.8119306 | -3.1063599 | -0.1902888 |
| H | -4.6782987 | -2.4611292 | -0.4012940 |
| C | -3.9586857 | -4.4541939 | 0.1903233 |
| H | -4.9699446 | -4.8800596 | 0.2778554 |
| C | -2.8330160 | -5.2545356 | 0.4562043 |
| H | -2.9630889 | -6.3066274 | 0.7524902 |
| C | -1.5331337 | -4.7260097 | 0.3445924 |
| H | -0.6345300 | -5.3274498 | 0.5489681 |
| F | -0.1644072 | -2.8066396 | -0.1619266 |
| F | -2.2948910 | -1.2824857 | -0.6517533 |
| Ba | 0.1534922 | 0.0172631 | -0.1093505 |

Vibrational analysis

| 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 | 8.25 | 0.10368 | YES | YES |
| 8 | a | 12.80 | 0.03774 | YES | YES |
| 9 | a | 14.66 | 0.04464 | YES | YES |
| 10 | a | 16.87 | 0.33786 | YES | YES |
| 11 | a | 20.11 | 0.68253 | YES | YES |
| 12 | a | 20.64 | 0.33130 | YES | YES |
| 13 | a | 27.44 | 0.02214 | YES | YES |
| 14 | a | 30.41 | 0.69285 | YES | YES |
| 15 | a | 31.77 | 0.48136 | YES | YES |
| 16 | a | 40.05 | 0.19350 | YES | YES |
| 17 | a | 45.64 | 0.49259 | YES | YES |
| 18 | a | 52.12 | 1.56908 | YES | YES |
| 19 | a | 55.27 | 0.06357 | YES | YES |
| 20 | a | 58.90 | 1.36898 | YES | YES |
| 21 | a | 61.23 | 0.57878 | YES | YES |
| 22 | a | 65.37 | 3.91281 | YES | YES |
| 23 | a | 69.62 | 0.90058 | YES | YES |
| 24 | a | 72.83 | 1.43005 | YES | YES |
| 25 | a | 76.28 | 0.67063 | YES | YES |
| 26 | a | 81.46 | 0.47924 | YES | YES |
| 27 | a | 82.19 | 0.68899 | YES | YES |
| 28 | a | 84.24 | 0.08962 | YES | YES |
| 29 | a | 87.49 | 1.32036 | YES | YES |
| 30 | a | 89.02 | 0.49685 | YES | YES |
| 31 | a | 95.74 | 2.83432 | YES | YES |
| 32 | a | 104.04 | 1.36213 | YES | YES |
| 33 | a | 112.97 | 0.85080 | YES | YES |
| 34 | a | 117.58 | 3.14174 | YES | YES |
| 35 | a | 120.17 | 6.49993 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 36 | a | 125.49 | 7.05260 | YES | YES |
| 37 | a | 129.47 | 8.56123 | YES | YES |
| 38 | a | 137.02 | 25.83530 | YES | YES |
| 39 | a | 138.56 | 4.30001 | YES | YES |
| 40 | a | 149.68 | 0.36582 | YES | YES |
| 41 | a | 157.38 | 3.63143 | YES | YES |
| 42 | a | 180.12 | 1.20019 | YES | YES |
| 43 | a | 197.95 | 0.12911 | YES | YES |
| 44 | a | 198.84 | 0.06105 | YES | YES |
| 45 | a | 203.53 | 0.48740 | YES | YES |
| 46 | a | 205.79 | 0.12740 | YES | YES |
| 47 | a | 240.86 | 38.52820 | YES | YES |
| 48 | a | 284.86 | 0.09482 | YES | YES |
| 49 | a | 286.23 | 1.02969 | YES | YES |
| 50 | a | 289.80 | 0.51535 | YES | YES |
| 51 | a | 293.25 | 2.03727 | YES | YES |
| 52 | a | 298.17 | 2.88415 | YES | YES |
| 53 | a | 299.40 | 1.26946 | YES | YES |
| 54 | a | 301.91 | 11.75610 | YES | YES |
| 55 | a | 305.10 | 3.30726 | YES | YES |
| 56 | a | 332.55 | 0.42992 | YES | YES |
| 57 | a | 348.63 | 0.48474 | YES | YES |
| 58 | a | 367.66 | 0.85590 | YES | YES |
| 59 | a | 379.15 | 1.46455 | YES | YES |
| 60 | a | 394.21 | 0.01623 | YES | YES |
| 61 | a | 409.45 | 0.01124 | YES | YES |
| 62 | a | 431.80 | 0.01151 | YES | YES |
| 63 | a | 432.04 | 0.05190 | YES | YES |
| 64 | a | 433.29 | 0.04361 | YES | YES |
| 65 | a | 433.69 | 0.09687 | YES | YES |
| 66 | a | 439.06 | 5.99227 | YES | YES |
| 67 | a | 440.21 | 0.31673 | YES | YES |
| 68 | a | 440.87 | 2.45738 | YES | YES |
| 69 | a | 442.06 | 0.09835 | YES | YES |
| 70 | a | 443.49 | 2.83676 | YES | YES |
| 71 | a | 443.98 | 0.02930 | YES | YES |
| 72 | a | 445.20 | 0.01294 | YES | YES |
| 73 | a | 532.73 | 1.92846 | YES | YES |
| 74 | a | 533.33 | 2.00200 | YES | YES |
| 75 | a | 533.74 | 3.32280 | YES | YES |
| 76 | a | 534.70 | 0.85502 | YES | YES |
| 77 | a | 537.46 | 4.94462 | YES | YES |
| 78 | a | 538.60 | 4.50592 | YES | YES |
| 79 | a | 539.24 | 0.94995 | YES | YES |
| 80 | a | 539.38 | 0.76584 | YES | YES |
| 81 | a | 548.27 | 2.04697 | YES | YES |
| 82 | a | 555.75 | 3.94094 | YES | YES |
| 83 | a | 556.80 | 53.54862 | YES | YES |
| 84 | a | 557.18 | 7.37191 | YES | YES |
| 85 | a | 558.10 | 18.75760 | YES | YES |
| 86 | a | 568.13 | 1.21435 | YES | YES |
| 87 | a | 570.01 | 0.37776 | YES | YES |
| 88 | a | 573.84 | 1.29645 | YES | YES |
| 89 | a | 580.35 | 1.12249 | YES | YES |
| 90 | a | 665.39 | 0.04924 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 91 | a | 667.18 | 0.05506 | YES | YES |
| 92 | a | 667.79 | 0.20970 | YES | YES |
| 93 | a | 670.09 | 0.03533 | YES | YES |
| 94 | a | 691.57 | 0.47711 | YES | YES |
| 95 | a | 745.92 | 30.20572 | YES | YES |
| 96 | a | 746.70 | 32.73657 | YES | YES |
| 97 | a | 748.89 | 150.61956 | YES | YES |
| 98 | a | 749.59 | 168.92380 | YES | YES |
| 99 | a | 750.88 | 140.05268 | YES | YES |
| 100 | a | 752.46 | 14.05212 | YES | YES |
| 101 | a | 752.85 | 32.52761 | YES | YES |
| 102 | a | 754.28 | 79.76607 | YES | YES |
| 103 | a | 793.64 | 1.28369 | YES | YES |
| 104 | a | 799.81 | 3.29087 | YES | YES |
| 105 | a | 813.78 | 1.28638 | YES | YES |
| 106 | a | 814.73 | 0.60547 | YES | YES |
| 107 | a | 815.53 | 24.53279 | YES | YES |
| 108 | a | 816.38 | 24.20661 | YES | YES |
| 109 | a | 837.94 | 0.09280 | YES | YES |
| 110 | a | 840.25 | 0.00479 | YES | YES |
| 111 | a | 840.51 | 0.27622 | YES | YES |
| 112 | a | 842.08 | 0.10510 | YES | YES |
| 113 | a | 932.51 | 3.67887 | YES | YES |
| 114 | a | 933.60 | 0.91464 | YES | YES |
| 115 | a | 933.81 | 2.05489 | YES | YES |
| 116 | a | 935.20 | 1.95409 | YES | YES |
| 117 | a | 955.27 | 0.29683 | YES | YES |
| 118 | a | 962.98 | 0.26605 | YES | YES |
| 119 | a | 973.29 | 4.71375 | YES | YES |
| 120 | a | 974.61 | 7.60396 | YES | YES |
| 121 | a | 981.52 | 0.07555 | YES | YES |
| 122 | a | 982.20 | 0.06408 | YES | YES |
| 123 | a | 982.96 | 0.02201 | YES | YES |
| 124 | a | 984.34 | 0.00373 | YES | YES |
| 125 | a | 998.98 | 2.04417 | YES | YES |
| 126 | a | 1000.80 | 0.61908 | YES | YES |
| 127 | a | 1016.67 | 3.81913 | YES | YES |
| 128 | a | 1017.10 | 0.69461 | YES | YES |
| 129 | a | 1017.79 | 7.20998 | YES | YES |
| 130 | a | 1017.88 | 2.51908 | YES | YES |
| 131 | a | 1026.54 | 2.08644 | YES | YES |
| 132 | a | 1026.79 | 1.61189 | YES | YES |
| 133 | a | 1027.62 | 4.36817 | YES | YES |
| 134 | a | 1051.50 | 18.33627 | YES | YES |
| 135 | a | 1052.29 | 13.72024 | YES | YES |
| 136 | a | 1074.24 | 0.72554 | YES | YES |
| 137 | a | 1074.43 | 1.75690 | YES | YES |
| 138 | a | 1076.56 | 4.89698 | YES | YES |
| 139 | a | 1077.98 | 26.90731 | YES | YES |
| 140 | a | 1078.32 | 1.11352 | YES | YES |
| 141 | a | 1079.26 | 27.08201 | YES | YES |
| 142 | a | 1080.87 | 50.95287 | YES | YES |
| 143 | a | 1134.62 | 5.05861 | YES | YES |
| 144 | a | 1136.49 | 1.57092 | YES | YES |
| 145 | a | 1139.20 | 10.32445 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 146 | a | 1141.06 | 6.00014 | YES | YES |
| 147 | a | 1141.21 | 5.31033 | YES | YES |
| 148 | a | 1141.42 | 0.10433 | YES | YES |
| 149 | a | 1141.54 | 4.16624 | YES | YES |
| 150 | a | 1143.49 | 20.68458 | YES | YES |
| 151 | a | 1230.64 | 1.34438 | YES | YES |
| 152 | a | 1231.70 | 67.33976 | YES | YES |
| 153 | a | 1237.97 | 383.35286 | YES | YES |
| 154 | a | 1244.25 | 49.86073 | YES | YES |
| 155 | a | 1244.77 | 1.14421 | YES | YES |
| 156 | a | 1244.89 | 8.83866 | YES | YES |
| 157 | a | 1245.53 | 6.30625 | YES | YES |
| 158 | a | 1246.29 | 83.69212 | YES | YES |
| 159 | a | 1252.31 | 0.60547 | YES | YES |
| 160 | a | 1301.95 | 3.66440 | YES | YES |
| 161 | a | 1316.67 | 0.66877 | YES | YES |
| 162 | a | 1359.55 | 0.77542 | YES | YES |
| 163 | a | 1359.75 | 2.32653 | YES | YES |
| 164 | a | 1365.18 | 3.77193 | YES | YES |
| 165 | a | 1368.59 | 6.90292 | YES | YES |
| 166 | a | 1369.37 | 16.48300 | YES | YES |
| 167 | a | 1375.35 | 3.31853 | YES | YES |
| 168 | a | 1378.84 | 1.91325 | YES | YES |
| 169 | a | 1379.77 | 7.35276 | YES | YES |
| 170 | a | 1380.04 | 2.22735 | YES | YES |
| 171 | a | 1380.69 | 1.66021 | YES | YES |
| 172 | a | 1384.39 | 0.09092 | YES | YES |
| 173 | a | 1389.56 | 7.65715 | YES | YES |
| 174 | a | 1401.08 | 0.08630 | YES | YES |
| 175 | a | 1405.59 | 0.03302 | YES | YES |
| 176 | a | 1416.98 | 9.97851 | YES | YES |
| 177 | a | 1419.18 | 69.75995 | YES | YES |
| 178 | a | 1425.21 | 4.11524 | YES | YES |
| 179 | a | 1434.25 | 1.75977 | YES | YES |
| 180 | a | 1439.08 | 0.65708 | YES | YES |
| 181 | a | 1443.33 | 49.52231 | YES | YES |
| 182 | a | 1449.35 | 61.85886 | YES | YES |
| 183 | a | 1456.42 | 12.84238 | YES | YES |
| 184 | a | 1457.02 | 2.88889 | YES | YES |
| 185 | a | 1457.59 | 15.10505 | YES | YES |
| 186 | a | 1457.71 | 3.77221 | YES | YES |
| 187 | a | 1458.11 | 2.29074 | YES | YES |
| 188 | a | 1466.70 | 10.79132 | YES | YES |
| 189 | a | 1476.75 | 4.45613 | YES | YES |
| 190 | a | 1488.19 | 15.18794 | YES | YES |
| 191 | a | 1489.47 | 120.88166 | YES | YES |
| 192 | a | 1489.92 | 542.04246 | YES | YES |
| 193 | a | 1494.13 | 191.06057 | YES | YES |
| 194 | a | 1553.02 | 0.03805 | YES | YES |
| 195 | a | 1556.38 | 0.20849 | YES | YES |
| 196 | a | 1605.87 | 0.27402 | YES | YES |
| 197 | a | 1606.13 | 0.06858 | YES | YES |
| 198 | a | 1607.19 | 0.18824 | YES | YES |
| 199 | a | 1608.32 | 0.99739 | YES | YES |
| 200 | a | 1632.84 | 13.16786 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 201 | a | 1633.50 | 9.72745 | YES | YES |
| 202 | a | 1634.70 | 12.02043 | YES | YES |
| 203 | a | 1635.66 | 9.04771 | YES | YES |
| 204 | a | 2942.97 | 4.51416 | YES | YES |
| 205 | a | 2948.35 | 3.02387 | YES | YES |
| 206 | a | 2951.73 | 4.69667 | YES | YES |
| 207 | a | 2953.09 | 1.94930 | YES | YES |
| 208 | a | 2957.03 | 0.99779 | YES | YES |
| 209 | a | 2957.50 | 5.41310 | YES | YES |
| 210 | a | 3027.79 | 6.62398 | YES | YES |
| 211 | a | 3029.97 | 7.83777 | YES | YES |
| 212 | a | 3033.10 | 2.26764 | YES | YES |
| 213 | a | 3036.03 | 1.76437 | YES | YES |
| 214 | a | 3039.07 | 2.61883 | YES | YES |
| 215 | a | 3047.88 | 5.29761 | YES | YES |
| 216 | a | 3073.88 | 4.18960 | YES | YES |
| 217 | a | 3080.57 | 3.16833 | YES | YES |
| 218 | a | 3082.77 | 3.61285 | YES | YES |
| 219 | a | 3088.25 | 2.78801 | YES | YES |
| 220 | a | 3093.13 | 5.45378 | YES | YES |
| 221 | a | 3094.71 | 3.56064 | YES | YES |
| 222 | a | 3125.46 | 0.57056 | YES | YES |
| 223 | a | 3125.75 | 0.56891 | YES | YES |
| 224 | a | 3125.95 | 0.40281 | YES | YES |
| 225 | a | 3126.57 | 0.56824 | YES | YES |
| 226 | a | 3132.99 | 1.19990 | YES | YES |
| 227 | a | 3133.43 | 0.84394 | YES | YES |
| 228 | a | 3133.75 | 1.07875 | YES | YES |
| 229 | a | 3134.05 | 0.85697 | YES | YES |
| 230 | a | 3138.32 | 4.19927 | YES | YES |
| 231 | a | 3138.94 | 4.05184 | YES | YES |
| 232 | a | 3138.95 | 3.71559 | YES | YES |
| 233 | a | 3139.60 | 3.72728 | YES | YES |
| 234 | a | 3144.12 | 2.85284 | YES | YES |
| 235 | a | 3144.51 | 2.68263 | YES | YES |
| 236 | a | 3144.72 | 2.91258 | YES | YES |
| 237 | a | 3144.83 | 3.09223 | YES | YES |

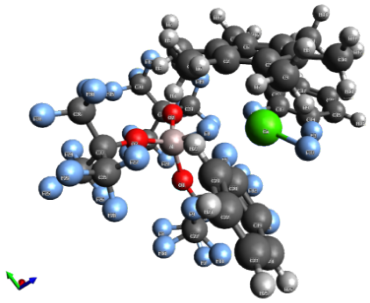
Charge analysis by NBO, PABOON & QTAIM

| Atom | Charge (NBO) | Charge (PABOON) | Charge (QTAIM) |
|---|---|---|---|
| 1 c | -0.06666 | 0.0563 | -0.067601 |
| 2 c | -0.07960 | 0.0213 | -0.083101 |
| 3 c | -0.06316 | 0.0725 | -0.061692 |
| 4 c | -0.07649 | 0.0704 | -0.074080 |
| 5 c | -0.06574 | 0.0753 | -0.069643 |
| 6 c | -0.07601 | 0.0286 | -0.072267 |
| 7 c | -0.65913 | -0.1966 | -0.048158 |
| 8 h | 0.25694 | 0.0541 | 0.067906 |
| 9 h | 0.23524 | 0.0482 | 0.035231 |
| 10 h | 0.24688 | 0.0487 | 0.059194 |
| 11 c | -0.66701 | -0.1944 | -0.056742 |
| 12 h | 0.24017 | 0.0413 | 0.045083 |
| 13 h | 0.24011 | 0.0424 | 0.039907 |
| 14 h | 0.26426 | 0.0658 | 0.076400 |
| 15 c | -0.65847 | -0.1993 | -0.046570 |

| | | | | |
|---|---|---|---|---|
| 16 | h | 0.24584 | 0.0505 | 0.057781 |
| 17 | h | 0.23483 | 0.0489 | 0.036874 |
| 18 | h | 0.25571 | 0.0509 | 0.066224 |
| 19 | c | -0.66667 | -0.1894 | -0.051137 |
| 20 | h | 0.26451 | 0.0672 | 0.075665 |
| 21 | h | 0.23748 | 0.0512 | 0.036954 |
| 22 | h | 0.23743 | 0.0492 | 0.046848 |
| 23 | c | -0.66134 | -0.1984 | -0.052111 |
| 24 | h | 0.25450 | 0.0542 | 0.065336 |
| 25 | h | 0.24917 | 0.0474 | 0.061299 |
| 26 | h | 0.23858 | 0.0559 | 0.036058 |
| 27 | c | -0.66523 | -0.2094 | -0.050075 |
| 28 | h | 0.26313 | 0.0620 | 0.074027 |
| 29 | h | 0.23850 | 0.0459 | 0.047491 |
| 30 | h | 0.23600 | 0.0442 | 0.039837 |
| 31 | c | 0.32678 | 0.2051 | 0.426127 |
| 32 | c | 0.32220 | 0.2064 | 0.424791 |
| 33 | c | -0.26045 | -0.0125 | -0.001068 |
| 34 | h | 0.26532 | 0.0279 | 0.119174 |
| 35 | c | -0.19697 | 0.0238 | -0.013373 |
| 36 | h | 0.25747 | 0.0318 | 0.107877 |
| 37 | c | -0.19877 | 0.0209 | -0.016861 |
| 38 | h | 0.25834 | 0.0334 | 0.110318 |
| 39 | c | -0.26489 | -0.0229 | -0.008066 |
| 40 | h | 0.26418 | 0.0282 | 0.117752 |
| 41 | f | -0.36693 | -0.2168 | -0.621410 |
| 42 | f | -0.36455 | -0.1963 | -0.618652 |
| 43 | c | 0.31762 | 0.1959 | 0.413730 |
| 44 | c | 0.32855 | 0.2174 | 0.430025 |
| 45 | c | -0.26154 | -0.0198 | -0.006935 |
| 46 | h | 0.26620 | 0.0302 | 0.122771 |
| 47 | c | -0.19716 | 0.0218 | -0.015176 |
| 48 | h | 0.25861 | 0.0338 | 0.110729 |
| 49 | c | -0.19627 | 0.0242 | -0.013384 |
| 50 | h | 0.25748 | 0.0318 | 0.108602 |
| 51 | c | -0.26286 | -0.0128 | -0.001476 |
| 52 | h | 0.26416 | 0.0263 | 0.116284 |
| 53 | f | -0.36689 | -0.2143 | -0.633773 |
| 54 | f | -0.36531 | -0.1741 | -0.615245 |
| 55 | c | 0.33033 | 0.2071 | 0.427061 |
| 56 | c | 0.32282 | 0.2046 | 0.428081 |
| 57 | c | -0.26157 | -0.0182 | -0.005302 |
| 58 | h | 0.26469 | 0.0285 | 0.119185 |
| 59 | c | -0.19854 | 0.0191 | -0.015261 |
| 60 | h | 0.25766 | 0.0326 | 0.109370 |
| 61 | c | -0.19710 | 0.0209 | -0.015195 |
| 62 | h | 0.25865 | 0.0341 | 0.111416 |
| 63 | c | -0.26413 | -0.0237 | -0.007255 |
| 64 | h | 0.26402 | 0.0282 | 0.118429 |
| 65 | f | -0.37019 | -0.2250 | -0.622087 |
| 66 | f | -0.36573 | -0.2132 | -0.618880 |
| 67 | c | 0.31667 | 0.1957 | 0.418354 |
| 68 | c | 0.33091 | 0.2150 | 0.422986 |
| 69 | c | -0.25899 | -0.0174 | -0.003978 |
| 70 | h | 0.26609 | 0.0302 | 0.123267 |

| | | | | |
|---|---|---|---|---|
| 71 | c | -0.19379 | 0.0246 | -0.011890 |
| 72 | h | 0.25931 | 0.0351 | 0.113300 |
| 73 | c | -0.19551 | 0.0226 | -0.013278 |
| 74 | h | 0.25798 | 0.0329 | 0.110809 |
| 75 | c | -0.26296 | -0.0159 | -0.005198 |
| 76 | h | 0.26358 | 0.0264 | 0.117321 |
| 77 | f | -0.36693 | -0.2046 | -0.637922 |
| 78 | f | -0.37070 | -0.2121 | -0.619995 |
| 79 | ba | 1.79533 | 1.4181 | 1.678964 |

F-Ca(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Ca | -0.43405 | -1.00428 | 1.61655 |
| F | -0.07355 | 0.02985 | -0.32367 |
| Al | 0.29743 | 0.26363 | -2.01001 |
| C | 0.27480 | 2.24627 | 1.68135 |
| C | -1.04482 | 2.05541 | 2.17920 |
| C | -1.25171 | 1.22588 | 3.31753 |
| C | -0.12851 | 0.66694 | 4.00236 |
| C | 1.19704 | 0.89588 | 3.52885 |
| C | 1.39489 | 1.68662 | 2.35707 |
| C | 0.49943 | 3.06185 | 0.42956 |
| H | 1.30911 | 2.64077 | -0.19654 |
| H | 0.79603 | 4.10874 | 0.67691 |
| H | -0.40352 | 3.11584 | -0.20432 |
| C | -2.18819 | 2.74950 | 1.47046 |
| H | -2.36807 | 2.32270 | 0.46088 |
| H | -1.96164 | 3.82700 | 1.32342 |
| H | -3.13575 | 2.69175 | 2.03836 |
| C | -2.62988 | 0.88839 | 3.84491 |
| H | -3.44384 | 1.26480 | 3.19898 |
| H | -2.79097 | 1.30428 | 4.86529 |
| H | -2.73989 | -0.21608 | 3.90723 |
| C | -0.39866 | -0.16595 | 5.23771 |
| H | -0.95354 | -1.08863 | 4.95284 |
| H | -1.03392 | 0.39128 | 5.96060 |
| H | 0.52288 | -0.46201 | 5.77198 |
| C | 2.36435 | 0.32660 | 4.31515 |
| H | 2.19974 | -0.73415 | 4.59474 |
| H | 2.51337 | 0.88858 | 5.26578 |
| H | 3.31928 | 0.36617 | 3.75937 |
| C | 2.76654 | 1.97872 | 1.78796 |
| H | 3.59157 | 1.55856 | 2.39281 |

| | | | |
|---|---|---|---|
| H | 2.93796 | 3.07525 | 1.71533 |
| H | 2.86610 | 1.58099 | 0.75604 |
| C | 3.06218 | -1.62715 | 1.61617 |
| C | 2.57806 | -2.56125 | 2.53704 |
| C | 3.44096 | -3.29042 | 3.35158 |
| H | 3.02630 | -4.01549 | 4.06790 |
| C | 4.82331 | -3.05815 | 3.22848 |
| H | 5.52388 | -3.62328 | 3.86252 |
| C | 5.31018 | -2.11307 | 2.30820 |
| H | 6.39332 | -1.93615 | 2.22113 |
| C | 4.42808 | -1.38390 | 1.48993 |
| H | 4.77910 | -0.63831 | 0.76398 |
| F | 2.14344 | -0.94517 | 0.88472 |
| F | 1.22465 | -2.70354 | 2.63252 |
| C | -3.99584 | -2.30071 | 0.81058 |
| C | -3.85477 | -0.90595 | 0.81841 |
| C | -4.94989 | -0.05885 | 0.97065 |
| H | -4.79152 | 1.02872 | 0.94470 |
| C | -6.22565 | -0.62615 | 1.13400 |
| H | -7.10065 | 0.03140 | 1.25297 |
| C | -6.37961 | -2.02286 | 1.14200 |
| H | -7.37830 | -2.46836 | 1.27190 |
| C | -5.26519 | -2.86341 | 0.97835 |
| H | -5.35799 | -3.96017 | 0.97391 |
| F | -2.92030 | -3.07803 | 0.62805 |
| F | -2.60722 | -0.36928 | 0.66285 |
| O | 0.33200 | -1.33094 | -2.74159 |
| C | -0.10292 | -2.60265 | -2.61782 |
| C | 0.42582 | -3.41816 | -3.86196 |
| F | 1.74320 | -3.67716 | -3.72399 |
| F | -0.21800 | -4.59876 | -3.99545 |
| F | 0.25579 | -2.71030 | -4.98240 |
| C | -1.67671 | -2.65660 | -2.58910 |
| F | -2.13733 | -1.67290 | -1.78017 |
| F | -2.18444 | -2.44512 | -3.81278 |
| F | -2.14900 | -3.83064 | -2.12838 |
| C | 0.47496 | -3.26767 | -1.30938 |
| F | -0.21897 | -2.82207 | -0.18963 |
| F | 0.38349 | -4.60094 | -1.29833 |
| F | 1.74973 | -2.91511 | -1.11829 |
| O | 1.93972 | 0.90332 | -1.95850 |
| C | 3.02158 | 1.06550 | -2.76329 |
| C | 3.31070 | 2.60699 | -2.90635 |
| F | 2.40009 | 3.17277 | -3.72128 |
| F | 4.54052 | 2.85663 | -3.40123 |
| F | 3.21854 | 3.21235 | -1.70674 |
| C | 4.25138 | 0.34817 | -2.09993 |
| F | 3.90900 | -0.88496 | -1.68795 |
| F | 4.67085 | 1.03103 | -1.00094 |
| F | 5.30072 | 0.24203 | -2.93619 |
| C | 2.79447 | 0.44666 | -4.19885 |
| F | 2.99210 | -0.88482 | -4.19440 |
| F | 3.60660 | 0.98378 | -5.12719 |
| F | 1.51725 | 0.66918 | -4.57442 |
| O | -0.89448 | 1.39781 | -2.55038 |

| | | | |
|---|---|---|---|
| C | -1.84233 | 1.98484 | -3.30860 |
| C | -1.62107 | 1.67254 | -4.83701 |
| F | -0.59684 | 2.39961 | -5.32559 |
| F | -2.71720 | 1.94696 | -5.57413 |
| F | -1.31762 | 0.37286 | -4.99735 |
| C | -3.26927 | 1.46423 | -2.88175 |
| F | -3.33884 | 1.35314 | -1.53752 |
| F | -3.50770 | 0.24280 | -3.39708 |
| F | -4.25812 | 2.28744 | -3.28258 |
| C | -1.76023 | 3.54097 | -3.07576 |
| F | -2.27907 | 3.86214 | -1.86299 |
| F | -2.43713 | 4.23813 | -4.00828 |
| F | -0.48197 | 3.94453 | -3.08379 |
| F | -1.60578 | -1.97924 | 2.92216 |

Vibrational analysis

| 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 | 8.12 | 0.22432 | YES | YES |
| 8 | a | 14.28 | 0.27226 | YES | YES |
| 9 | a | 18.06 | 0.76283 | YES | YES |
| 10 | a | 19.75 | 1.34408 | YES | YES |
| 11 | a | 21.25 | 0.81353 | YES | YES |
| 12 | a | 22.70 | 0.34642 | YES | YES |
| 13 | a | 24.17 | 0.17037 | YES | YES |
| 14 | a | 27.02 | 0.31529 | YES | YES |
| 15 | a | 28.42 | 0.13337 | YES | YES |
| 16 | a | 29.99 | 0.03676 | YES | YES |
| 17 | a | 33.92 | 0.25916 | YES | YES |
| 18 | a | 38.32 | 0.75117 | YES | YES |
| 19 | a | 40.57 | 0.49536 | YES | YES |
| 20 | a | 42.82 | 0.54981 | YES | YES |
| 21 | a | 44.42 | 0.62319 | YES | YES |
| 22 | a | 47.24 | 0.99774 | YES | YES |
| 23 | a | 48.78 | 0.16622 | YES | YES |
| 24 | a | 51.58 | 0.62181 | YES | YES |
| 25 | a | 55.50 | 2.49974 | YES | YES |
| 26 | a | 59.13 | 0.43375 | YES | YES |
| 27 | a | 62.19 | 0.16060 | YES | YES |
| 28 | a | 64.56 | 1.48953 | YES | YES |
| 29 | a | 67.84 | 1.63699 | YES | YES |
| 30 | a | 69.24 | 0.70990 | YES | YES |
| 31 | a | 71.22 | 1.70676 | YES | YES |
| 32 | a | 71.79 | 0.33416 | YES | YES |
| 33 | a | 74.14 | 0.48348 | YES | YES |
| 34 | a | 75.11 | 0.11235 | YES | YES |
| 35 | a | 75.83 | 0.11755 | YES | YES |
| 36 | a | 78.00 | 0.44727 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 37 | a | 80.16 | 0.21693 | YES | YES |
| 38 | a | 83.81 | 2.00626 | YES | YES |
| 39 | a | 84.32 | 0.51089 | YES | YES |
| 40 | a | 86.70 | 0.20793 | YES | YES |
| 41 | a | 88.14 | 1.34063 | YES | YES |
| 42 | a | 90.99 | 0.56774 | YES | YES |
| 43 | a | 91.83 | 0.54327 | YES | YES |
| 44 | a | 93.81 | 0.64027 | YES | YES |
| 45 | a | 97.08 | 1.11997 | YES | YES |
| 46 | a | 102.58 | 2.89566 | YES | YES |
| 47 | a | 104.90 | 1.51324 | YES | YES |
| 48 | a | 116.31 | 3.36578 | YES | YES |
| 49 | a | 121.25 | 7.48985 | YES | YES |
| 50 | a | 129.31 | 0.50366 | YES | YES |
| 51 | a | 131.57 | 11.12188 | YES | YES |
| 52 | a | 139.36 | 55.92803 | YES | YES |
| 53 | a | 147.39 | 11.99173 | YES | YES |
| 54 | a | 151.78 | 1.08121 | YES | YES |
| 55 | a | 154.55 | 5.39176 | YES | YES |
| 56 | a | 156.37 | 0.50780 | YES | YES |
| 57 | a | 157.13 | 0.67508 | YES | YES |
| 58 | a | 157.59 | 2.04202 | YES | YES |
| 59 | a | 162.17 | 0.73196 | YES | YES |
| 60 | a | 166.49 | 0.87416 | YES | YES |
| 61 | a | 168.67 | 10.11283 | YES | YES |
| 62 | a | 171.38 | 32.99594 | YES | YES |
| 63 | a | 179.99 | 1.72715 | YES | YES |
| 64 | a | 181.56 | 4.81724 | YES | YES |
| 65 | a | 193.30 | 20.83165 | YES | YES |
| 66 | a | 197.77 | 4.75145 | YES | YES |
| 67 | a | 200.77 | 1.80085 | YES | YES |
| 68 | a | 206.43 | 5.61386 | YES | YES |
| 69 | a | 207.31 | 2.58547 | YES | YES |
| 70 | a | 210.32 | 2.90563 | YES | YES |
| 71 | a | 217.08 | 6.41446 | YES | YES |
| 72 | a | 219.64 | 12.86147 | YES | YES |
| 73 | a | 254.42 | 9.94697 | YES | YES |
| 74 | a | 261.66 | 0.65596 | YES | YES |
| 75 | a | 265.46 | 3.38664 | YES | YES |
| 76 | a | 272.50 | 1.87086 | YES | YES |
| 77 | a | 276.51 | 8.06041 | YES | YES |
| 78 | a | 279.96 | 2.58178 | YES | YES |
| 79 | a | 282.77 | 1.52659 | YES | YES |
| 80 | a | 284.60 | 0.02434 | YES | YES |
| 81 | a | 284.91 | 0.58463 | YES | YES |
| 82 | a | 286.14 | 1.09043 | YES | YES |
| 83 | a | 288.11 | 0.29245 | YES | YES |
| 84 | a | 293.58 | 0.42157 | YES | YES |
| 85 | a | 300.42 | 0.57251 | YES | YES |
| 86 | a | 303.55 | 5.64834 | YES | YES |
| 87 | a | 305.81 | 6.09503 | YES | YES |
| 88 | a | 307.29 | 9.51677 | YES | YES |
| 89 | a | 308.19 | 0.61745 | YES | YES |
| 90 | a | 314.19 | 0.88054 | YES | YES |
| 91 | a | 315.58 | 1.06644 | YES | YES |

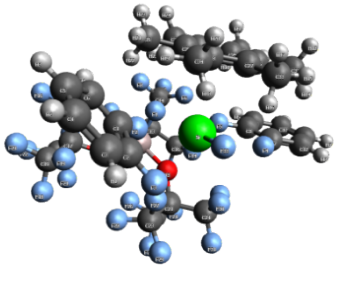
| | | | | | |
|---|---|---|---|---|---|
| 92 | a | 318.23 | 2.76938 | YES | YES |
| 93 | a | 319.54 | 1.10047 | YES | YES |
| 94 | a | 320.94 | 0.53487 | YES | YES |
| 95 | a | 327.59 | 0.95913 | YES | YES |
| 96 | a | 329.79 | 0.92479 | YES | YES |
| 97 | a | 334.77 | 4.04213 | YES | YES |
| 98 | a | 343.33 | 0.35600 | YES | YES |
| 99 | a | 345.98 | 0.83991 | YES | YES |
| 100 | a | 352.69 | 1.05350 | YES | YES |
| 101 | a | 354.00 | 1.79959 | YES | YES |
| 102 | a | 360.38 | 1.67130 | YES | YES |
| 103 | a | 365.12 | 9.65421 | YES | YES |
| 104 | a | 369.31 | 39.47896 | YES | YES |
| 105 | a | 376.46 | 1.57943 | YES | YES |
| 106 | a | 396.53 | 0.30278 | YES | YES |
| 107 | a | 402.18 | 35.97283 | YES | YES |
| 108 | a | 410.88 | 0.19769 | YES | YES |
| 109 | a | 436.64 | 0.02633 | YES | YES |
| 110 | a | 440.19 | 16.73962 | YES | YES |
| 111 | a | 440.24 | 40.75005 | YES | YES |
| 112 | a | 441.46 | 2.43920 | YES | YES |
| 113 | a | 443.62 | 0.59470 | YES | YES |
| 114 | a | 447.22 | 1.94521 | YES | YES |
| 115 | a | 450.57 | 0.25951 | YES | YES |
| 116 | a | 452.45 | 2.81281 | YES | YES |
| 117 | a | 454.22 | 41.34502 | YES | YES |
| 118 | a | 514.16 | 7.53213 | YES | YES |
| 119 | a | 516.59 | 1.56420 | YES | YES |
| 120 | a | 517.63 | 7.76400 | YES | YES |
| 121 | a | 518.31 | 1.48189 | YES | YES |
| 122 | a | 519.90 | 3.93910 | YES | YES |
| 123 | a | 520.82 | 3.66052 | YES | YES |
| 124 | a | 521.40 | 5.16445 | YES | YES |
| 125 | a | 523.95 | 0.84493 | YES | YES |
| 126 | a | 524.92 | 0.19444 | YES | YES |
| 127 | a | 526.90 | 1.59742 | YES | YES |
| 128 | a | 538.01 | 9.13205 | YES | YES |
| 129 | a | 539.39 | 83.23197 | YES | YES |
| 130 | a | 543.47 | 4.93007 | YES | YES |
| 131 | a | 546.30 | 0.58229 | YES | YES |
| 132 | a | 546.69 | 2.33716 | YES | YES |
| 133 | a | 550.45 | 12.83936 | YES | YES |
| 134 | a | 551.07 | 2.06804 | YES | YES |
| 135 | a | 551.40 | 6.74575 | YES | YES |
| 136 | a | 553.26 | 1.49706 | YES | YES |
| 137 | a | 553.60 | 1.58585 | YES | YES |
| 138 | a | 554.63 | 0.51728 | YES | YES |
| 139 | a | 555.27 | 0.48357 | YES | YES |
| 140 | a | 558.82 | 19.70551 | YES | YES |
| 141 | a | 560.99 | 12.23602 | YES | YES |
| 142 | a | 562.59 | 12.93713 | YES | YES |
| 143 | a | 563.34 | 6.82024 | YES | YES |
| 144 | a | 567.34 | 11.96179 | YES | YES |
| 145 | a | 570.65 | 1.12202 | YES | YES |
| 146 | a | 574.69 | 1.53913 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 147 | a | 586.57 | 0.31460 | YES | YES |
| 148 | a | 677.79 | 0.07276 | YES | YES |
| 149 | a | 682.27 | 0.41467 | YES | YES |
| 150 | a | 693.39 | 145.03410 | YES | YES |
| 151 | a | 694.73 | 0.99592 | YES | YES |
| 152 | a | 702.03 | 27.20898 | YES | YES |
| 153 | a | 706.40 | 19.74367 | YES | YES |
| 154 | a | 707.30 | 46.33856 | YES | YES |
| 155 | a | 707.65 | 14.95969 | YES | YES |
| 156 | a | 708.74 | 17.42864 | YES | YES |
| 157 | a | 710.88 | 110.62193 | YES | YES |
| 158 | a | 729.45 | 7.92267 | YES | YES |
| 159 | a | 735.59 | 2.50427 | YES | YES |
| 160 | a | 737.32 | 1.02709 | YES | YES |
| 161 | a | 741.52 | 69.29495 | YES | YES |
| 162 | a | 747.33 | 64.30898 | YES | YES |
| 163 | a | 760.46 | 73.78574 | YES | YES |
| 164 | a | 764.54 | 37.24540 | YES | YES |
| 165 | a | 790.63 | 0.22971 | YES | YES |
| 166 | a | 795.49 | 13.94530 | YES | YES |
| 167 | a | 802.44 | 5.76441 | YES | YES |
| 168 | a | 827.47 | 12.04490 | YES | YES |
| 169 | a | 830.58 | 35.25221 | YES | YES |
| 170 | a | 833.12 | 0.46477 | YES | YES |
| 171 | a | 834.01 | 14.62889 | YES | YES |
| 172 | a | 843.97 | 0.98330 | YES | YES |
| 173 | a | 861.11 | 19.11660 | YES | YES |
| 174 | a | 916.89 | 4.85295 | YES | YES |
| 175 | a | 929.04 | 1.79916 | YES | YES |
| 176 | a | 931.93 | 180.36385 | YES | YES |
| 177 | a | 951.26 | 2.84561 | YES | YES |
| 178 | a | 953.05 | 53.84645 | YES | YES |
| 179 | a | 956.04 | 47.64124 | YES | YES |
| 180 | a | 957.79 | 0.41685 | YES | YES |
| 181 | a | 960.92 | 301.62050 | YES | YES |
| 182 | a | 962.41 | 163.18782 | YES | YES |
| 183 | a | 963.11 | 210.09179 | YES | YES |
| 184 | a | 967.12 | 0.41542 | YES | YES |
| 185 | a | 968.47 | 4.42901 | YES | YES |
| 186 | a | 974.47 | 3.07455 | YES | YES |
| 187 | a | 983.36 | 24.80188 | YES | YES |
| 188 | a | 1003.94 | 4.74657 | YES | YES |
| 189 | a | 1008.46 | 1.43205 | YES | YES |
| 190 | a | 1020.72 | 6.15423 | YES | YES |
| 191 | a | 1024.19 | 8.97863 | YES | YES |
| 192 | a | 1026.40 | 0.71580 | YES | YES |
| 193 | a | 1032.26 | 1.44022 | YES | YES |
| 194 | a | 1034.89 | 0.65646 | YES | YES |
| 195 | a | 1047.57 | 14.56176 | YES | YES |
| 196 | a | 1049.59 | 27.02644 | YES | YES |
| 197 | a | 1054.07 | 11.28229 | YES | YES |
| 198 | a | 1075.35 | 0.07899 | YES | YES |
| 199 | a | 1077.61 | 1.66024 | YES | YES |
| 200 | a | 1084.58 | 2.48809 | YES | YES |
| 201 | a | 1086.67 | 8.54848 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 202 | a | 1088.19 | 17.99225 | YES | YES |
| 203 | a | 1094.41 | 5.23090 | YES | YES |
| 204 | a | 1098.52 | 0.11129 | YES | YES |
| 205 | a | 1133.30 | 2.69454 | YES | YES |
| 206 | a | 1135.59 | 21.13700 | YES | YES |
| 207 | a | 1136.37 | 2.37993 | YES | YES |
| 208 | a | 1145.65 | 38.20754 | YES | YES |
| 209 | a | 1151.52 | 19.43894 | YES | YES |
| 210 | a | 1156.48 | 26.93284 | YES | YES |
| 211 | a | 1157.90 | 25.79367 | YES | YES |
| 212 | a | 1166.85 | 34.73975 | YES | YES |
| 213 | a | 1170.72 | 6.02376 | YES | YES |
| 214 | a | 1174.71 | 3.45687 | YES | YES |
| 215 | a | 1177.82 | 17.48424 | YES | YES |
| 216 | a | 1178.95 | 35.34504 | YES | YES |
| 217 | a | 1185.13 | 29.96229 | YES | YES |
| 218 | a | 1194.65 | 17.45615 | YES | YES |
| 219 | a | 1198.99 | 102.07985 | YES | YES |
| 220 | a | 1199.53 | 29.10114 | YES | YES |
| 221 | a | 1210.41 | 58.00333 | YES | YES |
| 222 | a | 1213.03 | 52.59846 | YES | YES |
| 223 | a | 1220.98 | 259.31670 | YES | YES |
| 224 | a | 1229.43 | 244.50082 | YES | YES |
| 225 | a | 1232.34 | 383.41860 | YES | YES |
| 226 | a | 1237.57 | 652.49976 | YES | YES |
| 227 | a | 1239.83 | 474.68030 | YES | YES |
| 228 | a | 1243.66 | 1091.83204 | YES | YES |
| 229 | a | 1244.18 | 69.13297 | YES | YES |
| 230 | a | 1248.86 | 140.46447 | YES | YES |
| 231 | a | 1250.73 | 893.34928 | YES | YES |
| 232 | a | 1251.27 | 144.13792 | YES | YES |
| 233 | a | 1256.77 | 476.89795 | YES | YES |
| 234 | a | 1259.29 | 450.11366 | YES | YES |
| 235 | a | 1261.52 | 188.10248 | YES | YES |
| 236 | a | 1266.81 | 103.45202 | YES | YES |
| 237 | a | 1276.01 | 92.34084 | YES | YES |
| 238 | a | 1304.27 | 0.51843 | YES | YES |
| 239 | a | 1313.83 | 0.28904 | YES | YES |
| 240 | a | 1325.08 | 112.94105 | YES | YES |
| 241 | a | 1345.24 | 159.08519 | YES | YES |
| 242 | a | 1346.85 | 1.99644 | YES | YES |
| 243 | a | 1353.42 | 0.75886 | YES | YES |
| 244 | a | 1359.76 | 5.25207 | YES | YES |
| 245 | a | 1360.83 | 10.81424 | YES | YES |
| 246 | a | 1368.07 | 3.40377 | YES | YES |
| 247 | a | 1371.34 | 73.70711 | YES | YES |
| 248 | a | 1376.76 | 167.26893 | YES | YES |
| 249 | a | 1379.09 | 2.08284 | YES | YES |
| 250 | a | 1382.38 | 0.34108 | YES | YES |
| 251 | a | 1391.95 | 0.77642 | YES | YES |
| 252 | a | 1397.36 | 3.12885 | YES | YES |
| 253 | a | 1408.92 | 2.11043 | YES | YES |
| 254 | a | 1417.88 | 14.63663 | YES | YES |
| 255 | a | 1418.87 | 1.40342 | YES | YES |
| 256 | a | 1423.05 | 1.94974 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 257 | a | 1430.90 | 34.14886 | YES | YES |
| 258 | a | 1433.64 | 9.91564 | YES | YES |
| 259 | a | 1442.83 | 34.35675 | YES | YES |
| 260 | a | 1447.32 | 14.68086 | YES | YES |
| 261 | a | 1448.68 | 4.38300 | YES | YES |
| 262 | a | 1456.90 | 9.76409 | YES | YES |
| 263 | a | 1459.37 | 8.00584 | YES | YES |
| 264 | a | 1463.70 | 4.96726 | YES | YES |
| 265 | a | 1469.39 | 41.46468 | YES | YES |
| 266 | a | 1475.77 | 12.39815 | YES | YES |
| 267 | a | 1503.64 | 258.21706 | YES | YES |
| 268 | a | 1511.34 | 183.00820 | YES | YES |
| 269 | a | 1557.65 | 0.57902 | YES | YES |
| 270 | a | 1565.99 | 0.53325 | YES | YES |
| 271 | a | 1614.34 | 8.74393 | YES | YES |
| 272 | a | 1616.70 | 1.52586 | YES | YES |
| 273 | a | 1633.37 | 21.70765 | YES | YES |
| 274 | a | 1633.98 | 16.75892 | YES | YES |
| 275 | a | 2937.86 | 12.85846 | YES | YES |
| 276 | a | 2941.64 | 29.06600 | YES | YES |
| 277 | a | 2942.74 | 13.87409 | YES | YES |
| 278 | a | 2947.96 | 17.42202 | YES | YES |
| 279 | a | 2959.49 | 13.18227 | YES | YES |
| 280 | a | 2967.49 | 10.28625 | YES | YES |
| 281 | a | 3011.71 | 7.02110 | YES | YES |
| 282 | a | 3017.47 | 1.90862 | YES | YES |
| 283 | a | 3026.25 | 8.88931 | YES | YES |
| 284 | a | 3030.38 | 5.86199 | YES | YES |
| 285 | a | 3038.78 | 5.20651 | YES | YES |
| 286 | a | 3052.56 | 1.06470 | YES | YES |
| 287 | a | 3072.83 | 1.94422 | YES | YES |
| 288 | a | 3073.68 | 6.45756 | YES | YES |
| 289 | a | 3081.32 | 35.47456 | YES | YES |
| 290 | a | 3084.30 | 6.21604 | YES | YES |
| 291 | a | 3086.65 | 23.76255 | YES | YES |
| 292 | a | 3103.66 | 1.92060 | YES | YES |
| 293 | a | 3111.42 | 1.81179 | YES | YES |
| 294 | a | 3116.35 | 2.13570 | YES | YES |
| 295 | a | 3124.65 | 9.55418 | YES | YES |
| 296 | a | 3128.90 | 5.43584 | YES | YES |
| 297 | a | 3134.13 | 1.43608 | YES | YES |
| 298 | a | 3138.44 | 0.35815 | YES | YES |
| 299 | a | 3143.96 | 0.09898 | YES | YES |
| 300 | a | 3160.99 | 10.43615 | YES | YES |

F-Sr(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Sr | -0.22826 | -0.44811 | -1.46908 |
| Al | 0.60074 | -1.02766 | 1.83886 |
| F | 0.42651 | 0.36359 | 0.81577 |
| C | 3.50848 | -0.23097 | -2.19738 |
| C | 3.63535 | -1.09420 | -3.29612 |
| C | 4.73855 | -0.95734 | -4.14844 |
| H | 4.81661 | -1.63516 | -5.01227 |
| C | 5.70948 | 0.02160 | -3.88154 |
| H | 6.57543 | 0.12331 | -4.55435 |
| C | 5.58396 | 0.85820 | -2.75949 |
| H | 6.35240 | 1.61521 | -2.53903 |
| C | 4.47513 | 0.72998 | -1.90640 |
| H | 4.35198 | 1.35670 | -1.01359 |
| F | 2.40849 | -0.33917 | -1.38896 |
| F | 2.71837 | -2.03821 | -3.52006 |
| C | -3.92418 | -0.60882 | -1.53982 |
| C | -3.67356 | -0.15197 | -0.24297 |
| C | -4.71532 | 0.14310 | 0.63374 |
| H | -4.48446 | 0.48784 | 1.65087 |
| C | -6.03469 | -0.02245 | 0.17659 |
| H | -6.87170 | 0.20632 | 0.85419 |
| C | -6.28932 | -0.48041 | -1.12866 |
| H | -7.32617 | -0.60838 | -1.47619 |
| C | -5.22786 | -0.78060 | -2.00111 |
| H | -5.39458 | -1.13815 | -3.02826 |
| F | -2.85421 | -0.86154 | -2.34085 |
| F | -2.37465 | -0.00674 | 0.13132 |
| O | -0.19736 | -0.91157 | 3.37307 |
| C | -1.19882 | -0.43444 | 4.14829 |
| C | -1.45480 | 1.09079 | 3.85601 |
| F | -2.12660 | 1.23248 | 2.68012 |
| F | -2.18202 | 1.69186 | 4.81436 |
| F | -0.29113 | 1.74430 | 3.73100 |
| C | -0.77632 | -0.61216 | 5.65567 |
| F | -0.23607 | -1.82189 | 5.84476 |
| F | 0.13979 | 0.31493 | 5.99761 |
| F | -1.83531 | -0.48019 | 6.48488 |
| C | -2.52170 | -1.24631 | 3.87402 |
| F | -2.48546 | -2.44926 | 4.46944 |
| F | -3.62611 | -0.59605 | 4.30461 |
| F | -2.65845 | -1.45243 | 2.54620 |
| O | 2.28093 | -1.48127 | 1.94463 |

| | | | |
|---|---|---|---|
| C | 3.43721 | -1.11221 | 2.55488 |
| C | 3.59619 | 0.45285 | 2.53971 |
| F | 2.41716 | 1.03310 | 2.85771 |
| F | 4.52865 | 0.89781 | 3.39634 |
| F | 3.92584 | 0.89096 | 1.30016 |
| C | 4.62607 | -1.77182 | 1.76281 |
| F | 4.70311 | -3.08774 | 2.03333 |
| F | 4.43620 | -1.63682 | 0.43793 |
| F | 5.81136 | -1.20612 | 2.07577 |
| C | 3.45142 | -1.61945 | 4.04827 |
| F | 2.96280 | -2.86525 | 4.11610 |
| F | 4.69402 | -1.61672 | 4.57348 |
| F | 2.67305 | -0.82697 | 4.81712 |
| O | -0.17171 | -2.13628 | 0.63053 |
| C | -0.23581 | -3.49321 | 0.42940 |
| C | -0.35950 | -4.28608 | 1.77944 |
| F | -1.61039 | -4.22249 | 2.26919 |
| F | -0.03665 | -5.58215 | 1.62040 |
| F | 0.46888 | -3.74342 | 2.69200 |
| C | 1.06160 | -3.96000 | -0.34025 |
| F | 1.37634 | -3.01802 | -1.26601 |
| F | 2.10261 | -4.07278 | 0.49485 |
| F | 0.89447 | -5.12848 | -0.98001 |
| C | -1.50021 | -3.75652 | -0.45977 |
| F | -1.29045 | -3.19301 | -1.68994 |
| F | -1.76930 | -5.05345 | -0.63134 |
| F | -2.58495 | -3.15308 | 0.05425 |
| C | -1.95622 | 2.89203 | -1.06285 |
| C | -2.17667 | 2.46744 | -2.40663 |
| C | -1.06526 | 2.23214 | -3.26364 |
| C | 0.26930 | 2.39438 | -2.78103 |
| C | 0.48450 | 2.82651 | -1.44318 |
| C | -0.62881 | 3.06042 | -0.58688 |
| C | -3.10399 | 3.22610 | -0.12885 |
| H | -3.08988 | 4.30540 | 0.14420 |
| H | -3.03832 | 2.65580 | 0.82106 |
| H | -4.09710 | 3.01893 | -0.56763 |
| C | -3.57735 | 2.31154 | -2.97107 |
| H | -3.83994 | 3.16800 | -3.63428 |
| H | -4.35591 | 2.25505 | -2.18796 |
| H | -3.67148 | 1.39258 | -3.58363 |
| C | -1.24448 | 1.78110 | -4.69594 |
| H | -2.29658 | 1.80635 | -5.03470 |
| H | -0.86135 | 0.73740 | -4.79001 |
| H | -0.65789 | 2.41767 | -5.39373 |
| C | 1.40219 | 2.08756 | -3.73917 |
| H | 1.28460 | 1.05302 | -4.13068 |
| H | 2.40203 | 2.16173 | -3.27350 |
| H | 1.39066 | 2.77825 | -4.61258 |
| C | 1.86735 | 3.07361 | -0.88059 |
| H | 2.66193 | 2.97536 | -1.64224 |
| H | 2.09883 | 2.37139 | -0.05006 |
| H | 1.94368 | 4.09891 | -0.45639 |
| C | -0.35083 | 3.52419 | 0.82547 |
| H | 0.11425 | 4.53720 | 0.82962 |

| | | | |
|---|---|---|---|
| H | 0.35812 | 2.83889 | 1.33350 |
| H | -1.25850 | 3.57652 | 1.45202 |
| F | 0.05202 | -0.82289 | -3.58645 |

Vibrational analysis

| 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 | 6.47 | 0.29257 | YES | YES |
| 8 | a | 13.59 | 0.59582 | YES | YES |
| 9 | a | 17.39 | 0.73553 | YES | YES |
| 10 | a | 18.70 | 0.34617 | YES | YES |
| 11 | a | 22.44 | 0.07457 | YES | YES |
| 12 | a | 24.19 | 0.05599 | YES | YES |
| 13 | a | 25.07 | 0.45310 | YES | YES |
| 14 | a | 26.45 | 0.03499 | YES | YES |
| 15 | a | 29.17 | 0.21553 | YES | YES |
| 16 | a | 30.45 | 0.32831 | YES | YES |
| 17 | a | 31.87 | 0.62427 | YES | YES |
| 18 | a | 34.99 | 0.17557 | YES | YES |
| 19 | a | 36.30 | 0.35604 | YES | YES |
| 20 | a | 38.65 | 1.31703 | YES | YES |
| 21 | a | 42.82 | 1.12924 | YES | YES |
| 22 | a | 43.08 | 0.56479 | YES | YES |
| 23 | a | 46.65 | 0.46399 | YES | YES |
| 24 | a | 49.12 | 3.23772 | YES | YES |
| 25 | a | 51.87 | 0.15207 | YES | YES |
| 26 | a | 57.33 | 1.05414 | YES | YES |
| 27 | a | 58.02 | 0.92130 | YES | YES |
| 28 | a | 60.78 | 0.50297 | YES | YES |
| 29 | a | 62.26 | 1.22115 | YES | YES |
| 30 | a | 66.11 | 1.10538 | YES | YES |
| 31 | a | 67.71 | 0.37740 | YES | YES |
| 32 | a | 68.11 | 0.01684 | YES | YES |
| 33 | a | 70.15 | 0.33360 | YES | YES |
| 34 | a | 71.76 | 2.19470 | YES | YES |
| 35 | a | 72.85 | 0.17183 | YES | YES |
| 36 | a | 76.90 | 0.76574 | YES | YES |
| 37 | a | 77.95 | 0.04432 | YES | YES |
| 38 | a | 80.04 | 0.40829 | YES | YES |
| 39 | a | 81.62 | 0.39619 | YES | YES |
| 40 | a | 83.47 | 1.57452 | YES | YES |
| 41 | a | 83.98 | 1.35663 | YES | YES |
| 42 | a | 85.74 | 0.39160 | YES | YES |
| 43 | a | 90.16 | 12.81200 | YES | YES |
| 44 | a | 92.06 | 3.83410 | YES | YES |
| 45 | a | 94.19 | 3.82276 | YES | YES |
| 46 | a | 96.63 | 5.54416 | YES | YES |
| 47 | a | 103.40 | 4.47397 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 48 | a | 106.27 | 5.93255 | YES | YES |
| 49 | a | 109.94 | 0.66305 | YES | YES |
| 50 | a | 110.99 | 16.96167 | YES | YES |
| 51 | a | 127.24 | 19.35836 | YES | YES |
| 52 | a | 131.82 | 1.93173 | YES | YES |
| 53 | a | 142.52 | 1.94570 | YES | YES |
| 54 | a | 146.00 | 5.74452 | YES | YES |
| 55 | a | 154.54 | 14.49801 | YES | YES |
| 56 | a | 155.94 | 3.19684 | YES | YES |
| 57 | a | 158.38 | 0.22282 | YES | YES |
| 58 | a | 160.22 | 0.52166 | YES | YES |
| 59 | a | 164.21 | 3.05747 | YES | YES |
| 60 | a | 168.66 | 1.71626 | YES | YES |
| 61 | a | 169.73 | 1.55404 | YES | YES |
| 62 | a | 171.53 | 1.56313 | YES | YES |
| 63 | a | 178.40 | 1.83548 | YES | YES |
| 64 | a | 183.56 | 0.49894 | YES | YES |
| 65 | a | 193.84 | 5.74034 | YES | YES |
| 66 | a | 196.09 | 7.56771 | YES | YES |
| 67 | a | 196.60 | 17.61185 | YES | YES |
| 68 | a | 198.94 | 1.69401 | YES | YES |
| 69 | a | 201.40 | 0.87825 | YES | YES |
| 70 | a | 201.68 | 3.05524 | YES | YES |
| 71 | a | 231.53 | 1.00071 | YES | YES |
| 72 | a | 242.60 | 3.75811 | YES | YES |
| 73 | a | 263.35 | 10.52600 | YES | YES |
| 74 | a | 266.45 | 2.71457 | YES | YES |
| 75 | a | 270.48 | 5.25367 | YES | YES |
| 76 | a | 275.06 | 2.35418 | YES | YES |
| 77 | a | 277.96 | 2.18450 | YES | YES |
| 78 | a | 278.32 | 0.26412 | YES | YES |
| 79 | a | 282.15 | 2.09869 | YES | YES |
| 80 | a | 284.37 | 0.74963 | YES | YES |
| 81 | a | 285.34 | 0.13328 | YES | YES |
| 82 | a | 288.02 | 2.63238 | YES | YES |
| 83 | a | 291.99 | 2.78618 | YES | YES |
| 84 | a | 292.70 | 1.40302 | YES | YES |
| 85 | a | 294.64 | 0.35133 | YES | YES |
| 86 | a | 295.67 | 2.25948 | YES | YES |
| 87 | a | 306.78 | 1.03788 | YES | YES |
| 88 | a | 306.98 | 11.08218 | YES | YES |
| 89 | a | 308.56 | 5.13408 | YES | YES |
| 90 | a | 315.15 | 1.62777 | YES | YES |
| 91 | a | 319.06 | 1.72175 | YES | YES |
| 92 | a | 320.48 | 2.12264 | YES | YES |
| 93 | a | 321.65 | 1.13076 | YES | YES |
| 94 | a | 324.73 | 1.65381 | YES | YES |
| 95 | a | 327.42 | 0.67191 | YES | YES |
| 96 | a | 331.71 | 0.44448 | YES | YES |
| 97 | a | 332.03 | 0.82618 | YES | YES |
| 98 | a | 348.39 | 0.46232 | YES | YES |
| 99 | a | 348.67 | 1.12340 | YES | YES |
| 100 | a | 355.64 | 0.89719 | YES | YES |
| 101 | a | 359.37 | 6.32776 | YES | YES |
| 102 | a | 360.98 | 7.56327 | YES | YES |

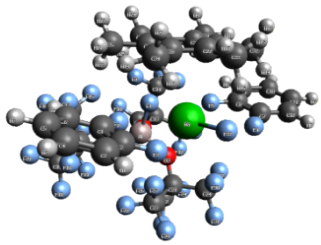
| | | | | | |
|---|---|---|---|---|---|
| 103 | a | 370.07 | 18.61246 | YES | YES |
| 104 | a | 370.93 | 13.55137 | YES | YES |
| 105 | a | 389.67 | 50.63860 | YES | YES |
| 106 | a | 393.19 | 1.08323 | YES | YES |
| 107 | a | 406.95 | 2.22842 | YES | YES |
| 108 | a | 408.49 | 5.15490 | YES | YES |
| 109 | a | 437.10 | 7.22133 | YES | YES |
| 110 | a | 437.85 | 1.60192 | YES | YES |
| 111 | a | 441.19 | 4.12678 | YES | YES |
| 112 | a | 443.02 | 77.78355 | YES | YES |
| 113 | a | 445.87 | 4.36318 | YES | YES |
| 114 | a | 449.43 | 2.23254 | YES | YES |
| 115 | a | 451.64 | 1.63117 | YES | YES |
| 116 | a | 453.20 | 42.53520 | YES | YES |
| 117 | a | 454.53 | 1.20064 | YES | YES |
| 118 | a | 468.49 | 26.36834 | YES | YES |
| 119 | a | 515.46 | 5.24318 | YES | YES |
| 120 | a | 516.79 | 4.14109 | YES | YES |
| 121 | a | 517.90 | 0.85979 | YES | YES |
| 122 | a | 518.71 | 5.22579 | YES | YES |
| 123 | a | 520.07 | 4.19182 | YES | YES |
| 124 | a | 520.73 | 5.10133 | YES | YES |
| 125 | a | 522.06 | 1.90282 | YES | YES |
| 126 | a | 524.07 | 0.54454 | YES | YES |
| 127 | a | 524.74 | 2.11808 | YES | YES |
| 128 | a | 527.64 | 1.35178 | YES | YES |
| 129 | a | 535.37 | 3.63390 | YES | YES |
| 130 | a | 543.22 | 3.53331 | YES | YES |
| 131 | a | 546.31 | 1.54337 | YES | YES |
| 132 | a | 546.82 | 9.81799 | YES | YES |
| 133 | a | 547.78 | 0.70760 | YES | YES |
| 134 | a | 552.51 | 2.41812 | YES | YES |
| 135 | a | 553.83 | 0.88888 | YES | YES |
| 136 | a | 554.05 | 0.28165 | YES | YES |
| 137 | a | 554.80 | 0.34851 | YES | YES |
| 138 | a | 555.67 | 0.79013 | YES | YES |
| 139 | a | 556.57 | 0.99571 | YES | YES |
| 140 | a | 559.47 | 0.06162 | YES | YES |
| 141 | a | 562.18 | 13.90308 | YES | YES |
| 142 | a | 563.82 | 22.97132 | YES | YES |
| 143 | a | 566.66 | 34.02892 | YES | YES |
| 144 | a | 567.60 | 1.26669 | YES | YES |
| 145 | a | 568.26 | 0.56917 | YES | YES |
| 146 | a | 580.39 | 0.21341 | YES | YES |
| 147 | a | 585.27 | 0.07524 | YES | YES |
| 148 | a | 681.29 | 0.02237 | YES | YES |
| 149 | a | 682.51 | 0.18861 | YES | YES |
| 150 | a | 687.69 | 94.10121 | YES | YES |
| 151 | a | 705.71 | 7.07607 | YES | YES |
| 152 | a | 706.35 | 27.98926 | YES | YES |
| 153 | a | 707.12 | 27.23705 | YES | YES |
| 154 | a | 708.09 | 0.04083 | YES | YES |
| 155 | a | 708.94 | 53.52108 | YES | YES |
| 156 | a | 709.56 | 30.38258 | YES | YES |
| 157 | a | 711.37 | 67.33923 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 158 | a | 726.20 | 10.90473 | YES | YES |
| 159 | a | 738.52 | 2.06359 | YES | YES |
| 160 | a | 739.31 | 11.98267 | YES | YES |
| 161 | a | 743.05 | 72.88029 | YES | YES |
| 162 | a | 746.10 | 80.28840 | YES | YES |
| 163 | a | 757.61 | 65.62598 | YES | YES |
| 164 | a | 764.01 | 45.56120 | YES | YES |
| 165 | a | 779.58 | 15.84401 | YES | YES |
| 166 | a | 789.47 | 0.31017 | YES | YES |
| 167 | a | 799.03 | 2.71355 | YES | YES |
| 168 | a | 828.21 | 19.07544 | YES | YES |
| 169 | a | 830.49 | 35.15286 | YES | YES |
| 170 | a | 833.84 | 9.50067 | YES | YES |
| 171 | a | 834.92 | 11.66804 | YES | YES |
| 172 | a | 841.58 | 0.59075 | YES | YES |
| 173 | a | 862.25 | 26.24354 | YES | YES |
| 174 | a | 918.17 | 10.74107 | YES | YES |
| 175 | a | 926.67 | 3.88584 | YES | YES |
| 176 | a | 949.64 | 0.12490 | YES | YES |
| 177 | a | 955.49 | 21.26738 | YES | YES |
| 178 | a | 956.39 | 19.82972 | YES | YES |
| 179 | a | 958.53 | 8.61241 | YES | YES |
| 180 | a | 959.98 | 165.94555 | YES | YES |
| 181 | a | 962.07 | 196.54337 | YES | YES |
| 182 | a | 964.48 | 2.58171 | YES | YES |
| 183 | a | 966.60 | 99.53946 | YES | YES |
| 184 | a | 966.99 | 106.42834 | YES | YES |
| 185 | a | 970.43 | 341.57613 | YES | YES |
| 186 | a | 972.77 | 6.01715 | YES | YES |
| 187 | a | 985.02 | 20.06850 | YES | YES |
| 188 | a | 1004.47 | 1.63321 | YES | YES |
| 189 | a | 1008.49 | 1.45654 | YES | YES |
| 190 | a | 1020.44 | 7.92991 | YES | YES |
| 191 | a | 1025.98 | 8.16953 | YES | YES |
| 192 | a | 1028.47 | 1.93974 | YES | YES |
| 193 | a | 1033.43 | 0.99015 | YES | YES |
| 194 | a | 1035.16 | 0.35527 | YES | YES |
| 195 | a | 1049.48 | 23.15694 | YES | YES |
| 196 | a | 1051.02 | 9.61872 | YES | YES |
| 197 | a | 1073.78 | 0.48518 | YES | YES |
| 198 | a | 1075.29 | 0.57477 | YES | YES |
| 199 | a | 1080.09 | 2.23740 | YES | YES |
| 200 | a | 1084.69 | 1.22131 | YES | YES |
| 201 | a | 1087.61 | 4.51742 | YES | YES |
| 202 | a | 1088.28 | 21.50733 | YES | YES |
| 203 | a | 1093.26 | 7.58874 | YES | YES |
| 204 | a | 1097.92 | 17.77349 | YES | YES |
| 205 | a | 1132.74 | 1.82606 | YES | YES |
| 206 | a | 1134.04 | 12.97830 | YES | YES |
| 207 | a | 1136.82 | 14.28484 | YES | YES |
| 208 | a | 1144.75 | 19.33167 | YES | YES |
| 209 | a | 1147.84 | 69.22934 | YES | YES |
| 210 | a | 1155.73 | 20.43727 | YES | YES |
| 211 | a | 1161.73 | 20.29138 | YES | YES |
| 212 | a | 1167.24 | 35.15692 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 213 | a | 1171.89 | 6.01208 | YES | YES |
| 214 | a | 1174.69 | 63.72134 | YES | YES |
| 215 | a | 1178.79 | 112.12309 | YES | YES |
| 216 | a | 1184.63 | 27.14826 | YES | YES |
| 217 | a | 1186.89 | 31.10282 | YES | YES |
| 218 | a | 1190.59 | 11.46289 | YES | YES |
| 219 | a | 1194.80 | 27.30522 | YES | YES |
| 220 | a | 1202.62 | 22.54723 | YES | YES |
| 221 | a | 1205.87 | 77.10100 | YES | YES |
| 222 | a | 1212.39 | 76.93453 | YES | YES |
| 223 | a | 1219.52 | 166.95277 | YES | YES |
| 224 | a | 1224.87 | 255.16361 | YES | YES |
| 225 | a | 1233.59 | 1005.84540 | YES | YES |
| 226 | a | 1235.20 | 423.44890 | YES | YES |
| 227 | a | 1241.81 | 184.29584 | YES | YES |
| 228 | a | 1243.01 | 309.20735 | YES | YES |
| 229 | a | 1246.66 | 28.03860 | YES | YES |
| 230 | a | 1247.48 | 483.97336 | YES | YES |
| 231 | a | 1248.69 | 250.66109 | YES | YES |
| 232 | a | 1249.77 | 758.24558 | YES | YES |
| 233 | a | 1256.06 | 439.62059 | YES | YES |
| 234 | a | 1259.43 | 259.62631 | YES | YES |
| 235 | a | 1262.17 | 908.17425 | YES | YES |
| 236 | a | 1268.27 | 68.22182 | YES | YES |
| 237 | a | 1279.79 | 92.63907 | YES | YES |
| 238 | a | 1301.52 | 18.56476 | YES | YES |
| 239 | a | 1302.14 | 0.16023 | YES | YES |
| 240 | a | 1318.72 | 0.52137 | YES | YES |
| 241 | a | 1331.77 | 122.91334 | YES | YES |
| 242 | a | 1342.47 | 2.24348 | YES | YES |
| 243 | a | 1350.06 | 2.57697 | YES | YES |
| 244 | a | 1354.13 | 153.32312 | YES | YES |
| 245 | a | 1356.71 | 7.74063 | YES | YES |
| 246 | a | 1359.16 | 7.83706 | YES | YES |
| 247 | a | 1366.35 | 1.50165 | YES | YES |
| 248 | a | 1371.83 | 5.89779 | YES | YES |
| 249 | a | 1377.54 | 2.28260 | YES | YES |
| 250 | a | 1382.85 | 0.59583 | YES | YES |
| 251 | a | 1394.05 | 0.60805 | YES | YES |
| 252 | a | 1399.69 | 1.70630 | YES | YES |
| 253 | a | 1409.81 | 0.61929 | YES | YES |
| 254 | a | 1418.55 | 0.22976 | YES | YES |
| 255 | a | 1419.31 | 15.16888 | YES | YES |
| 256 | a | 1425.01 | 1.93401 | YES | YES |
| 257 | a | 1430.13 | 16.18581 | YES | YES |
| 258 | a | 1435.53 | 19.56393 | YES | YES |
| 259 | a | 1439.26 | 35.28009 | YES | YES |
| 260 | a | 1444.77 | 1.21861 | YES | YES |
| 261 | a | 1452.62 | 6.17591 | YES | YES |
| 262 | a | 1455.01 | 15.81272 | YES | YES |
| 263 | a | 1456.11 | 4.86473 | YES | YES |
| 264 | a | 1459.72 | 7.99338 | YES | YES |
| 265 | a | 1472.61 | 30.70596 | YES | YES |
| 266 | a | 1474.84 | 19.94782 | YES | YES |
| 267 | a | 1504.30 | 243.83053 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 268 | a | 1511.58 | 166.93965 | YES | YES |
| 269 | a | 1563.64 | 1.18077 | YES | YES |
| 270 | a | 1570.63 | 0.58866 | YES | YES |
| 271 | a | 1611.67 | 9.24802 | YES | YES |
| 272 | a | 1617.67 | 1.05384 | YES | YES |
| 273 | a | 1633.31 | 25.98876 | YES | YES |
| 274 | a | 1634.18 | 14.66644 | YES | YES |
| 275 | a | 2926.14 | 32.34327 | YES | YES |
| 276 | a | 2938.53 | 20.29799 | YES | YES |
| 277 | a | 2942.66 | 25.90657 | YES | YES |
| 278 | a | 2945.63 | 17.42305 | YES | YES |
| 279 | a | 2952.78 | 18.08442 | YES | YES |
| 280 | a | 2953.79 | 18.53879 | YES | YES |
| 281 | a | 3004.83 | 14.57217 | YES | YES |
| 282 | a | 3009.56 | 2.08578 | YES | YES |
| 283 | a | 3016.96 | 6.81763 | YES | YES |
| 284 | a | 3028.04 | 3.84124 | YES | YES |
| 285 | a | 3029.88 | 17.67250 | YES | YES |
| 286 | a | 3034.15 | 2.52949 | YES | YES |
| 287 | a | 3071.31 | 6.61043 | YES | YES |
| 288 | a | 3077.06 | 4.21439 | YES | YES |
| 289 | a | 3081.55 | 24.71005 | YES | YES |
| 290 | a | 3084.10 | 12.73421 | YES | YES |
| 291 | a | 3087.66 | 21.27317 | YES | YES |
| 292 | a | 3099.63 | 9.29796 | YES | YES |
| 293 | a | 3110.79 | 2.53071 | YES | YES |
| 294 | a | 3115.79 | 1.83968 | YES | YES |
| 295 | a | 3124.54 | 8.13045 | YES | YES |
| 296 | a | 3128.44 | 6.55354 | YES | YES |
| 297 | a | 3133.58 | 1.64825 | YES | YES |
| 298 | a | 3138.10 | 0.19241 | YES | YES |
| 299 | a | 3157.29 | 1.99739 | YES | YES |
| 300 | a | 3164.34 | 0.75483 | YES | YES |

F-Sr(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Ba | 0.06490 | -1.11864 | -1.35708 |
| Al | -0.09932 | -0.14994 | 2.17220 |
| F | -0.09032 | 0.71932 | 0.68594 |
| C | 3.88019 | -0.59109 | -0.88379 |
| C | 3.92304 | -1.64259 | -1.80675 |
| C | 5.11915 | -1.99487 | -2.43243 |
| H | 5.11907 | -2.82107 | -3.15926 |

| | | | |
|---|---|---|---|
| C | 6.28282 | -1.27217 | -2.11597 |
| H | 7.23380 | -1.53831 | -2.60301 |
| C | 6.23704 | -0.21942 | -1.18504 |
| H | 7.15264 | 0.33962 | -0.93734 |
| C | 5.02811 | 0.12921 | -0.55740 |
| H | 4.96432 | 0.93923 | 0.18103 |
| F | 2.67472 | -0.28301 | -0.33201 |
| F | 2.76864 | -2.28839 | -2.09400 |
| C | -3.86515 | -1.59849 | -1.90393 |
| C | -3.78180 | -0.52452 | -1.01009 |
| C | -4.91533 | 0.18507 | -0.61852 |
| H | -4.81420 | 1.01321 | 0.09591 |
| C | -6.15850 | -0.19959 | -1.15173 |
| H | -7.06547 | 0.34815 | -0.85235 |
| C | -6.24784 | -1.27351 | -2.05484 |
| H | -7.22534 | -1.56736 | -2.46795 |
| C | -5.09564 | -1.98355 | -2.43756 |
| H | -5.13298 | -2.82789 | -3.14231 |
| F | -2.72168 | -2.23604 | -2.23797 |
| F | -2.54842 | -0.19145 | -0.54352 |
| O | -1.24774 | 0.44280 | 3.33756 |
| C | -2.43652 | 1.05805 | 3.54302 |
| C | -2.58184 | 2.32836 | 2.62365 |
| F | -2.88182 | 1.95161 | 1.34933 |
| F | -3.55328 | 3.16278 | 3.03693 |
| F | -1.42809 | 3.00770 | 2.57310 |
| C | -2.49843 | 1.50312 | 5.05286 |
| F | -2.04190 | 0.52449 | 5.84344 |
| F | -1.73262 | 2.59454 | 5.25162 |
| F | -3.76103 | 1.80500 | 5.42957 |
| C | -3.61732 | 0.05877 | 3.24085 |
| F | -3.77225 | -0.82406 | 4.24141 |
| F | -4.79668 | 0.69109 | 3.05121 |
| F | -3.33944 | -0.64102 | 2.11950 |
| O | 1.51537 | -0.27724 | 2.83238 |
| C | 2.43958 | 0.42528 | 3.53378 |
| C | 2.65764 | 1.84541 | 2.89214 |
| F | 1.46557 | 2.40007 | 2.59274 |
| F | 3.32794 | 2.69018 | 3.69267 |
| F | 3.34731 | 1.74656 | 1.72555 |
| C | 3.78589 | -0.38867 | 3.49063 |
| F | 3.73147 | -1.44331 | 4.32383 |
| F | 4.00517 | -0.86246 | 2.24864 |
| F | 4.84794 | 0.36979 | 3.83838 |
| C | 1.98835 | 0.60651 | 5.03559 |
| F | 1.45556 | -0.53229 | 5.49797 |
| F | 3.02111 | 0.95093 | 5.83417 |
| F | 1.05080 | 1.57303 | 5.13017 |
| O | -0.46061 | -1.75693 | 1.42394 |
| C | -0.42357 | -3.07046 | 1.80712 |
| C | -0.86279 | -3.26601 | 3.30385 |
| F | -2.19843 | -3.17264 | 3.42985 |
| F | -0.47724 | -4.46486 | 3.77987 |
| F | -0.30805 | -2.30372 | 4.06301 |
| C | 1.04116 | -3.62746 | 1.61559 |

| | | | |
|---|---|---|---|
| F | 1.56340 | -3.11045 | 0.46195 |
| F | 1.84124 | -3.24744 | 2.61751 |
| F | 1.08412 | -4.96448 | 1.51145 |
| C | -1.41123 | -3.85171 | 0.86828 |
| F | -0.89733 | -3.86674 | -0.40010 |
| F | -1.61232 | -5.11772 | 1.24969 |
| F | -2.59476 | -3.22464 | 0.79706 |
| C | -1.06123 | 2.01911 | -2.56460 |
| C | -1.00707 | 1.09506 | -3.64807 |
| C | 0.25367 | 0.69283 | -4.17746 |
| C | 1.46253 | 1.12517 | -3.55852 |
| C | 1.40682 | 2.02366 | -2.45420 |
| C | 0.14645 | 2.46068 | -1.95700 |
| C | -2.37422 | 2.58720 | -2.06478 |
| H | -2.37133 | 3.69685 | -2.14713 |
| H | -2.54875 | 2.34581 | -0.99600 |
| H | -3.24654 | 2.22371 | -2.63921 |
| C | -2.26295 | 0.50816 | -4.26587 |
| H | -2.51166 | 0.99145 | -5.23934 |
| H | -3.15009 | 0.61774 | -3.61275 |
| H | -2.13302 | -0.57604 | -4.46512 |
| C | 0.29680 | -0.25337 | -5.35544 |
| H | -0.54298 | -0.07703 | -6.05791 |
| H | 0.21976 | -1.30000 | -4.96319 |
| H | 1.23531 | -0.15924 | -5.93627 |
| C | 2.77842 | 0.60628 | -4.10780 |
| H | 2.73115 | -0.48771 | -4.29128 |
| H | 3.62983 | 0.78638 | -3.42497 |
| H | 3.03160 | 1.08522 | -5.08190 |
| C | 2.65115 | 2.58649 | -1.80013 |
| H | 3.58786 | 2.24360 | -2.27724 |
| H | 2.70328 | 2.31952 | -0.72320 |
| H | 2.64650 | 3.69840 | -1.84725 |
| C | 0.11539 | 3.42758 | -0.79412 |
| H | 0.37536 | 4.46165 | -1.12325 |
| H | 0.84104 | 3.14024 | -0.00797 |
| H | -0.87304 | 3.46962 | -0.30263 |
| F | 0.04919 | -2.43268 | -3.25740 |

Vibrational analysis

| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | -0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 12.67 | 0.03633 | YES | YES |
| 8 | a | 19.46 | 0.64607 | YES | YES |
| 9 | a | 19.58 | 0.55432 | YES | YES |
| 10 | a | 20.73 | 0.38668 | YES | YES |
| 11 | a | 24.25 | 0.24421 | YES | YES |
| 12 | a | 25.54 | 0.06153 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 13 | a | 27.85 | 0.03653 | YES | YES |
| 14 | a | 28.35 | 0.16383 | YES | YES |
| 15 | a | 30.77 | 0.04541 | YES | YES |
| 16 | a | 33.62 | 0.61310 | YES | YES |
| 17 | a | 34.79 | 0.11574 | YES | YES |
| 18 | a | 37.15 | 0.25499 | YES | YES |
| 19 | a | 38.99 | 0.98357 | YES | YES |
| 20 | a | 40.55 | 0.58705 | YES | YES |
| 21 | a | 42.86 | 0.78136 | YES | YES |
| 22 | a | 44.20 | 0.53658 | YES | YES |
| 23 | a | 45.66 | 0.89119 | YES | YES |
| 24 | a | 48.41 | 0.64567 | YES | YES |
| 25 | a | 50.62 | 0.52381 | YES | YES |
| 26 | a | 56.22 | 0.33845 | YES | YES |
| 27 | a | 58.27 | 0.77389 | YES | YES |
| 28 | a | 58.85 | 1.31445 | YES | YES |
| 29 | a | 60.70 | 0.97927 | YES | YES |
| 30 | a | 63.33 | 0.52912 | YES | YES |
| 31 | a | 65.68 | 1.07842 | YES | YES |
| 32 | a | 67.46 | 0.05993 | YES | YES |
| 33 | a | 71.18 | 0.06220 | YES | YES |
| 34 | a | 71.89 | 0.78300 | YES | YES |
| 35 | a | 72.05 | 0.28204 | YES | YES |
| 36 | a | 75.35 | 0.30380 | YES | YES |
| 37 | a | 77.65 | 0.33647 | YES | YES |
| 38 | a | 78.58 | 0.67386 | YES | YES |
| 39 | a | 80.68 | 0.61748 | YES | YES |
| 40 | a | 83.23 | 1.18343 | YES | YES |
| 41 | a | 84.22 | 0.78673 | YES | YES |
| 42 | a | 85.74 | 0.56226 | YES | YES |
| 43 | a | 91.42 | 1.55630 | YES | YES |
| 44 | a | 93.02 | 10.58023 | YES | YES |
| 45 | a | 95.15 | 0.27998 | YES | YES |
| 46 | a | 98.43 | 15.41469 | YES | YES |
| 47 | a | 99.48 | 0.44443 | YES | YES |
| 48 | a | 102.46 | 1.35749 | YES | YES |
| 49 | a | 103.70 | 3.27796 | YES | YES |
| 50 | a | 106.72 | 22.26351 | YES | YES |
| 51 | a | 115.14 | 4.21694 | YES | YES |
| 52 | a | 121.71 | 5.68466 | YES | YES |
| 53 | a | 141.11 | 1.76088 | YES | YES |
| 54 | a | 144.60 | 3.86178 | YES | YES |
| 55 | a | 154.30 | 0.21641 | YES | YES |
| 56 | a | 156.45 | 0.12067 | YES | YES |
| 57 | a | 160.37 | 0.56910 | YES | YES |
| 58 | a | 161.99 | 16.21918 | YES | YES |
| 59 | a | 162.88 | 2.87634 | YES | YES |
| 60 | a | 166.77 | 2.58279 | YES | YES |
| 61 | a | 170.70 | 1.78313 | YES | YES |
| 62 | a | 175.51 | 1.13675 | YES | YES |
| 63 | a | 176.42 | 1.10355 | YES | YES |
| 64 | a | 183.63 | 1.56863 | YES | YES |
| 65 | a | 188.38 | 0.07008 | YES | YES |
| 66 | a | 194.89 | 8.93603 | YES | YES |
| 67 | a | 195.18 | 1.25399 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 68 | a | 195.91 | 0.06127 | YES | YES |
| 69 | a | 199.06 | 1.19137 | YES | YES |
| 70 | a | 200.07 | 1.46451 | YES | YES |
| 71 | a | 210.47 | 5.40005 | YES | YES |
| 72 | a | 227.29 | 15.86005 | YES | YES |
| 73 | a | 242.84 | 19.21458 | YES | YES |
| 74 | a | 250.77 | 5.14857 | YES | YES |
| 75 | a | 269.27 | 2.02829 | YES | YES |
| 76 | a | 273.80 | 2.77456 | YES | YES |
| 77 | a | 278.00 | 1.86183 | YES | YES |
| 78 | a | 282.39 | 2.51027 | YES | YES |
| 79 | a | 284.24 | 0.26347 | YES | YES |
| 80 | a | 285.27 | 0.25234 | YES | YES |
| 81 | a | 287.20 | 2.80744 | YES | YES |
| 82 | a | 291.42 | 0.85009 | YES | YES |
| 83 | a | 291.68 | 3.88675 | YES | YES |
| 84 | a | 292.19 | 2.26564 | YES | YES |
| 85 | a | 292.60 | 0.28927 | YES | YES |
| 86 | a | 297.17 | 4.37615 | YES | YES |
| 87 | a | 299.86 | 1.72321 | YES | YES |
| 88 | a | 306.40 | 7.53302 | YES | YES |
| 89 | a | 307.28 | 5.23275 | YES | YES |
| 90 | a | 313.51 | 2.13623 | YES | YES |
| 91 | a | 317.93 | 0.41600 | YES | YES |
| 92 | a | 320.18 | 2.43133 | YES | YES |
| 93 | a | 321.25 | 1.82345 | YES | YES |
| 94 | a | 324.56 | 1.10477 | YES | YES |
| 95 | a | 326.57 | 1.78245 | YES | YES |
| 96 | a | 328.89 | 0.17071 | YES | YES |
| 97 | a | 330.74 | 0.65509 | YES | YES |
| 98 | a | 348.17 | 0.87231 | YES | YES |
| 99 | a | 354.83 | 1.22078 | YES | YES |
| 100 | a | 357.40 | 1.45451 | YES | YES |
| 101 | a | 358.29 | 6.28226 | YES | YES |
| 102 | a | 360.48 | 6.45248 | YES | YES |
| 103 | a | 368.14 | 31.07626 | YES | YES |
| 104 | a | 371.34 | 0.63948 | YES | YES |
| 105 | a | 385.25 | 48.58125 | YES | YES |
| 106 | a | 400.04 | 0.09731 | YES | YES |
| 107 | a | 404.97 | 64.34296 | YES | YES |
| 108 | a | 407.65 | 19.43140 | YES | YES |
| 109 | a | 413.53 | 1.03439 | YES | YES |
| 110 | a | 435.96 | 0.22367 | YES | YES |
| 111 | a | 437.00 | 0.21053 | YES | YES |
| 112 | a | 442.78 | 0.07293 | YES | YES |
| 113 | a | 446.37 | 0.16209 | YES | YES |
| 114 | a | 449.27 | 0.40327 | YES | YES |
| 115 | a | 449.43 | 3.66235 | YES | YES |
| 116 | a | 450.06 | 1.64678 | YES | YES |
| 117 | a | 452.39 | 47.98757 | YES | YES |
| 118 | a | 463.62 | 32.82655 | YES | YES |
| 119 | a | 515.15 | 5.64390 | YES | YES |
| 120 | a | 516.33 | 3.35894 | YES | YES |
| 121 | a | 517.97 | 0.98467 | YES | YES |
| 122 | a | 519.05 | 4.93934 | YES | YES |

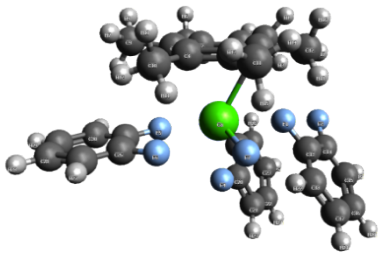
| | | | | | |
|---|---|---|---|---|---|
| 123 | a | 520.17 | 4.60891 | YES | YES |
| 124 | a | 520.68 | 4.59411 | YES | YES |
| 125 | a | 521.38 | 2.08273 | YES | YES |
| 126 | a | 524.13 | 0.29560 | YES | YES |
| 127 | a | 524.82 | 2.10800 | YES | YES |
| 128 | a | 527.30 | 1.10184 | YES | YES |
| 129 | a | 540.98 | 2.50309 | YES | YES |
| 130 | a | 542.46 | 2.99193 | YES | YES |
| 131 | a | 545.91 | 11.72468 | YES | YES |
| 132 | a | 547.15 | 0.59387 | YES | YES |
| 133 | a | 547.58 | 0.21843 | YES | YES |
| 134 | a | 552.37 | 2.95842 | YES | YES |
| 135 | a | 553.52 | 0.76165 | YES | YES |
| 136 | a | 553.90 | 0.51489 | YES | YES |
| 137 | a | 554.23 | 0.34776 | YES | YES |
| 138 | a | 555.11 | 0.41926 | YES | YES |
| 139 | a | 555.39 | 1.13590 | YES | YES |
| 140 | a | 562.12 | 33.51849 | YES | YES |
| 141 | a | 562.48 | 1.94256 | YES | YES |
| 142 | a | 562.82 | 13.14572 | YES | YES |
| 143 | a | 565.29 | 23.28622 | YES | YES |
| 144 | a | 566.22 | 0.13694 | YES | YES |
| 145 | a | 571.27 | 0.98984 | YES | YES |
| 146 | a | 580.88 | 0.83252 | YES | YES |
| 147 | a | 587.18 | 0.50050 | YES | YES |
| 148 | a | 681.06 | 0.11881 | YES | YES |
| 149 | a | 682.38 | 0.08402 | YES | YES |
| 150 | a | 703.00 | 27.92351 | YES | YES |
| 151 | a | 706.00 | 11.28489 | YES | YES |
| 152 | a | 706.79 | 36.93213 | YES | YES |
| 153 | a | 707.20 | 33.67436 | YES | YES |
| 154 | a | 709.00 | 36.60200 | YES | YES |
| 155 | a | 709.51 | 29.36176 | YES | YES |
| 156 | a | 709.59 | 0.46543 | YES | YES |
| 157 | a | 712.29 | 96.30851 | YES | YES |
| 158 | a | 727.50 | 7.09705 | YES | YES |
| 159 | a | 738.13 | 2.64930 | YES | YES |
| 160 | a | 742.61 | 14.04845 | YES | YES |
| 161 | a | 745.59 | 31.08003 | YES | YES |
| 162 | a | 746.17 | 123.95402 | YES | YES |
| 163 | a | 763.09 | 80.98031 | YES | YES |
| 164 | a | 765.32 | 30.70700 | YES | YES |
| 165 | a | 780.84 | 19.81413 | YES | YES |
| 166 | a | 793.55 | 0.11503 | YES | YES |
| 167 | a | 802.33 | 2.42067 | YES | YES |
| 168 | a | 829.15 | 33.52666 | YES | YES |
| 169 | a | 829.98 | 33.84450 | YES | YES |
| 170 | a | 830.81 | 6.03482 | YES | YES |
| 171 | a | 841.21 | 1.01140 | YES | YES |
| 172 | a | 841.36 | 0.67665 | YES | YES |
| 173 | a | 853.49 | 33.26929 | YES | YES |
| 174 | a | 925.68 | 4.43944 | YES | YES |
| 175 | a | 926.63 | 7.22569 | YES | YES |
| 176 | a | 950.80 | 39.40071 | YES | YES |
| 177 | a | 953.97 | 65.99729 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 178 | a | 954.41 | 8.88889 | YES | YES |
| 179 | a | 959.37 | 146.01701 | YES | YES |
| 180 | a | 960.10 | 187.32563 | YES | YES |
| 181 | a | 964.56 | 8.64535 | YES | YES |
| 182 | a | 964.89 | 16.71911 | YES | YES |
| 183 | a | 966.62 | 165.79227 | YES | YES |
| 184 | a | 968.28 | 11.54525 | YES | YES |
| 185 | a | 968.61 | 320.42211 | YES | YES |
| 186 | a | 975.61 | 2.84030 | YES | YES |
| 187 | a | 984.12 | 19.07204 | YES | YES |
| 188 | a | 1005.15 | 1.67688 | YES | YES |
| 189 | a | 1008.07 | 0.24480 | YES | YES |
| 190 | a | 1021.14 | 8.96596 | YES | YES |
| 191 | a | 1022.23 | 9.65190 | YES | YES |
| 192 | a | 1029.75 | 2.61406 | YES | YES |
| 193 | a | 1034.97 | 0.27040 | YES | YES |
| 194 | a | 1036.90 | 6.86388 | YES | YES |
| 195 | a | 1052.73 | 17.24400 | YES | YES |
| 196 | a | 1055.04 | 8.26494 | YES | YES |
| 197 | a | 1075.69 | 0.01916 | YES | YES |
| 198 | a | 1076.65 | 0.28877 | YES | YES |
| 199 | a | 1077.30 | 5.32935 | YES | YES |
| 200 | a | 1085.79 | 2.75233 | YES | YES |
| 201 | a | 1087.28 | 0.03203 | YES | YES |
| 202 | a | 1087.66 | 10.81675 | YES | YES |
| 203 | a | 1093.36 | 2.70905 | YES | YES |
| 204 | a | 1096.80 | 27.97960 | YES | YES |
| 205 | a | 1133.01 | 39.21973 | YES | YES |
| 206 | a | 1134.57 | 2.99146 | YES | YES |
| 207 | a | 1135.00 | 10.23620 | YES | YES |
| 208 | a | 1138.24 | 22.30440 | YES | YES |
| 209 | a | 1144.34 | 64.74489 | YES | YES |
| 210 | a | 1154.40 | 17.04067 | YES | YES |
| 211 | a | 1159.65 | 21.80366 | YES | YES |
| 212 | a | 1171.75 | 20.35879 | YES | YES |
| 213 | a | 1173.68 | 25.37253 | YES | YES |
| 214 | a | 1175.39 | 23.37870 | YES | YES |
| 215 | a | 1178.24 | 94.04573 | YES | YES |
| 216 | a | 1183.64 | 26.26486 | YES | YES |
| 217 | a | 1188.45 | 39.48877 | YES | YES |
| 218 | a | 1190.32 | 3.11986 | YES | YES |
| 219 | a | 1196.32 | 34.66142 | YES | YES |
| 220 | a | 1203.25 | 17.18663 | YES | YES |
| 221 | a | 1208.36 | 116.63768 | YES | YES |
| 222 | a | 1213.08 | 68.08396 | YES | YES |
| 223 | a | 1220.16 | 243.44079 | YES | YES |
| 224 | a | 1223.81 | 233.41843 | YES | YES |
| 225 | a | 1230.99 | 194.06763 | YES | YES |
| 226 | a | 1234.31 | 1332.75964 | YES | YES |
| 227 | a | 1241.86 | 490.86330 | YES | YES |
| 228 | a | 1246.40 | 831.71299 | YES | YES |
| 229 | a | 1248.49 | 128.40490 | YES | YES |
| 230 | a | 1248.99 | 16.49629 | YES | YES |
| 231 | a | 1249.52 | 247.91133 | YES | YES |
| 232 | a | 1250.37 | 37.68951 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 233 | a | 1256.54 | 345.80936 | YES | YES |
| 234 | a | 1261.26 | 1027.64853 | YES | YES |
| 235 | a | 1263.18 | 342.08917 | YES | YES |
| 236 | a | 1267.12 | 142.07506 | YES | YES |
| 237 | a | 1268.89 | 68.51859 | YES | YES |
| 238 | a | 1304.11 | 9.35272 | YES | YES |
| 239 | a | 1307.30 | 0.49713 | YES | YES |
| 240 | a | 1317.13 | 0.08020 | YES | YES |
| 241 | a | 1332.93 | 148.58835 | YES | YES |
| 242 | a | 1345.41 | 20.22914 | YES | YES |
| 243 | a | 1347.48 | 105.43763 | YES | YES |
| 244 | a | 1354.50 | 0.06532 | YES | YES |
| 245 | a | 1361.13 | 2.66513 | YES | YES |
| 246 | a | 1363.89 | 4.93658 | YES | YES |
| 247 | a | 1367.75 | 1.16658 | YES | YES |
| 248 | a | 1374.59 | 3.72978 | YES | YES |
| 249 | a | 1380.95 | 0.17825 | YES | YES |
| 250 | a | 1381.10 | 0.21816 | YES | YES |
| 251 | a | 1393.26 | 1.22696 | YES | YES |
| 252 | a | 1398.32 | 2.40802 | YES | YES |
| 253 | a | 1414.14 | 6.67327 | YES | YES |
| 254 | a | 1414.90 | 2.75392 | YES | YES |
| 255 | a | 1423.15 | 0.84871 | YES | YES |
| 256 | a | 1426.05 | 11.24288 | YES | YES |
| 257 | a | 1429.35 | 28.48668 | YES | YES |
| 258 | a | 1433.51 | 0.97257 | YES | YES |
| 259 | a | 1441.56 | 32.89334 | YES | YES |
| 260 | a | 1447.16 | 6.69394 | YES | YES |
| 261 | a | 1454.53 | 18.82428 | YES | YES |
| 262 | a | 1458.47 | 2.65637 | YES | YES |
| 263 | a | 1458.60 | 11.45396 | YES | YES |
| 264 | a | 1463.10 | 13.34451 | YES | YES |
| 265 | a | 1468.68 | 44.10575 | YES | YES |
| 266 | a | 1472.50 | 7.25489 | YES | YES |
| 267 | a | 1505.09 | 406.13125 | YES | YES |
| 268 | a | 1507.17 | 42.59677 | YES | YES |
| 269 | a | 1560.96 | 0.22390 | YES | YES |
| 270 | a | 1568.24 | 0.20332 | YES | YES |
| 271 | a | 1617.58 | 1.11255 | YES | YES |
| 272 | a | 1617.83 | 2.61596 | YES | YES |
| 273 | a | 1630.40 | 25.53975 | YES | YES |
| 274 | a | 1631.52 | 14.77699 | YES | YES |
| 275 | a | 2884.58 | 60.11936 | YES | YES |
| 276 | a | 2935.48 | 23.68503 | YES | YES |
| 277 | a | 2940.07 | 16.99884 | YES | YES |
| 278 | a | 2942.84 | 15.73132 | YES | YES |
| 279 | a | 2953.36 | 16.57123 | YES | YES |
| 280 | a | 2959.64 | 15.67329 | YES | YES |
| 281 | a | 3017.91 | 15.32164 | YES | YES |
| 282 | a | 3020.72 | 4.46854 | YES | YES |
| 283 | a | 3022.34 | 6.28608 | YES | YES |
| 284 | a | 3025.99 | 10.45170 | YES | YES |
| 285 | a | 3037.07 | 6.18395 | YES | YES |
| 286 | a | 3044.98 | 3.60560 | YES | YES |
| 287 | a | 3061.41 | 19.63749 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 288 | a | 3066.10 | 2.93783 | YES | YES |
| 289 | a | 3071.58 | 4.93755 | YES | YES |
| 290 | a | 3081.91 | 28.12769 | YES | YES |
| 291 | a | 3082.45 | 7.90960 | YES | YES |
| 292 | a | 3097.52 | 4.47453 | YES | YES |
| 293 | a | 3113.87 | 2.13140 | YES | YES |
| 294 | a | 3114.30 | 2.09220 | YES | YES |
| 295 | a | 3126.99 | 7.82664 | YES | YES |
| 296 | a | 3127.30 | 7.17049 | YES | YES |
| 297 | a | 3137.05 | 0.29413 | YES | YES |
| 298 | a | 3137.45 | 0.25088 | YES | YES |
| 299 | a | 3159.10 | 2.12677 | YES | YES |
| 300 | a | 3165.08 | 2.68619 | YES | YES |

F-Ba(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 1.34197 | -0.35056 | -2.23739 |
| C | 1.76387 | -1.43932 | -1.41944 |
| C | 0.92315 | -2.58211 | -1.26370 |
| C | -0.39419 | -2.57650 | -1.80685 |
| C | -0.81736 | -1.48886 | -2.62639 |
| C | 0.04692 | -0.37641 | -2.83508 |
| C | 2.26542 | 0.82007 | -2.50840 |
| H | 2.33559 | 1.01340 | -3.59992 |
| H | 3.29449 | 0.63892 | -2.14760 |
| H | 1.90055 | 1.75853 | -2.03625 |
| C | 3.11556 | -1.41269 | -0.73503 |
| H | 3.14377 | -2.08077 | 0.14745 |
| H | 3.37266 | -0.39594 | -0.37812 |
| H | 3.92991 | -1.73883 | -1.42227 |
| C | 1.48001 | -3.81910 | -0.58600 |
| H | 0.88739 | -4.72245 | -0.82343 |
| H | 1.52567 | -3.73711 | 0.52253 |
| H | 2.51583 | -4.01370 | -0.93475 |
| C | -1.35762 | -3.71296 | -1.53234 |
| H | -1.41366 | -4.41823 | -2.39311 |
| H | -2.38292 | -3.32951 | -1.35508 |
| H | -1.06956 | -4.30265 | -0.64080 |
| C | -2.19671 | -1.48726 | -3.24019 |
| H | -2.58901 | -2.51059 | -3.39586 |
| H | -2.20727 | -0.97831 | -4.22417 |
| H | -2.89717 | -0.94334 | -2.56317 |
| C | -0.43736 | 0.77619 | -3.68673 |

| | | | |
|---|---|---|---|
| H | -0.45754 | 0.49170 | -4.76380 |
| H | 0.19984 | 1.67402 | -3.59333 |
| H | -1.47091 | 1.06953 | -3.40817 |
| C | -0.96142 | 3.12883 | -0.53469 |
| C | -0.21465 | 4.31258 | -0.49071 |
| C | -0.82897 | 5.48791 | -0.04894 |
| H | -0.23913 | 6.41658 | -0.01535 |
| C | -2.18156 | 5.44975 | 0.33518 |
| H | -2.66833 | 6.37534 | 0.68012 |
| C | -2.91383 | 4.25052 | 0.27302 |
| H | -3.97472 | 4.23371 | 0.56713 |
| C | -2.30257 | 3.06339 | -0.17079 |
| H | -2.81464 | 2.08579 | -0.23164 |
| F | -0.29526 | 1.97987 | -0.92177 |
| F | 1.07900 | 4.29068 | -0.86053 |
| C | 1.23941 | 2.10688 | 1.66205 |
| C | -0.03520 | 2.14555 | 2.23715 |
| C | -0.46753 | 3.24560 | 2.97114 |
| H | -1.48330 | 3.25289 | 3.39266 |
| C | 0.42030 | 4.32534 | 3.12503 |
| H | 0.09799 | 5.20931 | 3.69604 |
| C | 1.70453 | 4.28588 | 2.55420 |
| H | 2.38942 | 5.13846 | 2.67888 |
| C | 2.12706 | 3.16857 | 1.81116 |
| H | 3.11835 | 3.12168 | 1.33687 |
| F | 1.56236 | 1.00704 | 0.90979 |
| F | -0.86466 | 1.07654 | 2.01110 |
| C | 0.29390 | -2.58404 | 2.45685 |
| C | -0.99212 | -2.98696 | 2.08686 |
| C | -1.54259 | -4.17170 | 2.56914 |
| H | -2.55804 | -4.46451 | 2.26242 |
| C | -0.76668 | -4.95324 | 3.44575 |
| H | -1.18269 | -5.89278 | 3.84051 |
| C | 0.52491 | -4.54355 | 3.82187 |
| H | 1.12019 | -5.16206 | 4.51086 |
| C | 1.07169 | -3.34511 | 3.32522 |
| H | 2.08095 | -3.00300 | 3.59983 |
| F | 0.76836 | -1.42255 | 1.90243 |
| F | -1.67612 | -2.17859 | 1.22470 |
| Ca | -0.52907 | -0.31651 | -0.07664 |
| F | -2.45668 | 0.04073 | -0.44951 |

Vibrational analysis

| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 9.66 | 0.05739 | YES | YES |
| 8 | a | 14.16 | 0.87588 | YES | YES |
| 9 | a | 22.63 | 0.53912 | YES | YES |
| 10 | a | 24.58 | 0.17508 | YES | YES |

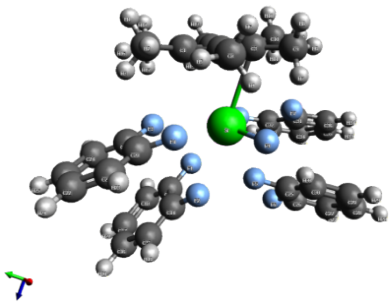
| | | | | | |
|---|---|---|---|---|---|
| 11 | a | 36.37 | 0.27180 | YES | YES |
| 12 | a | 43.76 | 0.35139 | YES | YES |
| 13 | a | 49.55 | 0.42378 | YES | YES |
| 14 | a | 50.37 | 1.02663 | YES | YES |
| 15 | a | 57.51 | 0.14541 | YES | YES |
| 16 | a | 64.40 | 0.18448 | YES | YES |
| 17 | a | 66.22 | 0.37606 | YES | YES |
| 18 | a | 70.36 | 0.91342 | YES | YES |
| 19 | a | 78.70 | 1.74277 | YES | YES |
| 20 | a | 83.45 | 0.02473 | YES | YES |
| 21 | a | 86.94 | 0.38941 | YES | YES |
| 22 | a | 91.16 | 0.42245 | YES | YES |
| 23 | a | 98.43 | 1.14380 | YES | YES |
| 24 | a | 103.04 | 2.33566 | YES | YES |
| 25 | a | 107.61 | 0.15726 | YES | YES |
| 26 | a | 118.15 | 0.57906 | YES | YES |
| 27 | a | 126.16 | 5.26699 | YES | YES |
| 28 | a | 129.47 | 1.11260 | YES | YES |
| 29 | a | 135.32 | 1.96926 | YES | YES |
| 30 | a | 140.13 | 2.75473 | YES | YES |
| 31 | a | 141.44 | 0.48758 | YES | YES |
| 32 | a | 156.23 | 11.04659 | YES | YES |
| 33 | a | 168.77 | 0.61587 | YES | YES |
| 34 | a | 181.54 | 2.65167 | YES | YES |
| 35 | a | 186.64 | 5.45969 | YES | YES |
| 36 | a | 189.85 | 31.68803 | YES | YES |
| 37 | a | 193.32 | 31.56570 | YES | YES |
| 38 | a | 198.43 | 1.32826 | YES | YES |
| 39 | a | 200.15 | 6.71857 | YES | YES |
| 40 | a | 207.91 | 26.26591 | YES | YES |
| 41 | a | 213.39 | 26.44234 | YES | YES |
| 42 | a | 256.55 | 73.58015 | YES | YES |
| 43 | a | 288.92 | 0.45641 | YES | YES |
| 44 | a | 290.37 | 0.26257 | YES | YES |
| 45 | a | 297.90 | 3.61511 | YES | YES |
| 46 | a | 300.77 | 1.49440 | YES | YES |
| 47 | a | 306.23 | 8.22816 | YES | YES |
| 48 | a | 308.06 | 1.99261 | YES | YES |
| 49 | a | 335.67 | 0.60885 | YES | YES |
| 50 | a | 345.47 | 1.12590 | YES | YES |
| 51 | a | 369.71 | 1.00105 | YES | YES |
| 52 | a | 379.96 | 1.93568 | YES | YES |
| 53 | a | 397.24 | 0.04012 | YES | YES |
| 54 | a | 405.72 | 0.03363 | YES | YES |
| 55 | a | 433.91 | 0.23235 | YES | YES |
| 56 | a | 435.58 | 1.13000 | YES | YES |
| 57 | a | 436.09 | 0.08221 | YES | YES |
| 58 | a | 440.23 | 0.21927 | YES | YES |
| 59 | a | 442.21 | 2.41284 | YES | YES |
| 60 | a | 442.60 | 2.79227 | YES | YES |
| 61 | a | 445.29 | 0.05606 | YES | YES |
| 62 | a | 446.19 | 0.39848 | YES | YES |
| 63 | a | 459.78 | 1.55263 | YES | YES |
| 64 | a | 535.25 | 2.15317 | YES | YES |
| 65 | a | 536.41 | 65.05326 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 66 | a | 540.17 | 15.50590 | YES | YES |
| 67 | a | 540.70 | 3.18947 | YES | YES |
| 68 | a | 542.98 | 2.44376 | YES | YES |
| 69 | a | 543.71 | 3.02571 | YES | YES |
| 70 | a | 545.13 | 0.25952 | YES | YES |
| 71 | a | 550.17 | 0.92639 | YES | YES |
| 72 | a | 558.15 | 22.35992 | YES | YES |
| 73 | a | 559.57 | 7.08122 | YES | YES |
| 74 | a | 561.44 | 9.73392 | YES | YES |
| 75 | a | 567.87 | 0.74915 | YES | YES |
| 76 | a | 572.05 | 4.16824 | YES | YES |
| 77 | a | 576.79 | 0.64437 | YES | YES |
| 78 | a | 584.05 | 1.04817 | YES | YES |
| 79 | a | 669.25 | 0.37036 | YES | YES |
| 80 | a | 680.52 | 0.05917 | YES | YES |
| 81 | a | 683.82 | 0.77702 | YES | YES |
| 82 | a | 695.94 | 0.13809 | YES | YES |
| 83 | a | 745.06 | 73.15021 | YES | YES |
| 84 | a | 748.24 | 70.77145 | YES | YES |
| 85 | a | 752.73 | 25.36753 | YES | YES |
| 86 | a | 755.33 | 138.00127 | YES | YES |
| 87 | a | 759.60 | 49.13350 | YES | YES |
| 88 | a | 761.70 | 49.63053 | YES | YES |
| 89 | a | 795.99 | 1.03634 | YES | YES |
| 90 | a | 802.20 | 2.17387 | YES | YES |
| 91 | a | 820.04 | 7.89617 | YES | YES |
| 92 | a | 822.29 | 11.92045 | YES | YES |
| 93 | a | 829.34 | 19.52184 | YES | YES |
| 94 | a | 833.36 | 1.92066 | YES | YES |
| 95 | a | 841.34 | 0.08123 | YES | YES |
| 96 | a | 865.44 | 0.25864 | YES | YES |
| 97 | a | 924.89 | 2.28113 | YES | YES |
| 98 | a | 929.84 | 3.23916 | YES | YES |
| 99 | a | 955.25 | 3.92136 | YES | YES |
| 100 | a | 960.89 | 1.19136 | YES | YES |
| 101 | a | 962.23 | 0.10477 | YES | YES |
| 102 | a | 972.02 | 0.10044 | YES | YES |
| 103 | a | 976.26 | 0.04783 | YES | YES |
| 104 | a | 978.34 | 16.49162 | YES | YES |
| 105 | a | 980.68 | 1.44607 | YES | YES |
| 106 | a | 995.60 | 4.68646 | YES | YES |
| 107 | a | 1001.70 | 0.52272 | YES | YES |
| 108 | a | 1005.37 | 0.40075 | YES | YES |
| 109 | a | 1016.55 | 4.37711 | YES | YES |
| 110 | a | 1018.16 | 3.12337 | YES | YES |
| 111 | a | 1022.98 | 12.19514 | YES | YES |
| 112 | a | 1027.04 | 3.02087 | YES | YES |
| 113 | a | 1031.44 | 3.66721 | YES | YES |
| 114 | a | 1033.32 | 1.54744 | YES | YES |
| 115 | a | 1054.05 | 10.72215 | YES | YES |
| 116 | a | 1056.40 | 23.62146 | YES | YES |
| 117 | a | 1076.87 | 1.34462 | YES | YES |
| 118 | a | 1077.96 | 9.26691 | YES | YES |
| 119 | a | 1080.89 | 10.28445 | YES | YES |
| 120 | a | 1082.81 | 11.55182 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 121 | a | 1083.78 | 2.21868 | YES | YES |
| 122 | a | 1084.49 | 23.34296 | YES | YES |
| 123 | a | 1136.20 | 2.79932 | YES | YES |
| 124 | a | 1138.42 | 1.95135 | YES | YES |
| 125 | a | 1138.94 | 2.18998 | YES | YES |
| 126 | a | 1148.96 | 4.73712 | YES | YES |
| 127 | a | 1154.75 | 15.47139 | YES | YES |
| 128 | a | 1158.49 | 71.01491 | YES | YES |
| 129 | a | 1243.02 | 179.82426 | YES | YES |
| 130 | a | 1245.84 | 1.07885 | YES | YES |
| 131 | a | 1246.42 | 39.13719 | YES | YES |
| 132 | a | 1248.31 | 6.67585 | YES | YES |
| 133 | a | 1251.13 | 73.28310 | YES | YES |
| 134 | a | 1253.11 | 5.19765 | YES | YES |
| 135 | a | 1267.64 | 54.34674 | YES | YES |
| 136 | a | 1305.71 | 0.73018 | YES | YES |
| 137 | a | 1319.88 | 0.27913 | YES | YES |
| 138 | a | 1349.02 | 7.96268 | YES | YES |
| 139 | a | 1361.24 | 5.75294 | YES | YES |
| 140 | a | 1361.75 | 3.16561 | YES | YES |
| 141 | a | 1366.77 | 4.53772 | YES | YES |
| 142 | a | 1368.72 | 6.41615 | YES | YES |
| 143 | a | 1373.32 | 4.26079 | YES | YES |
| 144 | a | 1378.23 | 1.14916 | YES | YES |
| 145 | a | 1380.77 | 2.42123 | YES | YES |
| 146 | a | 1381.81 | 1.42607 | YES | YES |
| 147 | a | 1391.50 | 1.15458 | YES | YES |
| 148 | a | 1396.41 | 5.93140 | YES | YES |
| 149 | a | 1408.16 | 1.52150 | YES | YES |
| 150 | a | 1410.57 | 0.87663 | YES | YES |
| 151 | a | 1415.63 | 45.66279 | YES | YES |
| 152 | a | 1422.61 | 6.50899 | YES | YES |
| 153 | a | 1433.31 | 1.80230 | YES | YES |
| 154 | a | 1435.15 | 7.55940 | YES | YES |
| 155 | a | 1440.38 | 5.74578 | YES | YES |
| 156 | a | 1450.34 | 31.86286 | YES | YES |
| 157 | a | 1453.38 | 12.86274 | YES | YES |
| 158 | a | 1453.71 | 40.83732 | YES | YES |
| 159 | a | 1458.00 | 7.93296 | YES | YES |
| 160 | a | 1459.27 | 9.05258 | YES | YES |
| 161 | a | 1462.03 | 7.42537 | YES | YES |
| 162 | a | 1464.53 | 10.18532 | YES | YES |
| 163 | a | 1476.75 | 8.24637 | YES | YES |
| 164 | a | 1493.91 | 266.99278 | YES | YES |
| 165 | a | 1497.67 | 142.11946 | YES | YES |
| 166 | a | 1504.64 | 199.94547 | YES | YES |
| 167 | a | 1558.61 | 0.23390 | YES | YES |
| 168 | a | 1560.91 | 1.21368 | YES | YES |
| 169 | a | 1607.88 | 7.19349 | YES | YES |
| 170 | a | 1611.71 | 0.42018 | YES | YES |
| 171 | a | 1613.75 | 1.18781 | YES | YES |
| 172 | a | 1632.87 | 11.42297 | YES | YES |
| 173 | a | 1633.23 | 12.46575 | YES | YES |
| 174 | a | 1634.77 | 13.55372 | YES | YES |
| 175 | a | 2942.69 | 8.80428 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 176 | a | 2952.09 | 7.68820 | YES | YES |
| 177 | a | 2952.31 | 6.94937 | YES | YES |
| 178 | a | 2953.18 | 2.40677 | YES | YES |
| 179 | a | 2961.67 | 5.76924 | YES | YES |
| 180 | a | 2964.42 | 4.73544 | YES | YES |
| 181 | a | 3030.55 | 5.06062 | YES | YES |
| 182 | a | 3032.10 | 4.22186 | YES | YES |
| 183 | a | 3034.72 | 0.28271 | YES | YES |
| 184 | a | 3036.47 | 4.07556 | YES | YES |
| 185 | a | 3042.48 | 4.03425 | YES | YES |
| 186 | a | 3045.97 | 4.45760 | YES | YES |
| 187 | a | 3068.44 | 4.47644 | YES | YES |
| 188 | a | 3071.83 | 81.96209 | YES | YES |
| 189 | a | 3072.76 | 11.64031 | YES | YES |
| 190 | a | 3078.73 | 6.91722 | YES | YES |
| 191 | a | 3082.60 | 3.66349 | YES | YES |
| 192 | a | 3088.86 | 7.92527 | YES | YES |
| 193 | a | 3094.39 | 4.43912 | YES | YES |
| 194 | a | 3116.26 | 0.15476 | YES | YES |
| 195 | a | 3123.19 | 0.66086 | YES | YES |
| 196 | a | 3123.33 | 0.83037 | YES | YES |
| 197 | a | 3128.56 | 3.98225 | YES | YES |
| 198 | a | 3132.35 | 2.35982 | YES | YES |
| 199 | a | 3134.26 | 1.44391 | YES | YES |
| 200 | a | 3136.50 | 0.15644 | YES | YES |
| 201 | a | 3138.39 | 1.98116 | YES | YES |
| 202 | a | 3142.96 | 1.99708 | YES | YES |
| 203 | a | 3143.39 | 0.64113 | YES | YES |
| 204 | a | 3146.66 | 1.03824 | YES | YES |

[F-Ca(HMB)oDFB$_3$]$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.61493 | 2.57770 | -2.25986 |
| C | 1.53879 | 1.55763 | -2.62852 |
| C | 1.06428 | 0.31770 | -3.17023 |
| C | -0.33425 | 0.09131 | -3.31960 |
| C | -1.25430 | 1.06676 | -2.83244 |
| C | -0.78410 | 2.30665 | -2.32195 |
| C | 1.07314 | 3.96569 | -1.85863 |
| H | 0.68359 | 4.72080 | -2.57694 |
| H | 2.17283 | 4.06838 | -1.84930 |
| H | 0.70564 | 4.26816 | -0.85465 |
| C | 3.03744 | 1.72607 | -2.49295 |

| | | | |
|---|---|---|---|
| H | 3.46193 | 0.90295 | -1.87802 |
| H | 3.32734 | 2.67719 | -2.01149 |
| H | 3.53859 | 1.68716 | -3.48565 |
| C | 2.10595 | -0.70490 | -3.57231 |
| H | 2.73835 | -0.96971 | -2.69666 |
| H | 2.78238 | -0.30093 | -4.35742 |
| H | 1.66889 | -1.64305 | -3.95787 |
| C | -0.88132 | -1.12726 | -4.03585 |
| H | -1.48121 | -0.81451 | -4.91892 |
| H | -1.55657 | -1.73595 | -3.39663 |
| H | -0.08711 | -1.79985 | -4.40545 |
| C | -2.74866 | 0.84026 | -2.92011 |
| H | -3.21205 | 1.51151 | -3.67926 |
| H | -3.25193 | 1.06628 | -1.95534 |
| H | -3.01355 | -0.19723 | -3.19426 |
| C | -1.80295 | 3.35038 | -1.91659 |
| H | -1.34669 | 4.25004 | -1.46525 |
| H | -2.53366 | 2.94543 | -1.18349 |
| H | -2.39741 | 3.68639 | -2.79653 |
| C | -1.19233 | 0.68726 | 3.12834 |
| C | 0.16311 | 0.81900 | 3.45348 |
| C | 0.56733 | 1.43722 | 4.63452 |
| H | 1.64133 | 1.53048 | 4.85407 |
| C | -0.42158 | 1.93211 | 5.50223 |
| H | -0.12036 | 2.42341 | 6.44006 |
| C | -1.78377 | 1.80149 | 5.17970 |
| H | -2.55297 | 2.18792 | 5.86599 |
| C | -2.17937 | 1.17469 | 3.98399 |
| H | -3.23855 | 1.05882 | 3.70821 |
| F | -1.51925 | 0.10701 | 1.93964 |
| F | 1.08674 | 0.36815 | 2.55407 |
| C | 0.16320 | 3.25246 | 1.60119 |
| C | 1.55670 | 3.14593 | 1.53712 |
| C | 2.36822 | 3.92743 | 2.35739 |
| H | 3.46201 | 3.82408 | 2.29309 |
| C | 1.75074 | 4.82567 | 3.24742 |
| H | 2.37746 | 5.45105 | 3.90169 |
| C | 0.34973 | 4.93087 | 3.30555 |
| H | -0.12249 | 5.63616 | 4.00629 |
| C | -0.46163 | 4.13802 | 2.47456 |
| H | -1.55996 | 4.18847 | 2.50637 |
| F | -0.56967 | 2.41920 | 0.79758 |
| F | 2.08539 | 2.23976 | 0.67162 |
| C | 0.63226 | -3.30721 | 1.45236 |
| C | -0.22734 | -4.31656 | 1.90479 |
| C | 0.17907 | -5.65071 | 1.80586 |
| H | -0.49899 | -6.44024 | 2.16407 |
| C | 1.43705 | -5.94453 | 1.24959 |
| H | 1.75882 | -6.99497 | 1.17279 |
| C | 2.28137 | -4.91432 | 0.79738 |
| H | 3.26421 | -5.15327 | 0.36242 |
| C | 1.88118 | -3.56923 | 0.89743 |
| H | 2.48234 | -2.71748 | 0.52474 |
| F | 0.17252 | -2.00726 | 1.52080 |
| F | -1.43084 | -3.98572 | 2.40352 |

| | | | |
|---|---|---|---|
| C | -0.66657 | -3.23652 | -1.29957 |
| C | -1.82774 | -2.68557 | -0.74706 |
| C | -2.92426 | -3.48169 | -0.42965 |
| H | -3.81951 | -3.02523 | 0.01800 |
| C | -2.83668 | -4.86234 | -0.68580 |
| H | -3.69064 | -5.51060 | -0.43679 |
| C | -1.67288 | -5.41495 | -1.24864 |
| H | -1.61407 | -6.49715 | -1.44042 |
| C | -0.57125 | -4.60018 | -1.56340 |
| H | 0.36068 | -5.00657 | -1.98259 |
| F | 0.37877 | -2.39619 | -1.53519 |
| F | -1.83754 | -1.33384 | -0.50839 |
| Sr | 0.55119 | 0.01369 | -0.13727 |
| F | 2.56054 | -0.75911 | -0.21095 |

Vibrational analysis

| 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 | 15.33 | 0.69057 | YES | YES |
| 8 | a | 16.58 | 0.31378 | YES | YES |
| 9 | a | 19.62 | 0.47694 | YES | YES |
| 10 | a | 25.94 | 0.28389 | YES | YES |
| 11 | a | 29.84 | 0.68123 | YES | YES |
| 12 | a | 32.57 | 0.21961 | YES | YES |
| 13 | a | 37.59 | 0.16876 | YES | YES |
| 14 | a | 39.80 | 0.12435 | YES | YES |
| 15 | a | 43.90 | 0.22317 | YES | YES |
| 16 | a | 52.50 | 0.34368 | YES | YES |
| 17 | a | 53.80 | 0.21586 | YES | YES |
| 18 | a | 56.51 | 0.91380 | YES | YES |
| 19 | a | 58.06 | 0.65425 | YES | YES |
| 20 | a | 62.04 | 0.25667 | YES | YES |
| 21 | a | 64.97 | 0.74549 | YES | YES |
| 22 | a | 70.41 | 0.24523 | YES | YES |
| 23 | a | 72.14 | 0.44242 | YES | YES |
| 24 | a | 75.07 | 0.20010 | YES | YES |
| 25 | a | 76.39 | 2.27811 | YES | YES |
| 26 | a | 80.96 | 0.65321 | YES | YES |
| 27 | a | 84.33 | 0.68808 | YES | YES |
| 28 | a | 87.28 | 0.44053 | YES | YES |
| 29 | a | 88.87 | 3.37792 | YES | YES |
| 30 | a | 93.97 | 1.79742 | YES | YES |
| 31 | a | 95.20 | 0.52155 | YES | YES |
| 32 | a | 100.79 | 3.98053 | YES | YES |
| 33 | a | 110.47 | 0.21260 | YES | YES |
| 34 | a | 116.52 | 17.70423 | YES | YES |
| 35 | a | 122.42 | 12.94897 | YES | YES |
| 36 | a | 123.74 | 25.40192 | YES | YES |

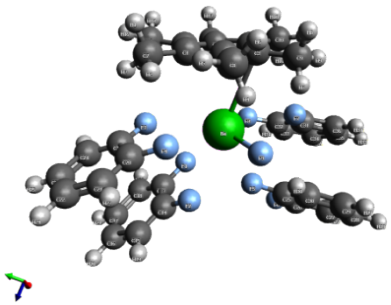
| | | | | | |
|---|---|---|---|---|---|
| 37 | a | 136.01 | 31.64804 | YES | YES |
| 38 | a | 138.56 | 0.36767 | YES | YES |
| 39 | a | 142.92 | 4.87269 | YES | YES |
| 40 | a | 149.05 | 54.62518 | YES | YES |
| 41 | a | 156.19 | 7.60895 | YES | YES |
| 42 | a | 197.41 | 1.88193 | YES | YES |
| 43 | a | 199.87 | 4.27145 | YES | YES |
| 44 | a | 201.66 | 9.26273 | YES | YES |
| 45 | a | 206.43 | 1.25961 | YES | YES |
| 46 | a | 211.61 | 0.78637 | YES | YES |
| 47 | a | 214.31 | 0.08899 | YES | YES |
| 48 | a | 219.87 | 0.91682 | YES | YES |
| 49 | a | 255.65 | 7.28356 | YES | YES |
| 50 | a | 288.75 | 0.51229 | YES | YES |
| 51 | a | 290.13 | 0.77376 | YES | YES |
| 52 | a | 294.63 | 2.34760 | YES | YES |
| 53 | a | 296.45 | 2.64010 | YES | YES |
| 54 | a | 297.39 | 5.51521 | YES | YES |
| 55 | a | 298.43 | 2.38928 | YES | YES |
| 56 | a | 304.30 | 0.86507 | YES | YES |
| 57 | a | 305.55 | 0.73525 | YES | YES |
| 58 | a | 326.43 | 0.52623 | YES | YES |
| 59 | a | 347.23 | 1.36783 | YES | YES |
| 60 | a | 366.08 | 0.63867 | YES | YES |
| 61 | a | 373.15 | 1.58375 | YES | YES |
| 62 | a | 389.57 | 0.03540 | YES | YES |
| 63 | a | 402.72 | 0.19244 | YES | YES |
| 64 | a | 433.74 | 0.09342 | YES | YES |
| 65 | a | 434.11 | 0.14073 | YES | YES |
| 66 | a | 435.30 | 0.02897 | YES | YES |
| 67 | a | 436.07 | 0.94509 | YES | YES |
| 68 | a | 436.58 | 0.76287 | YES | YES |
| 69 | a | 442.20 | 0.21191 | YES | YES |
| 70 | a | 443.64 | 4.57772 | YES | YES |
| 71 | a | 444.15 | 2.84360 | YES | YES |
| 72 | a | 447.25 | 0.03086 | YES | YES |
| 73 | a | 448.80 | 1.56530 | YES | YES |
| 74 | a | 450.64 | 58.11144 | YES | YES |
| 75 | a | 461.26 | 2.90626 | YES | YES |
| 76 | a | 535.97 | 1.91332 | YES | YES |
| 77 | a | 536.41 | 0.10944 | YES | YES |
| 78 | a | 537.40 | 4.91151 | YES | YES |
| 79 | a | 539.50 | 5.70744 | YES | YES |
| 80 | a | 543.58 | 1.12058 | YES | YES |
| 81 | a | 543.69 | 0.65736 | YES | YES |
| 82 | a | 543.78 | 1.72692 | YES | YES |
| 83 | a | 546.30 | 0.22014 | YES | YES |
| 84 | a | 552.96 | 1.49564 | YES | YES |
| 85 | a | 559.67 | 13.46647 | YES | YES |
| 86 | a | 559.72 | 6.23392 | YES | YES |
| 87 | a | 560.66 | 19.54886 | YES | YES |
| 88 | a | 561.81 | 1.25231 | YES | YES |
| 89 | a | 562.11 | 7.28683 | YES | YES |
| 90 | a | 572.43 | 0.19942 | YES | YES |
| 91 | a | 580.60 | 0.17790 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 92 | a | 585.93 | 0.02041 | YES | YES |
| 93 | a | 672.39 | 0.28095 | YES | YES |
| 94 | a | 672.81 | 0.34873 | YES | YES |
| 95 | a | 676.34 | 0.25689 | YES | YES |
| 96 | a | 679.44 | 0.34813 | YES | YES |
| 97 | a | 705.97 | 1.53988 | YES | YES |
| 98 | a | 744.57 | 38.89837 | YES | YES |
| 99 | a | 745.46 | 178.91931 | YES | YES |
| 100 | a | 749.30 | 1.46743 | YES | YES |
| 101 | a | 754.14 | 44.39079 | YES | YES |
| 102 | a | 755.78 | 11.54921 | YES | YES |
| 103 | a | 757.69 | 137.88035 | YES | YES |
| 104 | a | 760.82 | 10.74928 | YES | YES |
| 105 | a | 761.52 | 99.65564 | YES | YES |
| 106 | a | 789.84 | 0.56616 | YES | YES |
| 107 | a | 799.59 | 3.80913 | YES | YES |
| 108 | a | 822.67 | 5.99895 | YES | YES |
| 109 | a | 823.67 | 0.26348 | YES | YES |
| 110 | a | 825.95 | 17.95712 | YES | YES |
| 111 | a | 830.79 | 20.24898 | YES | YES |
| 112 | a | 834.83 | 1.11655 | YES | YES |
| 113 | a | 836.01 | 0.39431 | YES | YES |
| 114 | a | 838.92 | 0.33957 | YES | YES |
| 115 | a | 861.95 | 0.79926 | YES | YES |
| 116 | a | 924.61 | 2.94434 | YES | YES |
| 117 | a | 925.82 | 7.60889 | YES | YES |
| 118 | a | 927.09 | 0.78804 | YES | YES |
| 119 | a | 950.50 | 2.91333 | YES | YES |
| 120 | a | 951.53 | 7.26873 | YES | YES |
| 121 | a | 960.47 | 0.75700 | YES | YES |
| 122 | a | 970.60 | 4.05036 | YES | YES |
| 123 | a | 970.84 | 0.05673 | YES | YES |
| 124 | a | 971.41 | 0.20217 | YES | YES |
| 125 | a | 972.34 | 0.06690 | YES | YES |
| 126 | a | 983.06 | 15.10324 | YES | YES |
| 127 | a | 987.02 | 7.01019 | YES | YES |
| 128 | a | 1004.93 | 1.05293 | YES | YES |
| 129 | a | 1005.48 | 3.70240 | YES | YES |
| 130 | a | 1018.96 | 2.18691 | YES | YES |
| 131 | a | 1019.26 | 3.89439 | YES | YES |
| 132 | a | 1020.65 | 4.74565 | YES | YES |
| 133 | a | 1026.20 | 2.29881 | YES | YES |
| 134 | a | 1027.26 | 9.18714 | YES | YES |
| 135 | a | 1030.77 | 0.07814 | YES | YES |
| 136 | a | 1035.49 | 0.38446 | YES | YES |
| 137 | a | 1045.36 | 18.77988 | YES | YES |
| 138 | a | 1051.66 | 9.83996 | YES | YES |
| 139 | a | 1072.33 | 0.33057 | YES | YES |
| 140 | a | 1073.22 | 5.58497 | YES | YES |
| 141 | a | 1083.12 | 0.34629 | YES | YES |
| 142 | a | 1084.68 | 11.99400 | YES | YES |
| 143 | a | 1085.35 | 0.55769 | YES | YES |
| 144 | a | 1086.16 | 18.19938 | YES | YES |
| 145 | a | 1087.37 | 32.89247 | YES | YES |
| 146 | a | 1137.09 | 3.26104 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 147 | a | 1137.61 | 2.11656 | YES | YES |
| 148 | a | 1137.83 | 1.71271 | YES | YES |
| 149 | a | 1138.13 | 1.20556 | YES | YES |
| 150 | a | 1153.02 | 4.74113 | YES | YES |
| 151 | a | 1155.37 | 0.65911 | YES | YES |
| 152 | a | 1164.95 | 72.11969 | YES | YES |
| 153 | a | 1166.93 | 21.58276 | YES | YES |
| 154 | a | 1244.12 | 4.95307 | YES | YES |
| 155 | a | 1245.48 | 50.80528 | YES | YES |
| 156 | a | 1246.74 | 0.83971 | YES | YES |
| 157 | a | 1249.37 | 3.35116 | YES | YES |
| 158 | a | 1249.58 | 5.12214 | YES | YES |
| 159 | a | 1252.25 | 153.23514 | YES | YES |
| 160 | a | 1255.72 | 2.76147 | YES | YES |
| 161 | a | 1260.32 | 199.41025 | YES | YES |
| 162 | a | 1271.56 | 50.54662 | YES | YES |
| 163 | a | 1290.24 | 0.61744 | YES | YES |
| 164 | a | 1318.58 | 2.29563 | YES | YES |
| 165 | a | 1352.93 | 0.35267 | YES | YES |
| 166 | a | 1355.89 | 4.18734 | YES | YES |
| 167 | a | 1362.55 | 0.60326 | YES | YES |
| 168 | a | 1367.51 | 1.01647 | YES | YES |
| 169 | a | 1368.10 | 13.79993 | YES | YES |
| 170 | a | 1375.45 | 7.40437 | YES | YES |
| 171 | a | 1378.33 | 1.03493 | YES | YES |
| 172 | a | 1380.31 | 0.23329 | YES | YES |
| 173 | a | 1381.64 | 0.31400 | YES | YES |
| 174 | a | 1382.44 | 0.70376 | YES | YES |
| 175 | a | 1389.69 | 0.14149 | YES | YES |
| 176 | a | 1397.14 | 8.43758 | YES | YES |
| 177 | a | 1404.63 | 0.26207 | YES | YES |
| 178 | a | 1416.10 | 0.49703 | YES | YES |
| 179 | a | 1422.18 | 24.43147 | YES | YES |
| 180 | a | 1425.53 | 1.15766 | YES | YES |
| 181 | a | 1427.58 | 4.45007 | YES | YES |
| 182 | a | 1430.01 | 11.70298 | YES | YES |
| 183 | a | 1438.89 | 25.95702 | YES | YES |
| 184 | a | 1440.18 | 6.89522 | YES | YES |
| 185 | a | 1444.98 | 7.79764 | YES | YES |
| 186 | a | 1453.70 | 6.38790 | YES | YES |
| 187 | a | 1453.75 | 15.11777 | YES | YES |
| 188 | a | 1458.02 | 4.33769 | YES | YES |
| 189 | a | 1458.88 | 7.34721 | YES | YES |
| 190 | a | 1459.59 | 9.92938 | YES | YES |
| 191 | a | 1462.57 | 54.25683 | YES | YES |
| 192 | a | 1469.14 | 16.62566 | YES | YES |
| 193 | a | 1496.33 | 20.88743 | YES | YES |
| 194 | a | 1497.22 | 268.12048 | YES | YES |
| 195 | a | 1502.24 | 372.78542 | YES | YES |
| 196 | a | 1508.73 | 120.28010 | YES | YES |
| 197 | a | 1556.19 | 0.15960 | YES | YES |
| 198 | a | 1564.61 | 1.76001 | YES | YES |
| 199 | a | 1609.54 | 7.26157 | YES | YES |
| 200 | a | 1612.75 | 0.31291 | YES | YES |
| 201 | a | 1614.51 | 0.81372 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 202 | a | 1616.61 | 0.44311 | YES | YES |
| 203 | a | 1629.63 | 14.13797 | YES | YES |
| 204 | a | 1632.11 | 9.95386 | YES | YES |
| 205 | a | 1632.50 | 23.48476 | YES | YES |
| 206 | a | 1633.22 | 8.63354 | YES | YES |
| 207 | a | 2944.76 | 18.45047 | YES | YES |
| 208 | a | 2948.14 | 6.07204 | YES | YES |
| 209 | a | 2950.66 | 17.62048 | YES | YES |
| 210 | a | 2951.84 | 2.35882 | YES | YES |
| 211 | a | 2957.17 | 13.31134 | YES | YES |
| 212 | a | 2957.46 | 13.30103 | YES | YES |
| 213 | a | 3010.09 | 17.71563 | YES | YES |
| 214 | a | 3014.88 | 0.63406 | YES | YES |
| 215 | a | 3019.17 | 3.26040 | YES | YES |
| 216 | a | 3020.10 | 7.39027 | YES | YES |
| 217 | a | 3021.16 | 8.91856 | YES | YES |
| 218 | a | 3022.74 | 0.69380 | YES | YES |
| 219 | a | 3046.33 | 112.22574 | YES | YES |
| 220 | a | 3085.45 | 0.49951 | YES | YES |
| 221 | a | 3085.84 | 5.51103 | YES | YES |
| 222 | a | 3088.75 | 9.25027 | YES | YES |
| 223 | a | 3089.44 | 17.65615 | YES | YES |
| 224 | a | 3095.10 | 12.11742 | YES | YES |
| 225 | a | 3096.60 | 17.40803 | YES | YES |
| 226 | a | 3114.30 | 0.51542 | YES | YES |
| 227 | a | 3119.70 | 0.85514 | YES | YES |
| 228 | a | 3120.98 | 0.87867 | YES | YES |
| 229 | a | 3121.91 | 0.75022 | YES | YES |
| 230 | a | 3127.47 | 4.12686 | YES | YES |
| 231 | a | 3129.92 | 2.08371 | YES | YES |
| 232 | a | 3131.36 | 2.79115 | YES | YES |
| 233 | a | 3132.90 | 2.27699 | YES | YES |
| 234 | a | 3135.50 | 0.30669 | YES | YES |
| 235 | a | 3136.59 | 0.74217 | YES | YES |
| 236 | a | 3138.22 | 1.46283 | YES | YES |
| 237 | a | 3141.16 | 0.91087 | YES | YES |
| 238 | a | 3142.29 | 0.53716 | YES | YES |
| 239 | a | 3143.20 | 0.39845 | YES | YES |
| 240 | a | 3145.92 | 0.98689 | YES | YES |

[F-Sr(HMB)oDFB$_3$]$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.61493 | 2.57770 | -2.25986 |

| | | | |
|---|---|---|---|
| C | 1.53879 | 1.55763 | -2.62852 |
| C | 1.06428 | 0.31770 | -3.17023 |
| C | -0.33425 | 0.09131 | -3.31960 |
| C | -1.25430 | 1.06676 | -2.83244 |
| C | -0.78410 | 2.30665 | -2.32195 |
| C | 1.07314 | 3.96569 | -1.85863 |
| H | 0.68359 | 4.72080 | -2.57694 |
| H | 2.17283 | 4.06838 | -1.84930 |
| H | 0.70564 | 4.26816 | -0.85465 |
| C | 3.03744 | 1.72607 | -2.49295 |
| H | 3.46193 | 0.90295 | -1.87802 |
| H | 3.32734 | 2.67719 | -2.01149 |
| H | 3.53859 | 1.68716 | -3.48565 |
| C | 2.10595 | -0.70490 | -3.57231 |
| H | 2.73835 | -0.96971 | -2.69666 |
| H | 2.78238 | -0.30093 | -4.35742 |
| H | 1.66889 | -1.64305 | -3.95787 |
| C | -0.88132 | -1.12726 | -4.03585 |
| H | -1.48121 | -0.81451 | -4.91892 |
| H | -1.55657 | -1.73595 | -3.39663 |
| H | -0.08711 | -1.79985 | -4.40545 |
| C | -2.74866 | 0.84026 | -2.92011 |
| H | -3.21205 | 1.51151 | -3.67926 |
| H | -3.25193 | 1.06628 | -1.95534 |
| H | -3.01355 | -0.19723 | -3.19426 |
| C | -1.80295 | 3.35038 | -1.91659 |
| H | -1.34669 | 4.25004 | -1.46525 |
| H | -2.53366 | 2.94543 | -1.18349 |
| H | -2.39741 | 3.68639 | -2.79653 |
| C | -1.19233 | 0.68726 | 3.12834 |
| C | 0.16311 | 0.81900 | 3.45348 |
| C | 0.56733 | 1.43722 | 4.63452 |
| H | 1.64133 | 1.53048 | 4.85407 |
| C | -0.42158 | 1.93211 | 5.50223 |
| H | -0.12036 | 2.42341 | 6.44006 |
| C | -1.78377 | 1.80149 | 5.17970 |
| H | -2.55297 | 2.18792 | 5.86599 |
| C | -2.17937 | 1.17469 | 3.98399 |
| H | -3.23855 | 1.05882 | 3.70821 |
| F | -1.51925 | 0.10701 | 1.93964 |
| F | 1.08674 | 0.36815 | 2.55407 |
| C | 0.16320 | 3.25246 | 1.60119 |
| C | 1.55670 | 3.14593 | 1.53712 |
| C | 2.36822 | 3.92743 | 2.35739 |
| H | 3.46201 | 3.82408 | 2.29309 |
| C | 1.75074 | 4.82567 | 3.24742 |
| H | 2.37746 | 5.45105 | 3.90169 |
| C | 0.34973 | 4.93087 | 3.30555 |
| H | -0.12249 | 5.63616 | 4.00629 |
| C | -0.46163 | 4.13802 | 2.47456 |
| H | -1.55996 | 4.18847 | 2.50637 |
| F | -0.56967 | 2.41920 | 0.79758 |
| F | 2.08539 | 2.23976 | 0.67162 |
| C | 0.63226 | -3.30721 | 1.45236 |
| C | -0.22734 | -4.31656 | 1.90479 |

| | | | |
|---|---|---|---|
| C | 0.17907 | -5.65071 | 1.80586 |
| H | -0.49899 | -6.44024 | 2.16407 |
| C | 1.43705 | -5.94453 | 1.24959 |
| H | 1.75882 | -6.99497 | 1.17279 |
| C | 2.28137 | -4.91432 | 0.79738 |
| H | 3.26421 | -5.15327 | 0.36242 |
| C | 1.88118 | -3.56923 | 0.89743 |
| H | 2.48234 | -2.71748 | 0.52474 |
| F | 0.17252 | -2.00726 | 1.52080 |
| F | -1.43084 | -3.98572 | 2.40352 |
| C | -0.66657 | -3.23652 | -1.29957 |
| C | -1.82774 | -2.68557 | -0.74706 |
| C | -2.92426 | -3.48169 | -0.42965 |
| H | -3.81951 | -3.02523 | 0.01800 |
| C | -2.83668 | -4.86234 | -0.68580 |
| H | -3.69064 | -5.51060 | -0.43679 |
| C | -1.67288 | -5.41495 | -1.24864 |
| H | -1.61407 | -6.49715 | -1.44042 |
| C | -0.57125 | -4.60018 | -1.56340 |
| H | 0.36068 | -5.00657 | -1.98259 |
| F | 0.37877 | -2.39619 | -1.53519 |
| F | -1.83754 | -1.33384 | -0.50839 |
| Sr | 0.55119 | 0.01369 | -0.13727 |
| F | 2.56054 | -0.75911 | -0.21095 |

Vibrational analysis

| 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 | 15.33 | 0.69057 | YES | YES |
| 8 | a | 16.58 | 0.31378 | YES | YES |
| 9 | a | 19.62 | 0.47694 | YES | YES |
| 10 | a | 25.94 | 0.28389 | YES | YES |
| 11 | a | 29.84 | 0.68123 | YES | YES |
| 12 | a | 32.57 | 0.21961 | YES | YES |
| 13 | a | 37.59 | 0.16876 | YES | YES |
| 14 | a | 39.80 | 0.12435 | YES | YES |
| 15 | a | 43.90 | 0.22317 | YES | YES |
| 16 | a | 52.50 | 0.34368 | YES | YES |
| 17 | a | 53.80 | 0.21586 | YES | YES |
| 18 | a | 56.51 | 0.91380 | YES | YES |
| 19 | a | 58.06 | 0.65425 | YES | YES |
| 20 | a | 62.04 | 0.25667 | YES | YES |
| 21 | a | 64.97 | 0.74549 | YES | YES |
| 22 | a | 70.41 | 0.24523 | YES | YES |
| 23 | a | 72.14 | 0.44242 | YES | YES |
| 24 | a | 75.07 | 0.20010 | YES | YES |
| 25 | a | 76.39 | 2.27811 | YES | YES |
| 26 | a | 80.96 | 0.65321 | YES | YES |
| 27 | a | 84.33 | 0.68808 | YES | YES |

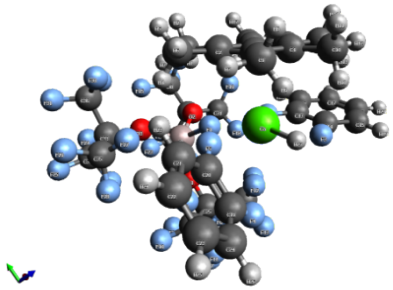
| | | | | | |
|---|---|---|---|---|---|
| 28 | a | 87.28 | 0.44053 | YES | YES |
| 29 | a | 88.87 | 3.37792 | YES | YES |
| 30 | a | 93.97 | 1.79742 | YES | YES |
| 31 | a | 95.20 | 0.52155 | YES | YES |
| 32 | a | 100.79 | 3.98053 | YES | YES |
| 33 | a | 110.47 | 0.21260 | YES | YES |
| 34 | a | 116.52 | 17.70423 | YES | YES |
| 35 | a | 122.42 | 12.94897 | YES | YES |
| 36 | a | 123.74 | 25.40192 | YES | YES |
| 37 | a | 136.01 | 31.64804 | YES | YES |
| 38 | a | 138.56 | 0.36767 | YES | YES |
| 39 | a | 142.92 | 4.87269 | YES | YES |
| 40 | a | 149.05 | 54.62518 | YES | YES |
| 41 | a | 156.19 | 7.60895 | YES | YES |
| 42 | a | 197.41 | 1.88193 | YES | YES |
| 43 | a | 199.87 | 4.27145 | YES | YES |
| 44 | a | 201.66 | 9.26273 | YES | YES |
| 45 | a | 206.43 | 1.25961 | YES | YES |
| 46 | a | 211.61 | 0.78637 | YES | YES |
| 47 | a | 214.31 | 0.08899 | YES | YES |
| 48 | a | 219.87 | 0.91682 | YES | YES |
| 49 | a | 255.65 | 7.28356 | YES | YES |
| 50 | a | 288.75 | 0.51229 | YES | YES |
| 51 | a | 290.13 | 0.77376 | YES | YES |
| 52 | a | 294.63 | 2.34760 | YES | YES |
| 53 | a | 296.45 | 2.64010 | YES | YES |
| 54 | a | 297.39 | 5.51521 | YES | YES |
| 55 | a | 298.43 | 2.38928 | YES | YES |
| 56 | a | 304.30 | 0.86507 | YES | YES |
| 57 | a | 305.55 | 0.73525 | YES | YES |
| 58 | a | 326.43 | 0.52623 | YES | YES |
| 59 | a | 347.23 | 1.36783 | YES | YES |
| 60 | a | 366.08 | 0.63867 | YES | YES |
| 61 | a | 373.15 | 1.58375 | YES | YES |
| 62 | a | 389.57 | 0.03540 | YES | YES |
| 63 | a | 402.72 | 0.19244 | YES | YES |
| 64 | a | 433.74 | 0.09342 | YES | YES |
| 65 | a | 434.11 | 0.14073 | YES | YES |
| 66 | a | 435.30 | 0.02897 | YES | YES |
| 67 | a | 436.07 | 0.94509 | YES | YES |
| 68 | a | 436.58 | 0.76287 | YES | YES |
| 69 | a | 442.20 | 0.21191 | YES | YES |
| 70 | a | 443.64 | 4.57772 | YES | YES |
| 71 | a | 444.15 | 2.84360 | YES | YES |
| 72 | a | 447.25 | 0.03086 | YES | YES |
| 73 | a | 448.80 | 1.56530 | YES | YES |
| 74 | a | 450.64 | 58.11144 | YES | YES |
| 75 | a | 461.26 | 2.90626 | YES | YES |
| 76 | a | 535.97 | 1.91332 | YES | YES |
| 77 | a | 536.41 | 0.10944 | YES | YES |
| 78 | a | 537.40 | 4.91151 | YES | YES |
| 79 | a | 539.50 | 5.70744 | YES | YES |
| 80 | a | 543.58 | 1.12058 | YES | YES |
| 81 | a | 543.69 | 0.65736 | YES | YES |
| 82 | a | 543.78 | 1.72692 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 83 | a | 546.30 | 0.22014 | YES | YES |
| 84 | a | 552.96 | 1.49564 | YES | YES |
| 85 | a | 559.67 | 13.46647 | YES | YES |
| 86 | a | 559.72 | 6.23392 | YES | YES |
| 87 | a | 560.66 | 19.54886 | YES | YES |
| 88 | a | 561.81 | 1.25231 | YES | YES |
| 89 | a | 562.11 | 7.28683 | YES | YES |
| 90 | a | 572.43 | 0.19942 | YES | YES |
| 91 | a | 580.60 | 0.17790 | YES | YES |
| 92 | a | 585.93 | 0.02041 | YES | YES |
| 93 | a | 672.39 | 0.28095 | YES | YES |
| 94 | a | 672.81 | 0.34873 | YES | YES |
| 95 | a | 676.34 | 0.25689 | YES | YES |
| 96 | a | 679.44 | 0.34813 | YES | YES |
| 97 | a | 705.97 | 1.53988 | YES | YES |
| 98 | a | 744.57 | 38.89837 | YES | YES |
| 99 | a | 745.46 | 178.91931 | YES | YES |
| 100 | a | 749.30 | 1.46743 | YES | YES |
| 101 | a | 754.14 | 44.39079 | YES | YES |
| 102 | a | 755.78 | 11.54921 | YES | YES |
| 103 | a | 757.69 | 137.88035 | YES | YES |
| 104 | a | 760.82 | 10.74928 | YES | YES |
| 105 | a | 761.52 | 99.65564 | YES | YES |
| 106 | a | 789.84 | 0.56616 | YES | YES |
| 107 | a | 799.59 | 3.80913 | YES | YES |
| 108 | a | 822.67 | 5.99895 | YES | YES |
| 109 | a | 823.67 | 0.26348 | YES | YES |
| 110 | a | 825.95 | 17.95712 | YES | YES |
| 111 | a | 830.79 | 20.24898 | YES | YES |
| 112 | a | 834.83 | 1.11655 | YES | YES |
| 113 | a | 836.01 | 0.39431 | YES | YES |
| 114 | a | 838.92 | 0.33957 | YES | YES |
| 115 | a | 861.95 | 0.79926 | YES | YES |
| 116 | a | 924.61 | 2.94434 | YES | YES |
| 117 | a | 925.82 | 7.60889 | YES | YES |
| 118 | a | 927.09 | 0.78804 | YES | YES |
| 119 | a | 950.50 | 2.91333 | YES | YES |
| 120 | a | 951.53 | 7.26873 | YES | YES |
| 121 | a | 960.47 | 0.75700 | YES | YES |
| 122 | a | 970.60 | 4.05036 | YES | YES |
| 123 | a | 970.84 | 0.05673 | YES | YES |
| 124 | a | 971.41 | 0.20217 | YES | YES |
| 125 | a | 972.34 | 0.06690 | YES | YES |
| 126 | a | 983.06 | 15.10324 | YES | YES |
| 127 | a | 987.02 | 7.01019 | YES | YES |
| 128 | a | 1004.93 | 1.05293 | YES | YES |
| 129 | a | 1005.48 | 3.70240 | YES | YES |
| 130 | a | 1018.96 | 2.18691 | YES | YES |
| 131 | a | 1019.26 | 3.89439 | YES | YES |
| 132 | a | 1020.65 | 4.74565 | YES | YES |
| 133 | a | 1026.20 | 2.29881 | YES | YES |
| 134 | a | 1027.26 | 9.18714 | YES | YES |
| 135 | a | 1030.77 | 0.07814 | YES | YES |
| 136 | a | 1035.49 | 0.38446 | YES | YES |
| 137 | a | 1045.36 | 18.77988 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 138 | a | 1051.66 | 9.83996 | YES | YES |
| 139 | a | 1072.33 | 0.33057 | YES | YES |
| 140 | a | 1073.22 | 5.58497 | YES | YES |
| 141 | a | 1083.12 | 0.34629 | YES | YES |
| 142 | a | 1084.68 | 11.99400 | YES | YES |
| 143 | a | 1085.35 | 0.55769 | YES | YES |
| 144 | a | 1086.16 | 18.19938 | YES | YES |
| 145 | a | 1087.37 | 32.89247 | YES | YES |
| 146 | a | 1137.09 | 3.26104 | YES | YES |
| 147 | a | 1137.61 | 2.11656 | YES | YES |
| 148 | a | 1137.83 | 1.71271 | YES | YES |
| 149 | a | 1138.13 | 1.20556 | YES | YES |
| 150 | a | 1153.02 | 4.74113 | YES | YES |
| 151 | a | 1155.37 | 0.65911 | YES | YES |
| 152 | a | 1164.95 | 72.11969 | YES | YES |
| 153 | a | 1166.93 | 21.58276 | YES | YES |
| 154 | a | 1244.12 | 4.95307 | YES | YES |
| 155 | a | 1245.48 | 50.80528 | YES | YES |
| 156 | a | 1246.74 | 0.83971 | YES | YES |
| 157 | a | 1249.37 | 3.35116 | YES | YES |
| 158 | a | 1249.58 | 5.12214 | YES | YES |
| 159 | a | 1252.25 | 153.23514 | YES | YES |
| 160 | a | 1255.72 | 2.76147 | YES | YES |
| 161 | a | 1260.32 | 199.41025 | YES | YES |
| 162 | a | 1271.56 | 50.54662 | YES | YES |
| 163 | a | 1290.24 | 0.61744 | YES | YES |
| 164 | a | 1318.58 | 2.29563 | YES | YES |
| 165 | a | 1352.93 | 0.35267 | YES | YES |
| 166 | a | 1355.89 | 4.18734 | YES | YES |
| 167 | a | 1362.55 | 0.60326 | YES | YES |
| 168 | a | 1367.51 | 1.01647 | YES | YES |
| 169 | a | 1368.10 | 13.79993 | YES | YES |
| 170 | a | 1375.45 | 7.40437 | YES | YES |
| 171 | a | 1378.33 | 1.03493 | YES | YES |
| 172 | a | 1380.31 | 0.23329 | YES | YES |
| 173 | a | 1381.64 | 0.31400 | YES | YES |
| 174 | a | 1382.44 | 0.70376 | YES | YES |
| 175 | a | 1389.69 | 0.14149 | YES | YES |
| 176 | a | 1397.14 | 8.43758 | YES | YES |
| 177 | a | 1404.63 | 0.26207 | YES | YES |
| 178 | a | 1416.10 | 0.49703 | YES | YES |
| 179 | a | 1422.18 | 24.43147 | YES | YES |
| 180 | a | 1425.53 | 1.15766 | YES | YES |
| 181 | a | 1427.58 | 4.45007 | YES | YES |
| 182 | a | 1430.01 | 11.70298 | YES | YES |
| 183 | a | 1438.89 | 25.95702 | YES | YES |
| 184 | a | 1440.18 | 6.89522 | YES | YES |
| 185 | a | 1444.98 | 7.79764 | YES | YES |
| 186 | a | 1453.70 | 6.38790 | YES | YES |
| 187 | a | 1453.75 | 15.11777 | YES | YES |
| 188 | a | 1458.02 | 4.33769 | YES | YES |
| 189 | a | 1458.88 | 7.34721 | YES | YES |
| 190 | a | 1459.59 | 9.92938 | YES | YES |
| 191 | a | 1462.57 | 54.25683 | YES | YES |
| 192 | a | 1469.14 | 16.62566 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 193 | a | 1496.33 | 20.88743 | YES | YES |
| 194 | a | 1497.22 | 268.12048 | YES | YES |
| 195 | a | 1502.24 | 372.78542 | YES | YES |
| 196 | a | 1508.73 | 120.28010 | YES | YES |
| 197 | a | 1556.19 | 0.15960 | YES | YES |
| 198 | a | 1564.61 | 1.76001 | YES | YES |
| 199 | a | 1609.54 | 7.26157 | YES | YES |
| 200 | a | 1612.75 | 0.31291 | YES | YES |
| 201 | a | 1614.51 | 0.81372 | YES | YES |
| 202 | a | 1616.61 | 0.44311 | YES | YES |
| 203 | a | 1629.63 | 14.13797 | YES | YES |
| 204 | a | 1632.11 | 9.95386 | YES | YES |
| 205 | a | 1632.50 | 23.48476 | YES | YES |
| 206 | a | 1633.22 | 8.63354 | YES | YES |
| 207 | a | 2944.76 | 18.45047 | YES | YES |
| 208 | a | 2948.14 | 6.07204 | YES | YES |
| 209 | a | 2950.66 | 17.62048 | YES | YES |
| 210 | a | 2951.84 | 2.35882 | YES | YES |
| 211 | a | 2957.17 | 13.31134 | YES | YES |
| 212 | a | 2957.46 | 13.30103 | YES | YES |
| 213 | a | 3010.09 | 17.71563 | YES | YES |
| 214 | a | 3014.88 | 0.63406 | YES | YES |
| 215 | a | 3019.17 | 3.26040 | YES | YES |
| 216 | a | 3020.10 | 7.39027 | YES | YES |
| 217 | a | 3021.16 | 8.91856 | YES | YES |
| 218 | a | 3022.74 | 0.69380 | YES | YES |
| 219 | a | 3046.33 | 112.22574 | YES | YES |
| 220 | a | 3085.45 | 0.49951 | YES | YES |
| 221 | a | 3085.84 | 5.51103 | YES | YES |
| 222 | a | 3088.75 | 9.25027 | YES | YES |
| 223 | a | 3089.44 | 17.65615 | YES | YES |
| 224 | a | 3095.10 | 12.11742 | YES | YES |
| 225 | a | 3096.60 | 17.40803 | YES | YES |
| 226 | a | 3114.30 | 0.51542 | YES | YES |
| 227 | a | 3119.70 | 0.85514 | YES | YES |
| 228 | a | 3120.98 | 0.87867 | YES | YES |
| 229 | a | 3121.91 | 0.75022 | YES | YES |
| 230 | a | 3127.47 | 4.12686 | YES | YES |
| 231 | a | 3129.92 | 2.08371 | YES | YES |
| 232 | a | 3131.36 | 2.79115 | YES | YES |
| 233 | a | 3132.90 | 2.27699 | YES | YES |
| 234 | a | 3135.50 | 0.30669 | YES | YES |
| 235 | a | 3136.59 | 0.74217 | YES | YES |
| 236 | a | 3138.22 | 1.46283 | YES | YES |
| 237 | a | 3141.16 | 0.91087 | YES | YES |
| 238 | a | 3142.29 | 0.53716 | YES | YES |
| 239 | a | 3143.20 | 0.39845 | YES | YES |
| 240 | a | 3145.92 | 0.98689 | YES | YES |

$[F\text{-}Ba(HMB)oDFB_3]^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| Ca | -0.40039 | -0.97054 | 1.58435 |
| F | -0.11580 | 0.02596 | -0.38450 |
| Al | 0.29833 | 0.26147 | -2.06320 |
| C | 0.24684 | 2.22317 | 1.68635 |
| C | -1.06833 | 2.05005 | 2.20439 |
| C | -1.26728 | 1.24760 | 3.36394 |
| C | -0.14008 | 0.69250 | 4.04412 |
| C | 1.18153 | 0.89952 | 3.54813 |
| C | 1.37231 | 1.66897 | 2.36003 |
| C | 0.45589 | 3.02064 | 0.42015 |
| H | 1.29412 | 2.62658 | -0.18431 |
| H | 0.69491 | 4.08626 | 0.64956 |
| H | -0.43900 | 3.01727 | -0.22793 |
| C | -2.21354 | 2.74317 | 1.49715 |
| H | -2.40896 | 2.30241 | 0.49640 |
| H | -1.97798 | 3.81572 | 1.32918 |
| H | -3.15510 | 2.70351 | 2.07630 |
| C | -2.64069 | 0.94849 | 3.92343 |
| H | -3.45934 | 1.29368 | 3.26585 |
| H | -2.78678 | 1.42191 | 4.92154 |
| H | -2.76100 | -0.15080 | 4.04419 |
| C | -0.39842 | -0.10144 | 5.30617 |
| H | -0.95058 | -1.03700 | 5.05340 |
| H | -1.03039 | 0.47597 | 6.01610 |
| H | 0.52797 | -0.37980 | 5.84171 |
| C | 2.35381 | 0.32545 | 4.32374 |
| H | 2.17251 | -0.72501 | 4.63057 |
| H | 2.53555 | 0.90556 | 5.25766 |
| H | 3.29711 | 0.33219 | 3.74684 |
| C | 2.74180 | 1.95211 | 1.77956 |
| H | 3.56846 | 1.53689 | 2.38560 |
| H | 2.91392 | 3.04787 | 1.69740 |
| H | 2.83816 | 1.54534 | 0.75101 |
| C | 3.06666 | -1.64225 | 1.60778 |
| C | 2.56587 | -2.55257 | 2.54262 |
| C | 3.41496 | -3.28321 | 3.36994 |
| H | 2.98810 | -3.99001 | 4.09725 |
| C | 4.80114 | -3.07558 | 3.24424 |
| H | 5.49178 | -3.64188 | 3.88807 |
| C | 5.30472 | -2.15350 | 2.30968 |
| H | 6.39075 | -1.99606 | 2.22145 |
| C | 4.43602 | -1.42283 | 1.47821 |

| | | | |
|---|---|---|---|
| H | 4.79984 | -0.69481 | 0.74079 |
| F | 2.15734 | -0.95671 | 0.86424 |
| F | 1.20725 | -2.66716 | 2.63825 |
| C | -3.96895 | -2.32709 | 0.82078 |
| C | -3.83383 | -0.93185 | 0.83366 |
| C | -4.93146 | -0.08952 | 0.99436 |
| H | -4.77713 | 0.99881 | 0.97262 |
| C | -6.20429 | -0.66231 | 1.16238 |
| H | -7.08123 | -0.00870 | 1.28871 |
| C | -6.35269 | -2.05952 | 1.16479 |
| H | -7.34896 | -2.50961 | 1.29748 |
| C | -5.23557 | -2.89496 | 0.99234 |
| H | -5.32439 | -3.99204 | 0.98534 |
| F | -2.89141 | -3.10048 | 0.62927 |
| F | -2.59141 | -0.38658 | 0.66055 |
| O | 0.28295 | -1.32741 | -2.80557 |
| C | -0.12216 | -2.60674 | -2.65851 |
| C | 0.40536 | -3.42587 | -3.90117 |
| F | 1.72942 | -3.65798 | -3.77841 |
| F | -0.21709 | -4.61988 | -4.01339 |
| F | 0.20706 | -2.73366 | -5.02668 |
| C | -1.69415 | -2.69104 | -2.60697 |
| F | -2.16397 | -1.71041 | -1.80107 |
| F | -2.22184 | -2.50095 | -3.82614 |
| F | -2.13577 | -3.87087 | -2.13060 |
| C | 0.48726 | -3.24692 | -1.35191 |
| F | -0.19796 | -2.80488 | -0.22524 |
| F | 0.42274 | -4.58150 | -1.32752 |
| F | 1.75773 | -2.86718 | -1.18373 |
| O | 1.95905 | 0.84793 | -1.95573 |
| C | 3.03585 | 1.04464 | -2.76057 |
| C | 3.30154 | 2.59242 | -2.88061 |
| F | 2.38121 | 3.15766 | -3.68470 |
| F | 4.52642 | 2.86768 | -3.37406 |
| F | 3.20325 | 3.17789 | -1.67137 |
| C | 4.27770 | 0.33632 | -2.11034 |
| F | 3.95601 | -0.90844 | -1.71753 |
| F | 4.68782 | 1.00822 | -1.00124 |
| F | 5.32700 | 0.26002 | -2.94998 |
| C | 2.81353 | 0.44492 | -4.20423 |
| F | 3.01418 | -0.88593 | -4.21597 |
| F | 3.62356 | 0.99676 | -5.12498 |
| F | 1.53461 | 0.66781 | -4.57786 |
| O | -0.82017 | 1.45528 | -2.62996 |
| C | -1.80626 | 2.02397 | -3.35351 |
| C | -1.60513 | 1.74251 | -4.89031 |
| F | -0.59638 | 2.49037 | -5.37926 |
| F | -2.71586 | 2.01751 | -5.60526 |
| F | -1.28918 | 0.44988 | -5.08041 |
| C | -3.20982 | 1.45891 | -2.90680 |
| F | -3.24585 | 1.31820 | -1.56373 |
| F | -3.42990 | 0.24267 | -3.44230 |
| F | -4.22754 | 2.26465 | -3.26860 |
| C | -1.76162 | 3.57770 | -3.09453 |
| F | -2.26527 | 3.86245 | -1.86603 |

| | | | |
|---|---|---|---|
| F | -2.47638 | 4.27173 | -4.00085 |
| F | -0.49619 | 4.01724 | -3.12022 |
| H | -1.59843 | -1.92098 | 2.91819 |

Vibrational analysis

| 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 | 6.05 | 0.34020 | YES | YES |
| 8 | a | 11.37 | 0.11497 | YES | YES |
| 9 | a | 17.78 | 0.24909 | YES | YES |
| 10 | a | 20.59 | 0.72819 | YES | YES |
| 11 | a | 21.43 | 1.32026 | YES | YES |
| 12 | a | 23.21 | 0.56845 | YES | YES |
| 13 | a | 23.59 | 0.05078 | YES | YES |
| 14 | a | 26.18 | 0.22185 | YES | YES |
| 15 | a | 28.75 | 0.17344 | YES | YES |
| 16 | a | 29.82 | 0.15408 | YES | YES |
| 17 | a | 31.86 | 0.37659 | YES | YES |
| 18 | a | 35.91 | 0.35815 | YES | YES |
| 19 | a | 39.75 | 0.42425 | YES | YES |
| 20 | a | 41.80 | 1.10483 | YES | YES |
| 21 | a | 43.28 | 0.60334 | YES | YES |
| 22 | a | 46.79 | 0.99197 | YES | YES |
| 23 | a | 49.96 | 0.39556 | YES | YES |
| 24 | a | 51.13 | 0.46422 | YES | YES |
| 25 | a | 55.68 | 1.08224 | YES | YES |
| 26 | a | 58.38 | 0.86557 | YES | YES |
| 27 | a | 62.21 | 0.12195 | YES | YES |
| 28 | a | 65.10 | 0.61763 | YES | YES |
| 29 | a | 67.67 | 0.43083 | YES | YES |
| 30 | a | 68.76 | 0.82095 | YES | YES |
| 31 | a | 69.59 | 1.62539 | YES | YES |
| 32 | a | 72.16 | 0.46638 | YES | YES |
| 33 | a | 73.77 | 0.60917 | YES | YES |
| 34 | a | 74.22 | 0.05874 | YES | YES |
| 35 | a | 75.58 | 0.02257 | YES | YES |
| 36 | a | 78.77 | 0.12825 | YES | YES |
| 37 | a | 81.90 | 0.72827 | YES | YES |
| 38 | a | 84.27 | 0.26164 | YES | YES |
| 39 | a | 85.24 | 0.12708 | YES | YES |
| 40 | a | 87.53 | 0.21107 | YES | YES |
| 41 | a | 88.99 | 2.77594 | YES | YES |
| 42 | a | 91.79 | 0.66023 | YES | YES |
| 43 | a | 94.37 | 1.76732 | YES | YES |
| 44 | a | 97.21 | 1.46544 | YES | YES |
| 45 | a | 98.41 | 1.29873 | YES | YES |
| 46 | a | 103.20 | 6.37450 | YES | YES |
| 47 | a | 104.11 | 0.19231 | YES | YES |
| 48 | a | 115.19 | 30.62767 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 49 | a | 116.73 | 0.62746 | YES | YES |
| 50 | a | 125.65 | 0.39108 | YES | YES |
| 51 | a | 137.59 | 22.71719 | YES | YES |
| 52 | a | 142.85 | 0.18195 | YES | YES |
| 53 | a | 151.23 | 1.09468 | YES | YES |
| 54 | a | 155.42 | 4.24548 | YES | YES |
| 55 | a | 156.86 | 0.71276 | YES | YES |
| 56 | a | 158.46 | 2.32895 | YES | YES |
| 57 | a | 162.48 | 1.14303 | YES | YES |
| 58 | a | 166.01 | 0.49183 | YES | YES |
| 59 | a | 168.16 | 3.00401 | YES | YES |
| 60 | a | 171.43 | 23.04900 | YES | YES |
| 61 | a | 176.90 | 4.45793 | YES | YES |
| 62 | a | 181.18 | 3.08703 | YES | YES |
| 63 | a | 184.26 | 2.93348 | YES | YES |
| 64 | a | 193.56 | 11.99008 | YES | YES |
| 65 | a | 199.09 | 0.27725 | YES | YES |
| 66 | a | 202.56 | 1.58804 | YES | YES |
| 67 | a | 204.69 | 8.35358 | YES | YES |
| 68 | a | 207.82 | 2.31572 | YES | YES |
| 69 | a | 212.59 | 1.33068 | YES | YES |
| 70 | a | 220.81 | 9.56240 | YES | YES |
| 71 | a | 247.85 | 8.76966 | YES | YES |
| 72 | a | 261.69 | 0.49840 | YES | YES |
| 73 | a | 265.54 | 4.73814 | YES | YES |
| 74 | a | 272.82 | 1.52620 | YES | YES |
| 75 | a | 276.95 | 4.44119 | YES | YES |
| 76 | a | 279.78 | 5.98929 | YES | YES |
| 77 | a | 282.90 | 2.29139 | YES | YES |
| 78 | a | 283.82 | 2.16097 | YES | YES |
| 79 | a | 284.55 | 0.52975 | YES | YES |
| 80 | a | 285.04 | 1.39640 | YES | YES |
| 81 | a | 288.30 | 0.67559 | YES | YES |
| 82 | a | 289.89 | 21.88823 | YES | YES |
| 83 | a | 292.77 | 0.59868 | YES | YES |
| 84 | a | 303.56 | 4.45869 | YES | YES |
| 85 | a | 306.03 | 7.73092 | YES | YES |
| 86 | a | 309.13 | 3.71109 | YES | YES |
| 87 | a | 309.40 | 2.79866 | YES | YES |
| 88 | a | 313.82 | 1.18396 | YES | YES |
| 89 | a | 315.65 | 0.92777 | YES | YES |
| 90 | a | 318.93 | 2.34357 | YES | YES |
| 91 | a | 319.67 | 1.78431 | YES | YES |
| 92 | a | 320.87 | 0.32862 | YES | YES |
| 93 | a | 327.28 | 0.69795 | YES | YES |
| 94 | a | 328.36 | 0.74613 | YES | YES |
| 95 | a | 337.72 | 1.59023 | YES | YES |
| 96 | a | 343.11 | 0.56819 | YES | YES |
| 97 | a | 347.30 | 1.11864 | YES | YES |
| 98 | a | 351.55 | 1.42257 | YES | YES |
| 99 | a | 353.92 | 0.95118 | YES | YES |
| 100 | a | 358.53 | 3.29468 | YES | YES |
| 101 | a | 364.96 | 6.45589 | YES | YES |
| 102 | a | 371.12 | 31.92829 | YES | YES |
| 103 | a | 373.85 | 1.43218 | YES | YES |

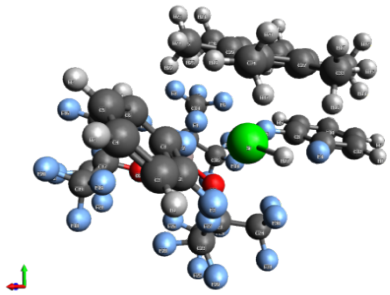
| | | | | | |
|---|---|---|---|---|---|
| 104 | a | 395.78 | 0.14133 | YES | YES |
| 105 | a | 404.84 | 30.41221 | YES | YES |
| 106 | a | 410.33 | 0.58170 | YES | YES |
| 107 | a | 434.02 | 4.42990 | YES | YES |
| 108 | a | 439.70 | 34.88741 | YES | YES |
| 109 | a | 439.85 | 5.31429 | YES | YES |
| 110 | a | 441.15 | 6.02968 | YES | YES |
| 111 | a | 443.22 | 2.44910 | YES | YES |
| 112 | a | 446.07 | 2.41599 | YES | YES |
| 113 | a | 449.16 | 8.85492 | YES | YES |
| 114 | a | 451.36 | 2.00605 | YES | YES |
| 115 | a | 455.05 | 30.76020 | YES | YES |
| 116 | a | 485.91 | 272.24332 | YES | YES |
| 117 | a | 514.23 | 5.20074 | YES | YES |
| 118 | a | 516.45 | 53.00746 | YES | YES |
| 119 | a | 517.59 | 12.84813 | YES | YES |
| 120 | a | 518.20 | 1.10099 | YES | YES |
| 121 | a | 520.01 | 118.24277 | YES | YES |
| 122 | a | 520.29 | 142.35251 | YES | YES |
| 123 | a | 520.67 | 9.18731 | YES | YES |
| 124 | a | 521.52 | 17.41541 | YES | YES |
| 125 | a | 523.88 | 4.21187 | YES | YES |
| 126 | a | 524.87 | 6.92388 | YES | YES |
| 127 | a | 527.33 | 20.86553 | YES | YES |
| 128 | a | 536.92 | 4.77023 | YES | YES |
| 129 | a | 542.40 | 2.28931 | YES | YES |
| 130 | a | 542.82 | 3.22268 | YES | YES |
| 131 | a | 546.45 | 4.20272 | YES | YES |
| 132 | a | 550.53 | 13.34618 | YES | YES |
| 133 | a | 551.08 | 1.23077 | YES | YES |
| 134 | a | 551.53 | 7.02674 | YES | YES |
| 135 | a | 553.47 | 1.48774 | YES | YES |
| 136 | a | 553.63 | 1.55232 | YES | YES |
| 137 | a | 554.17 | 1.15506 | YES | YES |
| 138 | a | 555.18 | 0.58302 | YES | YES |
| 139 | a | 558.66 | 25.26955 | YES | YES |
| 140 | a | 559.53 | 6.98193 | YES | YES |
| 141 | a | 563.29 | 19.54328 | YES | YES |
| 142 | a | 564.00 | 6.51145 | YES | YES |
| 143 | a | 566.14 | 0.44077 | YES | YES |
| 144 | a | 567.06 | 11.75228 | YES | YES |
| 145 | a | 570.31 | 12.15867 | YES | YES |
| 146 | a | 586.25 | 1.47094 | YES | YES |
| 147 | a | 674.27 | 0.05147 | YES | YES |
| 148 | a | 681.73 | 0.60487 | YES | YES |
| 149 | a | 687.46 | 195.23313 | YES | YES |
| 150 | a | 695.33 | 0.03062 | YES | YES |
| 151 | a | 701.76 | 29.18476 | YES | YES |
| 152 | a | 706.51 | 16.16210 | YES | YES |
| 153 | a | 707.24 | 37.48267 | YES | YES |
| 154 | a | 707.81 | 26.45430 | YES | YES |
| 155 | a | 708.67 | 17.84217 | YES | YES |
| 156 | a | 710.64 | 106.48939 | YES | YES |
| 157 | a | 728.66 | 7.54839 | YES | YES |
| 158 | a | 735.44 | 2.69085 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 159 | a | 737.33 | 0.93210 | YES | YES |
| 160 | a | 740.92 | 66.74386 | YES | YES |
| 161 | a | 747.00 | 64.25214 | YES | YES |
| 162 | a | 759.46 | 65.71515 | YES | YES |
| 163 | a | 761.65 | 29.91664 | YES | YES |
| 164 | a | 790.64 | 0.18415 | YES | YES |
| 165 | a | 794.18 | 17.01390 | YES | YES |
| 166 | a | 802.65 | 5.37183 | YES | YES |
| 167 | a | 825.01 | 13.29323 | YES | YES |
| 168 | a | 830.63 | 36.23175 | YES | YES |
| 169 | a | 831.74 | 1.77346 | YES | YES |
| 170 | a | 833.46 | 14.48790 | YES | YES |
| 171 | a | 843.60 | 0.96702 | YES | YES |
| 172 | a | 861.58 | 19.45107 | YES | YES |
| 173 | a | 915.68 | 4.40435 | YES | YES |
| 174 | a | 928.60 | 1.90852 | YES | YES |
| 175 | a | 931.25 | 192.45342 | YES | YES |
| 176 | a | 950.84 | 2.15887 | YES | YES |
| 177 | a | 953.27 | 52.18201 | YES | YES |
| 178 | a | 956.17 | 48.73367 | YES | YES |
| 179 | a | 957.35 | 0.11739 | YES | YES |
| 180 | a | 961.23 | 308.52348 | YES | YES |
| 181 | a | 962.68 | 165.84630 | YES | YES |
| 182 | a | 963.19 | 202.05135 | YES | YES |
| 183 | a | 966.02 | 1.87145 | YES | YES |
| 184 | a | 968.58 | 3.78873 | YES | YES |
| 185 | a | 974.64 | 1.59476 | YES | YES |
| 186 | a | 982.18 | 21.02037 | YES | YES |
| 187 | a | 1002.43 | 6.34208 | YES | YES |
| 188 | a | 1006.72 | 1.15671 | YES | YES |
| 189 | a | 1020.13 | 5.80759 | YES | YES |
| 190 | a | 1024.30 | 9.09864 | YES | YES |
| 191 | a | 1026.58 | 0.98646 | YES | YES |
| 192 | a | 1031.28 | 0.85146 | YES | YES |
| 193 | a | 1034.60 | 1.05523 | YES | YES |
| 194 | a | 1046.93 | 19.83510 | YES | YES |
| 195 | a | 1050.01 | 21.01666 | YES | YES |
| 196 | a | 1054.01 | 10.95506 | YES | YES |
| 197 | a | 1075.27 | 0.38589 | YES | YES |
| 198 | a | 1077.35 | 1.17338 | YES | YES |
| 199 | a | 1084.18 | 5.41432 | YES | YES |
| 200 | a | 1085.66 | 4.88930 | YES | YES |
| 201 | a | 1087.56 | 15.82984 | YES | YES |
| 202 | a | 1094.53 | 4.72822 | YES | YES |
| 203 | a | 1098.73 | 0.09305 | YES | YES |
| 204 | a | 1133.24 | 1.78516 | YES | YES |
| 205 | a | 1136.20 | 7.07216 | YES | YES |
| 206 | a | 1136.33 | 18.62672 | YES | YES |
| 207 | a | 1145.74 | 36.36678 | YES | YES |
| 208 | a | 1152.06 | 18.35521 | YES | YES |
| 209 | a | 1156.90 | 30.38542 | YES | YES |
| 210 | a | 1158.00 | 27.22954 | YES | YES |
| 211 | a | 1162.46 | 17.69605 | YES | YES |
| 212 | a | 1168.86 | 25.10754 | YES | YES |
| 213 | a | 1172.69 | 4.54431 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 214 | a | 1176.59 | 23.08065 | YES | YES |
| 215 | a | 1177.80 | 11.18358 | YES | YES |
| 216 | a | 1184.82 | 17.58230 | YES | YES |
| 217 | a | 1194.89 | 25.27568 | YES | YES |
| 218 | a | 1199.29 | 69.83146 | YES | YES |
| 219 | a | 1199.65 | 80.16578 | YES | YES |
| 220 | a | 1209.39 | 414.76656 | YES | YES |
| 221 | a | 1210.06 | 40.82231 | YES | YES |
| 222 | a | 1212.81 | 5.99628 | YES | YES |
| 223 | a | 1220.96 | 265.35372 | YES | YES |
| 224 | a | 1229.79 | 252.49821 | YES | YES |
| 225 | a | 1232.36 | 320.71417 | YES | YES |
| 226 | a | 1237.52 | 671.72517 | YES | YES |
| 227 | a | 1239.99 | 560.84381 | YES | YES |
| 228 | a | 1243.68 | 373.20480 | YES | YES |
| 229 | a | 1244.06 | 659.54759 | YES | YES |
| 230 | a | 1247.26 | 296.39938 | YES | YES |
| 231 | a | 1250.78 | 957.72903 | YES | YES |
| 232 | a | 1251.52 | 26.31170 | YES | YES |
| 233 | a | 1254.98 | 373.45853 | YES | YES |
| 234 | a | 1258.79 | 201.95079 | YES | YES |
| 235 | a | 1260.44 | 507.34406 | YES | YES |
| 236 | a | 1266.96 | 95.66486 | YES | YES |
| 237 | a | 1274.67 | 103.65712 | YES | YES |
| 238 | a | 1304.64 | 0.56381 | YES | YES |
| 239 | a | 1311.96 | 0.80338 | YES | YES |
| 240 | a | 1323.09 | 95.69192 | YES | YES |
| 241 | a | 1343.23 | 2.51183 | YES | YES |
| 242 | a | 1345.28 | 161.31824 | YES | YES |
| 243 | a | 1351.12 | 2.74360 | YES | YES |
| 244 | a | 1357.55 | 5.47419 | YES | YES |
| 245 | a | 1362.55 | 3.72856 | YES | YES |
| 246 | a | 1367.97 | 0.17426 | YES | YES |
| 247 | a | 1370.50 | 105.75399 | YES | YES |
| 248 | a | 1375.92 | 129.32082 | YES | YES |
| 249 | a | 1379.29 | 1.87705 | YES | YES |
| 250 | a | 1382.55 | 0.60855 | YES | YES |
| 251 | a | 1390.87 | 0.99321 | YES | YES |
| 252 | a | 1396.33 | 3.15948 | YES | YES |
| 253 | a | 1410.22 | 1.58622 | YES | YES |
| 254 | a | 1416.60 | 0.64300 | YES | YES |
| 255 | a | 1417.94 | 14.92686 | YES | YES |
| 256 | a | 1422.05 | 1.16592 | YES | YES |
| 257 | a | 1429.12 | 37.72359 | YES | YES |
| 258 | a | 1431.80 | 6.13926 | YES | YES |
| 259 | a | 1442.85 | 36.77715 | YES | YES |
| 260 | a | 1447.64 | 8.11746 | YES | YES |
| 261 | a | 1448.23 | 10.85469 | YES | YES |
| 262 | a | 1456.13 | 8.70280 | YES | YES |
| 263 | a | 1457.27 | 2.91366 | YES | YES |
| 264 | a | 1458.93 | 8.09928 | YES | YES |
| 265 | a | 1467.61 | 40.36384 | YES | YES |
| 266 | a | 1474.87 | 13.01384 | YES | YES |
| 267 | a | 1499.38 | 208.68942 | YES | YES |
| 268 | a | 1510.12 | 194.57191 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 269 | a | 1556.58 | 0.44305 | YES | YES |
| 270 | a | 1563.72 | 0.48350 | YES | YES |
| 271 | a | 1613.31 | 7.94350 | YES | YES |
| 272 | a | 1615.44 | 1.32328 | YES | YES |
| 273 | a | 1633.22 | 26.82292 | YES | YES |
| 274 | a | 1633.37 | 3.34064 | YES | YES |
| 275 | a | 2925.32 | 24.34659 | YES | YES |
| 276 | a | 2933.39 | 25.60229 | YES | YES |
| 277 | a | 2937.98 | 12.99025 | YES | YES |
| 278 | a | 2947.71 | 16.31224 | YES | YES |
| 279 | a | 2960.05 | 12.76770 | YES | YES |
| 280 | a | 2967.15 | 9.91801 | YES | YES |
| 281 | a | 3001.77 | 7.56786 | YES | YES |
| 282 | a | 3005.89 | 0.40251 | YES | YES |
| 283 | a | 3026.29 | 8.29572 | YES | YES |
| 284 | a | 3031.38 | 5.51362 | YES | YES |
| 285 | a | 3037.77 | 4.76803 | YES | YES |
| 286 | a | 3057.15 | 0.78428 | YES | YES |
| 287 | a | 3072.19 | 1.29220 | YES | YES |
| 288 | a | 3073.68 | 5.07865 | YES | YES |
| 289 | a | 3080.20 | 32.89962 | YES | YES |
| 290 | a | 3083.14 | 7.68894 | YES | YES |
| 291 | a | 3085.00 | 22.31461 | YES | YES |
| 292 | a | 3103.77 | 1.20630 | YES | YES |
| 293 | a | 3111.05 | 1.84943 | YES | YES |
| 294 | a | 3116.61 | 2.20203 | YES | YES |
| 295 | a | 3124.29 | 10.07498 | YES | YES |
| 296 | a | 3129.19 | 5.39454 | YES | YES |
| 297 | a | 3133.92 | 1.55487 | YES | YES |
| 298 | a | 3138.69 | 0.51973 | YES | YES |
| 299 | a | 3143.07 | 0.10572 | YES | YES |
| 300 | a | 3160.93 | 10.46687 | YES | YES |

H-Ca(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Sr | -0.26830 | -0.43406 | -1.43859 |
| Al | 0.61042 | -1.02892 | 1.85974 |
| F | 0.44841 | 0.36447 | 0.83538 |
| C | 3.47765 | -0.24340 | -2.19374 |
| C | 3.60932 | -1.09529 | -3.30060 |
| C | 4.72456 | -0.96011 | -4.13763 |
| H | 4.80630 | -1.62882 | -5.00819 |
| C | 5.70276 | 0.00473 | -3.84738 |

| | | | |
|---|---|---|---|
| H | 6.57833 | 0.10440 | -4.50793 |
| C | 5.57198 | 0.82960 | -2.71730 |
| H | 6.34587 | 1.57522 | -2.47787 |
| C | 4.45132 | 0.70325 | -1.87963 |
| H | 4.32537 | 1.31942 | -0.98011 |
| F | 2.36945 | -0.35154 | -1.39532 |
| F | 2.68482 | -2.02627 | -3.54949 |
| C | -3.96087 | -0.60480 | -1.51565 |
| C | -3.70975 | -0.17827 | -0.20914 |
| C | -4.74887 | 0.09483 | 0.67730 |
| H | -4.51639 | 0.41813 | 1.70113 |
| C | -6.06892 | -0.06318 | 0.21905 |
| H | -6.90504 | 0.14836 | 0.90332 |
| C | -6.32525 | -0.49094 | -1.09615 |
| H | -7.36267 | -0.61305 | -1.44416 |
| C | -5.26532 | -0.76842 | -1.97816 |
| H | -5.43391 | -1.10275 | -3.01278 |
| F | -2.88981 | -0.83841 | -2.32257 |
| F | -2.40769 | -0.03804 | 0.16402 |
| O | -0.19330 | -0.90962 | 3.39028 |
| C | -1.19088 | -0.43367 | 4.17096 |
| C | -1.45923 | 1.08783 | 3.87070 |
| F | -2.14065 | 1.21703 | 2.69874 |
| F | -2.18348 | 1.69017 | 4.83033 |
| F | -0.30117 | 1.74860 | 3.73254 |
| C | -0.75511 | -0.59863 | 5.67616 |
| F | -0.20625 | -1.80386 | 5.86896 |
| F | 0.15830 | 0.33610 | 6.00428 |
| F | -1.80810 | -0.46715 | 6.51297 |
| C | -2.51058 | -1.25607 | 3.91315 |
| F | -2.46088 | -2.45515 | 4.51537 |
| F | -3.61559 | -0.61062 | 4.34978 |
| F | -2.65786 | -1.47094 | 2.58803 |
| O | 2.28858 | -1.48721 | 1.97145 |
| C | 3.44500 | -1.11490 | 2.57959 |
| C | 3.59654 | 0.45099 | 2.57246 |
| F | 2.41594 | 1.02383 | 2.89788 |
| F | 4.52990 | 0.89524 | 3.42844 |
| F | 3.91991 | 0.89809 | 1.33441 |
| C | 4.63412 | -1.76489 | 1.78019 |
| F | 4.71757 | -3.08193 | 2.04310 |
| F | 4.43897 | -1.62320 | 0.45673 |
| F | 5.81804 | -1.19590 | 2.09228 |
| C | 3.46608 | -1.62983 | 4.07030 |
| F | 2.98276 | -2.87791 | 4.13325 |
| F | 4.71032 | -1.62469 | 4.59156 |
| F | 2.68692 | -0.84454 | 4.84571 |
| O | -0.16973 | -2.13077 | 0.64857 |
| C | -0.23871 | -3.48833 | 0.44661 |
| C | -0.34957 | -4.28315 | 1.79668 |
| F | -1.59607 | -4.22405 | 2.29765 |
| F | -0.02455 | -5.57798 | 1.63282 |
| F | 0.48526 | -3.73960 | 2.70305 |
| C | 1.05071 | -3.95404 | -0.33656 |
| F | 1.35232 | -3.01303 | -1.26762 |

| | | | |
|---|---|---|---|
| F | 2.10092 | -4.06169 | 0.48798 |
| F | 0.88014 | -5.12434 | -0.97159 |
| C | -1.51206 | -3.74754 | -0.43043 |
| F | -1.31670 | -3.16979 | -1.65740 |
| F | -1.77820 | -5.04341 | -0.61216 |
| F | -2.59355 | -3.15315 | 0.10054 |
| C | -1.93920 | 2.84990 | -1.10543 |
| C | -2.15382 | 2.46480 | -2.46229 |
| C | -1.03968 | 2.27545 | -3.32757 |
| C | 0.29263 | 2.42703 | -2.83841 |
| C | 0.50331 | 2.81676 | -1.48617 |
| C | -0.61285 | 3.02312 | -0.62509 |
| C | -3.09195 | 3.15207 | -0.16650 |
| H | -3.10888 | 4.23295 | 0.10115 |
| H | -3.00579 | 2.58901 | 0.78547 |
| H | -4.08040 | 2.91354 | -0.59997 |
| C | -3.55145 | 2.29620 | -3.02987 |
| H | -3.83429 | 3.16366 | -3.66996 |
| H | -4.32700 | 2.20441 | -2.24694 |
| H | -3.62534 | 1.39021 | -3.66478 |
| C | -1.22138 | 1.91112 | -4.78374 |
| H | -2.27049 | 1.98865 | -5.12477 |
| H | -0.87708 | 0.86035 | -4.94170 |
| H | -0.61087 | 2.56855 | -5.44029 |
| C | 1.42873 | 2.16672 | -3.80466 |
| H | 1.30930 | 1.15672 | -4.25812 |
| H | 2.42573 | 2.19985 | -3.32745 |
| H | 1.43200 | 2.90979 | -4.63482 |
| C | 1.88306 | 3.06412 | -0.91557 |
| H | 2.68253 | 2.96263 | -1.67150 |
| H | 2.10904 | 2.36588 | -0.08035 |
| H | 1.95700 | 4.09135 | -0.49485 |
| C | -0.34023 | 3.47293 | 0.79294 |
| H | 0.12020 | 4.48792 | 0.80598 |
| H | 0.37012 | 2.78671 | 1.29735 |
| H | -1.24983 | 3.51636 | 1.41721 |
| H | -0.03296 | -0.79119 | -3.60457 |

Vibrational analysis

| mode | symmetry | wave number | IR intensity | selection rules | |
|---|---|---|---|---|---|
| | | cm**(-1) | km/mol | IR | RAMAN |
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | -0.00 | 0.00000 | - | - |
| 5 | | -0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 11.66 | 1.91519 | YES | YES |
| 8 | a | 15.54 | 0.57148 | YES | YES |
| 9 | a | 17.81 | 0.17174 | YES | YES |
| 10 | a | 19.41 | 0.08586 | YES | YES |
| 11 | a | 22.00 | 0.12001 | YES | YES |
| 12 | a | 24.22 | 0.17826 | YES | YES |
| 13 | a | 24.73 | 0.56445 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 14 | a | 28.06 | 0.18811 | YES | YES |
| 15 | a | 28.93 | 0.18316 | YES | YES |
| 16 | a | 30.39 | 0.34670 | YES | YES |
| 17 | a | 32.49 | 0.47797 | YES | YES |
| 18 | a | 35.35 | 0.12716 | YES | YES |
| 19 | a | 36.84 | 0.99436 | YES | YES |
| 20 | a | 38.27 | 1.25884 | YES | YES |
| 21 | a | 42.81 | 1.38000 | YES | YES |
| 22 | a | 43.38 | 0.56331 | YES | YES |
| 23 | a | 49.12 | 2.64445 | YES | YES |
| 24 | a | 49.37 | 0.80486 | YES | YES |
| 25 | a | 54.32 | 0.30877 | YES | YES |
| 26 | a | 58.11 | 0.92987 | YES | YES |
| 27 | a | 60.93 | 0.83030 | YES | YES |
| 28 | a | 61.76 | 0.90896 | YES | YES |
| 29 | a | 63.84 | 1.78568 | YES | YES |
| 30 | a | 66.73 | 0.27560 | YES | YES |
| 31 | a | 68.06 | 0.20918 | YES | YES |
| 32 | a | 70.33 | 0.16465 | YES | YES |
| 33 | a | 70.62 | 0.34110 | YES | YES |
| 34 | a | 71.95 | 0.90532 | YES | YES |
| 35 | a | 73.87 | 1.14946 | YES | YES |
| 36 | a | 76.77 | 0.77561 | YES | YES |
| 37 | a | 78.24 | 0.20687 | YES | YES |
| 38 | a | 80.44 | 0.19204 | YES | YES |
| 39 | a | 82.42 | 0.16720 | YES | YES |
| 40 | a | 84.09 | 1.88608 | YES | YES |
| 41 | a | 84.49 | 0.56215 | YES | YES |
| 42 | a | 86.37 | 0.33929 | YES | YES |
| 43 | a | 93.49 | 6.83575 | YES | YES |
| 44 | a | 94.24 | 2.75877 | YES | YES |
| 45 | a | 96.34 | 5.53098 | YES | YES |
| 46 | a | 103.55 | 5.79433 | YES | YES |
| 47 | a | 105.90 | 3.14018 | YES | YES |
| 48 | a | 110.20 | 2.17984 | YES | YES |
| 49 | a | 114.43 | 3.44633 | YES | YES |
| 50 | a | 116.22 | 15.03446 | YES | YES |
| 51 | a | 129.06 | 19.37653 | YES | YES |
| 52 | a | 134.57 | 0.47857 | YES | YES |
| 53 | a | 142.52 | 0.86863 | YES | YES |
| 54 | a | 151.43 | 0.26032 | YES | YES |
| 55 | a | 155.97 | 0.49471 | YES | YES |
| 56 | a | 158.46 | 0.05478 | YES | YES |
| 57 | a | 160.46 | 0.62064 | YES | YES |
| 58 | a | 164.40 | 2.28535 | YES | YES |
| 59 | a | 168.68 | 0.20516 | YES | YES |
| 60 | a | 171.55 | 1.18599 | YES | YES |
| 61 | a | 174.01 | 6.02371 | YES | YES |
| 62 | a | 178.92 | 2.08252 | YES | YES |
| 63 | a | 184.12 | 4.56876 | YES | YES |
| 64 | a | 193.70 | 0.50061 | YES | YES |
| 65 | a | 195.73 | 9.26591 | YES | YES |
| 66 | a | 199.24 | 0.97060 | YES | YES |
| 67 | a | 201.42 | 0.47057 | YES | YES |
| 68 | a | 205.28 | 0.21362 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 69 | a | 216.02 | 3.69746 | YES | YES |
| 70 | a | 241.64 | 6.24866 | YES | YES |
| 71 | a | 257.63 | 11.32486 | YES | YES |
| 72 | a | 260.27 | 12.49197 | YES | YES |
| 73 | a | 269.14 | 2.29550 | YES | YES |
| 74 | a | 271.95 | 18.85654 | YES | YES |
| 75 | a | 275.44 | 4.02934 | YES | YES |
| 76 | a | 277.47 | 2.46355 | YES | YES |
| 77 | a | 281.84 | 2.56972 | YES | YES |
| 78 | a | 284.33 | 0.46584 | YES | YES |
| 79 | a | 285.21 | 0.06268 | YES | YES |
| 80 | a | 287.35 | 8.90967 | YES | YES |
| 81 | a | 288.09 | 1.53297 | YES | YES |
| 82 | a | 292.07 | 2.92337 | YES | YES |
| 83 | a | 293.59 | 0.71697 | YES | YES |
| 84 | a | 295.97 | 1.04424 | YES | YES |
| 85 | a | 306.90 | 6.50756 | YES | YES |
| 86 | a | 307.50 | 1.30459 | YES | YES |
| 87 | a | 308.44 | 4.36301 | YES | YES |
| 88 | a | 315.04 | 0.95307 | YES | YES |
| 89 | a | 318.99 | 1.17707 | YES | YES |
| 90 | a | 320.48 | 2.19142 | YES | YES |
| 91 | a | 321.60 | 0.65956 | YES | YES |
| 92 | a | 324.60 | 1.87562 | YES | YES |
| 93 | a | 327.44 | 0.11658 | YES | YES |
| 94 | a | 331.52 | 1.84627 | YES | YES |
| 95 | a | 331.96 | 0.97859 | YES | YES |
| 96 | a | 347.09 | 36.23683 | YES | YES |
| 97 | a | 348.35 | 1.01617 | YES | YES |
| 98 | a | 354.54 | 49.41552 | YES | YES |
| 99 | a | 358.04 | 135.00836 | YES | YES |
| 100 | a | 359.67 | 30.99364 | YES | YES |
| 101 | a | 360.71 | 5.64462 | YES | YES |
| 102 | a | 370.23 | 43.65101 | YES | YES |
| 103 | a | 371.67 | 24.33391 | YES | YES |
| 104 | a | 389.82 | 85.04398 | YES | YES |
| 105 | a | 393.89 | 2.69466 | YES | YES |
| 106 | a | 404.69 | 4.65631 | YES | YES |
| 107 | a | 407.77 | 5.17065 | YES | YES |
| 108 | a | 436.20 | 13.10625 | YES | YES |
| 109 | a | 437.19 | 1.89265 | YES | YES |
| 110 | a | 441.72 | 0.75675 | YES | YES |
| 111 | a | 444.97 | 5.01775 | YES | YES |
| 112 | a | 448.07 | 0.23139 | YES | YES |
| 113 | a | 450.48 | 52.05800 | YES | YES |
| 114 | a | 451.98 | 17.39015 | YES | YES |
| 115 | a | 454.10 | 64.67539 | YES | YES |
| 116 | a | 457.66 | 247.96417 | YES | YES |
| 117 | a | 467.79 | 56.22754 | YES | YES |
| 118 | a | 514.95 | 5.60135 | YES | YES |
| 119 | a | 516.67 | 4.57483 | YES | YES |
| 120 | a | 517.95 | 1.07223 | YES | YES |
| 121 | a | 518.71 | 6.01317 | YES | YES |
| 122 | a | 520.11 | 4.54636 | YES | YES |
| 123 | a | 520.74 | 5.14455 | YES | YES |

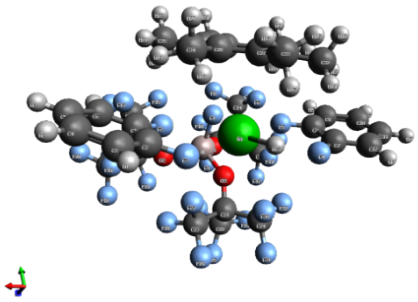
| | | | | | |
|---|---|---|---|---|---|
| 124 | a | 522.02 | 1.78356 | YES | YES |
| 125 | a | 523.93 | 0.67294 | YES | YES |
| 126 | a | 524.69 | 2.86039 | YES | YES |
| 127 | a | 527.57 | 1.77734 | YES | YES |
| 128 | a | 534.45 | 3.99915 | YES | YES |
| 129 | a | 542.96 | 3.89296 | YES | YES |
| 130 | a | 545.86 | 1.04871 | YES | YES |
| 131 | a | 546.41 | 11.49764 | YES | YES |
| 132 | a | 547.09 | 1.31178 | YES | YES |
| 133 | a | 552.49 | 2.74059 | YES | YES |
| 134 | a | 553.84 | 0.95812 | YES | YES |
| 135 | a | 554.06 | 0.22471 | YES | YES |
| 136 | a | 554.78 | 0.43956 | YES | YES |
| 137 | a | 555.45 | 0.58263 | YES | YES |
| 138 | a | 556.25 | 1.60584 | YES | YES |
| 139 | a | 560.46 | 1.11899 | YES | YES |
| 140 | a | 560.86 | 11.23863 | YES | YES |
| 141 | a | 563.35 | 25.65812 | YES | YES |
| 142 | a | 566.64 | 29.05260 | YES | YES |
| 143 | a | 566.87 | 4.52085 | YES | YES |
| 144 | a | 567.54 | 2.64366 | YES | YES |
| 145 | a | 577.37 | 1.67413 | YES | YES |
| 146 | a | 585.82 | 0.24192 | YES | YES |
| 147 | a | 681.05 | 0.23447 | YES | YES |
| 148 | a | 682.30 | 0.33601 | YES | YES |
| 149 | a | 685.00 | 113.15144 | YES | YES |
| 150 | a | 705.01 | 18.39158 | YES | YES |
| 151 | a | 706.11 | 19.37564 | YES | YES |
| 152 | a | 707.14 | 27.13373 | YES | YES |
| 153 | a | 708.37 | 0.18404 | YES | YES |
| 154 | a | 708.88 | 51.52551 | YES | YES |
| 155 | a | 709.54 | 30.31141 | YES | YES |
| 156 | a | 711.21 | 66.77601 | YES | YES |
| 157 | a | 725.84 | 11.84614 | YES | YES |
| 158 | a | 738.55 | 2.19008 | YES | YES |
| 159 | a | 738.99 | 13.07734 | YES | YES |
| 160 | a | 743.02 | 71.69578 | YES | YES |
| 161 | a | 745.78 | 81.38507 | YES | YES |
| 162 | a | 756.71 | 59.30708 | YES | YES |
| 163 | a | 761.68 | 42.06519 | YES | YES |
| 164 | a | 779.02 | 15.87554 | YES | YES |
| 165 | a | 790.49 | 0.29330 | YES | YES |
| 166 | a | 799.74 | 2.79007 | YES | YES |
| 167 | a | 826.35 | 15.45208 | YES | YES |
| 168 | a | 830.12 | 44.65944 | YES | YES |
| 169 | a | 833.63 | 13.56534 | YES | YES |
| 170 | a | 834.92 | 5.54893 | YES | YES |
| 171 | a | 841.15 | 0.54729 | YES | YES |
| 172 | a | 862.57 | 26.96689 | YES | YES |
| 173 | a | 918.31 | 10.84427 | YES | YES |
| 174 | a | 926.23 | 3.52844 | YES | YES |
| 175 | a | 950.40 | 0.07911 | YES | YES |
| 176 | a | 955.46 | 21.91679 | YES | YES |
| 177 | a | 956.40 | 21.29223 | YES | YES |
| 178 | a | 958.63 | 13.00729 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 179 | a | 959.88 | 156.41918 | YES | YES |
| 180 | a | 962.05 | 193.46388 | YES | YES |
| 181 | a | 964.69 | 2.25473 | YES | YES |
| 182 | a | 966.67 | 116.22529 | YES | YES |
| 183 | a | 967.07 | 84.22327 | YES | YES |
| 184 | a | 969.58 | 359.38651 | YES | YES |
| 185 | a | 972.39 | 4.93577 | YES | YES |
| 186 | a | 985.04 | 18.30018 | YES | YES |
| 187 | a | 1003.69 | 3.65262 | YES | YES |
| 188 | a | 1008.86 | 0.83553 | YES | YES |
| 189 | a | 1020.40 | 7.72544 | YES | YES |
| 190 | a | 1026.17 | 7.66095 | YES | YES |
| 191 | a | 1028.70 | 1.31072 | YES | YES |
| 192 | a | 1034.94 | 0.79780 | YES | YES |
| 193 | a | 1036.04 | 0.64135 | YES | YES |
| 194 | a | 1050.08 | 9.30130 | YES | YES |
| 195 | a | 1050.89 | 8.83458 | YES | YES |
| 196 | a | 1074.50 | 0.82792 | YES | YES |
| 197 | a | 1074.86 | 6.43047 | YES | YES |
| 198 | a | 1078.21 | 2.73447 | YES | YES |
| 199 | a | 1084.64 | 0.05291 | YES | YES |
| 200 | a | 1086.85 | 4.86364 | YES | YES |
| 201 | a | 1087.21 | 7.43976 | YES | YES |
| 202 | a | 1093.10 | 10.68296 | YES | YES |
| 203 | a | 1097.79 | 2.96783 | YES | YES |
| 204 | a | 1102.57 | 432.45898 | YES | YES |
| 205 | a | 1132.66 | 2.38894 | YES | YES |
| 206 | a | 1134.01 | 9.32290 | YES | YES |
| 207 | a | 1136.75 | 13.67117 | YES | YES |
| 208 | a | 1144.29 | 19.35149 | YES | YES |
| 209 | a | 1147.82 | 65.19492 | YES | YES |
| 210 | a | 1155.90 | 21.62325 | YES | YES |
| 211 | a | 1161.71 | 18.73968 | YES | YES |
| 212 | a | 1164.55 | 39.16769 | YES | YES |
| 213 | a | 1170.94 | 5.19444 | YES | YES |
| 214 | a | 1174.13 | 86.34005 | YES | YES |
| 215 | a | 1178.93 | 128.79872 | YES | YES |
| 216 | a | 1184.73 | 30.39370 | YES | YES |
| 217 | a | 1186.79 | 29.74233 | YES | YES |
| 218 | a | 1190.38 | 17.94767 | YES | YES |
| 219 | a | 1194.76 | 32.71976 | YES | YES |
| 220 | a | 1202.38 | 26.78632 | YES | YES |
| 221 | a | 1205.35 | 78.36470 | YES | YES |
| 222 | a | 1212.41 | 77.95531 | YES | YES |
| 223 | a | 1219.35 | 169.18761 | YES | YES |
| 224 | a | 1223.99 | 255.01860 | YES | YES |
| 225 | a | 1233.66 | 880.32139 | YES | YES |
| 226 | a | 1235.20 | 533.97512 | YES | YES |
| 227 | a | 1241.56 | 90.23519 | YES | YES |
| 228 | a | 1242.74 | 409.97752 | YES | YES |
| 229 | a | 1247.27 | 466.59739 | YES | YES |
| 230 | a | 1247.83 | 94.67871 | YES | YES |
| 231 | a | 1248.45 | 136.09893 | YES | YES |
| 232 | a | 1249.79 | 806.06488 | YES | YES |
| 233 | a | 1253.81 | 353.45224 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 234 | a | 1258.00 | 32.83686 | YES | YES |
| 235 | a | 1261.35 | 1167.24761 | YES | YES |
| 236 | a | 1267.93 | 63.09900 | YES | YES |
| 237 | a | 1278.26 | 100.40847 | YES | YES |
| 238 | a | 1299.67 | 29.83870 | YES | YES |
| 239 | a | 1303.63 | 0.48488 | YES | YES |
| 240 | a | 1316.75 | 0.67489 | YES | YES |
| 241 | a | 1331.82 | 121.24909 | YES | YES |
| 242 | a | 1342.91 | 1.47351 | YES | YES |
| 243 | a | 1350.44 | 1.52738 | YES | YES |
| 244 | a | 1354.85 | 143.46254 | YES | YES |
| 245 | a | 1356.69 | 14.88569 | YES | YES |
| 246 | a | 1359.58 | 6.77157 | YES | YES |
| 247 | a | 1366.76 | 1.42898 | YES | YES |
| 248 | a | 1371.91 | 6.84120 | YES | YES |
| 249 | a | 1377.56 | 2.18739 | YES | YES |
| 250 | a | 1382.93 | 0.84087 | YES | YES |
| 251 | a | 1392.69 | 0.62933 | YES | YES |
| 252 | a | 1398.86 | 0.85631 | YES | YES |
| 253 | a | 1410.37 | 0.44590 | YES | YES |
| 254 | a | 1417.94 | 1.11691 | YES | YES |
| 255 | a | 1420.17 | 11.35053 | YES | YES |
| 256 | a | 1423.29 | 2.22994 | YES | YES |
| 257 | a | 1430.02 | 0.53769 | YES | YES |
| 258 | a | 1432.02 | 35.54433 | YES | YES |
| 259 | a | 1438.03 | 37.55582 | YES | YES |
| 260 | a | 1445.12 | 0.89485 | YES | YES |
| 261 | a | 1451.59 | 7.96437 | YES | YES |
| 262 | a | 1453.26 | 6.72358 | YES | YES |
| 263 | a | 1455.51 | 10.09690 | YES | YES |
| 264 | a | 1459.18 | 7.27406 | YES | YES |
| 265 | a | 1463.29 | 12.89878 | YES | YES |
| 266 | a | 1472.85 | 37.79267 | YES | YES |
| 267 | a | 1500.50 | 194.82811 | YES | YES |
| 268 | a | 1510.32 | 178.10199 | YES | YES |
| 269 | a | 1562.79 | 1.06243 | YES | YES |
| 270 | a | 1569.08 | 0.49855 | YES | YES |
| 271 | a | 1611.25 | 8.44081 | YES | YES |
| 272 | a | 1616.67 | 0.90644 | YES | YES |
| 273 | a | 1632.83 | 22.70149 | YES | YES |
| 274 | a | 1633.98 | 11.58255 | YES | YES |
| 275 | a | 2908.89 | 31.78675 | YES | YES |
| 276 | a | 2927.39 | 27.54336 | YES | YES |
| 277 | a | 2943.43 | 26.94216 | YES | YES |
| 278 | a | 2945.25 | 16.26618 | YES | YES |
| 279 | a | 2951.53 | 15.99807 | YES | YES |
| 280 | a | 2952.85 | 19.85898 | YES | YES |
| 281 | a | 2993.95 | 5.64780 | YES | YES |
| 282 | a | 3000.71 | 7.33905 | YES | YES |
| 283 | a | 3016.02 | 6.40909 | YES | YES |
| 284 | a | 3027.51 | 7.24643 | YES | YES |
| 285 | a | 3031.19 | 12.24770 | YES | YES |
| 286 | a | 3036.06 | 2.12583 | YES | YES |
| 287 | a | 3070.68 | 9.19522 | YES | YES |
| 288 | a | 3073.03 | 5.71780 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 289 | a | 3078.41 | 15.88130 | YES | YES |
| 290 | a | 3083.62 | 16.47288 | YES | YES |
| 291 | a | 3087.72 | 18.05940 | YES | YES |
| 292 | a | 3101.09 | 9.23539 | YES | YES |
| 293 | a | 3110.72 | 2.64690 | YES | YES |
| 294 | a | 3115.70 | 1.92396 | YES | YES |
| 295 | a | 3124.47 | 8.19284 | YES | YES |
| 296 | a | 3128.45 | 6.64859 | YES | YES |
| 297 | a | 3133.47 | 1.75916 | YES | YES |
| 298 | a | 3138.24 | 0.28137 | YES | YES |
| 299 | a | 3156.74 | 1.80273 | YES | YES |
| 300 | a | 3166.34 | 0.90734 | YES | YES |

H-Sr(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Ba | 0.05835 | -1.11111 | -1.33807 |
| Al | -0.11898 | -0.13094 | 2.18771 |
| F | -0.13299 | 0.75016 | 0.70887 |
| C | 3.85272 | -0.61052 | -0.87464 |
| C | 3.87092 | -1.64638 | -1.81481 |
| C | 5.05805 | -2.02064 | -2.44415 |
| H | 5.03936 | -2.83457 | -3.18440 |
| C | 6.23904 | -1.33367 | -2.11193 |
| H | 7.18434 | -1.61644 | -2.60065 |
| C | 6.21800 | -0.29484 | -1.16449 |
| H | 7.14714 | 0.23645 | -0.90637 |
| C | 5.01714 | 0.07515 | -0.53337 |
| H | 4.97216 | 0.87481 | 0.21763 |
| F | 2.65213 | -0.28310 | -0.31936 |
| F | 2.69540 | -2.25261 | -2.12001 |
| C | -3.85770 | -1.60255 | -1.86286 |
| C | -3.78344 | -0.52933 | -0.96841 |
| C | -4.92191 | 0.17146 | -0.57586 |
| H | -4.82805 | 0.99985 | 0.13920 |
| C | -6.16153 | -0.22288 | -1.11061 |
| H | -7.07309 | 0.31727 | -0.81139 |
| C | -6.24182 | -1.29658 | -2.01501 |
| H | -7.21692 | -1.59749 | -2.42874 |
| C | -5.08409 | -1.99700 | -2.39901 |
| H | -5.11482 | -2.84091 | -3.10454 |
| F | -2.70502 | -2.22632 | -2.19841 |
| F | -2.55053 | -0.19104 | -0.49998 |
| O | -1.26555 | 0.44097 | 3.36544 |

| | | | |
|---|---|---|---|
| C | -2.45517 | 1.05375 | 3.57623 |
| C | -2.60760 | 2.32569 | 2.65983 |
| F | -2.91381 | 1.95230 | 1.38623 |
| F | -3.57813 | 3.15727 | 3.08074 |
| F | -1.45500 | 3.00697 | 2.60519 |
| C | -2.51269 | 1.49622 | 5.08708 |
| F | -2.04833 | 0.51847 | 5.87420 |
| F | -1.75125 | 2.59088 | 5.28459 |
| F | -3.77513 | 1.79152 | 5.46937 |
| C | -3.63373 | 0.05106 | 3.27734 |
| F | -3.78226 | -0.83322 | 4.27766 |
| F | -4.81561 | 0.67950 | 3.09203 |
| F | -3.35697 | -0.64725 | 2.15460 |
| O | 1.50070 | -0.24935 | 2.83785 |
| C | 2.42475 | 0.45297 | 3.53994 |
| C | 2.65366 | 1.86706 | 2.88888 |
| F | 1.46635 | 2.42743 | 2.58233 |
| F | 3.32763 | 2.71292 | 3.68515 |
| F | 3.34598 | 1.75486 | 1.72485 |
| C | 3.76708 | -0.36830 | 3.51007 |
| F | 3.70398 | -1.41517 | 4.35229 |
| F | 3.98899 | -0.85451 | 2.27311 |
| F | 4.83171 | 0.38763 | 3.85507 |
| C | 1.96726 | 0.64745 | 5.03816 |
| F | 1.42717 | -0.48550 | 5.50646 |
| F | 2.99807 | 0.99299 | 5.83872 |
| F | 1.03394 | 1.61893 | 5.12121 |
| O | -0.46263 | -1.74186 | 1.43342 |
| C | -0.41387 | -3.05562 | 1.81750 |
| C | -0.85541 | -3.25672 | 3.31254 |
| F | -2.19149 | -3.17196 | 3.43629 |
| F | -0.46327 | -4.45496 | 3.78508 |
| F | -0.30729 | -2.29363 | 4.07511 |
| C | 1.05682 | -3.59869 | 1.63058 |
| F | 1.57707 | -3.07435 | 0.47780 |
| F | 1.85063 | -3.21260 | 2.63431 |
| F | 1.11358 | -4.93450 | 1.52343 |
| C | -1.39034 | -3.84396 | 0.87354 |
| F | -0.87557 | -3.83457 | -0.39735 |
| F | -1.56933 | -5.11698 | 1.23893 |
| F | -2.58354 | -3.23604 | 0.80923 |
| C | -1.03848 | 1.97885 | -2.57723 |
| C | -0.97706 | 1.08454 | -3.68566 |
| C | 0.28684 | 0.71570 | -4.23200 |
| C | 1.49245 | 1.13116 | -3.59705 |
| C | 1.43087 | 2.00205 | -2.47039 |
| C | 0.16767 | 2.42602 | -1.96768 |
| C | -2.35615 | 2.52188 | -2.06182 |
| H | -2.38501 | 3.62948 | -2.16841 |
| H | -2.50251 | 2.29949 | -0.98507 |
| H | -3.22949 | 2.12201 | -2.60993 |
| C | -2.22180 | 0.49111 | -4.31702 |
| H | -2.47538 | 0.98548 | -5.28376 |
| H | -3.11321 | 0.57572 | -3.66529 |
| H | -2.06701 | -0.58882 | -4.52843 |

| | | | |
|---|---|---|---|
| C | 0.32964 | -0.13024 | -5.48583 |
| H | -0.48634 | 0.14360 | -6.18677 |
| H | 0.20598 | -1.20628 | -5.20807 |
| H | 1.28521 | -0.01822 | -6.03474 |
| C | 2.81146 | 0.62739 | -4.15222 |
| H | 2.74994 | -0.45406 | -4.39587 |
| H | 3.65104 | 0.75553 | -3.44295 |
| H | 3.09241 | 1.15756 | -5.09171 |
| C | 2.67374 | 2.56260 | -1.81093 |
| H | 3.61141 | 2.21509 | -2.28281 |
| H | 2.72050 | 2.30055 | -0.73277 |
| H | 2.67283 | 3.67451 | -1.86293 |
| C | 0.13121 | 3.39242 | -0.80453 |
| H | 0.37297 | 4.42891 | -1.14018 |
| H | 0.86722 | 3.11980 | -0.02317 |
| H | -0.85391 | 3.42184 | -0.30569 |
| H | -0.03234 | -2.39900 | -3.35049 |

Vibrational analysis

| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | -0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 13.15 | 0.02263 | YES | YES |
| 8 | a | 18.51 | 0.17355 | YES | YES |
| 9 | a | 19.85 | 1.15314 | YES | YES |
| 10 | a | 21.11 | 0.97693 | YES | YES |
| 11 | a | 22.61 | 0.30008 | YES | YES |
| 12 | a | 25.83 | 0.06622 | YES | YES |
| 13 | a | 28.20 | 0.02676 | YES | YES |
| 14 | a | 29.05 | 0.11980 | YES | YES |
| 15 | a | 31.35 | 0.11641 | YES | YES |
| 16 | a | 33.93 | 0.92143 | YES | YES |
| 17 | a | 34.83 | 0.16332 | YES | YES |
| 18 | a | 37.30 | 0.11544 | YES | YES |
| 19 | a | 38.72 | 1.45192 | YES | YES |
| 20 | a | 40.92 | 0.45210 | YES | YES |
| 21 | a | 43.07 | 0.41273 | YES | YES |
| 22 | a | 44.99 | 0.91226 | YES | YES |
| 23 | a | 45.75 | 1.14634 | YES | YES |
| 24 | a | 48.68 | 0.69189 | YES | YES |
| 25 | a | 51.59 | 0.28407 | YES | YES |
| 26 | a | 58.32 | 0.07698 | YES | YES |
| 27 | a | 59.46 | 0.18880 | YES | YES |
| 28 | a | 63.26 | 0.63280 | YES | YES |
| 29 | a | 63.78 | 0.74042 | YES | YES |
| 30 | a | 64.82 | 0.53841 | YES | YES |
| 31 | a | 67.69 | 0.72874 | YES | YES |
| 32 | a | 68.19 | 0.64058 | YES | YES |
| 33 | a | 71.58 | 0.08982 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 34 | a | 72.89 | 0.11497 | YES | YES |
| 35 | a | 73.90 | 0.32915 | YES | YES |
| 36 | a | 75.54 | 0.07312 | YES | YES |
| 37 | a | 77.96 | 0.30156 | YES | YES |
| 38 | a | 79.24 | 0.34737 | YES | YES |
| 39 | a | 81.44 | 0.40707 | YES | YES |
| 40 | a | 83.67 | 0.66055 | YES | YES |
| 41 | a | 85.60 | 1.31582 | YES | YES |
| 42 | a | 86.49 | 0.65415 | YES | YES |
| 43 | a | 93.66 | 1.08971 | YES | YES |
| 44 | a | 95.07 | 3.09480 | YES | YES |
| 45 | a | 96.91 | 7.65353 | YES | YES |
| 46 | a | 100.17 | 7.42707 | YES | YES |
| 47 | a | 102.10 | 2.70563 | YES | YES |
| 48 | a | 104.84 | 0.83834 | YES | YES |
| 49 | a | 109.39 | 13.18065 | YES | YES |
| 50 | a | 115.72 | 1.36448 | YES | YES |
| 51 | a | 120.75 | 0.10246 | YES | YES |
| 52 | a | 134.95 | 0.24366 | YES | YES |
| 53 | a | 140.72 | 2.58587 | YES | YES |
| 54 | a | 151.95 | 1.53842 | YES | YES |
| 55 | a | 154.20 | 0.42297 | YES | YES |
| 56 | a | 156.39 | 0.05873 | YES | YES |
| 57 | a | 160.21 | 0.43241 | YES | YES |
| 58 | a | 163.10 | 2.03588 | YES | YES |
| 59 | a | 166.87 | 0.73684 | YES | YES |
| 60 | a | 170.44 | 2.37901 | YES | YES |
| 61 | a | 174.80 | 13.84815 | YES | YES |
| 62 | a | 177.96 | 5.83240 | YES | YES |
| 63 | a | 185.01 | 2.05349 | YES | YES |
| 64 | a | 189.62 | 0.10748 | YES | YES |
| 65 | a | 194.29 | 10.61508 | YES | YES |
| 66 | a | 194.95 | 0.04265 | YES | YES |
| 67 | a | 195.44 | 0.41437 | YES | YES |
| 68 | a | 199.18 | 0.10498 | YES | YES |
| 69 | a | 213.36 | 1.75366 | YES | YES |
| 70 | a | 220.73 | 28.50262 | YES | YES |
| 71 | a | 238.84 | 7.04208 | YES | YES |
| 72 | a | 248.04 | 6.21684 | YES | YES |
| 73 | a | 269.37 | 1.98750 | YES | YES |
| 74 | a | 273.71 | 3.05196 | YES | YES |
| 75 | a | 277.89 | 1.69278 | YES | YES |
| 76 | a | 282.20 | 2.33007 | YES | YES |
| 77 | a | 284.11 | 0.18047 | YES | YES |
| 78 | a | 285.19 | 0.16962 | YES | YES |
| 79 | a | 287.28 | 2.33741 | YES | YES |
| 80 | a | 290.58 | 0.22756 | YES | YES |
| 81 | a | 291.37 | 1.73351 | YES | YES |
| 82 | a | 291.74 | 1.25275 | YES | YES |
| 83 | a | 292.45 | 1.70807 | YES | YES |
| 84 | a | 299.44 | 2.92347 | YES | YES |
| 85 | a | 302.12 | 1.49922 | YES | YES |
| 86 | a | 306.41 | 7.05434 | YES | YES |
| 87 | a | 307.06 | 4.58417 | YES | YES |
| 88 | a | 313.68 | 1.92961 | YES | YES |

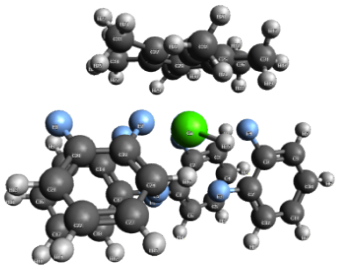
| | | | | | |
|---|---|---|---|---|---|
| 89 | a | 317.94 | 0.45383 | YES | YES |
| 90 | a | 320.14 | 2.31344 | YES | YES |
| 91 | a | 321.18 | 1.95342 | YES | YES |
| 92 | a | 324.42 | 1.05358 | YES | YES |
| 93 | a | 326.65 | 1.27846 | YES | YES |
| 94 | a | 328.95 | 0.15708 | YES | YES |
| 95 | a | 330.81 | 0.65986 | YES | YES |
| 96 | a | 348.25 | 0.69139 | YES | YES |
| 97 | a | 350.31 | 6.08632 | YES | YES |
| 98 | a | 355.21 | 1.02148 | YES | YES |
| 99 | a | 358.23 | 6.00991 | YES | YES |
| 100 | a | 360.37 | 6.56001 | YES | YES |
| 101 | a | 367.88 | 28.93711 | YES | YES |
| 102 | a | 373.57 | 0.87155 | YES | YES |
| 103 | a | 384.63 | 39.57990 | YES | YES |
| 104 | a | 396.54 | 0.10542 | YES | YES |
| 105 | a | 405.91 | 3.04699 | YES | YES |
| 106 | a | 413.99 | 1.00884 | YES | YES |
| 107 | a | 423.39 | 250.70422 | YES | YES |
| 108 | a | 435.63 | 2.79145 | YES | YES |
| 109 | a | 437.71 | 109.57495 | YES | YES |
| 110 | a | 440.29 | 5.27832 | YES | YES |
| 111 | a | 443.69 | 8.32213 | YES | YES |
| 112 | a | 447.80 | 17.13023 | YES | YES |
| 113 | a | 448.37 | 8.54050 | YES | YES |
| 114 | a | 449.07 | 2.00475 | YES | YES |
| 115 | a | 452.09 | 50.23100 | YES | YES |
| 116 | a | 460.09 | 230.31421 | YES | YES |
| 117 | a | 465.39 | 157.67109 | YES | YES |
| 118 | a | 514.64 | 7.05648 | YES | YES |
| 119 | a | 516.16 | 4.35172 | YES | YES |
| 120 | a | 518.03 | 1.03286 | YES | YES |
| 121 | a | 519.03 | 5.52474 | YES | YES |
| 122 | a | 520.15 | 4.62260 | YES | YES |
| 123 | a | 520.70 | 4.77376 | YES | YES |
| 124 | a | 521.50 | 1.99617 | YES | YES |
| 125 | a | 524.04 | 0.37101 | YES | YES |
| 126 | a | 524.83 | 2.51859 | YES | YES |
| 127 | a | 527.23 | 1.40860 | YES | YES |
| 128 | a | 540.41 | 3.29548 | YES | YES |
| 129 | a | 542.64 | 3.86759 | YES | YES |
| 130 | a | 545.26 | 13.87315 | YES | YES |
| 131 | a | 546.44 | 1.19616 | YES | YES |
| 132 | a | 547.40 | 0.52759 | YES | YES |
| 133 | a | 552.37 | 3.24251 | YES | YES |
| 134 | a | 553.48 | 0.88218 | YES | YES |
| 135 | a | 553.68 | 0.09841 | YES | YES |
| 136 | a | 554.18 | 0.20564 | YES | YES |
| 137 | a | 555.03 | 1.59595 | YES | YES |
| 138 | a | 555.36 | 1.15762 | YES | YES |
| 139 | a | 561.04 | 21.30205 | YES | YES |
| 140 | a | 561.28 | 2.98771 | YES | YES |
| 141 | a | 562.24 | 18.11052 | YES | YES |
| 142 | a | 565.13 | 27.50151 | YES | YES |
| 143 | a | 566.87 | 0.19302 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 144 | a | 572.09 | 1.05757 | YES | YES |
| 145 | a | 573.08 | 0.34921 | YES | YES |
| 146 | a | 586.59 | 1.48172 | YES | YES |
| 147 | a | 680.60 | 0.11123 | YES | YES |
| 148 | a | 683.07 | 0.06053 | YES | YES |
| 149 | a | 702.08 | 34.87004 | YES | YES |
| 150 | a | 705.67 | 25.43782 | YES | YES |
| 151 | a | 706.55 | 29.70281 | YES | YES |
| 152 | a | 707.03 | 0.93956 | YES | YES |
| 153 | a | 707.16 | 31.90595 | YES | YES |
| 154 | a | 708.97 | 35.21778 | YES | YES |
| 155 | a | 709.51 | 28.79048 | YES | YES |
| 156 | a | 712.15 | 100.72197 | YES | YES |
| 157 | a | 726.90 | 7.05396 | YES | YES |
| 158 | a | 738.12 | 2.82412 | YES | YES |
| 159 | a | 742.35 | 17.11079 | YES | YES |
| 160 | a | 745.06 | 31.68601 | YES | YES |
| 161 | a | 745.66 | 125.30704 | YES | YES |
| 162 | a | 760.54 | 59.57905 | YES | YES |
| 163 | a | 763.67 | 36.90215 | YES | YES |
| 164 | a | 779.76 | 19.81605 | YES | YES |
| 165 | a | 793.36 | 0.03004 | YES | YES |
| 166 | a | 802.13 | 3.15301 | YES | YES |
| 167 | a | 827.18 | 9.65037 | YES | YES |
| 168 | a | 828.37 | 63.44658 | YES | YES |
| 169 | a | 829.17 | 15.56672 | YES | YES |
| 170 | a | 840.51 | 1.52745 | YES | YES |
| 171 | a | 841.24 | 0.59150 | YES | YES |
| 172 | a | 853.16 | 39.55417 | YES | YES |
| 173 | a | 925.35 | 3.91887 | YES | YES |
| 174 | a | 925.95 | 6.61269 | YES | YES |
| 175 | a | 950.12 | 54.04562 | YES | YES |
| 176 | a | 953.88 | 80.38966 | YES | YES |
| 177 | a | 954.54 | 1.95757 | YES | YES |
| 178 | a | 959.21 | 128.82008 | YES | YES |
| 179 | a | 960.00 | 178.09975 | YES | YES |
| 180 | a | 964.51 | 7.37288 | YES | YES |
| 181 | a | 965.19 | 36.35358 | YES | YES |
| 182 | a | 966.52 | 203.71761 | YES | YES |
| 183 | a | 966.96 | 345.70564 | YES | YES |
| 184 | a | 967.25 | 22.75346 | YES | YES |
| 185 | a | 974.10 | 4.23279 | YES | YES |
| 186 | a | 983.07 | 65.79534 | YES | YES |
| 187 | a | 990.12 | 409.00306 | YES | YES |
| 188 | a | 1005.16 | 34.77622 | YES | YES |
| 189 | a | 1009.25 | 0.44330 | YES | YES |
| 190 | a | 1020.87 | 8.60424 | YES | YES |
| 191 | a | 1021.70 | 8.72071 | YES | YES |
| 192 | a | 1030.30 | 2.13548 | YES | YES |
| 193 | a | 1034.23 | 0.83079 | YES | YES |
| 194 | a | 1035.94 | 20.88751 | YES | YES |
| 195 | a | 1052.26 | 15.29740 | YES | YES |
| 196 | a | 1054.28 | 19.22563 | YES | YES |
| 197 | a | 1073.48 | 6.09399 | YES | YES |
| 198 | a | 1074.71 | 0.72137 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 199 | a | 1076.87 | 0.10110 | YES | YES |
| 200 | a | 1084.44 | 2.19648 | YES | YES |
| 201 | a | 1086.31 | 4.35829 | YES | YES |
| 202 | a | 1086.95 | 10.20608 | YES | YES |
| 203 | a | 1093.17 | 3.15206 | YES | YES |
| 204 | a | 1096.84 | 27.78499 | YES | YES |
| 205 | a | 1131.25 | 50.79043 | YES | YES |
| 206 | a | 1134.30 | 2.21450 | YES | YES |
| 207 | a | 1134.86 | 2.32907 | YES | YES |
| 208 | a | 1138.05 | 20.82329 | YES | YES |
| 209 | a | 1144.15 | 61.53095 | YES | YES |
| 210 | a | 1154.56 | 15.96031 | YES | YES |
| 211 | a | 1159.71 | 20.74487 | YES | YES |
| 212 | a | 1168.35 | 35.82474 | YES | YES |
| 213 | a | 1170.44 | 13.62462 | YES | YES |
| 214 | a | 1174.02 | 4.73397 | YES | YES |
| 215 | a | 1177.94 | 123.90209 | YES | YES |
| 216 | a | 1183.43 | 29.49644 | YES | YES |
| 217 | a | 1188.08 | 35.82756 | YES | YES |
| 218 | a | 1190.35 | 4.08244 | YES | YES |
| 219 | a | 1195.86 | 31.15447 | YES | YES |
| 220 | a | 1203.16 | 18.24923 | YES | YES |
| 221 | a | 1208.43 | 126.57840 | YES | YES |
| 222 | a | 1212.73 | 67.26307 | YES | YES |
| 223 | a | 1219.15 | 247.91114 | YES | YES |
| 224 | a | 1223.02 | 222.17719 | YES | YES |
| 225 | a | 1230.50 | 188.49851 | YES | YES |
| 226 | a | 1234.34 | 1309.45747 | YES | YES |
| 227 | a | 1241.75 | 507.88965 | YES | YES |
| 228 | a | 1246.33 | 789.62737 | YES | YES |
| 229 | a | 1248.17 | 42.97873 | YES | YES |
| 230 | a | 1248.58 | 23.39021 | YES | YES |
| 231 | a | 1249.42 | 197.03140 | YES | YES |
| 232 | a | 1250.15 | 89.10972 | YES | YES |
| 233 | a | 1255.63 | 239.73310 | YES | YES |
| 234 | a | 1257.14 | 552.86868 | YES | YES |
| 235 | a | 1260.80 | 531.98679 | YES | YES |
| 236 | a | 1263.61 | 590.98221 | YES | YES |
| 237 | a | 1269.51 | 82.99092 | YES | YES |
| 238 | a | 1301.77 | 14.20918 | YES | YES |
| 239 | a | 1307.51 | 0.93053 | YES | YES |
| 240 | a | 1315.28 | 0.19654 | YES | YES |
| 241 | a | 1332.58 | 146.80199 | YES | YES |
| 242 | a | 1339.55 | 6.69643 | YES | YES |
| 243 | a | 1346.28 | 110.81291 | YES | YES |
| 244 | a | 1354.44 | 0.10257 | YES | YES |
| 245 | a | 1361.39 | 4.22958 | YES | YES |
| 246 | a | 1363.87 | 2.72466 | YES | YES |
| 247 | a | 1367.23 | 0.95230 | YES | YES |
| 248 | a | 1374.55 | 5.78684 | YES | YES |
| 249 | a | 1381.37 | 0.40219 | YES | YES |
| 250 | a | 1381.68 | 0.41227 | YES | YES |
| 251 | a | 1391.64 | 1.21562 | YES | YES |
| 252 | a | 1397.03 | 2.40813 | YES | YES |
| 253 | a | 1412.48 | 2.36014 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 254 | a | 1414.63 | 4.35262 | YES | YES |
| 255 | a | 1418.68 | 1.10365 | YES | YES |
| 256 | a | 1425.34 | 10.18776 | YES | YES |
| 257 | a | 1430.48 | 27.60736 | YES | YES |
| 258 | a | 1433.75 | 3.14956 | YES | YES |
| 259 | a | 1440.72 | 32.29024 | YES | YES |
| 260 | a | 1447.40 | 3.13115 | YES | YES |
| 261 | a | 1452.76 | 18.67627 | YES | YES |
| 262 | a | 1456.98 | 11.69873 | YES | YES |
| 263 | a | 1458.24 | 12.33087 | YES | YES |
| 264 | a | 1458.33 | 4.47332 | YES | YES |
| 265 | a | 1467.57 | 19.23810 | YES | YES |
| 266 | a | 1469.91 | 26.99980 | YES | YES |
| 267 | a | 1500.35 | 293.25568 | YES | YES |
| 268 | a | 1503.02 | 99.91075 | YES | YES |
| 269 | a | 1560.19 | 0.07859 | YES | YES |
| 270 | a | 1566.51 | 0.17015 | YES | YES |
| 271 | a | 1616.24 | 0.29951 | YES | YES |
| 272 | a | 1616.60 | 2.20903 | YES | YES |
| 273 | a | 1630.22 | 16.72675 | YES | YES |
| 274 | a | 1631.47 | 13.82736 | YES | YES |
| 275 | a | 2891.80 | 45.05511 | YES | YES |
| 276 | a | 2934.69 | 24.84282 | YES | YES |
| 277 | a | 2935.05 | 20.19373 | YES | YES |
| 278 | a | 2941.15 | 17.62166 | YES | YES |
| 279 | a | 2952.63 | 16.78684 | YES | YES |
| 280 | a | 2957.32 | 16.06842 | YES | YES |
| 281 | a | 3010.11 | 10.56818 | YES | YES |
| 282 | a | 3014.67 | 7.00757 | YES | YES |
| 283 | a | 3019.29 | 3.80605 | YES | YES |
| 284 | a | 3022.90 | 6.47025 | YES | YES |
| 285 | a | 3037.08 | 5.16773 | YES | YES |
| 286 | a | 3046.74 | 3.57393 | YES | YES |
| 287 | a | 3058.54 | 21.47381 | YES | YES |
| 288 | a | 3060.88 | 1.80378 | YES | YES |
| 289 | a | 3068.89 | 5.37980 | YES | YES |
| 290 | a | 3081.47 | 20.95694 | YES | YES |
| 291 | a | 3082.71 | 11.47620 | YES | YES |
| 292 | a | 3098.18 | 4.08810 | YES | YES |
| 293 | a | 3113.79 | 2.29935 | YES | YES |
| 294 | a | 3114.61 | 2.17665 | YES | YES |
| 295 | a | 3127.02 | 7.94342 | YES | YES |
| 296 | a | 3127.64 | 7.32113 | YES | YES |
| 297 | a | 3137.38 | 0.32276 | YES | YES |
| 298 | a | 3138.08 | 0.27902 | YES | YES |
| 299 | a | 3159.51 | 2.09183 | YES | YES |
| 300 | a | 3164.88 | 2.65973 | YES | YES |

H-Ba(HMB)oDFB$_2${*f-al*}



Atomic coordinates

| | | | |
|---|---|---|---|
| Ca | -0.57705 | -0.09681 | -0.18652 |
| C | 2.03162 | 1.19455 | 2.93716 |
| C | 1.22821 | 2.01449 | 2.13435 |
| C | 0.62727 | 3.16989 | 2.62688 |
| H | 0.00673 | 3.78421 | 1.95772 |
| C | 0.82836 | 3.50834 | 3.97617 |
| H | 0.35726 | 4.41513 | 4.38393 |
| C | 1.62122 | 2.68820 | 4.79646 |
| H | 1.77571 | 2.95179 | 5.85407 |
| C | 2.22911 | 1.53032 | 4.28002 |
| H | 2.85976 | 0.87741 | 4.90275 |
| F | 2.58027 | 0.08876 | 2.40624 |
| F | 0.99433 | 1.61904 | 0.83584 |
| C | -1.36738 | 0.60139 | 3.27835 |
| C | -2.09906 | 1.55195 | 2.56196 |
| C | -2.90232 | 2.48815 | 3.20623 |
| H | -3.46771 | 3.22221 | 2.61276 |
| C | -2.95403 | 2.46137 | 4.61235 |
| H | -3.58504 | 3.19066 | 5.14321 |
| C | -2.21064 | 1.51344 | 5.33664 |
| H | -2.25742 | 1.50064 | 6.43639 |
| C | -1.40730 | 0.57008 | 4.67005 |
| H | -0.81564 | -0.18283 | 5.21153 |
| F | -0.58582 | -0.25966 | 2.57236 |
| F | -1.95426 | 1.56680 | 1.20148 |
| C | 1.96447 | -2.35917 | 0.58545 |
| C | 2.60806 | -1.61101 | -0.40369 |
| C | 3.79161 | -2.05568 | -0.98482 |
| H | 4.27282 | -1.45576 | -1.77135 |
| C | 4.32326 | -3.28289 | -0.54718 |
| H | 5.25619 | -3.65552 | -0.99711 |
| C | 3.67344 | -4.03359 | 0.44850 |
| H | 4.09670 | -4.99490 | 0.77757 |
| C | 2.47835 | -3.57302 | 1.02972 |
| H | 1.93686 | -4.14506 | 1.79716 |
| F | 0.78480 | -1.86698 | 1.07280 |
| F | 2.00679 | -0.44757 | -0.80096 |
| C | -0.03138 | -3.38545 | -1.45694 |
| C | 1.00420 | -4.05020 | -2.12684 |
| C | 1.22927 | -5.40484 | -1.86712 |
| H | 2.04510 | -5.91898 | -2.39749 |
| C | 0.41034 | -6.06811 | -0.93617 |

| | | | |
|---|---|---|---|
| H | 0.58449 | -7.13592 | -0.73101 |
| C | -0.62751 | -5.38466 | -0.27714 |
| H | -1.26874 | -5.91428 | 0.44437 |
| C | -0.85935 | -4.02201 | -0.53727 |
| H | -1.64644 | -3.42680 | -0.04196 |
| F | -0.18072 | -2.03655 | -1.69684 |
| F | 1.77625 | -3.36968 | -2.99513 |
| C | -2.28975 | 1.46770 | -1.93640 |
| C | -1.82033 | 0.40908 | -2.77973 |
| C | -0.49302 | 0.44257 | -3.29403 |
| C | 0.40983 | 1.44655 | -2.83656 |
| C | -0.05295 | 2.50074 | -2.00153 |
| C | -1.42139 | 2.54736 | -1.59736 |
| C | -3.72638 | 1.39323 | -1.46538 |
| H | -4.43014 | 1.39930 | -2.32715 |
| H | -4.01036 | 2.22386 | -0.79488 |
| H | -3.89673 | 0.44701 | -0.90606 |
| C | -2.78357 | -0.70728 | -3.11971 |
| H | -3.62604 | -0.33887 | -3.74793 |
| H | -3.22348 | -1.12967 | -2.19067 |
| H | -2.29966 | -1.54229 | -3.65756 |
| C | -0.01289 | -0.54015 | -4.34082 |
| H | 0.51497 | -0.00507 | -5.15861 |
| H | -0.84595 | -1.09876 | -4.80618 |
| H | 0.69703 | -1.28842 | -3.92690 |
| C | 1.84641 | 1.43575 | -3.31186 |
| H | 2.19380 | 0.41529 | -3.56442 |
| H | 2.53973 | 1.84481 | -2.55055 |
| H | 1.96864 | 2.06146 | -4.22690 |
| C | 0.90964 | 3.60412 | -1.61503 |
| H | 1.84022 | 3.19648 | -1.16645 |
| H | 0.48049 | 4.31576 | -0.88617 |
| H | 1.21982 | 4.19215 | -2.50854 |
| C | -1.91817 | 3.77066 | -0.85288 |
| H | -1.71182 | 4.69207 | -1.43945 |
| H | -1.42120 | 3.89659 | 0.13394 |
| H | -3.00715 | 3.74315 | -0.66853 |
| H | -2.21468 | -1.16607 | 0.20932 |

Vibrational analysis

| 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 | 10.57 | 0.08806 | YES | YES |
| 8 | a | 15.00 | 0.65859 | YES | YES |
| 9 | a | 18.59 | 0.07181 | YES | YES |
| 10 | a | 25.94 | 1.29842 | YES | YES |
| 11 | a | 28.32 | 0.74993 | YES | YES |
| 12 | a | 32.41 | 0.33237 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 13 | a | 35.07 | 0.48770 | YES | YES |
| 14 | a | 41.55 | 0.08611 | YES | YES |
| 15 | a | 44.23 | 0.88633 | YES | YES |
| 16 | a | 46.97 | 0.33469 | YES | YES |
| 17 | a | 48.08 | 0.09423 | YES | YES |
| 18 | a | 56.28 | 0.35191 | YES | YES |
| 19 | a | 57.21 | 0.34271 | YES | YES |
| 20 | a | 61.36 | 0.06828 | YES | YES |
| 21 | a | 66.30 | 0.61983 | YES | YES |
| 22 | a | 68.24 | 0.78082 | YES | YES |
| 23 | a | 72.85 | 1.42015 | YES | YES |
| 24 | a | 77.65 | 0.98383 | YES | YES |
| 25 | a | 78.17 | 1.47858 | YES | YES |
| 26 | a | 81.54 | 0.05656 | YES | YES |
| 27 | a | 85.55 | 0.07273 | YES | YES |
| 28 | a | 87.34 | 0.29020 | YES | YES |
| 29 | a | 88.37 | 0.70193 | YES | YES |
| 30 | a | 92.98 | 0.54382 | YES | YES |
| 31 | a | 96.65 | 0.77556 | YES | YES |
| 32 | a | 108.79 | 0.14886 | YES | YES |
| 33 | a | 122.21 | 5.34808 | YES | YES |
| 34 | a | 125.20 | 4.15775 | YES | YES |
| 35 | a | 127.31 | 3.70999 | YES | YES |
| 36 | a | 130.77 | 1.38400 | YES | YES |
| 37 | a | 144.40 | 0.23768 | YES | YES |
| 38 | a | 155.03 | 29.36721 | YES | YES |
| 39 | a | 171.44 | 44.28980 | YES | YES |
| 40 | a | 182.75 | 12.25079 | YES | YES |
| 41 | a | 193.39 | 3.61861 | YES | YES |
| 42 | a | 199.04 | 3.91574 | YES | YES |
| 43 | a | 202.37 | 2.30600 | YES | YES |
| 44 | a | 203.89 | 3.09713 | YES | YES |
| 45 | a | 207.92 | 1.28781 | YES | YES |
| 46 | a | 211.89 | 0.16587 | YES | YES |
| 47 | a | 244.43 | 13.43012 | YES | YES |
| 48 | a | 279.77 | 0.76285 | YES | YES |
| 49 | a | 288.11 | 8.07714 | YES | YES |
| 50 | a | 289.95 | 1.05309 | YES | YES |
| 51 | a | 296.65 | 10.98536 | YES | YES |
| 52 | a | 297.76 | 0.69987 | YES | YES |
| 53 | a | 301.21 | 0.33111 | YES | YES |
| 54 | a | 304.28 | 5.27117 | YES | YES |
| 55 | a | 309.62 | 1.28187 | YES | YES |
| 56 | a | 327.23 | 0.73102 | YES | YES |
| 57 | a | 346.20 | 0.85378 | YES | YES |
| 58 | a | 370.18 | 4.77253 | YES | YES |
| 59 | a | 372.86 | 3.25309 | YES | YES |
| 60 | a | 398.80 | 0.07986 | YES | YES |
| 61 | a | 403.12 | 0.07082 | YES | YES |
| 62 | a | 431.78 | 45.32201 | YES | YES |
| 63 | a | 432.40 | 28.81360 | YES | YES |
| 64 | a | 433.76 | 5.24214 | YES | YES |
| 65 | a | 435.18 | 8.77677 | YES | YES |
| 66 | a | 439.27 | 2.30869 | YES | YES |
| 67 | a | 442.13 | 1.95846 | YES | YES |

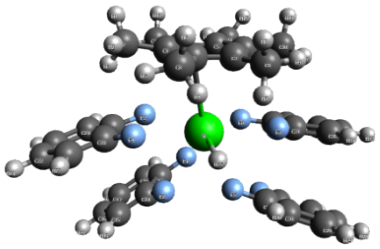
| | | | | | |
|---|---|---|---|---|---|
| 68 | a | 443.32 | 18.01090 | YES | YES |
| 69 | a | 444.14 | 6.81277 | YES | YES |
| 70 | a | 446.08 | 1.43808 | YES | YES |
| 71 | a | 450.04 | 124.96570 | YES | YES |
| 72 | a | 452.72 | 4.79612 | YES | YES |
| 73 | a | 460.86 | 74.27238 | YES | YES |
| 74 | a | 534.60 | 3.66927 | YES | YES |
| 75 | a | 537.59 | 3.12934 | YES | YES |
| 76 | a | 538.03 | 13.94830 | YES | YES |
| 77 | a | 538.51 | 6.95591 | YES | YES |
| 78 | a | 542.77 | 2.80532 | YES | YES |
| 79 | a | 543.82 | 0.76398 | YES | YES |
| 80 | a | 545.06 | 2.27526 | YES | YES |
| 81 | a | 545.58 | 0.87712 | YES | YES |
| 82 | a | 552.10 | 2.10464 | YES | YES |
| 83 | a | 558.59 | 19.66547 | YES | YES |
| 84 | a | 560.62 | 7.62678 | YES | YES |
| 85 | a | 561.17 | 9.53771 | YES | YES |
| 86 | a | 563.12 | 11.86851 | YES | YES |
| 87 | a | 564.89 | 0.00943 | YES | YES |
| 88 | a | 570.43 | 0.10681 | YES | YES |
| 89 | a | 572.16 | 0.53158 | YES | YES |
| 90 | a | 585.80 | 5.05665 | YES | YES |
| 91 | a | 603.30 | 385.15167 | YES | YES |
| 92 | a | 674.49 | 0.40315 | YES | YES |
| 93 | a | 677.02 | 0.15664 | YES | YES |
| 94 | a | 677.30 | 0.31664 | YES | YES |
| 95 | a | 680.93 | 0.15426 | YES | YES |
| 96 | a | 693.41 | 1.54703 | YES | YES |
| 97 | a | 742.51 | 108.81465 | YES | YES |
| 98 | a | 744.54 | 92.71073 | YES | YES |
| 99 | a | 746.85 | 1.62724 | YES | YES |
| 100 | a | 754.17 | 55.68274 | YES | YES |
| 101 | a | 754.79 | 37.83253 | YES | YES |
| 102 | a | 757.01 | 58.16954 | YES | YES |
| 103 | a | 758.30 | 87.43951 | YES | YES |
| 104 | a | 762.55 | 49.15192 | YES | YES |
| 105 | a | 792.22 | 0.44408 | YES | YES |
| 106 | a | 801.36 | 3.39992 | YES | YES |
| 107 | a | 821.83 | 4.50019 | YES | YES |
| 108 | a | 825.18 | 10.21286 | YES | YES |
| 109 | a | 828.48 | 22.32449 | YES | YES |
| 110 | a | 829.21 | 17.33940 | YES | YES |
| 111 | a | 833.14 | 1.13848 | YES | YES |
| 112 | a | 834.45 | 1.70391 | YES | YES |
| 113 | a | 838.23 | 0.54749 | YES | YES |
| 114 | a | 854.58 | 0.48408 | YES | YES |
| 115 | a | 920.75 | 4.31674 | YES | YES |
| 116 | a | 923.22 | 0.08296 | YES | YES |
| 117 | a | 923.64 | 2.89494 | YES | YES |
| 118 | a | 943.04 | 5.68675 | YES | YES |
| 119 | a | 952.61 | 2.55091 | YES | YES |
| 120 | a | 962.37 | 0.94897 | YES | YES |
| 121 | a | 967.52 | 0.12625 | YES | YES |
| 122 | a | 969.30 | 0.05993 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 123 | a | 970.56 | 0.11995 | YES | YES |
| 124 | a | 972.89 | 1.68605 | YES | YES |
| 125 | a | 975.90 | 0.99378 | YES | YES |
| 126 | a | 981.56 | 15.39186 | YES | YES |
| 127 | a | 1003.30 | 4.35718 | YES | YES |
| 128 | a | 1004.10 | 0.33822 | YES | YES |
| 129 | a | 1017.46 | 9.14523 | YES | YES |
| 130 | a | 1017.60 | 6.28499 | YES | YES |
| 131 | a | 1018.35 | 3.68805 | YES | YES |
| 132 | a | 1022.08 | 6.03322 | YES | YES |
| 133 | a | 1024.73 | 0.29189 | YES | YES |
| 134 | a | 1031.31 | 0.41616 | YES | YES |
| 135 | a | 1033.10 | 1.93439 | YES | YES |
| 136 | a | 1047.24 | 20.12015 | YES | YES |
| 137 | a | 1054.37 | 13.22723 | YES | YES |
| 138 | a | 1073.68 | 1.64409 | YES | YES |
| 139 | a | 1074.47 | 0.89557 | YES | YES |
| 140 | a | 1079.15 | 20.91063 | YES | YES |
| 141 | a | 1083.68 | 8.64109 | YES | YES |
| 142 | a | 1084.30 | 1.93221 | YES | YES |
| 143 | a | 1085.15 | 7.72362 | YES | YES |
| 144 | a | 1086.83 | 44.61521 | YES | YES |
| 145 | a | 1135.13 | 0.92347 | YES | YES |
| 146 | a | 1136.49 | 1.11502 | YES | YES |
| 147 | a | 1137.59 | 2.91262 | YES | YES |
| 148 | a | 1137.76 | 1.11612 | YES | YES |
| 149 | a | 1152.07 | 4.00283 | YES | YES |
| 150 | a | 1156.88 | 6.75479 | YES | YES |
| 151 | a | 1160.39 | 54.38866 | YES | YES |
| 152 | a | 1164.90 | 84.41151 | YES | YES |
| 153 | a | 1235.92 | 46.27920 | YES | YES |
| 154 | a | 1238.06 | 12.42765 | YES | YES |
| 155 | a | 1244.79 | 12.53690 | YES | YES |
| 156 | a | 1245.96 | 52.47181 | YES | YES |
| 157 | a | 1246.87 | 124.91019 | YES | YES |
| 158 | a | 1251.14 | 1.13099 | YES | YES |
| 159 | a | 1252.01 | 71.34959 | YES | YES |
| 160 | a | 1263.22 | 18.07914 | YES | YES |
| 161 | a | 1269.11 | 202.20719 | YES | YES |
| 162 | a | 1274.67 | 221.31108 | YES | YES |
| 163 | a | 1294.85 | 6.26195 | YES | YES |
| 164 | a | 1318.60 | 4.06972 | YES | YES |
| 165 | a | 1351.49 | 0.14564 | YES | YES |
| 166 | a | 1353.88 | 1.69925 | YES | YES |
| 167 | a | 1362.07 | 0.18615 | YES | YES |
| 168 | a | 1365.05 | 10.62186 | YES | YES |
| 169 | a | 1366.57 | 2.45121 | YES | YES |
| 170 | a | 1374.73 | 7.23571 | YES | YES |
| 171 | a | 1378.23 | 0.68107 | YES | YES |
| 172 | a | 1378.32 | 0.86199 | YES | YES |
| 173 | a | 1383.31 | 1.65734 | YES | YES |
| 174 | a | 1383.69 | 0.69854 | YES | YES |
| 175 | a | 1388.92 | 0.17460 | YES | YES |
| 176 | a | 1397.05 | 6.20124 | YES | YES |
| 177 | a | 1405.03 | 1.17549 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 178 | a | 1411.08 | 0.35849 | YES | YES |
| 179 | a | 1421.30 | 8.99550 | YES | YES |
| 180 | a | 1424.51 | 19.70862 | YES | YES |
| 181 | a | 1429.11 | 4.09695 | YES | YES |
| 182 | a | 1429.97 | 6.85258 | YES | YES |
| 183 | a | 1433.50 | 27.12643 | YES | YES |
| 184 | a | 1442.93 | 8.07162 | YES | YES |
| 185 | a | 1447.89 | 28.21657 | YES | YES |
| 186 | a | 1453.32 | 2.02289 | YES | YES |
| 187 | a | 1454.27 | 18.29358 | YES | YES |
| 188 | a | 1455.22 | 10.15585 | YES | YES |
| 189 | a | 1458.43 | 8.60215 | YES | YES |
| 190 | a | 1459.79 | 10.40970 | YES | YES |
| 191 | a | 1460.51 | 45.38971 | YES | YES |
| 192 | a | 1469.68 | 12.70559 | YES | YES |
| 193 | a | 1496.50 | 223.28194 | YES | YES |
| 194 | a | 1499.17 | 25.00068 | YES | YES |
| 195 | a | 1502.37 | 275.10277 | YES | YES |
| 196 | a | 1506.26 | 271.58392 | YES | YES |
| 197 | a | 1556.26 | 0.83719 | YES | YES |
| 198 | a | 1562.69 | 1.26136 | YES | YES |
| 199 | a | 1609.03 | 6.24397 | YES | YES |
| 200 | a | 1609.52 | 2.99181 | YES | YES |
| 201 | a | 1614.09 | 0.81673 | YES | YES |
| 202 | a | 1615.83 | 3.26430 | YES | YES |
| 203 | a | 1631.12 | 11.62204 | YES | YES |
| 204 | a | 1633.59 | 13.67270 | YES | YES |
| 205 | a | 1635.64 | 22.09369 | YES | YES |
| 206 | a | 1636.22 | 12.19961 | YES | YES |
| 207 | a | 2944.57 | 11.84217 | YES | YES |
| 208 | a | 2945.90 | 20.97046 | YES | YES |
| 209 | a | 2947.44 | 3.55437 | YES | YES |
| 210 | a | 2952.72 | 8.85866 | YES | YES |
| 211 | a | 2955.96 | 23.96165 | YES | YES |
| 212 | a | 2966.72 | 8.31689 | YES | YES |
| 213 | a | 3014.82 | 1.93754 | YES | YES |
| 214 | a | 3018.96 | 0.26443 | YES | YES |
| 215 | a | 3021.38 | 23.37231 | YES | YES |
| 216 | a | 3023.02 | 1.18435 | YES | YES |
| 217 | a | 3034.34 | 7.68064 | YES | YES |
| 218 | a | 3038.54 | 3.30211 | YES | YES |
| 219 | a | 3073.79 | 6.94639 | YES | YES |
| 220 | a | 3079.87 | 38.50147 | YES | YES |
| 221 | a | 3081.47 | 3.01954 | YES | YES |
| 222 | a | 3083.86 | 1.43291 | YES | YES |
| 223 | a | 3087.55 | 16.94457 | YES | YES |
| 224 | a | 3092.15 | 14.22459 | YES | YES |
| 225 | a | 3094.24 | 15.67425 | YES | YES |
| 226 | a | 3116.25 | 0.23215 | YES | YES |
| 227 | a | 3119.67 | 0.34882 | YES | YES |
| 228 | a | 3119.94 | 0.81654 | YES | YES |
| 229 | a | 3121.47 | 0.64180 | YES | YES |
| 230 | a | 3128.03 | 1.26933 | YES | YES |
| 231 | a | 3128.79 | 4.63898 | YES | YES |
| 232 | a | 3130.11 | 3.36841 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 233 | a | 3132.67 | 2.18949 | YES | YES |
| 234 | a | 3134.22 | 0.26197 | YES | YES |
| 235 | a | 3137.04 | 0.12613 | YES | YES |
| 236 | a | 3137.60 | 0.26638 | YES | YES |
| 237 | a | 3141.01 | 0.16592 | YES | YES |
| 238 | a | 3141.55 | 0.84852 | YES | YES |
| 239 | a | 3142.40 | 0.22700 | YES | YES |
| 240 | a | 3145.79 | 0.77512 | YES | YES |

[H-Ca(HMB)oDFB$_4$]$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.08074 | 2.10712 | -2.76151 |
| C | 1.10822 | 1.15950 | -3.03476 |
| C | 0.77524 | -0.21530 | -3.26233 |
| C | -0.57955 | -0.64066 | -3.17328 |
| C | -1.59384 | 0.29622 | -2.80869 |
| C | -1.26597 | 1.66178 | -2.59537 |
| C | 0.36773 | 3.59534 | -2.71631 |
| H | -0.26321 | 4.12975 | -3.45997 |
| H | 1.41924 | 3.83317 | -2.95731 |
| H | 0.14393 | 4.05374 | -1.72830 |
| C | 2.56585 | 1.55525 | -3.14561 |
| H | 3.20192 | 0.86069 | -2.55721 |
| H | 2.76769 | 2.57280 | -2.76457 |
| H | 2.91465 | 1.51578 | -4.20311 |
| C | 1.90126 | -1.15606 | -3.63364 |
| H | 2.63191 | -1.23854 | -2.79728 |
| H | 2.45693 | -0.77718 | -4.51910 |
| H | 1.55242 | -2.17579 | -3.87714 |
| C | -1.01083 | -2.05102 | -3.51513 |
| H | -1.53337 | -2.06728 | -4.49943 |
| H | -1.73124 | -2.46047 | -2.77687 |
| H | -0.16745 | -2.76101 | -3.58301 |
| C | -3.02912 | -0.18282 | -2.73969 |
| H | -3.74576 | 0.62998 | -2.52219 |
| H | -3.16631 | -0.96496 | -1.96038 |
| H | -3.33861 | -0.64246 | -3.70415 |
| C | -2.35973 | 2.65520 | -2.25307 |
| H | -1.95803 | 3.62849 | -1.91590 |
| H | -3.01704 | 2.27665 | -1.44240 |
| H | -3.01118 | 2.85910 | -3.13349 |
| C | -0.95727 | 1.21555 | 3.10679 |

| | | | |
|---|---|---|---|
| C | 0.38607 | 1.58975 | 3.22996 |
| C | 0.79772 | 2.50126 | 4.19959 |
| H | 1.86050 | 2.77855 | 4.26296 |
| C | -0.17197 | 3.04559 | 5.05952 |
| H | 0.13514 | 3.76764 | 5.83147 |
| C | -1.52228 | 2.67306 | 4.93868 |
| H | -2.27577 | 3.10061 | 5.61799 |
| C | -1.92529 | 1.75066 | 3.95579 |
| H | -2.97536 | 1.44169 | 3.84050 |
| F | -1.29737 | 0.34885 | 2.11218 |
| F | 1.28175 | 1.07193 | 2.33755 |
| C | -0.10588 | 3.53187 | 0.92333 |
| C | 1.27595 | 3.58415 | 0.71324 |
| C | 2.03664 | 4.62388 | 1.24499 |
| H | 3.12320 | 4.64374 | 1.07142 |
| C | 1.37874 | 5.61764 | 1.99351 |
| H | 1.96491 | 6.44621 | 2.41995 |
| C | -0.01132 | 5.56161 | 2.19826 |
| H | -0.51488 | 6.34381 | 2.78654 |
| C | -0.77115 | 4.50849 | 1.65864 |
| H | -1.85744 | 4.42976 | 1.81269 |
| F | -0.78020 | 2.45441 | 0.40939 |
| F | 1.84852 | 2.57549 | 0.00120 |
| C | 1.17168 | -2.85045 | 2.07068 |
| C | 0.32950 | -3.77297 | 2.70632 |
| C | 0.73216 | -5.10728 | 2.81355 |
| H | 0.06514 | -5.82483 | 3.31489 |
| C | 1.97284 | -5.49285 | 2.27563 |
| H | 2.29330 | -6.54299 | 2.36065 |
| C | 2.80238 | -4.55323 | 1.63747 |
| H | 3.77241 | -4.86364 | 1.21925 |
| C | 2.40295 | -3.20876 | 1.52962 |
| H | 2.99761 | -2.43641 | 1.01057 |
| F | 0.71368 | -1.55852 | 1.94535 |
| F | -0.85885 | -3.36014 | 3.18090 |
| C | -0.26458 | -3.48236 | -0.56216 |
| C | -1.45155 | -2.99018 | -0.01151 |
| C | -2.44274 | -3.84762 | 0.45588 |
| H | -3.36094 | -3.43289 | 0.89743 |
| C | -2.21919 | -5.23327 | 0.35546 |
| H | -2.98805 | -5.93016 | 0.72265 |
| C | -1.02813 | -5.72885 | -0.20349 |
| H | -0.86325 | -6.81486 | -0.27374 |
| C | -0.03435 | -4.85095 | -0.67141 |
| H | 0.91342 | -5.20914 | -1.09886 |
| F | 0.66789 | -2.57317 | -0.96634 |
| F | -1.59609 | -1.62660 | 0.06700 |
| Sr | 0.56623 | 0.06402 | -0.14805 |
| H | 2.66709 | -0.43510 | -0.31266 |

Vibrational analysis

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

| | | | | | |
|---|---|---|---|---|---|
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 14.34 | 0.37768 | YES | YES |
| 8 | a | 16.62 | 0.95168 | YES | YES |
| 9 | a | 18.83 | 0.10885 | YES | YES |
| 10 | a | 23.81 | 0.73978 | YES | YES |
| 11 | a | 26.61 | 0.73619 | YES | YES |
| 12 | a | 31.33 | 0.05793 | YES | YES |
| 13 | a | 35.34 | 0.11087 | YES | YES |
| 14 | a | 41.66 | 0.75109 | YES | YES |
| 15 | a | 48.59 | 0.20656 | YES | YES |
| 16 | a | 50.99 | 0.39796 | YES | YES |
| 17 | a | 53.01 | 0.39926 | YES | YES |
| 18 | a | 57.45 | 0.66420 | YES | YES |
| 19 | a | 61.63 | 0.22987 | YES | YES |
| 20 | a | 62.79 | 0.32610 | YES | YES |
| 21 | a | 65.58 | 0.35251 | YES | YES |
| 22 | a | 67.93 | 1.57165 | YES | YES |
| 23 | a | 72.65 | 0.88084 | YES | YES |
| 24 | a | 73.53 | 0.88838 | YES | YES |
| 25 | a | 75.97 | 0.85664 | YES | YES |
| 26 | a | 78.16 | 0.39029 | YES | YES |
| 27 | a | 85.09 | 0.22128 | YES | YES |
| 28 | a | 86.94 | 0.17403 | YES | YES |
| 29 | a | 88.75 | 0.37190 | YES | YES |
| 30 | a | 92.75 | 2.51698 | YES | YES |
| 31 | a | 96.46 | 1.53847 | YES | YES |
| 32 | a | 104.36 | 0.78289 | YES | YES |
| 33 | a | 111.69 | 22.18319 | YES | YES |
| 34 | a | 125.81 | 11.58341 | YES | YES |
| 35 | a | 129.11 | 1.44862 | YES | YES |
| 36 | a | 135.46 | 11.71372 | YES | YES |
| 37 | a | 142.18 | 4.05293 | YES | YES |
| 38 | a | 153.32 | 2.92589 | YES | YES |
| 39 | a | 165.43 | 0.13887 | YES | YES |
| 40 | a | 181.01 | 3.43004 | YES | YES |
| 41 | a | 194.98 | 4.67410 | YES | YES |
| 42 | a | 196.54 | 0.87233 | YES | YES |
| 43 | a | 199.83 | 0.26660 | YES | YES |
| 44 | a | 208.69 | 2.18242 | YES | YES |
| 45 | a | 210.20 | 0.07892 | YES | YES |
| 46 | a | 215.15 | 0.31753 | YES | YES |
| 47 | a | 248.40 | 7.43656 | YES | YES |
| 48 | a | 285.14 | 4.15381 | YES | YES |
| 49 | a | 288.97 | 0.04166 | YES | YES |
| 50 | a | 294.96 | 2.25527 | YES | YES |
| 51 | a | 296.20 | 2.55664 | YES | YES |
| 52 | a | 298.05 | 4.15521 | YES | YES |
| 53 | a | 299.52 | 0.71944 | YES | YES |
| 54 | a | 304.25 | 0.45562 | YES | YES |
| 55 | a | 305.96 | 1.18686 | YES | YES |
| 56 | a | 330.29 | 0.71040 | YES | YES |

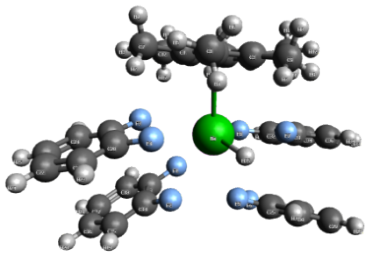
| | | | | | |
|---|---|---|---|---|---|
| 57 | a | 341.69 | 0.43543 | YES | YES |
| 58 | a | 364.69 | 5.49054 | YES | YES |
| 59 | a | 370.35 | 6.40178 | YES | YES |
| 60 | a | 394.72 | 0.46483 | YES | YES |
| 61 | a | 405.04 | 1.10118 | YES | YES |
| 62 | a | 427.54 | 105.34114 | YES | YES |
| 63 | a | 432.59 | 32.00468 | YES | YES |
| 64 | a | 433.80 | 13.53938 | YES | YES |
| 65 | a | 434.81 | 2.38807 | YES | YES |
| 66 | a | 436.37 | 24.76124 | YES | YES |
| 67 | a | 440.80 | 120.16064 | YES | YES |
| 68 | a | 443.33 | 5.25197 | YES | YES |
| 69 | a | 443.40 | 12.81678 | YES | YES |
| 70 | a | 444.98 | 36.53771 | YES | YES |
| 71 | a | 445.63 | 7.31658 | YES | YES |
| 72 | a | 448.36 | 1.33998 | YES | YES |
| 73 | a | 454.21 | 252.43451 | YES | YES |
| 74 | a | 462.73 | 189.94567 | YES | YES |
| 75 | a | 536.13 | 0.51454 | YES | YES |
| 76 | a | 536.52 | 1.71146 | YES | YES |
| 77 | a | 537.02 | 5.07773 | YES | YES |
| 78 | a | 538.86 | 2.59189 | YES | YES |
| 79 | a | 542.76 | 1.94051 | YES | YES |
| 80 | a | 543.59 | 1.86014 | YES | YES |
| 81 | a | 543.88 | 0.67630 | YES | YES |
| 82 | a | 545.88 | 0.67471 | YES | YES |
| 83 | a | 552.27 | 0.74882 | YES | YES |
| 84 | a | 558.82 | 4.94465 | YES | YES |
| 85 | a | 559.01 | 14.95585 | YES | YES |
| 86 | a | 560.15 | 18.12137 | YES | YES |
| 87 | a | 561.54 | 5.72266 | YES | YES |
| 88 | a | 562.06 | 0.40191 | YES | YES |
| 89 | a | 571.99 | 0.69382 | YES | YES |
| 90 | a | 574.09 | 0.31058 | YES | YES |
| 91 | a | 584.13 | 0.27074 | YES | YES |
| 92 | a | 672.13 | 0.05011 | YES | YES |
| 93 | a | 675.36 | 0.34168 | YES | YES |
| 94 | a | 675.87 | 0.43071 | YES | YES |
| 95 | a | 679.50 | 0.10081 | YES | YES |
| 96 | a | 705.21 | 0.29934 | YES | YES |
| 97 | a | 744.63 | 48.44842 | YES | YES |
| 98 | a | 745.55 | 182.72903 | YES | YES |
| 99 | a | 748.97 | 3.68546 | YES | YES |
| 100 | a | 754.12 | 22.08038 | YES | YES |
| 101 | a | 754.70 | 34.54512 | YES | YES |
| 102 | a | 756.36 | 60.64651 | YES | YES |
| 103 | a | 757.27 | 127.59635 | YES | YES |
| 104 | a | 760.20 | 36.74848 | YES | YES |
| 105 | a | 792.97 | 1.30720 | YES | YES |
| 106 | a | 796.10 | 3.59674 | YES | YES |
| 107 | a | 821.43 | 6.76843 | YES | YES |
| 108 | a | 822.55 | 1.15698 | YES | YES |
| 109 | a | 825.29 | 13.59709 | YES | YES |
| 110 | a | 830.34 | 17.44602 | YES | YES |
| 111 | a | 835.01 | 0.98751 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 112 | a | 835.80 | 0.54423 | YES | YES |
| 113 | a | 838.58 | 0.34707 | YES | YES |
| 114 | a | 851.14 | 1.65182 | YES | YES |
| 115 | a | 924.34 | 2.75346 | YES | YES |
| 116 | a | 925.55 | 7.82717 | YES | YES |
| 117 | a | 926.60 | 0.46746 | YES | YES |
| 118 | a | 937.85 | 9.13103 | YES | YES |
| 119 | a | 950.35 | 4.33503 | YES | YES |
| 120 | a | 961.22 | 1.64271 | YES | YES |
| 121 | a | 969.77 | 0.70321 | YES | YES |
| 122 | a | 970.58 | 0.05401 | YES | YES |
| 123 | a | 971.32 | 0.74239 | YES | YES |
| 124 | a | 972.01 | 0.02449 | YES | YES |
| 125 | a | 972.44 | 1.58662 | YES | YES |
| 126 | a | 981.02 | 13.10526 | YES | YES |
| 127 | a | 1002.08 | 0.97455 | YES | YES |
| 128 | a | 1005.62 | 3.05374 | YES | YES |
| 129 | a | 1018.73 | 2.43873 | YES | YES |
| 130 | a | 1018.74 | 3.60929 | YES | YES |
| 131 | a | 1020.64 | 4.52464 | YES | YES |
| 132 | a | 1021.93 | 9.25471 | YES | YES |
| 133 | a | 1027.22 | 1.43426 | YES | YES |
| 134 | a | 1029.98 | 0.30088 | YES | YES |
| 135 | a | 1033.18 | 1.12724 | YES | YES |
| 136 | a | 1047.21 | 10.52073 | YES | YES |
| 137 | a | 1051.43 | 16.52677 | YES | YES |
| 138 | a | 1072.07 | 3.04820 | YES | YES |
| 139 | a | 1074.06 | 0.43520 | YES | YES |
| 140 | a | 1081.00 | 0.49312 | YES | YES |
| 141 | a | 1083.80 | 18.30209 | YES | YES |
| 142 | a | 1084.03 | 12.05362 | YES | YES |
| 143 | a | 1084.61 | 2.85575 | YES | YES |
| 144 | a | 1086.93 | 27.69250 | YES | YES |
| 145 | a | 1135.91 | 3.55051 | YES | YES |
| 146 | a | 1137.53 | 6.64557 | YES | YES |
| 147 | a | 1137.74 | 2.81758 | YES | YES |
| 148 | a | 1137.80 | 0.72071 | YES | YES |
| 149 | a | 1144.26 | 206.60702 | YES | YES |
| 150 | a | 1151.86 | 41.47952 | YES | YES |
| 151 | a | 1153.93 | 11.14102 | YES | YES |
| 152 | a | 1166.66 | 47.57960 | YES | YES |
| 153 | a | 1169.26 | 155.99318 | YES | YES |
| 154 | a | 1241.81 | 9.88663 | YES | YES |
| 155 | a | 1243.95 | 80.88230 | YES | YES |
| 156 | a | 1246.15 | 37.19834 | YES | YES |
| 157 | a | 1246.71 | 1.06935 | YES | YES |
| 158 | a | 1248.72 | 33.41511 | YES | YES |
| 159 | a | 1249.05 | 15.51116 | YES | YES |
| 160 | a | 1249.31 | 43.04388 | YES | YES |
| 161 | a | 1258.42 | 171.24052 | YES | YES |
| 162 | a | 1269.85 | 53.81454 | YES | YES |
| 163 | a | 1289.89 | 0.31442 | YES | YES |
| 164 | a | 1321.64 | 1.79092 | YES | YES |
| 165 | a | 1353.73 | 0.06627 | YES | YES |
| 166 | a | 1355.89 | 1.48413 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 167 | a | 1361.59 | 4.28046 | YES | YES |
| 168 | a | 1365.29 | 7.19196 | YES | YES |
| 169 | a | 1366.21 | 3.06268 | YES | YES |
| 170 | a | 1375.43 | 10.88837 | YES | YES |
| 171 | a | 1378.26 | 0.84268 | YES | YES |
| 172 | a | 1380.26 | 0.26732 | YES | YES |
| 173 | a | 1381.86 | 0.35328 | YES | YES |
| 174 | a | 1383.31 | 0.94572 | YES | YES |
| 175 | a | 1392.59 | 1.20241 | YES | YES |
| 176 | a | 1395.05 | 1.07189 | YES | YES |
| 177 | a | 1411.40 | 15.45987 | YES | YES |
| 178 | a | 1414.09 | 4.87069 | YES | YES |
| 179 | a | 1417.55 | 1.48232 | YES | YES |
| 180 | a | 1419.99 | 9.92839 | YES | YES |
| 181 | a | 1424.58 | 3.75103 | YES | YES |
| 182 | a | 1432.45 | 10.31647 | YES | YES |
| 183 | a | 1439.95 | 14.82512 | YES | YES |
| 184 | a | 1441.83 | 27.17182 | YES | YES |
| 185 | a | 1450.03 | 3.18370 | YES | YES |
| 186 | a | 1451.19 | 13.40445 | YES | YES |
| 187 | a | 1454.82 | 16.31981 | YES | YES |
| 188 | a | 1457.81 | 4.21883 | YES | YES |
| 189 | a | 1458.41 | 12.04297 | YES | YES |
| 190 | a | 1459.35 | 6.62560 | YES | YES |
| 191 | a | 1460.13 | 31.22259 | YES | YES |
| 192 | a | 1470.02 | 12.37508 | YES | YES |
| 193 | a | 1494.42 | 66.45255 | YES | YES |
| 194 | a | 1494.83 | 183.82125 | YES | YES |
| 195 | a | 1500.15 | 364.41302 | YES | YES |
| 196 | a | 1505.65 | 118.32572 | YES | YES |
| 197 | a | 1559.46 | 2.00631 | YES | YES |
| 198 | a | 1563.56 | 1.82357 | YES | YES |
| 199 | a | 1609.34 | 6.43133 | YES | YES |
| 200 | a | 1612.23 | 0.56728 | YES | YES |
| 201 | a | 1613.55 | 0.78111 | YES | YES |
| 202 | a | 1615.93 | 0.41438 | YES | YES |
| 203 | a | 1629.41 | 13.39250 | YES | YES |
| 204 | a | 1631.00 | 9.75398 | YES | YES |
| 205 | a | 1632.33 | 14.73438 | YES | YES |
| 206 | a | 1634.19 | 9.81639 | YES | YES |
| 207 | a | 2942.64 | 20.81536 | YES | YES |
| 208 | a | 2944.80 | 4.32910 | YES | YES |
| 209 | a | 2947.66 | 16.93803 | YES | YES |
| 210 | a | 2950.50 | 9.99729 | YES | YES |
| 211 | a | 2952.08 | 9.88587 | YES | YES |
| 212 | a | 2956.43 | 13.07708 | YES | YES |
| 213 | a | 3012.64 | 2.48421 | YES | YES |
| 214 | a | 3014.08 | 13.38108 | YES | YES |
| 215 | a | 3018.72 | 9.72880 | YES | YES |
| 216 | a | 3021.69 | 6.09592 | YES | YES |
| 217 | a | 3023.76 | 0.57085 | YES | YES |
| 218 | a | 3025.24 | 5.30246 | YES | YES |
| 219 | a | 3078.79 | 41.10302 | YES | YES |
| 220 | a | 3080.52 | 6.46243 | YES | YES |
| 221 | a | 3083.44 | 13.73465 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 222 | a | 3085.27 | 3.39578 | YES | YES |
| 223 | a | 3089.49 | 5.91964 | YES | YES |
| 224 | a | 3093.77 | 9.78842 | YES | YES |
| 225 | a | 3094.58 | 17.69971 | YES | YES |
| 226 | a | 3115.19 | 0.32260 | YES | YES |
| 227 | a | 3119.57 | 0.89080 | YES | YES |
| 228 | a | 3120.78 | 0.90444 | YES | YES |
| 229 | a | 3121.34 | 0.77182 | YES | YES |
| 230 | a | 3128.35 | 4.62040 | YES | YES |
| 231 | a | 3129.81 | 2.14405 | YES | YES |
| 232 | a | 3131.26 | 2.81584 | YES | YES |
| 233 | a | 3132.57 | 2.37805 | YES | YES |
| 234 | a | 3136.41 | 0.72464 | YES | YES |
| 235 | a | 3136.60 | 0.17057 | YES | YES |
| 236 | a | 3138.22 | 1.43456 | YES | YES |
| 237 | a | 3141.35 | 1.11195 | YES | YES |
| 238 | a | 3142.16 | 0.44942 | YES | YES |
| 239 | a | 3142.94 | 0.24939 | YES | YES |
| 240 | a | 3145.89 | 1.04597 | YES | YES |

[H-Ba(HMB)oDFB$_4$]$^+$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.62393 | 2.54012 | -2.32691 |
| C | 1.53050 | 1.53551 | -2.77540 |
| C | 1.03847 | 0.29032 | -3.27662 |
| C | -0.36504 | 0.06528 | -3.36715 |
| C | -1.26775 | 1.05363 | -2.87679 |
| C | -0.78052 | 2.30051 | -2.39623 |
| C | 1.13646 | 3.86773 | -1.80213 |
| H | 1.17064 | 4.63487 | -2.60984 |
| H | 2.15699 | 3.78637 | -1.38513 |
| H | 0.49079 | 4.27463 | -0.99880 |
| C | 3.02940 | 1.75119 | -2.76412 |
| H | 3.51356 | 1.11633 | -1.98653 |
| H | 3.31278 | 2.80232 | -2.57321 |
| H | 3.47541 | 1.46721 | -3.74100 |
| C | 2.05128 | -0.74792 | -3.70979 |
| H | 2.84135 | -0.86293 | -2.93807 |
| H | 2.55108 | -0.45436 | -4.66159 |
| H | 1.60331 | -1.74662 | -3.86261 |
| C | -0.94049 | -1.16784 | -4.03427 |
| H | -1.62907 | -0.87260 | -4.85604 |
| H | -1.53740 | -1.79835 | -3.33896 |

| | | | |
|---|---|---|---|
| H | -0.16312 | -1.81476 | -4.47913 |
| C | -2.76170 | 0.80717 | -2.91955 |
| H | -3.21899 | 1.24334 | -3.83872 |
| H | -3.28077 | 1.26804 | -2.05403 |
| H | -3.01133 | -0.27154 | -2.91715 |
| C | -1.78480 | 3.37152 | -2.01847 |
| H | -1.32186 | 4.37019 | -1.91370 |
| H | -2.30219 | 3.14422 | -1.05870 |
| H | -2.57479 | 3.46092 | -2.79419 |
| C | -1.25296 | 0.90934 | 3.36657 |
| C | 0.11341 | 0.99661 | 3.66154 |
| C | 0.56273 | 1.65333 | 4.80556 |
| H | 1.64312 | 1.70739 | 5.00572 |
| C | -0.38798 | 2.23457 | 5.66212 |
| H | -0.04885 | 2.75699 | 6.56967 |
| C | -1.75991 | 2.15017 | 5.36725 |
| H | -2.49953 | 2.60381 | 6.04484 |
| C | -2.20289 | 1.48282 | 4.21083 |
| H | -3.27083 | 1.39867 | 3.95809 |
| F | -1.62720 | 0.27896 | 2.21673 |
| F | 0.99901 | 0.45530 | 2.77721 |
| C | 0.15444 | 3.45640 | 1.75818 |
| C | 1.53870 | 3.26180 | 1.69151 |
| C | 2.39793 | 3.97195 | 2.52845 |
| H | 3.48266 | 3.79904 | 2.45983 |
| C | 1.84083 | 4.88796 | 3.43939 |
| H | 2.50674 | 5.45670 | 4.10652 |
| C | 0.44955 | 5.08070 | 3.50226 |
| H | 0.02288 | 5.79792 | 4.21992 |
| C | -0.40989 | 4.36087 | 2.65387 |
| H | -1.50264 | 4.48263 | 2.68654 |
| F | -0.63506 | 2.69713 | 0.93620 |
| F | 2.01528 | 2.33974 | 0.81135 |
| C | 0.57761 | -3.35882 | 1.55196 |
| C | -0.34559 | -4.37035 | 1.85270 |
| C | 0.00561 | -5.70607 | 1.63654 |
| H | -0.72480 | -6.49270 | 1.87895 |
| C | 1.27582 | -6.00409 | 1.11230 |
| H | 1.55521 | -7.05584 | 0.94326 |
| C | 2.18419 | -4.97567 | 0.80474 |
| H | 3.17562 | -5.21596 | 0.39045 |
| C | 1.83733 | -3.63022 | 1.02495 |
| H | 2.50075 | -2.78411 | 0.76459 |
| F | 0.17873 | -2.05611 | 1.74559 |
| F | -1.55849 | -4.03444 | 2.32489 |
| C | -0.59737 | -3.40809 | -1.34669 |
| C | -1.81684 | -3.00628 | -0.78971 |
| C | -2.85634 | -3.91248 | -0.59978 |
| H | -3.79922 | -3.57201 | -0.14678 |
| C | -2.65207 | -5.24894 | -0.98896 |
| H | -3.46098 | -5.98133 | -0.84414 |
| C | -1.43012 | -5.65112 | -1.55559 |
| H | -1.28006 | -6.69977 | -1.85462 |
| C | -0.38662 | -4.72720 | -1.74001 |
| H | 0.58525 | -5.01465 | -2.16677 |

| | | | |
|---|---|---|---|
| F | 0.38347 | -2.47108 | -1.47712 |
| F | -1.94942 | -1.69185 | -0.42121 |
| Ba | 0.33820 | 0.08223 | -0.08214 |
| H | 2.54449 | -0.64834 | -0.18270 |

Vibrational analysis

| 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 | 11.95 | 0.39342 | YES | YES |
| 8 | a | 12.83 | 0.72125 | YES | YES |
| 9 | a | 18.42 | 1.16956 | YES | YES |
| 10 | a | 19.63 | 0.01898 | YES | YES |
| 11 | a | 22.78 | 0.63724 | YES | YES |
| 12 | a | 26.37 | 0.25849 | YES | YES |
| 13 | a | 31.61 | 0.78285 | YES | YES |
| 14 | a | 41.05 | 1.52087 | YES | YES |
| 15 | a | 42.89 | 0.48623 | YES | YES |
| 16 | a | 47.45 | 0.80772 | YES | YES |
| 17 | a | 52.58 | 0.68007 | YES | YES |
| 18 | a | 53.12 | 0.29301 | YES | YES |
| 19 | a | 56.17 | 0.37195 | YES | YES |
| 20 | a | 58.86 | 0.29837 | YES | YES |
| 21 | a | 62.43 | 0.14690 | YES | YES |
| 22 | a | 65.40 | 0.76657 | YES | YES |
| 23 | a | 67.86 | 0.07688 | YES | YES |
| 24 | a | 71.82 | 0.70366 | YES | YES |
| 25 | a | 73.60 | 0.66229 | YES | YES |
| 26 | a | 76.07 | 0.29787 | YES | YES |
| 27 | a | 78.05 | 0.54694 | YES | YES |
| 28 | a | 79.49 | 0.05840 | YES | YES |
| 29 | a | 83.09 | 0.37189 | YES | YES |
| 30 | a | 86.30 | 2.03097 | YES | YES |
| 31 | a | 93.36 | 1.17480 | YES | YES |
| 32 | a | 95.73 | 6.52615 | YES | YES |
| 33 | a | 102.78 | 3.55498 | YES | YES |
| 34 | a | 108.10 | 0.51213 | YES | YES |
| 35 | a | 112.72 | 4.33523 | YES | YES |
| 36 | a | 119.29 | 4.42126 | YES | YES |
| 37 | a | 124.21 | 9.01844 | YES | YES |
| 38 | a | 133.06 | 0.52041 | YES | YES |
| 39 | a | 145.72 | 1.21177 | YES | YES |
| 40 | a | 163.05 | 3.31483 | YES | YES |
| 41 | a | 170.01 | 0.23479 | YES | YES |
| 42 | a | 193.75 | 0.40722 | YES | YES |
| 43 | a | 196.54 | 0.13013 | YES | YES |
| 44 | a | 203.78 | 0.81146 | YES | YES |
| 45 | a | 204.83 | 0.43189 | YES | YES |
| 46 | a | 216.65 | 3.83321 | YES | YES |

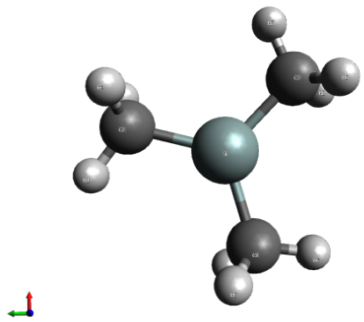
| | | | | | |
|---|---|---|---|---|---|
| 47 | a | 229.92 | 8.20217 | YES | YES |
| 48 | a | 283.85 | 2.10411 | YES | YES |
| 49 | a | 285.82 | 0.01480 | YES | YES |
| 50 | a | 289.98 | 1.36833 | YES | YES |
| 51 | a | 292.99 | 2.43867 | YES | YES |
| 52 | a | 293.44 | 2.19686 | YES | YES |
| 53 | a | 295.57 | 1.08531 | YES | YES |
| 54 | a | 300.61 | 0.03870 | YES | YES |
| 55 | a | 302.90 | 0.56176 | YES | YES |
| 56 | a | 328.55 | 0.40794 | YES | YES |
| 57 | a | 348.29 | 1.67304 | YES | YES |
| 58 | a | 357.91 | 12.73093 | YES | YES |
| 59 | a | 369.17 | 0.31372 | YES | YES |
| 60 | a | 385.50 | 270.66134 | YES | YES |
| 61 | a | 391.31 | 1.71602 | YES | YES |
| 62 | a | 409.31 | 8.24718 | YES | YES |
| 63 | a | 417.15 | 406.38491 | YES | YES |
| 64 | a | 433.83 | 5.79363 | YES | YES |
| 65 | a | 433.98 | 1.31848 | YES | YES |
| 66 | a | 434.27 | 1.17193 | YES | YES |
| 67 | a | 435.83 | 9.20069 | YES | YES |
| 68 | a | 440.69 | 2.56194 | YES | YES |
| 69 | a | 443.16 | 5.90846 | YES | YES |
| 70 | a | 445.28 | 0.75078 | YES | YES |
| 71 | a | 446.82 | 4.36554 | YES | YES |
| 72 | a | 447.44 | 0.88515 | YES | YES |
| 73 | a | 448.59 | 0.05439 | YES | YES |
| 74 | a | 457.88 | 8.93733 | YES | YES |
| 75 | a | 535.50 | 0.13768 | YES | YES |
| 76 | a | 535.91 | 1.42051 | YES | YES |
| 77 | a | 536.56 | 5.03518 | YES | YES |
| 78 | a | 537.97 | 5.34927 | YES | YES |
| 79 | a | 541.07 | 1.37460 | YES | YES |
| 80 | a | 542.58 | 0.08634 | YES | YES |
| 81 | a | 542.95 | 1.07960 | YES | YES |
| 82 | a | 546.14 | 0.13559 | YES | YES |
| 83 | a | 549.61 | 1.01190 | YES | YES |
| 84 | a | 559.53 | 2.06137 | YES | YES |
| 85 | a | 559.75 | 24.53678 | YES | YES |
| 86 | a | 560.24 | 10.16897 | YES | YES |
| 87 | a | 561.12 | 10.01675 | YES | YES |
| 88 | a | 563.87 | 0.83322 | YES | YES |
| 89 | a | 567.22 | 0.27253 | YES | YES |
| 90 | a | 571.93 | 0.59313 | YES | YES |
| 91 | a | 582.44 | 0.68273 | YES | YES |
| 92 | a | 671.69 | 0.05809 | YES | YES |
| 93 | a | 673.97 | 0.44926 | YES | YES |
| 94 | a | 675.26 | 0.37492 | YES | YES |
| 95 | a | 679.63 | 0.08183 | YES | YES |
| 96 | a | 698.35 | 0.21704 | YES | YES |
| 97 | a | 744.49 | 78.34997 | YES | YES |
| 98 | a | 745.51 | 152.41510 | YES | YES |
| 99 | a | 749.09 | 0.80638 | YES | YES |
| 100 | a | 754.07 | 25.53644 | YES | YES |
| 101 | a | 754.89 | 13.66529 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 102 | a | 756.56 | 146.34699 | YES | YES |
| 103 | a | 757.07 | 37.95820 | YES | YES |
| 104 | a | 759.28 | 60.42639 | YES | YES |
| 105 | a | 791.85 | 0.70189 | YES | YES |
| 106 | a | 799.98 | 4.01145 | YES | YES |
| 107 | a | 822.82 | 6.15649 | YES | YES |
| 108 | a | 823.37 | 0.35140 | YES | YES |
| 109 | a | 825.70 | 11.92253 | YES | YES |
| 110 | a | 830.18 | 19.25313 | YES | YES |
| 111 | a | 834.51 | 1.27414 | YES | YES |
| 112 | a | 835.61 | 0.48373 | YES | YES |
| 113 | a | 838.40 | 0.50270 | YES | YES |
| 114 | a | 852.22 | 2.63162 | YES | YES |
| 115 | a | 923.63 | 2.67883 | YES | YES |
| 116 | a | 925.04 | 6.75691 | YES | YES |
| 117 | a | 926.25 | 0.75527 | YES | YES |
| 118 | a | 938.90 | 12.58074 | YES | YES |
| 119 | a | 952.33 | 0.97683 | YES | YES |
| 120 | a | 962.62 | 0.45387 | YES | YES |
| 121 | a | 969.36 | 0.05660 | YES | YES |
| 122 | a | 970.31 | 0.37850 | YES | YES |
| 123 | a | 971.02 | 0.03917 | YES | YES |
| 124 | a | 972.16 | 0.90196 | YES | YES |
| 125 | a | 972.88 | 5.55396 | YES | YES |
| 126 | a | 979.80 | 12.36561 | YES | YES |
| 127 | a | 1002.66 | 4.01559 | YES | YES |
| 128 | a | 1003.70 | 2.30069 | YES | YES |
| 129 | a | 1019.39 | 4.26949 | YES | YES |
| 130 | a | 1019.51 | 1.17607 | YES | YES |
| 131 | a | 1020.88 | 4.90354 | YES | YES |
| 132 | a | 1025.31 | 9.42928 | YES | YES |
| 133 | a | 1026.99 | 2.40934 | YES | YES |
| 134 | a | 1030.90 | 1.59748 | YES | YES |
| 135 | a | 1032.69 | 0.74463 | YES | YES |
| 136 | a | 1048.75 | 4.31196 | YES | YES |
| 137 | a | 1052.24 | 17.63425 | YES | YES |
| 138 | a | 1059.47 | 398.01241 | YES | YES |
| 139 | a | 1073.37 | 2.09727 | YES | YES |
| 140 | a | 1074.04 | 1.83090 | YES | YES |
| 141 | a | 1081.26 | 2.72689 | YES | YES |
| 142 | a | 1084.80 | 21.94991 | YES | YES |
| 143 | a | 1085.20 | 0.39229 | YES | YES |
| 144 | a | 1087.34 | 40.45248 | YES | YES |
| 145 | a | 1088.08 | 35.58358 | YES | YES |
| 146 | a | 1137.00 | 4.43325 | YES | YES |
| 147 | a | 1137.20 | 2.17933 | YES | YES |
| 148 | a | 1137.50 | 0.49588 | YES | YES |
| 149 | a | 1137.60 | 0.71842 | YES | YES |
| 150 | a | 1155.04 | 5.55969 | YES | YES |
| 151 | a | 1156.95 | 0.15381 | YES | YES |
| 152 | a | 1167.92 | 31.08018 | YES | YES |
| 153 | a | 1169.00 | 72.70208 | YES | YES |
| 154 | a | 1243.42 | 11.68888 | YES | YES |
| 155 | a | 1244.80 | 55.29388 | YES | YES |
| 156 | a | 1246.48 | 1.54769 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 157 | a | 1247.98 | 3.37576 | YES | YES |
| 158 | a | 1248.61 | 5.64936 | YES | YES |
| 159 | a | 1250.14 | 114.75435 | YES | YES |
| 160 | a | 1250.29 | 30.68106 | YES | YES |
| 161 | a | 1259.04 | 201.60039 | YES | YES |
| 162 | a | 1270.47 | 50.11626 | YES | YES |
| 163 | a | 1299.06 | 1.40886 | YES | YES |
| 164 | a | 1318.14 | 1.47096 | YES | YES |
| 165 | a | 1352.73 | 0.17507 | YES | YES |
| 166 | a | 1357.03 | 3.23897 | YES | YES |
| 167 | a | 1363.40 | 0.91345 | YES | YES |
| 168 | a | 1364.85 | 13.18665 | YES | YES |
| 169 | a | 1366.83 | 6.15318 | YES | YES |
| 170 | a | 1373.62 | 6.11340 | YES | YES |
| 171 | a | 1377.99 | 0.81997 | YES | YES |
| 172 | a | 1380.03 | 0.17785 | YES | YES |
| 173 | a | 1381.36 | 0.27556 | YES | YES |
| 174 | a | 1382.47 | 0.42226 | YES | YES |
| 175 | a | 1389.13 | 0.49954 | YES | YES |
| 176 | a | 1395.44 | 3.32436 | YES | YES |
| 177 | a | 1405.57 | 1.22536 | YES | YES |
| 178 | a | 1413.50 | 2.83384 | YES | YES |
| 179 | a | 1415.56 | 1.83027 | YES | YES |
| 180 | a | 1421.93 | 38.97760 | YES | YES |
| 181 | a | 1426.17 | 7.17478 | YES | YES |
| 182 | a | 1432.61 | 10.38363 | YES | YES |
| 183 | a | 1440.62 | 21.36082 | YES | YES |
| 184 | a | 1444.86 | 15.75310 | YES | YES |
| 185 | a | 1450.13 | 27.46455 | YES | YES |
| 186 | a | 1454.16 | 16.00188 | YES | YES |
| 187 | a | 1455.07 | 10.79208 | YES | YES |
| 188 | a | 1457.67 | 4.54119 | YES | YES |
| 189 | a | 1458.37 | 6.09742 | YES | YES |
| 190 | a | 1459.03 | 8.75881 | YES | YES |
| 191 | a | 1463.23 | 24.53449 | YES | YES |
| 192 | a | 1472.63 | 7.88210 | YES | YES |
| 193 | a | 1495.66 | 136.70540 | YES | YES |
| 194 | a | 1495.99 | 118.64949 | YES | YES |
| 195 | a | 1501.35 | 397.02716 | YES | YES |
| 196 | a | 1506.64 | 111.27442 | YES | YES |
| 197 | a | 1558.18 | 0.29093 | YES | YES |
| 198 | a | 1562.51 | 1.08804 | YES | YES |
| 199 | a | 1609.62 | 6.85498 | YES | YES |
| 200 | a | 1613.34 | 0.44936 | YES | YES |
| 201 | a | 1614.50 | 0.27664 | YES | YES |
| 202 | a | 1616.61 | 0.33410 | YES | YES |
| 203 | a | 1628.29 | 12.56328 | YES | YES |
| 204 | a | 1629.82 | 10.04051 | YES | YES |
| 205 | a | 1630.60 | 21.50035 | YES | YES |
| 206 | a | 1631.23 | 7.92219 | YES | YES |
| 207 | a | 2940.79 | 11.91724 | YES | YES |
| 208 | a | 2942.10 | 15.99150 | YES | YES |
| 209 | a | 2945.05 | 5.16163 | YES | YES |
| 210 | a | 2949.74 | 10.19130 | YES | YES |
| 211 | a | 2952.10 | 10.19039 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 212 | a | 2954.61 | 11.80079 | YES | YES |
| 213 | a | 3016.75 | 10.79922 | YES | YES |
| 214 | a | 3018.58 | 5.85180 | YES | YES |
| 215 | a | 3019.99 | 8.75166 | YES | YES |
| 216 | a | 3026.06 | 0.71998 | YES | YES |
| 217 | a | 3027.48 | 2.63840 | YES | YES |
| 218 | a | 3040.11 | 11.84276 | YES | YES |
| 219 | a | 3048.75 | 73.31159 | YES | YES |
| 220 | a | 3068.53 | 8.50811 | YES | YES |
| 221 | a | 3078.94 | 1.15959 | YES | YES |
| 222 | a | 3082.89 | 6.77014 | YES | YES |
| 223 | a | 3085.07 | 12.90257 | YES | YES |
| 224 | a | 3091.49 | 7.47532 | YES | YES |
| 225 | a | 3092.80 | 12.53287 | YES | YES |
| 226 | a | 3114.21 | 0.48549 | YES | YES |
| 227 | a | 3119.23 | 0.94513 | YES | YES |
| 228 | a | 3120.18 | 0.93826 | YES | YES |
| 229 | a | 3120.69 | 0.79285 | YES | YES |
| 230 | a | 3127.64 | 4.91011 | YES | YES |
| 231 | a | 3129.54 | 1.86345 | YES | YES |
| 232 | a | 3130.71 | 3.18157 | YES | YES |
| 233 | a | 3132.09 | 2.55687 | YES | YES |
| 234 | a | 3136.37 | 0.65567 | YES | YES |
| 235 | a | 3136.50 | 0.14038 | YES | YES |
| 236 | a | 3137.64 | 1.23681 | YES | YES |
| 237 | a | 3141.16 | 1.04230 | YES | YES |
| 238 | a | 3142.38 | 0.49004 | YES | YES |
| 239 | a | 3142.58 | 0.17178 | YES | YES |
| 240 | a | 3145.60 | 0.90965 | YES | YES |

TMS$^{+}$



Atomic coordinates

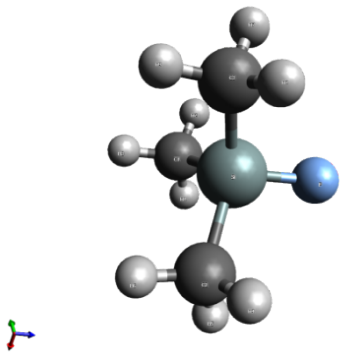
| | | | |
|---|---|---|---|
| C | -1.77202 | -0.51312 | -0.00109 |
| Si | -0.00000 | 0.00000 | -0.00303 |
| C | 0.44164 | 1.79117 | -0.00109 |
| H | -0.44385 | 2.46070 | -0.01115 |
| H | 1.08733 | 2.02055 | -0.88338 |
| H | 1.06582 | 2.02144 | 0.89663 |
| H | -2.29352 | -0.06862 | -0.88338 |
| H | -2.28353 | -0.08769 | 0.89663 |
| H | -1.90910 | -1.61473 | -0.01115 |
| C | 1.33038 | -1.27806 | -0.00109 |
| H | 2.35295 | -0.84597 | -0.01115 |

| | | | |
|---|---|---|---|
| H | 1.20618 | -1.95193 | -0.88338 |
| H | 1.21771 | -1.93375 | 0.89663 |

Vibrational analysis

| 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 | e | 41.97 | 0.00121 | YES | YES |
| 8 | e | 41.97 | 0.00121 | YES | YES |
| 9 | a | 71.31 | 2.66890 | YES | YES |
| 10 | e | 210.22 | 2.17958 | YES | YES |
| 11 | e | 210.22 | 2.17958 | YES | YES |
| 12 | a | 214.38 | 1.30854 | YES | YES |
| 13 | a | 594.49 | 0.00127 | YES | YES |
| 14 | e | 621.71 | 0.00091 | YES | YES |
| 15 | e | 621.71 | 0.00091 | YES | YES |
| 16 | a | 696.30 | 0.00028 | YES | YES |
| 17 | e | 744.25 | 7.79635 | YES | YES |
| 18 | e | 744.25 | 7.79635 | YES | YES |
| 19 | a | 817.45 | 83.61421 | YES | YES |
| 20 | e | 884.17 | 133.09786 | YES | YES |
| 21 | e | 884.17 | 133.09786 | YES | YES |
| 22 | e | 1240.82 | 78.24857 | YES | YES |
| 23 | e | 1240.82 | 78.24857 | YES | YES |
| 24 | a | 1246.85 | 0.01078 | YES | YES |
| 25 | e | 1360.82 | 11.77859 | YES | YES |
| 26 | e | 1360.82 | 11.77859 | YES | YES |
| 27 | e | 1362.48 | 0.03821 | YES | YES |
| 28 | e | 1362.48 | 0.03821 | YES | YES |
| 29 | a | 1368.79 | 30.43935 | YES | YES |
| 30 | a | 1370.52 | 16.92580 | YES | YES |
| 31 | e | 2924.99 | 45.94410 | YES | YES |
| 32 | e | 2924.99 | 45.94410 | YES | YES |
| 33 | a | 2930.16 | 0.01873 | YES | YES |
| 34 | a | 3000.05 | 44.64866 | YES | YES |
| 35 | e | 3000.43 | 0.00312 | YES | YES |
| 36 | e | 3000.43 | 0.00312 | YES | YES |
| 37 | e | 3067.24 | 14.43421 | YES | YES |
| 38 | e | 3067.24 | 14.43421 | YES | YES |
| 39 | a | 3067.87 | 0.00009 | YES | YES |

TMSF



Atomic coordinates

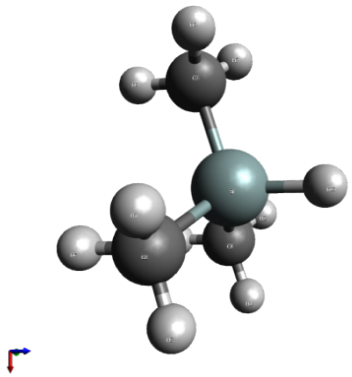
| | | | |
|---|---|---|---|
| Si | 0.00000 | 0.00000 | 0.43656 |
| C | 0.89918 | 1.55743 | -0.12081 |
| H | 1.94641 | 1.57282 | 0.25497 |
| H | 0.38890 | 2.47205 | 0.25497 |
| H | 0.93549 | 1.62032 | -1.23189 |
| C | 0.89918 | -1.55743 | -0.12081 |
| H | 0.38890 | -2.47205 | 0.25497 |
| H | 1.94641 | -1.57282 | 0.25497 |
| H | 0.93549 | -1.62032 | -1.23189 |
| C | -1.79837 | 0.00000 | -0.12081 |
| H | -2.33531 | 0.89923 | 0.25497 |
| H | -2.33531 | -0.89923 | 0.25497 |
| H | -1.87098 | 0.00000 | -1.23189 |
| F | -0.00000 | 0.00000 | 2.09200 |

Vibrational analysis

| 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 | a2 | 135.92 | 0.00000 | NO | NO |
| 8 | e | 155.63 | 0.00402 | YES | YES |
| 9 | e | 155.63 | 0.00402 | YES | YES |
| 10 | e | 186.86 | 0.07200 | YES | YES |
| 11 | e | 186.86 | 0.07200 | YES | YES |
| 12 | a1 | 224.21 | 0.11033 | YES | YES |
| 13 | e | 265.24 | 12.10160 | YES | YES |
| 14 | e | 265.24 | 12.10160 | YES | YES |
| 15 | a1 | 589.66 | 0.03853 | YES | YES |
| 16 | a2 | 666.55 | 0.00000 | NO | NO |
| 17 | e | 676.35 | 2.60368 | YES | YES |
| 18 | e | 676.35 | 2.60368 | YES | YES |
| 19 | e | 753.74 | 29.29597 | YES | YES |
| 20 | e | 753.74 | 29.29597 | YES | YES |
| 21 | a1 | 770.19 | 3.59849 | YES | YES |
| 22 | e | 853.03 | 137.48691 | YES | YES |
| 23 | e | 853.03 | 137.48691 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 24 | a1 | 909.11 | 168.56407 | YES | YES |
| 25 | e | 1246.92 | 46.83500 | YES | YES |
| 26 | e | 1246.92 | 46.83500 | YES | YES |
| 27 | a1 | 1254.34 | 16.08381 | YES | YES |
| 28 | a2 | 1390.64 | 0.00000 | NO | NO |
| 29 | e | 1398.14 | 0.06431 | YES | YES |
| 30 | e | 1398.14 | 0.06431 | YES | YES |
| 31 | e | 1404.35 | 4.83497 | YES | YES |
| 32 | e | 1404.35 | 4.83497 | YES | YES |
| 33 | a1 | 1415.88 | 15.92780 | YES | YES |
| 34 | e | 2941.28 | 3.39472 | YES | YES |
| 35 | e | 2941.28 | 3.39472 | YES | YES |
| 36 | a1 | 2943.45 | 1.24516 | YES | YES |
| 37 | e | 3031.56 | 0.75640 | YES | YES |
| 38 | e | 3031.56 | 0.75640 | YES | YES |
| 39 | a1 | 3034.00 | 16.62908 | YES | YES |
| 40 | a2 | 3038.02 | 0.00000 | NO | NO |
| 41 | e | 3038.66 | 8.78859 | YES | YES |
| 42 | e | 3038.66 | 8.78859 | YES | YES |

TMSH



Atomic coordinates

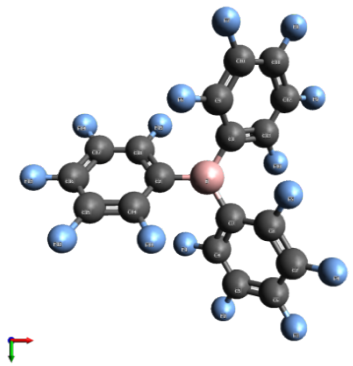
| | | | |
|---|---|---|---|
| Si | 0.00000 | 0.00000 | 0.49410 |
| C | 0.89905 | 1.55720 | -0.11149 |
| H | 1.95111 | 1.58171 | 0.25071 |
| H | 0.39424 | 2.48057 | 0.25071 |
| H | 0.92177 | 1.59656 | -1.22407 |
| C | 0.89905 | -1.55720 | -0.11149 |
| H | 0.39424 | -2.48057 | 0.25071 |
| H | 1.95111 | -1.58171 | 0.25071 |
| H | 0.92177 | -1.59656 | -1.22407 |
| C | -1.79810 | 0.00000 | -0.11149 |
| H | -2.34536 | 0.89886 | 0.25071 |
| H | -2.34536 | -0.89886 | 0.25071 |
| H | -1.84354 | 0.00000 | -1.22407 |
| H | 0.00000 | 0.00000 | 2.00859 |

Vibrational analysis

| 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 | a2 | 154.19 | 0.00000 | NO | NO |
| 8 | e | 167.58 | 0.00016 | YES | YES |
| 9 | e | 167.58 | 0.00016 | YES | YES |
| 10 | e | 199.14 | 0.60512 | YES | YES |
| 11 | e | 199.14 | 0.60512 | YES | YES |
| 12 | a1 | 230.68 | 0.91663 | YES | YES |
| 13 | a1 | 599.53 | 1.44165 | YES | YES |
| 14 | e | 603.12 | 7.13510 | YES | YES |
| 15 | e | 603.12 | 7.13510 | YES | YES |
| 16 | a2 | 669.19 | 0.00000 | NO | NO |
| 17 | e | 689.08 | 11.15726 | YES | YES |
| 18 | e | 689.08 | 11.15726 | YES | YES |
| 19 | e | 834.77 | 15.44621 | YES | YES |
| 20 | e | 834.77 | 15.44621 | YES | YES |
| 21 | a1 | 857.13 | 69.93309 | YES | YES |
| 22 | e | 889.84 | 163.14323 | YES | YES |
| 23 | e | 889.84 | 163.14323 | YES | YES |
| 24 | e | 1239.93 | 30.83601 | YES | YES |
| 25 | e | 1239.93 | 30.83601 | YES | YES |
| 26 | a1 | 1250.47 | 6.02253 | YES | YES |
| 27 | a2 | 1395.73 | 0.00000 | NO | NO |
| 28 | e | 1400.44 | 0.32430 | YES | YES |
| 29 | e | 1400.44 | 0.32430 | YES | YES |
| 30 | e | 1409.47 | 4.98149 | YES | YES |
| 31 | e | 1409.47 | 4.98149 | YES | YES |
| 32 | a1 | 1417.04 | 13.85350 | YES | YES |
| 33 | a1 | 2135.76 | 162.32938 | YES | YES |
| 34 | e | 2938.17 | 8.17543 | YES | YES |
| 35 | e | 2938.17 | 8.17543 | YES | YES |
| 36 | a1 | 2939.07 | 2.70072 | YES | YES |
| 37 | e | 3028.28 | 0.80092 | YES | YES |
| 38 | e | 3028.28 | 0.80092 | YES | YES |
| 39 | a1 | 3029.72 | 21.92102 | YES | YES |
| 40 | a2 | 3033.35 | 0.00000 | NO | NO |
| 41 | e | 3033.77 | 12.29847 | YES | YES |
| 42 | e | 3033.77 | 12.29847 | YES | YES |

$B(C_6F_5)_3$



Atomic coordinates

| | | | |
|---|---|---|---|
| B | 0.0000000 | 0.0000000 | 0.0000000 |
| C | 0.7834617 | -1.3569954 | 0.0000000 |
| C | -1.5669234 | 0.0000000 | 0.0000000 |
| C | 0.7834617 | 1.3569954 | 0.0000000 |
| C | 0.3339335 | 2.4787778 | 0.7306595 |
| C | 1.0258822 | 3.6981330 | 0.7514839 |
| C | 2.2084332 | 3.8251184 | 0.0000000 |
| C | 2.6897360 | 2.7375066 | -0.7514839 |
| C | 1.9797178 | 1.5285838 | -0.7306595 |
| C | 0.3339335 | -2.4787778 | -0.7306595 |
| C | 1.0258822 | -3.6981330 | -0.7514839 |
| C | 2.2084332 | -3.8251184 | 0.0000000 |
| C | 2.6897360 | -2.7375066 | 0.7514839 |
| C | 1.9797178 | -1.5285838 | 0.7306595 |
| C | -2.3136513 | 0.9501940 | -0.7306595 |
| C | -3.7156182 | 0.9606264 | -0.7514839 |
| C | -4.4168663 | 0.0000000 | 0.0000000 |
| C | -3.7156182 | -0.9606264 | 0.7514839 |
| C | -2.3136513 | -0.9501940 | 0.7306595 |
| F | -0.7819149 | 2.4000971 | 1.4733842 |
| F | 0.5803408 | 4.7319535 | 1.4701518 |
| F | 2.8741026 | 4.9780917 | 0.0000000 |
| F | 3.8078215 | 2.8685667 | -1.4701518 |
| F | 2.4695026 | 0.5228904 | -1.4733842 |
| F | -0.7819149 | -2.4000971 | -1.4733842 |
| F | 0.5803408 | -4.7319535 | -1.4701518 |
| F | 2.8741026 | -4.9780917 | 0.0000000 |
| F | 3.8078215 | -2.8685667 | 1.4701518 |
| F | 2.4695026 | -0.5228904 | 1.4733842 |
| F | -1.6875876 | 1.8772068 | -1.4733842 |
| F | -4.3881624 | 1.8633869 | -1.4701518 |
| F | -5.7482051 | 0.0000000 | 0.0000000 |
| F | -4.3881624 | -1.8633869 | 1.4701518 |
| F | -1.6875876 | -1.8772068 | 1.4733842 |

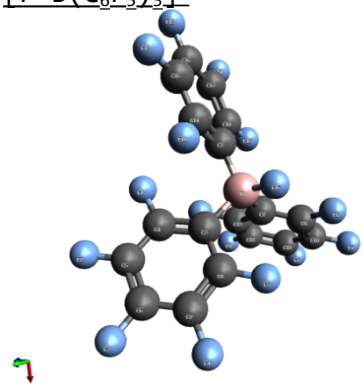
Vibrational analysis

| 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 | e | 18.72 | 0.46396 | YES | YES |
| 8 | e | 18.72 | 0.46396 | YES | YES |
| 9 | a2 | 31.36 | 0.00737 | YES | NO |
| 10 | e | 31.47 | 0.01787 | YES | YES |
| 11 | e | 31.47 | 0.01787 | YES | YES |
| 12 | a1 | 36.98 | 0.00000 | NO | YES |
| 13 | a2 | 101.19 | 0.06859 | YES | NO |
| 14 | e | 106.24 | 0.07407 | YES | YES |
| 15 | e | 106.24 | 0.07407 | YES | YES |
| 16 | e | 124.89 | 0.42610 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 17 | e | 124.89 | 0.42610 | YES | YES |
| 18 | a1 | 125.98 | 0.00000 | NO | YES |
| 19 | e | 141.95 | 0.02937 | YES | YES |
| 20 | e | 141.95 | 0.02937 | YES | YES |
| 21 | a2 | 147.19 | 0.00466 | YES | NO |
| 22 | e | 153.84 | 0.16692 | YES | YES |
| 23 | e | 153.84 | 0.16692 | YES | YES |
| 24 | a1 | 156.14 | 0.00000 | NO | YES |
| 25 | a2 | 219.51 | 3.77763 | YES | NO |
| 26 | e | 223.95 | 3.58364 | YES | YES |
| 27 | e | 223.95 | 3.58364 | YES | YES |
| 28 | a2 | 262.81 | 0.02089 | YES | NO |
| 29 | e | 263.01 | 0.24328 | YES | YES |
| 30 | e | 263.01 | 0.24328 | YES | YES |
| 31 | e | 269.81 | 0.14677 | YES | YES |
| 32 | e | 269.81 | 0.14677 | YES | YES |
| 33 | a1 | 271.07 | 0.00000 | NO | YES |
| 34 | e | 307.44 | 0.06713 | YES | YES |
| 35 | e | 307.44 | 0.06713 | YES | YES |
| 36 | a2 | 307.45 | 1.57146 | YES | NO |
| 37 | e | 340.61 | 2.73309 | YES | YES |
| 38 | e | 340.61 | 2.73309 | YES | YES |
| 39 | a2 | 345.31 | 0.05154 | YES | NO |
| 40 | a1 | 349.72 | 0.00000 | NO | YES |
| 41 | e | 377.20 | 6.46685 | YES | YES |
| 42 | e | 377.20 | 6.46685 | YES | YES |
| 43 | e | 390.68 | 1.32793 | YES | YES |
| 44 | e | 390.68 | 1.32793 | YES | YES |
| 45 | a1 | 391.44 | 0.00000 | NO | YES |
| 46 | a2 | 429.96 | 0.46799 | YES | NO |
| 47 | e | 431.25 | 0.26410 | YES | YES |
| 48 | e | 431.25 | 0.26410 | YES | YES |
| 49 | e | 460.04 | 4.51967 | YES | YES |
| 50 | e | 460.04 | 4.51967 | YES | YES |
| 51 | a1 | 486.24 | 0.00000 | NO | YES |
| 52 | a2 | 493.67 | 0.07742 | YES | NO |
| 53 | e | 505.74 | 0.02409 | YES | YES |
| 54 | e | 505.74 | 0.02409 | YES | YES |
| 55 | a2 | 533.28 | 1.87280 | YES | NO |
| 56 | e | 564.02 | 2.96581 | YES | YES |
| 57 | e | 564.02 | 2.96581 | YES | YES |
| 58 | a1 | 566.58 | 0.00000 | NO | YES |
| 59 | e | 617.53 | 26.76263 | YES | YES |
| 60 | e | 617.53 | 26.76263 | YES | YES |
| 61 | e | 631.38 | 1.83876 | YES | YES |
| 62 | e | 631.38 | 1.83876 | YES | YES |
| 63 | a1 | 633.74 | 0.00000 | NO | YES |
| 64 | e | 664.87 | 24.48621 | YES | YES |
| 65 | e | 664.87 | 24.48621 | YES | YES |
| 66 | a2 | 675.85 | 6.62506 | YES | NO |
| 67 | e | 770.59 | 23.92494 | YES | YES |
| 68 | e | 770.59 | 23.92494 | YES | YES |
| 69 | a2 | 773.30 | 2.69285 | YES | NO |
| 70 | a1 | 855.79 | 0.00000 | NO | YES |
| 71 | a2 | 982.48 | 183.87296 | YES | NO |

| | | | | | |
|---|---|---|---|---|---|
| 72 | e | 984.07 | 64.04209 | YES | YES |
| 73 | e | 984.07 | 64.04209 | YES | YES |
| 74 | e | 1024.00 | 126.53424 | YES | YES |
| 75 | e | 1024.00 | 126.53424 | YES | YES |
| 76 | a1 | 1116.35 | 0.00000 | NO | YES |
| 77 | a2 | 1151.47 | 7.06988 | YES | NO |
| 78 | e | 1154.83 | 14.98724 | YES | YES |
| 79 | e | 1154.83 | 14.98724 | YES | YES |
| 80 | e | 1185.19 | 181.69897 | YES | YES |
| 81 | e | 1185.19 | 181.69897 | YES | YES |
| 82 | a1 | 1302.18 | 0.00000 | NO | YES |
| 83 | e | 1318.04 | 162.25277 | YES | YES |
| 84 | e | 1318.04 | 162.25277 | YES | YES |
| 85 | a2 | 1347.57 | 0.01812 | YES | NO |
| 86 | e | 1351.63 | 6.56530 | YES | YES |
| 87 | e | 1351.63 | 6.56530 | YES | YES |
| 88 | e | 1382.76 | 323.51309 | YES | YES |
| 89 | e | 1382.76 | 323.51309 | YES | YES |
| 90 | a1 | 1399.11 | 0.00000 | NO | YES |
| 91 | a2 | 1472.65 | 456.85941 | YES | NO |
| 92 | e | 1482.35 | 628.43438 | YES | YES |
| 93 | e | 1482.35 | 628.43438 | YES | YES |
| 94 | e | 1518.16 | 241.50454 | YES | YES |
| 95 | e | 1518.16 | 241.50454 | YES | YES |
| 96 | a1 | 1520.14 | 0.00000 | NO | YES |
| 97 | a2 | 1608.75 | 21.07254 | YES | NO |
| 98 | e | 1611.12 | 5.93169 | YES | YES |
| 99 | e | 1611.12 | 5.93169 | YES | YES |
| 100 | e | 1631.96 | 198.22814 | YES | YES |
| 101 | e | 1631.96 | 198.22814 | YES | YES |
| 102 | a1 | 1633.40 | 0.00000 | NO | YES |

$[F\text{-}B(C_6F_5)_3]^-$



Atomic coordinates

| | | | |
|---|---|---|---|
| B | -0.22898 | -0.07327 | -0.90178 |
| C | 0.65568 | -1.37570 | -0.38619 |
| C | -1.74794 | -0.00998 | -0.24435 |
| C | 0.70832 | 1.24821 | -0.51289 |
| C | 0.48745 | 2.16586 | 0.52455 |
| C | 1.34226 | 3.25005 | 0.79472 |
| C | 2.49361 | 3.42987 | 0.01464 |
| C | 2.76868 | 2.52675 | -1.02317 |
| C | 1.88498 | 1.45745 | -1.25334 |

| | | | |
|---|---|---|---|
| C | 1.12093 | -2.40063 | -1.22465 |
| C | 1.94643 | -3.44712 | -0.76632 |
| C | 2.32953 | -3.49130 | 0.58125 |
| C | 1.87839 | -2.49197 | 1.45820 |
| C | 1.06239 | -1.46814 | 0.95423 |
| C | -2.54643 | 1.11597 | -0.51065 |
| C | -3.87351 | 1.25225 | -0.07469 |
| C | -4.46199 | 0.20809 | 0.65657 |
| C | -3.71204 | -0.94182 | 0.93655 |
| C | -2.38428 | -1.03144 | 0.47416 |
| F | -0.58363 | 2.05764 | 1.34056 |
| F | 1.07682 | 4.11147 | 1.79706 |
| F | 3.32640 | 4.45983 | 0.25809 |
| F | 3.88068 | 2.68581 | -1.76852 |
| F | 2.23444 | 0.60516 | -2.23798 |
| F | 0.79282 | -2.45131 | -2.52897 |
| F | 2.37146 | -4.41107 | -1.60816 |
| F | 3.11565 | -4.48733 | 1.03321 |
| F | 2.23131 | -2.53336 | 2.75850 |
| F | 0.63950 | -0.54439 | 1.84829 |
| F | -2.04177 | 2.15627 | -1.20686 |
| F | -4.58996 | 2.36090 | -0.34687 |
| F | -5.73503 | 0.31117 | 1.08258 |
| F | -4.27506 | -1.95305 | 1.62769 |
| F | -1.75270 | -2.19056 | 0.76751 |
| F | -0.41443 | -0.10028 | -2.31296 |

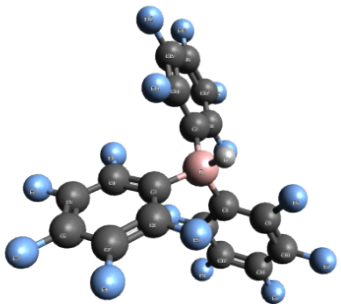
Vibrational analysis

| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 16.74 | 0.00971 | YES | YES |
| 8 | a | 22.68 | 0.03094 | YES | YES |
| 9 | a | 26.55 | 0.00676 | YES | YES |
| 10 | a | 31.42 | 0.00421 | YES | YES |
| 11 | a | 38.20 | 0.09017 | YES | YES |
| 12 | a | 40.18 | 0.02233 | YES | YES |
| 13 | a | 94.70 | 0.18485 | YES | YES |
| 14 | a | 105.12 | 0.15464 | YES | YES |
| 15 | a | 112.02 | 0.08971 | YES | YES |
| 16 | a | 123.02 | 0.03298 | YES | YES |
| 17 | a | 126.03 | 0.03316 | YES | YES |
| 18 | a | 131.28 | 0.17122 | YES | YES |
| 19 | a | 133.05 | 0.02901 | YES | YES |
| 20 | a | 145.05 | 0.18440 | YES | YES |
| 21 | a | 147.57 | 0.10397 | YES | YES |
| 22 | a | 157.25 | 0.01410 | YES | YES |
| 23 | a | 158.57 | 0.08667 | YES | YES |
| 24 | a | 164.28 | 0.08317 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 25 | a | 201.41 | 2.69124 | YES | YES |
| 26 | a | 215.30 | 1.67158 | YES | YES |
| 27 | a | 225.96 | 1.80099 | YES | YES |
| 28 | a | 236.92 | 0.64783 | YES | YES |
| 29 | a | 246.63 | 0.90606 | YES | YES |
| 30 | a | 261.19 | 0.06193 | YES | YES |
| 31 | a | 261.63 | 0.05858 | YES | YES |
| 32 | a | 261.81 | 0.07653 | YES | YES |
| 33 | a | 270.09 | 0.12558 | YES | YES |
| 34 | a | 271.00 | 0.05817 | YES | YES |
| 35 | a | 272.12 | 0.12344 | YES | YES |
| 36 | a | 305.97 | 0.39144 | YES | YES |
| 37 | a | 307.86 | 0.20251 | YES | YES |
| 38 | a | 308.48 | 0.31106 | YES | YES |
| 39 | a | 315.04 | 1.06823 | YES | YES |
| 40 | a | 340.91 | 3.55914 | YES | YES |
| 41 | a | 345.12 | 2.29898 | YES | YES |
| 42 | a | 349.87 | 0.78970 | YES | YES |
| 43 | a | 367.04 | 0.30311 | YES | YES |
| 44 | a | 385.00 | 0.06783 | YES | YES |
| 45 | a | 387.28 | 0.08366 | YES | YES |
| 46 | a | 388.53 | 0.11373 | YES | YES |
| 47 | a | 397.79 | 1.16029 | YES | YES |
| 48 | a | 426.66 | 0.37649 | YES | YES |
| 49 | a | 434.05 | 0.05532 | YES | YES |
| 50 | a | 434.88 | 0.19232 | YES | YES |
| 51 | a | 435.33 | 0.09541 | YES | YES |
| 52 | a | 465.13 | 2.10995 | YES | YES |
| 53 | a | 467.86 | 1.25645 | YES | YES |
| 54 | a | 483.80 | 0.02273 | YES | YES |
| 55 | a | 494.72 | 0.19477 | YES | YES |
| 56 | a | 496.26 | 0.07702 | YES | YES |
| 57 | a | 503.03 | 0.03609 | YES | YES |
| 58 | a | 562.39 | 5.08093 | YES | YES |
| 59 | a | 563.33 | 3.29133 | YES | YES |
| 60 | a | 565.00 | 0.06943 | YES | YES |
| 61 | a | 593.21 | 20.47027 | YES | YES |
| 62 | a | 614.35 | 35.56013 | YES | YES |
| 63 | a | 626.22 | 0.66747 | YES | YES |
| 64 | a | 629.04 | 0.30157 | YES | YES |
| 65 | a | 630.80 | 0.03494 | YES | YES |
| 66 | a | 645.58 | 4.86504 | YES | YES |
| 67 | a | 683.01 | 60.93894 | YES | YES |
| 68 | a | 706.08 | 92.55773 | YES | YES |
| 69 | a | 747.54 | 4.45169 | YES | YES |
| 70 | a | 751.69 | 34.39234 | YES | YES |
| 71 | a | 759.33 | 33.92413 | YES | YES |
| 72 | a | 811.58 | 10.40171 | YES | YES |
| 73 | a | 905.13 | 8.12259 | YES | YES |
| 74 | a | 936.78 | 23.67051 | YES | YES |
| 75 | a | 968.89 | 75.17850 | YES | YES |
| 76 | a | 972.73 | 243.23854 | YES | YES |
| 77 | a | 980.23 | 218.82513 | YES | YES |
| 78 | a | 1029.17 | 5.88795 | YES | YES |
| 79 | a | 1084.21 | 189.02098 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 80 | a | 1087.12 | 109.33459 | YES | YES |
| 81 | a | 1096.23 | 399.25044 | YES | YES |
| 82 | a | 1124.08 | 2.12866 | YES | YES |
| 83 | a | 1129.41 | 3.24181 | YES | YES |
| 84 | a | 1132.96 | 2.42007 | YES | YES |
| 85 | a | 1262.04 | 45.30432 | YES | YES |
| 86 | a | 1265.08 | 57.75380 | YES | YES |
| 87 | a | 1266.75 | 39.83310 | YES | YES |
| 88 | a | 1349.56 | 5.80585 | YES | YES |
| 89 | a | 1352.56 | 5.39959 | YES | YES |
| 90 | a | 1354.51 | 1.38633 | YES | YES |
| 91 | a | 1370.03 | 23.24218 | YES | YES |
| 92 | a | 1376.71 | 18.58981 | YES | YES |
| 93 | a | 1385.46 | 0.31978 | YES | YES |
| 94 | a | 1455.43 | 219.96879 | YES | YES |
| 95 | a | 1465.45 | 328.57673 | YES | YES |
| 96 | a | 1469.75 | 749.70441 | YES | YES |
| 97 | a | 1504.21 | 172.36132 | YES | YES |
| 98 | a | 1505.68 | 247.07692 | YES | YES |
| 99 | a | 1508.45 | 23.85032 | YES | YES |
| 100 | a | 1614.26 | 6.97706 | YES | YES |
| 101 | a | 1616.05 | 8.81057 | YES | YES |
| 102 | a | 1617.86 | 3.16168 | YES | YES |
| 103 | a | 1622.03 | 48.57268 | YES | YES |
| 104 | a | 1624.77 | 49.14303 | YES | YES |
| 105 | a | 1626.74 | 12.58045 | YES | YES |

$[H\text{-}B(C_6F_5)_3]^-$



Atomic coordinates

| | | | |
|---|---|---|---|
| B | -0.16240 | -0.07625 | -0.78713 |
| C | 0.69245 | -1.38524 | -0.30467 |
| C | -1.69811 | -0.00872 | -0.23284 |
| C | 0.72744 | 1.25840 | -0.44325 |
| C | 0.48189 | 2.17877 | 0.58787 |
| C | 1.28864 | 3.30555 | 0.82958 |
| C | 2.41721 | 3.52972 | 0.02736 |
| C | 2.71381 | 2.62989 | -1.00813 |
| C | 1.87397 | 1.52181 | -1.21366 |
| C | 1.00742 | -2.43911 | -1.17603 |
| C | 1.79634 | -3.54154 | -0.79685 |
| C | 2.29985 | -3.61024 | 0.51046 |
| C | 2.00385 | -2.58247 | 1.42027 |
| C | 1.21470 | -1.50270 | 0.99313 |

| | | | |
|---|---|---|---|
| C | -2.51061 | 1.07657 | -0.61109 |
| C | -3.85827 | 1.21443 | -0.24564 |
| C | -4.45817 | 0.21891 | 0.54234 |
| C | -3.69604 | -0.88768 | 0.94019 |
| C | -2.34630 | -0.97878 | 0.54816 |
| F | -0.56973 | 2.02211 | 1.42111 |
| F | 1.00325 | 4.16358 | 1.82995 |
| F | 3.20742 | 4.59917 | 0.24628 |
| F | 3.79856 | 2.83776 | -1.78245 |
| F | 2.22260 | 0.68877 | -2.21800 |
| F | 0.55121 | -2.44881 | -2.44568 |
| F | 2.07523 | -4.53171 | -1.66947 |
| F | 3.05553 | -4.65796 | 0.89338 |
| F | 2.47621 | -2.65217 | 2.68122 |
| F | 0.94097 | -0.55589 | 1.91779 |
| F | -1.99455 | 2.06766 | -1.37210 |
| F | -4.58342 | 2.28176 | -0.63736 |
| F | -5.75152 | 0.32492 | 0.90617 |
| F | -4.26389 | -1.85159 | 1.69334 |
| F | -1.69632 | -2.08635 | 0.97519 |
| H | -0.25921 | -0.12258 | -2.01943 |

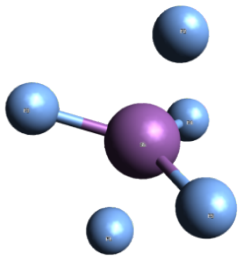
Vibrational analysis

| 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 | 11.40 | 0.00781 | YES | YES |
| 8 | a | 19.58 | 0.01224 | YES | YES |
| 9 | a | 24.07 | 0.01246 | YES | YES |
| 10 | a | 28.61 | 0.01668 | YES | YES |
| 11 | a | 36.95 | 0.01281 | YES | YES |
| 12 | a | 38.25 | 0.09055 | YES | YES |
| 13 | a | 96.85 | 0.16457 | YES | YES |
| 14 | a | 102.00 | 0.06658 | YES | YES |
| 15 | a | 111.70 | 0.08953 | YES | YES |
| 16 | a | 123.83 | 0.01042 | YES | YES |
| 17 | a | 124.69 | 0.00284 | YES | YES |
| 18 | a | 129.59 | 0.00716 | YES | YES |
| 19 | a | 132.89 | 0.03931 | YES | YES |
| 20 | a | 144.54 | 0.12206 | YES | YES |
| 21 | a | 146.81 | 0.02650 | YES | YES |
| 22 | a | 157.76 | 0.02121 | YES | YES |
| 23 | a | 160.38 | 0.01506 | YES | YES |
| 24 | a | 163.82 | 0.04614 | YES | YES |
| 25 | a | 218.10 | 1.52328 | YES | YES |
| 26 | a | 219.32 | 1.21943 | YES | YES |
| 27 | a | 227.97 | 1.81053 | YES | YES |
| 28 | a | 260.64 | 0.02972 | YES | YES |
| 29 | a | 260.86 | 0.03173 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 30 | a | 261.38 | 0.03451 | YES | YES |
| 31 | a | 268.32 | 0.06824 | YES | YES |
| 32 | a | 269.84 | 0.04760 | YES | YES |
| 33 | a | 271.14 | 0.06670 | YES | YES |
| 34 | a | 304.11 | 0.36433 | YES | YES |
| 35 | a | 305.68 | 0.86366 | YES | YES |
| 36 | a | 307.60 | 0.30772 | YES | YES |
| 37 | a | 333.93 | 0.25530 | YES | YES |
| 38 | a | 337.78 | 1.73722 | YES | YES |
| 39 | a | 338.98 | 2.25438 | YES | YES |
| 40 | a | 351.58 | 0.19553 | YES | YES |
| 41 | a | 359.15 | 0.89434 | YES | YES |
| 42 | a | 379.01 | 0.09106 | YES | YES |
| 43 | a | 386.37 | 0.05820 | YES | YES |
| 44 | a | 387.44 | 0.30900 | YES | YES |
| 45 | a | 388.46 | 0.05406 | YES | YES |
| 46 | a | 433.02 | 0.01199 | YES | YES |
| 47 | a | 433.63 | 0.05768 | YES | YES |
| 48 | a | 434.40 | 0.14924 | YES | YES |
| 49 | a | 453.74 | 1.48491 | YES | YES |
| 50 | a | 455.31 | 1.64226 | YES | YES |
| 51 | a | 470.34 | 0.00919 | YES | YES |
| 52 | a | 492.61 | 0.04975 | YES | YES |
| 53 | a | 496.54 | 0.00668 | YES | YES |
| 54 | a | 505.75 | 0.07610 | YES | YES |
| 55 | a | 529.85 | 0.85258 | YES | YES |
| 56 | a | 560.01 | 5.52809 | YES | YES |
| 57 | a | 561.16 | 4.53377 | YES | YES |
| 58 | a | 564.53 | 0.06618 | YES | YES |
| 59 | a | 584.69 | 8.93178 | YES | YES |
| 60 | a | 592.69 | 11.97998 | YES | YES |
| 61 | a | 624.57 | 0.20766 | YES | YES |
| 62 | a | 626.40 | 0.62963 | YES | YES |
| 63 | a | 630.10 | 0.39271 | YES | YES |
| 64 | a | 644.50 | 25.36682 | YES | YES |
| 65 | a | 663.25 | 3.19942 | YES | YES |
| 66 | a | 688.37 | 34.13539 | YES | YES |
| 67 | a | 740.26 | 11.95791 | YES | YES |
| 68 | a | 755.28 | 13.45912 | YES | YES |
| 69 | a | 769.22 | 1.85668 | YES | YES |
| 70 | a | 835.32 | 3.21874 | YES | YES |
| 71 | a | 889.21 | 69.88553 | YES | YES |
| 72 | a | 909.35 | 108.07630 | YES | YES |
| 73 | a | 960.34 | 93.63068 | YES | YES |
| 74 | a | 971.86 | 260.94870 | YES | YES |
| 75 | a | 976.72 | 189.66353 | YES | YES |
| 76 | a | 1028.69 | 8.59580 | YES | YES |
| 77 | a | 1042.63 | 58.79993 | YES | YES |
| 78 | a | 1080.39 | 18.51629 | YES | YES |
| 79 | a | 1094.39 | 178.35320 | YES | YES |
| 80 | a | 1108.35 | 235.26091 | YES | YES |
| 81 | a | 1123.57 | 3.97248 | YES | YES |
| 82 | a | 1127.94 | 5.78757 | YES | YES |
| 83 | a | 1129.80 | 6.42974 | YES | YES |
| 84 | a | 1262.04 | 30.99396 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 85 | a | 1263.10 | 7.40646 | YES | YES |
| 86 | a | 1265.25 | 46.34944 | YES | YES |
| 87 | a | 1350.00 | 13.19832 | YES | YES |
| 88 | a | 1353.29 | 6.24188 | YES | YES |
| 89 | a | 1354.49 | 1.84392 | YES | YES |
| 90 | a | 1375.78 | 13.19973 | YES | YES |
| 91 | a | 1380.20 | 3.46623 | YES | YES |
| 92 | a | 1384.98 | 4.31574 | YES | YES |
| 93 | a | 1458.68 | 309.41682 | YES | YES |
| 94 | a | 1465.98 | 253.77436 | YES | YES |
| 95 | a | 1469.56 | 548.85500 | YES | YES |
| 96 | a | 1501.21 | 223.58684 | YES | YES |
| 97 | a | 1502.48 | 304.66458 | YES | YES |
| 98 | a | 1506.01 | 30.78507 | YES | YES |
| 99 | a | 1612.36 | 3.26708 | YES | YES |
| 100 | a | 1615.05 | 4.03735 | YES | YES |
| 101 | a | 1615.76 | 5.68092 | YES | YES |
| 102 | a | 1620.56 | 27.54753 | YES | YES |
| 103 | a | 1622.47 | 26.41400 | YES | YES |
| 104 | a | 1624.25 | 5.55063 | YES | YES |
| 105 | a | 2392.69 | 84.22793 | YES | YES |

$SbF_5$



Atomic coordinates

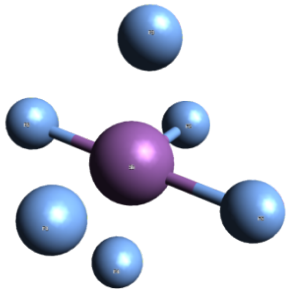
| | | | |
|---|---|---|---|
| Sb | -0.00000 | 0.00000 | 0.00000 |
| F | 0.00000 | 0.00000 | -1.92422 |
| F | 0.00000 | 0.00000 | 1.92422 |
| F | -0.95686 | -1.65733 | 0.00000 |
| F | -0.95686 | 1.65733 | 0.00000 |
| F | 1.91372 | 0.00000 | 0.00000 |

Vibrational analysis

| 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 | e' | 91.81 | 0.61255 | YES | YES |
| 8 | e' | 91.81 | 0.61255 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 9 | e' | 236.60 | 40.54739 | YES | YES |
| 10 | e' | 236.60 | 40.54739 | YES | YES |
| 11 | e" | 246.90 | 0.00000 | NO | YES |
| 12 | e" | 246.90 | 0.00000 | NO | YES |
| 13 | a2" | 259.74 | 41.65984 | YES | NO |
| 14 | a1' | 597.49 | 0.00000 | NO | YES |
| 15 | a1' | 603.26 | 0.00000 | NO | YES |
| 16 | a2" | 663.38 | 73.29589 | YES | NO |
| 17 | e' | 666.88 | 65.05131 | YES | YES |
| 18 | e' | 666.88 | 65.05131 | YES | YES |

$[SbF_6]^-$



Atomic coordinates

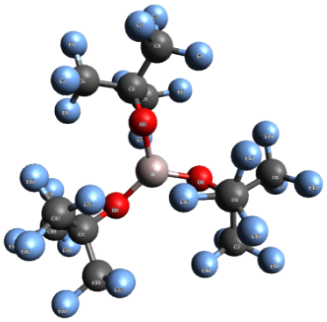
| | | | |
|---|---|---|---|
| Sb | -0.00000 | 0.00000 | 0.00000 |
| F | 1.38218 | -1.38218 | -0.00000 |
| F | -1.38218 | 1.38218 | -0.00000 |
| F | 0.00000 | 0.00000 | 1.95575 |
| F | 0.00000 | 0.00000 | -1.95575 |
| F | 1.38218 | 1.38218 | -0.00000 |
| F | -1.38218 | -1.38218 | -0.00000 |

Vibrational analysis

| 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 | e | 148.50 | 0.06118 | YES | YES |
| 8 | e | 148.50 | 0.06118 | YES | YES |
| 9 | b2 | 150.46 | 0.00000 | NO | YES |
| 10 | e | 244.82 | 0.00000 | YES | YES |
| 11 | e | 244.82 | 0.00000 | YES | YES |
| 12 | b1 | 248.29 | 0.00000 | NO | YES |
| 13 | e | 268.66 | 53.77941 | YES | YES |
| 14 | e | 268.66 | 53.77941 | YES | YES |
| 15 | a1 | 270.08 | 53.71609 | YES | YES |
| 16 | a1 | 551.14 | 0.00000 | YES | YES |
| 17 | b2 | 551.58 | 0.00000 | NO | YES |
| 18 | a1 | 568.35 | 0.00000 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 19 | a1 | 616.56 | 114.51528 | YES | YES |
| 20 | e | 617.28 | 114.38467 | YES | YES |
| 21 | e | 617.28 | 114.38467 | YES | YES |

$Al(OR^F)_3$



Atomic coordinates

| | | | |
|---|---|---|---|
| Al | 0.12634 | -0.02702 | 0.17021 |
| O | 1.78305 | 0.07559 | 0.75076 |
| O | -0.84295 | 1.38409 | 0.27881 |
| O | -0.46148 | -1.61339 | -0.29868 |
| C | -0.98357 | -2.53448 | 0.57299 |
| C | 2.86539 | 0.30165 | -0.05731 |
| C | -1.76216 | 2.17694 | -0.34843 |
| C | -0.44248 | -3.95828 | 0.19021 |
| F | 0.87717 | -3.90046 | -0.04033 |
| F | -1.04467 | -4.41104 | -0.92048 |
| F | -0.66768 | -4.84034 | 1.18899 |
| C | -0.53210 | -2.18764 | 2.04287 |
| F | -1.38106 | -2.52547 | 2.99967 |
| F | -0.42434 | -0.76476 | 2.08489 |
| F | 0.68113 | -2.64036 | 2.33996 |
| C | -2.55389 | -2.49732 | 0.48501 |
| F | -2.94446 | -2.49182 | -0.79212 |
| F | -3.00382 | -1.36207 | 1.06787 |
| F | -3.11960 | -3.54646 | 1.11095 |
| C | 3.25262 | 1.82566 | 0.00414 |
| F | 2.32737 | 2.54643 | -0.67156 |
| F | 4.45717 | 2.06374 | -0.54806 |
| F | 3.26262 | 2.24811 | 1.27066 |
| C | 4.06202 | -0.59131 | 0.43035 |
| F | 5.03070 | -0.64715 | -0.51084 |
| F | 3.63381 | -1.83720 | 0.67778 |
| F | 4.59319 | -0.09546 | 1.55847 |
| C | 2.50225 | -0.09002 | -1.53873 |
| F | 1.10153 | 0.19631 | -1.67383 |
| F | 2.61273 | -1.38979 | -1.78317 |
| F | 3.11136 | 0.59848 | -2.48790 |
| C | -2.82195 | 2.63493 | 0.71908 |
| F | -3.91366 | 3.16225 | 0.12978 |
| F | -2.29677 | 3.56112 | 1.54201 |
| F | -3.20250 | 1.58737 | 1.46743 |
| C | -1.01676 | 3.42856 | -0.94349 |
| F | -1.87188 | 4.39996 | -1.31011 |

| | | | |
|---|---|---|---|
| F | -0.30354 | 3.05691 | -2.03202 |
| F | -0.15971 | 3.92881 | -0.04455 |
| C | -2.48204 | 1.38981 | -1.50648 |
| F | -1.56944 | 0.61690 | -2.14724 |
| F | -3.05118 | 2.20222 | -2.40830 |
| F | -3.42679 | 0.56598 | -1.01927 |

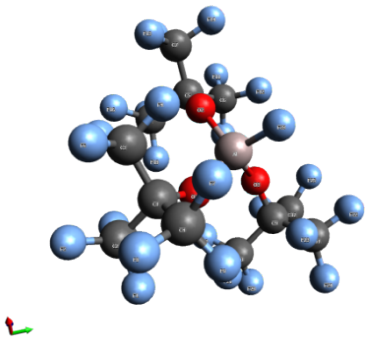
Vibrational analysis

| 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 | 18.74 | 0.04076 | YES | YES |
| 8 | a | 23.10 | 0.02245 | YES | YES |
| 9 | a | 24.03 | 0.03849 | YES | YES |
| 10 | a | 26.29 | 0.03613 | YES | YES |
| 11 | a | 28.94 | 0.02549 | YES | YES |
| 12 | a | 37.32 | 0.00794 | YES | YES |
| 13 | a | 43.29 | 0.11897 | YES | YES |
| 14 | a | 60.29 | 1.05660 | YES | YES |
| 15 | a | 63.49 | 0.06219 | YES | YES |
| 16 | a | 64.47 | 0.19701 | YES | YES |
| 17 | a | 66.55 | 0.01455 | YES | YES |
| 18 | a | 69.56 | 0.08257 | YES | YES |
| 19 | a | 75.54 | 0.11595 | YES | YES |
| 20 | a | 77.31 | 0.22796 | YES | YES |
| 21 | a | 79.96 | 1.28430 | YES | YES |
| 22 | a | 86.82 | 0.63740 | YES | YES |
| 23 | a | 91.82 | 0.69710 | YES | YES |
| 24 | a | 99.86 | 0.19143 | YES | YES |
| 25 | a | 106.89 | 0.02967 | YES | YES |
| 26 | a | 111.37 | 1.05316 | YES | YES |
| 27 | a | 135.01 | 2.53377 | YES | YES |
| 28 | a | 149.78 | 3.04633 | YES | YES |
| 29 | a | 155.61 | 0.76361 | YES | YES |
| 30 | a | 156.76 | 0.68852 | YES | YES |
| 31 | a | 159.87 | 0.10534 | YES | YES |
| 32 | a | 162.98 | 1.62117 | YES | YES |
| 33 | a | 166.59 | 0.62736 | YES | YES |
| 34 | a | 186.06 | 5.84518 | YES | YES |
| 35 | a | 189.37 | 15.42632 | YES | YES |
| 36 | a | 203.07 | 88.02604 | YES | YES |
| 37 | a | 216.66 | 0.01407 | YES | YES |
| 38 | a | 262.77 | 1.69903 | YES | YES |
| 39 | a | 269.61 | 1.36239 | YES | YES |
| 40 | a | 272.68 | 4.40420 | YES | YES |
| 41 | a | 281.68 | 4.46958 | YES | YES |
| 42 | a | 285.65 | 0.33372 | YES | YES |
| 43 | a | 286.84 | 9.47569 | YES | YES |
| 44 | a | 288.23 | 1.52253 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 45 | a | 297.41 | 0.45117 | YES | YES |
| 46 | a | 300.02 | 15.63770 | YES | YES |
| 47 | a | 303.93 | 22.84447 | YES | YES |
| 48 | a | 308.21 | 7.19096 | YES | YES |
| 49 | a | 313.75 | 0.58299 | YES | YES |
| 50 | a | 316.24 | 1.70143 | YES | YES |
| 51 | a | 318.46 | 6.48519 | YES | YES |
| 52 | a | 323.62 | 3.62754 | YES | YES |
| 53 | a | 326.68 | 0.12902 | YES | YES |
| 54 | a | 335.97 | 4.69452 | YES | YES |
| 55 | a | 339.29 | 6.19669 | YES | YES |
| 56 | a | 346.83 | 6.92827 | YES | YES |
| 57 | a | 354.20 | 7.50642 | YES | YES |
| 58 | a | 369.82 | 3.00604 | YES | YES |
| 59 | a | 374.20 | 15.71110 | YES | YES |
| 60 | a | 400.43 | 39.16739 | YES | YES |
| 61 | a | 438.76 | 27.40306 | YES | YES |
| 62 | a | 470.39 | 2.16195 | YES | YES |
| 63 | a | 478.35 | 1.18688 | YES | YES |
| 64 | a | 502.49 | 4.80907 | YES | YES |
| 65 | a | 506.19 | 9.41010 | YES | YES |
| 66 | a | 517.24 | 4.16070 | YES | YES |
| 67 | a | 517.89 | 4.89544 | YES | YES |
| 68 | a | 518.66 | 7.74224 | YES | YES |
| 69 | a | 521.56 | 5.03377 | YES | YES |
| 70 | a | 522.63 | 4.04887 | YES | YES |
| 71 | a | 523.10 | 0.64996 | YES | YES |
| 72 | a | 523.91 | 2.22491 | YES | YES |
| 73 | a | 533.23 | 0.44622 | YES | YES |
| 74 | a | 549.94 | 2.44190 | YES | YES |
| 75 | a | 550.93 | 1.76472 | YES | YES |
| 76 | a | 551.45 | 1.17453 | YES | YES |
| 77 | a | 552.00 | 0.67722 | YES | YES |
| 78 | a | 554.62 | 0.54252 | YES | YES |
| 79 | a | 557.31 | 0.59010 | YES | YES |
| 80 | a | 588.08 | 45.96212 | YES | YES |
| 81 | a | 600.08 | 31.02718 | YES | YES |
| 82 | a | 695.99 | 30.62335 | YES | YES |
| 83 | a | 698.90 | 36.06275 | YES | YES |
| 84 | a | 707.99 | 26.79940 | YES | YES |
| 85 | a | 708.57 | 33.04617 | YES | YES |
| 86 | a | 709.94 | 10.65241 | YES | YES |
| 87 | a | 710.67 | 51.91885 | YES | YES |
| 88 | a | 714.41 | 15.43531 | YES | YES |
| 89 | a | 733.01 | 6.35216 | YES | YES |
| 90 | a | 740.49 | 1.46777 | YES | YES |
| 91 | a | 775.89 | 3.59208 | YES | YES |
| 92 | a | 842.04 | 44.12147 | YES | YES |
| 93 | a | 884.63 | 25.85356 | YES | YES |
| 94 | a | 896.78 | 197.61231 | YES | YES |
| 95 | a | 909.80 | 265.41453 | YES | YES |
| 96 | a | 963.02 | 63.89741 | YES | YES |
| 97 | a | 966.69 | 149.65345 | YES | YES |
| 98 | a | 971.44 | 125.27107 | YES | YES |
| 99 | a | 972.85 | 254.16031 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 100 | a | 1035.94 | 35.83706 | YES | YES |
| 101 | a | 1040.79 | 57.54039 | YES | YES |
| 102 | a | 1106.22 | 1.48454 | YES | YES |
| 103 | a | 1140.79 | 5.98620 | YES | YES |
| 104 | a | 1143.08 | 29.38634 | YES | YES |
| 105 | a | 1156.50 | 17.47458 | YES | YES |
| 106 | a | 1164.52 | 13.66258 | YES | YES |
| 107 | a | 1164.90 | 41.31380 | YES | YES |
| 108 | a | 1170.36 | 23.79844 | YES | YES |
| 109 | a | 1177.34 | 289.85908 | YES | YES |
| 110 | a | 1182.65 | 68.77437 | YES | YES |
| 111 | a | 1187.19 | 15.55794 | YES | YES |
| 112 | a | 1202.91 | 19.00765 | YES | YES |
| 113 | a | 1206.69 | 103.81777 | YES | YES |
| 114 | a | 1208.97 | 100.24123 | YES | YES |
| 115 | a | 1217.35 | 35.78669 | YES | YES |
| 116 | a | 1222.20 | 641.14265 | YES | YES |
| 117 | a | 1224.16 | 319.43051 | YES | YES |
| 118 | a | 1226.02 | 657.28022 | YES | YES |
| 119 | a | 1228.42 | 519.07935 | YES | YES |
| 120 | a | 1248.14 | 179.33566 | YES | YES |
| 121 | a | 1256.38 | 202.08105 | YES | YES |
| 122 | a | 1262.55 | 481.28262 | YES | YES |
| 123 | a | 1270.73 | 775.47830 | YES | YES |
| 124 | a | 1273.30 | 260.12141 | YES | YES |
| 125 | a | 1291.04 | 929.10954 | YES | YES |
| 126 | a | 1298.94 | 189.41464 | YES | YES |
| 127 | a | 1305.49 | 19.12762 | YES | YES |
| 128 | a | 1306.92 | 23.61437 | YES | YES |
| 129 | a | 1337.88 | 143.68836 | YES | YES |

$[F\text{-}Al(OR^F)_3]^-$



Atomic coordinates

| | | | |
|---|---|---|---|
| O | 0.44082 | -0.46646 | -1.39941 |
| C | 1.12091 | -1.36165 | -2.14177 |
| C | 0.20130 | -2.62441 | -2.34283 |
| F | -0.77825 | -2.36914 | -3.23744 |
| F | 0.89347 | -3.70043 | -2.79768 |
| F | -0.38235 | -2.96841 | -1.18639 |
| C | 2.45805 | -1.80797 | -1.43814 |
| F | 3.10152 | -0.73392 | -0.94674 |
| F | 2.20640 | -2.64278 | -0.41034 |
| F | 3.30531 | -2.44424 | -2.28472 |

| | | | |
|---|---|---|---|
| C | 1.46187 | -0.73722 | -3.54903 |
| F | 2.49749 | 0.12452 | -3.45141 |
| F | 1.79939 | -1.67717 | -4.46917 |
| F | 0.40972 | -0.05539 | -4.02543 |
| O | 1.34859 | 0.13100 | 1.26947 |
| C | 1.14709 | -0.18196 | 2.56180 |
| C | 0.25997 | 0.89640 | 3.30301 |
| F | -1.05309 | 0.68890 | 3.08358 |
| F | 0.44838 | 0.88063 | 4.64847 |
| F | 0.56619 | 2.12658 | 2.86047 |
| C | 2.55982 | -0.24305 | 3.25667 |
| F | 3.43985 | -0.89430 | 2.48138 |
| F | 3.04129 | 1.00434 | 3.45913 |
| F | 2.52661 | -0.86897 | 4.46001 |
| C | 0.44787 | -1.58850 | 2.68098 |
| F | 1.31746 | -2.58378 | 2.40084 |
| F | -0.04284 | -1.81954 | 3.92549 |
| F | -0.56838 | -1.67884 | 1.81024 |
| O | -1.00707 | 1.33352 | 0.21885 |
| C | -2.18317 | 1.64696 | -0.36150 |
| C | -2.93725 | 0.34676 | -0.84907 |
| F | -2.79388 | -0.63727 | 0.04983 |
| F | -4.26857 | 0.56124 | -1.02330 |
| F | -2.44634 | -0.09124 | -2.02567 |
| C | -1.97621 | 2.60857 | -1.59096 |
| F | -1.64387 | 3.85091 | -1.17902 |
| F | -0.97555 | 2.15729 | -2.36765 |
| F | -3.08426 | 2.71692 | -2.36422 |
| C | -3.06708 | 2.37696 | 0.71886 |
| F | -2.33765 | 3.27782 | 1.39378 |
| F | -4.12438 | 3.02859 | 0.17041 |
| F | -3.55836 | 1.49306 | 1.61416 |
| F | 1.59146 | 2.10716 | -0.72932 |
| Al | 0.63772 | 0.81850 | -0.19620 |

Vibrational analysis

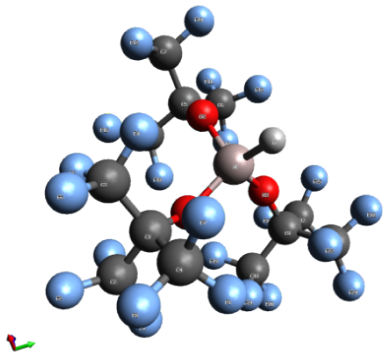
| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 10.11 | 0.05188 | YES | YES |
| 8 | a | 11.87 | 0.01513 | YES | YES |
| 9 | a | 13.87 | 0.00826 | YES | YES |
| 10 | a | 17.15 | 0.01773 | YES | YES |
| 11 | a | 23.78 | 0.24360 | YES | YES |
| 12 | a | 26.18 | 0.03809 | YES | YES |
| 13 | a | 31.68 | 0.07018 | YES | YES |
| 14 | a | 44.14 | 0.03883 | YES | YES |
| 15 | a | 57.02 | 0.11397 | YES | YES |
| 16 | a | 63.74 | 0.02799 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 17 | a | 66.28 | 0.25133 | YES | YES |
| 18 | a | 67.78 | 0.07023 | YES | YES |
| 19 | a | 70.30 | 0.01740 | YES | YES |
| 20 | a | 72.68 | 0.13673 | YES | YES |
| 21 | a | 75.70 | 0.12235 | YES | YES |
| 22 | a | 80.71 | 0.03444 | YES | YES |
| 23 | a | 82.22 | 0.01401 | YES | YES |
| 24 | a | 84.01 | 0.20217 | YES | YES |
| 25 | a | 88.93 | 0.38712 | YES | YES |
| 26 | a | 92.54 | 0.24913 | YES | YES |
| 27 | a | 99.00 | 0.37325 | YES | YES |
| 28 | a | 136.39 | 1.37007 | YES | YES |
| 29 | a | 140.94 | 0.63843 | YES | YES |
| 30 | a | 148.93 | 0.30736 | YES | YES |
| 31 | a | 156.50 | 0.27719 | YES | YES |
| 32 | a | 157.68 | 0.19378 | YES | YES |
| 33 | a | 161.63 | 0.22148 | YES | YES |
| 34 | a | 166.35 | 1.84618 | YES | YES |
| 35 | a | 167.99 | 0.92914 | YES | YES |
| 36 | a | 186.74 | 1.21944 | YES | YES |
| 37 | a | 195.27 | 7.14382 | YES | YES |
| 38 | a | 200.19 | 6.75326 | YES | YES |
| 39 | a | 236.65 | 0.27237 | YES | YES |
| 40 | a | 262.22 | 1.68075 | YES | YES |
| 41 | a | 270.75 | 0.53623 | YES | YES |
| 42 | a | 275.32 | 3.35599 | YES | YES |
| 43 | a | 277.62 | 4.34264 | YES | YES |
| 44 | a | 280.45 | 3.96430 | YES | YES |
| 45 | a | 283.51 | 0.18532 | YES | YES |
| 46 | a | 283.87 | 0.09570 | YES | YES |
| 47 | a | 284.34 | 0.14518 | YES | YES |
| 48 | a | 289.26 | 3.93202 | YES | YES |
| 49 | a | 303.66 | 9.82295 | YES | YES |
| 50 | a | 304.62 | 9.97936 | YES | YES |
| 51 | a | 308.69 | 0.14747 | YES | YES |
| 52 | a | 314.53 | 0.22511 | YES | YES |
| 53 | a | 317.76 | 0.68170 | YES | YES |
| 54 | a | 319.56 | 1.30904 | YES | YES |
| 55 | a | 321.83 | 2.86866 | YES | YES |
| 56 | a | 322.95 | 2.69760 | YES | YES |
| 57 | a | 327.49 | 0.17329 | YES | YES |
| 58 | a | 343.17 | 0.83189 | YES | YES |
| 59 | a | 353.25 | 4.65556 | YES | YES |
| 60 | a | 356.38 | 9.43498 | YES | YES |
| 61 | a | 363.84 | 28.97129 | YES | YES |
| 62 | a | 369.37 | 26.55365 | YES | YES |
| 63 | a | 407.56 | 10.86083 | YES | YES |
| 64 | a | 449.09 | 65.33209 | YES | YES |
| 65 | a | 452.31 | 56.09370 | YES | YES |
| 66 | a | 515.91 | 0.38248 | YES | YES |
| 67 | a | 516.61 | 4.01766 | YES | YES |
| 68 | a | 517.28 | 5.37347 | YES | YES |
| 69 | a | 517.65 | 4.78778 | YES | YES |
| 70 | a | 519.16 | 4.90209 | YES | YES |
| 71 | a | 519.41 | 5.58407 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 72 | a | 519.67 | 5.84670 | YES | YES |
| 73 | a | 522.97 | 1.92894 | YES | YES |
| 74 | a | 523.19 | 2.62390 | YES | YES |
| 75 | a | 526.87 | 0.19124 | YES | YES |
| 76 | a | 547.60 | 20.50946 | YES | YES |
| 77 | a | 549.04 | 20.76864 | YES | YES |
| 78 | a | 551.87 | 1.37550 | YES | YES |
| 79 | a | 553.00 | 0.33981 | YES | YES |
| 80 | a | 553.06 | 0.60566 | YES | YES |
| 81 | a | 554.52 | 0.16412 | YES | YES |
| 82 | a | 556.88 | 24.16976 | YES | YES |
| 83 | a | 559.86 | 27.36268 | YES | YES |
| 84 | a | 705.31 | 4.39604 | YES | YES |
| 85 | a | 705.62 | 2.43967 | YES | YES |
| 86 | a | 706.03 | 9.54257 | YES | YES |
| 87 | a | 706.96 | 62.49001 | YES | YES |
| 88 | a | 707.77 | 59.75348 | YES | YES |
| 89 | a | 708.25 | 66.87308 | YES | YES |
| 90 | a | 716.98 | 5.09569 | YES | YES |
| 91 | a | 734.21 | 6.69308 | YES | YES |
| 92 | a | 734.62 | 6.34880 | YES | YES |
| 93 | a | 760.18 | 11.91838 | YES | YES |
| 94 | a | 811.65 | 31.94216 | YES | YES |
| 95 | a | 817.21 | 32.46202 | YES | YES |
| 96 | a | 849.91 | 57.29140 | YES | YES |
| 97 | a | 953.43 | 31.73135 | YES | YES |
| 98 | a | 955.22 | 44.61639 | YES | YES |
| 99 | a | 958.18 | 55.46450 | YES | YES |
| 100 | a | 959.95 | 239.22036 | YES | YES |
| 101 | a | 963.94 | 297.27867 | YES | YES |
| 102 | a | 964.32 | 208.24046 | YES | YES |
| 103 | a | 1103.99 | 11.24707 | YES | YES |
| 104 | a | 1105.45 | 10.36676 | YES | YES |
| 105 | a | 1110.91 | 3.16486 | YES | YES |
| 106 | a | 1124.61 | 3.75704 | YES | YES |
| 107 | a | 1127.05 | 25.82396 | YES | YES |
| 108 | a | 1129.38 | 2.92069 | YES | YES |
| 109 | a | 1130.88 | 12.78537 | YES | YES |
| 110 | a | 1132.87 | 28.97947 | YES | YES |
| 111 | a | 1135.04 | 13.96048 | YES | YES |
| 112 | a | 1190.74 | 11.99196 | YES | YES |
| 113 | a | 1193.97 | 25.58747 | YES | YES |
| 114 | a | 1195.76 | 40.85179 | YES | YES |
| 115 | a | 1201.16 | 39.65866 | YES | YES |
| 116 | a | 1204.42 | 10.38482 | YES | YES |
| 117 | a | 1206.26 | 38.16633 | YES | YES |
| 118 | a | 1214.16 | 886.79886 | YES | YES |
| 119 | a | 1216.15 | 1152.43123 | YES | YES |
| 120 | a | 1227.50 | 452.42724 | YES | YES |
| 121 | a | 1228.70 | 297.45653 | YES | YES |
| 122 | a | 1232.78 | 66.79091 | YES | YES |
| 123 | a | 1234.75 | 158.19286 | YES | YES |
| 124 | a | 1240.55 | 100.89622 | YES | YES |
| 125 | a | 1244.44 | 82.61423 | YES | YES |
| 126 | a | 1248.82 | 400.00465 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 127 | a | 1253.51 | 492.20381 | YES | YES |
| 128 | a | 1255.56 | 595.02304 | YES | YES |
| 129 | a | 1262.07 | 786.56683 | YES | YES |
| 130 | a | 1334.22 | 227.39354 | YES | YES |
| 131 | a | 1340.54 | 270.74734 | YES | YES |
| 132 | a | 1359.42 | 92.79016 | YES | YES |

[H-Al(OR$^F$)$_3$]$^-$



Atomic coordinates

| | | | |
|---|---|---|---|
| O | 0.46781 | -0.62916 | -1.21177 |
| C | 1.08292 | -1.47444 | -2.05951 |
| C | 0.15009 | -2.72935 | -2.25184 |
| F | -0.90148 | -2.42880 | -3.04508 |
| F | 0.80201 | -3.77521 | -2.82420 |
| F | -0.33396 | -3.14289 | -1.07303 |
| C | 2.47164 | -1.95188 | -1.48587 |
| F | 3.14682 | -0.90472 | -0.97700 |
| F | 2.30138 | -2.84824 | -0.49287 |
| F | 3.25816 | -2.53098 | -2.42747 |
| C | 1.31949 | -0.78945 | -3.46161 |
| F | 2.37087 | 0.05918 | -3.40810 |
| F | 1.57338 | -1.68722 | -4.44785 |
| F | 0.24240 | -0.07637 | -3.82359 |
| O | 1.41856 | 0.40180 | 1.34380 |
| C | 1.17001 | -0.05719 | 2.58458 |
| C | 0.21337 | 0.91800 | 3.38094 |
| F | -1.07923 | 0.70205 | 3.06616 |
| F | 0.32776 | 0.76740 | 4.72744 |
| F | 0.50401 | 2.19514 | 3.08754 |
| C | 2.55157 | -0.13986 | 3.33783 |
| F | 3.48860 | -0.68697 | 2.54816 |
| F | 2.98062 | 1.09721 | 3.67930 |
| F | 2.48908 | -0.87655 | 4.47545 |
| C | 0.51778 | -1.49088 | 2.55023 |
| F | 1.43318 | -2.42656 | 2.21605 |
| F | -0.00659 | -1.84981 | 3.75063 |
| F | -0.46483 | -1.53736 | 1.63975 |
| O | -0.94091 | 1.40467 | 0.14084 |
| C | -2.13585 | 1.68326 | -0.41374 |
| C | -2.80433 | 0.39367 | -1.03612 |
| F | -2.61622 | -0.66415 | -0.23678 |
| F | -4.14442 | 0.54693 | -1.21437 |
| F | -2.27346 | 0.10634 | -2.24213 |

| | | | |
|---|---|---|---|
| C | -1.99099 | 2.77431 | -1.54145 |
| F | -1.73732 | 3.98831 | -1.00339 |
| F | -0.96137 | 2.47198 | -2.35380 |
| F | -3.10111 | 2.89355 | -2.31002 |
| C | -3.07447 | 2.24413 | 0.72173 |
| F | -2.41139 | 3.11897 | 1.49287 |
| F | -4.16839 | 2.87927 | 0.22625 |
| F | -3.51496 | 1.24588 | 1.51727 |
| H | 1.66037 | 1.95332 | -0.90986 |
| Al | 0.71940 | 0.85266 | -0.23536 |

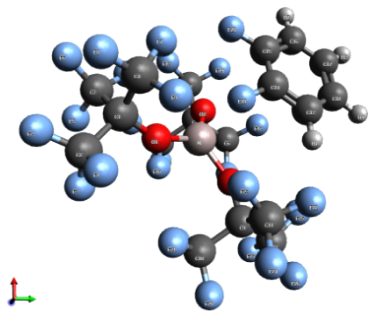
Vibrational analysis

| 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 | 10.75 | 0.01535 | YES | YES |
| 8 | a | 11.13 | 0.01199 | YES | YES |
| 9 | a | 16.70 | 0.00428 | YES | YES |
| 10 | a | 24.79 | 0.05444 | YES | YES |
| 11 | a | 29.36 | 0.09406 | YES | YES |
| 12 | a | 32.04 | 0.13548 | YES | YES |
| 13 | a | 34.07 | 0.09546 | YES | YES |
| 14 | a | 47.33 | 0.07381 | YES | YES |
| 15 | a | 57.02 | 0.08341 | YES | YES |
| 16 | a | 63.83 | 0.15017 | YES | YES |
| 17 | a | 65.22 | 0.05367 | YES | YES |
| 18 | a | 67.54 | 0.06569 | YES | YES |
| 19 | a | 68.49 | 0.00270 | YES | YES |
| 20 | a | 72.17 | 0.17301 | YES | YES |
| 21 | a | 73.56 | 0.08588 | YES | YES |
| 22 | a | 80.63 | 0.04344 | YES | YES |
| 23 | a | 81.95 | 0.07806 | YES | YES |
| 24 | a | 83.95 | 0.00826 | YES | YES |
| 25 | a | 87.64 | 0.15103 | YES | YES |
| 26 | a | 90.88 | 0.39348 | YES | YES |
| 27 | a | 99.28 | 0.50768 | YES | YES |
| 28 | a | 151.26 | 0.10530 | YES | YES |
| 29 | a | 152.77 | 0.07311 | YES | YES |
| 30 | a | 155.08 | 0.04232 | YES | YES |
| 31 | a | 158.55 | 0.31958 | YES | YES |
| 32 | a | 159.93 | 0.71014 | YES | YES |
| 33 | a | 161.18 | 0.30648 | YES | YES |
| 34 | a | 182.93 | 2.73960 | YES | YES |
| 35 | a | 187.32 | 1.97720 | YES | YES |
| 36 | a | 194.42 | 0.36851 | YES | YES |
| 37 | a | 245.97 | 0.22955 | YES | YES |
| 38 | a | 256.96 | 0.48838 | YES | YES |
| 39 | a | 259.36 | 0.97983 | YES | YES |
| 40 | a | 272.36 | 2.94741 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 41 | a | 274.83 | 1.89406 | YES | YES |
| 42 | a | 277.66 | 3.04386 | YES | YES |
| 43 | a | 283.55 | 0.17473 | YES | YES |
| 44 | a | 283.87 | 0.06484 | YES | YES |
| 45 | a | 284.16 | 0.05268 | YES | YES |
| 46 | a | 297.59 | 5.48984 | YES | YES |
| 47 | a | 301.39 | 7.12160 | YES | YES |
| 48 | a | 301.58 | 7.99770 | YES | YES |
| 49 | a | 308.13 | 0.25794 | YES | YES |
| 50 | a | 309.63 | 0.47057 | YES | YES |
| 51 | a | 312.29 | 0.08739 | YES | YES |
| 52 | a | 317.53 | 0.97029 | YES | YES |
| 53 | a | 319.47 | 0.74262 | YES | YES |
| 54 | a | 322.21 | 1.74962 | YES | YES |
| 55 | a | 330.06 | 1.21296 | YES | YES |
| 56 | a | 334.55 | 0.62243 | YES | YES |
| 57 | a | 341.88 | 1.39487 | YES | YES |
| 58 | a | 347.87 | 6.72344 | YES | YES |
| 59 | a | 355.56 | 7.69104 | YES | YES |
| 60 | a | 364.26 | 11.24481 | YES | YES |
| 61 | a | 403.78 | 13.44849 | YES | YES |
| 62 | a | 438.36 | 26.03518 | YES | YES |
| 63 | a | 441.35 | 35.17300 | YES | YES |
| 64 | a | 516.50 | 0.64381 | YES | YES |
| 65 | a | 516.66 | 5.26041 | YES | YES |
| 66 | a | 517.27 | 5.54456 | YES | YES |
| 67 | a | 518.14 | 2.63900 | YES | YES |
| 68 | a | 518.72 | 10.71504 | YES | YES |
| 69 | a | 519.20 | 0.88506 | YES | YES |
| 70 | a | 520.48 | 4.30825 | YES | YES |
| 71 | a | 522.43 | 1.22833 | YES | YES |
| 72 | a | 522.53 | 2.13104 | YES | YES |
| 73 | a | 528.74 | 2.54697 | YES | YES |
| 74 | a | 537.38 | 5.15934 | YES | YES |
| 75 | a | 539.95 | 5.94036 | YES | YES |
| 76 | a | 551.84 | 0.21444 | YES | YES |
| 77 | a | 552.05 | 0.72393 | YES | YES |
| 78 | a | 552.95 | 0.36429 | YES | YES |
| 79 | a | 554.08 | 1.07612 | YES | YES |
| 80 | a | 554.23 | 2.05885 | YES | YES |
| 81 | a | 554.99 | 2.37992 | YES | YES |
| 82 | a | 656.54 | 243.67256 | YES | YES |
| 83 | a | 677.73 | 196.37891 | YES | YES |
| 84 | a | 705.12 | 8.38145 | YES | YES |
| 85 | a | 705.60 | 4.51095 | YES | YES |
| 86 | a | 706.62 | 18.00378 | YES | YES |
| 87 | a | 707.27 | 87.13427 | YES | YES |
| 88 | a | 708.09 | 68.22597 | YES | YES |
| 89 | a | 708.47 | 62.63864 | YES | YES |
| 90 | a | 724.43 | 1.03745 | YES | YES |
| 91 | a | 732.27 | 20.53342 | YES | YES |
| 92 | a | 733.09 | 20.61998 | YES | YES |
| 93 | a | 775.94 | 2.11345 | YES | YES |
| 94 | a | 795.05 | 39.58847 | YES | YES |
| 95 | a | 801.09 | 34.82029 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 96 | a | 951.63 | 30.14316 | YES | YES |
| 97 | a | 953.50 | 44.88816 | YES | YES |
| 98 | a | 957.43 | 183.68125 | YES | YES |
| 99 | a | 959.30 | 116.88847 | YES | YES |
| 100 | a | 962.51 | 178.76915 | YES | YES |
| 101 | a | 963.50 | 311.78297 | YES | YES |
| 102 | a | 1102.24 | 12.37235 | YES | YES |
| 103 | a | 1104.06 | 14.02876 | YES | YES |
| 104 | a | 1108.90 | 4.07879 | YES | YES |
| 105 | a | 1120.98 | 5.35831 | YES | YES |
| 106 | a | 1124.57 | 35.45643 | YES | YES |
| 107 | a | 1127.51 | 1.42160 | YES | YES |
| 108 | a | 1128.52 | 7.13866 | YES | YES |
| 109 | a | 1130.95 | 35.34591 | YES | YES |
| 110 | a | 1133.41 | 12.81682 | YES | YES |
| 111 | a | 1189.18 | 17.33315 | YES | YES |
| 112 | a | 1193.97 | 18.82649 | YES | YES |
| 113 | a | 1194.99 | 73.63362 | YES | YES |
| 114 | a | 1198.63 | 19.09107 | YES | YES |
| 115 | a | 1203.13 | 14.88523 | YES | YES |
| 116 | a | 1206.45 | 49.91127 | YES | YES |
| 117 | a | 1212.83 | 894.32629 | YES | YES |
| 118 | a | 1213.43 | 1128.26919 | YES | YES |
| 119 | a | 1226.14 | 375.16996 | YES | YES |
| 120 | a | 1228.12 | 313.40371 | YES | YES |
| 121 | a | 1231.17 | 22.79628 | YES | YES |
| 122 | a | 1233.51 | 273.69972 | YES | YES |
| 123 | a | 1240.17 | 89.81242 | YES | YES |
| 124 | a | 1241.70 | 73.69692 | YES | YES |
| 125 | a | 1247.41 | 441.10575 | YES | YES |
| 126 | a | 1251.96 | 569.71050 | YES | YES |
| 127 | a | 1255.11 | 486.94669 | YES | YES |
| 128 | a | 1262.02 | 721.85106 | YES | YES |
| 129 | a | 1331.24 | 223.02646 | YES | YES |
| 130 | a | 1332.01 | 272.32132 | YES | YES |
| 131 | a | 1348.17 | 72.62193 | YES | YES |
| 132 | a | 1903.33 | 216.97770 | YES | YES |

*o*DFB·AlOR$^{F}_{3}$



Atomic coordinates

| | | | |
|---|---|---|---|
| O | -0.42583 | -1.88011 | -0.92437 |
| C | 0.09429 | -2.98119 | -1.53943 |
| C | -1.09763 | -3.96512 | -1.83189 |

| | | | |
|---|---|---|---|
| F | -1.84683 | -3.50738 | -2.85273 |
| F | -0.65066 | -5.19571 | -2.15536 |
| F | -1.88560 | -4.06686 | -0.75234 |
| C | 1.14566 | -3.67866 | -0.60000 |
| F | 1.95367 | -2.74338 | -0.05847 |
| F | 0.52837 | -4.31442 | 0.41346 |
| F | 1.90904 | -4.56696 | -1.25907 |
| C | 0.78396 | -2.55104 | -2.88547 |
| F | 1.95725 | -1.92916 | -2.62477 |
| F | 1.03156 | -3.59895 | -3.68940 |
| F | 0.00599 | -1.67770 | -3.54606 |
| O | 1.13281 | -0.02870 | 0.96698 |
| C | 1.25161 | -0.05303 | 2.32839 |
| C | 0.66714 | 1.28022 | 2.92958 |
| F | -0.68244 | 1.25060 | 2.88585 |
| F | 1.04409 | 1.47196 | 4.20692 |
| F | 1.07647 | 2.33027 | 2.20021 |
| C | 2.77602 | -0.18025 | 2.67647 |
| F | 3.35049 | -1.12982 | 1.92996 |
| F | 3.40945 | 0.98552 | 2.42481 |
| F | 2.95439 | -0.48468 | 3.97839 |
| C | 0.45937 | -1.28754 | 2.89985 |
| F | 1.16492 | -2.42141 | 2.81976 |
| F | 0.04444 | -1.12626 | 4.15873 |
| F | -0.65603 | -1.45906 | 2.10741 |
| O | -1.55436 | 0.64025 | 0.04534 |
| C | -2.85704 | 0.83206 | -0.31114 |
| C | -3.72061 | -0.44537 | 0.01438 |
| F | -3.34789 | -0.95699 | 1.19961 |
| F | -5.03567 | -0.16570 | 0.06159 |
| F | -3.52476 | -1.39598 | -0.92232 |
| C | -2.95129 | 1.14605 | -1.84966 |
| F | -2.51288 | 2.40413 | -2.10789 |
| F | -2.15856 | 0.30305 | -2.53798 |
| F | -4.20286 | 1.04051 | -2.32070 |
| C | -3.38770 | 2.05759 | 0.52028 |
| F | -2.47392 | 3.04588 | 0.52131 |
| F | -4.53639 | 2.54541 | 0.01260 |
| F | -3.60564 | 1.69944 | 1.79832 |
| Al | -0.18649 | -0.39713 | -0.10923 |
| C | 0.66338 | 3.02498 | -0.99144 |
| H | -0.41268 | 3.01894 | -1.20930 |
| C | 1.40527 | 1.86051 | -1.11490 |
| F | 0.74997 | 0.67041 | -1.51301 |
| C | 2.76723 | 1.76640 | -0.81285 |
| F | 3.40274 | 0.59923 | -0.93036 |
| C | 3.42672 | 2.91964 | -0.37492 |
| H | 4.49588 | 2.84921 | -0.12387 |
| C | 2.70936 | 4.12175 | -0.25007 |
| H | 3.23222 | 5.02515 | 0.10064 |
| C | 1.33953 | 4.17901 | -0.55645 |
| H | 0.78045 | 5.12042 | -0.44540 |

Vibrational analysis

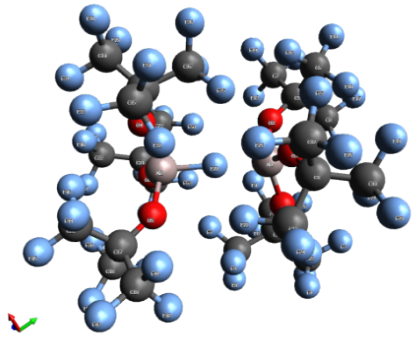
| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 6.11 | 0.01127 | YES | YES |
| 8 | a | 14.71 | 0.04418 | YES | YES |
| 9 | a | 21.14 | 0.07461 | YES | YES |
| 10 | a | 21.82 | 0.18145 | YES | YES |
| 11 | a | 25.59 | 0.27390 | YES | YES |
| 12 | a | 29.45 | 0.18221 | YES | YES |
| 13 | a | 36.52 | 0.93755 | YES | YES |
| 14 | a | 42.33 | 0.18201 | YES | YES |
| 15 | a | 43.34 | 0.39333 | YES | YES |
| 16 | a | 48.43 | 0.78822 | YES | YES |
| 17 | a | 51.93 | 1.15275 | YES | YES |
| 18 | a | 57.48 | 1.82802 | YES | YES |
| 19 | a | 58.53 | 0.27203 | YES | YES |
| 20 | a | 61.09 | 0.58735 | YES | YES |
| 21 | a | 66.24 | 0.08951 | YES | YES |
| 22 | a | 69.47 | 0.17481 | YES | YES |
| 23 | a | 72.08 | 0.91269 | YES | YES |
| 24 | a | 74.56 | 0.09856 | YES | YES |
| 25 | a | 75.11 | 0.46664 | YES | YES |
| 26 | a | 76.48 | 0.01097 | YES | YES |
| 27 | a | 82.59 | 0.58673 | YES | YES |
| 28 | a | 83.33 | 0.79275 | YES | YES |
| 29 | a | 84.06 | 0.24020 | YES | YES |
| 30 | a | 90.19 | 1.88879 | YES | YES |
| 31 | a | 94.89 | 1.05046 | YES | YES |
| 32 | a | 103.90 | 4.53577 | YES | YES |
| 33 | a | 128.44 | 9.09449 | YES | YES |
| 34 | a | 154.86 | 3.56643 | YES | YES |
| 35 | a | 156.88 | 0.07703 | YES | YES |
| 36 | a | 158.96 | 0.49302 | YES | YES |
| 37 | a | 162.19 | 0.20739 | YES | YES |
| 38 | a | 162.50 | 1.56355 | YES | YES |
| 39 | a | 165.75 | 0.36775 | YES | YES |
| 40 | a | 181.10 | 10.91628 | YES | YES |
| 41 | a | 187.22 | 5.23202 | YES | YES |
| 42 | a | 199.09 | 12.59108 | YES | YES |
| 43 | a | 228.67 | 5.44222 | YES | YES |
| 44 | a | 264.64 | 6.12414 | YES | YES |
| 45 | a | 270.09 | 0.52944 | YES | YES |
| 46 | a | 272.80 | 1.51271 | YES | YES |
| 47 | a | 277.77 | 10.05341 | YES | YES |
| 48 | a | 281.01 | 4.47670 | YES | YES |
| 49 | a | 282.46 | 17.05138 | YES | YES |
| 50 | a | 284.38 | 1.13337 | YES | YES |
| 51 | a | 285.66 | 0.37267 | YES | YES |
| 52 | a | 287.54 | 6.12299 | YES | YES |
| 53 | a | 292.08 | 6.79915 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 54 | a | 296.16 | 1.07013 | YES | YES |
| 55 | a | 308.30 | 6.51256 | YES | YES |
| 56 | a | 309.05 | 5.47678 | YES | YES |
| 57 | a | 313.02 | 0.63980 | YES | YES |
| 58 | a | 318.95 | 0.47435 | YES | YES |
| 59 | a | 319.33 | 0.84196 | YES | YES |
| 60 | a | 321.36 | 2.52984 | YES | YES |
| 61 | a | 321.50 | 2.32315 | YES | YES |
| 62 | a | 326.32 | 0.07021 | YES | YES |
| 63 | a | 335.46 | 2.28559 | YES | YES |
| 64 | a | 348.18 | 17.82160 | YES | YES |
| 65 | a | 351.77 | 3.87337 | YES | YES |
| 66 | a | 358.43 | 12.97798 | YES | YES |
| 67 | a | 360.08 | 17.97076 | YES | YES |
| 68 | a | 367.43 | 8.37521 | YES | YES |
| 69 | a | 373.04 | 42.12784 | YES | YES |
| 70 | a | 412.13 | 18.39749 | YES | YES |
| 71 | a | 433.65 | 3.98541 | YES | YES |
| 72 | a | 450.40 | 35.82061 | YES | YES |
| 73 | a | 455.88 | 9.32674 | YES | YES |
| 74 | a | 471.87 | 17.23065 | YES | YES |
| 75 | a | 513.05 | 4.79641 | YES | YES |
| 76 | a | 518.96 | 2.33490 | YES | YES |
| 77 | a | 519.70 | 1.69443 | YES | YES |
| 78 | a | 519.78 | 3.68620 | YES | YES |
| 79 | a | 520.31 | 3.73320 | YES | YES |
| 80 | a | 521.21 | 10.53861 | YES | YES |
| 81 | a | 521.37 | 3.01174 | YES | YES |
| 82 | a | 523.60 | 1.12985 | YES | YES |
| 83 | a | 524.65 | 1.38798 | YES | YES |
| 84 | a | 527.98 | 0.63080 | YES | YES |
| 85 | a | 532.50 | 7.54744 | YES | YES |
| 86 | a | 543.79 | 0.81257 | YES | YES |
| 87 | a | 552.54 | 0.74982 | YES | YES |
| 88 | a | 553.75 | 1.02451 | YES | YES |
| 89 | a | 554.65 | 0.56817 | YES | YES |
| 90 | a | 554.89 | 0.54445 | YES | YES |
| 91 | a | 556.03 | 0.29802 | YES | YES |
| 92 | a | 556.35 | 0.50348 | YES | YES |
| 93 | a | 559.60 | 14.49158 | YES | YES |
| 94 | a | 568.78 | 23.22919 | YES | YES |
| 95 | a | 586.73 | 37.58899 | YES | YES |
| 96 | a | 670.78 | 0.13125 | YES | YES |
| 97 | a | 705.73 | 15.99500 | YES | YES |
| 98 | a | 707.85 | 3.96991 | YES | YES |
| 99 | a | 708.80 | 59.53678 | YES | YES |
| 100 | a | 709.77 | 21.51395 | YES | YES |
| 101 | a | 710.50 | 20.75939 | YES | YES |
| 102 | a | 711.07 | 75.88343 | YES | YES |
| 103 | a | 727.17 | 1.51785 | YES | YES |
| 104 | a | 735.31 | 64.46517 | YES | YES |
| 105 | a | 740.04 | 3.29954 | YES | YES |
| 106 | a | 741.34 | 55.43215 | YES | YES |
| 107 | a | 742.46 | 25.20961 | YES | YES |
| 108 | a | 793.60 | 2.78133 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 109 | a | 827.02 | 12.00464 | YES | YES |
| 110 | a | 831.49 | 3.15872 | YES | YES |
| 111 | a | 873.24 | 22.59766 | YES | YES |
| 112 | a | 899.43 | 24.25628 | YES | YES |
| 113 | a | 919.34 | 4.02050 | YES | YES |
| 114 | a | 952.13 | 98.50927 | YES | YES |
| 115 | a | 960.25 | 67.04056 | YES | YES |
| 116 | a | 963.84 | 3.72878 | YES | YES |
| 117 | a | 964.13 | 68.53033 | YES | YES |
| 118 | a | 967.38 | 160.25532 | YES | YES |
| 119 | a | 970.39 | 228.12225 | YES | YES |
| 120 | a | 971.27 | 231.27917 | YES | YES |
| 121 | a | 1026.16 | 8.35300 | YES | YES |
| 122 | a | 1069.60 | 56.31000 | YES | YES |
| 123 | a | 1086.42 | 25.65334 | YES | YES |
| 124 | a | 1101.52 | 9.69151 | YES | YES |
| 125 | a | 1109.01 | 1.62197 | YES | YES |
| 126 | a | 1123.92 | 30.23962 | YES | YES |
| 127 | a | 1138.84 | 9.82003 | YES | YES |
| 128 | a | 1140.52 | 25.88095 | YES | YES |
| 129 | a | 1154.32 | 12.80453 | YES | YES |
| 130 | a | 1159.63 | 29.66661 | YES | YES |
| 131 | a | 1163.69 | 4.85933 | YES | YES |
| 132 | a | 1166.89 | 1.01717 | YES | YES |
| 133 | a | 1170.90 | 4.52210 | YES | YES |
| 134 | a | 1178.15 | 43.81557 | YES | YES |
| 135 | a | 1188.71 | 17.97495 | YES | YES |
| 136 | a | 1191.96 | 11.91211 | YES | YES |
| 137 | a | 1194.84 | 14.65264 | YES | YES |
| 138 | a | 1202.40 | 1.48448 | YES | YES |
| 139 | a | 1205.67 | 139.42884 | YES | YES |
| 140 | a | 1209.10 | 92.31604 | YES | YES |
| 141 | a | 1213.65 | 22.18365 | YES | YES |
| 142 | a | 1222.49 | 60.33808 | YES | YES |
| 143 | a | 1234.41 | 1086.93650 | YES | YES |
| 144 | a | 1237.96 | 239.53590 | YES | YES |
| 145 | a | 1242.83 | 225.26914 | YES | YES |
| 146 | a | 1245.26 | 200.32079 | YES | YES |
| 147 | a | 1246.43 | 1064.20024 | YES | YES |
| 148 | a | 1252.76 | 279.68402 | YES | YES |
| 149 | a | 1256.49 | 546.97068 | YES | YES |
| 150 | a | 1261.33 | 1158.41754 | YES | YES |
| 151 | a | 1264.76 | 302.06305 | YES | YES |
| 152 | a | 1272.07 | 409.43403 | YES | YES |
| 153 | a | 1285.08 | 123.04506 | YES | YES |
| 154 | a | 1317.95 | 40.01856 | YES | YES |
| 155 | a | 1334.78 | 141.92433 | YES | YES |
| 156 | a | 1345.85 | 159.57202 | YES | YES |
| 157 | a | 1379.85 | 6.41352 | YES | YES |
| 158 | a | 1455.91 | 10.61101 | YES | YES |
| 159 | a | 1506.63 | 157.44247 | YES | YES |
| 160 | a | 1602.68 | 1.99213 | YES | YES |
| 161 | a | 1649.18 | 24.75118 | YES | YES |
| 162 | a | 3116.86 | 3.06963 | YES | YES |
| 163 | a | 3131.45 | 3.73491 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 164 | a | 3138.28 | 0.24810 | YES | YES |
| 165 | a | 3164.27 | 17.53559 | YES | YES |

[μF-{Al(OR$^F$)$_3$}$_2$]$^-$



Atomic coordinates

| | | | |
|---|---|---|---|
| O | -2.51851 | 1.21475 | -0.40729 |
| C | -3.54134 | 0.60541 | 0.24149 |
| C | -4.87112 | 0.95401 | -0.52084 |
| F | -4.96713 | 0.24793 | -1.66550 |
| F | -5.96428 | 0.67311 | 0.22825 |
| F | -4.90373 | 2.25596 | -0.83768 |
| C | -3.63466 | 1.12127 | 1.72637 |
| F | -2.39756 | 1.21505 | 2.24863 |
| F | -4.19071 | 2.34971 | 1.77359 |
| F | -4.36636 | 0.30633 | 2.51363 |
| C | -3.32431 | -0.95328 | 0.24080 |
| F | -2.37417 | -1.27795 | 1.14662 |
| F | -4.44739 | -1.63310 | 0.55195 |
| F | -2.90026 | -1.36092 | -0.96202 |
| O | -0.11370 | 2.62723 | 0.74500 |
| C | -0.00456 | 3.95096 | 1.03078 |
| C | 0.85879 | 4.69373 | -0.06030 |
| F | 0.13303 | 4.89209 | -1.18096 |
| F | 1.28954 | 5.90290 | 0.36906 |
| F | 1.93270 | 3.96374 | -0.38860 |
| C | 0.69818 | 4.07876 | 2.43199 |
| F | 0.16203 | 3.21926 | 3.30740 |
| F | 2.01403 | 3.80532 | 2.33193 |
| F | 0.57316 | 5.32888 | 2.94051 |
| C | -1.42801 | 4.62131 | 1.09797 |
| F | -2.06606 | 4.29168 | 2.23731 |
| F | -1.37437 | 5.96839 | 1.02922 |
| F | -2.18087 | 4.18119 | 0.06812 |
| O | -0.31629 | 1.99663 | -2.04031 |
| C | -0.61397 | 1.87303 | -3.35791 |
| C | -1.56279 | 3.04801 | -3.79795 |
| F | -0.88294 | 4.21049 | -3.88035 |
| F | -2.12928 | 2.81677 | -5.00524 |
| F | -2.54572 | 3.21423 | -2.89840 |
| C | -1.31425 | 0.49291 | -3.66725 |
| F | -0.76917 | -0.46595 | -2.89832 |
| F | -2.63206 | 0.54218 | -3.38830 |
| F | -1.18223 | 0.12692 | -4.96015 |

| | | | |
|---|---|---|---|
| C | 0.73956 | 1.95943 | -4.15656 |
| F | 1.42708 | 0.80505 | -4.04153 |
| F | 0.53727 | 2.19273 | -5.47505 |
| F | 1.50719 | 2.94565 | -3.67324 |
| Al | -0.81383 | 1.55187 | -0.43604 |
| F | 0.00000 | -0.00000 | 0.00000 |
| O | 2.51851 | -1.21475 | 0.40729 |
| C | 3.54134 | -0.60541 | -0.24149 |
| C | 4.87112 | -0.95401 | 0.52084 |
| F | 4.96713 | -0.24793 | 1.66550 |
| F | 5.96428 | -0.67311 | -0.22825 |
| F | 4.90373 | -2.25596 | 0.83768 |
| C | 3.63466 | -1.12127 | -1.72637 |
| F | 2.39756 | -1.21505 | -2.24863 |
| F | 4.19071 | -2.34971 | -1.77359 |
| F | 4.36636 | -0.30633 | -2.51363 |
| C | 3.32431 | 0.95328 | -0.24080 |
| F | 2.37417 | 1.27795 | -1.14662 |
| F | 4.44739 | 1.63310 | -0.55195 |
| F | 2.90026 | 1.36092 | 0.96202 |
| O | 0.11370 | -2.62723 | -0.74500 |
| C | 0.00456 | -3.95096 | -1.03078 |
| C | -0.85879 | -4.69373 | 0.06030 |
| F | -0.13303 | -4.89209 | 1.18096 |
| F | -1.28954 | -5.90290 | -0.36906 |
| F | -1.93270 | -3.96374 | 0.38860 |
| C | -0.69818 | -4.07876 | -2.43199 |
| F | -0.16203 | -3.21926 | -3.30740 |
| F | -2.01403 | -3.80532 | -2.33193 |
| F | -0.57316 | -5.32888 | -2.94051 |
| C | 1.42801 | -4.62131 | -1.09797 |
| F | 2.06606 | -4.29168 | -2.23731 |
| F | 1.37437 | -5.96839 | -1.02922 |
| F | 2.18087 | -4.18119 | -0.06812 |
| O | 0.31629 | -1.99663 | 2.04031 |
| C | 0.61397 | -1.87303 | 3.35791 |
| C | 1.56279 | -3.04801 | 3.79795 |
| F | 0.88294 | -4.21049 | 3.88035 |
| F | 2.12928 | -2.81677 | 5.00524 |
| F | 2.54572 | -3.21423 | 2.89840 |
| C | 1.31425 | -0.49291 | 3.66725 |
| F | 0.76917 | 0.46595 | 2.89832 |
| F | 2.63206 | -0.54218 | 3.38830 |
| F | 1.18223 | -0.12692 | 4.96015 |
| C | -0.73956 | -1.95943 | 4.15656 |
| F | -1.42708 | -0.80505 | 4.04153 |
| F | -0.53727 | -2.19273 | 5.47505 |
| F | -1.50719 | -2.94565 | 3.67324 |
| Al | 0.81383 | -1.55187 | 0.43604 |

Vibrational analysis

| 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 | 5.94 | 0.00888 | YES | NO |
| 8 | au | 11.29 | 0.00634 | YES | NO |
| 9 | ag | 11.40 | 0.00000 | NO | YES |
| 10 | ag | 13.65 | 0.00000 | NO | YES |
| 11 | au | 18.31 | 0.00782 | YES | NO |
| 12 | ag | 21.10 | 0.00000 | NO | YES |
| 13 | au | 22.90 | 0.13822 | YES | NO |
| 14 | au | 25.40 | 0.01215 | YES | NO |
| 15 | au | 26.99 | 0.04041 | YES | NO |
| 16 | ag | 27.06 | 0.00000 | NO | YES |
| 17 | ag | 29.07 | 0.00000 | NO | YES |
| 18 | ag | 32.42 | 0.00000 | NO | YES |
| 19 | au | 34.15 | 0.02169 | YES | NO |
| 20 | au | 35.89 | 0.06529 | YES | NO |
| 21 | au | 37.66 | 0.03532 | YES | NO |
| 22 | au | 39.47 | 0.13293 | YES | NO |
| 23 | ag | 42.40 | 0.00000 | NO | YES |
| 24 | au | 46.66 | 0.01983 | YES | NO |
| 25 | ag | 47.32 | 0.00000 | NO | YES |
| 26 | ag | 48.77 | 0.00000 | NO | YES |
| 27 | ag | 51.56 | 0.00000 | NO | YES |
| 28 | ag | 58.22 | 0.00000 | NO | YES |
| 29 | au | 62.72 | 0.81582 | YES | NO |
| 30 | ag | 65.16 | 0.00000 | NO | YES |
| 31 | au | 65.91 | 0.36694 | YES | NO |
| 32 | ag | 68.09 | 0.00000 | NO | YES |
| 33 | au | 68.59 | 0.29482 | YES | NO |
| 34 | au | 70.40 | 0.49921 | YES | NO |
| 35 | ag | 71.01 | 0.00000 | NO | YES |
| 36 | au | 71.52 | 0.04875 | YES | NO |
| 37 | ag | 71.65 | 0.00000 | NO | YES |
| 38 | ag | 73.13 | 0.00000 | NO | YES |
| 39 | au | 74.76 | 0.33129 | YES | NO |
| 40 | ag | 75.28 | 0.00000 | NO | YES |
| 41 | au | 76.84 | 0.28987 | YES | NO |
| 42 | ag | 78.45 | 0.00000 | NO | YES |
| 43 | au | 78.64 | 0.01765 | YES | NO |
| 44 | ag | 82.31 | 0.00000 | NO | YES |
| 45 | ag | 83.45 | 0.00000 | NO | YES |
| 46 | au | 83.80 | 0.14817 | YES | NO |
| 47 | au | 85.53 | 0.42880 | YES | NO |
| 48 | ag | 86.95 | 0.00000 | NO | YES |
| 49 | au | 88.30 | 1.16063 | YES | NO |
| 50 | ag | 91.31 | 0.00000 | NO | YES |
| 51 | ag | 93.81 | 0.00000 | NO | YES |
| 52 | au | 95.03 | 1.42235 | YES | NO |
| 53 | au | 105.28 | 3.04029 | YES | NO |
| 54 | ag | 109.61 | 0.00000 | NO | YES |
| 55 | au | 148.52 | 1.81439 | YES | NO |
| 56 | au | 151.13 | 1.89487 | YES | NO |

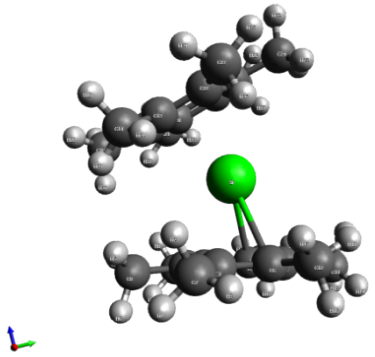
| | | | | | |
|---|---|---|---|---|---|
| 57 | ag | 154.16 | 0.00000 | NO | YES |
| 58 | au | 155.12 | 0.85692 | YES | NO |
| 59 | ag | 156.60 | 0.00000 | NO | YES |
| 60 | au | 160.15 | 2.07224 | YES | NO |
| 61 | ag | 160.22 | 0.00000 | NO | YES |
| 62 | ag | 161.01 | 0.00000 | NO | YES |
| 63 | au | 161.65 | 1.81452 | YES | NO |
| 64 | ag | 162.69 | 0.00000 | NO | YES |
| 65 | au | 164.33 | 1.27903 | YES | NO |
| 66 | ag | 166.24 | 0.00000 | NO | YES |
| 67 | au | 170.36 | 9.39120 | YES | NO |
| 68 | au | 178.82 | 7.01450 | YES | NO |
| 69 | au | 185.24 | 10.13773 | YES | NO |
| 70 | ag | 187.98 | 0.00000 | NO | YES |
| 71 | ag | 190.70 | 0.00000 | NO | YES |
| 72 | au | 201.46 | 11.56042 | YES | NO |
| 73 | au | 210.06 | 8.97200 | YES | NO |
| 74 | ag | 212.13 | 0.00000 | NO | YES |
| 75 | au | 246.74 | 16.28009 | YES | NO |
| 76 | ag | 266.06 | 0.00000 | NO | YES |
| 77 | au | 266.46 | 2.10372 | YES | NO |
| 78 | ag | 270.16 | 0.00000 | NO | YES |
| 79 | ag | 272.14 | 0.00000 | NO | YES |
| 80 | au | 272.22 | 13.18201 | YES | NO |
| 81 | au | 273.36 | 3.38380 | YES | NO |
| 82 | ag | 278.68 | 0.00000 | NO | YES |
| 83 | ag | 279.81 | 0.00000 | NO | YES |
| 84 | au | 281.59 | 3.81976 | YES | NO |
| 85 | au | 283.21 | 10.75543 | YES | NO |
| 86 | ag | 284.14 | 0.00000 | NO | YES |
| 87 | au | 285.97 | 4.79051 | YES | NO |
| 88 | ag | 286.04 | 0.00000 | NO | YES |
| 89 | au | 286.32 | 6.40694 | YES | NO |
| 90 | ag | 286.82 | 0.00000 | NO | YES |
| 91 | au | 286.89 | 1.41697 | YES | NO |
| 92 | ag | 287.91 | 0.00000 | NO | YES |
| 93 | au | 291.35 | 13.57462 | YES | NO |
| 94 | ag | 305.85 | 0.00000 | NO | YES |
| 95 | au | 306.64 | 14.50222 | YES | NO |
| 96 | ag | 307.63 | 0.00000 | NO | YES |
| 97 | au | 307.88 | 9.66664 | YES | NO |
| 98 | ag | 311.72 | 0.00000 | NO | YES |
| 99 | au | 312.82 | 1.54502 | YES | NO |
| 100 | ag | 317.51 | 0.00000 | NO | YES |
| 101 | au | 317.85 | 0.56626 | YES | NO |
| 102 | ag | 317.91 | 0.00000 | NO | YES |
| 103 | au | 319.09 | 2.98500 | YES | NO |
| 104 | ag | 320.81 | 0.00000 | NO | YES |
| 105 | au | 321.41 | 5.15909 | YES | NO |
| 106 | ag | 321.97 | 0.00000 | NO | YES |
| 107 | au | 324.25 | 2.11333 | YES | NO |
| 108 | ag | 324.33 | 0.00000 | NO | YES |
| 109 | au | 324.83 | 2.67766 | YES | NO |
| 110 | ag | 328.09 | 0.00000 | NO | YES |
| 111 | au | 329.95 | 1.93832 | YES | NO |

| | | | | | |
|---|---|---|---|---|---|
| 112 | ag | 345.60 | 0.00000 | NO | YES |
| 113 | au | 346.38 | 1.36097 | YES | NO |
| 114 | ag | 351.77 | 0.00000 | NO | YES |
| 115 | au | 352.73 | 9.19508 | YES | NO |
| 116 | ag | 353.55 | 0.00000 | NO | YES |
| 117 | au | 358.27 | 3.22394 | YES | NO |
| 118 | ag | 359.09 | 0.00000 | NO | YES |
| 119 | au | 366.13 | 35.81050 | YES | NO |
| 120 | ag | 367.91 | 0.00000 | NO | YES |
| 121 | au | 375.37 | 84.70424 | YES | NO |
| 122 | ag | 393.96 | 0.00000 | NO | YES |
| 123 | au | 407.22 | 14.33834 | YES | NO |
| 124 | ag | 443.67 | 0.00000 | NO | YES |
| 125 | ag | 449.65 | 0.00000 | NO | YES |
| 126 | au | 450.76 | 89.18994 | YES | NO |
| 127 | au | 453.93 | 88.96293 | YES | NO |
| 128 | ag | 472.89 | 0.00000 | NO | YES |
| 129 | au | 517.48 | 3.99575 | YES | NO |
| 130 | ag | 517.48 | 0.00000 | NO | YES |
| 131 | au | 518.18 | 11.59830 | YES | NO |
| 132 | ag | 518.22 | 0.00000 | NO | YES |
| 133 | au | 518.60 | 7.35187 | YES | NO |
| 134 | ag | 518.77 | 0.00000 | NO | YES |
| 135 | au | 519.86 | 15.74568 | YES | NO |
| 136 | ag | 520.17 | 0.00000 | NO | YES |
| 137 | ag | 520.41 | 0.00000 | NO | YES |
| 138 | au | 520.44 | 9.01922 | YES | NO |
| 139 | au | 520.49 | 10.31307 | YES | NO |
| 140 | ag | 521.47 | 0.00000 | NO | YES |
| 141 | au | 521.65 | 6.11686 | YES | NO |
| 142 | ag | 523.89 | 0.00000 | NO | YES |
| 143 | au | 524.27 | 1.99155 | YES | NO |
| 144 | ag | 524.35 | 0.00000 | NO | YES |
| 145 | au | 524.74 | 1.35318 | YES | NO |
| 146 | ag | 524.94 | 0.00000 | NO | YES |
| 147 | au | 528.04 | 0.93678 | YES | NO |
| 148 | ag | 535.70 | 0.00000 | NO | YES |
| 149 | ag | 551.92 | 0.00000 | NO | YES |
| 150 | au | 552.25 | 10.95707 | YES | NO |
| 151 | ag | 552.79 | 0.00000 | NO | YES |
| 152 | au | 553.12 | 3.61828 | YES | NO |
| 153 | au | 554.20 | 1.37731 | YES | NO |
| 154 | ag | 554.26 | 0.00000 | NO | YES |
| 155 | au | 554.35 | 0.19746 | YES | NO |
| 156 | ag | 554.37 | 0.00000 | NO | YES |
| 157 | au | 554.96 | 2.58946 | YES | NO |
| 158 | ag | 555.08 | 0.00000 | NO | YES |
| 159 | ag | 556.30 | 0.00000 | NO | YES |
| 160 | au | 556.33 | 0.14542 | YES | NO |
| 161 | ag | 562.92 | 0.00000 | NO | YES |
| 162 | au | 563.67 | 47.69356 | YES | NO |
| 163 | ag | 567.02 | 0.00000 | NO | YES |
| 164 | au | 569.70 | 68.54847 | YES | NO |
| 165 | au | 673.76 | 259.71161 | YES | NO |
| 166 | ag | 705.15 | 0.00000 | NO | YES |

| | | | | | |
|---|---|---|---|---|---|
| 167 | au | 706.21 | 23.04772 | YES | NO |
| 168 | ag | 707.12 | 0.00000 | NO | YES |
| 169 | au | 707.13 | 9.00736 | YES | NO |
| 170 | ag | 707.83 | 0.00000 | NO | YES |
| 171 | au | 708.37 | 154.49098 | YES | NO |
| 172 | ag | 708.44 | 0.00000 | NO | YES |
| 173 | au | 708.95 | 45.87446 | YES | NO |
| 174 | au | 709.44 | 72.47322 | YES | NO |
| 175 | ag | 709.62 | 0.00000 | NO | YES |
| 176 | ag | 710.22 | 0.00000 | NO | YES |
| 177 | au | 710.24 | 136.24866 | YES | NO |
| 178 | au | 730.34 | 12.45939 | YES | NO |
| 179 | ag | 730.80 | 0.00000 | NO | YES |
| 180 | ag | 738.65 | 0.00000 | NO | YES |
| 181 | au | 739.21 | 3.97495 | YES | NO |
| 182 | ag | 739.66 | 0.00000 | NO | YES |
| 183 | au | 739.88 | 3.70230 | YES | NO |
| 184 | au | 792.07 | 7.42730 | YES | NO |
| 185 | ag | 796.73 | 0.00000 | NO | YES |
| 186 | ag | 850.43 | 0.00000 | NO | YES |
| 187 | au | 853.21 | 43.07776 | YES | NO |
| 188 | ag | 858.97 | 0.00000 | NO | YES |
| 189 | au | 863.15 | 63.21366 | YES | NO |
| 190 | ag | 954.51 | 0.00000 | NO | YES |
| 191 | au | 957.50 | 30.20122 | YES | NO |
| 192 | ag | 959.01 | 0.00000 | NO | YES |
| 193 | au | 959.12 | 79.97029 | YES | NO |
| 194 | ag | 961.33 | 0.00000 | NO | YES |
| 195 | ag | 964.06 | 0.00000 | NO | YES |
| 196 | au | 964.63 | 435.11440 | YES | NO |
| 197 | au | 965.17 | 294.03699 | YES | NO |
| 198 | au | 967.25 | 253.51473 | YES | NO |
| 199 | ag | 968.42 | 0.00000 | NO | YES |
| 200 | ag | 969.95 | 0.00000 | NO | YES |
| 201 | au | 970.46 | 592.15533 | YES | NO |
| 202 | au | 1102.77 | 2.80096 | YES | NO |
| 203 | ag | 1104.61 | 0.00000 | NO | YES |
| 204 | ag | 1107.23 | 0.00000 | NO | YES |
| 205 | au | 1108.05 | 8.77261 | YES | NO |
| 206 | ag | 1112.34 | 0.00000 | NO | YES |
| 207 | au | 1113.53 | 3.16462 | YES | NO |
| 208 | ag | 1135.30 | 0.00000 | NO | YES |
| 209 | au | 1136.62 | 14.80126 | YES | NO |
| 210 | ag | 1137.69 | 0.00000 | NO | YES |
| 211 | au | 1139.67 | 18.59505 | YES | NO |
| 212 | ag | 1143.29 | 0.00000 | NO | YES |
| 213 | au | 1144.62 | 60.77711 | YES | NO |
| 214 | au | 1145.39 | 16.84675 | YES | NO |
| 215 | ag | 1146.01 | 0.00000 | NO | YES |
| 216 | ag | 1147.14 | 0.00000 | NO | YES |
| 217 | au | 1147.69 | 26.02008 | YES | NO |
| 218 | au | 1154.50 | 48.39632 | YES | NO |
| 219 | ag | 1154.75 | 0.00000 | NO | YES |
| 220 | ag | 1184.81 | 0.00000 | NO | YES |
| 221 | au | 1186.21 | 27.99365 | YES | NO |

| | | | | | |
|---|---|---|---|---|---|
| 222 | au | 1190.48 | 47.39151 | YES | NO |
| 223 | ag | 1190.60 | 0.00000 | NO | YES |
| 224 | ag | 1193.16 | 0.00000 | NO | YES |
| 225 | au | 1193.82 | 21.18910 | YES | NO |
| 226 | au | 1196.61 | 95.67532 | YES | NO |
| 227 | ag | 1198.65 | 0.00000 | NO | YES |
| 228 | au | 1202.09 | 13.99509 | YES | NO |
| 229 | ag | 1204.77 | 0.00000 | NO | YES |
| 230 | ag | 1207.92 | 0.00000 | NO | YES |
| 231 | au | 1209.67 | 153.86905 | YES | NO |
| 232 | ag | 1211.49 | 0.00000 | NO | YES |
| 233 | au | 1211.98 | 440.53965 | YES | NO |
| 234 | ag | 1213.58 | 0.00000 | NO | YES |
| 235 | au | 1214.05 | 419.97017 | YES | NO |
| 236 | au | 1225.54 | 658.48738 | YES | NO |
| 237 | ag | 1227.02 | 0.00000 | NO | YES |
| 238 | ag | 1229.73 | 0.00000 | NO | YES |
| 239 | ag | 1231.93 | 0.00000 | NO | YES |
| 240 | au | 1233.55 | 2521.84707 | YES | NO |
| 241 | au | 1236.30 | 1796.14276 | YES | NO |
| 242 | ag | 1237.66 | 0.00000 | NO | YES |
| 243 | au | 1239.06 | 1031.86133 | YES | NO |
| 244 | ag | 1242.61 | 0.00000 | NO | YES |
| 245 | ag | 1244.90 | 0.00000 | NO | YES |
| 246 | au | 1246.06 | 460.19351 | YES | NO |
| 247 | au | 1249.25 | 95.00754 | YES | NO |
| 248 | au | 1252.07 | 500.08174 | YES | NO |
| 249 | au | 1256.74 | 975.21199 | YES | NO |
| 250 | ag | 1257.18 | 0.00000 | NO | YES |
| 251 | ag | 1259.92 | 0.00000 | NO | YES |
| 252 | au | 1260.11 | 1003.63786 | YES | NO |
| 253 | au | 1260.76 | 1393.40094 | YES | NO |
| 254 | ag | 1261.89 | 0.00000 | NO | YES |
| 255 | ag | 1265.19 | 0.00000 | NO | YES |
| 256 | au | 1332.06 | 360.92258 | YES | NO |
| 257 | ag | 1332.38 | 0.00000 | NO | YES |
| 258 | ag | 1337.62 | 0.00000 | NO | YES |
| 259 | au | 1338.50 | 445.89694 | YES | NO |
| 260 | au | 1347.73 | 159.81710 | YES | NO |
| 261 | ag | 1352.29 | 0.00000 | NO | YES |

$[Sr(HMB)_2]^{2+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 1.47645 | -0.35665 | -2.18734 |
| C | 0.39336 | -1.28878 | -2.14175 |
| C | -0.94218 | -0.85639 | -2.41163 |
| C | -1.20071 | 0.52346 | -2.68849 |
| C | -0.11210 | 1.44864 | -2.77291 |
| C | 1.21847 | 1.02254 | -2.46308 |
| C | 2.89229 | -0.86338 | -2.00683 |
| H | 3.04174 | -1.80828 | -2.56906 |
| H | 3.13826 | -1.08729 | -0.94260 |
| H | 3.64814 | -0.14767 | -2.37918 |
| C | 0.67922 | -2.74973 | -1.87603 |
| H | -0.19847 | -3.29039 | -1.47290 |
| H | 1.52197 | -2.89305 | -1.17050 |
| H | 0.96549 | -3.26765 | -2.82154 |
| C | -2.05665 | -1.88191 | -2.46576 |
| H | -2.96621 | -1.49265 | -2.95853 |
| H | -2.35699 | -2.25116 | -1.45705 |
| H | -1.73617 | -2.77250 | -3.04550 |
| C | -2.61851 | 1.00832 | -2.91944 |
| H | -2.90672 | 0.90761 | -3.99170 |
| H | -2.74696 | 2.07736 | -2.65621 |
| H | -3.36367 | 0.42978 | -2.33649 |
| C | -0.36225 | 2.87173 | -3.23125 |
| H | -1.21447 | 2.92321 | -3.93664 |
| H | 0.51717 | 3.28393 | -3.76328 |
| H | -0.59240 | 3.57408 | -2.39433 |
| C | 2.34986 | 2.03134 | -2.45561 |
| H | 2.82918 | 2.10345 | -3.45955 |
| H | 3.15273 | 1.75959 | -1.74084 |
| H | 2.00345 | 3.05195 | -2.19616 |
| Sr | -0.19700 | 0.59366 | 0.01035 |
| C | 0.97896 | -0.91919 | 2.19318 |
| C | 2.17006 | -1.81614 | 1.93209 |
| H | 2.49699 | -2.32488 | 2.86899 |
| H | 1.94074 | -2.61491 | 1.19913 |
| H | 3.04738 | -1.25308 | 1.55619 |
| C | -0.34677 | -1.44681 | 2.10853 |
| C | -1.26663 | 0.77194 | 2.71071 |
| C | 0.06042 | 1.30121 | 2.79255 |
| H | 0.37790 | 2.90241 | 4.23687 |
| H | 1.18579 | 3.17986 | 2.67227 |
| H | -0.58372 | 3.39674 | 2.82013 |
| C | -2.45099 | 1.63940 | 3.08790 |
| H | -3.29525 | 1.03183 | 3.46708 |
| H | -2.18409 | 2.35261 | 3.89267 |
| H | -2.84421 | 2.24668 | 2.23741 |
| C | -0.56084 | -2.92628 | 1.86524 |
| H | 0.27651 | -3.52700 | 2.27079 |
| H | -1.48252 | -3.28797 | 2.36131 |
| H | -0.64837 | -3.18133 | 0.78370 |
| C | -1.47081 | -0.58713 | 2.31568 |
| C | -2.87642 | -1.12712 | 2.14513 |
| H | -3.26689 | -1.54097 | 3.10398 |
| H | -2.92205 | -1.94986 | 1.40322 |
| H | -3.59297 | -0.34473 | 1.82272 |

| | | | |
|---|---|---|---|
| C | 1.18432 | 0.44469 | 2.57154 |
| C | 2.59507 | 0.95461 | 2.78806 |
| H | 3.22638 | 0.17805 | 3.26534 |
| H | 2.61918 | 1.83775 | 3.45379 |
| H | 3.10760 | 1.24379 | 1.83961 |
| C | 0.26891 | 2.76266 | 3.13601 |

Vibrational analysis

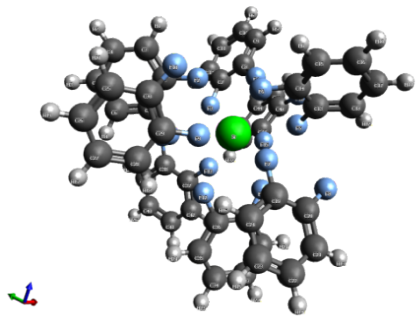
| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
| 5 | | 0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 8.77 | 0.18762 | YES | YES |
| 8 | a | 10.87 | 0.98490 | YES | YES |
| 9 | a | 31.16 | 0.69472 | YES | YES |
| 10 | a | 39.22 | 0.45948 | YES | YES |
| 11 | a | 59.82 | 0.20062 | YES | YES |
| 12 | a | 63.44 | 0.04904 | YES | YES |
| 13 | a | 64.13 | 0.11729 | YES | YES |
| 14 | a | 70.76 | 0.05382 | YES | YES |
| 15 | a | 73.05 | 0.55402 | YES | YES |
| 16 | a | 77.88 | 0.10124 | YES | YES |
| 17 | a | 81.46 | 0.07319 | YES | YES |
| 18 | a | 96.70 | 0.02269 | YES | YES |
| 19 | a | 100.80 | 0.56156 | YES | YES |
| 20 | a | 106.82 | 0.23593 | YES | YES |
| 21 | a | 111.39 | 0.09234 | YES | YES |
| 22 | a | 113.54 | 0.08271 | YES | YES |
| 23 | a | 117.94 | 0.37724 | YES | YES |
| 24 | a | 129.19 | 0.01475 | YES | YES |
| 25 | a | 135.19 | 0.15857 | YES | YES |
| 26 | a | 142.66 | 0.14781 | YES | YES |
| 27 | a | 149.51 | 0.63547 | YES | YES |
| 28 | a | 153.08 | 0.50883 | YES | YES |
| 29 | a | 155.09 | 1.70224 | YES | YES |
| 30 | a | 157.35 | 1.47477 | YES | YES |
| 31 | a | 163.19 | 0.11040 | YES | YES |
| 32 | a | 176.56 | 1.24412 | YES | YES |
| 33 | a | 177.81 | 0.33260 | YES | YES |
| 34 | a | 248.93 | 1.77513 | YES | YES |
| 35 | a | 272.77 | 98.93500 | YES | YES |
| 36 | a | 336.79 | 0.57355 | YES | YES |
| 37 | a | 339.69 | 0.37957 | YES | YES |
| 38 | a | 343.18 | 0.21424 | YES | YES |
| 39 | a | 345.85 | 0.25310 | YES | YES |
| 40 | a | 374.15 | 1.12058 | YES | YES |
| 41 | a | 375.67 | 1.97566 | YES | YES |
| 42 | a | 377.13 | 1.65908 | YES | YES |
| 43 | a | 381.90 | 0.85278 | YES | YES |
| 44 | a | 400.79 | 0.00655 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 45 | a | 404.06 | 0.00996 | YES | YES |
| 46 | a | 405.87 | 0.02628 | YES | YES |
| 47 | a | 406.73 | 0.01201 | YES | YES |
| 48 | a | 439.71 | 0.07603 | YES | YES |
| 49 | a | 441.04 | 0.09658 | YES | YES |
| 50 | a | 441.59 | 0.08685 | YES | YES |
| 51 | a | 442.08 | 0.05222 | YES | YES |
| 52 | a | 445.17 | 0.01595 | YES | YES |
| 53 | a | 445.80 | 0.08267 | YES | YES |
| 54 | a | 544.47 | 1.42991 | YES | YES |
| 55 | a | 545.42 | 0.06458 | YES | YES |
| 56 | a | 569.40 | 0.70266 | YES | YES |
| 57 | a | 571.83 | 0.89811 | YES | YES |
| 58 | a | 574.17 | 1.52121 | YES | YES |
| 59 | a | 574.36 | 2.30112 | YES | YES |
| 60 | a | 575.13 | 1.22793 | YES | YES |
| 61 | a | 576.13 | 0.73207 | YES | YES |
| 62 | a | 577.95 | 1.71203 | YES | YES |
| 63 | a | 578.03 | 0.89854 | YES | YES |
| 64 | a | 695.37 | 0.47691 | YES | YES |
| 65 | a | 695.83 | 0.70657 | YES | YES |
| 66 | a | 792.73 | 2.13680 | YES | YES |
| 67 | a | 795.12 | 1.90065 | YES | YES |
| 68 | a | 796.25 | 1.89501 | YES | YES |
| 69 | a | 797.19 | 2.99740 | YES | YES |
| 70 | a | 955.95 | 0.35868 | YES | YES |
| 71 | a | 957.66 | 0.09512 | YES | YES |
| 72 | a | 959.28 | 0.41214 | YES | YES |
| 73 | a | 959.87 | 0.02985 | YES | YES |
| 74 | a | 968.53 | 10.65130 | YES | YES |
| 75 | a | 969.34 | 0.56733 | YES | YES |
| 76 | a | 972.99 | 1.22615 | YES | YES |
| 77 | a | 973.70 | 0.13367 | YES | YES |
| 78 | a | 994.73 | 3.16720 | YES | YES |
| 79 | a | 996.04 | 2.22182 | YES | YES |
| 80 | a | 996.70 | 2.49705 | YES | YES |
| 81 | a | 997.00 | 3.69351 | YES | YES |
| 82 | a | 1022.75 | 0.23873 | YES | YES |
| 83 | a | 1023.55 | 4.33100 | YES | YES |
| 84 | a | 1024.13 | 1.78326 | YES | YES |
| 85 | a | 1024.20 | 5.23056 | YES | YES |
| 86 | a | 1024.49 | 3.24194 | YES | YES |
| 87 | a | 1025.65 | 2.83761 | YES | YES |
| 88 | a | 1049.63 | 5.16315 | YES | YES |
| 89 | a | 1050.28 | 8.36119 | YES | YES |
| 90 | a | 1050.87 | 23.25830 | YES | YES |
| 91 | a | 1051.38 | 15.51832 | YES | YES |
| 92 | a | 1071.61 | 0.78046 | YES | YES |
| 93 | a | 1072.36 | 0.12882 | YES | YES |
| 94 | a | 1073.95 | 0.02578 | YES | YES |
| 95 | a | 1074.28 | 0.03659 | YES | YES |
| 96 | a | 1074.89 | 0.09506 | YES | YES |
| 97 | a | 1075.54 | 0.09016 | YES | YES |
| 98 | a | 1253.80 | 0.27698 | YES | YES |
| 99 | a | 1254.37 | 1.07211 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 100 | a | 1295.28 | 8.44285 | YES | YES |
| 101 | a | 1297.11 | 0.32390 | YES | YES |
| 102 | a | 1305.62 | 0.30194 | YES | YES |
| 103 | a | 1307.17 | 0.15453 | YES | YES |
| 104 | a | 1355.70 | 4.01598 | YES | YES |
| 105 | a | 1358.53 | 4.86473 | YES | YES |
| 106 | a | 1359.69 | 2.74902 | YES | YES |
| 107 | a | 1361.01 | 4.07668 | YES | YES |
| 108 | a | 1363.88 | 9.02967 | YES | YES |
| 109 | a | 1364.54 | 0.98299 | YES | YES |
| 110 | a | 1366.98 | 4.47873 | YES | YES |
| 111 | a | 1367.27 | 1.26703 | YES | YES |
| 112 | a | 1370.08 | 48.42694 | YES | YES |
| 113 | a | 1371.08 | 38.88846 | YES | YES |
| 114 | a | 1373.60 | 16.09014 | YES | YES |
| 115 | a | 1375.26 | 2.16538 | YES | YES |
| 116 | a | 1376.13 | 5.35640 | YES | YES |
| 117 | a | 1376.80 | 3.11952 | YES | YES |
| 118 | a | 1378.97 | 8.87990 | YES | YES |
| 119 | a | 1384.13 | 16.29103 | YES | YES |
| 120 | a | 1397.62 | 0.02676 | YES | YES |
| 121 | a | 1397.79 | 0.62842 | YES | YES |
| 122 | a | 1399.24 | 1.19460 | YES | YES |
| 123 | a | 1399.83 | 0.66839 | YES | YES |
| 124 | a | 1412.90 | 5.60889 | YES | YES |
| 125 | a | 1413.25 | 59.11112 | YES | YES |
| 126 | a | 1415.11 | 70.10044 | YES | YES |
| 127 | a | 1415.56 | 17.39139 | YES | YES |
| 128 | a | 1427.32 | 1.20290 | YES | YES |
| 129 | a | 1428.67 | 1.01096 | YES | YES |
| 130 | a | 1431.09 | 5.78354 | YES | YES |
| 131 | a | 1432.06 | 0.92859 | YES | YES |
| 132 | a | 1433.39 | 0.23189 | YES | YES |
| 133 | a | 1435.19 | 1.15581 | YES | YES |
| 134 | a | 1442.56 | 80.19441 | YES | YES |
| 135 | a | 1443.04 | 50.55634 | YES | YES |
| 136 | a | 1443.60 | 85.15845 | YES | YES |
| 137 | a | 1444.77 | 19.07471 | YES | YES |
| 138 | a | 1460.60 | 3.29140 | YES | YES |
| 139 | a | 1463.58 | 2.67724 | YES | YES |
| 140 | a | 1464.14 | 0.19643 | YES | YES |
| 141 | a | 1465.52 | 1.09123 | YES | YES |
| 142 | a | 1478.28 | 1.52888 | YES | YES |
| 143 | a | 1479.81 | 1.16018 | YES | YES |
| 144 | a | 1542.55 | 0.09214 | YES | YES |
| 145 | a | 1543.76 | 0.25822 | YES | YES |
| 146 | a | 1544.27 | 0.50673 | YES | YES |
| 147 | a | 1544.73 | 0.50188 | YES | YES |
| 148 | a | 2934.48 | 5.80179 | YES | YES |
| 149 | a | 2934.70 | 1.81421 | YES | YES |
| 150 | a | 2937.04 | 4.59627 | YES | YES |
| 151 | a | 2942.11 | 4.38375 | YES | YES |
| 152 | a | 2947.50 | 3.06343 | YES | YES |
| 153 | a | 2950.21 | 1.17904 | YES | YES |
| 154 | a | 2950.36 | 2.36273 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 155 | a | 2950.86 | 2.72368 | YES | YES |
| 156 | a | 2951.20 | 4.73620 | YES | YES |
| 157 | a | 2951.80 | 1.17242 | YES | YES |
| 158 | a | 2952.13 | 4.85981 | YES | YES |
| 159 | a | 2952.90 | 0.34414 | YES | YES |
| 160 | a | 3030.56 | 3.53477 | YES | YES |
| 161 | a | 3032.34 | 2.40593 | YES | YES |
| 162 | a | 3032.70 | 2.39708 | YES | YES |
| 163 | a | 3033.07 | 4.24691 | YES | YES |
| 164 | a | 3034.21 | 2.37718 | YES | YES |
| 165 | a | 3035.01 | 6.46790 | YES | YES |
| 166 | a | 3035.19 | 3.23834 | YES | YES |
| 167 | a | 3040.12 | 1.83861 | YES | YES |
| 168 | a | 3040.50 | 0.39132 | YES | YES |
| 169 | a | 3042.76 | 0.25598 | YES | YES |
| 170 | a | 3044.02 | 0.27748 | YES | YES |
| 171 | a | 3047.55 | 0.26631 | YES | YES |
| 172 | a | 3062.74 | 1.14358 | YES | YES |
| 173 | a | 3063.44 | 0.49828 | YES | YES |
| 174 | a | 3064.98 | 2.92045 | YES | YES |
| 175 | a | 3065.19 | 3.61802 | YES | YES |
| 176 | a | 3071.12 | 2.84415 | YES | YES |
| 177 | a | 3079.43 | 2.77179 | YES | YES |
| 178 | a | 3083.85 | 0.04220 | YES | YES |
| 179 | a | 3084.77 | 0.06301 | YES | YES |
| 180 | a | 3084.85 | 0.00162 | YES | YES |
| 181 | a | 3088.72 | 0.50201 | YES | YES |
| 182 | a | 3093.89 | 0.83521 | YES | YES |
| 183 | a | 3096.02 | 1.16583 | YES | YES |

$[Sr(oDFB)_8]^{2+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | -1.93825 | 2.55549 | 0.42523 |
| C | -1.74989 | 2.40387 | 1.80007 |
| C | -2.28565 | 3.30962 | 2.70931 |
| H | -2.13038 | 3.15834 | 3.78794 |
| C | -3.03385 | 4.38720 | 2.19983 |
| H | -3.47102 | 5.11689 | 2.89849 |
| C | -3.22876 | 4.53570 | 0.81490 |
| H | -3.81971 | 5.38102 | 0.43055 |
| C | -2.67684 | 3.61316 | -0.09298 |
| H | -2.81641 | 3.70384 | -1.17993 |
| F | -1.38792 | 1.59846 | -0.39723 |

| | | | |
|---|---|---|---|
| F | -1.05329 | 1.29875 | 2.22388 |
| C | 1.87215 | 2.29039 | 2.03829 |
| C | 1.90449 | 1.35918 | 3.07795 |
| C | 2.56566 | 1.63268 | 4.27054 |
| H | 2.58740 | 0.87735 | 5.07020 |
| C | 3.20431 | 2.88083 | 4.39694 |
| H | 3.73544 | 3.12043 | 5.33089 |
| C | 3.17008 | 3.81734 | 3.34822 |
| H | 3.67516 | 4.78871 | 3.46165 |
| C | 2.49603 | 3.52808 | 2.14722 |
| H | 2.45634 | 4.23576 | 1.30636 |
| F | 1.21315 | 1.92562 | 0.88697 |
| F | 1.29215 | 0.15126 | 2.85940 |
| C | 0.98607 | -3.10853 | 2.73880 |
| C | -0.20479 | -2.68011 | 3.32890 |
| C | -0.75361 | -3.34921 | 4.41847 |
| H | -1.69515 | -2.99339 | 4.86349 |
| C | -0.06926 | -4.47582 | 4.91261 |
| H | -0.48368 | -5.02186 | 5.77385 |
| C | 1.12937 | -4.90715 | 4.31668 |
| H | 1.65344 | -5.79093 | 4.71152 |
| C | 1.67165 | -4.22144 | 3.21370 |
| H | 2.60482 | -4.53916 | 2.72534 |
| F | 1.45301 | -2.39118 | 1.66030 |
| F | -0.82362 | -1.57626 | 2.78466 |
| C | -1.21011 | -3.84119 | -0.57229 |
| C | -0.17513 | -4.74959 | -0.83222 |
| C | -0.28920 | -5.62641 | -1.91573 |
| H | 0.52883 | -6.33650 | -2.11216 |
| C | -1.44318 | -5.58429 | -2.71717 |
| H | -1.53453 | -6.27731 | -3.56756 |
| C | -2.48114 | -4.68040 | -2.43148 |
| H | -3.39054 | -4.66639 | -3.05128 |
| C | -2.36927 | -3.79735 | -1.34331 |
| H | -3.16536 | -3.08327 | -1.08574 |
| F | -1.04058 | -2.93882 | 0.45787 |
| F | 0.92159 | -4.74203 | -0.05686 |
| Sr | 0.05413 | -0.47710 | 0.50674 |
| C | -5.38025 | 1.46881 | 1.49878 |
| C | -5.90732 | 1.75615 | 0.22868 |
| C | -5.34810 | 1.18042 | -0.92571 |
| H | -5.77238 | 1.40213 | -1.91693 |
| C | -4.24752 | 0.31195 | -0.82010 |
| H | -3.77921 | -0.14623 | -1.70314 |
| C | -3.73458 | 0.04269 | 0.44648 |
| F | -2.62544 | -0.76949 | 0.58157 |
| H | -6.77090 | 2.43355 | 0.14375 |
| C | -4.28779 | 0.60237 | 1.60619 |
| F | -3.74014 | 0.32121 | 2.79952 |
| H | -5.80441 | 1.90268 | 2.41696 |
| F | 1.06201 | -2.06422 | -1.41354 |
| C | 0.56002 | -2.15499 | -2.68804 |
| C | 1.25433 | -2.82782 | -3.68898 |
| H | 2.21585 | -3.31048 | -3.45769 |
| C | 0.68523 | -2.86507 | -4.97613 |

| | | | |
|---|---|---|---|
| H | 1.21521 | -3.39279 | -5.78377 |
| C | -0.54719 | -2.23858 | -5.23442 |
| H | -0.98230 | -2.27458 | -6.24486 |
| C | -1.23742 | -1.56259 | -4.21135 |
| H | -2.20094 | -1.06233 | -4.39014 |
| C | -0.66417 | -1.53472 | -2.94405 |
| F | -1.27320 | -0.88378 | -1.89906 |
| F | 0.97000 | 0.79152 | -1.66689 |
| C | 0.92407 | 1.63537 | -2.75979 |
| C | 0.65410 | 2.99614 | -2.55351 |
| C | 0.60859 | 3.86149 | -3.65195 |
| H | 0.39706 | 4.92768 | -3.47646 |
| C | 0.84324 | 3.35570 | -4.94182 |
| H | 0.81058 | 4.03905 | -5.80427 |
| C | 1.12911 | 1.99270 | -5.13173 |
| H | 1.32607 | 1.60102 | -6.14121 |
| F | 0.45103 | 3.46162 | -1.30692 |
| C | 1.17445 | 1.11971 | -4.03078 |
| H | 1.40878 | 0.05156 | -4.15104 |
| H | 5.95863 | 1.20816 | 2.79748 |
| C | 5.41675 | 1.29131 | 1.84332 |
| C | 5.70007 | 2.30469 | 0.91283 |
| H | 6.48766 | 3.03990 | 1.13873 |
| C | 4.99567 | 2.37800 | -0.30167 |
| H | 5.23084 | 3.16625 | -1.03309 |
| C | 3.99253 | 1.43822 | -0.59659 |
| H | 3.42981 | 1.47020 | -1.54021 |
| C | 3.71798 | 0.44585 | 0.34155 |
| F | 2.70657 | -0.46656 | 0.10883 |
| C | 4.41923 | 0.35572 | 1.55205 |
| F | 4.10364 | -0.61389 | 2.42730 |

Vibrational analysis

| mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules IR | RAMAN |
|---|---|---|---|---|---|
| 1 | | -0.00 | 0.00000 | - | - |
| 2 | | -0.00 | 0.00000 | - | - |
| 3 | | -0.00 | 0.00000 | - | - |
| 4 | | -0.00 | 0.00000 | - | - |
| 5 | | -0.00 | 0.00000 | - | - |
| 6 | | 0.00 | 0.00000 | - | - |
| 7 | a | 9.40 | 0.20188 | YES | YES |
| 8 | a | 12.90 | 0.14350 | YES | YES |
| 9 | a | 13.97 | 0.15909 | YES | YES |
| 10 | a | 17.69 | 0.71841 | YES | YES |
| 11 | a | 19.45 | 0.16194 | YES | YES |
| 12 | a | 22.76 | 0.15309 | YES | YES |
| 13 | a | 25.04 | 0.68511 | YES | YES |
| 14 | a | 28.10 | 0.56066 | YES | YES |
| 15 | a | 28.93 | 1.05944 | YES | YES |
| 16 | a | 32.54 | 0.00887 | YES | YES |
| 17 | a | 36.40 | 0.12945 | YES | YES |
| 18 | a | 38.91 | 0.16873 | YES | YES |
| 19 | a | 43.36 | 0.57441 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 20 | a | 45.83 | 0.61483 | YES | YES |
| 21 | a | 46.73 | 0.33659 | YES | YES |
| 22 | a | 49.81 | 0.80895 | YES | YES |
| 23 | a | 51.74 | 0.36637 | YES | YES |
| 24 | a | 53.27 | 0.18476 | YES | YES |
| 25 | a | 58.56 | 1.50823 | YES | YES |
| 26 | a | 59.46 | 1.96207 | YES | YES |
| 27 | a | 63.17 | 0.25399 | YES | YES |
| 28 | a | 65.24 | 2.48780 | YES | YES |
| 29 | a | 66.58 | 0.26028 | YES | YES |
| 30 | a | 69.21 | 0.86909 | YES | YES |
| 31 | a | 70.53 | 1.19590 | YES | YES |
| 32 | a | 72.12 | 0.61588 | YES | YES |
| 33 | a | 73.43 | 1.45105 | YES | YES |
| 34 | a | 75.73 | 1.50943 | YES | YES |
| 35 | a | 78.22 | 0.59911 | YES | YES |
| 36 | a | 79.15 | 0.12888 | YES | YES |
| 37 | a | 81.73 | 0.79810 | YES | YES |
| 38 | a | 83.74 | 0.93454 | YES | YES |
| 39 | a | 87.72 | 0.51895 | YES | YES |
| 40 | a | 93.40 | 3.93349 | YES | YES |
| 41 | a | 94.30 | 0.85331 | YES | YES |
| 42 | a | 98.05 | 0.15816 | YES | YES |
| 43 | a | 103.10 | 0.52844 | YES | YES |
| 44 | a | 107.07 | 9.74544 | YES | YES |
| 45 | a | 108.69 | 2.05110 | YES | YES |
| 46 | a | 117.49 | 15.66631 | YES | YES |
| 47 | a | 132.81 | 2.47670 | YES | YES |
| 48 | a | 139.00 | 36.56283 | YES | YES |
| 49 | a | 144.69 | 39.46512 | YES | YES |
| 50 | a | 148.83 | 13.61788 | YES | YES |
| 51 | a | 155.37 | 47.18294 | YES | YES |
| 52 | a | 197.41 | 0.15828 | YES | YES |
| 53 | a | 199.48 | 0.60841 | YES | YES |
| 54 | a | 200.76 | 3.03129 | YES | YES |
| 55 | a | 201.58 | 0.88792 | YES | YES |
| 56 | a | 203.61 | 0.52733 | YES | YES |
| 57 | a | 209.01 | 0.31106 | YES | YES |
| 58 | a | 210.64 | 0.33917 | YES | YES |
| 59 | a | 216.43 | 0.42551 | YES | YES |
| 60 | a | 276.59 | 0.67047 | YES | YES |
| 61 | a | 279.85 | 0.50665 | YES | YES |
| 62 | a | 280.77 | 1.05129 | YES | YES |
| 63 | a | 284.86 | 0.96082 | YES | YES |
| 64 | a | 286.36 | 1.05038 | YES | YES |
| 65 | a | 288.03 | 1.03579 | YES | YES |
| 66 | a | 289.55 | 1.41475 | YES | YES |
| 67 | a | 290.84 | 2.08472 | YES | YES |
| 68 | a | 293.95 | 1.38413 | YES | YES |
| 69 | a | 300.00 | 1.60470 | YES | YES |
| 70 | a | 303.27 | 3.79248 | YES | YES |
| 71 | a | 304.53 | 0.25385 | YES | YES |
| 72 | a | 307.63 | 4.14686 | YES | YES |
| 73 | a | 309.11 | 3.12224 | YES | YES |
| 74 | a | 311.47 | 7.12165 | YES | YES |

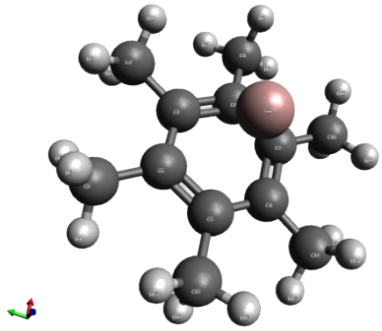
| | | | | | |
|---|---|---|---|---|---|
| 75 | a | 315.37 | 3.01696 | YES | YES |
| 76 | a | 431.43 | 1.05972 | YES | YES |
| 77 | a | 431.97 | 0.65109 | YES | YES |
| 78 | a | 434.23 | 0.64029 | YES | YES |
| 79 | a | 434.46 | 0.44982 | YES | YES |
| 80 | a | 434.99 | 0.15183 | YES | YES |
| 81 | a | 435.55 | 0.38120 | YES | YES |
| 82 | a | 436.44 | 0.08175 | YES | YES |
| 83 | a | 437.77 | 0.12472 | YES | YES |
| 84 | a | 440.74 | 1.05919 | YES | YES |
| 85 | a | 441.38 | 3.73806 | YES | YES |
| 86 | a | 441.46 | 0.73918 | YES | YES |
| 87 | a | 442.47 | 2.63785 | YES | YES |
| 88 | a | 451.90 | 5.13010 | YES | YES |
| 89 | a | 452.70 | 0.55865 | YES | YES |
| 90 | a | 454.20 | 0.23354 | YES | YES |
| 91 | a | 454.70 | 2.20483 | YES | YES |
| 92 | a | 532.04 | 1.49137 | YES | YES |
| 93 | a | 532.30 | 4.44960 | YES | YES |
| 94 | a | 533.63 | 0.08812 | YES | YES |
| 95 | a | 534.30 | 9.85707 | YES | YES |
| 96 | a | 534.73 | 5.68655 | YES | YES |
| 97 | a | 535.57 | 0.08686 | YES | YES |
| 98 | a | 535.76 | 0.67692 | YES | YES |
| 99 | a | 535.96 | 1.14852 | YES | YES |
| 100 | a | 539.66 | 2.42122 | YES | YES |
| 101 | a | 540.00 | 3.65897 | YES | YES |
| 102 | a | 540.48 | 7.78088 | YES | YES |
| 103 | a | 540.91 | 2.12542 | YES | YES |
| 104 | a | 541.45 | 2.62551 | YES | YES |
| 105 | a | 543.06 | 0.24234 | YES | YES |
| 106 | a | 543.12 | 0.26860 | YES | YES |
| 107 | a | 544.08 | 0.10491 | YES | YES |
| 108 | a | 557.78 | 15.24513 | YES | YES |
| 109 | a | 558.38 | 25.67234 | YES | YES |
| 110 | a | 558.83 | 22.20575 | YES | YES |
| 111 | a | 559.76 | 10.68422 | YES | YES |
| 112 | a | 561.83 | 12.07210 | YES | YES |
| 113 | a | 562.18 | 11.71211 | YES | YES |
| 114 | a | 563.24 | 8.07145 | YES | YES |
| 115 | a | 564.93 | 12.19620 | YES | YES |
| 116 | a | 663.01 | 0.31530 | YES | YES |
| 117 | a | 664.18 | 0.20306 | YES | YES |
| 118 | a | 667.42 | 0.01188 | YES | YES |
| 119 | a | 669.63 | 0.02351 | YES | YES |
| 120 | a | 670.75 | 0.18293 | YES | YES |
| 121 | a | 671.09 | 0.03199 | YES | YES |
| 122 | a | 673.81 | 0.17203 | YES | YES |
| 123 | a | 674.43 | 0.09651 | YES | YES |
| 124 | a | 745.14 | 127.59181 | YES | YES |
| 125 | a | 745.87 | 43.22491 | YES | YES |
| 126 | a | 747.61 | 35.75457 | YES | YES |
| 127 | a | 748.01 | 89.62476 | YES | YES |
| 128 | a | 749.22 | 128.24377 | YES | YES |
| 129 | a | 749.43 | 78.38238 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 130 | a | 749.60 | 59.32348 | YES | YES |
| 131 | a | 750.31 | 41.88187 | YES | YES |
| 132 | a | 750.32 | 19.15937 | YES | YES |
| 133 | a | 751.17 | 19.17517 | YES | YES |
| 134 | a | 751.62 | 40.76422 | YES | YES |
| 135 | a | 752.56 | 9.85453 | YES | YES |
| 136 | a | 753.37 | 64.16104 | YES | YES |
| 137 | a | 754.07 | 133.28967 | YES | YES |
| 138 | a | 755.68 | 227.86848 | YES | YES |
| 139 | a | 761.81 | 12.00802 | YES | YES |
| 140 | a | 816.07 | 5.17497 | YES | YES |
| 141 | a | 817.98 | 6.33392 | YES | YES |
| 142 | a | 818.95 | 13.42704 | YES | YES |
| 143 | a | 819.77 | 23.26121 | YES | YES |
| 144 | a | 826.58 | 19.71005 | YES | YES |
| 145 | a | 827.39 | 17.79510 | YES | YES |
| 146 | a | 827.85 | 27.56666 | YES | YES |
| 147 | a | 828.88 | 8.45173 | YES | YES |
| 148 | a | 832.94 | 0.91005 | YES | YES |
| 149 | a | 833.92 | 1.33747 | YES | YES |
| 150 | a | 836.67 | 0.06073 | YES | YES |
| 151 | a | 836.72 | 1.57636 | YES | YES |
| 152 | a | 837.79 | 0.73401 | YES | YES |
| 153 | a | 839.23 | 0.24402 | YES | YES |
| 154 | a | 840.97 | 1.37334 | YES | YES |
| 155 | a | 842.59 | 0.09192 | YES | YES |
| 156 | a | 924.26 | 2.37350 | YES | YES |
| 157 | a | 925.87 | 2.80442 | YES | YES |
| 158 | a | 927.61 | 5.65350 | YES | YES |
| 159 | a | 928.32 | 2.61207 | YES | YES |
| 160 | a | 929.87 | 2.45188 | YES | YES |
| 161 | a | 930.84 | 0.59323 | YES | YES |
| 162 | a | 931.86 | 0.70515 | YES | YES |
| 163 | a | 932.04 | 7.60241 | YES | YES |
| 164 | a | 972.47 | 0.05166 | YES | YES |
| 165 | a | 973.18 | 0.07314 | YES | YES |
| 166 | a | 974.16 | 0.00663 | YES | YES |
| 167 | a | 977.49 | 0.08939 | YES | YES |
| 168 | a | 977.76 | 0.07346 | YES | YES |
| 169 | a | 978.10 | 0.07445 | YES | YES |
| 170 | a | 979.65 | 0.01527 | YES | YES |
| 171 | a | 979.80 | 0.01704 | YES | YES |
| 172 | a | 1015.98 | 4.02951 | YES | YES |
| 173 | a | 1017.34 | 6.20912 | YES | YES |
| 174 | a | 1017.45 | 3.06620 | YES | YES |
| 175 | a | 1017.85 | 2.15010 | YES | YES |
| 176 | a | 1022.36 | 2.96376 | YES | YES |
| 177 | a | 1022.86 | 4.83163 | YES | YES |
| 178 | a | 1023.50 | 2.23927 | YES | YES |
| 179 | a | 1026.08 | 4.31639 | YES | YES |
| 180 | a | 1077.81 | 16.58676 | YES | YES |
| 181 | a | 1079.70 | 13.60400 | YES | YES |
| 182 | a | 1080.91 | 38.70175 | YES | YES |
| 183 | a | 1082.32 | 49.40236 | YES | YES |
| 184 | a | 1086.95 | 53.50158 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 185 | a | 1087.39 | 14.93527 | YES | YES |
| 186 | a | 1087.87 | 20.67573 | YES | YES |
| 187 | a | 1088.79 | 26.73194 | YES | YES |
| 188 | a | 1137.14 | 6.42494 | YES | YES |
| 189 | a | 1138.02 | 6.05137 | YES | YES |
| 190 | a | 1138.69 | 0.91050 | YES | YES |
| 191 | a | 1138.87 | 3.02154 | YES | YES |
| 192 | a | 1139.00 | 6.85202 | YES | YES |
| 193 | a | 1139.44 | 1.87184 | YES | YES |
| 194 | a | 1140.05 | 3.22363 | YES | YES |
| 195 | a | 1140.29 | 3.17975 | YES | YES |
| 196 | a | 1140.46 | 1.01881 | YES | YES |
| 197 | a | 1140.98 | 2.22886 | YES | YES |
| 198 | a | 1143.41 | 25.23709 | YES | YES |
| 199 | a | 1145.95 | 42.56018 | YES | YES |
| 200 | a | 1152.39 | 35.51222 | YES | YES |
| 201 | a | 1155.44 | 85.77020 | YES | YES |
| 202 | a | 1162.19 | 57.01703 | YES | YES |
| 203 | a | 1164.45 | 5.83251 | YES | YES |
| 204 | a | 1235.96 | 11.42343 | YES | YES |
| 205 | a | 1237.35 | 177.39111 | YES | YES |
| 206 | a | 1238.01 | 72.38970 | YES | YES |
| 207 | a | 1238.80 | 18.22370 | YES | YES |
| 208 | a | 1240.21 | 69.16162 | YES | YES |
| 209 | a | 1240.35 | 36.06904 | YES | YES |
| 210 | a | 1243.35 | 156.42746 | YES | YES |
| 211 | a | 1246.10 | 0.17758 | YES | YES |
| 212 | a | 1246.12 | 8.04176 | YES | YES |
| 213 | a | 1246.39 | 1.15933 | YES | YES |
| 214 | a | 1246.79 | 7.04731 | YES | YES |
| 215 | a | 1250.99 | 34.14822 | YES | YES |
| 216 | a | 1266.94 | 80.45049 | YES | YES |
| 217 | a | 1270.12 | 77.32678 | YES | YES |
| 218 | a | 1271.48 | 9.56281 | YES | YES |
| 219 | a | 1272.83 | 136.11234 | YES | YES |
| 220 | a | 1374.14 | 1.03703 | YES | YES |
| 221 | a | 1376.93 | 1.20446 | YES | YES |
| 222 | a | 1377.60 | 1.68473 | YES | YES |
| 223 | a | 1377.66 | 1.65699 | YES | YES |
| 224 | a | 1380.70 | 4.01182 | YES | YES |
| 225 | a | 1381.93 | 1.85255 | YES | YES |
| 226 | a | 1383.26 | 1.94245 | YES | YES |
| 227 | a | 1383.62 | 1.92053 | YES | YES |
| 228 | a | 1453.59 | 10.21149 | YES | YES |
| 229 | a | 1455.69 | 19.17319 | YES | YES |
| 230 | a | 1456.38 | 12.57782 | YES | YES |
| 231 | a | 1456.62 | 13.71409 | YES | YES |
| 232 | a | 1458.17 | 0.94239 | YES | YES |
| 233 | a | 1458.41 | 17.90035 | YES | YES |
| 234 | a | 1459.38 | 9.87295 | YES | YES |
| 235 | a | 1459.78 | 12.40830 | YES | YES |
| 236 | a | 1491.77 | 198.75431 | YES | YES |
| 237 | a | 1492.11 | 188.93000 | YES | YES |
| 238 | a | 1493.68 | 269.48638 | YES | YES |
| 239 | a | 1495.09 | 92.77024 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 240 | a | 1499.39 | 113.38756 | YES | YES |
| 241 | a | 1502.45 | 115.21100 | YES | YES |
| 242 | a | 1503.14 | 279.86302 | YES | YES |
| 243 | a | 1507.43 | 252.19120 | YES | YES |
| 244 | a | 1605.46 | 1.62378 | YES | YES |
| 245 | a | 1607.30 | 5.71898 | YES | YES |
| 246 | a | 1607.96 | 3.15184 | YES | YES |
| 247 | a | 1608.82 | 1.32574 | YES | YES |
| 248 | a | 1608.97 | 0.61874 | YES | YES |
| 249 | a | 1610.17 | 1.34637 | YES | YES |
| 250 | a | 1610.89 | 0.99409 | YES | YES |
| 251 | a | 1611.46 | 2.07496 | YES | YES |
| 252 | a | 1629.78 | 22.34416 | YES | YES |
| 253 | a | 1631.78 | 13.90763 | YES | YES |
| 254 | a | 1632.74 | 6.93468 | YES | YES |
| 255 | a | 1633.03 | 24.81998 | YES | YES |
| 256 | a | 1637.04 | 17.34278 | YES | YES |
| 257 | a | 1637.34 | 14.61006 | YES | YES |
| 258 | a | 1638.46 | 9.70899 | YES | YES |
| 259 | a | 1638.77 | 7.46999 | YES | YES |
| 260 | a | 3121.14 | 0.18153 | YES | YES |
| 261 | a | 3121.21 | 0.47784 | YES | YES |
| 262 | a | 3121.49 | 0.44317 | YES | YES |
| 263 | a | 3122.11 | 1.35743 | YES | YES |
| 264 | a | 3124.65 | 0.40641 | YES | YES |
| 265 | a | 3124.68 | 0.29375 | YES | YES |
| 266 | a | 3125.04 | 0.21702 | YES | YES |
| 267 | a | 3125.56 | 0.54018 | YES | YES |
| 268 | a | 3129.12 | 1.77560 | YES | YES |
| 269 | a | 3130.22 | 1.25630 | YES | YES |
| 270 | a | 3131.55 | 1.72639 | YES | YES |
| 271 | a | 3131.98 | 1.28550 | YES | YES |
| 272 | a | 3132.90 | 1.21639 | YES | YES |
| 273 | a | 3134.29 | 1.37643 | YES | YES |
| 274 | a | 3134.57 | 2.18880 | YES | YES |
| 275 | a | 3134.72 | 0.63888 | YES | YES |
| 276 | a | 3134.94 | 0.99132 | YES | YES |
| 277 | a | 3136.45 | 0.82683 | YES | YES |
| 278 | a | 3138.48 | 3.58419 | YES | YES |
| 279 | a | 3139.37 | 0.69832 | YES | YES |
| 280 | a | 3140.14 | 1.41813 | YES | YES |
| 281 | a | 3140.54 | 2.76679 | YES | YES |
| 282 | a | 3141.57 | 0.36275 | YES | YES |
| 283 | a | 3141.95 | 3.88206 | YES | YES |
| 284 | a | 3141.99 | 0.22745 | YES | YES |
| 285 | a | 3142.16 | 2.53532 | YES | YES |
| 286 | a | 3143.66 | 2.68544 | YES | YES |
| 287 | a | 3143.90 | 0.92989 | YES | YES |
| 288 | a | 3145.48 | 1.96605 | YES | YES |
| 289 | a | 3146.36 | 0.63419 | YES | YES |
| 290 | a | 3146.40 | 2.06558 | YES | YES |
| 291 | a | 3146.58 | 1.96782 | YES | YES |

[Ga(HMB)]$^{+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.71600 | 1.24015 | -0.03007 |
| C | 1.43182 | 0.00000 | -0.06345 |
| C | 0.71600 | -1.24015 | -0.03007 |
| C | -0.71591 | -1.23999 | -0.06345 |
| C | -1.43200 | 0.00000 | -0.03007 |
| C | -0.71591 | 1.23999 | -0.06345 |
| C | 1.47211 | 2.54977 | 0.01852 |
| C | -1.47082 | 2.54754 | -0.16722 |
| C | 2.94164 | 0.00000 | -0.16722 |
| C | 1.47211 | -2.54977 | 0.01852 |
| C | -1.47082 | -2.54754 | -0.16722 |
| C | -2.94422 | 0.00000 | 0.01852 |
| Ga | 0.00000 | 0.00000 | 2.29154 |
| H | 2.44365 | 2.44816 | 0.54073 |
| H | 1.68846 | 2.92449 | -1.00881 |
| H | 0.89834 | 3.34034 | 0.54073 |
| H | -2.42535 | 2.41975 | -0.71411 |
| H | -1.71841 | 2.97637 | 0.83103 |
| H | -0.88289 | 3.31029 | -0.71411 |
| H | 3.30824 | 0.89054 | -0.71411 |
| H | 3.43682 | 0.00000 | 0.83103 |
| H | 3.30824 | -0.89054 | -0.71411 |
| H | 2.44365 | -2.44816 | 0.54073 |
| H | 0.89834 | -3.34034 | 0.54073 |
| H | 1.68846 | -2.92449 | -1.00881 |
| H | -0.88289 | -3.31029 | -0.71411 |
| H | -1.71841 | -2.97637 | 0.83103 |
| H | -2.42535 | -2.41975 | -0.71411 |
| H | -3.34199 | -0.89218 | 0.54073 |
| H | -3.34199 | 0.89218 | 0.54073 |
| H | -3.37692 | 0.00000 | -1.00881 |

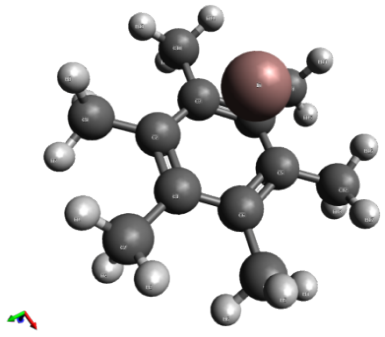
Vibrational analysis

| 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 | a2 | 17.10 | 0.00000 | NO | NO |

| | | | | | |
|---|---|---|---|---|---|
| 8 | e | 39.29 | 0.40972 | YES | YES |
| 9 | e | 39.29 | 0.40972 | YES | YES |
| 10 | e | 95.69 | 0.02304 | YES | YES |
| 11 | e | 95.69 | 0.02304 | YES | YES |
| 12 | e | 110.47 | 0.10515 | YES | YES |
| 13 | e | 110.47 | 0.10515 | YES | YES |
| 14 | a2 | 133.38 | 0.00000 | NO | NO |
| 15 | e | 145.87 | 0.59474 | YES | YES |
| 16 | e | 145.87 | 0.59474 | YES | YES |
| 17 | a1 | 162.14 | 0.04559 | YES | YES |
| 18 | a1 | 168.64 | 0.25698 | YES | YES |
| 19 | e | 342.61 | 0.13378 | YES | YES |
| 20 | e | 342.61 | 0.13378 | YES | YES |
| 21 | a1 | 355.03 | 58.38031 | YES | YES |
| 22 | e | 381.99 | 0.18164 | YES | YES |
| 23 | e | 381.99 | 0.18164 | YES | YES |
| 24 | e | 405.37 | 0.00392 | YES | YES |
| 25 | e | 405.37 | 0.00392 | YES | YES |
| 26 | e | 443.47 | 0.00282 | YES | YES |
| 27 | e | 443.47 | 0.00282 | YES | YES |
| 28 | a2 | 445.45 | 0.00000 | NO | NO |
| 29 | a1 | 554.53 | 0.02623 | YES | YES |
| 30 | e | 554.73 | 2.01013 | YES | YES |
| 31 | e | 554.73 | 2.01013 | YES | YES |
| 32 | a2 | 573.50 | 0.00000 | NO | NO |
| 33 | a1 | 582.40 | 1.63982 | YES | YES |
| 34 | a1 | 681.61 | 0.34470 | YES | YES |
| 35 | e | 797.63 | 3.18282 | YES | YES |
| 36 | e | 797.63 | 3.18282 | YES | YES |
| 37 | e | 958.63 | 0.00605 | YES | YES |
| 38 | e | 958.63 | 0.00605 | YES | YES |
| 39 | a1 | 974.40 | 1.47265 | YES | YES |
| 40 | a2 | 975.95 | 0.00000 | NO | NO |
| 41 | e | 999.64 | 0.35826 | YES | YES |
| 42 | e | 999.64 | 0.35826 | YES | YES |
| 43 | e | 1023.60 | 6.37292 | YES | YES |
| 44 | e | 1023.60 | 6.37292 | YES | YES |
| 45 | a1 | 1025.73 | 0.09295 | YES | YES |
| 46 | e | 1054.11 | 15.66944 | YES | YES |
| 47 | e | 1054.11 | 15.66944 | YES | YES |
| 48 | a2 | 1076.05 | 0.00000 | NO | NO |
| 49 | e | 1076.90 | 0.01781 | YES | YES |
| 50 | e | 1076.90 | 0.01781 | YES | YES |
| 51 | a1 | 1259.21 | 0.75813 | YES | YES |
| 52 | a1 | 1308.15 | 11.04513 | YES | YES |
| 53 | a2 | 1317.65 | 0.00000 | NO | NO |
| 54 | e | 1359.07 | 0.24696 | YES | YES |
| 55 | e | 1359.07 | 0.24696 | YES | YES |
| 56 | a1 | 1366.04 | 3.67542 | YES | YES |
| 57 | e | 1366.58 | 21.64440 | YES | YES |
| 58 | e | 1366.58 | 21.64440 | YES | YES |
| 59 | a1 | 1372.68 | 3.32361 | YES | YES |
| 60 | e | 1378.72 | 9.47173 | YES | YES |
| 61 | e | 1378.72 | 9.47173 | YES | YES |
| 62 | e | 1398.03 | 0.15370 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 63 | e | 1398.03 | 0.15370 | YES | YES |
| 64 | a1 | 1416.50 | 67.35523 | YES | YES |
| 65 | a2 | 1417.77 | 0.00000 | NO | NO |
| 66 | a2 | 1428.30 | 0.00000 | NO | NO |
| 67 | e | 1434.07 | 0.08650 | YES | YES |
| 68 | e | 1434.07 | 0.08650 | YES | YES |
| 69 | e | 1444.20 | 81.64438 | YES | YES |
| 70 | e | 1444.20 | 81.64438 | YES | YES |
| 71 | e | 1464.00 | 0.10035 | YES | YES |
| 72 | e | 1464.00 | 0.10035 | YES | YES |
| 73 | a1 | 1479.00 | 0.00673 | YES | YES |
| 74 | e | 1538.80 | 0.22939 | YES | YES |
| 75 | e | 1538.80 | 0.22939 | YES | YES |
| 76 | a1 | 2952.12 | 0.00919 | YES | YES |
| 77 | e | 2952.45 | 1.44287 | YES | YES |
| 78 | e | 2952.45 | 1.44287 | YES | YES |
| 79 | e | 2953.95 | 0.55182 | YES | YES |
| 80 | e | 2953.95 | 0.55182 | YES | YES |
| 81 | a1 | 2954.73 | 0.10959 | YES | YES |
| 82 | a1 | 3040.81 | 1.92025 | YES | YES |
| 83 | e | 3042.37 | 0.76562 | YES | YES |
| 84 | e | 3042.37 | 0.76562 | YES | YES |
| 85 | e | 3047.27 | 2.00782 | YES | YES |
| 86 | e | 3047.27 | 2.00782 | YES | YES |
| 87 | a1 | 3049.78 | 0.46181 | YES | YES |
| 88 | a2 | 3071.98 | 0.00000 | NO | NO |
| 89 | e | 3075.33 | 4.90670 | YES | YES |
| 90 | e | 3075.33 | 4.90670 | YES | YES |
| 91 | e | 3082.19 | 0.08931 | YES | YES |
| 92 | e | 3082.19 | 0.08931 | YES | YES |
| 93 | a2 | 3084.04 | 0.00000 | NO | NO |

[In(HMB)]$^{+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.3666003 | 1.3837988 | 0.0218599 |
| C | -1.0137973 | 1.0102967 | 0.0502848 |
| C | -1.3817050 | -0.3744142 | 0.0218599 |
| C | -0.3680439 | -1.3831226 | 0.0502848 |
| C | 1.0151047 | -1.0093845 | 0.0218599 |
| C | 1.3818413 | 0.3728259 | 0.0502848 |
| C | 0.7682516 | 2.8434543 | -0.0016915 |
| C | 2.8345355 | 0.7851011 | 0.1678604 |

| | | | |
|---|---|---|---|
| C | -2.0971852 | 2.0622292 | 0.1678604 |
| C | -2.8466294 | -0.7564017 | -0.0016915 |
| C | -0.7373503 | -2.8473302 | 0.1678604 |
| C | 2.0783778 | -2.0870525 | -0.0016915 |
| In | 0.0000000 | 0.0000000 | -2.5706268 |
| H | 0.0305095 | 3.4712954 | -0.5391957 |
| H | 0.8549253 | 3.2516176 | 1.0320829 |
| H | 1.7494979 | 2.9958453 | -0.4924493 |
| H | 3.4730782 | -0.0396070 | 0.5357104 |
| H | 3.2620635 | 1.1292891 | -0.8016013 |
| H | 2.9464114 | 1.6250738 | 0.8840150 |
| H | -1.7022384 | 3.0275774 | 0.5357104 |
| H | -2.6090248 | 2.2603853 | -0.8016013 |
| H | -2.8805609 | 1.7391302 | 0.8840150 |
| H | -3.4692270 | 0.0171870 | -0.4924493 |
| H | -3.0214847 | -1.7092257 | -0.5391957 |
| H | -3.2434461 | -0.8854218 | 1.0320829 |
| H | -1.7708398 | -2.9879704 | 0.5357104 |
| H | -0.6530387 | -3.3896744 | -0.8016013 |
| H | -0.0658505 | -3.3642040 | 0.8840150 |
| H | 1.7197292 | -3.0130322 | -0.4924493 |
| H | 2.9909752 | -1.7620697 | -0.5391957 |
| H | 2.3885208 | -2.3661958 | 1.0320829 |

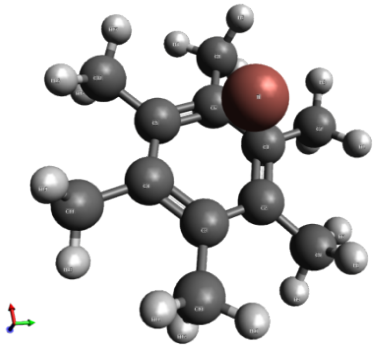
Vibrational analysis

| 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 | e | 63.36 | 0.15536 | YES | YES |
| 8 | e | 63.36 | 0.15536 | YES | YES |
| 9 | a | 63.91 | 0.69001 | YES | YES |
| 10 | e | 80.65 | 0.01268 | YES | YES |
| 11 | e | 80.65 | 0.01268 | YES | YES |
| 12 | e | 116.64 | 0.08450 | YES | YES |
| 13 | e | 116.64 | 0.08450 | YES | YES |
| 14 | a | 127.47 | 0.02175 | YES | YES |
| 15 | e | 143.75 | 0.48247 | YES | YES |
| 16 | e | 143.75 | 0.48247 | YES | YES |
| 17 | a | 154.02 | 0.16327 | YES | YES |
| 18 | a | 168.94 | 0.02109 | YES | YES |
| 19 | a | 319.50 | 55.67923 | YES | YES |
| 20 | e | 341.11 | 0.19766 | YES | YES |
| 21 | e | 341.11 | 0.19766 | YES | YES |
| 22 | e | 375.47 | 0.38772 | YES | YES |
| 23 | e | 375.47 | 0.38772 | YES | YES |
| 24 | e | 403.47 | 0.01758 | YES | YES |
| 25 | e | 403.47 | 0.01758 | YES | YES |
| 26 | a | 442.06 | 0.02164 | YES | YES |
| 27 | e | 443.58 | 0.00779 | YES | YES |
| 28 | e | 443.58 | 0.00779 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 29 | a | 553.10 | 0.71898 | YES | YES |
| 30 | e | 560.74 | 1.58312 | YES | YES |
| 31 | e | 560.74 | 1.58312 | YES | YES |
| 32 | a | 570.54 | 0.01602 | YES | YES |
| 33 | a | 581.74 | 1.40352 | YES | YES |
| 34 | a | 689.44 | 0.31655 | YES | YES |
| 35 | e | 795.85 | 4.03007 | YES | YES |
| 36 | e | 795.85 | 4.03007 | YES | YES |
| 37 | e | 957.43 | 0.32185 | YES | YES |
| 38 | e | 957.43 | 0.32185 | YES | YES |
| 39 | a | 973.23 | 0.02270 | YES | YES |
| 40 | a | 976.06 | 1.77019 | YES | YES |
| 41 | e | 999.87 | 1.02606 | YES | YES |
| 42 | e | 999.87 | 1.02606 | YES | YES |
| 43 | e | 1024.05 | 5.07655 | YES | YES |
| 44 | e | 1024.05 | 5.07655 | YES | YES |
| 45 | a | 1024.84 | 0.06914 | YES | YES |
| 46 | e | 1052.84 | 14.23618 | YES | YES |
| 47 | e | 1052.84 | 14.23618 | YES | YES |
| 48 | e | 1076.14 | 0.15584 | YES | YES |
| 49 | e | 1076.14 | 0.15584 | YES | YES |
| 50 | a | 1076.34 | 0.32286 | YES | YES |
| 51 | a | 1257.78 | 0.59222 | YES | YES |
| 52 | a | 1301.86 | 12.13487 | YES | YES |
| 53 | a | 1314.90 | 4.38497 | YES | YES |
| 54 | e | 1359.62 | 0.01585 | YES | YES |
| 55 | e | 1359.62 | 0.01585 | YES | YES |
| 56 | e | 1366.14 | 19.28903 | YES | YES |
| 57 | e | 1366.14 | 19.28903 | YES | YES |
| 58 | a | 1366.98 | 1.93926 | YES | YES |
| 59 | a | 1373.80 | 1.61410 | YES | YES |
| 60 | e | 1380.89 | 10.66879 | YES | YES |
| 61 | e | 1380.89 | 10.66879 | YES | YES |
| 62 | e | 1401.37 | 2.06593 | YES | YES |
| 63 | e | 1401.37 | 2.06593 | YES | YES |
| 64 | a | 1414.57 | 52.81971 | YES | YES |
| 65 | a | 1418.18 | 2.54136 | YES | YES |
| 66 | a | 1432.67 | 12.24236 | YES | YES |
| 67 | e | 1432.97 | 1.38001 | YES | YES |
| 68 | e | 1432.97 | 1.38001 | YES | YES |
| 69 | e | 1443.51 | 68.92992 | YES | YES |
| 70 | e | 1443.51 | 68.92992 | YES | YES |
| 71 | e | 1462.58 | 3.44274 | YES | YES |
| 72 | e | 1462.58 | 3.44274 | YES | YES |
| 73 | a | 1477.15 | 0.04358 | YES | YES |
| 74 | e | 1540.09 | 0.60628 | YES | YES |
| 75 | e | 1540.09 | 0.60628 | YES | YES |
| 76 | a | 2951.24 | 0.07607 | YES | YES |
| 77 | e | 2951.32 | 3.59803 | YES | YES |
| 78 | e | 2951.32 | 3.59803 | YES | YES |
| 79 | e | 2953.29 | 2.47249 | YES | YES |
| 80 | e | 2953.29 | 2.47249 | YES | YES |
| 81 | a | 2953.81 | 0.03569 | YES | YES |
| 82 | a | 3034.32 | 3.16001 | YES | YES |
| 83 | e | 3035.26 | 0.14199 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 84 | e | 3035.26 | 0.14199 | YES | YES |
| 85 | e | 3042.02 | 2.65967 | YES | YES |
| 86 | e | 3042.02 | 2.65967 | YES | YES |
| 87 | a | 3043.46 | 0.04502 | YES | YES |
| 88 | a | 3071.45 | 0.06419 | YES | YES |
| 89 | e | 3073.14 | 4.90370 | YES | YES |
| 90 | e | 3073.14 | 4.90370 | YES | YES |
| 91 | e | 3087.10 | 2.87759 | YES | YES |
| 92 | e | 3087.10 | 2.87759 | YES | YES |
| 93 | a | 3087.74 | 0.38896 | YES | YES |

[Tl(HMB)]$^{+}$



Atomic coordinates

| | | | |
|---|---|---|---|
| C | 0.36616 | 1.38255 | 0.01930 |
| C | -1.01300 | 1.00939 | 0.04666 |
| C | -1.38041 | -0.37418 | 0.01930 |
| C | -0.36766 | -1.38198 | 0.04666 |
| C | 1.01425 | -1.00838 | 0.01930 |
| C | 1.38066 | 0.37258 | 0.04666 |
| C | 0.76828 | 2.84281 | 0.00155 |
| C | 2.83350 | 0.78521 | 0.17040 |
| C | -2.09676 | 2.06128 | 0.17040 |
| C | -2.84608 | -0.75605 | 0.00155 |
| C | -0.73674 | -2.84648 | 0.17040 |
| C | 2.07780 | -2.08675 | 0.00155 |
| Tl | 0.00000 | 0.00000 | -2.65388 |
| H | 0.03096 | 3.47350 | -0.53334 |
| H | 0.85567 | 3.24827 | 1.03634 |
| H | 1.74970 | 2.99728 | -0.48853 |
| H | 3.47115 | -0.03999 | 0.53892 |
| H | 3.26619 | 1.13244 | -0.79573 |
| H | 2.94326 | 1.62316 | 0.88931 |
| H | -1.70094 | 3.02609 | 0.53892 |
| H | -2.61382 | 2.26238 | -0.79573 |
| H | -2.87733 | 1.73736 | 0.88931 |
| H | -3.47057 | 0.01665 | -0.48853 |
| H | -3.02362 | -1.70994 | -0.53334 |
| H | -3.24092 | -0.88310 | 1.03634 |
| H | -1.77020 | -2.98611 | 0.53892 |
| H | -0.65237 | -3.39482 | -0.79573 |
| H | -0.06593 | -3.36052 | 0.88931 |
| H | 1.72087 | -3.01392 | -0.48853 |

| | | | |
|---|---|---|---|
| H | 2.99266 | -1.76356 | -0.53334 |
| H | 2.38525 | -2.36516 | 1.03634 |

Vibrational analysis

| 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 | 60.39 | 0.70805 | YES | YES |
| 8 | e | 60.39 | 0.19844 | YES | YES |
| 9 | e | 60.39 | 0.19844 | YES | YES |
| 10 | e | 73.06 | 0.00644 | YES | YES |
| 11 | e | 73.06 | 0.00644 | YES | YES |
| 12 | e | 114.73 | 0.06845 | YES | YES |
| 13 | e | 114.73 | 0.06845 | YES | YES |
| 14 | a | 123.12 | 0.07466 | YES | YES |
| 15 | a | 126.48 | 0.39903 | YES | YES |
| 16 | e | 141.84 | 0.46741 | YES | YES |
| 17 | e | 141.84 | 0.46741 | YES | YES |
| 18 | a | 166.62 | 0.28166 | YES | YES |
| 19 | a | 260.30 | 42.54619 | YES | YES |
| 20 | e | 340.87 | 0.29990 | YES | YES |
| 21 | e | 340.87 | 0.29990 | YES | YES |
| 22 | e | 371.38 | 0.15785 | YES | YES |
| 23 | e | 371.38 | 0.15785 | YES | YES |
| 24 | e | 403.32 | 0.01471 | YES | YES |
| 25 | e | 403.32 | 0.01471 | YES | YES |
| 26 | a | 441.94 | 0.02767 | YES | YES |
| 27 | e | 443.86 | 0.00306 | YES | YES |
| 28 | e | 443.86 | 0.00306 | YES | YES |
| 29 | a | 551.69 | 1.25437 | YES | YES |
| 30 | e | 566.86 | 1.79321 | YES | YES |
| 31 | e | 566.86 | 1.79321 | YES | YES |
| 32 | a | 570.34 | 0.02776 | YES | YES |
| 33 | a | 581.80 | 1.27091 | YES | YES |
| 34 | a | 697.13 | 0.32428 | YES | YES |
| 35 | e | 795.74 | 3.60868 | YES | YES |
| 36 | e | 795.74 | 3.60868 | YES | YES |
| 37 | e | 957.32 | 0.35311 | YES | YES |
| 38 | e | 957.32 | 0.35311 | YES | YES |
| 39 | a | 972.53 | 0.00258 | YES | YES |
| 40 | a | 975.58 | 2.19303 | YES | YES |
| 41 | e | 1000.01 | 0.93577 | YES | YES |
| 42 | e | 1000.01 | 0.93577 | YES | YES |
| 43 | e | 1025.40 | 5.38191 | YES | YES |
| 44 | e | 1025.40 | 5.38191 | YES | YES |
| 45 | a | 1027.20 | 0.06546 | YES | YES |
| 46 | e | 1052.25 | 14.60630 | YES | YES |
| 47 | e | 1052.25 | 14.60630 | YES | YES |
| 48 | e | 1075.65 | 0.17913 | YES | YES |
| 49 | e | 1075.65 | 0.17913 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 50 | a | 1076.20 | 0.32599 | YES | YES |
| 51 | a | 1256.23 | 0.56791 | YES | YES |
| 52 | a | 1300.25 | 13.67261 | YES | YES |
| 53 | a | 1315.42 | 3.31159 | YES | YES |
| 54 | e | 1360.09 | 0.20497 | YES | YES |
| 55 | e | 1360.09 | 0.20497 | YES | YES |
| 56 | e | 1367.02 | 15.61416 | YES | YES |
| 57 | e | 1367.02 | 15.61416 | YES | YES |
| 58 | a | 1367.13 | 1.05155 | YES | YES |
| 59 | a | 1374.87 | 1.73172 | YES | YES |
| 60 | e | 1382.73 | 8.44395 | YES | YES |
| 61 | e | 1382.73 | 8.44395 | YES | YES |
| 62 | e | 1402.75 | 1.98370 | YES | YES |
| 63 | e | 1402.75 | 1.98370 | YES | YES |
| 64 | a | 1414.80 | 53.11522 | YES | YES |
| 65 | a | 1418.78 | 1.32809 | YES | YES |
| 66 | e | 1433.28 | 1.25467 | YES | YES |
| 67 | e | 1433.28 | 1.25467 | YES | YES |
| 68 | a | 1433.43 | 11.85460 | YES | YES |
| 69 | e | 1444.48 | 66.23854 | YES | YES |
| 70 | e | 1444.48 | 66.23854 | YES | YES |
| 71 | e | 1462.65 | 3.48599 | YES | YES |
| 72 | e | 1462.65 | 3.48599 | YES | YES |
| 73 | a | 1477.13 | 0.00821 | YES | YES |
| 74 | e | 1543.60 | 0.57413 | YES | YES |
| 75 | e | 1543.60 | 0.57413 | YES | YES |
| 76 | a | 2950.28 | 0.11260 | YES | YES |
| 77 | e | 2950.35 | 5.77681 | YES | YES |
| 78 | e | 2950.35 | 5.77681 | YES | YES |
| 79 | e | 2952.12 | 3.23338 | YES | YES |
| 80 | e | 2952.12 | 3.23338 | YES | YES |
| 81 | a | 2952.67 | 0.00007 | YES | YES |
| 82 | a | 3032.69 | 4.48845 | YES | YES |
| 83 | e | 3033.69 | 0.21129 | YES | YES |
| 84 | e | 3033.69 | 0.21129 | YES | YES |
| 85 | e | 3040.13 | 3.02094 | YES | YES |
| 86 | e | 3040.13 | 3.02094 | YES | YES |
| 87 | a | 3041.66 | 0.04557 | YES | YES |
| 88 | a | 3069.14 | 0.07450 | YES | YES |
| 89 | e | 3070.86 | 6.10208 | YES | YES |
| 90 | e | 3070.86 | 6.10208 | YES | YES |
| 91 | e | 3085.74 | 3.32557 | YES | YES |
| 92 | e | 3085.74 | 3.32557 | YES | YES |
| 93 | a | 3086.33 | 0.43237 | YES | YES |

# S-4 References


1 J. Cosier and A. M. Glazer, *J. Appl. Crystallogr.*, 1986, **19**, 105–107.

2 a) G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 2008, **64**, 112–122; b) D. Kratzert, J. J. Holstein and I. Krossing, *J. Appl. Crystallogr.*, 2015, **48**, 933–938;

3 Daniel Kratzert, available at: https://www.xs3.uni-freiburg.de/research/finalcif.

4 G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176–2179.

5 a) M. von Arnim and R. Ahlrichs, *J. Chem. Phys.*, 1999, **111**, 9183–9190; b) Becke, *Physical review. A, General physics*, 1988, **38**, 3098–3100; c) A. Schäfer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571–2577; d) H. Schröder, A. Creon and T. Schwabe, *J. Chem. Theory Comput.*, 2015, **11**, 3163–3170; e) R. Ahlrichs, M. Bär, M. Häser, H. Horn and C. Kölmel, *Chem. Phys. Lett.*, 1989, **162**, 165–169;

6 P. Deglmann, F. Furche and R. Ahlrichs, *Chem. Phys. Lett.*, 2002, **362**, 511–518.

7 A. E. Reed, R. B. Weinstock and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 735–746.

8 C. Ehrhardt and R. Ahlrichs, *Theor. Chim. Acta*, 1985, **68**, 231–245.

9 R. F. W. Bader, *Chem. Rev.*, 1991, **91**, 893–928.

10 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.

11 A. Klamt and G. Schüürmann, *J. Chem. Soc., Perkin Trans. 2*, 1993, 799–805.

12 M. Schorpp, S. Rein, S. Weber, H. Scherer and I. Krossing, *Chem. Commun.*, 2018, **54**, 10036–10039.