# Supporting Information

## *Bis(amidophenolate)-supported Pnictoranides: Lewis Acid-induced Electromerism in a Bismuth Complex*

Simon B. H. Karnbrock,[a] Jan F. Köster,[a] Isabelle Becker,[b] Christopher Golz, [a] Franc Meyer,[b] Martí Gimferrer,[c] and Manuel Alcarazo *[a]

[a] Institute of Organic and Biomolecular Chemistry, University of Göttingen, Tammanstraße 2, 37077 Göttingen, Germany.

[b] Institute of Inorganic Chemistry, University of Göttingen, Tammanstraße 4, 37077 Göttingen, Germany.

[c] Institute of Physical Chemistry, University of Göttingen, Tammanstraße 6, 37077 Göttingen, Germany.

* corresponding author, E-mail: manuel.alcarazo@chemie.uni-goettingen.de

## Contents

## General Information

Working methods:

Unless otherwise stated, all manipulations were carried out under a nitrogen atmosphere in flame-dried glassware on a Schlenk line or under nitrogen atmosphere in an MBraun UNIlab plus glovebox. Dry solvents were obtained using an MBraun MB-SPS-7 solvent purification system (THF, diethyl ether, toluene, pentane, dichloromethane, acetonitrile), deoxygenated in a nitrogen stream and stored over 3 Å molecular sieves under a nitrogen atmosphere. Benzene was distilled over Na/benzophenone and stored over a Na-mirror. 1,2-Dichlorobenzene (*o*DCB), $CHCl_3$ and fluorobenzene were deoxygenated in a nitrogen stream and dried over 3 Å molecular sieves under a nitrogen atmosphere.

Starting materials:

Unless otherwise specified, all reagents were used as received from commercial suppliers (ABCR, AcrosOrganics, Alfa Aesar, Chempur GmbH, J and K Scientific, Sigma Aldrich, Thermo Fisher Scientific, Tokyo Chemical Industry). Triethylamine and DIPEA were dried over 3 Å molecular sieves and deoxygenated in a nitrogen stream. $SbCl_3$ and $BiCl_3$ were purified under nitrogen atmosphere by sublimation at 80 °C and $10^{-3}$ mbar and stored in a nitrogen-filled glovebox. *N,N'*-bis(3,5-di-*tert*-butyl-2-hydroxyphenyl)-1,2-phenylenediamine (**1**),[1] $Bi(NMe_2)_3$,[2] **2a**,[3] **2b**,[4] **3b**,[4] $CpFe(CO)_2I$[5] and $CpFe(CO)_2(thf)BF_4$[6] were synthesized according to the published procedures.

NMR spectroscopy:

The NMR spectra were recorded on a Bruker Avance III 300 MHz, Bruker Avance III HD 300 MHz, Bruker Avance III 400, Bruker Avance III HD 400 MHz or Bruker Avance Neo 400 MHz at 298 K. $^{1}H$ and $^{13}C$ chemical shifts are given in ppm relative to TMS, using the solvent signals as references and converting the chemical shifts to the TMS scale. $^{11}B$ and $^{19}F$ chemical shifts are given in ppm relative to $BF_3{\cdot}OEt_2$ and $CFCl_3$, respectively (external standard). The chemical shifts are given in parts per million (ppm), and the coupling constants (*J*) in Hertz (Hz). Solvents for NMR spectroscopy were deoxygenated in a nitrogen stream or alternatively by three freeze-pump-thaw cycles and stored over 3 Å molecular sieves in a glove box.

Mass spectrometry:

Mass spectrometry analyses were performed using the following equipment: Bruker Daltronik microTOF (ESI), Bruker Daltronik maXis (ESI), Joel AccuTOF (LIFDI).

Infrared spectroscopy:

Neat samples were measured on a JASCO FT/IR-4100 or JASCO FT/IR-4600 at room temperature. The vibrational frequencies are reported in wavenumbers ($cm^{-1}$). Solution state spectra were recorded at a concentration of 1 mg/mL in DCM.

UV/vis spectroscopy:

UV/vis spectra were measured on a Jasco J-1500 spectrometer using a 10 mm quartz sample cell with a Teflon cap. Dried and deoxygenated solvents were used, and measurements were performed at ambient temperature.

Elemental analyses:

Elemental analyses were obtained from the Analytisches Labor, Georg-August-Universität, Göttingen, using an Elementar Vario EL 3 analyzer.

Mössbauer spectroscopy:

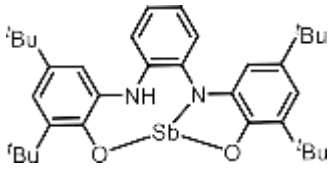
Zero-field $^{57}$Fe Mössbauer spectra were recorded with a $^{57}$Co source in a Rh matrix using an alternating constant acceleration Wissel Mössbauer spectrometer operated in the transmission mode and equipped with a Janis closed-cycle helium cryostat. Isomer shifts are given relative to iron metal at ambient temperature. Simulation of the experimental data was performed with the mf2.SL program (E. Bill, Max-Planck Institute for Chemical Energy Conversion, Mülheim/Ruhr, Germany) using Lorentzian line doublets.

Cyclic voltammetry:

Cyclic voltammetry was performed in a nitrogen-filled glovebox using a WaveNow wireless potentiostat (Pine Research) in combination with the Aftermath Blue software (version 2.1.13189). A standard three electrode setup was used with a platinum working electrode, a platinum counter electrode and a silver/silver chloride pseudo-reference electrode. Internal referencing was performed to ferrocene or cobaltocene.

## Experimental Procedures

Synthesis of Stibine **2c**




A Schlenk flask equipped with a magnetic stirring bar was charged with **1** (250 mg, 484 µmol, 1.00 equiv.). Afterwards $Et_2O$ (5 mL) was added, and the solution was cooled to –78 °C using a dry ice/acetone bath. $NEt_3$ (202 µL, 1.45 mmol, 3.00 equiv.) was added *via* syringe. $SbCl_3$ (110 mg, 484 µmol, 1.00 equiv.) in $Et_2O$ (1 mL) was added slowly *via* syringe under rigorous stirring resulting in the formation of a colorless precipitate. The mixture was allowed to warm to room temperature over the course of 3 h. The mixture was filtered and extracted with $Et_2O$ (2 x 2 mL). All volatiles were removed *in vacuo* to yield the title compound as a yellow solid (289 mg, 455 µmol, 94%).

**m. p.** 127 °C (decomp.).

**$^1$H NMR** (400 MHz, $CD_2Cl_2$): δ (ppm) = 7.65 – 7.59 (m, 1H), 7.57 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.31 – 7.22 (m, 2H), 7.19 (d, *J* = 2.4 Hz, 1H), 7.16 (d, *J* = 2.4 Hz, 1H), 6.90 (td, *J* = 7.6, 1.3 Hz, 1H), 6.81 (d, *J* = 2.2 Hz, 1H), 5.11 (s, 1H), 1.48 (s, 9H), 1.26 (s, 9H), 1.25 (s, 9H), 1.20 (s, 9H).

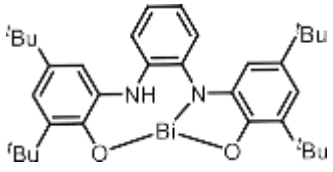
**$^{13}$C{$^1$H} NMR** (101 MHz, $CD_2Cl_2$): δ (ppm) = 154.6, 150.0, 142.3, 141.7, 140.4, 140.4, 136.5, 135.6, 135.1, 130.1, 128.6, 125.6, 124.3, 121.1, 120.2, 118.4, 115.1, 106.8, 35.8, 35.4, 34.9, 34.8, 32.2, 31.8, 30.0, 29.7.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 3206, 2952, 2904, 2866, 1596, 1566, 1488, 1470, 1420, 1359, 1337, 1236, 1120, 995, 829, 741, 666, 586, 545, 499.

**HR-MS-ESI(+)** m/z calcd. for $C_{34}H_{45}N_2O_2SbNa^+$ $[M+Na]^+$ 634.2513, found 634.2544.

**Anal.** calcd. for $C_{34}H_{45}N_2O_2Sb$: C 64.26, H 7.14, N 4.41, found: C 64.28, H 7.25, N 4.49.

Synthesis of Bismuthine **2d**




A Schlenk flask equipped with a magnetic stirring bar was charged with **1** (2.00 g, 3.87 mmol, 1.00 equiv.). Afterwards $Et_2O$ (12 mL) was added, and the solution was cooled to –78 °C using a dry ice/acetone bath. A solution of $Bi(NMe_2)_3$ (1.32 g, 3.87 mmol, 1.00 equiv.) in $Et_2O$ (5.0 mL) was cooled to –78 °C and added slowly *via* cannula resulting in a color change to red. The mixture was allowed to warm to room temperature over the course of 30 min. All volatiles were removed *in vacuo* to yield the title compound as an orange solid (2.49 g, 3.45 mmol, 89%).

**m. p.** 182 °C (decomposition).

**$^1$H NMR** (300 MHz, $C_6D_6$): δ (ppm) = 7.67 (d, *J* = 8.2 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.14 – 7.09 (m, 3H), 6.86 (d, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 2.3 Hz, 1H), 6.55 (t, *J* = 7.3 Hz, 1H), 3.12 (s, 1H), 1.93 (s, 9H), 1.48 (s, 9H), 1.17 (s, 9H), 1.10 (s, 9H).

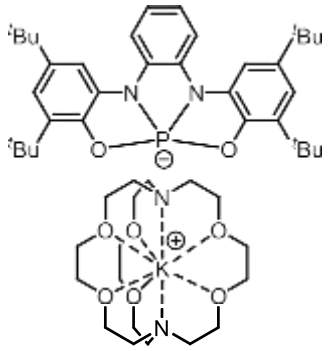
**$^{13}$C{$^1$H} NMR** (101 MHz, $C_6D_6$): δ (ppm) = 157.2, 155.0, 146.3, 142.7, 142.5, 139.8, 139.6, 139.0, 136.8, 134.4, 127.1, 124.6, 123.5, 122.3, 119.0, 118.9, 115.3, 112.4, 35.5, 35.3, 34.2, 34.1, 32.1, 31.7, 30.4, 30.0.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 3310, 2958, 2904, 2868, 1592, 1548, 1479, 1434, 1415, 1354, 1335, 1303, 1238, 1200, 1126, 1038, 992, 964, 922, 903, 858, 835, 824, 807, 754, 739, 678, 650, 602, 579, 533, 487, 457.

**HR-MS-ESI(+)** m/z calcd. for $C_{34}H_{45}N_2O_2Bi^+$ $[M]^+$ 722.3279, found 722.3265.

**Anal.** calcd. for $C_{34}H_{45}N_2O_2Bi$: C 56.50, H 6.28, N 3.88, found: C 56.65, H 6.54, N 3.66.

## Synthesis of Potassium Phosphoranide **3a**



In a Schlenk flask containing a magnetic stirring bar, **2a** (300 mg, 551 µmol, 1.00 equiv.) and [2.2.2]-cryptand (207 mg, 551 µmol, 1.00 equiv.) were dissolved in $Et_2O$ (6 mL). KHMDS (110 mg, 551 µmol, 1.00 equiv.) in $Et_2O$ (2 mL) was added dropwise *via* syringe under rigorous stirring resulting in precipitation of a white solid. The mixture was stirred for 20 min at room temperature. Afterwards, the mixture was filtered and washed with $Et_2O$ (2 x 2 mL). The residue was dried *in vacuo* to yield the target compound as a pale yellow solid (425 mg, 443 µmol, 81%).

**m. p.** 123 °C.

**$^1$H NMR** (400 MHz, $C_6D_6$): δ (ppm) = 7.60 – 7.54 (m, 2H), 7.50 (d, *J* = 2.1 Hz, 2H), 6.99 (d, *J* = 2.0 Hz, 2H), 6.97 – 6.92 (m, 2H), 2.96 (s, 12H), 2.88 (t, *J* = 4.7 Hz, 12H), 1.92 (t, *J* = 4.7 Hz, 12H), 1.83 – 1.78 (m, 18H), 1.50 (s, 18H).

**$^{13}$C{$^1$H} NMR** (101 MHz, $C_6D_6$): δ (ppm) = 147.5 (d, *J* = 8.7 Hz), 138.8 (d, *J* = 7.1 Hz), 138.6, 137.0 (d, *J* = 1.8 Hz), 131.2 (d, *J* = 2.6 Hz), 118.2, 112.9, 111.5, 107.0, 70.23, 67.5, 53.7, 35.1, 34.9, 32.6, 30.5.

**$^{31}$P{$^1$H} NMR** (162 MHz, $C_6D_6$): δ 76.6.

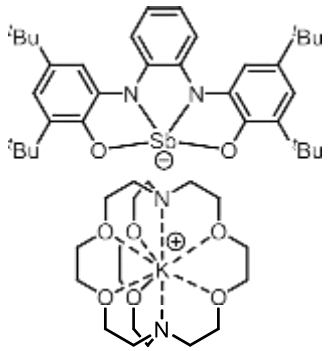
**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2951, 2869, 2813, 1577, 1560, 1475, 1435, 1354, 1290, 1259, 1100, 996, 948, 829, 724, 537, 475.

**HR-MS-ESI(–)** *m*/*z* calcd. for $C_{34}H_{46}N_2O_3P^-$ $[M–K\text{-crypt}+H_2O]^-$ 561.3252, found 561.3247.

**Anal.** calcd. for $C_{52}H_{80}PKN_4O_8$: C 65.11, H 8.41, N 5.84, found: C 65.09, H 8.57, N 5.77.

**UV/Vis** (MeCN, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 250 (22900), 301 (23800).

## Synthesis of Potassium Stiboranide **3c**



In a Schlenk flask containing a magnetic stirring bar, **2c** (279 mg, 438 µmol, 1.00 equiv.) and [2.2.2]-cryptand (165 mg, 438 µmol, 1.00 equiv.) were dissolved in $Et_2O$ (12 mL). KHMDS (87.4 mg, 438 µmol, 1.00 equiv.) in $Et_2O$ (1 mL) was added dropwise *via* syringe under rigorous stirring resulting in precipitation of a colorless solid. The mixture was stirred for 20 min at room temperature. Afterwards, the mixture was filtered and washed with $Et_2O$ (2 x 3 mL). The residue was dried *in vacuo* to yield the target compound as a colorless solid (422 mg, 402 µmol, 92%).

**m. p.** 127 °C (decomp.).

**$^1$H NMR** (400 MHz, $C_6D_6$): δ (ppm) = 7.92 – 7.85 (m, 2H), 7.74 (d, *J* = 2.3 Hz, 2H), 7.04 – 6.99 (m, 4H), 2.94 (s, 12H), 2.83 (t, *J* = 4.6 Hz, 12H), 1.89 – 1.80 (m, 30H), 1.53 (s, 18H).

**$^{13}C\{^1H\}$ NMR** (101 MHz, $C_6D_6$): δ (ppm) = 150.3, 143.0, 141.3, 136.8, 133.5, 118.4, 116.6, 113.0, 110.0, 70.3, 67.5, 53.5, 35.6, 34.7, 32.7, 30.6.

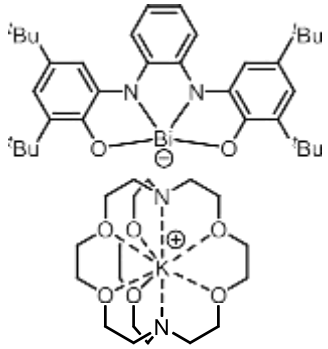
**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2948, 2878, 2814, 1552, 1473, 1417, 1353, 1251, 1100, 987, 948, 827, 736, 649, 592, 521, 494, 460.

**HR-MS-ESI(–)** *m*/*z* calcd. for $C_{34}H_{44}N_2O_2Sb^-$ [M–K-crypt]$^-$ 633.2446, found 633.2444.

**Anal.** calcd. for $C_{52}H_{80}SbKN_4O_8$: C 59.48, H 7.68, N 5.34, found: C 59.16, H 7.67, N 5.24.

**UV/Vis** (MeCN, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 223 (39700), 321 (14700).

## Synthesis of Potassium Bismuthoranide **3d**



In a Schlenk flask containing a magnetic stirring bar, **2d** (50.0 mg, 69.2 µmol, 1.00 equiv.) and [2.2.2]-cryptand (26.1 mg, 69.3 µmol, 1.00 equiv.) were dissolved in $Et_2O$ (2 mL). KHMDS (13.8 mg, 69.2 µmol, 1.00 equiv.) in $Et_2O$ (0.5 mL) was added dropwise with a syringe under rigorous stirring resulting in brown solid precipitating out of the orange reaction mixture. The mixture was stirred for 1.5 h at room temperature. Afterwards, the mixture was filtered and washed with $Et_2O$ (2 x 1 mL). The residue was dried under reduced pressure to yield the target compound as an orange-brown solid (69.4 mg, 61.0 µmol, 88%).

**m. p.** 237 °C (decomp.).

**$^1H$ NMR** (500 MHz, $CD_3CN$): δ (ppm) = 7.26 (s, 2H), 7.17 (s, 2H), 6.67 (s, 2H), 6.63 – 6.56 (m, 2H), 3.54 (s, 12H), 3.51 – 3.47 (m, 12H), 2.52 – 2.47 (m, 12H), 1.41 (s, 18H), 1.29 (s, 18H).

**$^{13}C\{^1H\}$ NMR** (126 MHz, $CD_3CN$): δ (ppm) = 154.0, 150.6, 147.1, 136.9, 136.5, 119.8, 119.0, 117.4, 114.9, 71.2, 68.4, 54.7, 35.6, 34.7, 32.4, 30.1.

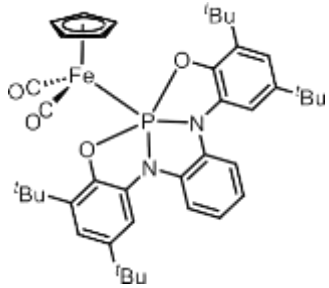
**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2947, 2868, 2815, 1544, 1463, 1414, 1354, 1324, 1247, 1098, 984, 945, 849, 823, 740, 682, 647, 583, 517, 486, 454.

**HR-MS-ESI(–)** *m*/*z* calcd. for $C_{34}H_{44}N_2O_2Bi^-$ [M–K-crypt]$^-$ 721.3212 found 721.3234.

**Anal.** calcd. for $C_{52}H_{80}BiKN_4O_8$: C 54.92, H 7.09, N 4.93, found: C 54.72, H 7.04, N 4.85.

**UV/Vis** (MeCN, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 225 (47600), 328 (13500).

## Synthesis of Fe-complex **4a**



In a Schlenk flask equipped with a magnetic stirring bar, **3a** (50.0 mg, 52.1 µmol, 1.10 equiv.) was dissolved in THF (2 mL) and a solution of cyclopentadienyliron(II) dicarbonyl iodide (14.4 mg, 47.4 µmol, 1.00 equiv.) in THF (0.5 mL) was added dropwise. The reaction mixture was stirred for 1 h at 21 °C and afterwards evaporated to dryness. The resulting red-orange solid was extracted with pentane (3 x 1 mL). Removal of all volatiles under reduced pressure yielded the target compound as a red-orange solid (21.8 mg, 30.3 µmol, 64%).

**m. p.** 110 °C (decomp.).

**$^{1}$H NMR** (400 MHz, $CDCl_3$): δ (ppm) = 7.57 – 7.51 (m, 2H), 7.38 (d, *J* = 2.0 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.92 (dd, *J* = 2.0, 1.1 Hz, 2H), 4.77 (d, *J* = 1.0 Hz, 5H), 1.52 (s, 18H), 1.39 (s, 18H).

**$^{13}$C{$^{1}$H} NMR** (101 MHz, $CDCl_3$): δ (ppm) = 211.5 (d, *J* = 41.9 Hz), 142.9, 141.5 (d, *J* = 3.9 Hz), 132.4 (d, *J* = 6.2 Hz), 131.5 (d, *J* = 12.3 Hz), 130.6 (d, *J* = 17.7 Hz), 120.3, 115.0, 110.9 (d, *J* = 7.1 Hz), 105.5 (d, *J* = 8.7 Hz), 84.4 (d, *J* = 1.6 Hz), 35.1, 34.6, 32.1, 23.0.

**$^{31}$P{$^{1}$H} NMR** (162 MHz, $CDCl_3$): δ (ppm) = 33.5.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2954, 2905, 2867, 2027 (CO), 1979 (CO), 1953, 1578, 1503, 1480, 1436, 1360, 1300, 1270, 1224, 1121, 1001, 885, 838, 764, 737, 704, 588, 577, 539, 497.

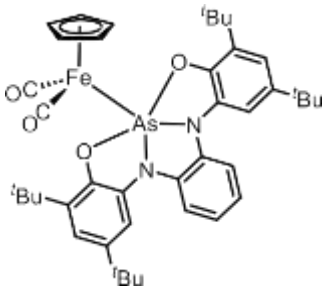
**IR** (DCM) [$cm^{-1}$] $\tilde{\nu}$ = 2028 (CO), 1979 (CO).

**HR-MS-ESI(+)** *m*/*z* calcd. for $C_{41}H_{50}FeN_2O_4P^+$ $[M+H]^+$ 721.2853, found 721.2833.

**Anal.** calcd. for $C_{41}H_{49}FeN_2O_4P$: C 68.33, H 6.85, N 3.89, found: C 68.20, H 6.65, N 3.93.

**UV/Vis** (DCM, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 303 (22000).

## Synthesis of Fe-complex **4b**




In a Schlenk flask containing a magnetic stirring bar, **3b** (143.8 mg, 136.9 µmol, 1.00 equiv.) was dissolved in DCM (1 mL). The solution was cooled to –78 °C using a dry ice/acetone bath. $[FeCp(CO)_2thf][BF_4]$ (46.0 mg, 136.9 µmol, 1.00 equiv.) in DCM (1 mL) was added dropwise with a syringe under rigorous stirring resulting in a color change to violet. The dry ice/acetone bath was removed, and the mixture was allowed to reach room temperature under continuous stirring over the course of 1 h. Afterwards the solvent was removed *in vacuo*. The residue was extracted with $Et_2O$ (3 x 3 mL) and the filtrate evaporated to dryness. The remaining solid was washed with acetonitrile (1 x 1 mL) at –20°C. Lyophilization from benzene yielded the target compound as a violet solid (48.8 mg, 63.8 µmol, 47%).

**m. p.** 125 °C (decomp.).

**$^{1}$H NMR** (300 MHz, $C_6D_6$): δ (ppm) = 7.95 – 7.85 (m, 2H), 7.81 (d, *J* = 2.1 Hz, 2H), 7.22 (d, *J* = 2.1 Hz, 2H), 7.06 – 6.97 (m, 2H), 3.95 (s, 5H), 1.76 (s, 18H), 1.46 (s, 18H).

**$^{13}$C{$^{1}$H} NMR** (75 MHz, $C_6D_6$): δ (ppm) = 209.1, 144.7, 141.0, 135.0, 133.2, 132.8, 120.2, 115.2, 112.1, 107.9, 84.3, 35.3, 35.0, 32.2, 30.2.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2952, 2904, 2867, 2043 (CO), 2002 (CO), 1780, 1573, 1480, 1422, 1359, 1286, 1264, 1237, 1119, 994, 921, 832, 732, 677, 650, 612, 573, 549.

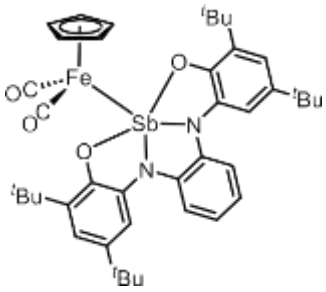
**IR** (DCM) [$cm^{-1}$] $\tilde{\nu}$ = 2047 (CO), 2005 (CO).

**MS-LIFDI(**toluene**)** *m*/*z* = 764.0 (100%, $[M]^+$).

**Anal.** calcd. for $C_{41}H_{49}FeN_2O_4As$: C 64.40, H 6.46, N 3.66, found: C 64.13, H 6.36, N 3.57.

**UV/Vis** (DCM, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 312 (25900), 556 (3200).

Synthesis of Fe-complex **4c**



In a Schlenk flask containing a magnetic stirring bar, **3c** (228.3 mg, 217.4 µmol, 1.00 equiv.) was dissolved in DCM (2 mL). The solution was cooled to –78 °C using a dry ice/acetone bath. $[FeCp(CO)_2thf][BF_4]$ (73.0 mg, 217.4 µmol, 1.00 equiv.) in DCM (1 mL) was added dropwise with a syringe under rigorous stirring resulting in a color change to dark blue. The dry ice/acetone bath was removed, and the mixture was allowed to reach room temperature under continuous stirring over the course of 1 h. Afterwards the solvent was removed *in vacuo*. The residue was extracted with $Et_2O$ (5 x 5 mL) and the filtrate evaporated to dryness. The residue was crystallized by slow evaporation of an acetonitrile/DCM solution inside a nitrogen-filled glovebox. Dark blue crystals formed over the course of 3 days. The crystals were collected by filtration, washed with acetonitrile (4 x 0.25 mL) and dried under reduced pressure to yield the target compound as a blue crystalline solid (127.0 mg, 156.5 µmol, 72%).

**m. p.** 183 °C.

**$^1$H NMR** (300 MHz, $C_6D_6$): δ (ppm) = 8.06 – 7.98 (m, 2H), 7.90 (d, *J* = 2.2 Hz, 2H), 7.18 (d, *J* = 2.2 Hz, 2H), 7.07 – 6.97 (m, 2H), 3.79 (s, 5H), 1.74 (s, 18H), 1.45 (s, 18H).

**$^{13}$C{$^1$H} NMR** (101 MHz, $C_6D_6$): δ (ppm) = 207.5, 147.0, 140.7, 138.6, 136.8, 134.8, 120.4, 115.8, 115.1, 110.2, 83.4, 35.6, 34.9, 32.2, 30.2.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2952, 2903, 2867, 2044 (CO), 2006 (CO), 1565, 1473, 1417, 1332, 1254, 1236, 1111, 987, 816, 734, 610, 573, 548.

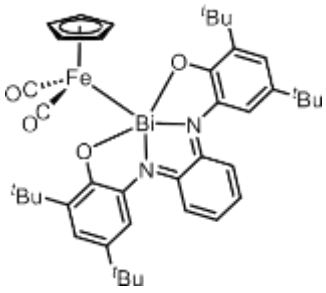
**IR** (DCM) [$cm^{-1}$] $\tilde{\nu}$ = 2049 (CO), 2009 (CO).

**MS-LIFDI(**toluene**)** *m*/*z* = 810.0 (100%, $[M]^+$).

**Anal.** calcd. for $C_{41}H_{49}FeN_2O_4Sb$: C 60.69, H 6.09, N 3.45, found: C 60.28, H 6.09, N 3.57.

**UV/Vis** (DCM, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ ($\varepsilon$) = 313 (32400), 622 (3100).

Synthesis of Fe-complex **4d'**



In a Schlenk flask containing a magnetic stirring bar, **3d** (338.6 mg, 297.7 µmol, 1.00 equiv.) was dissolved in DCM (20 mL). The solution was cooled to –78 °C using a dry ice/acetone bath. $[FeCp(CO)_2thf][BF_4]$ (100.0 mg, 297.7 µmol, 1.00 equiv.) in DCM (3 mL) was added dropwise with a syringe under rigorous stirring resulting in a color change to dark violet. The dry ice/acetone bath was removed, and the mixture was allowed to reach room temperature under continuous stirring over the course of 15 min. Afterwards the solvent was removed *in vacuo*. The residue was extracted with $Et_2O$ (6 x 8 mL) and all volatiles were removed *in vacuo*. The residue was washed with acetonitrile (4 x 3 mL) and drying under reduced pressure yielded the target compound as a dark violet solid (172.1 mg, 191.5 µmol, 64%).

**m. p.** 105 °C (decomp.).

**$^1$H NMR** (400 MHz, $CD_2Cl_2$): δ (ppm) = 7.91 – 7.78 (m, 2H), 7.73 (s, 2H), 7.26 (s, 2H), 6.87 – 6.71 (m, 2H), 4.91 (s, 5H), 1.52 (s, 18H), 1.37 (s, 18H).

**$^{13}C\{^1H\}$ NMR** (101 MHz, $CD_2Cl_2$): δ (ppm) = 203.3, 169.6, 150.6, 142.8, 141.9, 141.1, 125.7, 124.7, 122.1, 115.9, 84.5, 36.1, 35.2, 31.6, 30.0.

**IR** (ATR, neat) [$cm^{-1}$] $\tilde{\nu}$ = 2948, 2900, 2866, 2006 (CO), 1959 (CO), 1517, 1437, 1354, 1295, 1256, 1194,1158, 1110, 1019, 988, 949, 931, 909, 870, 839, 781, 744, 731, 665, 645, 627, 566, 537, 499,457, 415.

**IR** (DCM) [$cm^{-1}$] $\tilde{\nu}$ = 2004 (CO), 1962 (CO).

**MS-LIFDI(**toluene**)** *m*/*z* = 898.1 (100%, $[M]^+$).

**Anal.** calcd. for $C_{41}H_{49}FeN_2O_4Bi$: C 54.80, H 5.50, N 3.12, found: C 54.45, H 5.63, N 3.02.

**UV/Vis** (DCM, nm ($M^{-1}$ $cm^{-1}$): $\lambda_{max}$ (**ε**) = 323 (26300), 448 (7400), 516 (7900), 803 (5900), 1090 (22900).

# Crystallographic Supplement

## General Information

Data collection was done on two dual source equipped *Bruker D8 Venture* four-circle-diffractometer from *Bruker AXS GmbH*; used X-ray sources: microfocus *IμS 2.0* Cu/Mo and microfocus *IμS 3.0* Ag/Mo from *Incoatec GmbH* with mirror optics *HELIOS* and single-hole collimator from *Bruker AXS GmbH;* used detector: *Photon III CE14* (Cu/Mo) and Photon III HE (Ag/Mo) from *Bruker AXS GmbH.*

Used programs: *APEX6 Suite* (v2024.9-1-9.0.61) for data collection and therein integrated programs *SAINT* V8.40B (Integration) und *SADABS* 2016/2 (Absorption correction) from *Bruker AXS GmbH*; structure solution was done with *SHELXT*, refinement with *SHELXL*-2018/3.[7] OLEX[2] [8] and FinalCif[9] were used for data finalization.

Special Utilities: SMZ1270 stereomicroscope from Nikon Metrology GmbH was used for sample preparation; crystals were mounted on MicroMounts or MicroLoops from MiTeGen in NVH oil; crystals were cooled to given temperature with Cryostream 800 from Oxford Cryosystems.

This supplement contains in the following the refinement detail tables, a figure of the complete asymmetric unit and a microscope picture of the crystal used for data collection. The picture of the single crystals was cropped and auto-adjusted for brightness, graduation curve and white balance in Adobe Photoshop (Version 24.1.0). Further crystallographic details can be obtained from the crystallographic information files (CIFs) uploaded to the *Cambridge Crystallographic Data Centre* (CCDC), where they can be obtained free of charge.

| Identifier | CCDC number | Identifier | CCDC number |
|---|---|---|---|
| **2c** | 2448026 | **3d** | 2448031 |
| **2d** | 2448027 | **4a** | 2448032 |
| **3a I** | 2448028 | **4b** | 2448033 |
| **3a II** | 2448029 | **4c** | 2448034 |
| **3c** | 2448030 | **4d** | 2448035 |

The solid-state structures of **2a** (CCDC: 2153554),[3] **2b** (CCDC: 2416702)[4] and **3b** (CCDC: 2416703)[4] were already reported in previous publications.

Refinement details for **2c**

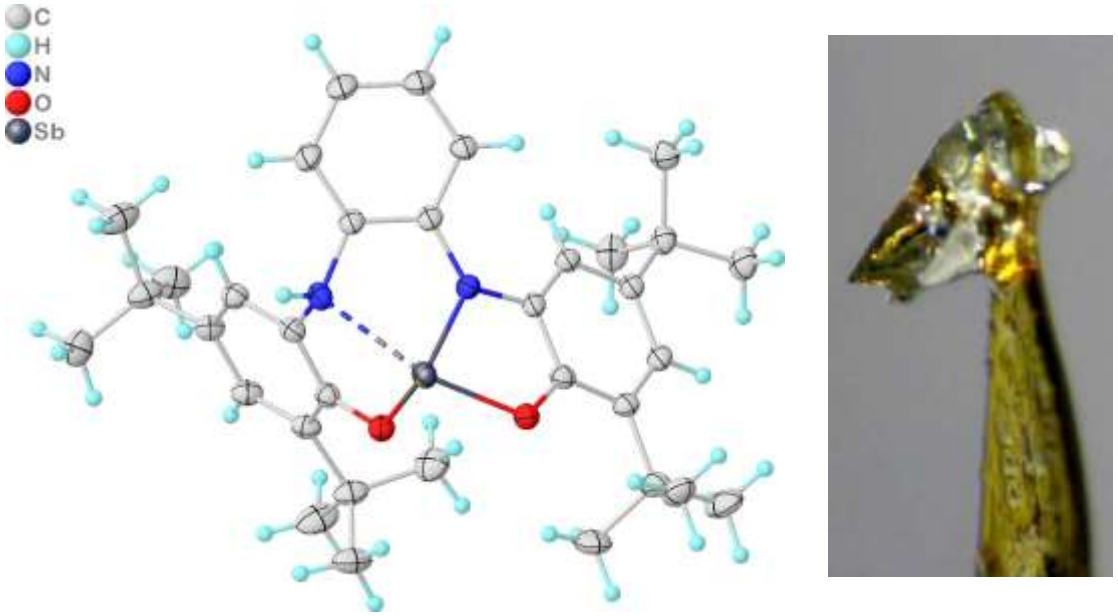



*Figure S 1*: Full asymmetric unit of **2c**. Anisotropic displacement ellipsoids drawn at 50% probability level. The HN···Sb contact is drawn as stippled bond. Single crystals were obtained from a solution in methanol.

| | |
|---|---|
| CCDC number | 2448026 |
| Empirical formula | $C_{34}H_{45}N_2O_2Sb$ |
| Formula weight | 635.47 |
| Temperature [K] | 100.00 |
| Crystal system | Tetragonal |
| Space group (number) | $P\bar{4}2_1c$ (114) |
| *a* [Å] | 18.2827(6) |
| *b* [Å] | 18.2827(6) |
| *c* [Å] | 20.6322(11) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 90 |
| Volume [Å$^3$] | 6896.5(6) |
| *Z* | 8 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.224 |
| $\mu$ [mm$^{-1}$] | 0.829 |
| *F*(000) | 2640 |
| Crystal size [mm$^3$] | 0.71×0.262×0.233 |
| Crystal color | Yellow |
| Crystal shape | Block |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.53 to 63.07 (0.68 Å) |
| Index ranges | −24 ≤ h ≤ 26<br>−26 ≤ k ≤ 26<br>−29 ≤ l ≤ 30 |
| Reflections collected | 87023 |
| Independent reflections | 11477<br>$R_{int}$ = 0.0358<br>$R_{sigma}$ = 0.0183 |
| Completeness to θ = 25.242° | 99.5 % |
| Data / Restraints / Parameters | 11477/0/368 |
| Goodness-of-fit on $F^2$ | 1.086 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0235<br>w$R_2$ = 0.0670 |
| Final *R* indexes [all data] | $R_1$ = 0.0248<br>w$R_2$ = 0.0683 |
| Largest peak/hole [eÅ$^{-3}$] | 0.90/-0.76 |
| Flack X parameter | -0.030(4) |

Refinement details for **2d**

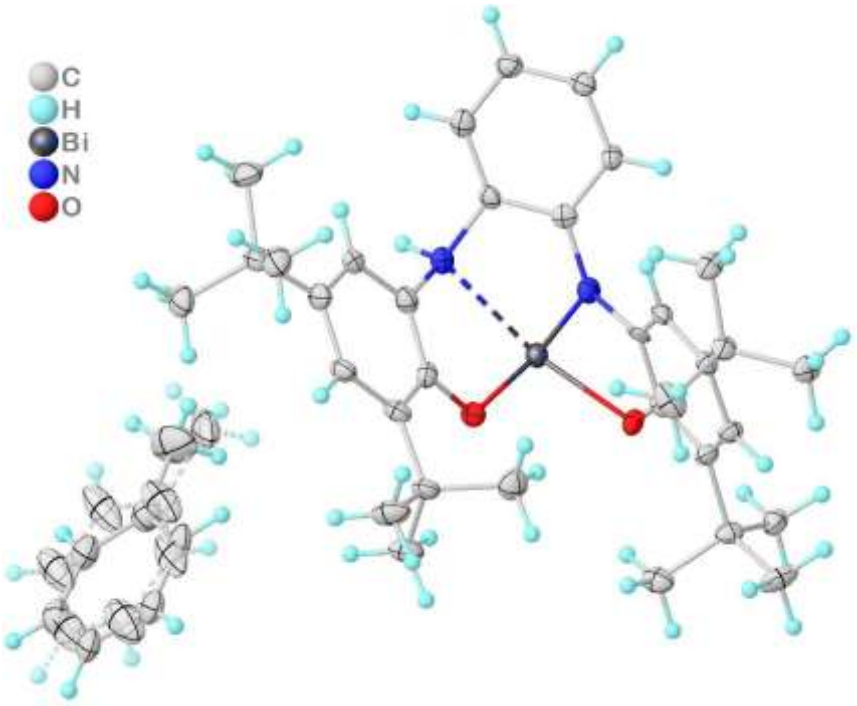



*Figure S 2:* Full asymmetric unit of **2d**◦toluene. Anisotropic displacement ellipsoids drawn at 50% probability level. The HN···Bi contact is drawn as stippled bond. The co-crystallized molecule of toluene is disordered; the minor disorder part is drawn translucent with stippled bonds. Single crystals were obtained from a solution in toluene.

| | |
|---|---|
| CCDC number | 2448027 |
| Empirical formula | $C_{41}H_{53}BiN_2O_2$ |
| Formula weight | 814.83 |
| Temperature [K] | 100.00 |
| Crystal system | Orthorhombic |
| Space group (number) | $P2_12_12_1$ (19) |
| *a* [Å] | 10.186(4) |
| *b* [Å] | 18.226(14) |
| *c* [Å] | 19.858(15) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 90 |
| Volume [Å$^3$] | 3687(4) |
| *Z* | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.468 |
| $\mu$ [mm$^{-1}$] | 4.818 |
| *F*(000) | 1648 |
| Crystal size [mm$^3$] | 0.406×0.023×0.02 |
| Crystal color | Orange |
| Crystal shape | Needle |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.10 to 57.45 (0.74 Å) |
| Index ranges | −13 ≤ h ≤ 13<br>−24 ≤ k ≤ 24<br>−25 ≤ l ≤ 26 |
| Reflections collected | 46132 |
| Independent reflections | 9412<br>$R_{int}$ = 0.0550<br>$R_{sigma}$ = 0.0526 |
| Completeness to θ = 25.242° | 100.0 % |
| Data / Restraints / Parameters | 9412/105/497 |
| Goodness-of-fit on $F^2$ | 1.076 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0357<br>w$R_2$ = 0.0735 |
| Final *R* indexes [all data] | $R_1$ = 0.0460<br>w$R_2$ = 0.0778 |
| Largest peak/hole [eÅ$^{-3}$] | 3.35/-1.29 |
| Flack X parameter | -0.053(4) |

Refinement details for **3a l**

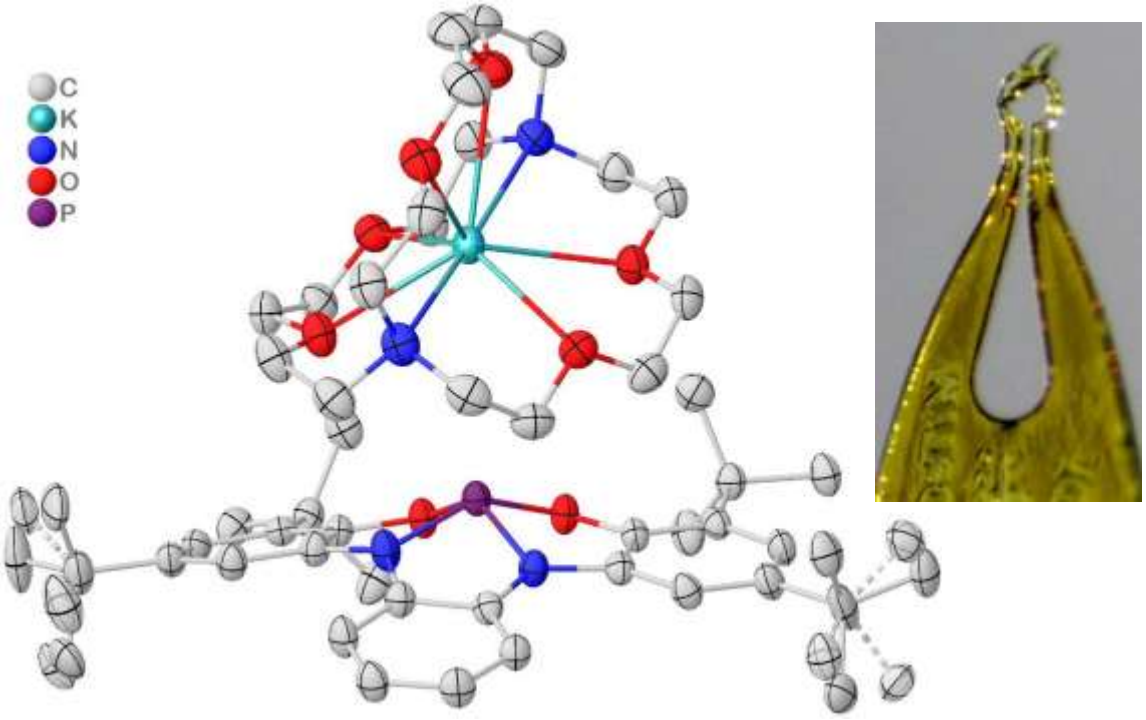



*Figure S 3:* Full asymmetric unit of **3a**. Hydrogen atoms omitted for clarity. Anisotropic displacement ellipsoids drawn at 50% probability level. Some of the *tert*-butyl groups are disordered; the minor disorder part is drawn translucent with stippled bonds. Single crystals were obtained from a solution in acetonitrile after storing it at −20 °C.

| | |
|---|---|
| CCDC number | 2448028 |
| Empirical formula | $C_{52}H_{80}KN_4O_8P$ |
| Formula weight | 959.27 |
| Temperature [K] | 100.0 |
| Crystal system | Hexagonal |
| Space group (number) | $P6_1$ (169) |
| *a* [Å] | 13.68860(10) |
| *b* [Å] | 13.68860(10) |
| *c* [Å] | 49.9629(9) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 120 |
| Volume [Å$^3$] | 8107.67(19) |
| *Z* | 6 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.179 |
| $\mu$ [mm$^{-1}$] | 1.564 |
| *F*(000) | 3108 |
| Crystal size [mm$^3$] | 0.057×0.062×0.192 |
| Crystal color | Yellow |
| Crystal shape | Needle |
| Radiation | Cu$K_\alpha$ (λ=1.54178 Å) |
| 2θ range [°] | 7.46 to 158.47 (0.78 Å) |

| | |
|---|---|
| Index ranges | −17 ≤ h ≤ 16<br>−17 ≤ k ≤ 17<br>−60 ≤ l ≤ 63 |
| Reflections collected | 216313 |
| Independent reflections | 11488<br>$R_{int}$ = 0.1083<br>$R_{sigma}$ = 0.0360 |
| Completeness to θ = 67.679° | 100.0 % |
| Data / Restraints / Parameters | 11488 / 19 / 669 |
| Absorption correction $T_{min}/T_{max}$ (method) | 0.7011 / 0.8959 (numerical) |
| Goodness-of-fit on $F^2$ | 1.026 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0486<br>w$R_2$ = 0.1264 |
| Final *R* indexes [all data] | $R_1$ = 0.0554<br>w$R_2$ = 0.1325 |
| Largest peak/hole [eÅ$^{-3}$] | 0.77/−0.30 |
| Flack X parameter | -0.004(6) |

Refinement details for **3a II**

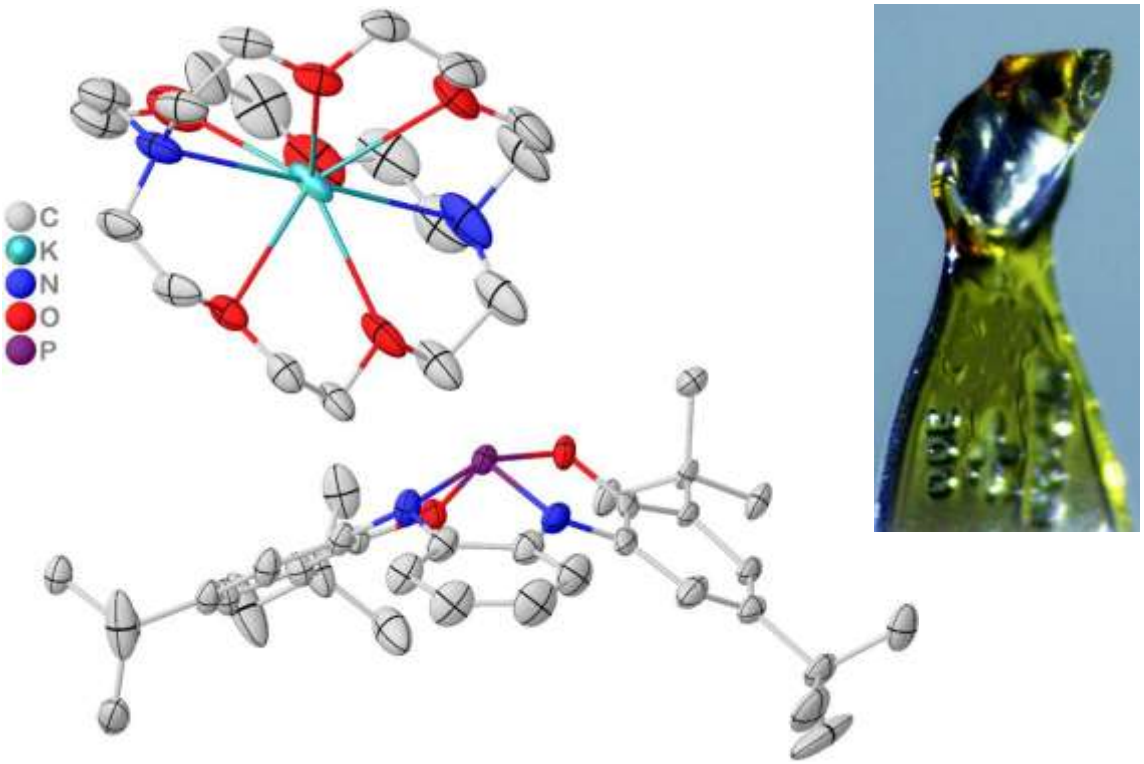



*Figure S 4:* Asymmetric unit of **3a**, showing only the first Part with the whole model being disordered. The crystals of **3a** in the monoclinic form are most likely modulated, showing typical satellites that indicate a supercell with tripled volume. While structure solution in the supercell is possible, the refinement was found to be considerably less stable and poorly converging. Due to that, the satellites were ignored during data integration, instead a model was built that is effectively a whole molecule disorder, that includes the geometric alteration of the modulation. Hydrogen atoms are omitted for clarity. Anisotropic displacement ellipsoids are drawn at 50% probability level. Single crystals were obtained from a solution in toluene.

| | |
|---|---|
| CCDC number | 2448029 |
| Empirical formula | $C_{52}H_{80}KN_4O_8P$ |
| Formula weight | 959.27 |
| Temperature [K] | 100.00 |
| Crystal system | Monoclinic |
| Space group (number) | $P2_1/c$ (14) |
| *a* [Å] | 14.9091(6) |
| *b* [Å] | 16.9235(8) |
| *c* [Å] | 21.9544(9) |
| α [°] | 90 |
| β [°] | 103.203(2) |
| γ [°] | 90 |
| Volume [Å$^3$] | 5393.0(4) |
| *Z* | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.181 |
| $\mu$ [mm$^{-1}$] | 0.181 |
| *F*(000) | 2072 |
| Crystal size [mm$^3$] | 0.216×0.284×0.514 |
| Crystal color | Colorless |
| Crystal shape | Block |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 3.85 to 56.57 (0.75 Å) |
| Index ranges | −19 ≤ h ≤ 19<br>−22 ≤ k ≤ 22<br>−29 ≤ l ≤ 28 |
| Reflections collected | 189301 |
| Independent reflections | 13376<br>$R_{int}$ = 0.0237<br>$R_{sigma}$ = 0.0081 |
| Completeness to θ = 25.242° | 100.0 % |
| Data / Restraints / Parameters | 13376 / 1801 / 1065 |
| Absorption correction $T_{min}/T_{max}$ (method) | 0.9373 / 0.9839 (multi-scan) |
| Goodness-of-fit on $F^2$ | 1.022 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0724<br>w$R_2$ = 0.1776 |
| Final *R* indexes [all data] | $R_1$ = 0.0779<br>w$R_2$ = 0.1824 |
| Largest peak/hole [eÅ$^{-3}$] | 0.89/−0.59 |

## Refinement details for **3c**

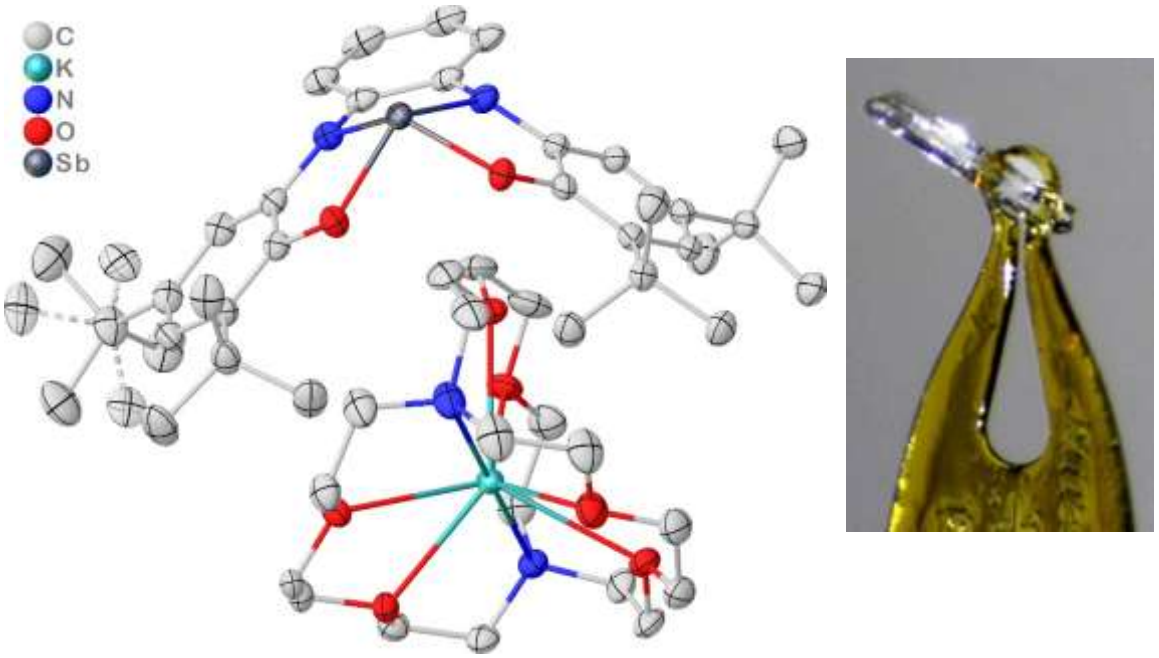



*Figure S 5:* Full asymmetric unit of **3c**. Hydrogen atoms omitted for clarity. Anisotropic displacement ellipsoids drawn at 50% probability level. Solvent mask was applied to treat a solvent channel that contains presumably 1.25 equiv. of toluene according to the number of electrons found. One of the *tert*-butyl groups is disordered; the minor disorder part is drawn translucent with stippled bonds. Single crystals were obtained by layering a solution in a mixture of toluene and dichloromethane with diethyl ether at −20 °C.

| | |
|---|---|
| CCDC number | 2448030 |
| Empirical formula | $C_{60.75}H_{90}KN_4O_8Sb$ |
| Formula weight | 1165.21 |
| Temperature [K] | 100.00 |
| Crystal system | Monoclinic |
| Space group (number) | $C2/c$ (15) |
| *a* [Å] | 19.5035(10) |
| *b* [Å] | 19.1189(12) |
| *c* [Å] | 34.1547(18) |
| α [°] | 90 |
| β [°] | 91.153(2) |
| γ [°] | 90 |
| Volume [Å$^3$] | 12733.2(12) |
| *Z* | 8 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.216 |
| $\mu$ [mm$^{-1}$] | 0.551 |
| *F*(000) | 4932 |
| Crystal size [mm$^3$] | 0.61×0.111×0.096 |
| Crystal color | Colorless |
| Crystal shape | Needle |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.18 to 59.25 (0.72 Å) |
| Index ranges | −26 ≤ h ≤ 27<br>−26 ≤ k ≤ 26<br>−47 ≤ l ≤ 47 |
| Reflections collected | 146960 |
| Independent reflections | 17874<br>$R_{int}$ = 0.0379<br>$R_{sigma}$ = 0.0214 |
| Completeness to θ = 25.242° | 99.9 % |
| Data / Restraints / Parameters | 17874/24/638 |
| Goodness-of-fit on $F^2$ | 1.104 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0327<br>w$R_2$ = 0.0772 |
| Final *R* indexes [all data] | $R_1$ = 0.0380<br>w$R_2$ = 0.0793 |
| Largest peak/hole [eÅ$^{-3}$] | 0.45/-0.89 |

## Refinement details for **3d**

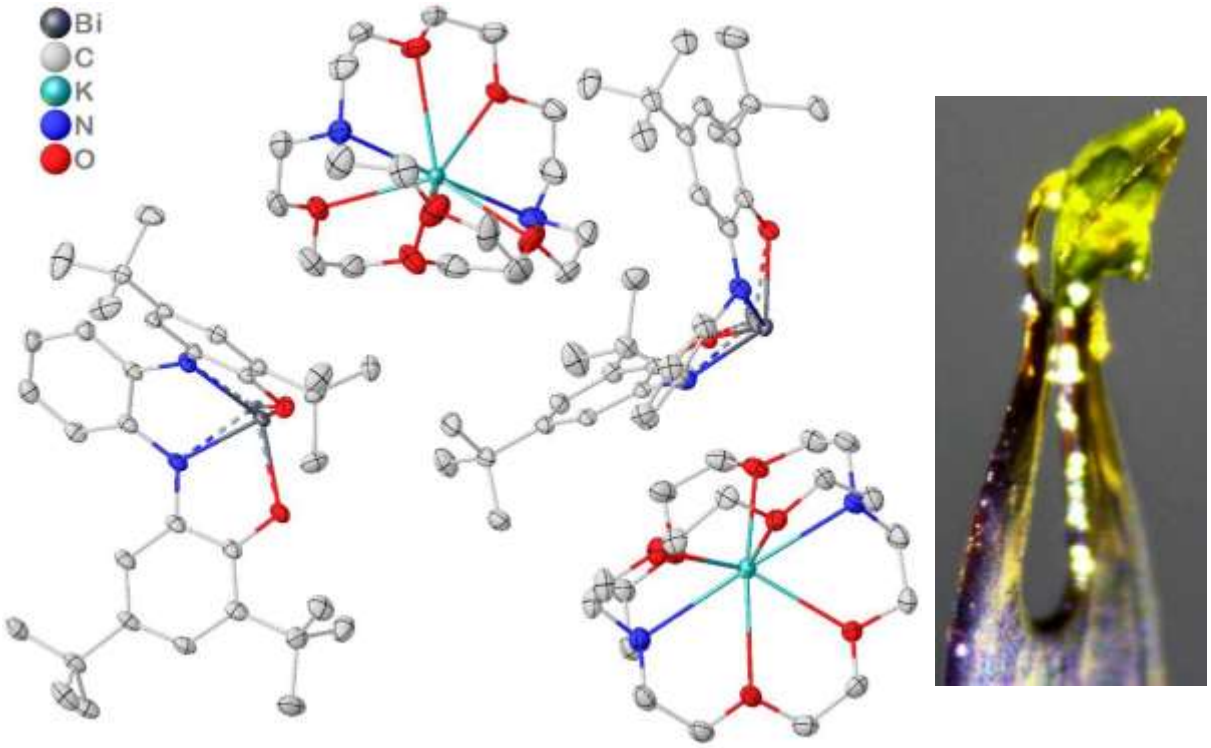



*Figure S 6:* Full asymmetric unit of **3d** (Z'=2). Hydrogen atoms omitted for clarity. Anisotropic displacement ellipsoids drawn at 50% probability level. The bismuth was modelled with positional disorder to remedy high residual densities. However, whether this is a true disorder or rather an absorption effect is unclear. The minor disorder part is drawn translucent with stippled bonds. Single crystals were obtained from diethyl ether at −20 °C.

| | |
|---|---|
| CCDC number | 2448031 |
| Empirical formula | $C_{52}H_{79.50}BiKN_4O_8$ |
| Formula weight | 1136.77 |
| Temperature [K] | 100.00 |
| Crystal system | Monoclinic |
| Space group (number) | $C2$ (5) |
| *a* [Å] | 33.0221(10) |
| *b* [Å] | 18.8484(5) |
| *c* [Å] | 19.1838(6) |
| α [°] | 90 |
| β [°] | 115.6180(10) |
| γ [°] | 90 |
| Volume [Å$^3$] | 10766.5(6) |
| *Z* | 8 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.403 |
| $\mu$ [mm$^{-1}$] | 3.406 |
| *F*(000) | 4684 |
| Crystal size [mm$^3$] | 0.406×0.198×0.164 |
| Crystal color | Orange |
| Crystal shape | Block |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 3.86 to 63.08 (0.68 Å) |
| Index ranges | −48 ≤ h ≤ 47<br>−26 ≤ k ≤ 27<br>−28 ≤ l ≤ 27 |
| Reflections collected | 250538 |
| Independent reflections | 34370<br>$R_{int}$ = 0.0254<br>$R_{sigma}$ = 0.0161 |
| Completeness to θ = 25.242° | 100.0 % |
| Data / Restraints / Parameters | 34370/1/1232 |
| Goodness-of-fit on $F^2$ | 1.042 |
| Final *R* indexes [$I$≥2σ($I$)] | $R_1$ = 0.0254<br>w$R_2$ = 0.0679 |
| Final *R* indexes [all data] | $R_1$ = 0.0267<br>w$R_2$ = 0.0686 |
| Largest peak/hole [eÅ$^{-3}$] | 1.81/-1.07 |
| Flack X parameter | -0.0232(8) |

## Refinement details for **4a**

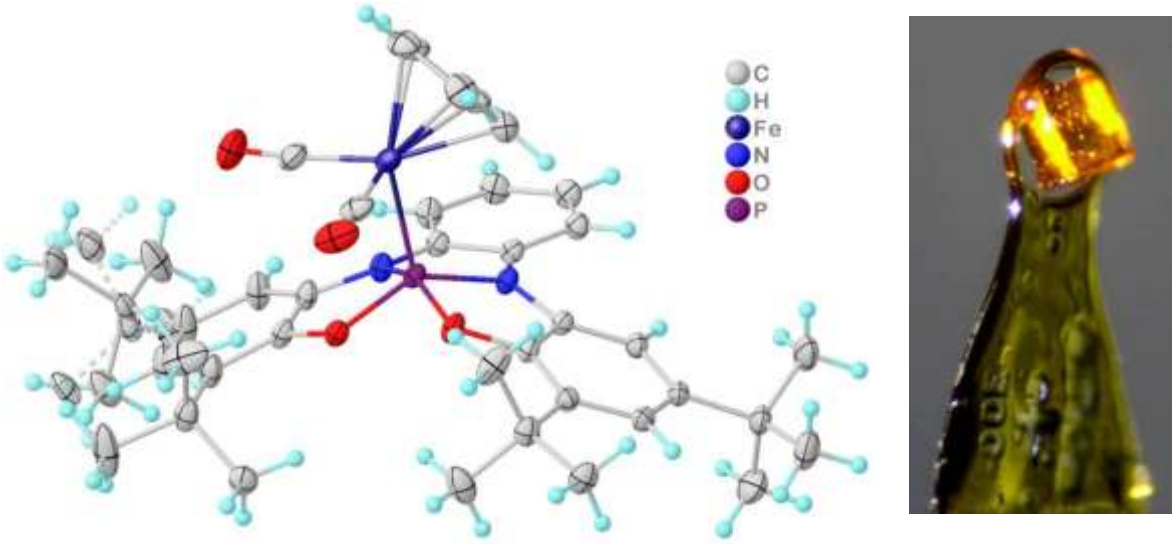



*Figure S 7:* Full asymmetric unit of **4a**. Anisotropic displacement ellipsoids drawn at 50% probability level. One of the *tert*-butyl groups is disordered; the minor disorder part is drawn translucent with stippled bonds. Single crystals were obtained from a solution in acetonitrile.

| | |
|---|---|
| CCDC number | 2448032 |
| Empirical formula | $C_{41}H_{49}FeN_2O_4P$ |
| Formula weight | 720.64 |
| Temperature [K] | 100.0 |
| Crystal system | Monoclinic |
| Space group (number) | $P2_1/c$ (14) |
| *a* [Å] | 11.2137(10) |
| *b* [Å] | 22.3307(12) |
| *c* [Å] | 15.4939(15) |
| α [°] | 90 |
| β [°] | 105.942(2) |
| γ [°] | 90 |
| Volume [Å$^3$] | 3730.6(5) |
| *Z* | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.283 |
| $\mu$ [mm$^{-1}$] | 0.490 |
| *F*(000) | 1528 |
| Crystal size [mm$^3$] | 0.134×0.224×0.259 |
| Crystal color | Orange |
| Crystal shape | Block |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.19 to 61.07 (0.70 Å) |
| Index ranges | −16 ≤ h ≤ 16<br>−31 ≤ k ≤ 31<br>−22 ≤ l ≤ 22 |
| Reflections collected | 107045 |
| Independent reflections | 11366<br>$R_{int}$ = 0.0244<br>$R_{sigma}$ = 0.0143 |
| Completeness to θ = 25.242° | 99.9 % |
| Data / Restraints / Parameters | 11366 / 10 / 494 |
| Absorption correction $T_{min}/T_{max}$ (method) | 0.8946 / 0.9991 (numerical) |
| Goodness-of-fit on $F^2$ | 1.013 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0350<br>w$R_2$ = 0.0940 |
| Final *R* indexes [all data] | $R_1$ = 0.0401<br>w$R_2$ = 0.0984 |
| Largest peak/hole [eÅ$^{-3}$] | 0.92/−0.44 |

Refinement details for **4b**

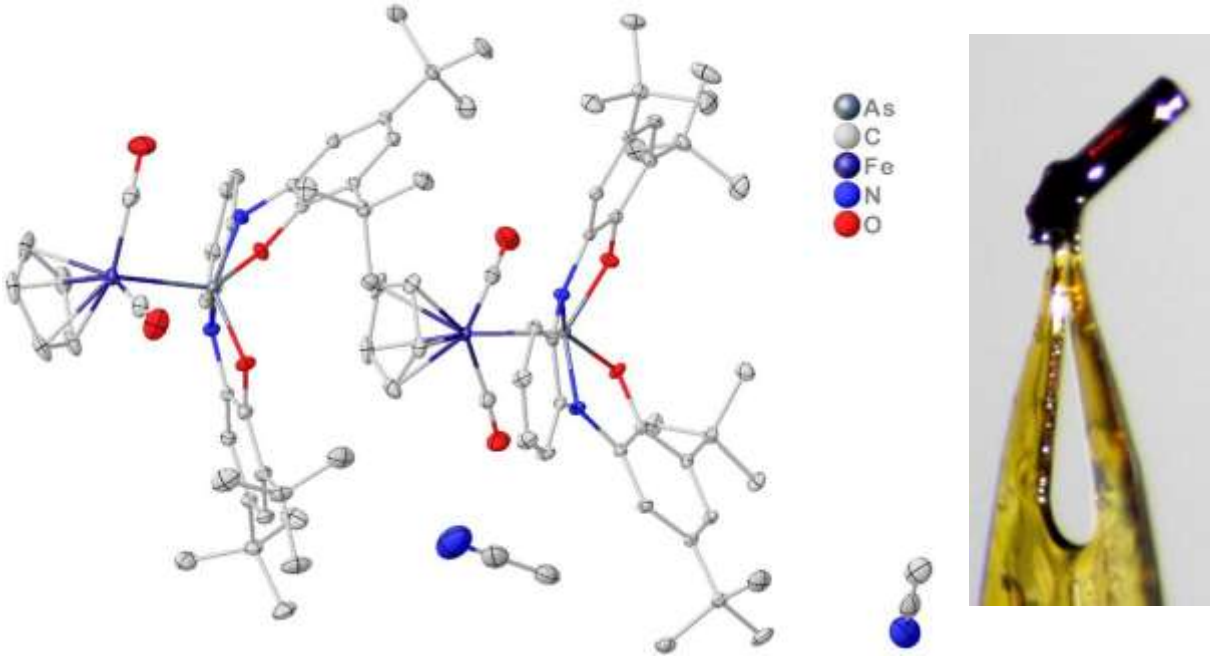



*Figure S 8:* Full asymmetric unit of **4b**◦MeCN (Z'=2). Hydrogen atoms omitted for clarity. Anisotropic displacement ellipsoids drawn at 50% probability level. Single crystals were obtained from a solution in acetonitrile.

| | |
|---|---|
| CCDC number | 2448033 |
| Empirical formula | $C_{170}H_{205}As_4Fe_4N_{11}O_{16}$ |
| Formula weight | 3181.52 |
| Temperature [K] | 100.00 |
| Crystal system | Monoclinic |
| Space group (number) | $P2_1/c$ (14) |
| *a* [Å] | 11.1002(7) |
| *b* [Å] | 24.3068(19) |
| *c* [Å] | 29.174(2) |
| α [°] | 90 |
| β [°] | 90.710(2) |
| γ [°] | 90 |
| Volume [Å$^3$] | 7870.9(10) |
| *Z* | 2 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.342 |
| $\mu$ [mm$^{-1}$] | 1.262 |
| *F*(000) | 3332 |
| Crystal size [mm$^3$] | 0.487×0.086×0.077 |
| Crystal color | Red |
| Crystal shape | Needle |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.25 to 65.19 (0.66 Å) |
| Index ranges | −16 ≤ h ≤ 12<br>−36 ≤ k ≤ 32<br>−43 ≤ l ≤ 41 |
| Reflections collected | 153146 |
| Independent reflections | 26489<br>$R_{int}$ = 0.0522<br>$R_{sigma}$ = 0.0343 |
| Completeness to θ = 25.242° | 99.9 % |
| Data / Restraints / Parameters | 26489/3/963 |
| Goodness-of-fit on $F^2$ | 1.059 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0346<br>w$R_2$ = 0.0807 |
| Final *R* indexes [all data] | $R_1$ = 0.0438<br>w$R_2$ = 0.0844 |
| Largest peak/hole [eÅ$^{-3}$] | 0.58/-0.83 |

Refinement details for **4c**

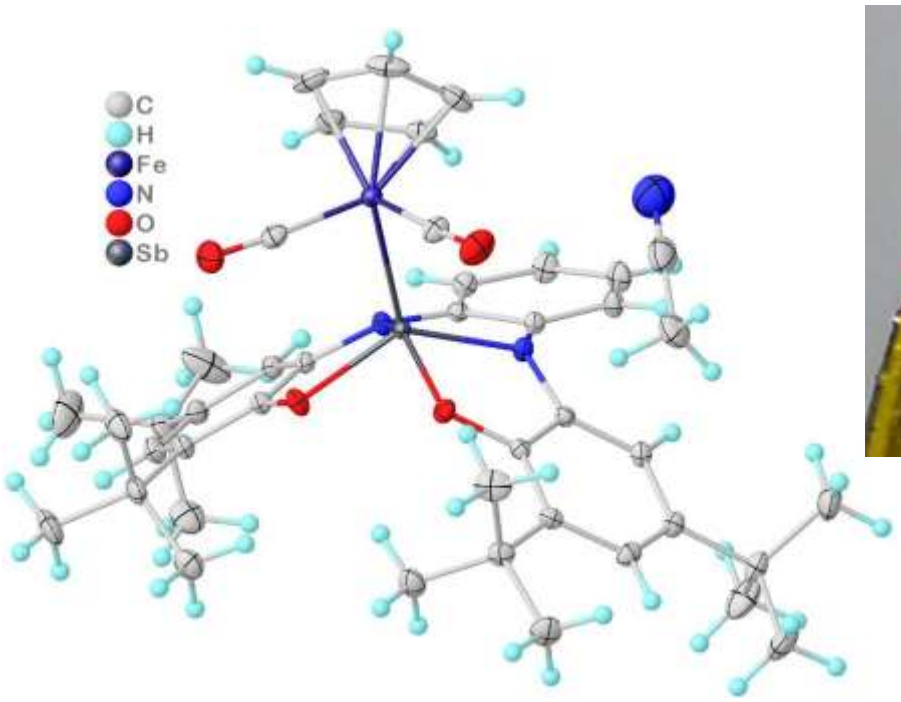



*Figure S 9:* Full asymmetric unit of **4c**◦MeCN. Anisotropic displacement ellipsoids drawn at 50% probability level. Single crystals were obtained from a solution in acetonitrile.

| | |
|---|---|
| CCDC number | 2448034 |
| Empirical formula | $C_{43}H_{52}FeN_3O_4Sb$ |
| Formula weight | 852.47 |
| Temperature [K] | 100.00 |
| Crystal system | Orthorhombic |
| Space group (number) | $P2_12_12_1$ (19) |
| *a* [Å] | 11.0459(6) |
| *b* [Å] | 15.0934(5) |
| *c* [Å] | 24.3347(11) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 90 |
| Volume [Å$^3$] | 4057.1(3) |
| *Z* | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.396 |
| $\mu$ [mm$^{-1}$] | 1.067 |
| *F*(000) | 1760 |
| Crystal size [mm$^3$] | 0.195×0.141×0.094 |
| Crystal color | Dark blue |
| Crystal shape | Block |
| Radiation | Mo$K_\alpha$ (λ=0.71073 Å) |

| | |
|---|---|
| 2θ range [°] | 4.30 to 65.21 (0.66 Å) |
| Index ranges | −16 ≤ h ≤ 15<br>−16 ≤ k ≤ 22<br>−36 ≤ l ≤ 36 |
| Reflections collected | 90796 |
| Independent reflections | 14093<br>$R_{int}$ = 0.0409<br>$R_{sigma}$ = 0.0248 |
| Completeness to θ = 25.242° | 99.9 % |
| Data / Restraints / Parameters | 14093/0/482 |
| Goodness-of-fit on $F^2$ | 1.033 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0202<br>w$R_2$ = 0.0494 |
| Final *R* indexes [all data] | $R_1$ = 0.0213<br>w$R_2$ = 0.0501 |
| Largest peak/hole [eÅ$^{-3}$] | 0.82/-0.53 |
| Flack X parameter | -0.009(4) |

## Refinement details for **4d**

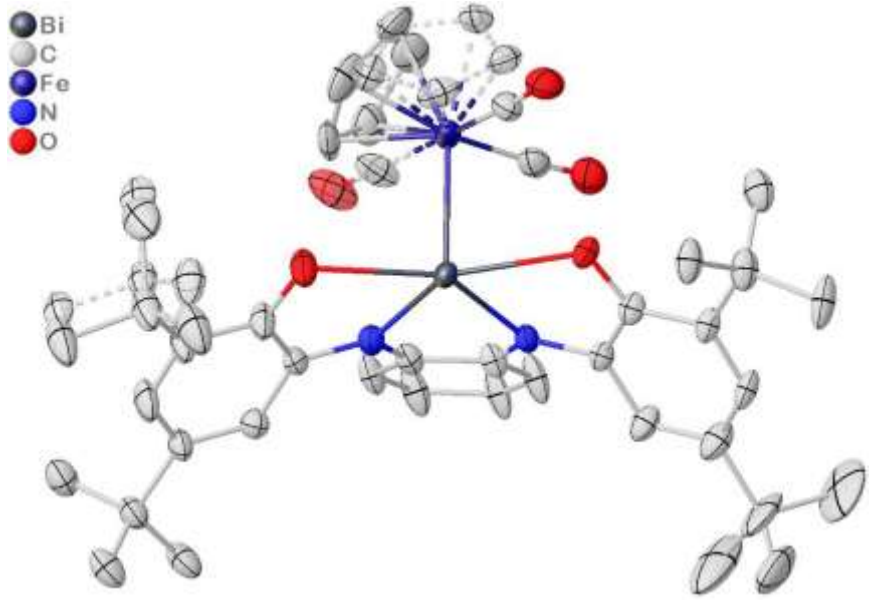



*Figure S10:* Full asymmetric unit of **4d**. Anisotropic displacement ellipsoids drawn at 50% probability level. Hydrogen atoms are omitted for clarity. One of the *tert*-butyl groups is disordered and the Cp and one CO ligand swap positions in a equally occupied disorder; the minor disorder part is drawn translucent with stippled bonds. Crystals were obtained from a mixture of acetonitrile and dichloromethane. Non-merohedral twinning was found and two unit cells were indexed that are related by (0 0.312 -0.031 | 0.125 -1 0.156 | 0.062 -1.906 0.258). For final refinement against HKLF5 data, both domains were used with a refined batch scale factor of 0.4245(9).

| | |
|---|---|
| CCDC number | 2448035 |
| Empirical formula | $C_{41}H_{49}BiFeN_2O_4$ |
| Formula weight | 898.65 |
| Temperature [K] | 100.00 |
| Crystal system | Orthorhombic |
| Space group (number) | $P2_12_12_1$ (19) |
| *a* [Å] | 12.6242(7) |
| *b* [Å] | 16.1575(10) |
| *c* [Å] | 18.7294(12) |
| α [°] | 90 |
| β [°] | 90 |
| γ [°] | 90 |
| Volume [Å$^3$] | 3820.3(4) |
| *Z* | 4 |
| $\rho_{calc}$ [gcm$^{-3}$] | 1.562 |
| $\mu$ [mm$^{-1}$] | 2.723 |
| *F*(000) | 1800 |
| Crystal size [mm$^3$] | 0.667×0.41×0.372 |
| Crystal color | Black |
| Crystal shape | Block |
| Radiation | Ag$K_\alpha$ (λ=0.56086 Å) |
| 2θ range [°] | 3.66 to 47.29 (0.70 Å) |

| | |
|---|---|
| Index ranges | −18 ≤ h ≤ 18<br>−23 ≤ k ≤ 23<br>−26 ≤ l ≤ 26 |
| Reflections collected | 16183 |
| Independent reflections | 16183<br>$R_{int}$ = 0.0605<br>$R_{sigma}$ = 0.0343 |
| Completeness to θ = 19.665° | 99.9 % |
| Data / Restraints / Parameters | 16183/621/540 |
| Absorption correction $T_{min}/T_{max}$ (method) | 0.023650/0.050160 (multi-scan) |
| Goodness-of-fit on $F^2$ | 1.037 |
| Final *R* indexes [$I \geq 2\sigma(I)$] | $R_1$ = 0.0353<br>w$R_2$ = 0.0850 |
| Final *R* indexes [all data] | $R_1$ = 0.0411<br>w$R_2$ = 0.0890 |
| Largest peak/hole [eÅ$^{-3}$] | 1.77/−1.05 |
| Flack X parameter | −0.051(6) |

## UV/vis Spectroscopy

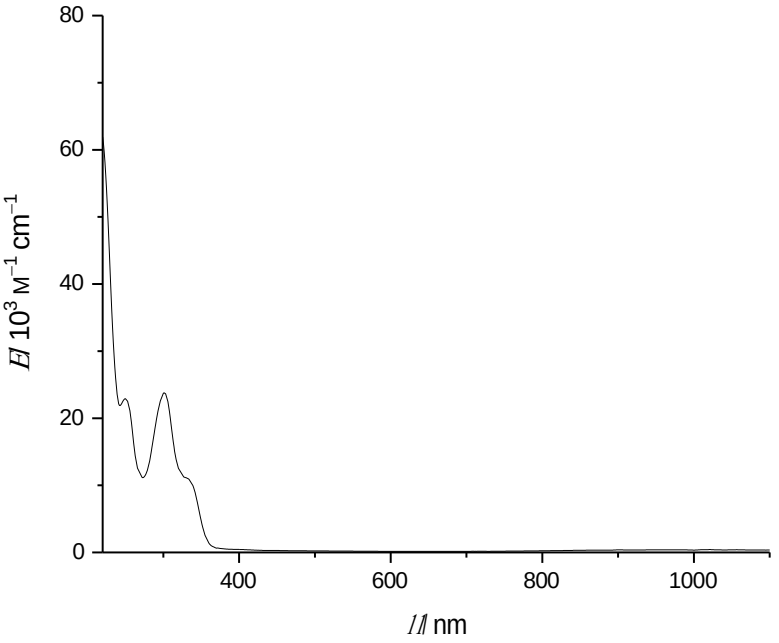



*Figure S11* UV/vis spectrum of **3a** in MeCN (0.01 mM).

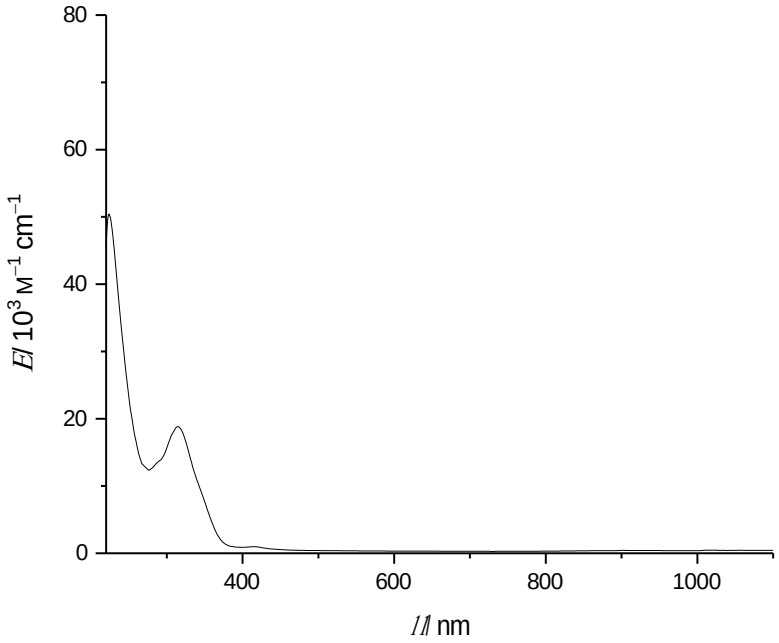



*Figure S12* UV/vis spectrum of **3b** in MeCN (0.01 mM).

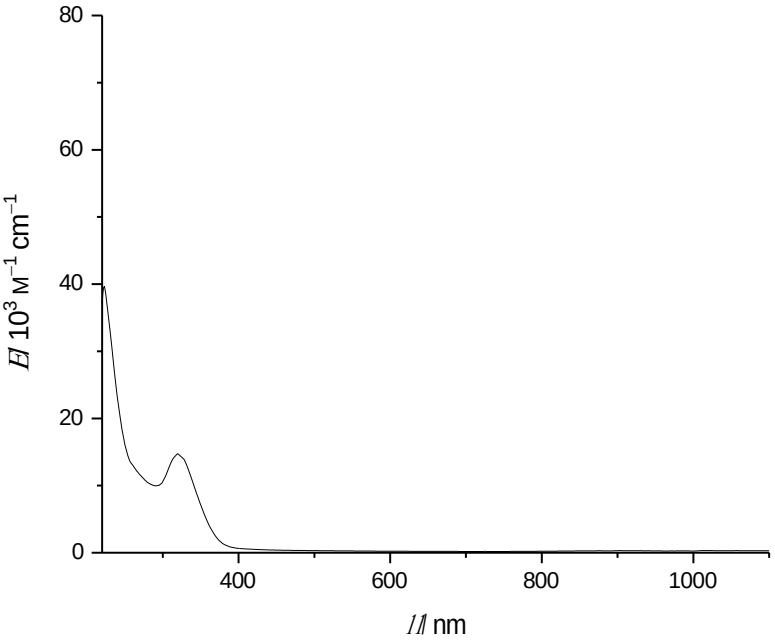



*Figure S13* UV/vis spectrum of **3c** in MeCN (0.01 mM).

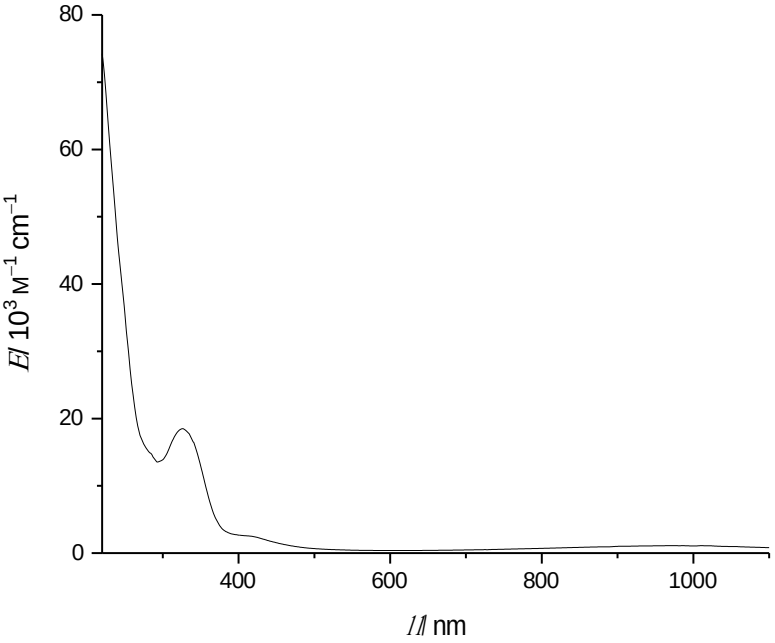



*Figure S14* UV/vis spectrum of **3d** in MeCN (0.01 mM).

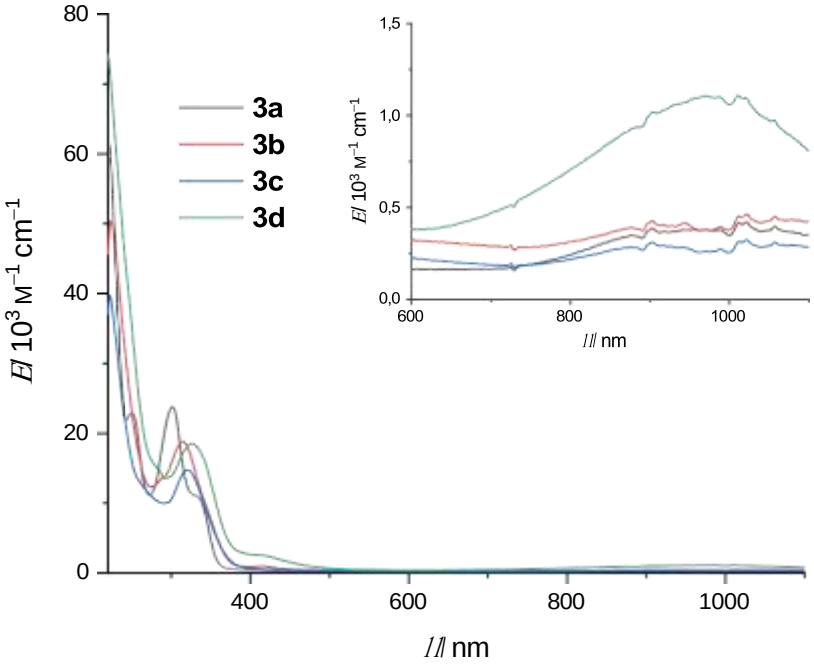



*Figure S15* Superimposed UV/vis spectra of **3a-d** in MeCN (0.01 mM). The inset shows a weak absorption in the NIR region for solutions of **3d**. This is attributed to small quantities of **3d'** available in solution.

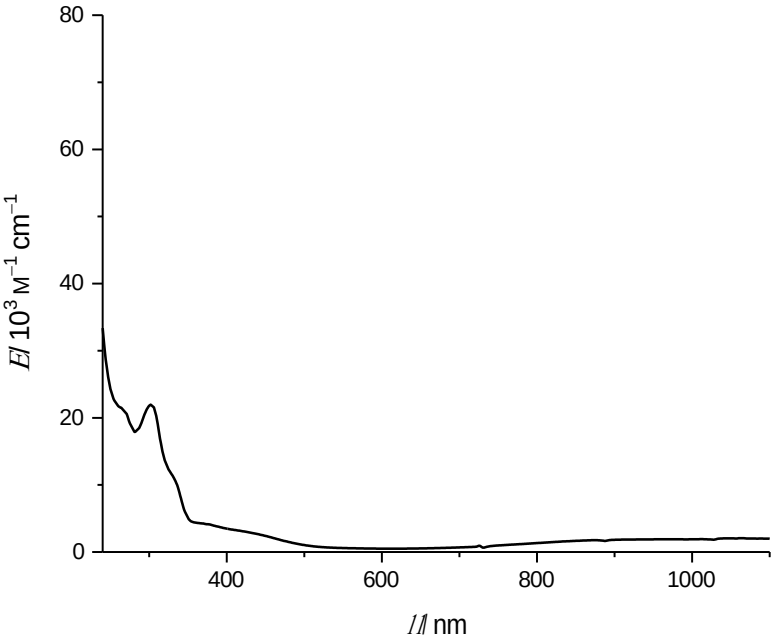



*Figure S16* UV/vis spectrum of **4a** in DCM (0.01 мм).

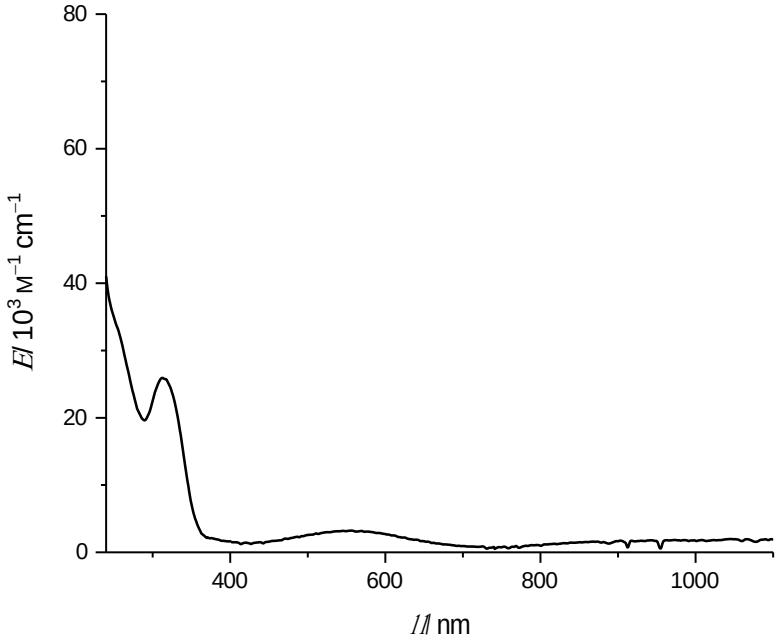



*Figure S17* UV/vis spectrum of **4b** in DCM (0.01 mM).

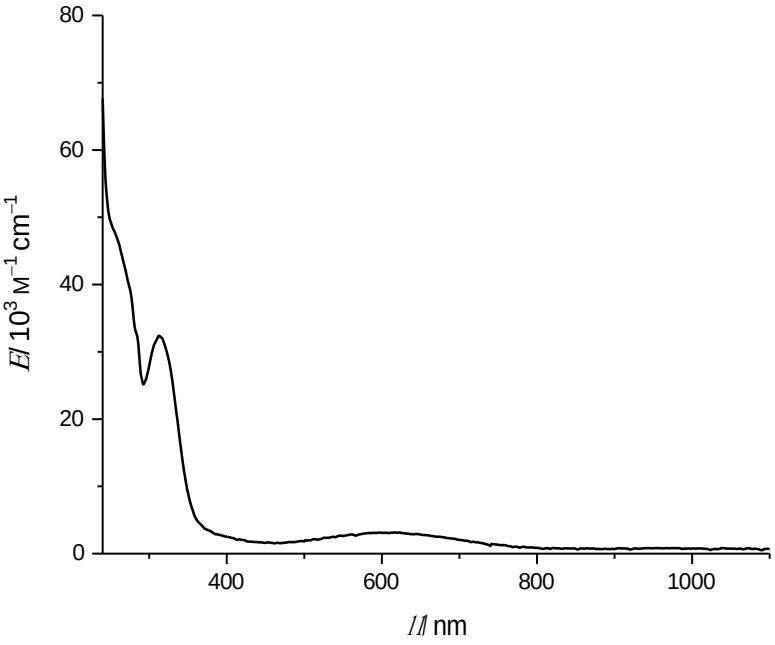



*Figure S18* UV/vis spectrum of **4c** in DCM (0.01 mM).

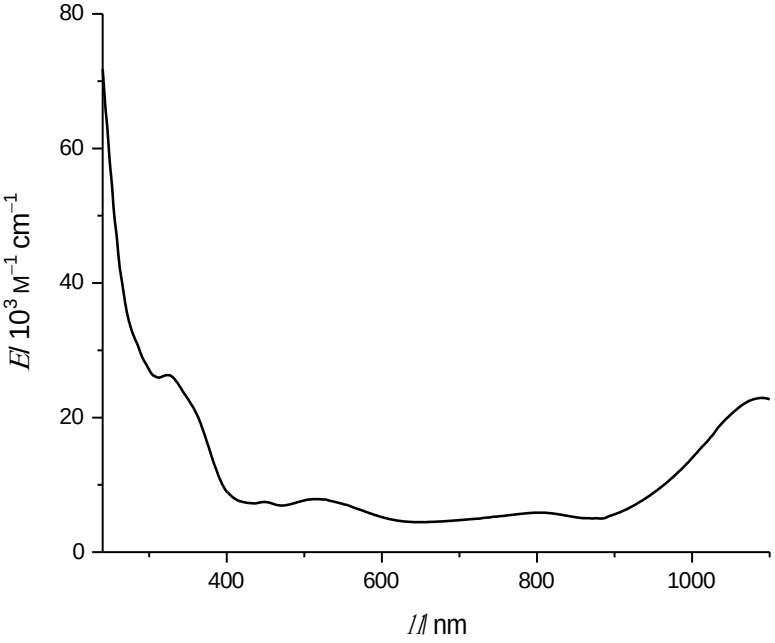



*Figure S19* UV/vis spectrum of **4d'** in DCM (0.01 mM).

## Mössbauer Spectroscopy

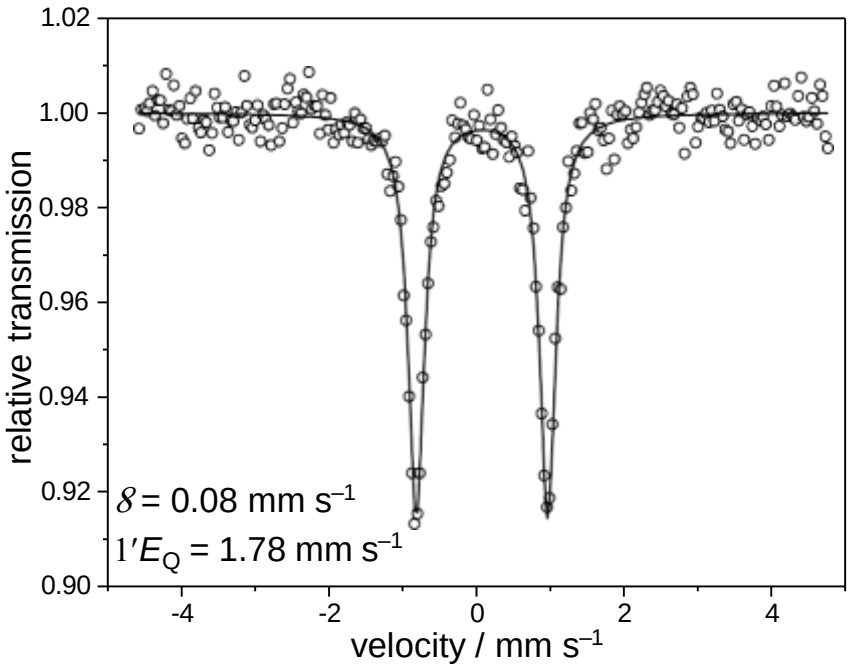



*Figure S20:* Zero-field $^{57}$Fe Mössbauer spectrum of solid **4a** at 80 K.

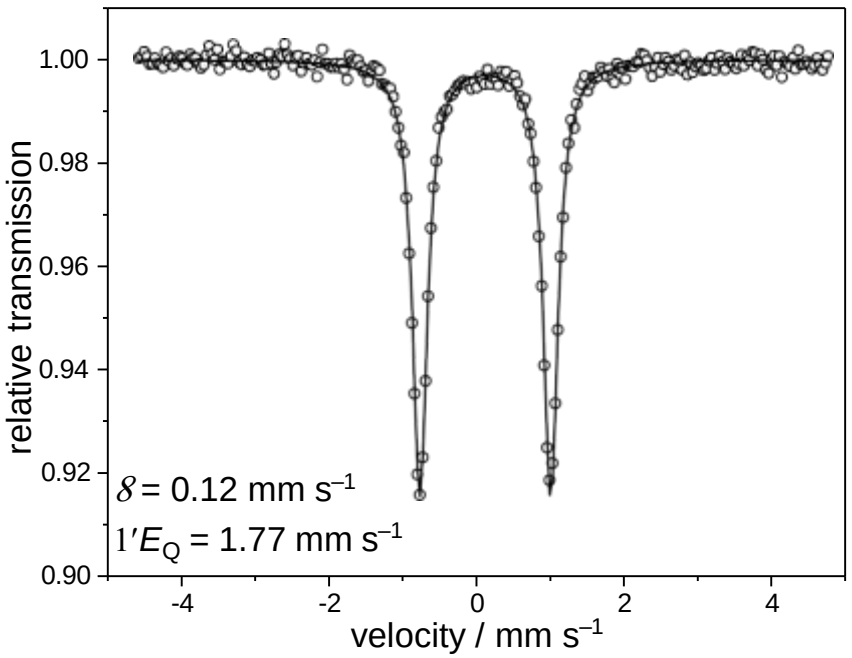



*Figure S21:* Zero-field $^{57}$Fe Mössbauer spectrum of solid **4b** at 80 K.

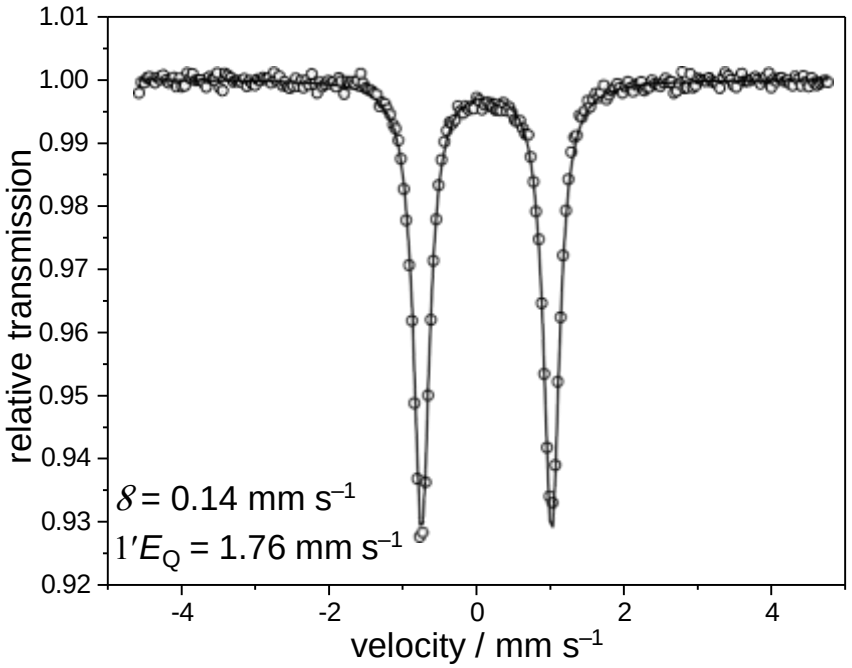



*Figure S22:* Zero-field $^{57}$Fe Mössbauer spectrum of solid **4c** at 80 K.

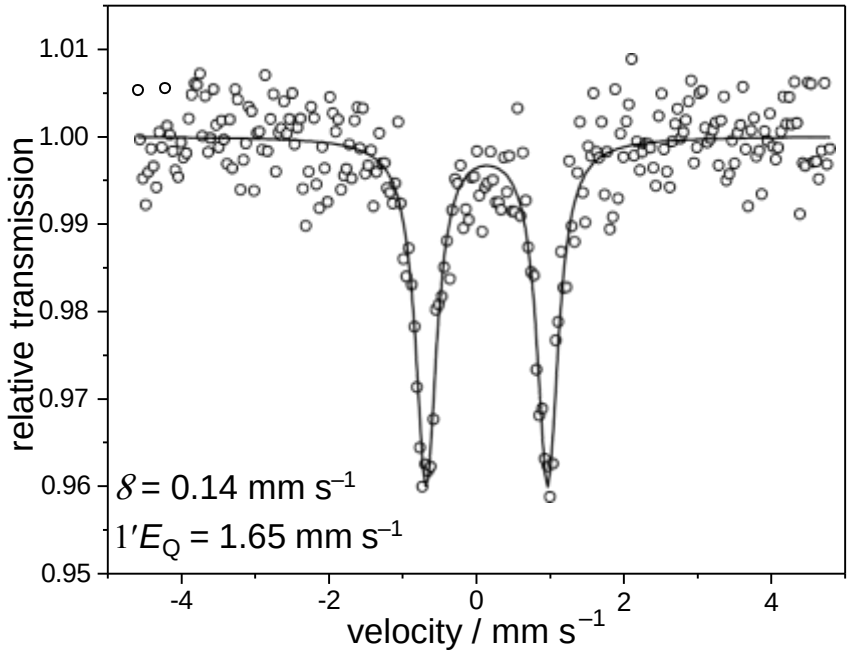



*Figure S23:* Zero-field $^{57}$Fe Mössbauer spectrum of solid **4d'** at 80 K.

## Cyclic Voltammetry

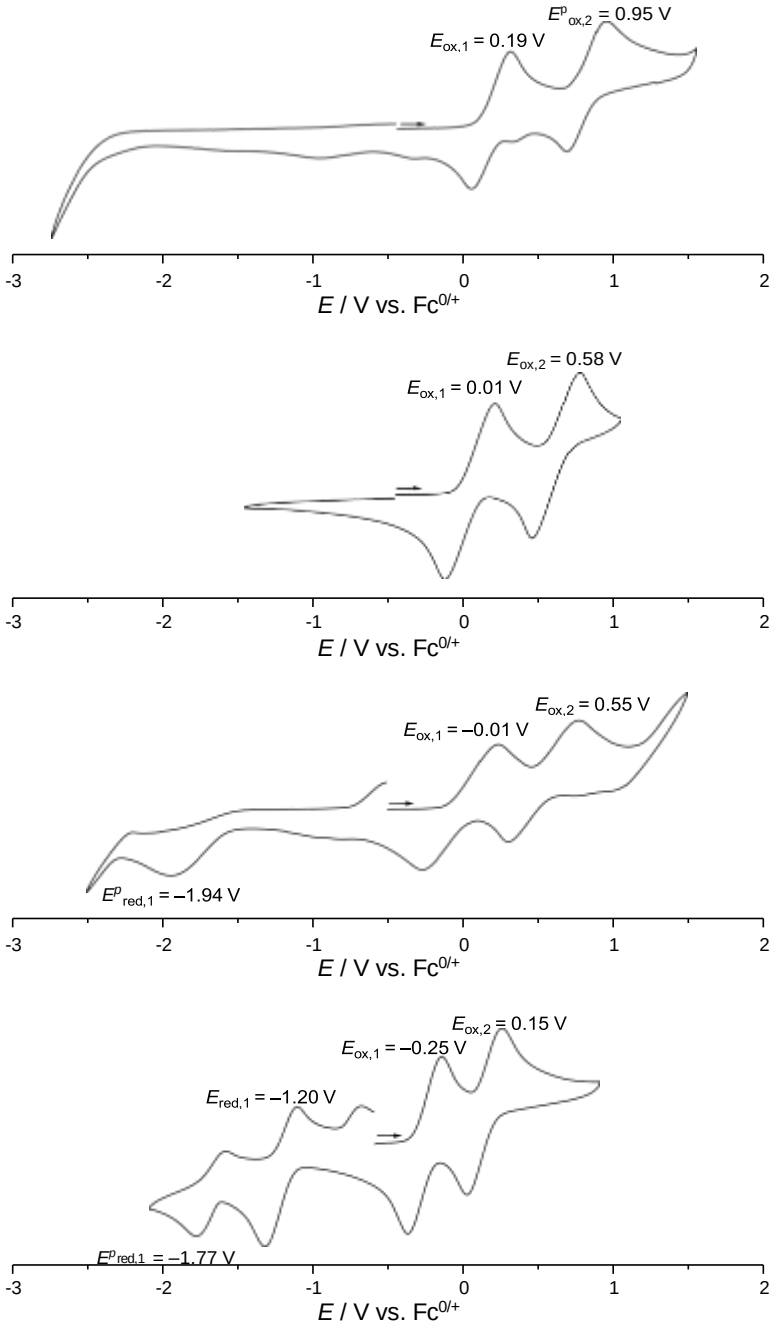



*Figure S24* Cyclic voltammograms of **4a**, **4b**, **4c** and **4d'** (top to bottom). DCM, 0.1 M $NBu_4PF_6$.

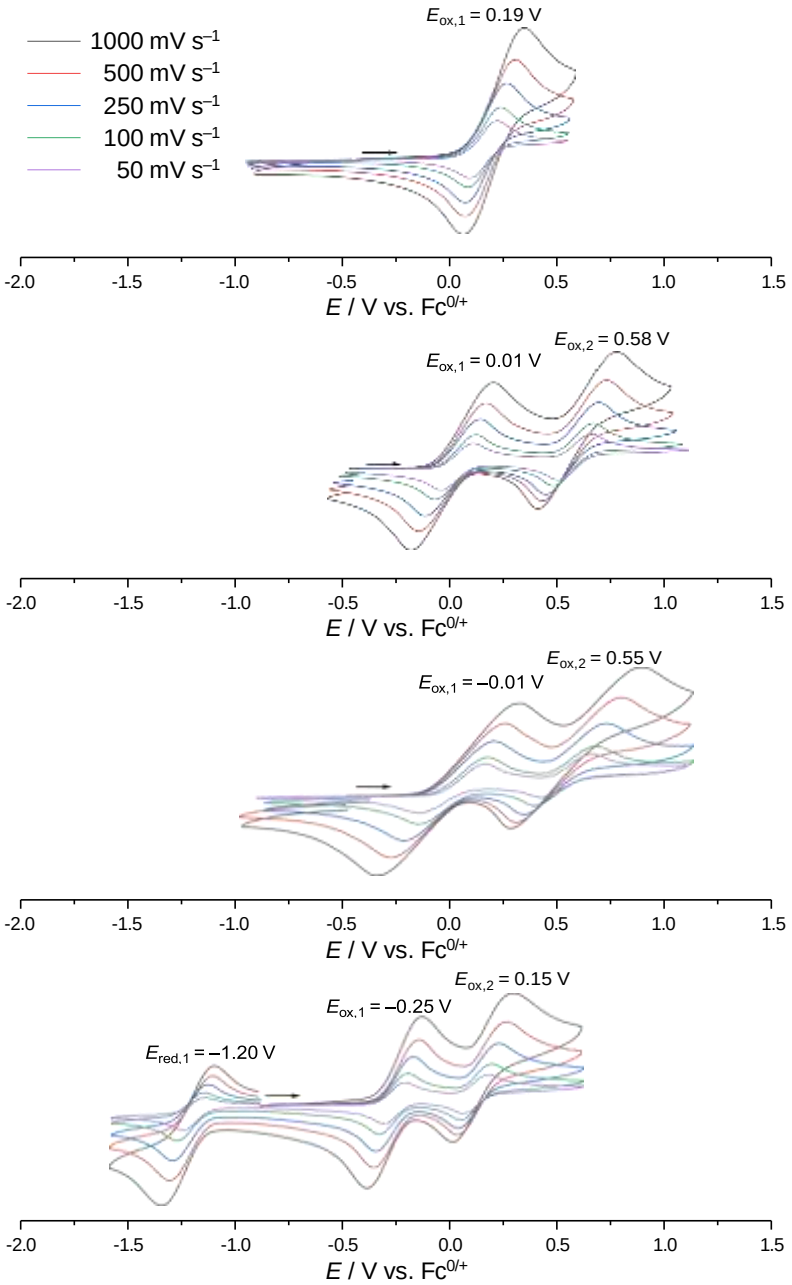



*Figure 25* Cyclic voltammograms of **4a**, **4b**, **4c** and **4d'** (top to bottom) at multiple scan rates. DCM, 0.1 M $NBu_4PF_6$.

## IR Data of Selected Pnictogen-Iron Carbonyl Complexes

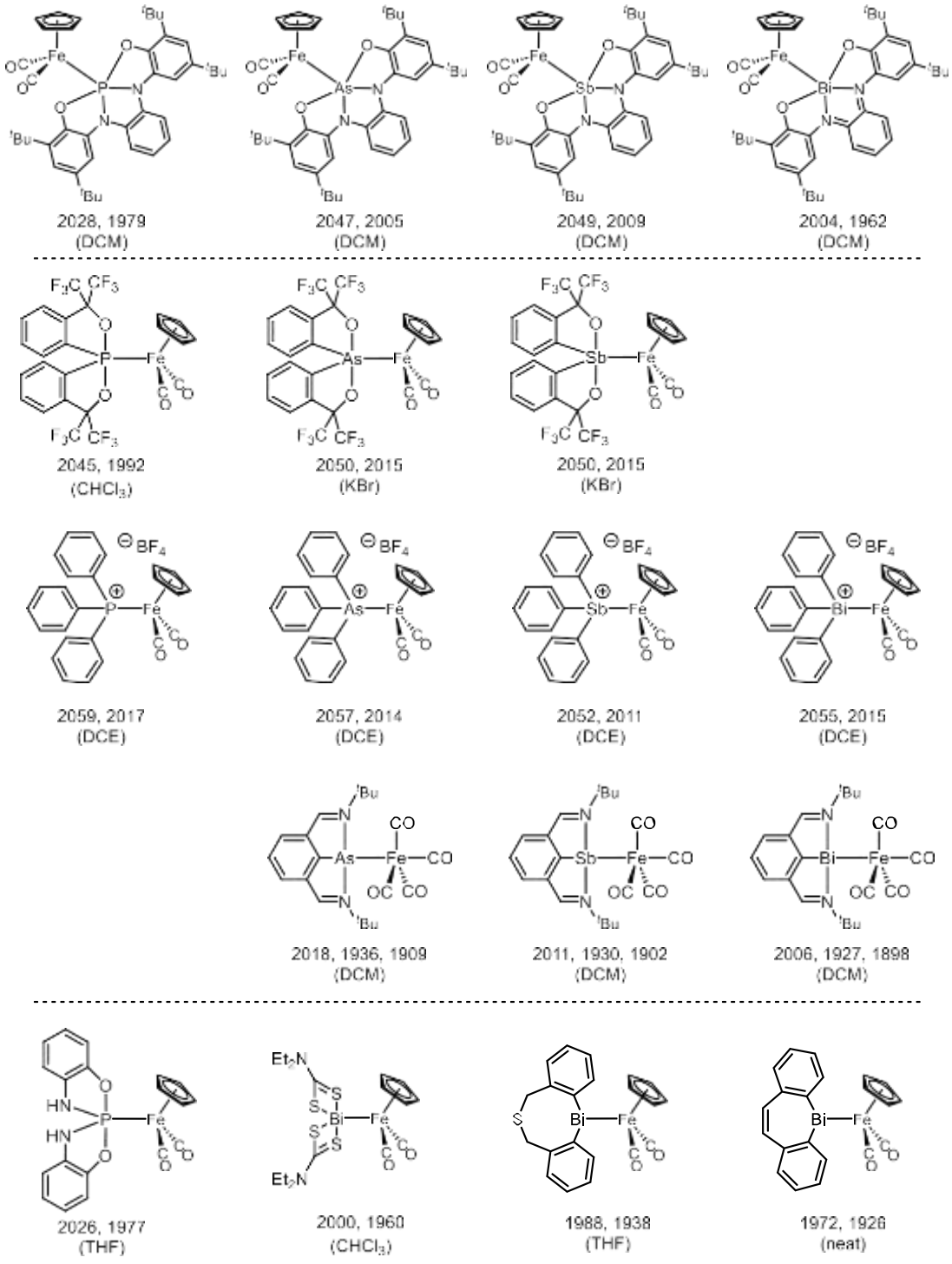



*Figure S26* Selected pnictogen-iron carbonyl complexes and their CO stretching frequencies in $cm^{-1}$.[10]

## Computational Details

All density functional theory (DFT) calculations were performed with the Gaussian16 (revision A.03) package.[11] Geometry optimizations were carried out without symmetry constraints using the TPSS density functional[12] coupled to the def2-TZVP full electron basis set for all atoms.[13] Normal mode analysis was computed to confirm minima on the potential energy surface. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298 K and 1 atm using the standard statistical mechanics relationship for an ideal gas. Accurate electronic energies were obtained via single-point calculations on the TPSS-optimized geometries using the PBE0 functional[14] coupled to the def2-TZVP basis set.[13] Solvent effects on the electronic energy were estimated with the polarizable continuum model (PCM) using acetonitrile as the solvent.[15] Dispersion correction through Grimme's D3, together with the Becke-Johnson damping function, was included in all cases.[16] Reported Gibbs free energies were obtained by adding the thermal and entropy corrections obtained (gas-phase) at the TPSS-D3(BJ)/def2-TZVP level on top of the PBE0-D3(BJ)/def2-TZVP(PCM) electronic energies. TD-DFT calculations were performed on the PBE0-D3(BJ)/def2-TZVP(PCM) level of theory making use of the Tamm-Dancoff approximation. All species coincide in the singlet spin state being the most stable electronic configuration. However, stability analysis revealed that, in species **4c'** and **4d',** the closed-shell wavefunction was not stable. In both cases, an open-shell singlet solution lower in energy (and stable) was found.

Topological analysis of the electron densities of all species was performed according to the quantum theory of atoms in molecules (QTAIM)[17] with the program Multiwfn.[18] Effective fragment orbitals (EFOs)[19] and effective oxidation states (EOS)[20] were evaluated with the APOST-3D software,[21] using the topological fuzzy Voronoi cells (TFVC)[22] real-space atomic definition and the default integration setup for the numerical integrations.

### Interconversion of **3d** and **3d'**

In order to explore the interconversion of **3d** and **3d'**, a relaxed coordinate scan in analogy to previous work by Chitnis and co-workers[23] was performed at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory (Figure S27). From the obtained maximum energy structure, the transition state for the interconversion **TS-3d-3d'** could be located as confirmed by frequency calculations. At the PBE0-D3(BJ)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level of theory, the transition state is 2.4 kcal $mol^{-1}$ higher in Gibbs free energy than **3d**. **3d'** lies 2.1 kcal $mol^{-1}$ higher in free energy than **3d**. After solvent correction (PCM:MeCN), **TS-3d-3d'** exhibits a free energy of 2.9 kcal $mol^{-1}$ relative to **3d** while **3d'** is at 4.0 kcal $mol^{-1}$ (Figure S28). This indicates that the interconversion of **3d** and **3d'** is barrierless in solution.

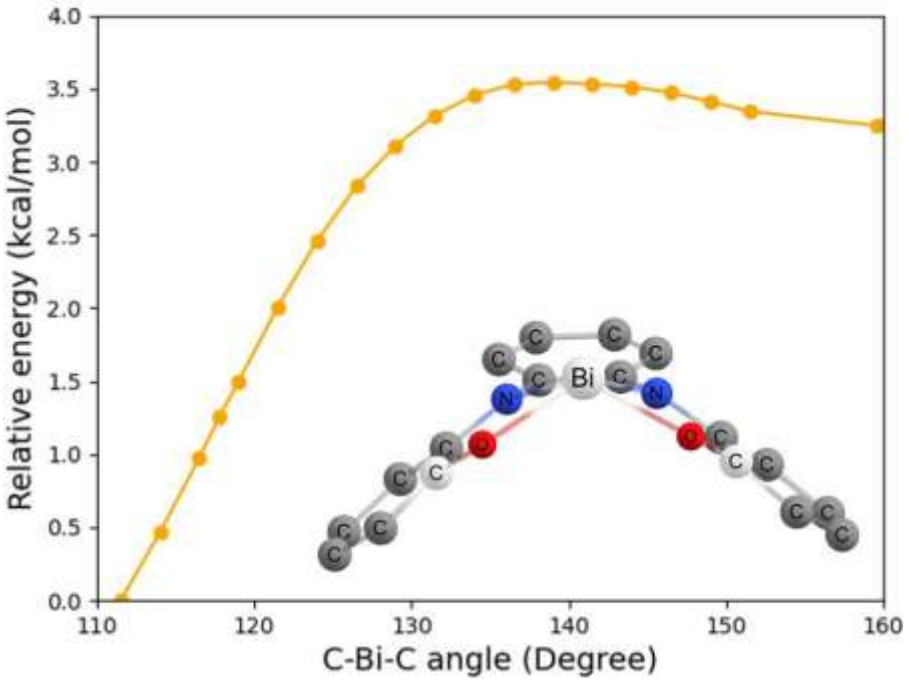



*Figure S27:* Electronic energies of the relaxed scan of the C-Bi-C angle (atoms forming the scanned angle represented in light grey), including solvent corrections at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. The ending points of the scan correspond to both minima (**3d** and **3d'**), while the gas-phase obtained **TS-3d-3d'** geometry (TPSS-D3(BJ)/def2-TZVP) is the point at x = 117.8º. Methyl groups and hydrogen atoms are visually omitted for clarity.

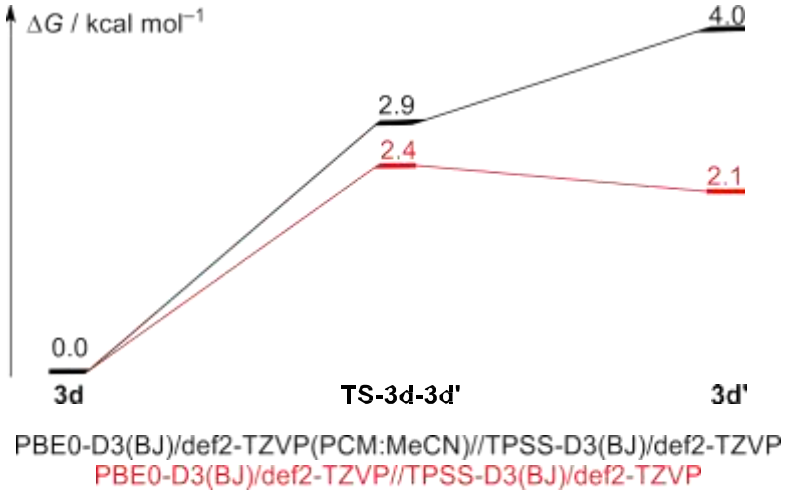



*Figure S28:* Gibbs free energies of **3d**, **3d'** and the transition state for their interconversion **TS-3d-3d'** with (black) and without (red) solvent correction.

## EOS results

*Table S1:* EOS analysis results for all studied systems. OS = oxidation state, LO = last occupied, FU = first unoccupied.

| | Pn OS | Fe OS | Fp OS | CO OS | Cp OS | LO EFO (α) | FU EFO (α) | LO EFO (β) | FU EFO (β) | *R(%)* (α) | R(%) (β) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **3d** | 3 | - | -4 | - | - | 0.610 | 0.390 | - | - | 71.9 | - |
| **3d'** | 3 | - | -4 | - | - | 0.741 | 0.259 | - | - | 98.2 | - |
| **4a** | 3 | 2 | -4 | 0 | -1 | 0.516 | 0.448 | - | - | 56.9 | - |
| **4b** | 3 | 2 | -4 | 0 | -1 | 0.630 | 0.430 | - | - | 70.0 | - |
| **4c** | 3 | 2 | -4 | 0 | -1 | 0.636 | 0.447 | - | - | 68.9 | - |
| **4b'** | 1 | 2 | -2 | 0 | -1 | 0.422 | 0.405 | - | - | 51.8 | - |
| **4c'** | 3 | 0 | -2 | 0 | -1 | 0.448 | 0.407 | 0.448 | 0.405 | 54.1 | 54.3 |
| **4d'** | 3 | 0 | -2 | 0 | -1 | 0.474 | 0.408 | 0.468 | 0.404 | 56.6 | 56.4 |

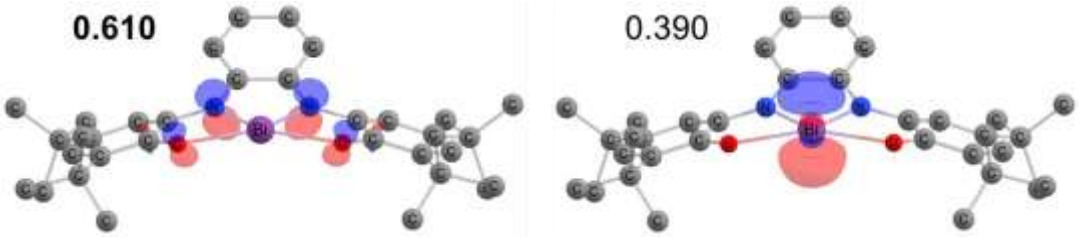



*Figure S29:* Frontier effective fragment orbitals and their associated occupation values for system **3d'**. Formally occupied EFO in bold. As defined, the resulting R(%) value from the difference in occupations is 71.9 (see equation in the main manuscript).

## QTAIM results

*Table S2:* Selected QTAIM Data: Electron Density ($\rho$), Laplacian of the Electron Density ($\nabla^2\rho$), Ellipticity ($\varepsilon$), relative Total Energy Density ($H/\rho$), relative Kinetic Energy Density ($G/\rho$) and Ratio of Potential and Kinetic Energy Density ($|V|/G$) at the Pnictogen–Iron Bond Critical Point, Pnictogen–Iron Delocalization Index (DI), Bond Distance ($d$) and AIM Charges $q$.

| | $\rho$ / a.u. | $\nabla^2\rho$ / a.u. | $\varepsilon$ | $H/\rho$ / a.u. | $G/\rho$ / a.u. | $\|V\|/G$ | DI | $d$ / Å | $q_{AIM}$ (Pn) | $q_{AIM}$ (Fe) |
|---|---|---|---|---|---|---|---|---|---|---|
| **4a** | 0.094 | 0.066 | 0.03 | –0.40 | 0.58 | 1.70 | 0.72 | 2.286 | 2.54 | 0.73 |
| **4b** | 0.083 | 0.073 | 0.06 | –0.39 | 0.61 | 1.64 | 0.70 | 2.355 | 1.94 | 0.72 |
| **4c** | 0.069 | 0.056 | 0.09 | –0.35 | 0.55 | 1.63 | 0.68 | 2.506 | 2.07 | 0.66 |
| **4b'** | 0.073 | 0.070 | 0.07 | –0.36 | 0.60 | 1.60 | 0.64 | 2.407 | 1.24 | 0.75 |
| **4c'** | 0.062 | 0.034 | 0.10 | –0.32 | 0.45 | 1.70 | 0.66 | 2.585 | 1.37 | 0.67 |
| **4d'** | 0.057 | 0.043 | 0.09 | –0.28 | 0.47 | 1.60 | 0.69 | 2.665 | 1.34 | 0.65 |

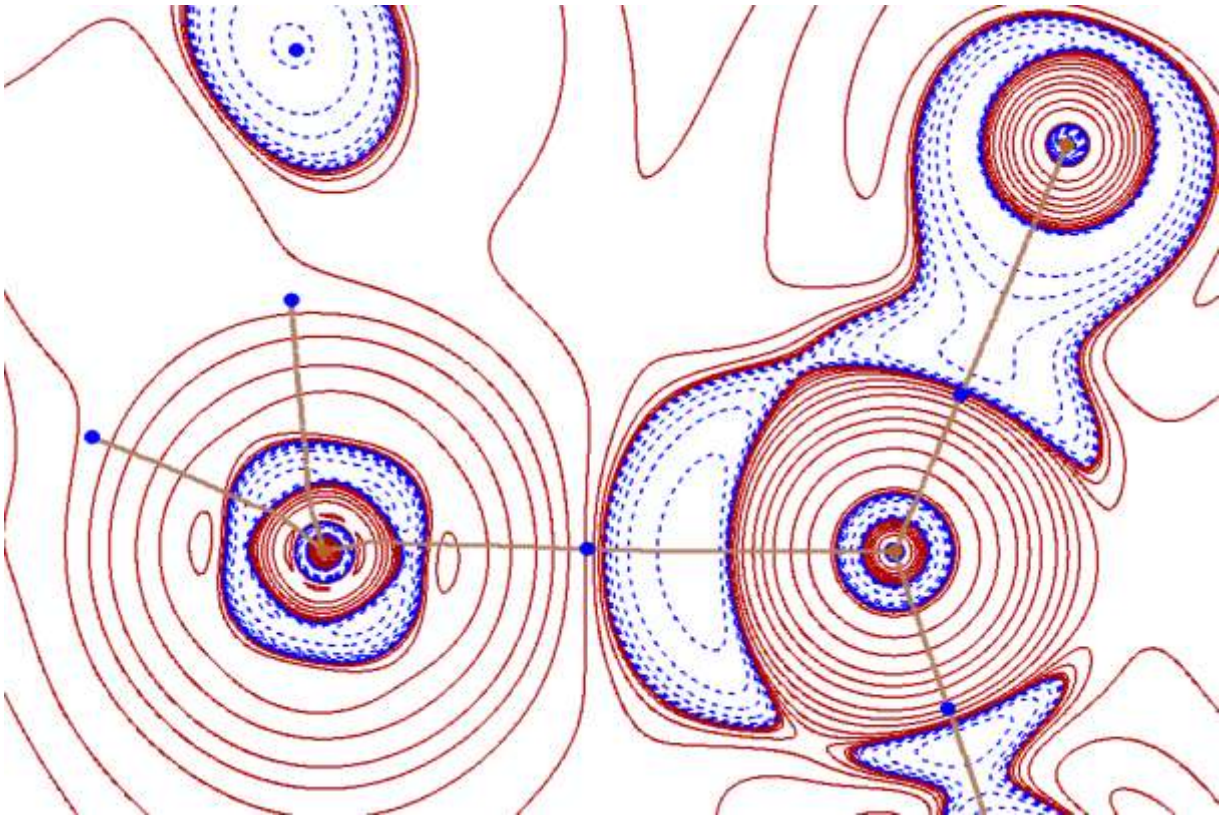


*Figure S30:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4a** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

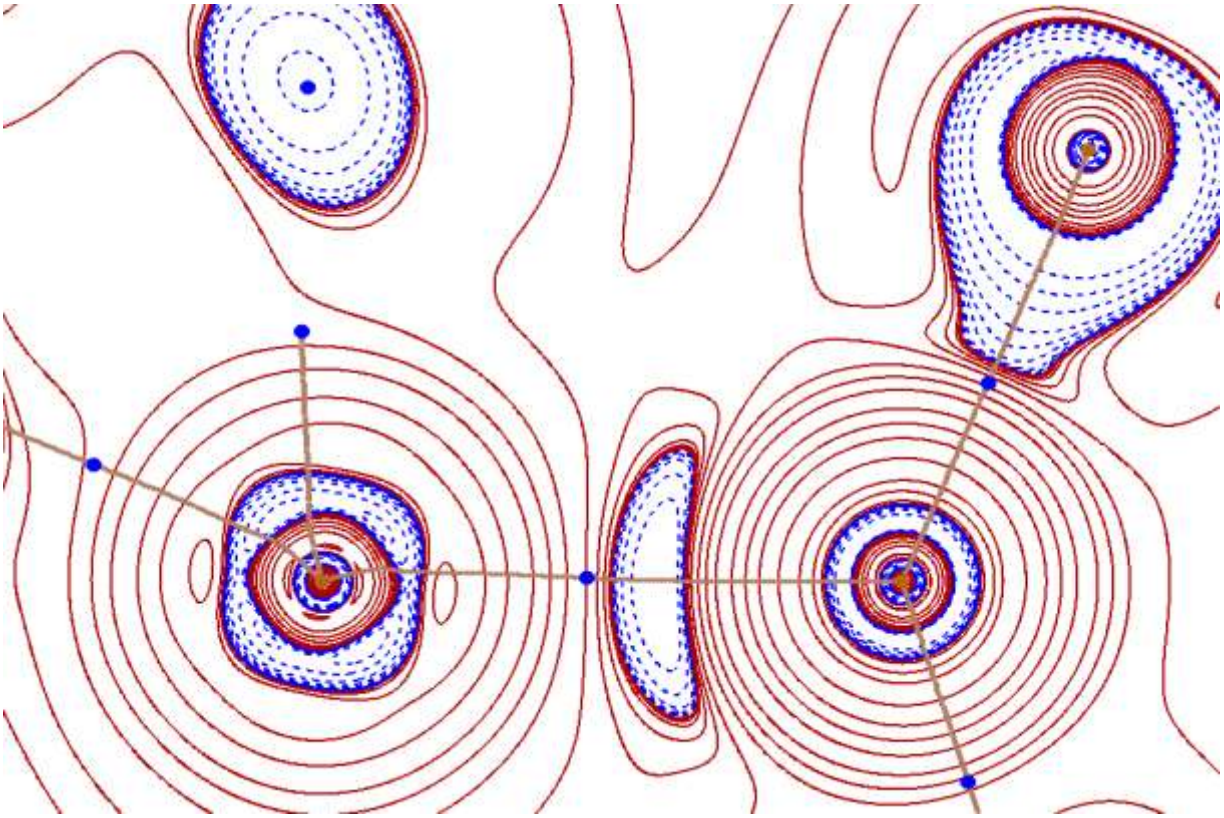


*Figure S31:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4b** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

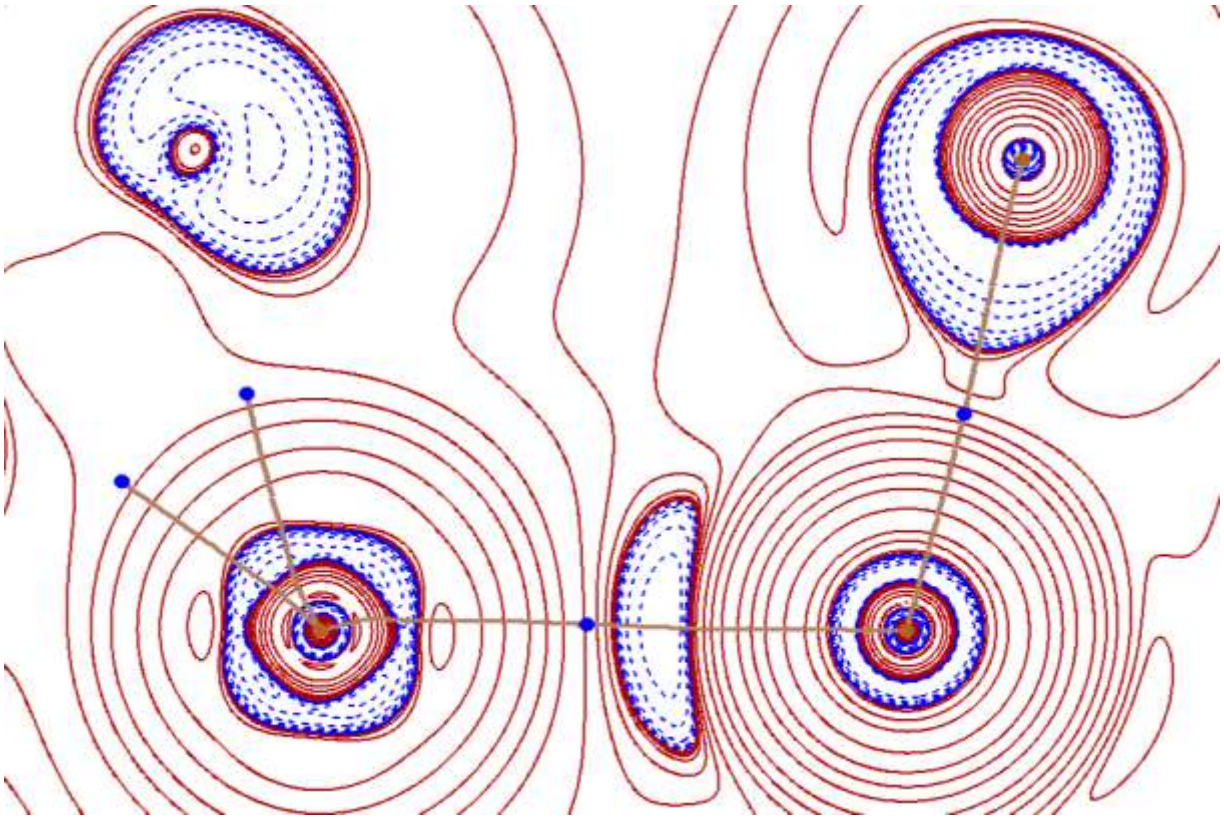


*Figure S32:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4b'** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

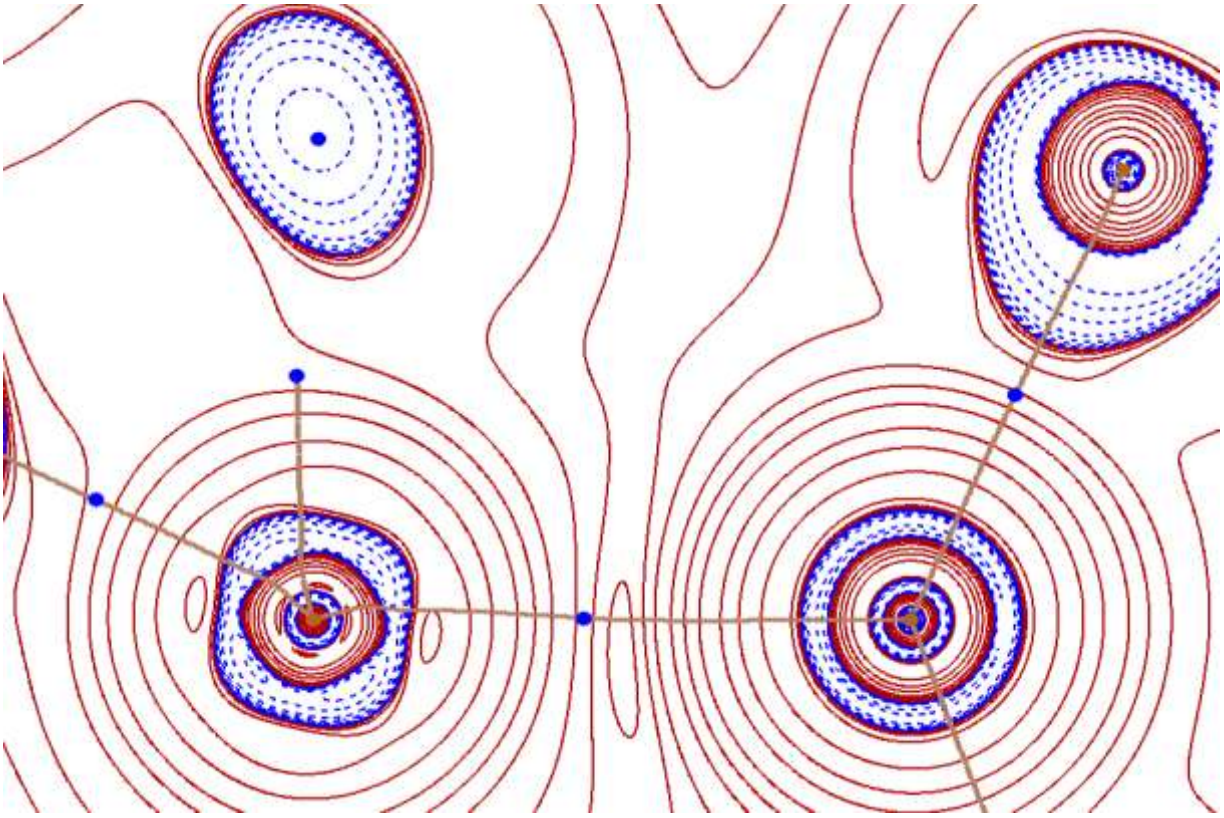


*Figure S33:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4c** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

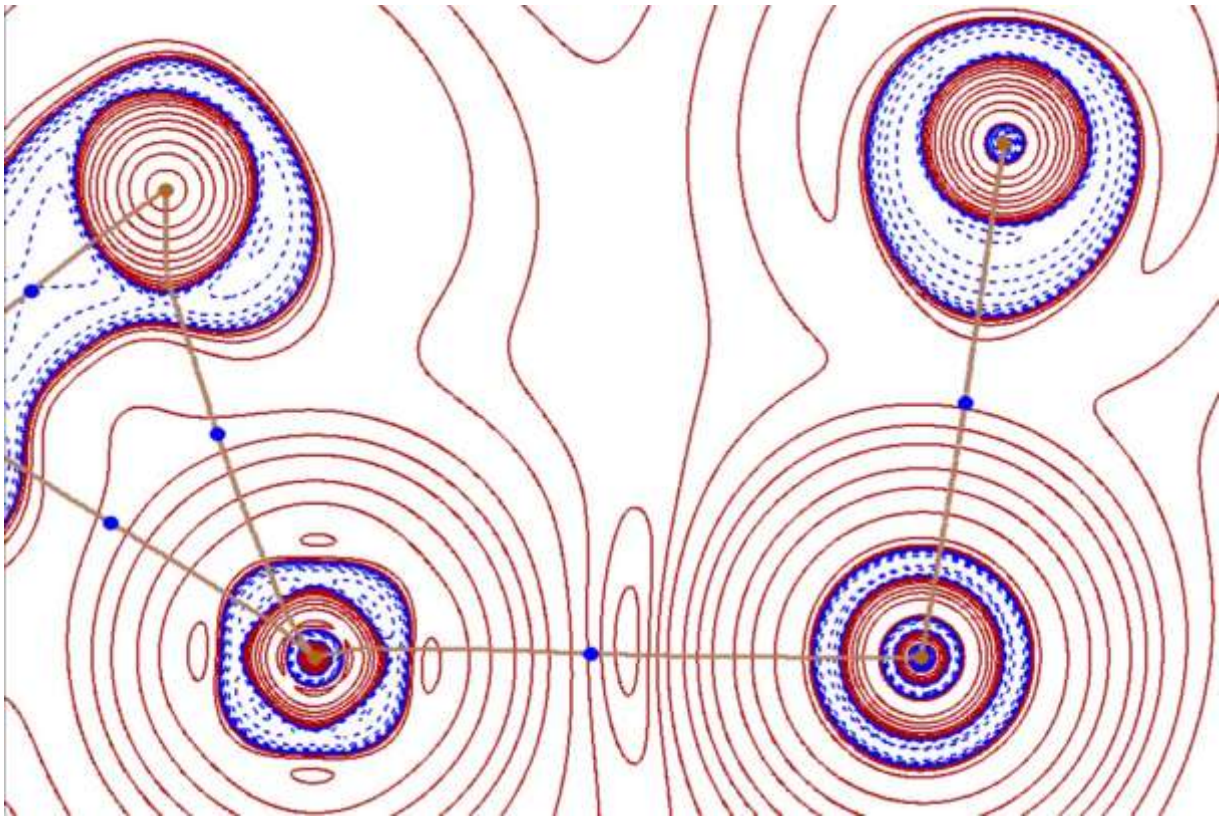


*Figure S34:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4c'** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

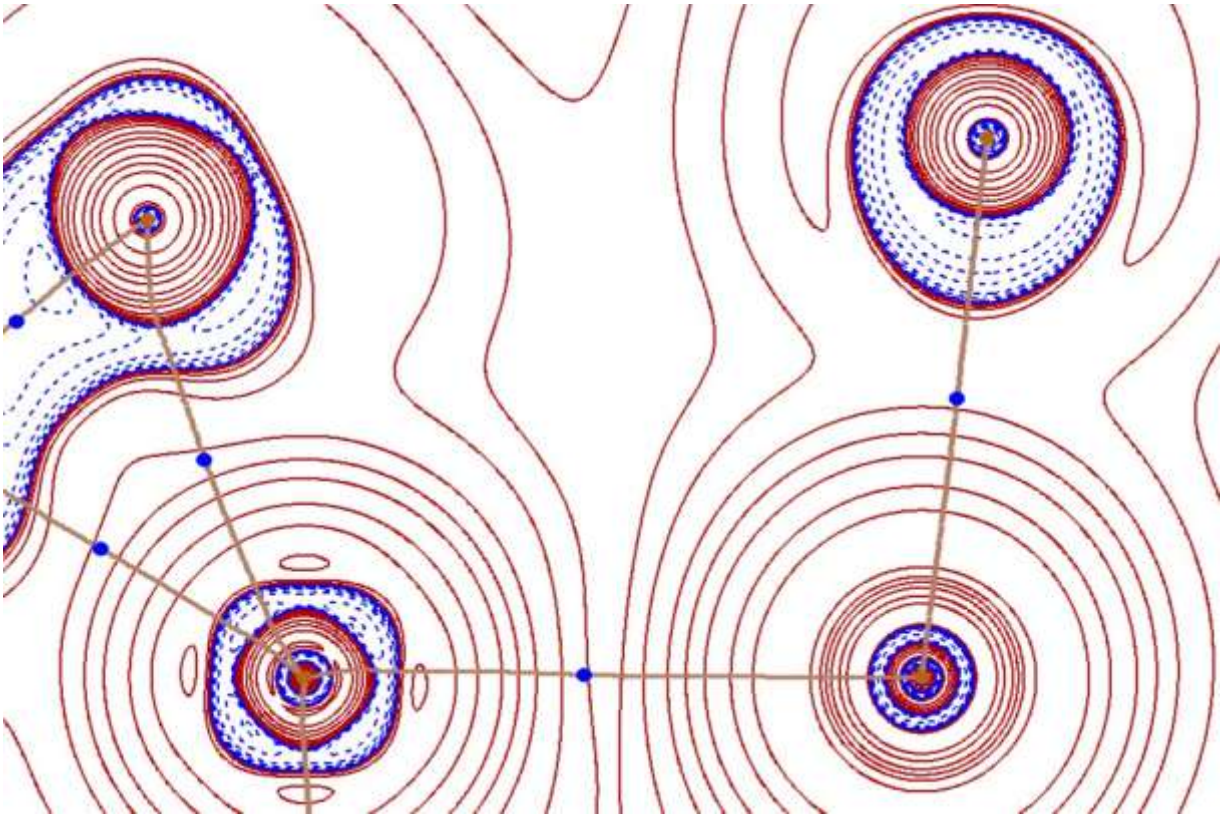


*Figure S35:* Contour plot of the Laplacian of the electron density $\nabla^2\rho$ for **4d'** calculated at the PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP level of theory. Blue: Charge accumulation ($\nabla^2\rho<0$). Red: Charge depletion ($\nabla^2\rho>0$).

## Frontier Molecular Orbitals of Iron Complexes

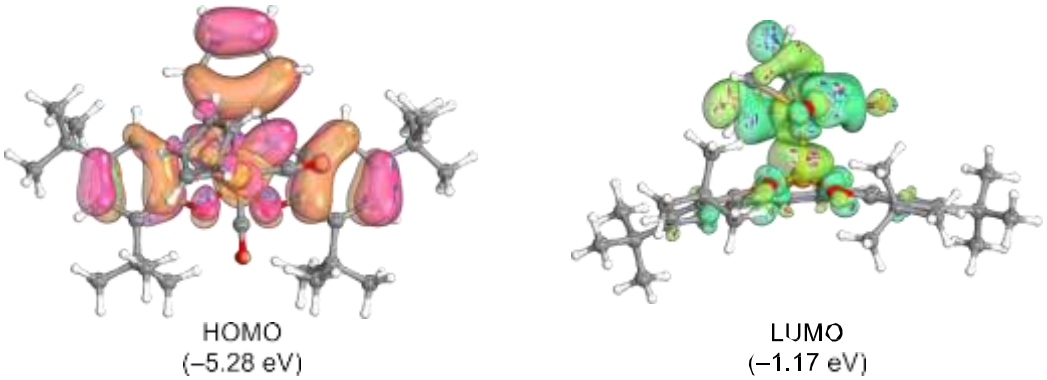



*Figure S36:* Frontier molecular orbitals of **4a**. Theory level: PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP.

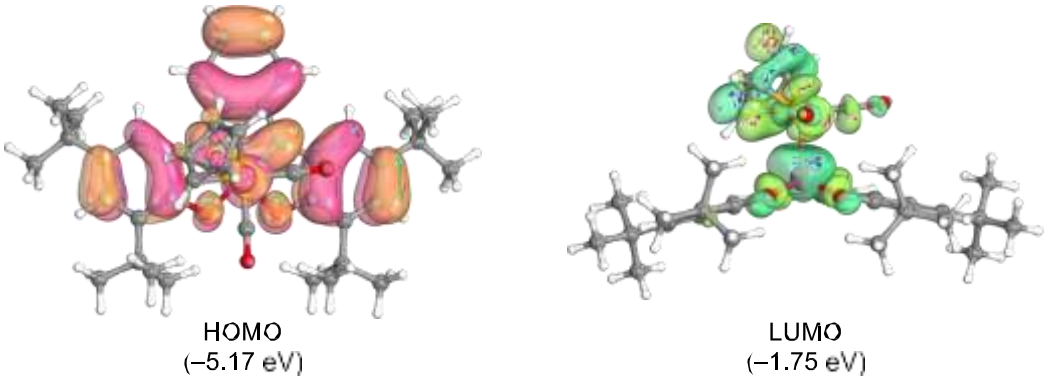



*Figure S37:* Frontier molecular orbitals of **4b**. Theory level: PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP.

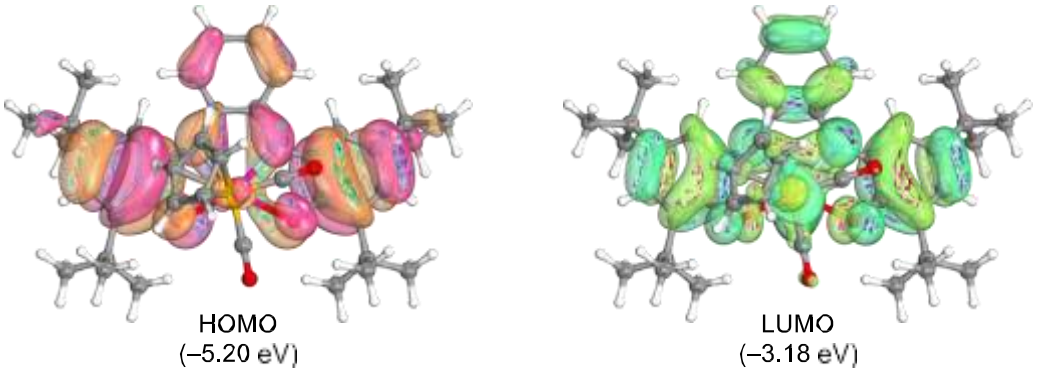



*Figure S38:* Frontier molecular orbitals of **4b'**. Theory level: PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP.

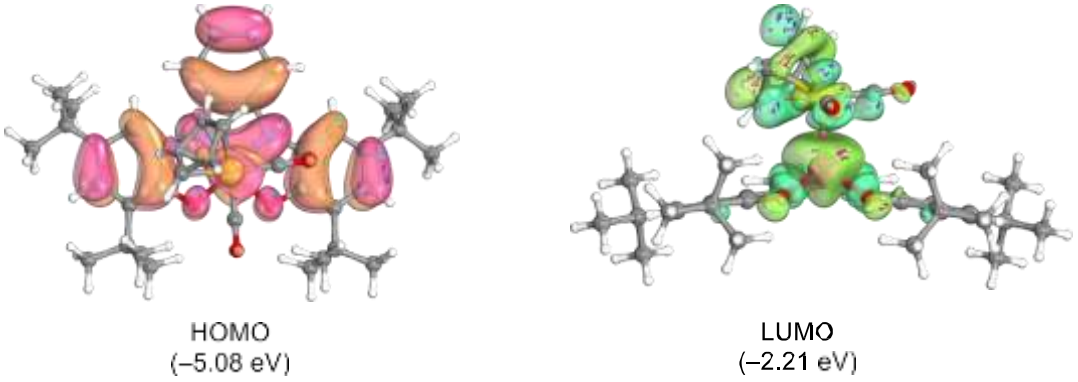



*Figure S39:* Frontier molecular orbitals of **4c**. Theory level: PBE0-D3(BJ)/def2-TZVP(PCM)//TPSS-D3(BJ)/def2-TZVP.

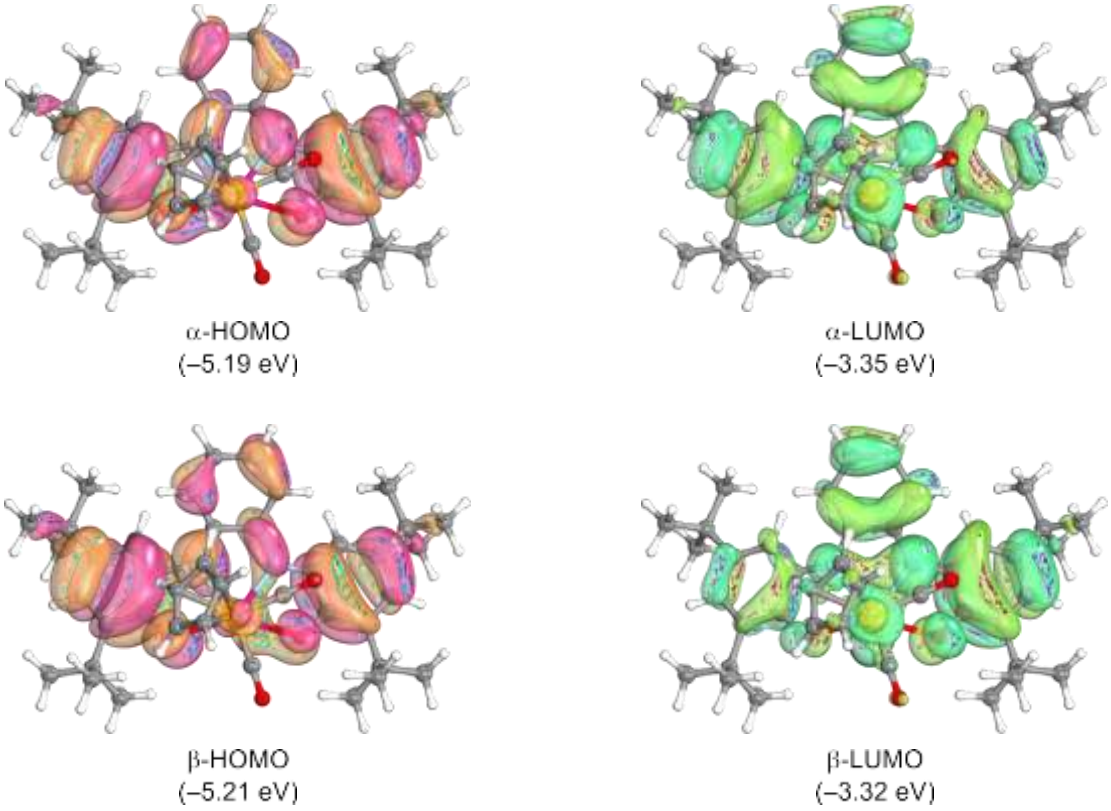



*Figure S40:* Frontier molecular orbitals of **4c'**. Theory level: UPBE0-D3(BJ)/def2-TZVP(PCM)//UTPSS-D3(BJ)/def2-TZVP.

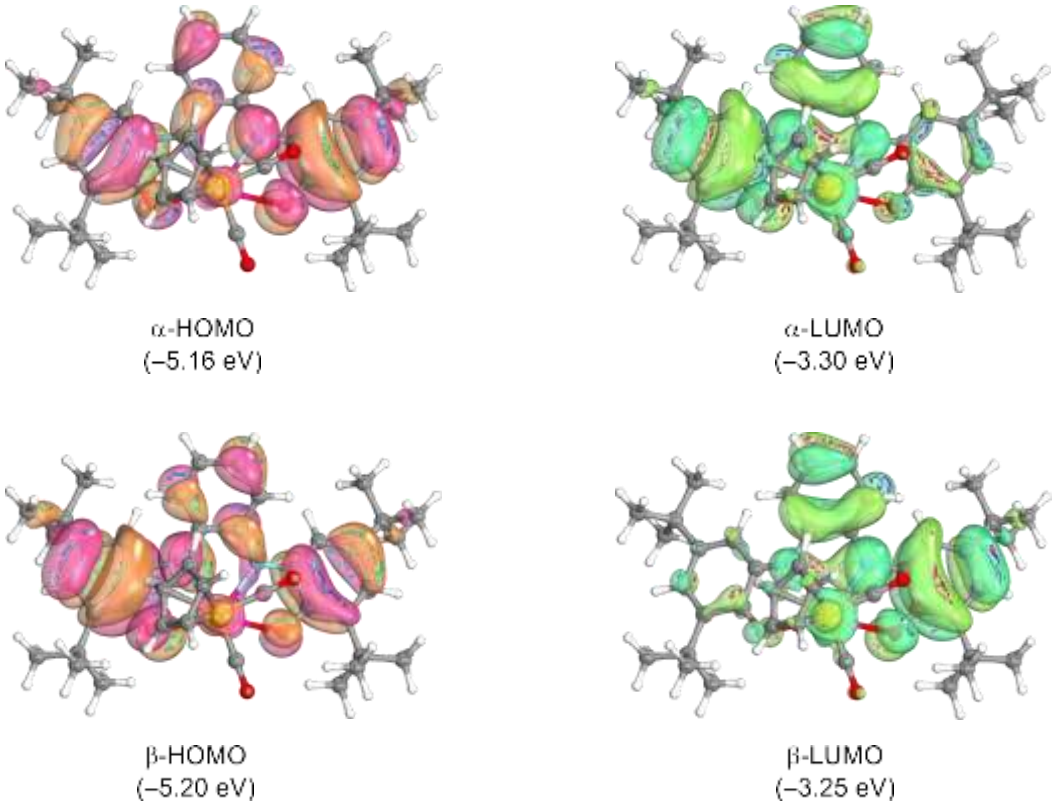
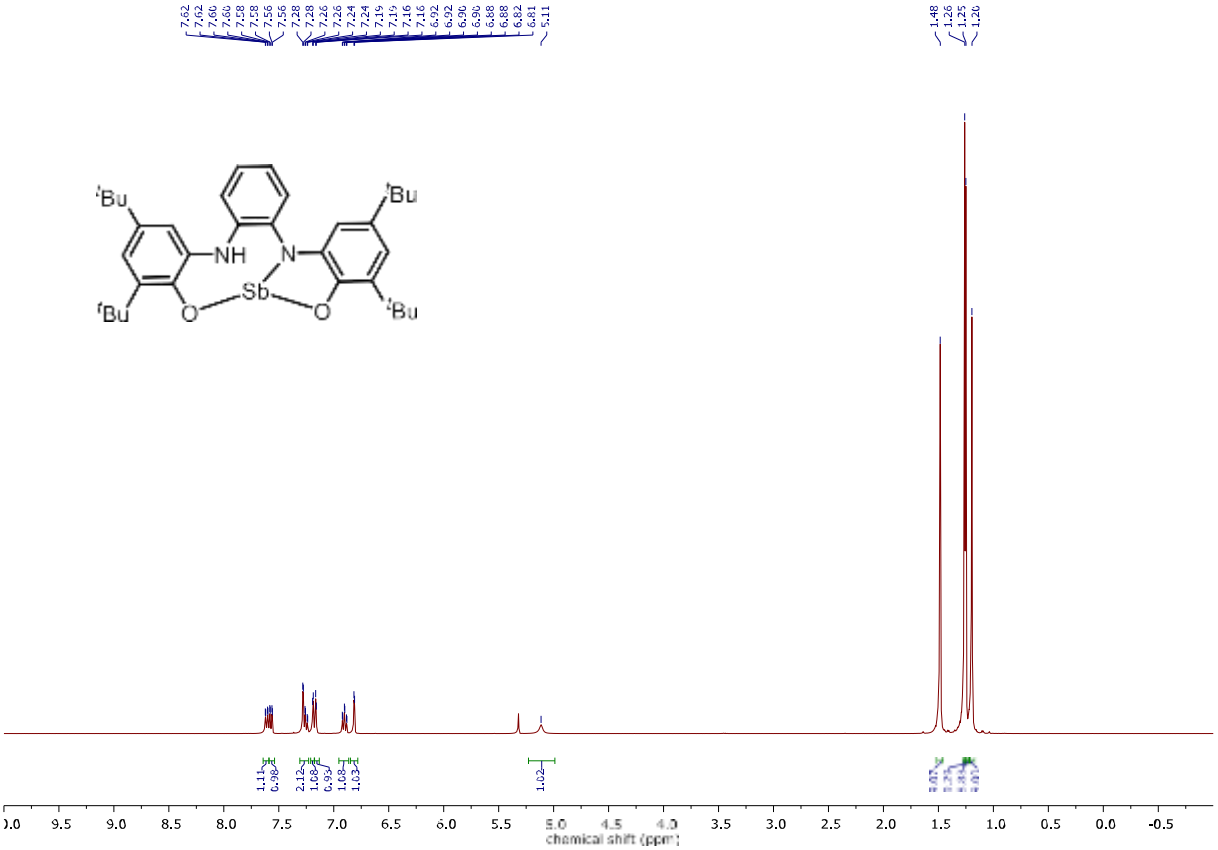



*Figure S41:* Frontier molecular orbitals of **4d'**. Theory level: UPBE0-D3(BJ)/def2-TZVP(PCM)//UTPSS-D3(BJ)/def2-TZVP.

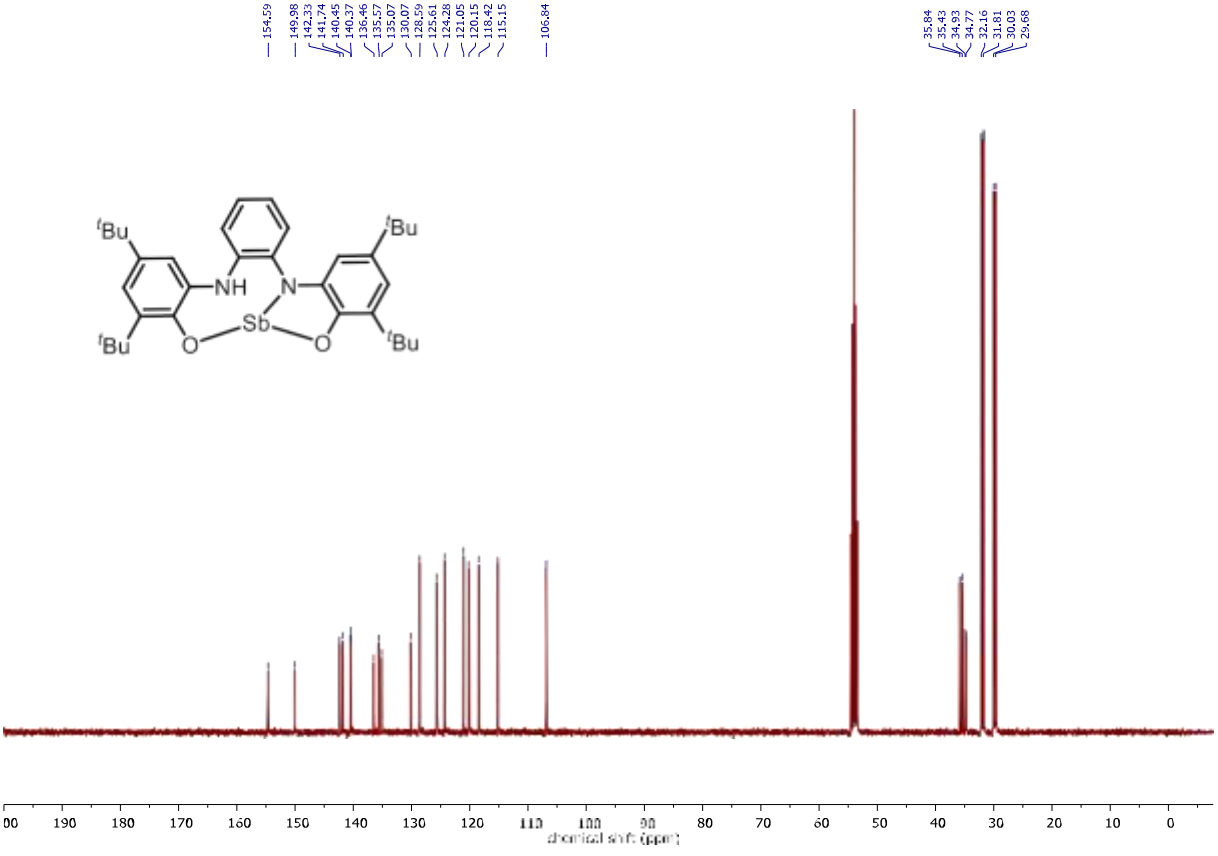
## NMR Spectra

Compound **2c**

**$^{1}$H NMR** (400 MHz, $CD_2Cl_2$)

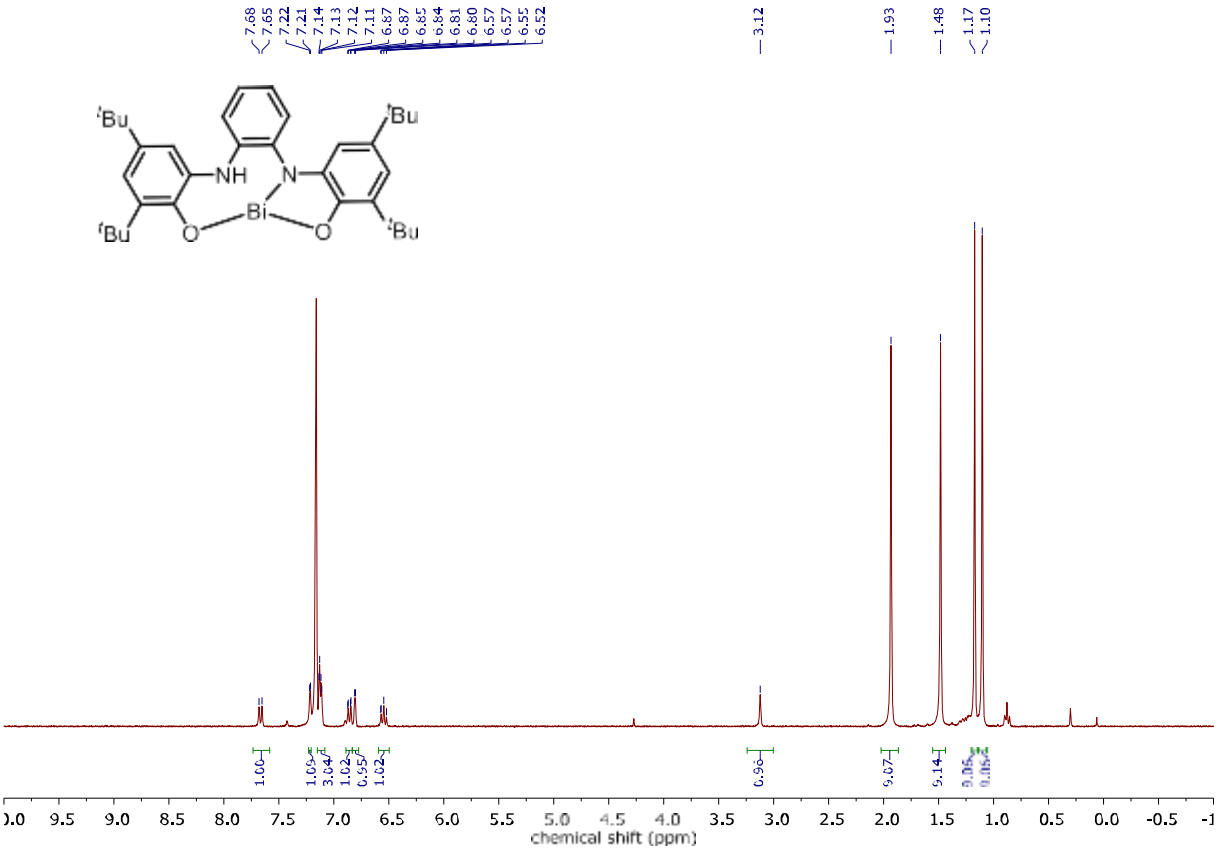



**$^{13}$C{$^{1}$H} NMR** (101 MHz, $CD_2Cl_2$)

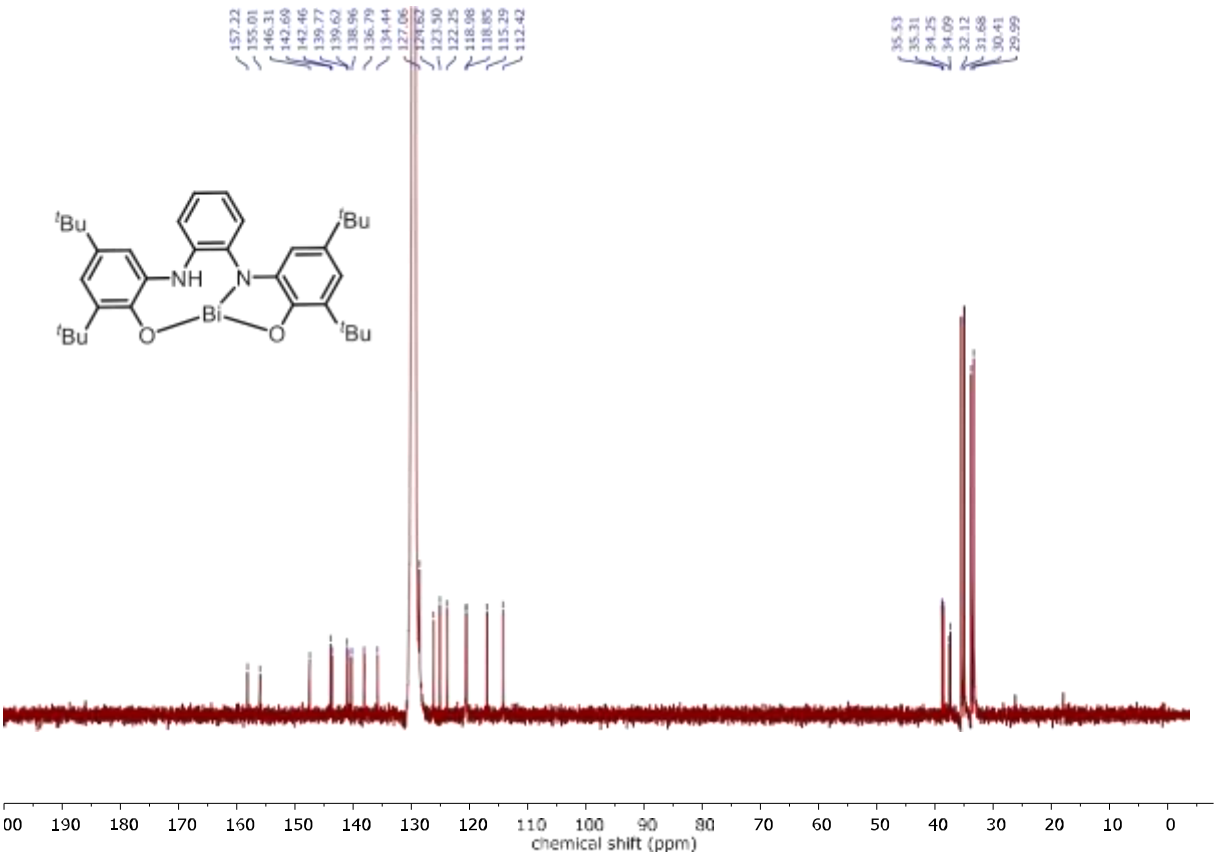


Compound **2d**

**$^{1}$H NMR** (300 MHz, $C_6D_6$)

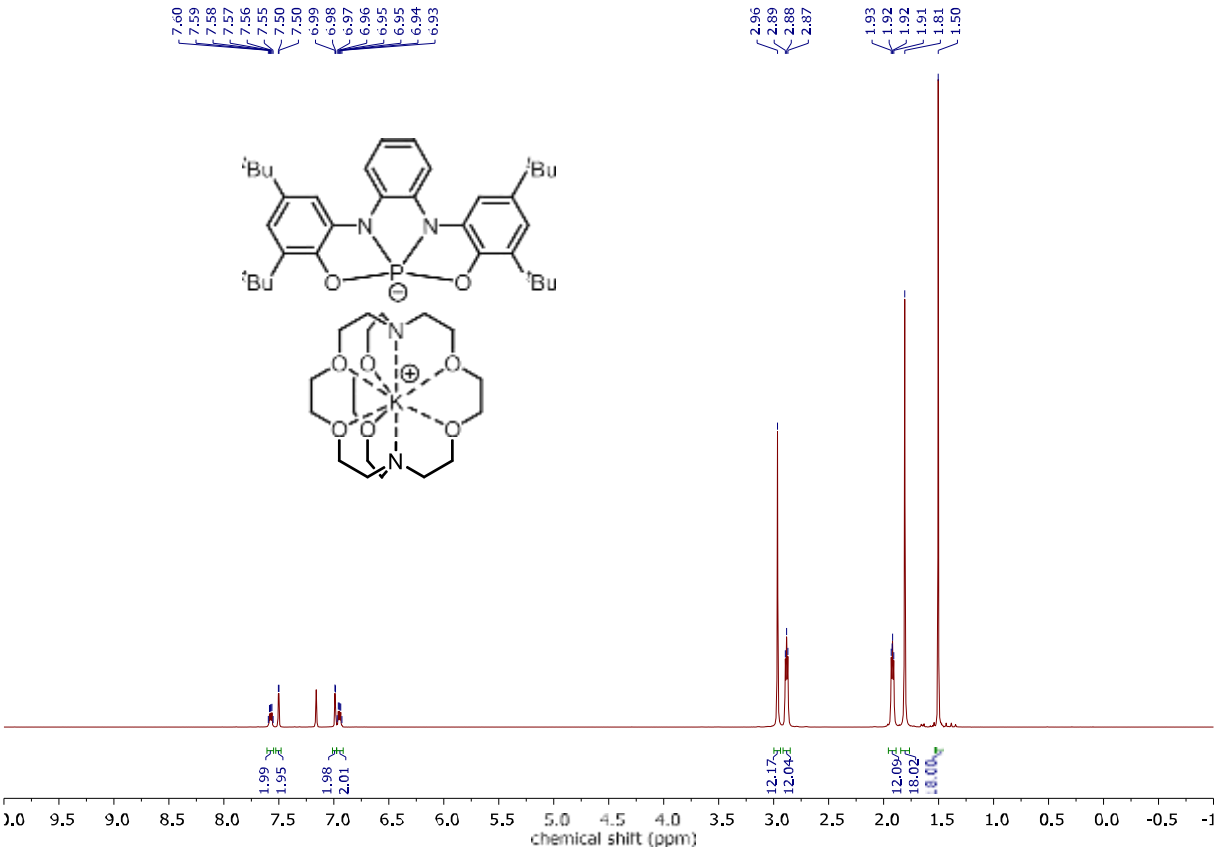



**$^{13}$C{$^{1}$H} NMR** (101 MHz, $C_6D_6$)

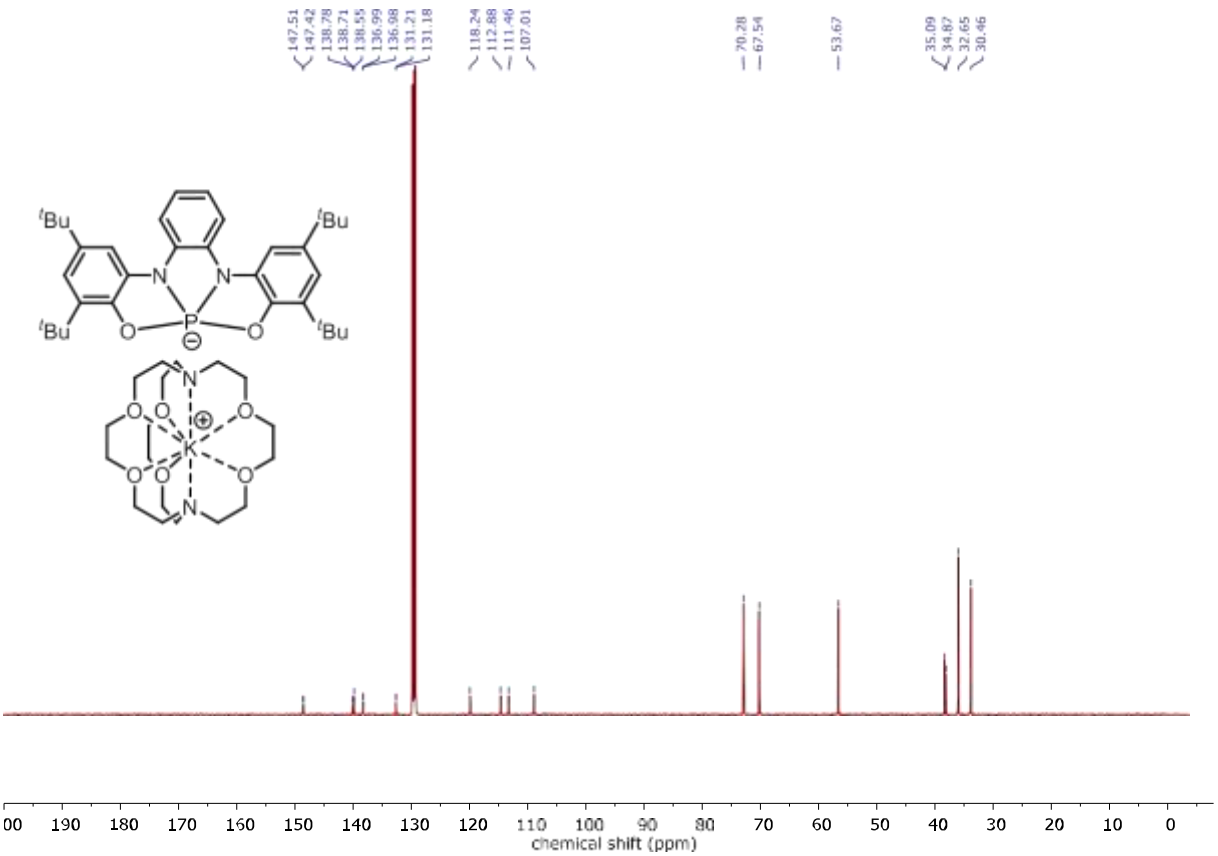


Compound **3a**

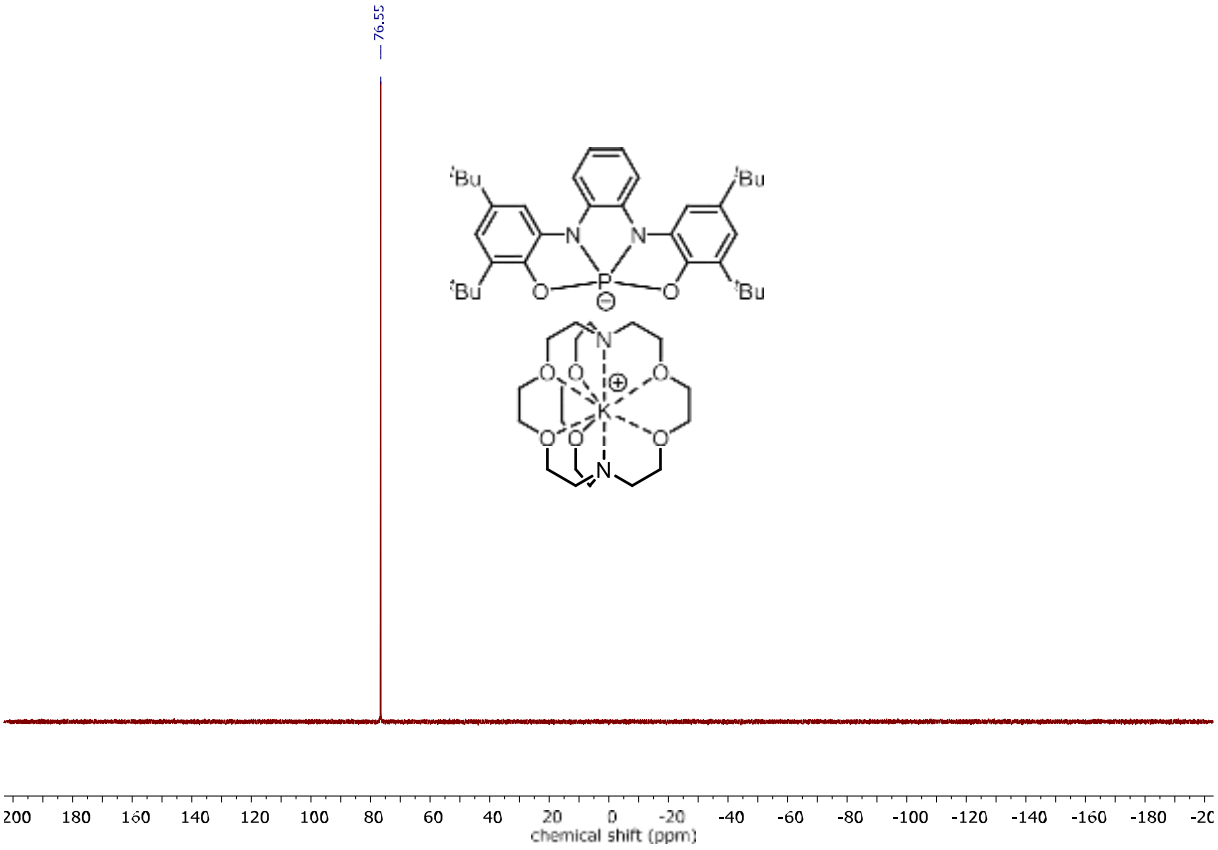
**$^{1}$H NMR** (400 MHz, $C_6D_6$)




**$^{13}$C{$^{1}$H} NMR** (101 MHz, $C_6D_6$)

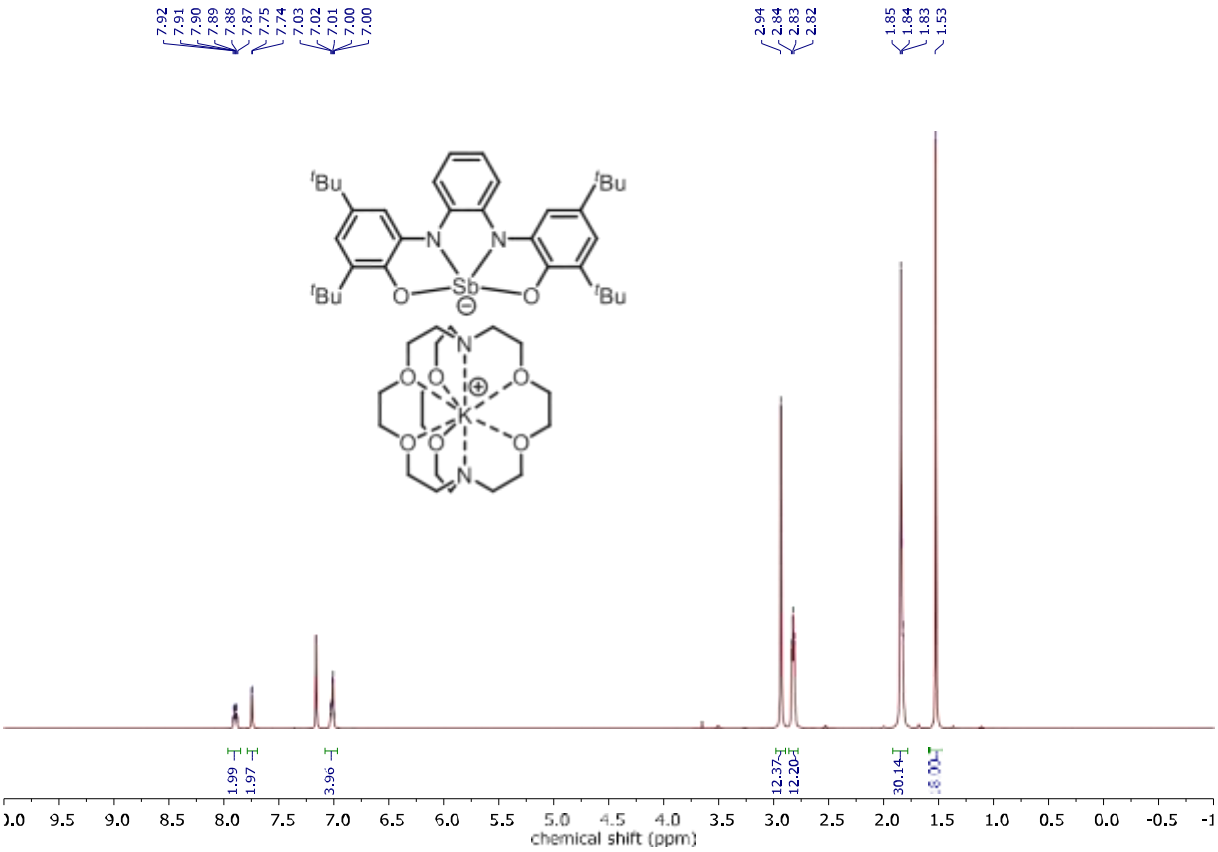


**$^{31}P\{^{1}H\}$ NMR** (162 MHz, $C_6D_6$)

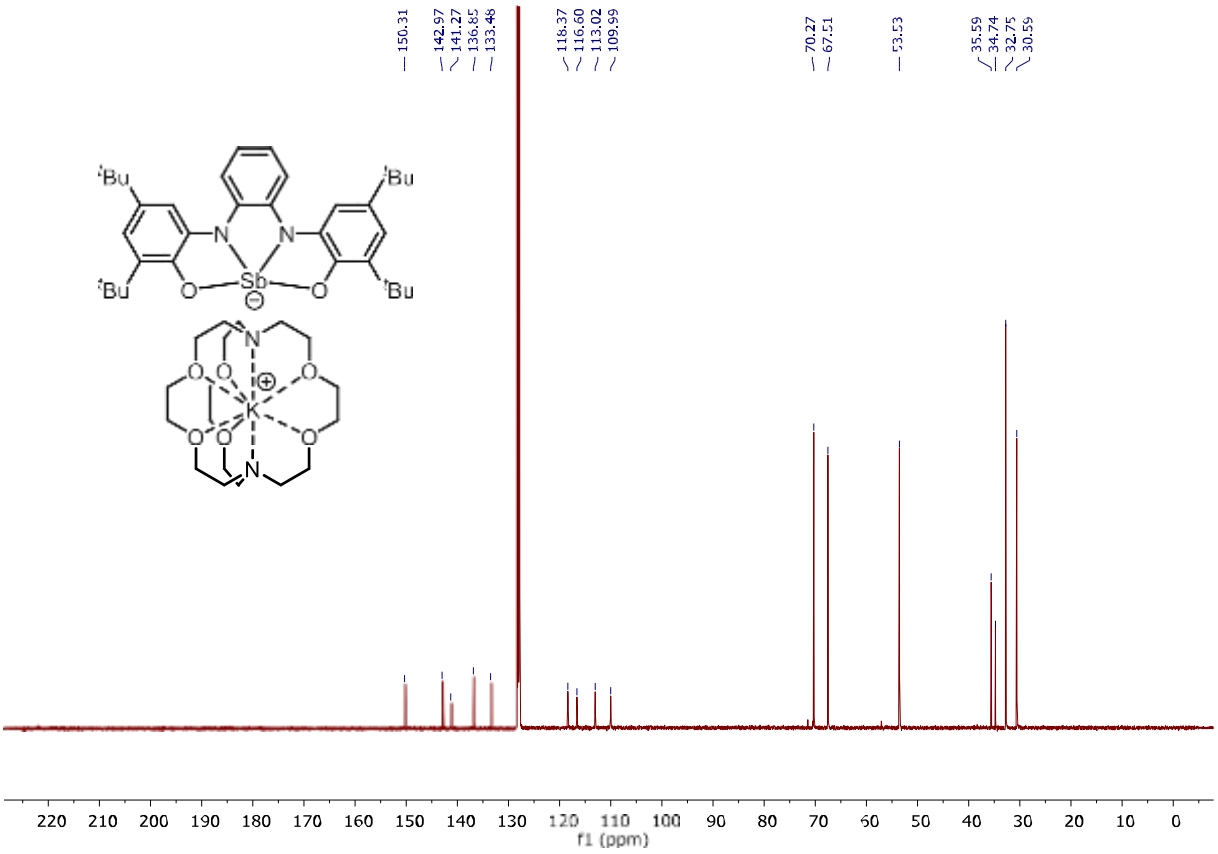



Compound **3c**

**$^{1}H$ NMR** (400 MHz, $C_6D_6$)

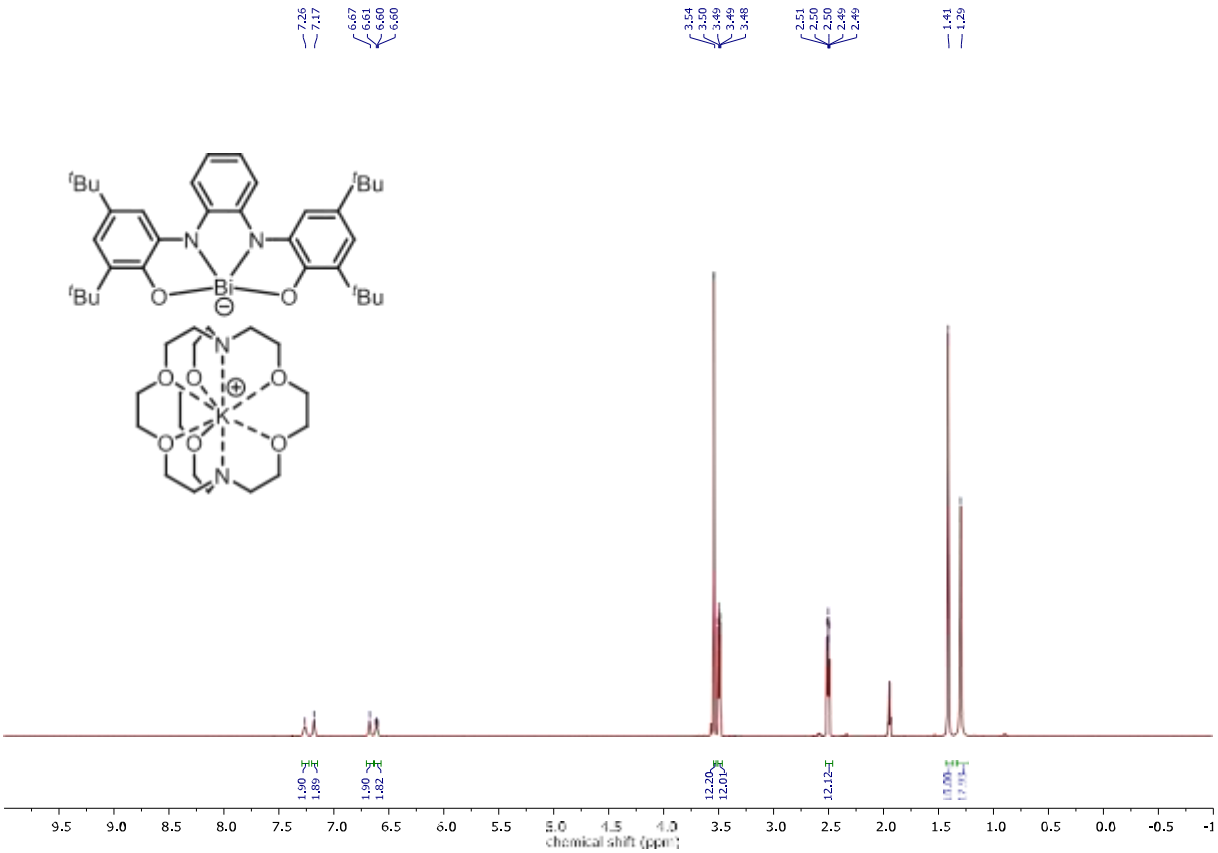


**$^{13}C\{^{1}H\}$ NMR** (101 MHz, $C_6D_6$)

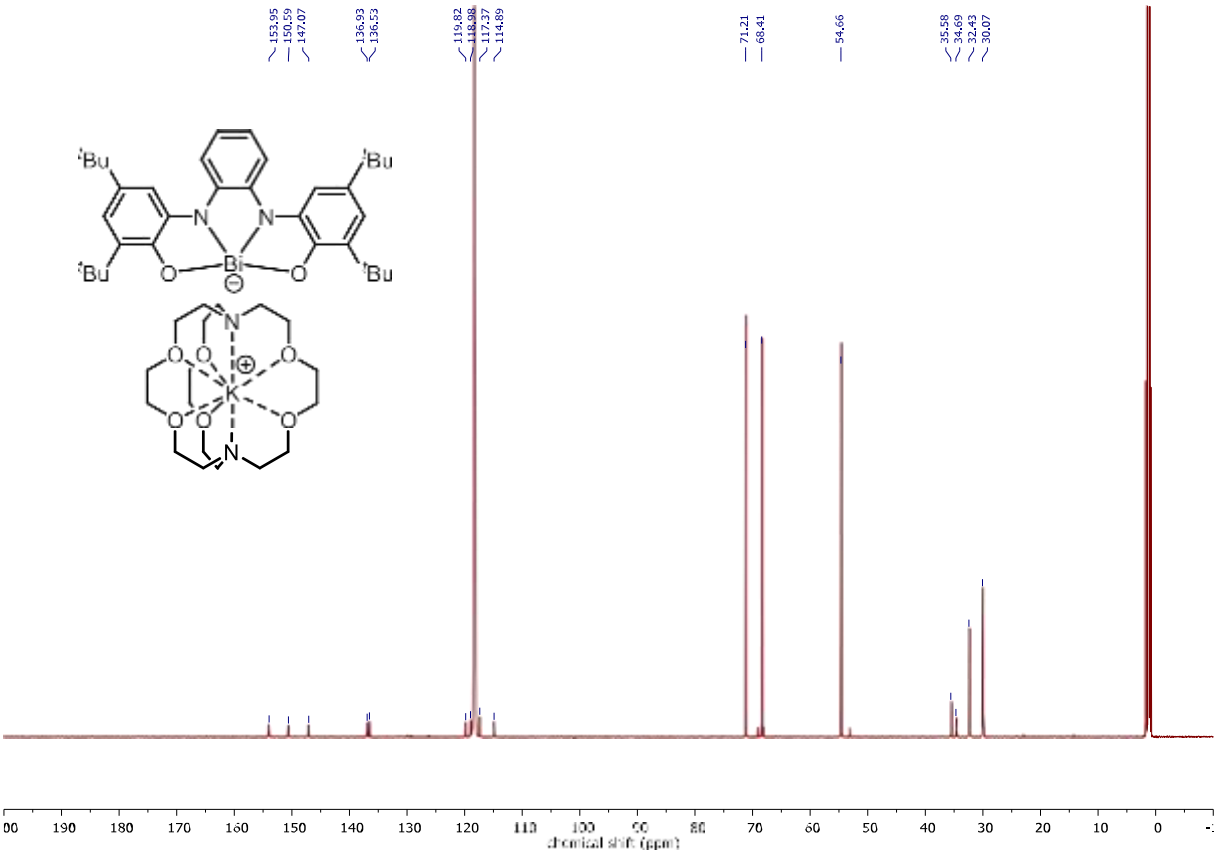



Compound **3d**

**$^{1}H$ NMR** (500 MHz, $CD_3CN$)

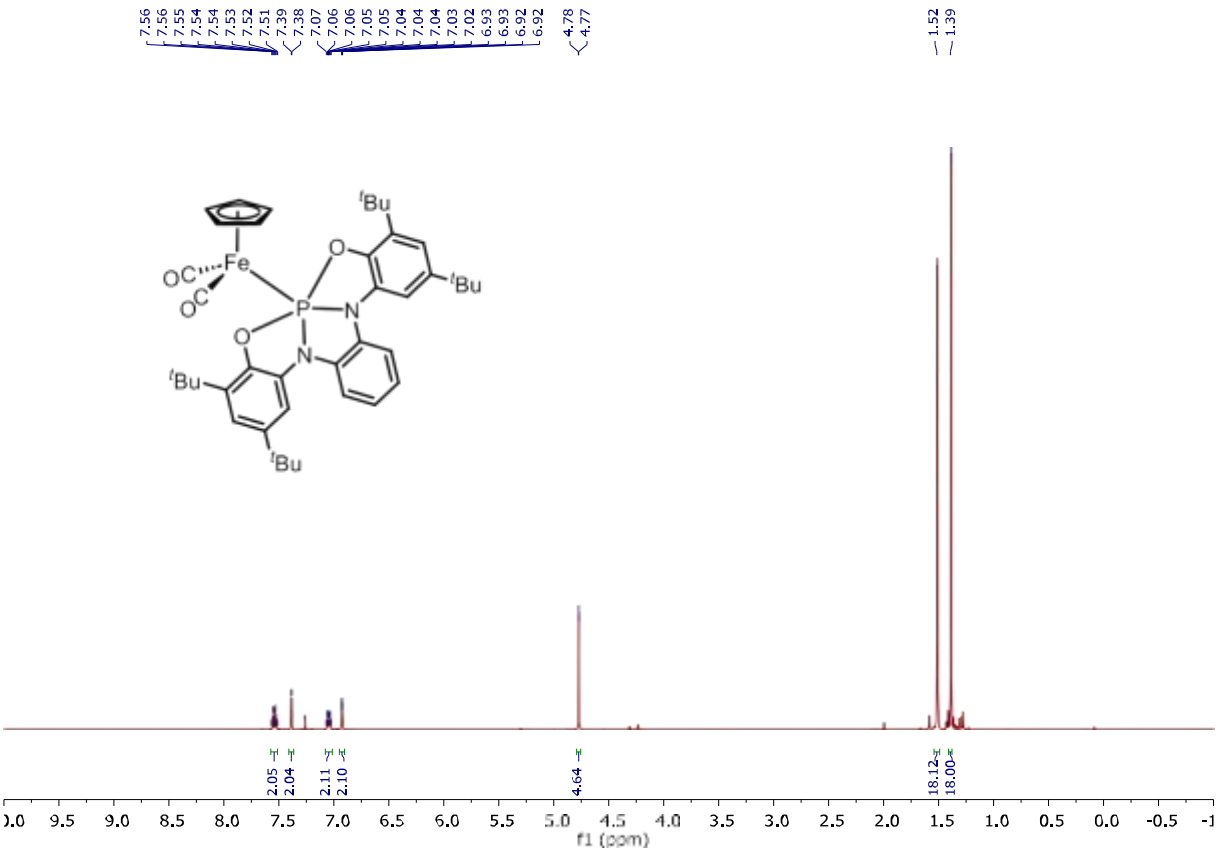


**$^{13}C\{^{1}H\}$ NMR** (101 MHz, $CD_3CN$)

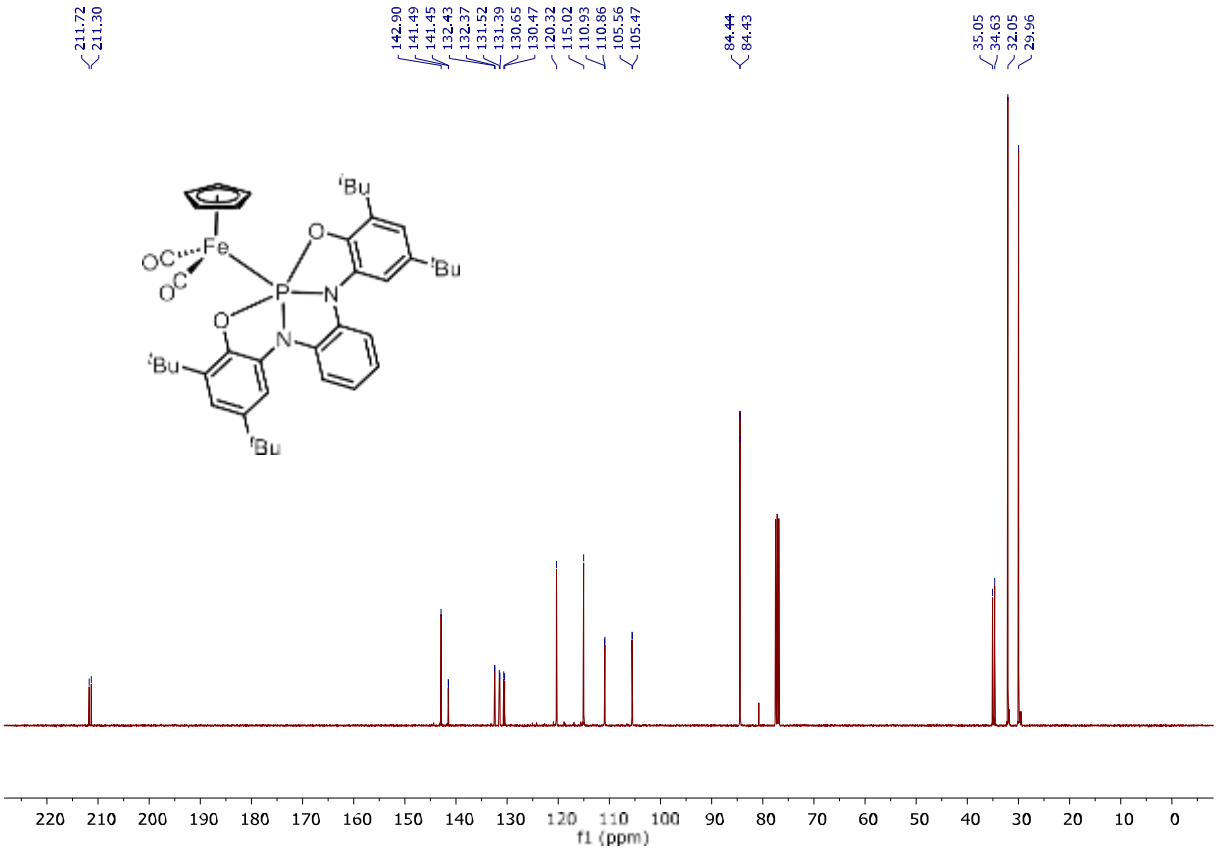



Compound **4a**

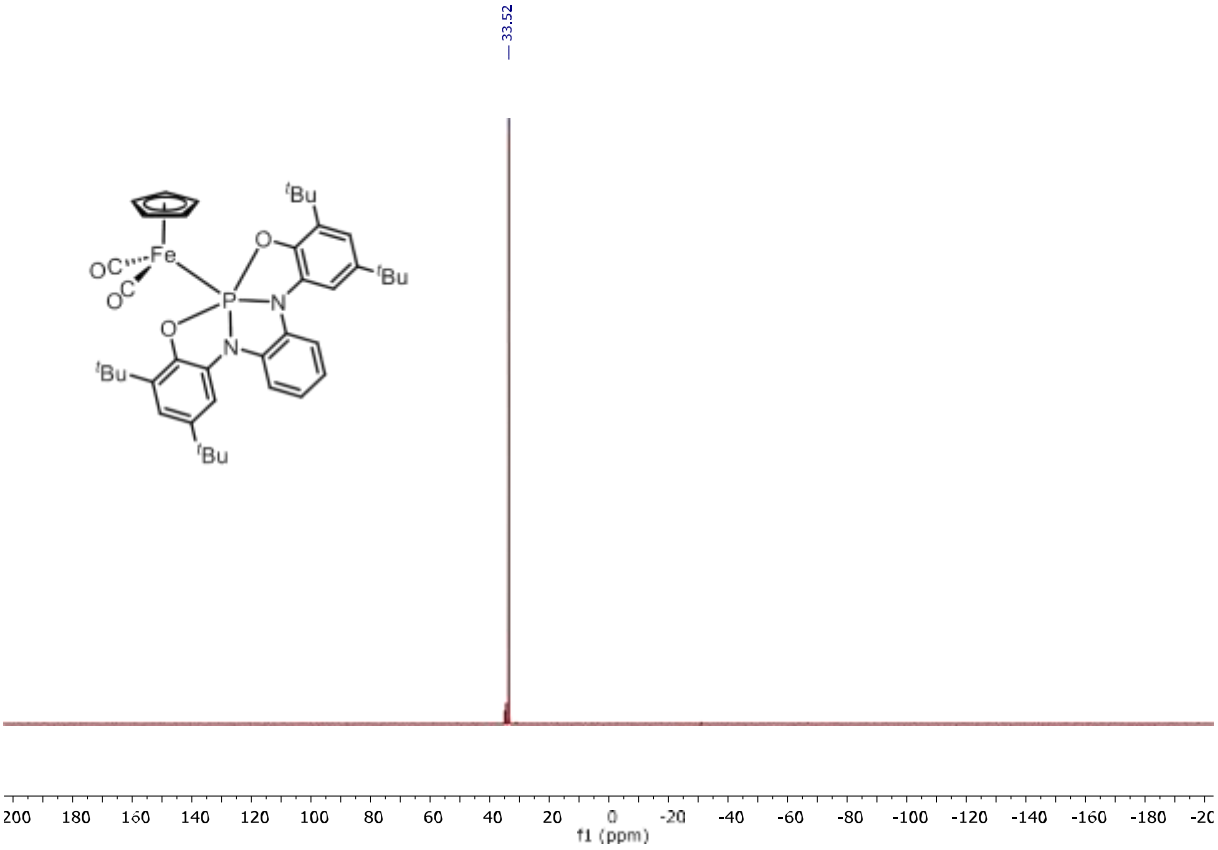
**$^{1}H$ NMR** (400 MHz, $CDCl_3$)



**$^{13}C\{^{1}H\}$ NMR** (101 MHz, $CDCl_3$)

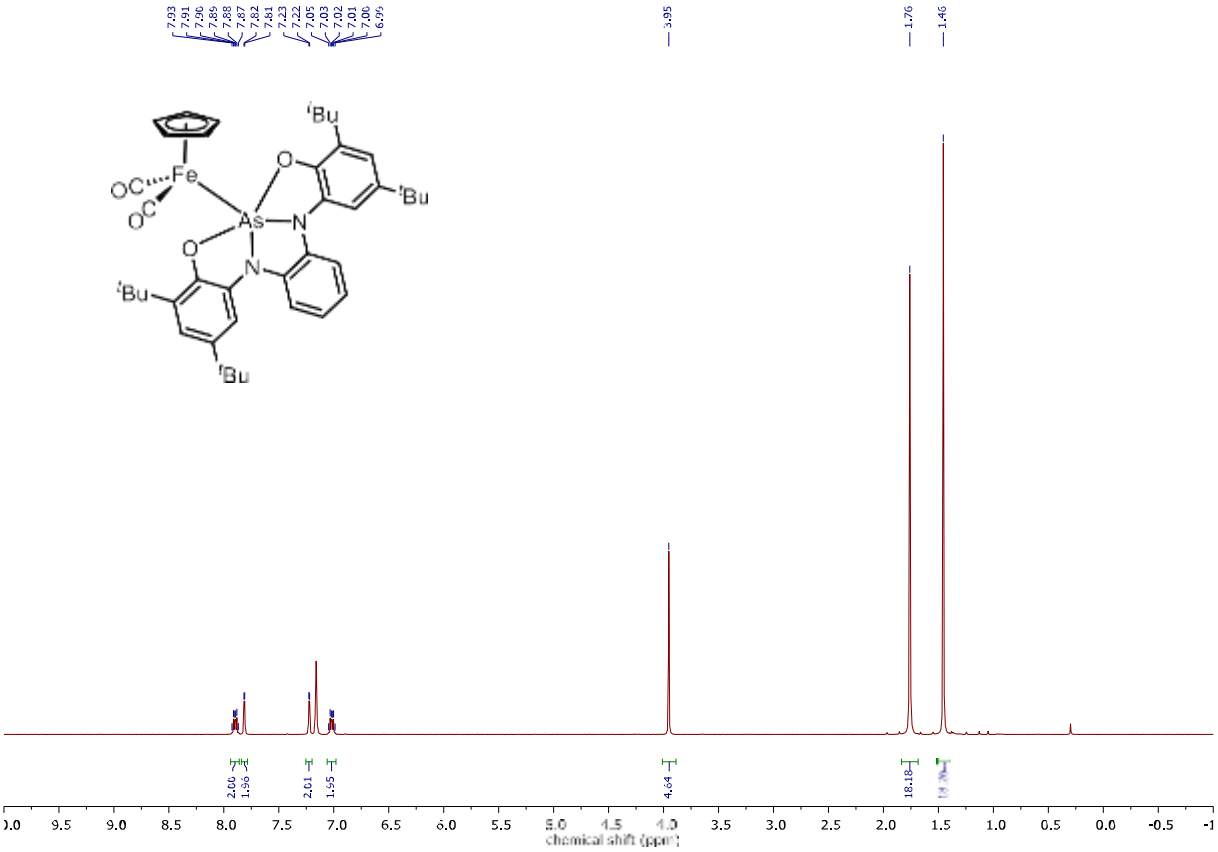



**$^{31}P\{^{1}H\}$ NMR** (162 MHz, $CDCl_3$)

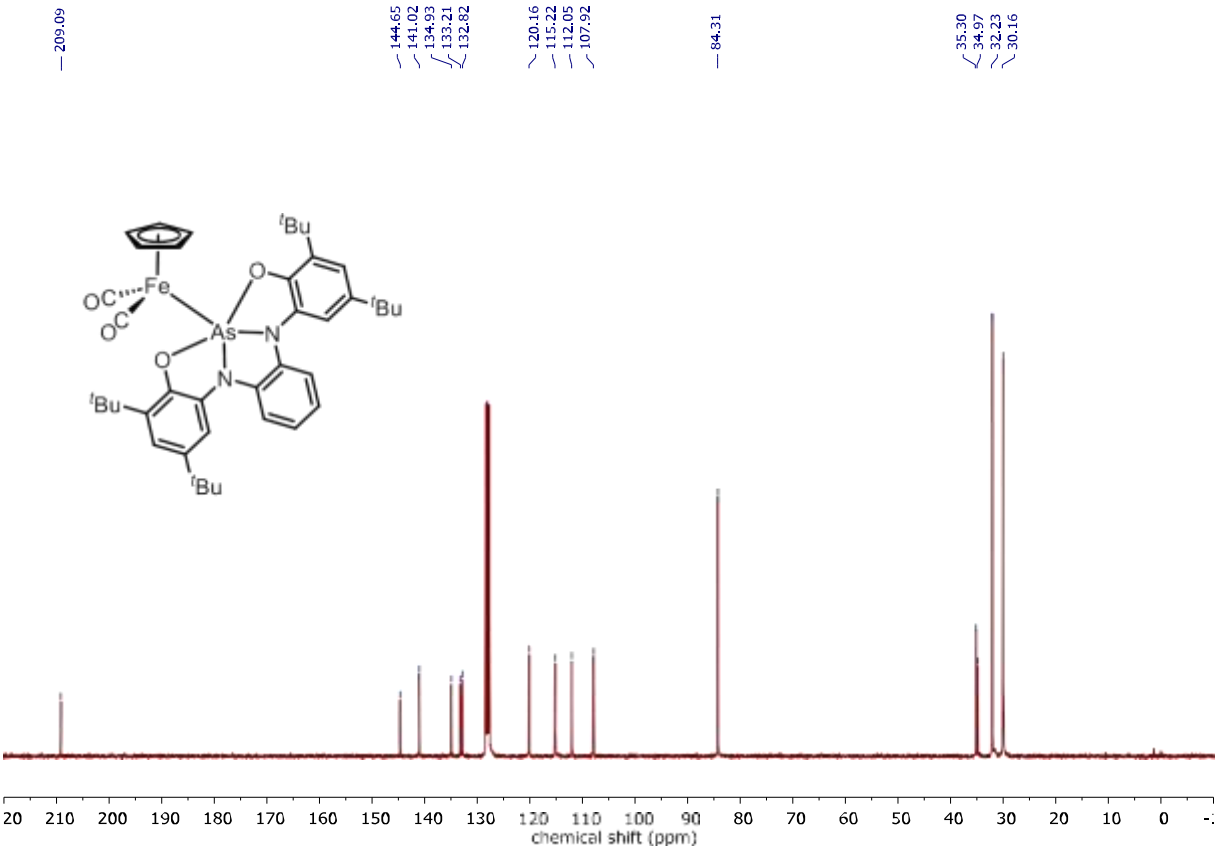


Compound **4b**

**$^{1}$H NMR** (300 MHz, $C_6D_6$)

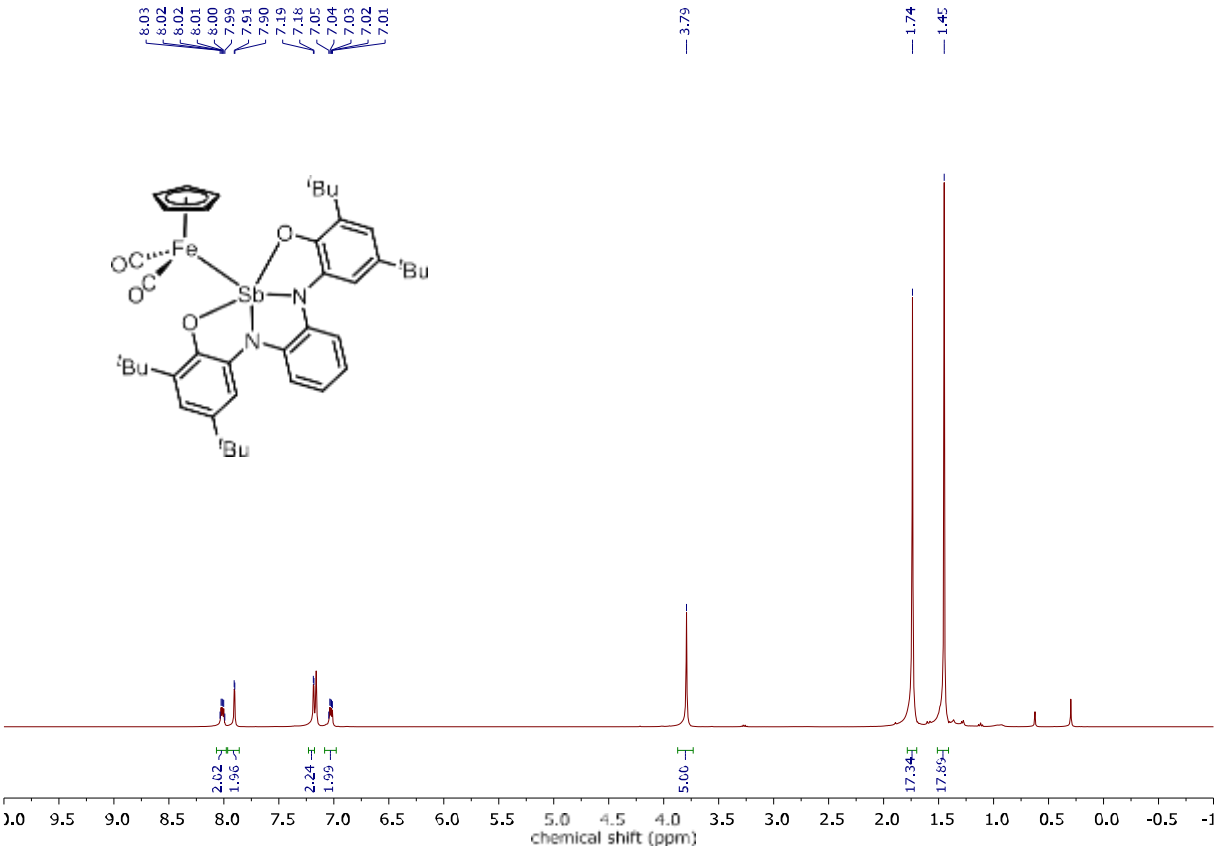



**$^{13}$C{$^{1}$H} NMR** (75 MHz, $C_6D_6$)

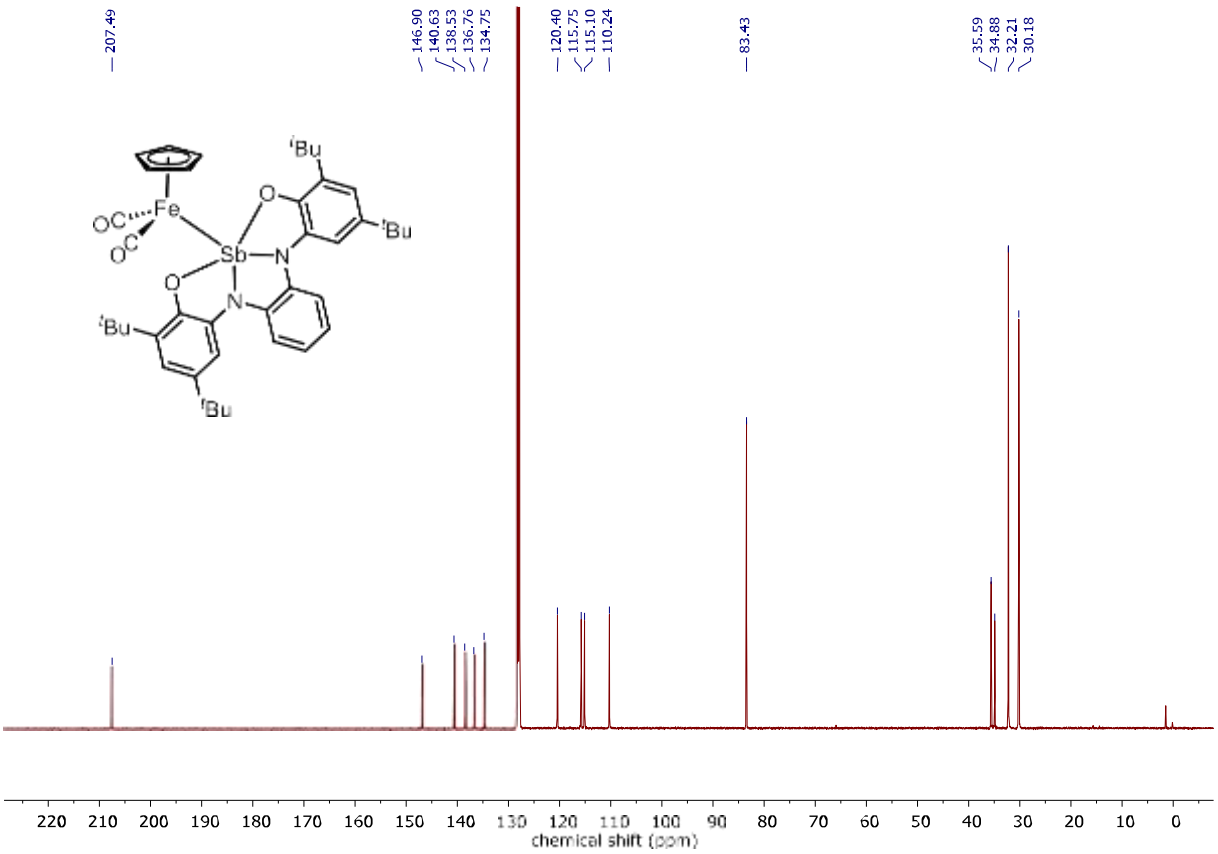


Compound **4c**

**$^{1}$H NMR** (300 MHz, $C_6D_6$)

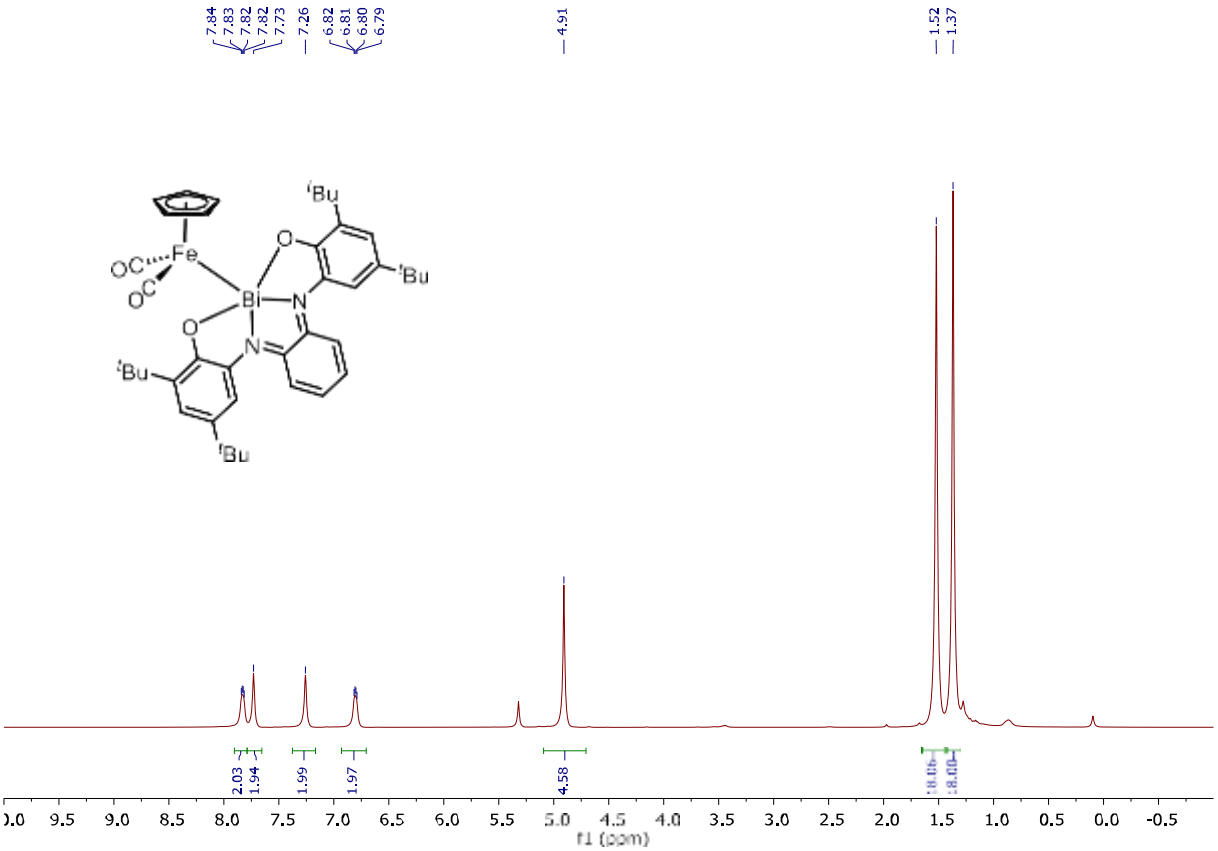



**$^{13}$C{$^{1}$H} NMR** (101 MHz, $C_6D_6$)

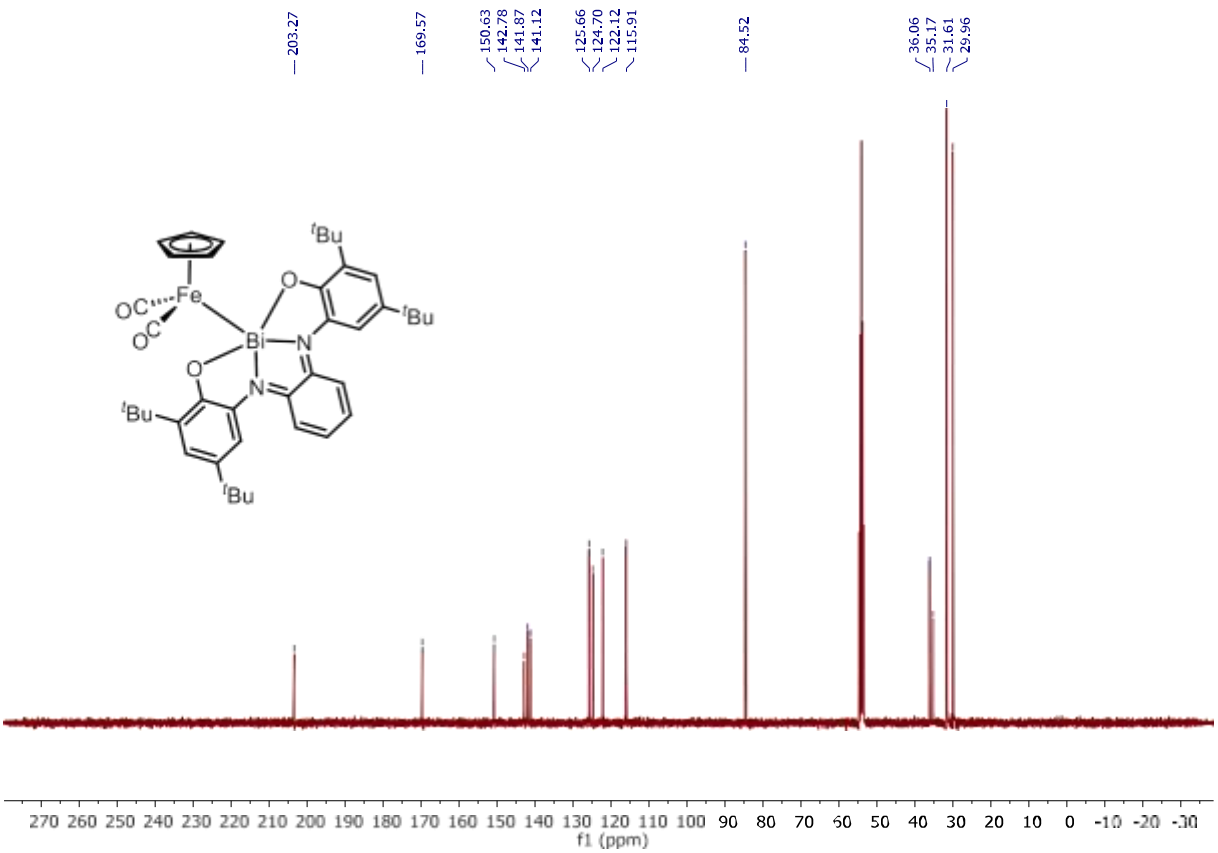


Compound **4d'**

**$^{1}$H NMR** (400 MHz, $CD_2Cl_2$)




**$^{13}$C{$^{1}$H} NMR** (101 MHz, $CD_2Cl_2$)



## Cartesian Coordinates of Optimized Geometries

**3d**

| | | | |
|---|---|---|---|
| Bi | -0.000289989 | -0.784111035 | -1.943766992 |
| O | 1.728671257 | -1.703002985 | -0.876750921 |
| O | -1.733494178 | -1.700428009 | -0.880531892 |
| N | 1.334572851 | 0.899576981 | -1.288185173 |
| N | -1.331416309 | 0.901334908 | -1.285554104 |
| C | 2.534782307 | -0.853352819 | -0.215979990 |
| C | 3.497031337 | -1.320879331 | 0.707506278 |
| C | 4.306859327 | -0.379864067 | 1.355988125 |
| H | 5.068917429 | -0.733432259 | 2.042988255 |
| C | 4.164446088 | 0.999787277 | 1.163908955 |
| C | 3.190718145 | 1.450343074 | 0.271247791 |
| H | 3.027366420 | 2.510787293 | 0.137941163 |
| C | 2.377662173 | 0.550358098 | -0.436442111 |
| C | 5.065947157 | 1.966919026 | 1.942849928 |
| C | 4.849453336 | 1.768782363 | 3.459566117 |
| H | 3.807220223 | 1.974693169 | 3.725877213 |
| H | 5.497479562 | 2.444251192 | 4.034816183 |
| H | 5.075146375 | 0.739807257 | 3.757376489 |
| C | 4.774175227 | 3.438275199 | 1.606574190 |
| H | 4.937610562 | 3.644345287 | 0.542907811 |
| H | 5.442618169 | 4.087778359 | 2.185466054 |
| H | 3.741554089 | 3.708647202 | 1.851503880 |
| C | 6.546515249 | 1.682710096 | 1.606326006 |
| H | 6.816197204 | 0.651679136 | 1.856513072 |
| H | 7.207147535 | 2.357330125 | 2.168121212 |
| H | 6.729316354 | 1.827987243 | 0.535906796 |
| C | 3.630020459 | -2.823763356 | 0.991356954 |
| C | 3.984814225 | -3.583092491 | -0.306969901 |
| H | 3.217074347 | -3.422354373 | -1.066114882 |
| H | 4.066999156 | -4.659496167 | -0.102681024 |
| H | 4.946898152 | -3.232996232 | -0.700161297 |
| C | 4.732964490 | -3.124632373 | 2.021120005 |
| H | 5.718092499 | -2.796194280 | 1.669199143 |
| H | 4.778342498 | -4.207483544 | 2.190319139 |
| H | 4.530818252 | -2.640945317 | 2.983627274 |
| C | 2.297920982 | -3.363465412 | 1.561373986 |
| H | 2.060859100 | -2.863554310 | 2.507530207 |
| H | 2.379603195 | -4.442235568 | 1.752360935 |
| H | 1.479502328 | -3.188072258 | 0.861099974 |
| C | 0.722208938 | 2.147811389 | -1.367420999 |
| C | 1.397152294 | 3.367356981 | -1.522363040 |
| H | 2.480320972 | 3.365391088 | -1.582289188 |
| C | 0.700332222 | 4.572030576 | -1.648969226 |
| H | 1.252239221 | 5.501015524 | -1.771340935 |
| C | -0.693234896 | 4.572899485 | -1.647407094 |
| H | -1.244223244 | 5.502597235 | -1.768516187 |
| C | -1.391413896 | 3.369206985 | -1.519212847 |
| H | -2.474707988 | 3.368786289 | -1.576678851 |

| | | | |
|---|---|---|---|
| C | -0.717726807 | 2.148706228 | -1.365881094 |
| C | -2.375860324 | 0.553600896 | -0.435100118 |
| C | -2.537156196 | -0.850179872 | -0.217798243 |
| C | -3.500907031 | -1.316884043 | 0.704520130 |
| C | -4.308016109 | -0.374909910 | 1.355005972 |
| H | -5.071316190 | -0.727728257 | 2.041017070 |
| C | -4.161397498 | 1.004758897 | 1.166101865 |
| C | -3.186187329 | 1.454457957 | 0.274620767 |
| H | -3.019573226 | 2.514710084 | 0.143891761 |
| C | -5.059852623 | 1.972789189 | 1.947410377 |
| C | -6.541390696 | 1.693297875 | 1.611346311 |
| H | -6.724466445 | 1.840807091 | 0.541275828 |
| H | -7.199756516 | 2.368864072 | 2.174644380 |
| H | -6.813906396 | 0.662644218 | 1.860074964 |
| C | -4.842851321 | 1.770982153 | 3.463620144 |
| H | -5.071377574 | 0.742070019 | 3.759457214 |
| H | -5.488451269 | 2.447201355 | 4.040717038 |
| H | -3.799805392 | 1.973267036 | 3.729553408 |
| C | -4.764319300 | 3.444020477 | 1.613867311 |
| H | -3.730949377 | 3.711243346 | 1.859057356 |
| H | -5.430935523 | 4.094141186 | 2.194175253 |
| H | -4.927485284 | 3.652509433 | 0.550629036 |
| C | -3.638523279 | -2.820059116 | 0.984593010 |
| C | -2.308237293 | -3.365085223 | 1.553769180 |
| H | -2.392894011 | -4.444190349 | 1.741546139 |
| H | -2.070341956 | -2.868586257 | 2.501510287 |
| H | -1.489012173 | -3.189847119 | 0.854384186 |
| C | -4.742801366 | -3.120316403 | 2.013091328 |
| H | -5.726718617 | -2.787691460 | 1.661703876 |
| H | -4.539474533 | -2.640008144 | 2.977039017 |
| H | -4.791724332 | -4.203493548 | 2.179227055 |
| C | -3.994957494 | -3.575037355 | -0.315806103 |
| H | -4.080698496 | -4.651682335 | -0.114236139 |
| H | -3.226278327 | -3.414810422 | -1.074103342 |
| H | -4.955671381 | -3.220903473 | -0.708729206 |

**3d'**

| | | | |
|---|---|---|---|
| Bi | -0.000034926 | -1.258190348 | -0.523790225 |
| C | 4.815182230 | 1.312501926 | 0.590054858 |
| C | 5.298582472 | -0.009942182 | 0.586979809 |
| H | 6.334087626 | -0.178658177 | 0.867179162 |
| C | 3.141629017 | -0.884223962 | -0.098312137 |
| O | 2.303849355 | -1.862417102 | -0.334236288 |
| C | 4.503570386 | -1.108370215 | 0.273945007 |
| C | -0.722158137 | 1.756970069 | -0.974729147 |
| N | 1.328129060 | 0.599731922 | -0.549834212 |
| C | 3.498354280 | 1.531774986 | 0.202276945 |
| H | 3.079400418 | 2.528186112 | 0.248424905 |
| N | -1.328171923 | 0.599781136 | -0.549994024 |
| C | -5.298613164 | -0.009948003 | 0.586948058 |
| H | -6.334102443 | -0.178696807 | 0.867190275 |
| C | -3.141639071 | -0.884164165 | -0.098321133 |

| | | | |
|---|---|---|---|
| C | 2.662568029 | 0.468054102 | -0.190320185 |
| O | -2.303822367 | -1.862349897 | -0.334202950 |
| C | 5.046302510 | -2.540795348 | 0.341714092 |
| C | -3.498447415 | 1.531822083 | 0.202122954 |
| H | -3.079558113 | 2.528253318 | 0.248271973 |
| C | -0.700807952 | 3.952876261 | -2.046659158 |
| H | -1.250568079 | 4.781346108 | -2.486903407 |
| C | 1.394876303 | 2.868402103 | -1.530791246 |
| H | 2.473954969 | 2.835120029 | -1.617723955 |
| C | -4.815259490 | 1.312507218 | 0.589935793 |
| C | -4.503550277 | -1.108359102 | 0.273978875 |
| C | 0.701195839 | 3.952895311 | -2.046407269 |
| H | 1.251094082 | 4.781387383 | -2.486440377 |
| C | -5.743752304 | 2.451549075 | 1.026750974 |
| C | 5.743651231 | 2.451554367 | 1.026885915 |
| C | -5.046218371 | -2.540805402 | 0.341877078 |
| C | -1.394641877 | 2.868381465 | -1.531244221 |
| H | -2.473682443 | 2.835073991 | -1.618578047 |
| C | -2.662602954 | 0.468123953 | -0.190439250 |
| C | 0.722217934 | 1.756951018 | -0.974571981 |
| C | 6.230430269 | 2.203827976 | 2.472070040 |
| H | 6.762285684 | 1.250208239 | 2.550644395 |
| H | 6.910628355 | 3.004214386 | 2.793500239 |
| H | 5.379608505 | 2.172154071 | 3.161213338 |
| C | 5.047253442 | 3.821094192 | 0.984400919 |
| H | 4.701872152 | 4.063918286 | -0.026511780 |
| H | 4.182605334 | 3.852048415 | 1.656134286 |
| H | 5.750369665 | 4.601818492 | 1.299786326 |
| C | 6.969572350 | 2.506735383 | 0.087957196 |
| H | 7.656688370 | 3.306501068 | 0.396018261 |
| H | 7.518808592 | 1.559768992 | 0.100820966 |
| H | 6.652361282 | 2.697950407 | -0.943002325 |
| C | 6.537379533 | -2.582032014 | 0.716992309 |
| H | 7.153899603 | -2.042859136 | -0.012032961 |
| H | 6.719032324 | -2.151312955 | 1.708695345 |
| H | 6.873002265 | -3.626107193 | 0.737104220 |
| C | 4.268208221 | -3.342310493 | 1.410574875 |
| H | 4.405535538 | -2.888149411 | 2.399112373 |
| H | 3.202737347 | -3.353524288 | 1.173556914 |
| H | 4.639988577 | -4.375388310 | 1.450981262 |
| C | 4.888344160 | -3.227896021 | -1.033816020 |
| H | 3.839294185 | -3.235357421 | -1.335868277 |
| H | 5.471125477 | -2.693625441 | -1.793711374 |
| H | 5.255685248 | -4.261965517 | -0.981888915 |
| C | -4.888172177 | -3.228052129 | -1.033571011 |
| H | -5.470926506 | -2.693879446 | -1.793557913 |
| H | -3.839104211 | -3.235514057 | -1.335559237 |
| H | -5.255486277 | -4.262125329 | -0.981555004 |
| C | -6.537312327 | -2.582060060 | 0.717087032 |
| H | -6.872882671 | -3.626149527 | 0.737360871 |
| H | -6.719033382 | -2.151181190 | 1.708708045 |
| H | -7.153824460 | -2.043042231 | -0.012058891 |

| | | | |
|---|---|---|---|
| C | -4.268155303 | -3.342180315 | 1.410866981 |
| H | -3.202675434 | -3.353409456 | 1.173896117 |
| H | -4.405529188 | -2.887902285 | 2.399344152 |
| H | -4.639922429 | -4.375258133 | 1.451385024 |
| C | -6.230305384 | 2.203954978 | 2.472034056 |
| H | -6.910514582 | 3.004328159 | 2.793473251 |
| H | -6.762077718 | 1.250304020 | 2.550790447 |
| H | -5.379380429 | 2.172421306 | 3.161056172 |
| C | -5.047462467 | 3.821134410 | 0.984000332 |
| H | -4.182720166 | 3.852239448 | 1.655602992 |
| H | -4.702245222 | 4.063856372 | -0.026994919 |
| H | -5.750590332 | 4.601846539 | 1.299388914 |
| C | -6.969809422 | 2.506533237 | 0.087991064 |
| H | -7.518978458 | 1.559530862 | 0.101034754 |
| H | -7.656937613 | 3.306284106 | 0.396064829 |
| H | -6.652761340 | 2.697660947 | -0.943035134 |

**4a**

| | | | |
|---|---|---|---|
| P | 0.004475252 | -0.037938834 | 0.176230841 |
| Fe | 0.103656827 | -0.216200128 | 2.453213338 |
| O | 1.071088090 | -1.161398009 | -0.505682837 |
| O | -1.206129891 | -1.210252181 | -0.186829203 |
| O | 2.994222990 | 0.130439017 | 2.605544947 |
| O | 0.263972133 | -3.119156447 | 2.307229210 |
| N | 1.225614197 | 1.219145005 | -0.231219236 |
| N | -1.159732159 | 1.184087012 | -0.373810280 |
| C | 2.356736917 | -0.697832918 | -0.704864096 |
| C | 2.472122958 | 0.694838304 | -0.545407115 |
| C | 3.699179163 | 1.321633938 | -0.733206829 |
| H | 3.797524108 | 2.392175388 | -0.614445167 |
| C | 4.814389523 | 0.546945963 | -1.085539921 |
| C | 4.656133245 | -0.831268136 | -1.255077199 |
| H | 5.518834510 | -1.421937898 | -1.531510927 |
| C | 3.428197019 | -1.500612267 | -1.086770258 |
| C | 3.273853478 | -3.003788398 | -1.338521042 |
| C | 6.168617604 | 1.244153922 | -1.267115981 |
| C | 0.735959080 | 2.510016282 | -0.269771916 |
| C | 1.420428155 | 3.724066369 | -0.202025057 |
| H | 2.498227271 | 3.748307449 | -0.110291122 |
| C | 0.693700043 | 4.919510583 | -0.225494068 |
| H | 1.225263352 | 5.864883622 | -0.172836169 |
| C | -0.697378883 | 4.904104117 | -0.295970952 |
| H | -1.253709275 | 5.836455691 | -0.295252859 |
| C | -1.396808329 | 3.692004048 | -0.356007169 |
| H | -2.477903161 | 3.699331036 | -0.376620211 |
| C | -0.683208046 | 2.494673317 | -0.357350221 |
| C | -2.436129380 | 0.693341790 | -0.648640071 |
| C | -2.431877969 | -0.707214172 | -0.515412290 |
| C | -3.572052266 | -1.480979262 | -0.730391077 |
| C | -4.731797125 | -0.772716790 | -1.098480950 |
| H | -5.638073490 | -1.339041224 | -1.266321157 |
| C | -4.767039272 | 0.614347798 | -1.263444020 |

| | | | |
|---|---|---|---|
| C | -3.596580161 | 1.356283935 | -1.035558071 |
| H | -3.600440509 | 2.426570322 | -1.186993254 |
| C | -6.039598370 | 1.358763130 | -1.687627211 |
| C | -3.553104016 | -3.003171377 | -0.565795785 |
| C | 1.854919190 | -0.010470830 | 2.473306198 |
| C | 0.209406021 | -1.965033038 | 2.314049247 |
| C | -0.071705105 | 1.238181098 | 3.979166316 |
| H | 0.769884104 | 1.781040225 | 4.388072160 |
| C | -0.844737284 | 1.638598939 | 2.845327329 |
| H | -0.708994853 | 2.540942988 | 2.267096408 |
| C | -1.837290179 | 0.634001970 | 2.626773950 |
| H | -2.583715327 | 0.629067922 | 1.845451151 |
| C | -1.662503992 | -0.378209859 | 3.610133449 |
| H | -2.247371326 | -1.284630160 | 3.688224135 |
| C | -0.572956083 | -0.004239239 | 4.459803194 |
| H | -0.189940236 | -0.569769907 | 5.297184386 |
| C | -5.782215552 | 2.093971308 | -3.021788362 |
| H | -6.681074440 | 2.638734944 | -3.334247419 |
| H | -4.963769381 | 2.815140942 | -2.929516254 |
| H | -5.516862266 | 1.381327248 | -3.809707356 |
| C | -6.416478407 | 2.393191408 | -0.603983862 |
| H | -6.608339556 | 1.897067099 | 0.353533266 |
| H | -5.614293323 | 3.122746385 | -0.452412151 |
| H | -7.320126348 | 2.939992376 | -0.898426021 |
| C | -7.233160301 | 0.410439929 | -1.882544359 |
| H | -7.035934353 | -0.329333990 | -2.665912429 |
| H | -7.479976507 | -0.122147868 | -0.957525065 |
| H | -8.113224400 | 0.990074228 | -2.181803089 |
| C | -4.918789315 | -3.631445004 | -0.887785854 |
| H | -5.221929560 | -3.432987131 | -1.921665375 |
| H | -4.850829197 | -4.717130448 | -0.759797986 |
| H | -5.704594245 | -3.263535051 | -0.218550204 |
| C | -3.196645459 | -3.350770449 | 0.897135886 |
| H | -2.215367215 | -2.955946012 | 1.163584040 |
| H | -3.944884097 | -2.933796240 | 1.581401229 |
| H | -3.177027271 | -4.438709131 | 1.030712924 |
| C | -2.503333303 | -3.623427439 | -1.516201300 |
| H | -2.748851437 | -3.393173422 | -2.558695297 |
| H | -1.501402858 | -3.245839364 | -1.303775264 |
| H | -2.497033977 | -4.713449492 | -1.397588336 |
| C | 2.783075976 | -3.708199518 | -0.055880059 |
| H | 3.477837020 | -3.532312113 | 0.772746953 |
| H | 1.795365053 | -3.351429275 | 0.235415083 |
| H | 2.719946189 | -4.789258366 | -0.227880128 |
| C | 2.247366034 | -3.229040103 | -2.472828351 |
| H | 1.270812284 | -2.815748438 | -2.210972398 |
| H | 2.589472246 | -2.755498433 | -3.399596047 |
| H | 2.130385053 | -4.303495348 | -2.658019221 |
| C | 4.602714390 | -3.651556385 | -1.761470192 |
| H | 4.436600359 | -4.719723417 | -1.937984143 |
| H | 4.992001516 | -3.214682465 | -2.687645209 |
| H | 5.367558610 | -3.555000059 | -0.982835084 |

| | | | |
|---|---|---|---|
| C | 7.287173423 | 0.260744152 | -1.646260896 |
| H | 7.432845336 | -0.501046186 | -0.872658264 |
| H | 7.075115694 | -0.244777816 | -2.594701046 |
| H | 8.229165548 | 0.808265859 | -1.760656317 |
| C | 6.564190298 | 1.940362265 | 0.054171875 |
| H | 5.819982403 | 2.687083223 | 0.349244284 |
| H | 6.647927306 | 1.209584889 | 0.865381018 |
| H | 7.529478393 | 2.448299927 | -0.058797942 |
| C | 6.055784314 | 2.303852001 | -2.385246341 |
| H | 5.781241337 | 1.834328903 | -3.335756103 |
| H | 5.295870439 | 3.055382121 | -2.148358029 |
| H | 7.014380434 | 2.819874433 | -2.516617239 |

**4b**

| | | | |
|---|---|---|---|
| As | 0.015758898 | -0.109299973 | 0.201208007 |
| Fe | -0.006232120 | -0.531742171 | 2.518249222 |
| O | 1.257438917 | -1.236938061 | -0.568605187 |
| O | -1.253594973 | -1.263365173 | -0.518674139 |
| O | 2.885520458 | -0.187846811 | 2.741914453 |
| O | 0.153913849 | -3.415132161 | 2.103774317 |
| N | 1.277511139 | 1.260023948 | -0.207323179 |
| N | -1.211051239 | 1.250987188 | -0.331110967 |
| C | 2.488734361 | -0.645394098 | -0.728155303 |
| C | 2.531483416 | 0.757488127 | -0.532714270 |
| C | 3.731395474 | 1.444491962 | -0.701323900 |
| H | 3.768205043 | 2.516956442 | -0.568230001 |
| C | 4.891655222 | 0.747606271 | -1.063859000 |
| C | 4.814199548 | -0.634303072 | -1.248608007 |
| H | 5.710698305 | -1.173092297 | -1.523973326 |
| C | 3.625061010 | -1.370224051 | -1.095558834 |
| C | 3.571313006 | -2.883921284 | -1.333457874 |
| C | 6.200172443 | 1.528732217 | -1.237244984 |
| C | 0.743941190 | 2.535010382 | -0.149413196 |
| C | 1.424310200 | 3.746305043 | 0.001210758 |
| H | 2.502263306 | 3.760284318 | 0.089155254 |
| C | 0.709674846 | 4.946438297 | 0.061355985 |
| H | 1.250462244 | 5.881518309 | 0.172128130 |
| C | -0.681129967 | 4.944055411 | -0.001691780 |
| H | -1.233661925 | 5.876823448 | 0.058879965 |
| C | -1.383828140 | 3.741234466 | -0.130385041 |
| H | -2.464886988 | 3.756789102 | -0.146866266 |
| C | -0.688533157 | 2.532583046 | -0.220345173 |
| C | -2.469199253 | 0.756749925 | -0.653171945 |
| C | -2.461058920 | -0.660111047 | -0.733831258 |
| C | -3.619878248 | -1.383840840 | -1.032216317 |
| C | -4.787397249 | -0.635135997 | -1.266433342 |
| H | -5.696372419 | -1.173070071 | -1.499603126 |
| C | -4.825686399 | 0.759894296 | -1.216521344 |
| C | -3.650079452 | 1.455640139 | -0.900507804 |
| H | -3.659700423 | 2.536238073 | -0.874306122 |
| C | -6.105362402 | 1.558673066 | -1.493983264 |
| C | -3.607184344 | -2.915307316 | -1.100323016 |

| | | | |
|---|---|---|---|
| C | 1.748141275 | -0.324729090 | 2.604921047 |
| C | 0.103226077 | -2.268655364 | 2.223502257 |
| C | -0.269344870 | 0.849390869 | 4.090081338 |
| H | 0.541792835 | 1.398716013 | 4.548704443 |
| C | -1.019374243 | 1.275656902 | 2.951927969 |
| H | -0.888526173 | 2.203060139 | 2.411793047 |
| C | -1.973624230 | 0.252393206 | 2.654874321 |
| H | -2.690484245 | 0.261300846 | 1.845195029 |
| C | -1.798354375 | -0.796471028 | 3.601612107 |
| H | -2.357162905 | -1.722338064 | 3.621720314 |
| C | -0.747228968 | -0.429949106 | 4.500216461 |
| H | -0.375914288 | -1.018701130 | 5.326686547 |
| C | -6.462189266 | 2.407628422 | -0.253644181 |
| H | -5.657085241 | 3.106072010 | -0.003162892 |
| H | -7.371134272 | 2.991605150 | -0.441100988 |
| H | -6.636469560 | 1.765490881 | 0.616529067 |
| C | -5.872506420 | 2.496523321 | -2.699280229 |
| H | -5.623271344 | 1.918187093 | -3.595099523 |
| H | -6.776208338 | 3.082809378 | -2.904312071 |
| H | -5.050913232 | 3.194589076 | -2.509238921 |
| C | -7.302260266 | 0.649531206 | -1.814874231 |
| H | -7.118223532 | 0.042266974 | -2.707710023 |
| H | -7.533122308 | -0.022390019 | -0.980900941 |
| H | -8.187430397 | 1.266503194 | -2.004502252 |
| C | -4.990211309 | -3.484443268 | -1.458469120 |
| H | -5.747015210 | -3.216928294 | -0.712460964 |
| H | -5.330848526 | -3.135659369 | -2.439529343 |
| H | -4.926499427 | -4.577341399 | -1.494590230 |
| C | -3.199427344 | -3.488417390 | 0.276022028 |
| H | -2.200796319 | -3.153314309 | 0.558967811 |
| H | -3.912469345 | -3.172748344 | 1.046944907 |
| H | -3.197896434 | -4.584148206 | 0.239265906 |
| C | -2.604791398 | -3.388641019 | -2.177927395 |
| H | -2.893384032 | -3.003339127 | -3.161999166 |
| H | -1.591242867 | -3.049654307 | -1.955423179 |
| H | -2.603918256 | -4.484211495 | -2.225077088 |
| C | 2.575313050 | -3.198363168 | -2.473419971 |
| H | 1.569297887 | -2.851383234 | -2.228624163 |
| H | 2.894321205 | -2.715378331 | -3.403625202 |
| H | 2.538351078 | -4.281141313 | -2.643659996 |
| C | 3.122700347 | -3.601713180 | -0.041381132 |
| H | 3.810038092 | -3.377256300 | 0.781948816 |
| H | 2.117211185 | -3.295727019 | 0.247974046 |
| H | 3.119381347 | -4.686596392 | -0.200791015 |
| C | 4.943986618 | -3.449014322 | -1.735557970 |
| H | 4.849532184 | -4.528179245 | -1.897877270 |
| H | 5.312177565 | -3.000713349 | -2.664926042 |
| H | 5.693949316 | -3.291637009 | -0.952349182 |
| C | 6.019797616 | 2.596366367 | -2.338962382 |
| H | 5.216709226 | 3.297065309 | -2.088801246 |
| H | 6.945050277 | 3.171285168 | -2.465513005 |
| H | 5.770351398 | 2.125168953 | -3.295533341 |

| | | | |
|---|---|---|---|
| C | 6.558714372 | 2.228479169 | 0.092567918 |
| H | 5.770720235 | 2.922760249 | 0.401972034 |
| H | 6.692528481 | 1.492124264 | 0.892078010 |
| H | 7.489784279 | 2.797657984 | -0.016264792 |
| C | 7.374029401 | 0.619995178 | -1.634834901 |
| H | 7.569589499 | -0.141953914 | -0.872432305 |
| H | 7.186732406 | 0.115052130 | -2.588741981 |
| H | 8.280861402 | 1.224564838 | -1.746491301 |

**4b'**

| | | | |
|---|---|---|---|
| As | -0.022175173 | -0.604955960 | -0.025762994 |
| Fe | -0.013131004 | -2.090906313 | 1.867851224 |
| O | 2.771579071 | -1.415998942 | 2.419596295 |
| C | -4.619151164 | 1.795342299 | -0.840753109 |
| C | -4.915622189 | 0.555632936 | -1.453003248 |
| H | -5.865532393 | 0.458878168 | -1.967456140 |
| C | -2.831920094 | -0.392824147 | -0.727124995 |
| O | -1.926855016 | -1.338889350 | -0.639353011 |
| C | -4.050915342 | -0.529867825 | -1.453502263 |
| C | 1.679517041 | -1.666163253 | 2.140152077 |
| C | 0.733467184 | 1.809056985 | 1.312071176 |
| N | -1.275240969 | 0.849359119 | 0.513214088 |
| C | -3.417436199 | 1.931927180 | -0.160813791 |
| H | -3.137453279 | 2.887031259 | 0.259412213 |
| N | 1.307404891 | 0.799795848 | 0.580335989 |
| C | 4.944875107 | 0.527792921 | -1.380710228 |
| H | 5.896740621 | 0.443858001 | -1.893908970 |
| C | 2.866535166 | -0.439873826 | -0.662080115 |
| C | -2.533197950 | 0.841527295 | -0.066542981 |
| O | 1.975970073 | -1.382908959 | -0.583977787 |
| C | -4.373889151 | -1.839044931 | -2.177745358 |
| C | 3.442033416 | 1.888516124 | -0.072016790 |
| H | 3.159246386 | 2.836876369 | 0.362019152 |
| C | 0.715305821 | 3.629537320 | 2.914139951 |
| H | 1.254918975 | 4.296363097 | 3.579914253 |
| C | -1.388529880 | 2.781116433 | 2.063289082 |
| H | -2.470466104 | 2.762677251 | 2.096851091 |
| C | 4.641593571 | 1.762735984 | -0.751931237 |
| C | 4.089023513 | -0.559782215 | -1.395833055 |
| C | -0.687699173 | 3.662276458 | 2.871700465 |
| H | -1.234291116 | 4.356091333 | 3.503539159 |
| C | 5.643255194 | 2.914629440 | -0.864334306 |
| C | -5.623027394 | 2.945242344 | -0.965652169 |
| C | 4.422304107 | -1.861872050 | -2.126405111 |
| C | 1.418092367 | 2.716142462 | 2.145003045 |
| H | 2.494397086 | 2.640997176 | 2.238407063 |
| C | 2.561168142 | 0.792468860 | 0.011877913 |
| C | -0.700832823 | 1.838785105 | 1.271729348 |
| C | -0.352281761 | -2.121130272 | 3.927766271 |
| H | 0.441120038 | -2.099586408 | 4.662471201 |
| C | -0.992557128 | -0.974679933 | 3.350090986 |
| H | -0.787814217 | 0.060398174 | 3.583564517 |

| | | | |
|---|---|---|---|
| C | -1.955703114 | -1.451462284 | 2.410412953 |
| H | -2.595510158 | -0.841544229 | 1.791150156 |
| C | -1.900107223 | -2.867975057 | 2.387696432 |
| H | -2.489983219 | -3.510322153 | 1.749562116 |
| C | -0.902277902 | -3.289598089 | 3.332954110 |
| H | -0.609832858 | -4.309001437 | 3.542070142 |
| O | 0.576342817 | -4.298154362 | 0.047783118 |
| C | 0.360241116 | -3.399742100 | 0.738343024 |
| C | -5.138033270 | 4.221312533 | -0.260040875 |
| H | -4.987697188 | 4.055065150 | 0.812691898 |
| H | -4.198841551 | 4.587694223 | -0.688884001 |
| H | -5.889235300 | 5.010222147 | -0.374634208 |
| C | -6.966163391 | 2.520401386 | -0.330508764 |
| H | -7.701054591 | 3.328892145 | -0.423550824 |
| H | -7.375761398 | 1.631530189 | -0.820437994 |
| H | -6.835156567 | 2.291717967 | 0.732626851 |
| C | -5.849109377 | 3.271311310 | -2.458925277 |
| H | -6.231042527 | 2.402276323 | -3.003640228 |
| H | -6.577374749 | 4.084459359 | -2.562520190 |
| H | -4.911722152 | 3.582458008 | -2.931903373 |
| C | -5.750407237 | -1.791523226 | -2.860667119 |
| H | -6.558782636 | -1.636874350 | -2.136732005 |
| H | -5.801956509 | -0.997869009 | -3.614439364 |
| H | -5.931339288 | -2.745855236 | -3.366871196 |
| C | -4.382477169 | -3.012499185 | -1.170526316 |
| H | -4.638103118 | -3.944102502 | -1.689297295 |
| H | -3.400678214 | -3.128587444 | -0.707108866 |
| H | -5.128945180 | -2.840818210 | -0.386249120 |
| C | -3.305894102 | -2.100992961 | -3.264916203 |
| H | -3.309315233 | -1.293290146 | -4.005155269 |
| H | -2.309379257 | -2.169493368 | -2.824526430 |
| H | -3.527757485 | -3.042007167 | -3.782562151 |
| C | 3.347994386 | -2.137210381 | -3.204242328 |
| H | 2.357607943 | -2.226280966 | -2.754283971 |
| H | 3.329603359 | -1.326829929 | -3.941662466 |
| H | 3.582265387 | -3.072072372 | -3.727436169 |
| C | 4.459390436 | -3.036089377 | -1.120705866 |
| H | 4.719459358 | -3.962763409 | -1.646240259 |
| H | 5.214271307 | -2.855763234 | -0.347130221 |
| H | 3.489047110 | -3.168481058 | -0.639363065 |
| C | 5.790688209 | -1.791194078 | -2.823656462 |
| H | 5.824420613 | -0.991396113 | -3.572288279 |
| H | 6.604696700 | -1.632123926 | -2.107036165 |
| H | 5.978380500 | -2.739714134 | -3.338189260 |
| C | 5.871592531 | 3.254854427 | -2.354264072 |
| H | 6.600110320 | 4.068923244 | -2.448010996 |
| H | 6.254605732 | 2.391550959 | -2.907192383 |
| H | 4.935075274 | 3.571075405 | -2.825642994 |
| C | 5.155566500 | 4.183076302 | -0.147137205 |
| H | 4.216239311 | 4.551949358 | -0.573564107 |
| H | 5.004159363 | 4.005966498 | 0.923593161 |
| H | 5.905830299 | 4.974065582 | -0.253329849 |

| | | | |
|---|---|---|---|
| C | 6.985537628 | 2.483993991 | -0.230609095 |
| H | 7.397853490 | 1.601351211 | -0.729314201 |
| H | 7.718920673 | 3.294953362 | -0.313370829 |
| H | 6.852110347 | 2.243160133 | 0.829375798 |

**4c**

| | | | |
|---|---|---|---|
| Sb | 0.034463198 | -0.263482115 | 0.136103859 |
| Fe | -0.117526034 | -1.132312310 | 2.481942371 |
| O | 1.484349063 | -1.202316110 | -0.879330130 |
| O | -1.373402290 | -1.183503859 | -0.971186834 |
| O | 2.756438252 | -0.781777892 | 2.885683974 |
| O | 0.129821996 | -3.907438456 | 1.604760171 |
| N | 1.334027269 | 1.316159070 | -0.194453059 |
| N | -1.223303280 | 1.335350212 | -0.302894178 |
| C | 2.665589102 | -0.494405012 | -0.874686071 |
| C | 2.615994081 | 0.887831892 | -0.521721142 |
| C | 3.786915163 | 1.646381020 | -0.570239816 |
| H | 3.751315293 | 2.703639062 | -0.346436999 |
| C | 5.001528294 | 1.060120892 | -0.942904956 |
| C | 5.020586613 | -0.303103203 | -1.244679924 |
| H | 5.960744610 | -0.762857160 | -1.517245896 |
| C | 3.873330337 | -1.113940864 | -1.217618329 |
| C | 3.935360494 | -2.608315189 | -1.561258097 |
| C | 6.261057461 | 1.933546992 | -0.999479296 |
| C | 0.772962857 | 2.539889925 | 0.133970217 |
| C | 1.445643980 | 3.695432059 | 0.550711059 |
| H | 2.522995942 | 3.689288311 | 0.644855925 |
| C | 0.736670823 | 4.855993438 | 0.866038256 |
| H | 1.280325833 | 5.745567382 | 1.170136313 |
| C | -0.655309821 | 4.867926385 | 0.809939118 |
| H | -1.206803004 | 5.767402293 | 1.067252084 |
| C | -1.356708335 | 3.719347166 | 0.435973260 |
| H | -2.437943928 | 3.737456141 | 0.435489063 |
| C | -0.672331866 | 2.552358400 | 0.073561988 |
| C | -2.496731287 | 0.916249240 | -0.667502065 |
| C | -2.547525424 | -0.474383062 | -0.996958824 |
| C | -3.757700345 | -1.097115144 | -1.330977091 |
| C | -4.901692127 | -0.283237889 | -1.393026299 |
| H | -5.840834632 | -0.745530309 | -1.665068385 |
| C | -4.878286617 | 1.087678326 | -1.127589933 |
| C | -3.665649434 | 1.677073300 | -0.750472295 |
| H | -3.630030513 | 2.739062187 | -0.551354009 |
| C | -6.130495675 | 1.967501121 | -1.229724846 |
| C | -3.822577476 | -2.602829209 | -1.619862360 |
| C | 1.626492951 | -0.915107275 | 2.690392168 |
| C | 0.046426837 | -2.798633258 | 1.915886230 |
| C | -0.528167050 | -0.011388953 | 4.214792540 |
| H | 0.234927181 | 0.449174116 | 4.827448559 |
| C | -1.175957262 | 0.601213090 | 3.096315040 |
| H | -1.005878107 | 1.604596126 | 2.729127943 |
| C | -2.098480956 | -0.348524074 | 2.556013956 |
| H | -2.749835178 | -0.195825216 | 1.704892148 |

| | | | |
|---|---|---|---|
| C | -2.001511342 | -1.540289977 | 3.331781453 |
| H | -2.558565120 | -2.449963131 | 3.153496346 |
| C | -1.039525313 | -1.332592140 | 4.370889245 |
| H | -0.746672273 | -2.048704957 | 5.125105470 |
| C | -6.406111295 | 2.634503113 | 0.136100155 |
| H | -6.577607587 | 1.876622336 | 0.908253900 |
| H | -5.563412401 | 3.257051042 | 0.453747266 |
| H | -7.294908406 | 3.273697371 | 0.074454181 |
| C | -7.377095454 | 1.163495138 | -1.631984223 |
| H | -8.240621706 | 1.835196225 | -1.689414243 |
| H | -7.252528717 | 0.691718804 | -2.612643330 |
| H | -7.607054720 | 0.382380834 | -0.898928210 |
| C | -5.897891582 | 3.065293082 | -2.291377176 |
| H | -5.705840458 | 2.618254197 | -3.272367019 |
| H | -6.781154558 | 3.710354328 | -2.370203949 |
| H | -5.039623235 | 3.693896386 | -2.033451952 |
| C | -5.251852417 | -3.060618330 | -1.957630377 |
| H | -5.947750662 | -2.868716964 | -1.133162169 |
| H | -5.634411584 | -2.566520241 | -2.857368228 |
| H | -5.243751242 | -4.139626087 | -2.146011128 |
| C | -3.362361019 | -3.387861012 | -0.369383183 |
| H | -2.334006108 | -3.137347973 | -0.104508802 |
| H | -4.015308064 | -3.161522377 | 0.482311195 |
| H | -3.416663071 | -4.465453220 | -0.563806079 |
| C | -2.918473384 | -2.957030296 | -2.822522965 |
| H | -3.251354449 | -2.421529908 | -3.718375067 |
| H | -1.876744047 | -2.695816235 | -2.628641417 |
| H | -2.978180982 | -4.033266223 | -3.024608348 |
| C | 5.368636544 | -3.060701411 | -1.889802025 |
| H | 5.358009606 | -4.131379389 | -2.121044016 |
| H | 5.772095566 | -2.533865242 | -2.761545341 |
| H | 6.048335615 | -2.906134029 | -1.044394273 |
| C | 3.446047226 | -3.442251437 | -0.355144081 |
| H | 4.060894038 | -3.235965974 | 0.528116778 |
| H | 2.405333380 | -3.217743227 | -0.118384888 |
| H | 3.523977042 | -4.511200064 | -0.586692995 |
| C | 3.053428399 | -2.906096457 | -2.795435969 |
| H | 2.010338019 | -2.641523179 | -2.612057002 |
| H | 3.409313328 | -2.340149327 | -3.663432181 |
| H | 3.105760325 | -3.974508498 | -3.037713422 |
| C | 6.517326361 | 2.558640263 | 0.389718935 |
| H | 5.674235347 | 3.179781109 | 0.709087988 |
| H | 6.665766400 | 1.777555064 | 1.142922314 |
| H | 7.413096441 | 3.190709149 | 0.362565263 |
| C | 6.054870425 | 3.062921310 | -2.032951879 |
| H | 6.943433640 | 3.704180417 | -2.077391126 |
| H | 5.877733633 | 2.645680924 | -3.029841382 |
| H | 5.196010458 | 3.689693131 | -1.772316209 |
| C | 7.508884402 | 1.132131332 | -1.403198144 |
| H | 7.720405545 | 0.329131844 | -0.688608829 |
| H | 7.397954563 | 0.688935860 | -2.398795395 |
| H | 8.377896635 | 1.798930120 | -1.426923277 |

**4c'**

| | | | |
|---|---|---|---|
| Sb | -0.025512164 | -0.753557928 | -0.401571976 |
| Fe | 0.080746098 | -2.253279060 | 1.700726994 |
| O | 2.741188422 | -1.242891305 | 2.337075336 |
| C | -4.748736089 | 1.940367028 | -0.647312895 |
| C | -5.168884303 | 0.714486126 | -1.220211826 |
| H | -6.169531493 | 0.668668901 | -1.635892197 |
| C | -3.061685152 | -0.342382972 | -0.724828895 |
| O | -2.219056109 | -1.339742913 | -0.745960001 |
| C | -4.366705570 | -0.411499871 | -1.307712872 |
| C | 1.696473996 | -1.621008029 | 2.016727305 |
| C | 0.702396013 | 1.752347176 | 1.212267288 |
| N | -1.340209118 | 0.852228318 | 0.374273839 |
| C | -3.482834040 | 2.010336960 | -0.092401227 |
| H | -3.107812474 | 2.948425345 | 0.293240927 |
| N | 1.307404891 | 0.854312218 | 0.384602850 |
| C | 5.138507413 | 0.741612810 | -1.185942837 |
| H | 6.144460663 | 0.704198920 | -1.589528862 |
| C | 3.035277090 | -0.326312917 | -0.710279166 |
| C | -2.638891051 | 0.879960910 | -0.089379096 |
| O | 2.203708382 | -1.321032263 | -0.736738029 |
| C | -4.837506102 | -1.697148168 | -1.993499070 |
| C | 3.435494373 | 2.032097258 | -0.070136094 |
| H | 3.052879113 | 2.966586179 | 0.317080891 |
| C | 0.679746168 | 3.385277039 | 3.015006427 |
| H | 1.218995248 | 3.980038400 | 3.746304513 |
| C | -1.425292353 | 2.594712159 | 2.115884009 |
| H | -2.505877058 | 2.545026120 | 2.167649186 |
| C | 4.702334123 | 1.968882273 | -0.618283289 |
| C | 4.349638545 | -0.389785082 | -1.278920338 |
| C | -0.729203074 | 3.393036365 | 3.001699206 |
| H | -1.274956271 | 3.996400031 | 3.721284484 |
| C | 5.643638318 | 3.174463407 | -0.654673221 |
| C | -5.697182589 | 3.141222080 | -0.685532192 |
| C | 4.841323586 | -1.681099281 | -1.936828949 |
| C | 1.380056165 | 2.580438132 | 2.139186329 |
| H | 2.458692439 | 2.512101240 | 2.208185221 |
| C | 2.598598966 | 0.895117075 | -0.074320828 |
| C | -0.742516115 | 1.754045306 | 1.202862221 |
| C | -0.321117984 | -2.461475382 | 3.735398170 |
| H | 0.445477284 | -2.532085090 | 4.494686558 |
| C | -0.915819018 | -1.246914110 | 3.246638421 |
| H | -0.688375991 | -0.243588225 | 3.578431498 |
| C | -1.859083286 | -1.601086093 | 2.239916277 |
| H | -2.475162023 | -0.917347282 | 1.678298875 |
| C | -1.838551208 | -3.014185143 | 2.082288133 |
| H | -2.428536215 | -3.576272455 | 1.373350960 |
| C | -0.888833095 | -3.548837260 | 3.018726013 |
| H | -0.630190836 | -4.591833447 | 3.138039079 |
| O | 0.996936070 | -4.419226412 | -0.027671208 |
| C | 0.644040992 | -3.534177463 | 0.627581992 |

| | | | |
|---|---|---|---|
| C | -6.048424517 | 3.473827444 | -2.153075115 |
| H | -6.527264310 | 2.625026078 | -2.651212414 |
| H | -6.738665329 | 4.324829128 | -2.193026410 |
| H | -5.145752378 | 3.732331059 | -2.716601259 |
| C | -5.079094566 | 4.391291145 | -0.040140740 |
| H | -4.833200186 | 4.220101247 | 1.013954939 |
| H | -4.168157208 | 4.705680111 | -0.561199881 |
| H | -5.794955494 | 5.219029139 | -0.087187244 |
| C | -6.993625573 | 2.789818223 | 0.078624097 |
| H | -7.691120346 | 3.635279422 | 0.047593143 |
| H | -7.493715536 | 1.921335168 | -0.361392077 |
| H | -6.773828628 | 2.559861075 | 1.126697211 |
| C | -6.278257309 | -1.573877916 | -2.516424089 |
| H | -6.990349437 | -1.379896882 | -1.706007125 |
| H | -6.373359457 | -0.776164909 | -3.261683989 |
| H | -6.565096249 | -2.515577935 | -2.996675197 |
| C | -3.916704350 | -2.006509951 | -3.196626409 |
| H | -3.961149418 | -1.193750847 | -3.930052317 |
| H | -2.881863314 | -2.131333338 | -2.872747178 |
| H | -4.246749554 | -2.929964468 | -3.687635161 |
| C | -4.795842389 | -2.877089077 | -0.995055903 |
| H | -5.437860336 | -2.673089131 | -0.130421025 |
| H | -5.158667478 | -3.788887407 | -1.484331071 |
| H | -3.775686022 | -3.048015445 | -0.646857273 |
| C | 4.814410161 | -2.837298123 | -0.909783223 |
| H | 3.800042463 | -3.019104375 | -0.551845086 |
| H | 5.190307515 | -3.754319432 | -1.379096237 |
| H | 5.454034639 | -2.603082156 | -0.051458254 |
| C | 3.932402393 | -2.032769313 | -3.137437404 |
| H | 2.899706112 | -2.177119342 | -2.815668003 |
| H | 3.961152064 | -1.233430145 | -3.886577231 |
| H | 4.286701378 | -2.957354153 | -3.608732187 |
| C | 6.282074265 | -1.544077299 | -2.456331250 |
| H | 6.368459275 | -0.757521995 | -3.214796239 |
| H | 6.987700376 | -1.326280114 | -1.646315931 |
| H | 6.585211335 | -2.489445046 | -2.918879263 |
| C | 6.935113386 | 2.833116035 | 0.122802989 |
| H | 7.444654455 | 1.966145898 | -0.309110952 |
| H | 7.627320621 | 3.682968347 | 0.094330078 |
| H | 6.706929511 | 2.605734392 | 1.169492304 |
| C | 6.005685517 | 3.501163153 | -2.121048249 |
| H | 6.692101435 | 4.355306563 | -2.158647351 |
| H | 6.493081576 | 2.652617380 | -2.611171159 |
| H | 5.106720264 | 3.752886420 | -2.693532306 |
| C | 5.013125214 | 4.424216553 | -0.020934252 |
| H | 4.104134169 | 4.729889441 | -0.550550189 |
| H | 4.760611355 | 4.257327278 | 1.032203088 |
| H | 5.724350549 | 5.255959361 | -0.067457928 |

**4d'**

| | | | |
|---|---|---|---|
| Bi | -0.031407199 | -0.829990173 | -0.530175277 |
| Fe | 0.137688745 | -2.222716958 | 1.736125248 |

| | | | |
|---|---|---|---|
| O | 2.750999368 | -1.073234962 | 2.331605231 |
| C | -4.795309508 | 2.055730314 | -0.564859142 |
| C | -5.280054389 | 0.830146809 | -1.088494317 |
| H | -6.303007458 | 0.806227998 | -1.448240124 |
| C | -3.169487024 | -0.282195939 | -0.705576897 |
| O | -2.373404942 | -1.309223144 | -0.769629041 |
| C | -4.517008313 | -0.319564849 | -1.197424925 |
| C | 1.721545356 | -1.504299045 | 2.026777968 |
| C | 0.695140993 | 1.768714099 | 1.160238052 |
| N | -1.370856947 | 0.909078888 | 0.304545211 |
| C | -3.501859021 | 2.094770895 | -0.080001017 |
| H | -3.077514960 | 3.026092161 | 0.271428240 |
| N | 1.313415286 | 0.924874300 | 0.298253823 |
| C | 5.221266501 | 0.881219822 | -1.076557137 |
| H | 6.248743506 | 0.867706223 | -1.423767264 |
| C | 3.112620049 | -0.240034271 | -0.729793107 |
| C | -2.682761962 | 0.943421962 | -0.106784265 |
| O | 2.325940388 | -1.261640055 | -0.814445062 |
| C | -5.070032406 | -1.604491349 | -1.821878950 |
| C | 3.430034322 | 2.132843081 | -0.066310143 |
| H | 3.000726049 | 3.057287160 | 0.297001789 |
| C | 0.672683240 | 3.313594160 | 3.045569059 |
| H | 1.211744990 | 3.869169416 | 3.807309125 |
| C | -1.435625068 | 2.566264119 | 2.116687300 |
| H | -2.516170084 | 2.510794173 | 2.168904923 |
| C | 4.723598582 | 2.102860957 | -0.544682142 |
| C | 4.468994474 | -0.269897860 | -1.204932892 |
| C | -0.740189852 | 3.320971420 | 3.035084999 |
| H | -1.283846978 | 3.886134310 | 3.786753235 |
| C | 5.633328358 | 3.332488434 | -0.542502990 |
| C | -5.708886402 | 3.283356443 | -0.579171799 |
| C | 5.036748215 | -1.552608165 | -1.818510208 |
| C | 1.369689053 | 2.554596290 | 2.132482182 |
| H | 2.448432221 | 2.481062349 | 2.197033340 |
| C | 2.614796023 | 0.977720056 | -0.114489085 |
| C | -0.758446996 | 1.765508873 | 1.156710027 |
| C | -0.302409981 | -2.393863993 | 3.766400019 |
| H | 0.447341046 | -2.453293244 | 4.543108393 |
| C | -0.883840308 | -1.186668868 | 3.243821081 |
| H | -0.657574171 | -0.178266057 | 3.561044321 |
| C | -1.809529011 | -1.552883867 | 2.225399357 |
| H | -2.416914424 | -0.878127311 | 1.644422006 |
| C | -1.789719261 | -2.970185114 | 2.092739383 |
| H | -2.370977077 | -3.543099391 | 1.385134150 |
| C | -0.861652964 | -3.490855309 | 3.057843325 |
| H | -0.609823862 | -4.532729111 | 3.199909424 |
| O | 1.180742083 | -4.431394314 | 0.139825034 |
| C | 0.773841292 | -3.530301240 | 0.742825155 |
| C | -6.126973471 | 3.598459269 | -2.032956113 |
| H | -6.655078607 | 2.754763935 | -2.488227409 |
| H | -6.793956414 | 4.468484347 | -2.054711119 |
| H | -5.247995244 | 3.819555345 | -2.647580141 |

| | | | |
|---|---|---|---|
| C | -5.021316348 | 4.525851394 | 0.007754034 |
| H | -4.724417219 | 4.366485432 | 1.050494099 |
| H | -4.130526355 | 4.802762440 | -0.566660990 |
| H | -5.714154362 | 5.373893391 | -0.017869787 |
| C | -6.973187689 | 2.985972058 | 0.258343804 |
| H | -7.646928754 | 3.850975244 | 0.245396953 |
| H | -7.520590332 | 2.124215375 | -0.136283250 |
| H | -6.705427706 | 2.770476266 | 1.298303042 |
| C | -6.536440243 | -1.446890193 | -2.257214022 |
| H | -7.189655581 | -1.209312892 | -1.409674215 |
| H | -6.653615432 | -0.665683812 | -3.016778112 |
| H | -6.882298322 | -2.390561927 | -2.692734307 |
| C | -4.240151243 | -1.973389276 | -3.073366210 |
| H | -4.304126127 | -1.175971021 | -3.822171068 |
| H | -3.191771207 | -2.127861407 | -2.812224117 |
| H | -4.633085459 | -2.894924996 | -3.519745212 |
| C | -5.003875195 | -2.760996055 | -0.797512978 |
| H | -3.971083133 | -2.950810347 | -0.500269883 |
| H | -5.591871554 | -2.517959233 | 0.094968266 |
| H | -5.417432507 | -3.673983446 | -1.242494951 |
| C | 4.969808351 | -2.702741049 | -0.786303945 |
| H | 5.545802441 | -2.446890199 | 0.110060930 |
| H | 3.938826076 | -2.907069085 | -0.494276951 |
| H | 5.398694341 | -3.612904221 | -1.222447071 |
| C | 6.505992442 | -1.382335860 | -2.239244221 |
| H | 6.864577763 | -2.323880301 | -2.668774219 |
| H | 6.624612285 | -0.601433227 | -2.999264991 |
| H | 7.148060662 | -1.137998849 | -1.385126212 |
| C | 4.224346306 | -1.936071167 | -3.077176286 |
| H | 3.176174237 | -2.107230373 | -2.826643139 |
| H | 4.283912085 | -1.140381205 | -3.828497382 |
| H | 4.636053085 | -2.852968119 | -3.515787495 |
| C | 6.062331295 | 3.659203526 | -1.990660034 |
| H | 6.728041566 | 4.530355222 | -1.999602071 |
| H | 6.595613372 | 2.820244328 | -2.448562928 |
| H | 5.188030465 | 3.884194346 | -2.610540380 |
| C | 4.937931243 | 4.568537477 | 0.048552013 |
| H | 4.050270275 | 4.846779404 | -0.530076850 |
| H | 4.634544401 | 4.400585085 | 1.087986836 |
| H | 5.628446169 | 5.418696182 | 0.033753042 |
| C | 6.891334553 | 3.030590167 | 0.303313816 |
| H | 7.445192628 | 2.174366032 | -0.094169208 |
| H | 7.561952413 | 3.898061436 | 0.303422826 |
| H | 6.615212510 | 2.804737317 | 1.338724246 |

Scan-3d-3d'-CBiC-113.953

| | | | |
|---|---|---|---|
| Bi | 0.000008000 | -0.816583000 | -1.882484000 |
| O | 1.768925000 | -1.713543000 | -0.846018000 |
| O | -1.768882000 | -1.713478000 | -0.845898000 |
| N | 1.331386000 | 0.880694000 | -1.251484000 |
| N | -1.331092000 | 0.880751000 | -1.251100000 |
| C | 2.579065000 | -0.854035000 | -0.206605000 |

| | | | |
|---|---|---|---|
| C | 3.568273000 | -1.307151000 | 0.696183000 |
| C | 4.382192000 | -0.355096000 | 1.322174000 |
| H | 5.165178000 | -0.697593000 | 1.991053000 |
| C | 4.218462000 | 1.022501000 | 1.130374000 |
| C | 3.218472000 | 1.459137000 | 0.260519000 |
| H | 3.038568000 | 2.517224000 | 0.130979000 |
| C | 2.400066000 | 0.547683000 | -0.426880000 |
| C | 5.126538000 | 2.002145000 | 1.885567000 |
| C | 4.948068000 | 1.805544000 | 3.407482000 |
| H | 3.910097000 | 2.000284000 | 3.697776000 |
| H | 5.601635000 | 2.489906000 | 3.965665000 |
| H | 5.192512000 | 0.780015000 | 3.702344000 |
| C | 4.810008000 | 3.469124000 | 1.552581000 |
| H | 4.945241000 | 3.673929000 | 0.484732000 |
| H | 5.484909000 | 4.127756000 | 2.113352000 |
| H | 3.780687000 | 3.728719000 | 1.821834000 |
| C | 6.602018000 | 1.734189000 | 1.515044000 |
| H | 6.889833000 | 0.707254000 | 1.761868000 |
| H | 7.267667000 | 2.418297000 | 2.059111000 |
| H | 6.757957000 | 1.878115000 | 0.440201000 |
| C | 3.726060000 | -2.807608000 | 0.979740000 |
| C | 4.058062000 | -3.565928000 | -0.325183000 |
| H | 3.270091000 | -3.416142000 | -1.065593000 |
| H | 4.158260000 | -4.640736000 | -0.120542000 |
| H | 5.005934000 | -3.205319000 | -0.742604000 |
| C | 4.857054000 | -3.093224000 | 1.983060000 |
| H | 5.829462000 | -2.754392000 | 1.606505000 |
| H | 4.919075000 | -4.175053000 | 2.153474000 |
| H | 4.672912000 | -2.609526000 | 2.949178000 |
| C | 2.414516000 | -3.361299000 | 1.583161000 |
| H | 2.195877000 | -2.862862000 | 2.534536000 |
| H | 2.512734000 | -4.438883000 | 1.773006000 |
| H | 1.577154000 | -3.195552000 | 0.902995000 |
| C | 0.720389000 | 2.126981000 | -1.348670000 |
| C | 1.394383000 | 3.344765000 | -1.523294000 |
| H | 2.477305000 | 3.342896000 | -1.585018000 |
| C | 0.697003000 | 4.546444000 | -1.670917000 |
| H | 1.248645000 | 5.473351000 | -1.809208000 |
| C | -0.696653000 | 4.546472000 | -1.670752000 |
| H | -1.248283000 | 5.473405000 | -1.808929000 |
| C | -1.394075000 | 3.344843000 | -1.522953000 |
| H | -2.477008000 | 3.343062000 | -1.584442000 |
| C | -0.720110000 | 2.127009000 | -1.348482000 |
| C | -2.399895000 | 0.547778000 | -0.426659000 |
| C | -2.579002000 | -0.853949000 | -0.206496000 |
| C | -3.568328000 | -1.307067000 | 0.696161000 |
| C | -4.382257000 | -0.355006000 | 1.322131000 |
| H | -5.165355000 | -0.697500000 | 1.990880000 |
| C | -4.218424000 | 1.022593000 | 1.130446000 |
| C | -3.218320000 | 1.459231000 | 0.260723000 |
| H | -3.038333000 | 2.517316000 | 0.131300000 |
| C | -5.126628000 | 2.002231000 | 1.885491000 |

| | | | |
|---|---|---|---|
| C | -6.602024000 | 1.734295000 | 1.514588000 |
| H | -6.757685000 | 1.878253000 | 0.439710000 |
| H | -7.267817000 | 2.418381000 | 2.058508000 |
| H | -6.889876000 | 0.707343000 | 1.761305000 |
| C | -4.948546000 | 1.805590000 | 3.407440000 |
| H | -5.193115000 | 0.780076000 | 3.702247000 |
| H | -5.602220000 | 2.489976000 | 3.965464000 |
| H | -3.910639000 | 2.000279000 | 3.698004000 |
| C | -4.809991000 | 3.469217000 | 1.552635000 |
| H | -3.780673000 | 3.728728000 | 1.821986000 |
| H | -5.484901000 | 4.127846000 | 2.113399000 |
| H | -4.945131000 | 3.674116000 | 0.484794000 |
| C | -3.726225000 | -2.807541000 | 0.979567000 |
| C | -2.414767000 | -3.361362000 | 1.583049000 |
| H | -2.513052000 | -4.438965000 | 1.772747000 |
| H | -2.196205000 | -2.863055000 | 2.534510000 |
| H | -1.577326000 | -3.195561000 | 0.902993000 |
| C | -4.857326000 | -3.093220000 | 1.982750000 |
| H | -5.829685000 | -2.754296000 | 1.606150000 |
| H | -4.673246000 | -2.609650000 | 2.948944000 |
| H | -4.919418000 | -4.175067000 | 2.153026000 |
| C | -4.058130000 | -3.565706000 | -0.325472000 |
| H | -4.158396000 | -4.640532000 | -0.120960000 |
| H | -3.270074000 | -3.415872000 | -1.065783000 |
| H | -5.005942000 | -3.205006000 | -0.742949000 |

Scan-3d-3d'-CBiC-116.453

| | | | |
|---|---|---|---|
| Bi | 0.000009000 | -0.858092000 | -1.819420000 |
| O | 1.811963000 | -1.728536000 | -0.813757000 |
| O | -1.812066000 | -1.728471000 | -0.813877000 |
| N | 1.329558000 | 0.854682000 | -1.220526000 |
| N | -1.329478000 | 0.854717000 | -1.220417000 |
| C | 2.622332000 | -0.857271000 | -0.195147000 |
| C | 3.636560000 | -1.291874000 | 0.690010000 |
| C | 4.450571000 | -0.325919000 | 1.293023000 |
| H | 5.252934000 | -0.654061000 | 1.945954000 |
| C | 4.263839000 | 1.048728000 | 1.098210000 |
| C | 3.240267000 | 1.467411000 | 0.247715000 |
| H | 3.042446000 | 2.522295000 | 0.118930000 |
| C | 2.420698000 | 0.541299000 | -0.419273000 |
| C | 5.175140000 | 2.044055000 | 1.828508000 |
| C | 5.037780000 | 1.849518000 | 3.354881000 |
| H | 4.004669000 | 2.029897000 | 3.670696000 |
| H | 5.694923000 | 2.545242000 | 3.894453000 |
| H | 5.304805000 | 0.828735000 | 3.646573000 |
| C | 4.828644000 | 3.505139000 | 1.499583000 |
| H | 4.935033000 | 3.709086000 | 0.428333000 |
| H | 5.506829000 | 4.175396000 | 2.042302000 |
| H | 3.802278000 | 3.750019000 | 1.792877000 |
| C | 6.644782000 | 1.796611000 | 1.421827000 |
| H | 6.953602000 | 0.774689000 | 1.664095000 |
| H | 7.313802000 | 2.491981000 | 1.947152000 |

| | | | |
|---|---|---|---|
| H | 6.771623000 | 1.939455000 | 0.343028000 |
| C | 3.821821000 | -2.788606000 | 0.976024000 |
| C | 4.136778000 | -3.547496000 | -0.332822000 |
| H | 3.331392000 | -3.411299000 | -1.056954000 |
| H | 4.256132000 | -4.620006000 | -0.126392000 |
| H | 5.070614000 | -3.175558000 | -0.771380000 |
| C | 4.977656000 | -3.054207000 | 1.956239000 |
| H | 5.937032000 | -2.703603000 | 1.557691000 |
| H | 5.058384000 | -4.134344000 | 2.129569000 |
| H | 4.807451000 | -2.569022000 | 2.924192000 |
| C | 2.531269000 | -3.358164000 | 1.609076000 |
| H | 2.325962000 | -2.859059000 | 2.563092000 |
| H | 2.648526000 | -4.433536000 | 1.800630000 |
| H | 1.677709000 | -3.206537000 | 0.945845000 |
| C | 0.720464000 | 2.098576000 | -1.340992000 |
| C | 1.394301000 | 3.312847000 | -1.541638000 |
| H | 2.476958000 | 3.309679000 | -1.605855000 |
| C | 0.696996000 | 4.510675000 | -1.715329000 |
| H | 1.248619000 | 5.434228000 | -1.874504000 |
| C | -0.696893000 | 4.510692000 | -1.715207000 |
| H | -1.248521000 | 5.434261000 | -1.874274000 |
| C | -1.394208000 | 3.312887000 | -1.541409000 |
| H | -2.476877000 | 3.309762000 | -1.605437000 |
| C | -0.720374000 | 2.098586000 | -1.340906000 |
| C | -2.420657000 | 0.541362000 | -0.419238000 |
| C | -2.622386000 | -0.857216000 | -0.195200000 |
| C | -3.636639000 | -1.291805000 | 0.689928000 |
| C | -4.450604000 | -0.325831000 | 1.292982000 |
| H | -5.252995000 | -0.653959000 | 1.945884000 |
| C | -4.263787000 | 1.048815000 | 1.098248000 |
| C | -3.240183000 | 1.467486000 | 0.247782000 |
| H | -3.042307000 | 2.522369000 | 0.119042000 |
| C | -5.175040000 | 2.044153000 | 1.828595000 |
| C | -6.644711000 | 1.796689000 | 1.422048000 |
| H | -6.771662000 | 1.939562000 | 0.343266000 |
| H | -7.313696000 | 2.492028000 | 1.947459000 |
| H | -6.953489000 | 0.774754000 | 1.664315000 |
| C | -5.037547000 | 1.849639000 | 3.354963000 |
| H | -5.304531000 | 0.828855000 | 3.646687000 |
| H | -5.694654000 | 2.545361000 | 3.894582000 |
| H | -4.004410000 | 2.030038000 | 3.670682000 |
| C | -4.828590000 | 3.505238000 | 1.499624000 |
| H | -3.802207000 | 3.750139000 | 1.792838000 |
| H | -5.506746000 | 4.175490000 | 2.042387000 |
| H | -4.935064000 | 3.709170000 | 0.428379000 |
| C | -3.821989000 | -2.788544000 | 0.975854000 |
| C | -2.531472000 | -3.358210000 | 1.608877000 |
| H | -2.648786000 | -4.433590000 | 1.800353000 |
| H | -2.326150000 | -2.859184000 | 2.562931000 |
| H | -1.677897000 | -3.206577000 | 0.945667000 |
| C | -4.977848000 | -3.054139000 | 1.956044000 |
| H | -5.937190000 | -2.703395000 | 1.557539000 |

| | | | |
|---|---|---|---|
| H | -4.807591000 | -2.569082000 | 2.924052000 |
| H | -5.058683000 | -4.134288000 | 2.129253000 |
| C | -4.136973000 | -3.547332000 | -0.333043000 |
| H | -4.256392000 | -4.619849000 | -0.126685000 |
| H | -3.331568000 | -3.411137000 | -1.057156000 |
| H | -5.070780000 | -3.175310000 | -0.771591000 |

Scan-3d-3d'-CBiC-118.953

| | | | |
|---|---|---|---|
| Bi | -0.000010000 | -0.907910000 | -1.754759000 |
| O | 1.859227000 | -1.746295000 | -0.782213000 |
| O | -1.859512000 | -1.746254000 | -0.782603000 |
| N | 1.327774000 | 0.822807000 | -1.194853000 |
| N | -1.328049000 | 0.822816000 | -1.195251000 |
| C | 2.665745000 | -0.861417000 | -0.183554000 |
| C | 3.703656000 | -1.273193000 | 0.686458000 |
| C | 4.512482000 | -0.290317000 | 1.267359000 |
| H | 5.332769000 | -0.600599000 | 1.906649000 |
| C | 4.299445000 | 1.080337000 | 1.067770000 |
| C | 3.254613000 | 1.476830000 | 0.233297000 |
| H | 3.036166000 | 2.527471000 | 0.103385000 |
| C | 2.439042000 | 0.532819000 | -0.414107000 |
| C | 5.207641000 | 2.094676000 | 1.775269000 |
| C | 5.107008000 | 1.903555000 | 3.304892000 |
| H | 4.077893000 | 2.066317000 | 3.642586000 |
| H | 5.762840000 | 2.613328000 | 3.827433000 |
| H | 5.399105000 | 0.889088000 | 3.594512000 |
| C | 4.827489000 | 3.547955000 | 1.449049000 |
| H | 4.907969000 | 3.750348000 | 0.375272000 |
| H | 5.504130000 | 4.232483000 | 1.975619000 |
| H | 3.802978000 | 3.774782000 | 1.762663000 |
| C | 6.672393000 | 1.872109000 | 1.337479000 |
| H | 7.004494000 | 0.856625000 | 1.576082000 |
| H | 7.340163000 | 2.581059000 | 1.845949000 |
| H | 6.773143000 | 2.013441000 | 0.255746000 |
| C | 3.920681000 | -2.764772000 | 0.976148000 |
| C | 4.224103000 | -3.524314000 | -0.335082000 |
| H | 3.403073000 | -3.404897000 | -1.044494000 |
| H | 4.365506000 | -4.593690000 | -0.126314000 |
| H | 5.143152000 | -3.138671000 | -0.792602000 |
| C | 5.099171000 | -3.005287000 | 1.935612000 |
| H | 6.044585000 | -2.640041000 | 1.517360000 |
| H | 5.202083000 | -4.082972000 | 2.112425000 |
| H | 4.938788000 | -2.518309000 | 2.904368000 |
| C | 2.652427000 | -3.353762000 | 1.635655000 |
| H | 2.455727000 | -2.853350000 | 2.590827000 |
| H | 2.792261000 | -4.425885000 | 1.830249000 |
| H | 1.784703000 | -3.220538000 | 0.986980000 |
| C | 0.720390000 | 2.063048000 | -1.344103000 |
| C | 1.394251000 | 3.272211000 | -1.575929000 |
| H | 2.476709000 | 3.267107000 | -1.641971000 |
| C | 0.697083000 | 4.464580000 | -1.781276000 |
| H | 1.248651000 | 5.383490000 | -1.965476000 |

| | | | |
|---|---|---|---|
| C | -0.697161000 | 4.464587000 | -1.781462000 |
| H | -1.248675000 | 5.383505000 | -1.965783000 |
| C | -1.394376000 | 3.272211000 | -1.576302000 |
| H | -2.476819000 | 3.267084000 | -1.642614000 |
| C | -0.720578000 | 2.063052000 | -1.344302000 |
| C | -2.439228000 | 0.532843000 | -0.414371000 |
| C | -2.665936000 | -0.861403000 | -0.183807000 |
| C | -3.703709000 | -1.273161000 | 0.686366000 |
| C | -4.512468000 | -0.290283000 | 1.267358000 |
| H | -5.332646000 | -0.600563000 | 1.906789000 |
| C | -4.299459000 | 1.080368000 | 1.067723000 |
| C | -3.254715000 | 1.476856000 | 0.233135000 |
| H | -3.036307000 | 2.527498000 | 0.103166000 |
| C | -5.207414000 | 2.094716000 | 1.775529000 |
| C | -6.672380000 | 1.872032000 | 1.338569000 |
| H | -6.773764000 | 2.013292000 | 0.256884000 |
| H | -7.339888000 | 2.580990000 | 1.847370000 |
| H | -7.004343000 | 0.856565000 | 1.577427000 |
| C | -5.105932000 | 1.903716000 | 3.305125000 |
| H | -5.397728000 | 0.889210000 | 3.594920000 |
| H | -5.761571000 | 2.613429000 | 3.827994000 |
| H | -4.076650000 | 2.066625000 | 3.642231000 |
| C | -4.827560000 | 3.547993000 | 1.448954000 |
| H | -3.803014000 | 3.775055000 | 1.762281000 |
| H | -5.504175000 | 4.232515000 | 1.975564000 |
| H | -4.908328000 | 3.750151000 | 0.375153000 |
| C | -3.920700000 | -2.764738000 | 0.976086000 |
| C | -2.652338000 | -3.353725000 | 1.635387000 |
| H | -2.792132000 | -4.425849000 | 1.830006000 |
| H | -2.455476000 | -2.853310000 | 2.590524000 |
| H | -1.784721000 | -3.220497000 | 0.986570000 |
| C | -5.099040000 | -3.005247000 | 1.935734000 |
| H | -6.044498000 | -2.639889000 | 1.517679000 |
| H | -4.938452000 | -2.518368000 | 2.904506000 |
| H | -5.202005000 | -4.082939000 | 2.112473000 |
| C | -4.224316000 | -3.524270000 | -0.335102000 |
| H | -4.365659000 | -4.593654000 | -0.126325000 |
| H | -3.403403000 | -3.404825000 | -1.044645000 |
| H | -5.143451000 | -3.138648000 | -0.792469000 |

Scan-3d-3d'-CBiC-121.453

| | | | |
|---|---|---|---|
| Bi | 0.000020000 | -0.960092000 | -1.689550000 |
| O | 1.908419000 | -1.764255000 | -0.753826000 |
| O | -1.908425000 | -1.764312000 | -0.753902000 |
| N | 1.326467000 | 0.789178000 | -1.172525000 |
| N | -1.326594000 | 0.789118000 | -1.172763000 |
| C | 2.708779000 | -0.865583000 | -0.174013000 |
| C | 3.768440000 | -1.253033000 | 0.682561000 |
| C | 4.569013000 | -0.252642000 | 1.243087000 |
| H | 5.405129000 | -0.543906000 | 1.870798000 |
| C | 4.328958000 | 1.113405000 | 1.038273000 |
| C | 3.265140000 | 1.486308000 | 0.217817000 |

| | | | |
|---|---|---|---|
| H | 3.025393000 | 2.532100000 | 0.086291000 |
| C | 2.456188000 | 0.523664000 | -0.411183000 |
| C | 5.229957000 | 2.147519000 | 1.725943000 |
| C | 5.158140000 | 1.962299000 | 3.257912000 |
| H | 4.131974000 | 2.108085000 | 3.611950000 |
| H | 5.809475000 | 2.686508000 | 3.766028000 |
| H | 5.473509000 | 0.954839000 | 3.547566000 |
| C | 4.817918000 | 3.591987000 | 1.399281000 |
| H | 4.877137000 | 3.790677000 | 0.323453000 |
| H | 5.490297000 | 4.291357000 | 1.911591000 |
| H | 3.794643000 | 3.801559000 | 1.728555000 |
| C | 6.691047000 | 1.949346000 | 1.264828000 |
| H | 7.045400000 | 0.941115000 | 1.502227000 |
| H | 7.354157000 | 2.672550000 | 1.759083000 |
| H | 6.771249000 | 2.087572000 | 0.180989000 |
| C | 4.017645000 | -2.738618000 | 0.976397000 |
| C | 4.312782000 | -3.499312000 | -0.336090000 |
| H | 3.477911000 | -3.397898000 | -1.032054000 |
| H | 4.476728000 | -4.564931000 | -0.124584000 |
| H | 5.217040000 | -3.099737000 | -0.810781000 |
| C | 5.216076000 | -2.952323000 | 1.917231000 |
| H | 6.147523000 | -2.572204000 | 1.481294000 |
| H | 5.341720000 | -4.026932000 | 2.097983000 |
| H | 5.062924000 | -2.462919000 | 2.885957000 |
| C | 2.771410000 | -3.347214000 | 1.659434000 |
| H | 2.580526000 | -2.845000000 | 2.614872000 |
| H | 2.934317000 | -4.415416000 | 1.857642000 |
| H | 1.891577000 | -3.233723000 | 1.023415000 |
| C | 0.720404000 | 2.024607000 | -1.352126000 |
| C | 1.394351000 | 3.227540000 | -1.616846000 |
| H | 2.476632000 | 3.220120000 | -1.684644000 |
| C | 0.697290000 | 4.413136000 | -1.855186000 |
| H | 1.248726000 | 5.326422000 | -2.065797000 |
| C | -0.697467000 | 4.413103000 | -1.855329000 |
| H | -1.248906000 | 5.326362000 | -2.066046000 |
| C | -1.394497000 | 3.227458000 | -1.617129000 |
| H | -2.476766000 | 3.219952000 | -1.685133000 |
| C | -0.720528000 | 2.024580000 | -1.352261000 |
| C | -2.456266000 | 0.523592000 | -0.411337000 |
| C | -2.708789000 | -0.865656000 | -0.174082000 |
| C | -3.768386000 | -1.253091000 | 0.682596000 |
| C | -4.568959000 | -0.252698000 | 1.243107000 |
| H | -5.405017000 | -0.543965000 | 1.870898000 |
| C | -4.328983000 | 1.113346000 | 1.038179000 |
| C | -3.265224000 | 1.486240000 | 0.217647000 |
| H | -3.025544000 | 2.532037000 | 0.086036000 |
| C | -5.229954000 | 2.147470000 | 1.725869000 |
| C | -6.691153000 | 1.948983000 | 1.265246000 |
| H | -6.771727000 | 2.086977000 | 0.181404000 |
| H | -7.354219000 | 2.672184000 | 1.759566000 |
| H | -7.045293000 | 0.940750000 | 1.502957000 |
| C | -5.157647000 | 1.962597000 | 3.257863000 |

| | | | |
|---|---|---|---|
| H | -5.472812000 | 0.955161000 | 3.547818000 |
| H | -5.808906000 | 2.686844000 | 3.766023000 |
| H | -4.131387000 | 2.108575000 | 3.611546000 |
| C | -4.818238000 | 3.591926000 | 1.398751000 |
| H | -3.794872000 | 3.801717000 | 1.727601000 |
| H | -5.490531000 | 4.291309000 | 1.911156000 |
| H | -4.877882000 | 3.790369000 | 0.322901000 |
| C | -4.017563000 | -2.738650000 | 0.976590000 |
| C | -2.771312000 | -3.347174000 | 1.659669000 |
| H | -2.934236000 | -4.415341000 | 1.858046000 |
| H | -2.580377000 | -2.844821000 | 2.615024000 |
| H | -1.891507000 | -3.233810000 | 1.023589000 |
| C | -5.215952000 | -2.952194000 | 1.917507000 |
| H | -6.147409000 | -2.572125000 | 1.481546000 |
| H | -5.062755000 | -2.462637000 | 2.886149000 |
| H | -5.341603000 | -4.026772000 | 2.098435000 |
| C | -4.312808000 | -3.499517000 | -0.335776000 |
| H | -4.476786000 | -4.565101000 | -0.124113000 |
| H | -3.477981000 | -3.398230000 | -1.031809000 |
| H | -5.217079000 | -3.099973000 | -0.810471000 |

Scan-3d-3d'-CBiC-123.953

| | | | |
|---|---|---|---|
| Bi | -0.000022000 | -1.009438000 | -1.623428000 |
| O | 1.956319000 | -1.780615000 | -0.727742000 |
| O | -1.956270000 | -1.780455000 | -0.727679000 |
| N | 1.325617000 | 0.757037000 | -1.149887000 |
| N | -1.325308000 | 0.757195000 | -1.149459000 |
| C | 2.750596000 | -0.869425000 | -0.166265000 |
| C | 3.831079000 | -1.233512000 | 0.676340000 |
| C | 4.622922000 | -0.216743000 | 1.217730000 |
| H | 5.473686000 | -0.489767000 | 1.833989000 |
| C | 4.356791000 | 1.144562000 | 1.009072000 |
| C | 3.275044000 | 1.494935000 | 0.203022000 |
| H | 3.014838000 | 2.535797000 | 0.071043000 |
| C | 2.472852000 | 0.514831000 | -0.408334000 |
| C | 5.249790000 | 2.197126000 | 1.678711000 |
| C | 5.202097000 | 2.019103000 | 3.212539000 |
| H | 4.178637000 | 2.150053000 | 3.579956000 |
| H | 5.848371000 | 2.756622000 | 3.707772000 |
| H | 5.537938000 | 1.018529000 | 3.503048000 |
| C | 4.809140000 | 3.632686000 | 1.350151000 |
| H | 4.849519000 | 3.826246000 | 0.272522000 |
| H | 5.477051000 | 4.345999000 | 1.848873000 |
| H | 3.787373000 | 3.827250000 | 1.693048000 |
| C | 6.707497000 | 2.020907000 | 1.198469000 |
| H | 7.082119000 | 1.020035000 | 1.435928000 |
| H | 7.365004000 | 2.757641000 | 1.680007000 |
| H | 6.770523000 | 2.154941000 | 0.112974000 |
| C | 4.111035000 | -2.712865000 | 0.972983000 |
| C | 4.397855000 | -3.474283000 | -0.340956000 |
| H | 3.549845000 | -3.390349000 | -1.023274000 |
| H | 4.583844000 | -4.535926000 | -0.127688000 |

| | | | |
|---|---|---|---|
| H | 5.287035000 | -3.061194000 | -0.832253000 |
| C | 5.328089000 | -2.900923000 | 1.895132000 |
| H | 6.245438000 | -2.506442000 | 1.442386000 |
| H | 5.475797000 | -3.972227000 | 2.078728000 |
| H | 5.181936000 | -2.409545000 | 2.863958000 |
| C | 2.886779000 | -3.340024000 | 1.678427000 |
| H | 2.701738000 | -2.836429000 | 2.634326000 |
| H | 3.071787000 | -4.404145000 | 1.879189000 |
| H | 1.995668000 | -3.245256000 | 1.055131000 |
| C | 0.720659000 | 1.987008000 | -1.358794000 |
| C | 1.394760000 | 3.182901000 | -1.655603000 |
| H | 2.476851000 | 3.172873000 | -1.725287000 |
| C | 0.697917000 | 4.361076000 | -1.925771000 |
| H | 1.249154000 | 5.268110000 | -2.162270000 |
| C | -0.697373000 | 4.361165000 | -1.925532000 |
| H | -1.248570000 | 5.268273000 | -2.161845000 |
| C | -1.394328000 | 3.183112000 | -1.655143000 |
| H | -2.476439000 | 3.173312000 | -1.724505000 |
| C | -0.720330000 | 1.987079000 | -1.358570000 |
| C | -2.472633000 | 0.515006000 | -0.408056000 |
| C | -2.750524000 | -0.869239000 | -0.166156000 |
| C | -3.831169000 | -1.233344000 | 0.676209000 |
| C | -4.622964000 | -0.216568000 | 1.217669000 |
| H | -5.473842000 | -0.489593000 | 1.833774000 |
| C | -4.356647000 | 1.144736000 | 1.009272000 |
| C | -3.274800000 | 1.495108000 | 0.203346000 |
| H | -3.014449000 | 2.535948000 | 0.071537000 |
| C | -5.249745000 | 2.197271000 | 1.678847000 |
| C | -6.707308000 | 2.021178000 | 1.198098000 |
| H | -6.769917000 | 2.155260000 | 0.112585000 |
| H | -7.364930000 | 2.757945000 | 1.679425000 |
| H | -7.082053000 | 1.020313000 | 1.435389000 |
| C | -5.202567000 | 2.018986000 | 3.212640000 |
| H | -5.538626000 | 1.018418000 | 3.502926000 |
| H | -5.848906000 | 2.756510000 | 3.707780000 |
| H | -4.179210000 | 2.149752000 | 3.580420000 |
| C | -4.808943000 | 3.632884000 | 1.350705000 |
| H | -3.787305000 | 3.827365000 | 1.694034000 |
| H | -5.477026000 | 4.346127000 | 1.849302000 |
| H | -4.848910000 | 3.826658000 | 0.273101000 |
| C | -4.111341000 | -2.712711000 | 0.972549000 |
| C | -2.887247000 | -3.340193000 | 1.677975000 |
| H | -3.072441000 | -4.404327000 | 1.878482000 |
| H | -2.702218000 | -2.836838000 | 2.634006000 |
| H | -1.996052000 | -3.245405000 | 1.054799000 |
| C | -5.328503000 | -2.900785000 | 1.894547000 |
| H | -6.245811000 | -2.506328000 | 1.441699000 |
| H | -5.182463000 | -2.409395000 | 2.863385000 |
| H | -5.476214000 | -3.972093000 | 2.078123000 |
| C | -4.398140000 | -3.473815000 | -0.341583000 |
| H | -4.584233000 | -4.535495000 | -0.128576000 |
| H | -3.550064000 | -3.389803000 | -1.023805000 |

| | | | |
|---|---|---|---|
| H | -5.287247000 | -3.060540000 | -0.832852000 |

Scan-3d-3d'-CBiC-126.453

| | | | |
|---|---|---|---|
| Bi | 0.000032000 | -1.054079000 | -1.555454000 |
| O | 2.001358000 | -1.794721000 | -0.701909000 |
| O | -2.001061000 | -1.794849000 | -0.701569000 |
| N | 1.324622000 | 0.728302000 | -1.123447000 |
| N | -1.324617000 | 0.728232000 | -1.123440000 |
| C | 2.790906000 | -0.872271000 | -0.159237000 |
| C | 3.892856000 | -1.214927000 | 0.666328000 |
| C | 4.676966000 | -0.183634000 | 1.189348000 |
| H | 5.542262000 | -0.440048000 | 1.792480000 |
| C | 4.385582000 | 1.173057000 | 0.979852000 |
| C | 3.285684000 | 1.502774000 | 0.190689000 |
| H | 3.005878000 | 2.538798000 | 0.060502000 |
| C | 2.488889000 | 0.507098000 | -0.403410000 |
| C | 5.271906000 | 2.242040000 | 1.631953000 |
| C | 5.249888000 | 2.069505000 | 3.166993000 |
| H | 4.230154000 | 2.186371000 | 3.549249000 |
| H | 5.892141000 | 2.818738000 | 3.649687000 |
| H | 5.605278000 | 1.075340000 | 3.456299000 |
| C | 4.804091000 | 3.669227000 | 1.304453000 |
| H | 4.824649000 | 3.858767000 | 0.225559000 |
| H | 5.468596000 | 4.394846000 | 1.789775000 |
| H | 3.784941000 | 3.849658000 | 1.662539000 |
| C | 6.724849000 | 2.086633000 | 1.130532000 |
| H | 7.118927000 | 1.092872000 | 1.366331000 |
| H | 7.377659000 | 2.835696000 | 1.599215000 |
| H | 6.769452000 | 2.217135000 | 0.043704000 |
| C | 4.202493000 | -2.688328000 | 0.962448000 |
| C | 4.477642000 | -3.449018000 | -0.354442000 |
| H | 3.615888000 | -3.380745000 | -1.021131000 |
| H | 4.684763000 | -4.506829000 | -0.141612000 |
| H | 5.350839000 | -3.023113000 | -0.863141000 |
| C | 5.438893000 | -2.853252000 | 1.862911000 |
| H | 6.341292000 | -2.445501000 | 1.392236000 |
| H | 5.607490000 | -3.921311000 | 2.047380000 |
| H | 5.302348000 | -2.360788000 | 2.832610000 |
| C | 3.001377000 | -3.333145000 | 1.691253000 |
| H | 2.824850000 | -2.829605000 | 2.648823000 |
| H | 3.207302000 | -4.393464000 | 1.891785000 |
| H | 2.098422000 | -3.254645000 | 1.082899000 |
| C | 0.720444000 | 1.952160000 | -1.359660000 |
| C | 1.394592000 | 3.141045000 | -1.686034000 |
| H | 2.476518000 | 3.128721000 | -1.757051000 |
| C | 0.697876000 | 4.311254000 | -1.985945000 |
| H | 1.248953000 | 5.211819000 | -2.246290000 |
| C | -0.698033000 | 4.311212000 | -1.986000000 |
| H | -1.249142000 | 5.211741000 | -2.246405000 |
| C | -1.394703000 | 3.140963000 | -1.686132000 |
| H | -2.476620000 | 3.128574000 | -1.757242000 |
| C | -0.720507000 | 1.952126000 | -1.359688000 |

| | | | |
|---|---|---|---|
| C | -2.488860000 | 0.506970000 | -0.403362000 |
| C | -2.790703000 | -0.872397000 | -0.159013000 |
| C | -3.892653000 | -1.215082000 | 0.666551000 |
| C | -4.676924000 | -0.183824000 | 1.189386000 |
| H | -5.542268000 | -0.440276000 | 1.792437000 |
| C | -4.385668000 | 1.172876000 | 0.979780000 |
| C | -3.285785000 | 1.502623000 | 0.190607000 |
| H | -3.006100000 | 2.538661000 | 0.060297000 |
| C | -5.272255000 | 2.241827000 | 1.631580000 |
| C | -6.725088000 | 2.086049000 | 1.129943000 |
| H | -6.769528000 | 2.216362000 | 0.043086000 |
| H | -7.378137000 | 2.835050000 | 1.598393000 |
| H | -7.118978000 | 1.092235000 | 1.365839000 |
| C | -5.250473000 | 2.069596000 | 3.166651000 |
| H | -5.605714000 | 1.075426000 | 3.456116000 |
| H | -5.892967000 | 2.818797000 | 3.649072000 |
| H | -4.230835000 | 2.186755000 | 3.549074000 |
| C | -4.804645000 | 3.669041000 | 1.303901000 |
| H | -3.785581000 | 3.849709000 | 1.662111000 |
| H | -5.469354000 | 4.394626000 | 1.788991000 |
| H | -4.825073000 | 3.858397000 | 0.224972000 |
| C | -4.202192000 | -2.688468000 | 0.962813000 |
| C | -3.001093000 | -3.333131000 | 1.691789000 |
| H | -3.206960000 | -4.393450000 | 1.892386000 |
| H | -2.824705000 | -2.829503000 | 2.649339000 |
| H | -2.098080000 | -3.254611000 | 1.083526000 |
| C | -5.438645000 | -2.853329000 | 1.863216000 |
| H | -6.340966000 | -2.445362000 | 1.392574000 |
| H | -5.302054000 | -2.361033000 | 2.832993000 |
| H | -5.607410000 | -3.921389000 | 2.047522000 |
| C | -4.477220000 | -3.449325000 | -0.354007000 |
| H | -4.684344000 | -4.507111000 | -0.141058000 |
| H | -3.615411000 | -3.381129000 | -1.020633000 |
| H | -5.350382000 | -3.023496000 | -0.862831000 |

Scan-3d-3d'-CBiC-128.953

| | | | |
|---|---|---|---|
| Bi | -0.000010000 | -1.092701000 | -1.485910000 |
| O | 2.041943000 | -1.806668000 | -0.675734000 |
| O | -2.042203000 | -1.806569000 | -0.676050000 |
| N | 1.324025000 | 0.703377000 | -1.093573000 |
| N | -1.324025000 | 0.703421000 | -1.093614000 |
| C | 2.829080000 | -0.874679000 | -0.152675000 |
| C | 3.952941000 | -1.198601000 | 0.652623000 |
| C | 4.731393000 | -0.154926000 | 1.157342000 |
| H | 5.611458000 | -0.396863000 | 1.744977000 |
| C | 4.416504000 | 1.197522000 | 0.950172000 |
| C | 3.298132000 | 1.509228000 | 0.180694000 |
| H | 3.000385000 | 2.540773000 | 0.054494000 |
| C | 2.504784000 | 0.500258000 | -0.396349000 |
| C | 5.298452000 | 2.280391000 | 1.584846000 |
| C | 5.303620000 | 2.112068000 | 3.120528000 |
| H | 4.288746000 | 2.216576000 | 3.518978000 |

| | | | |
|---|---|---|---|
| H | 5.943599000 | 2.871115000 | 3.590724000 |
| H | 5.676801000 | 1.123523000 | 3.406720000 |
| C | 4.805964000 | 3.700038000 | 1.260891000 |
| H | 4.805499000 | 3.886196000 | 0.181215000 |
| H | 5.468797000 | 4.436137000 | 1.732499000 |
| H | 3.790763000 | 3.868086000 | 1.635842000 |
| C | 6.745120000 | 2.143401000 | 1.060390000 |
| H | 7.156771000 | 1.155902000 | 1.292415000 |
| H | 7.394923000 | 2.902702000 | 1.516561000 |
| H | 6.770419000 | 2.271472000 | -0.027343000 |
| C | 4.289919000 | -2.666499000 | 0.945335000 |
| C | 4.548689000 | -3.425787000 | -0.375719000 |
| H | 3.672293000 | -3.370957000 | -1.024344000 |
| H | 4.775314000 | -4.480101000 | -0.165440000 |
| H | 5.404978000 | -2.988438000 | -0.903099000 |
| C | 5.546776000 | -2.811572000 | 1.820482000 |
| H | 6.433146000 | -2.391102000 | 1.330895000 |
| H | 5.735113000 | -3.876700000 | 2.002790000 |
| H | 5.422868000 | -2.319734000 | 2.792221000 |
| C | 3.113257000 | -3.326957000 | 1.699541000 |
| H | 2.949346000 | -2.824420000 | 2.659913000 |
| H | 3.338177000 | -4.383956000 | 1.897175000 |
| H | 2.197213000 | -3.261856000 | 1.109422000 |
| C | 0.720554000 | 1.921197000 | -1.354079000 |
| C | 1.394793000 | 3.103016000 | -1.707369000 |
| H | 2.476524000 | 3.088350000 | -1.779920000 |
| C | 0.698302000 | 4.265430000 | -2.033860000 |
| H | 1.249205000 | 5.159514000 | -2.315972000 |
| C | -0.698185000 | 4.265456000 | -2.033839000 |
| H | -1.249063000 | 5.159564000 | -2.315925000 |
| C | -1.394705000 | 3.103064000 | -1.707335000 |
| H | -2.476440000 | 3.088426000 | -1.779840000 |
| C | -0.720494000 | 1.921219000 | -1.354078000 |
| C | -2.504791000 | 0.500360000 | -0.396395000 |
| C | -2.829235000 | -0.874578000 | -0.152871000 |
| C | -3.953108000 | -1.198453000 | 0.652429000 |
| C | -4.731421000 | -0.154743000 | 1.157292000 |
| H | -5.611479000 | -0.396644000 | 1.744953000 |
| C | -4.416387000 | 1.197693000 | 0.950259000 |
| C | -3.297999000 | 1.509358000 | 0.180786000 |
| H | -3.000138000 | 2.540884000 | 0.054685000 |
| C | -5.298118000 | 2.280590000 | 1.585189000 |
| C | -6.744912000 | 2.143805000 | 1.061051000 |
| H | -6.770453000 | 2.271975000 | -0.026665000 |
| H | -7.394515000 | 2.903148000 | 1.517436000 |
| H | -7.156648000 | 1.156343000 | 1.293084000 |
| C | -5.302954000 | 2.112101000 | 3.120861000 |
| H | -5.676185000 | 1.123561000 | 3.407005000 |
| H | -5.942733000 | 2.871169000 | 3.591297000 |
| H | -4.287973000 | 2.216438000 | 3.519082000 |
| C | -4.805570000 | 3.700221000 | 1.261254000 |
| H | -3.790301000 | 3.868179000 | 1.636064000 |

| | | | |
|---|---|---|---|
| H | -5.468276000 | 4.436339000 | 1.733010000 |
| H | -4.805252000 | 3.886438000 | 0.181588000 |
| C | -4.290240000 | -2.666350000 | 0.944987000 |
| C | -3.113631000 | -3.327014000 | 1.699094000 |
| H | -3.338648000 | -4.384014000 | 1.896608000 |
| H | -2.949648000 | -2.824605000 | 2.659520000 |
| H | -2.197594000 | -3.261932000 | 1.108960000 |
| C | -5.547094000 | -2.811396000 | 1.820140000 |
| H | -6.433427000 | -2.390769000 | 1.330619000 |
| H | -5.423114000 | -2.319688000 | 2.791936000 |
| H | -5.735544000 | -3.876525000 | 2.002324000 |
| C | -4.549112000 | -3.425463000 | -0.376146000 |
| H | -4.775849000 | -4.479777000 | -0.165984000 |
| H | -3.672717000 | -3.370656000 | -1.024775000 |
| H | -5.405358000 | -2.987962000 | -0.903468000 |

Scan-3d-3d'-CBiC-131.453

| | | | |
|---|---|---|---|
| Bi | 0.000013000 | -1.126900000 | -1.414009000 |
| O | 2.079586000 | -1.816903000 | -0.648765000 |
| O | -2.079824000 | -1.816885000 | -0.649002000 |
| N | 1.323568000 | 0.681430000 | -1.059819000 |
| N | -1.323580000 | 0.681405000 | -1.059953000 |
| C | 2.865794000 | -0.876559000 | -0.146018000 |
| C | 4.012419000 | -1.183519000 | 0.635486000 |
| C | 4.786435000 | -0.128920000 | 1.122129000 |
| H | 5.681724000 | -0.357798000 | 1.691784000 |
| C | 4.448792000 | 1.219497000 | 0.920555000 |
| C | 3.311413000 | 1.514958000 | 0.173609000 |
| H | 2.996522000 | 2.542201000 | 0.053649000 |
| C | 2.520313000 | 0.494305000 | -0.386594000 |
| C | 5.328232000 | 2.314506000 | 1.537374000 |
| C | 5.365630000 | 2.147636000 | 3.072780000 |
| H | 4.357479000 | 2.239410000 | 3.490972000 |
| H | 6.004807000 | 2.915307000 | 3.529848000 |
| H | 5.757119000 | 1.164268000 | 3.352319000 |
| C | 4.810755000 | 3.727137000 | 1.221975000 |
| H | 4.786198000 | 3.911960000 | 0.142356000 |
| H | 5.473118000 | 4.472454000 | 1.679520000 |
| H | 3.801145000 | 3.882293000 | 1.617063000 |
| C | 6.766144000 | 2.196181000 | 0.984913000 |
| H | 7.195359000 | 1.214445000 | 1.209453000 |
| H | 7.414539000 | 2.964365000 | 1.427991000 |
| H | 6.768656000 | 2.323707000 | -0.103172000 |
| C | 4.376168000 | -2.646242000 | 0.921144000 |
| C | 4.614980000 | -3.402448000 | -0.405449000 |
| H | 3.723245000 | -3.359353000 | -1.033757000 |
| H | 4.860400000 | -4.453563000 | -0.200337000 |
| H | 5.453119000 | -2.953871000 | -0.952195000 |
| C | 5.654427000 | -2.773591000 | 1.767537000 |
| H | 6.523481000 | -2.340674000 | 1.258131000 |
| H | 5.861854000 | -3.835965000 | 1.945165000 |
| H | 5.545792000 | -2.283631000 | 2.742082000 |

| | | | |
|---|---|---|---|
| C | 3.225964000 | -3.322409000 | 1.701775000 |
| H | 3.077193000 | -2.822085000 | 2.665789000 |
| H | 3.469529000 | -4.376280000 | 1.893955000 |
| H | 2.296142000 | -3.269411000 | 1.132366000 |
| C | 0.720571000 | 1.893085000 | -1.342563000 |
| C | 1.394842000 | 3.067937000 | -1.720700000 |
| H | 2.476381000 | 3.051116000 | -1.794616000 |
| C | 0.698531000 | 4.222480000 | -2.071679000 |
| H | 1.249258000 | 5.110099000 | -2.373811000 |
| C | -0.698554000 | 4.222468000 | -2.071718000 |
| H | -1.249279000 | 5.110073000 | -2.373889000 |
| C | -1.394841000 | 3.067899000 | -1.720776000 |
| H | -2.476378000 | 3.051006000 | -1.794720000 |
| C | -0.720543000 | 1.893079000 | -1.342611000 |
| C | -2.520323000 | 0.494347000 | -0.386679000 |
| C | -2.865924000 | -0.876502000 | -0.146209000 |
| C | -4.012594000 | -1.183376000 | 0.635290000 |
| C | -4.786450000 | -0.128722000 | 1.122059000 |
| H | -5.681754000 | -0.357539000 | 1.691717000 |
| C | -4.448629000 | 1.219679000 | 0.920641000 |
| C | -3.311241000 | 1.515054000 | 0.173673000 |
| H | -2.996197000 | 2.542258000 | 0.053781000 |
| C | -5.327850000 | 2.314723000 | 1.537728000 |
| C | -6.765924000 | 2.196522000 | 0.985682000 |
| H | -6.768749000 | 2.324115000 | -0.102396000 |
| H | -7.414131000 | 2.964728000 | 1.428995000 |
| H | -7.195159000 | 1.214811000 | 1.210290000 |
| C | -5.364834000 | 2.147745000 | 3.073134000 |
| H | -5.756310000 | 1.164375000 | 3.352685000 |
| H | -6.003829000 | 2.915423000 | 3.530450000 |
| H | -4.356557000 | 2.239410000 | 3.491045000 |
| C | -4.810408000 | 3.727354000 | 1.222268000 |
| H | -3.800741000 | 3.882509000 | 1.617204000 |
| H | -5.472691000 | 4.472677000 | 1.679924000 |
| H | -4.786015000 | 3.912177000 | 0.142647000 |
| C | -4.376539000 | -2.646082000 | 0.920803000 |
| C | -3.226432000 | -3.322468000 | 1.701392000 |
| H | -3.470127000 | -4.376331000 | 1.893459000 |
| H | -3.077622000 | -2.822260000 | 2.665460000 |
| H | -2.296594000 | -3.269520000 | 1.132004000 |
| C | -5.654827000 | -2.773363000 | 1.767158000 |
| H | -6.523815000 | -2.340276000 | 1.257786000 |
| H | -5.546148000 | -2.283530000 | 2.741762000 |
| H | -5.862395000 | -3.835731000 | 1.944663000 |
| C | -4.615418000 | -3.402135000 | -0.405865000 |
| H | -4.860987000 | -4.453236000 | -0.200857000 |
| H | -3.723659000 | -3.359101000 | -1.034141000 |
| H | -5.453482000 | -2.953394000 | -0.952591000 |

Scan-3d-3d'-CBiC-133.953

| | | | |
|---|---|---|---|
| Bi | -0.000042000 | -1.156783000 | -1.340339000 |
| O | 2.114184000 | -1.825655000 | -0.621722000 |

| | | | |
|---|---|---|---|
| O | -2.113867000 | -1.825614000 | -0.621476000 |
| N | 1.323312000 | 0.662344000 | -1.023373000 |
| N | -1.323282000 | 0.662417000 | -1.023196000 |
| C | 2.900755000 | -0.877965000 | -0.139735000 |
| C | 4.070272000 | -1.169791000 | 0.615156000 |
| C | 4.840889000 | -0.105653000 | 1.084361000 |
| H | 5.751452000 | -0.322883000 | 1.634076000 |
| C | 4.481507000 | 1.238987000 | 0.891415000 |
| C | 3.325130000 | 1.519943000 | 0.169164000 |
| H | 2.993994000 | 2.543056000 | 0.057392000 |
| C | 2.535353000 | 0.489125000 | -0.374841000 |
| C | 5.359946000 | 2.344511000 | 1.490460000 |
| C | 5.433784000 | 2.176355000 | 3.024386000 |
| H | 4.434153000 | 2.254657000 | 3.465179000 |
| H | 6.073076000 | 2.951688000 | 3.468133000 |
| H | 5.844113000 | 1.197848000 | 3.293788000 |
| C | 4.817518000 | 3.750643000 | 1.188506000 |
| H | 4.766335000 | 3.936182000 | 0.109963000 |
| H | 5.480346000 | 4.503979000 | 1.632005000 |
| H | 3.815123000 | 3.892426000 | 1.606361000 |
| C | 6.786698000 | 2.245187000 | 0.906018000 |
| H | 7.233202000 | 1.268704000 | 1.119510000 |
| H | 7.434973000 | 3.020964000 | 1.335823000 |
| H | 6.763504000 | 2.374075000 | -0.181657000 |
| C | 4.459783000 | -2.627682000 | 0.890551000 |
| C | 4.676106000 | -3.379195000 | -0.442579000 |
| H | 3.768881000 | -3.346360000 | -1.048964000 |
| H | 4.939514000 | -4.427404000 | -0.245066000 |
| H | 5.495143000 | -2.919443000 | -1.008640000 |
| C | 5.759560000 | -2.739170000 | 1.705785000 |
| H | 6.610294000 | -2.293878000 | 1.176495000 |
| H | 5.985377000 | -3.798941000 | 1.876403000 |
| H | 5.667895000 | -2.252245000 | 2.683623000 |
| C | 3.337461000 | -3.319671000 | 1.697453000 |
| H | 3.205401000 | -2.822630000 | 2.665619000 |
| H | 3.599183000 | -4.370555000 | 1.882000000 |
| H | 2.393856000 | -3.277687000 | 1.150246000 |
| C | 0.720627000 | 1.867941000 | -1.326181000 |
| C | 1.394970000 | 3.035853000 | -1.727343000 |
| H | 2.476315000 | 3.016864000 | -1.802580000 |
| C | 0.698897000 | 4.182678000 | -2.100715000 |
| H | 1.249455000 | 5.063865000 | -2.421389000 |
| C | -0.698771000 | 4.182714000 | -2.100672000 |
| H | -1.249303000 | 5.063937000 | -2.421294000 |
| C | -1.394901000 | 3.035936000 | -1.727257000 |
| H | -2.476246000 | 3.017051000 | -1.802475000 |
| C | -0.720613000 | 1.867973000 | -1.326128000 |
| C | -2.535325000 | 0.489122000 | -0.374739000 |
| C | -2.900588000 | -0.877990000 | -0.139507000 |
| C | -4.070033000 | -1.169949000 | 0.615373000 |
| C | -4.840864000 | -0.105882000 | 1.084424000 |
| H | -5.751406000 | -0.323204000 | 1.634136000 |

| | | | |
|---|---|---|---|
| C | -4.481713000 | 1.238779000 | 0.891294000 |
| C | -3.325342000 | 1.519864000 | 0.169069000 |
| H | -2.994414000 | 2.543029000 | 0.057209000 |
| C | -5.360437000 | 2.344234000 | 1.490055000 |
| C | -6.787052000 | 2.244595000 | 0.905327000 |
| H | -6.763653000 | 2.373388000 | -0.182354000 |
| H | -7.435560000 | 3.020289000 | 1.334927000 |
| H | -7.233411000 | 1.268044000 | 1.118814000 |
| C | -5.434559000 | 2.176238000 | 3.023980000 |
| H | -5.844724000 | 1.197672000 | 3.293422000 |
| H | -6.074124000 | 2.951476000 | 3.467495000 |
| H | -4.435041000 | 2.254827000 | 3.464980000 |
| C | -4.818178000 | 3.750423000 | 1.188052000 |
| H | -3.815872000 | 3.892408000 | 1.606051000 |
| H | -5.481197000 | 4.503694000 | 1.631374000 |
| H | -4.766859000 | 3.935874000 | 0.109500000 |
| C | -4.459298000 | -2.627874000 | 0.890920000 |
| C | -3.336831000 | -3.319591000 | 1.697849000 |
| H | -3.598377000 | -4.370497000 | 1.882519000 |
| H | -3.204808000 | -2.822425000 | 2.665955000 |
| H | -2.393251000 | -3.277523000 | 1.150606000 |
| C | -5.759029000 | -2.739480000 | 1.706214000 |
| H | -6.609859000 | -2.294405000 | 1.176897000 |
| H | -5.667412000 | -2.252413000 | 2.683985000 |
| H | -5.984655000 | -3.799268000 | 1.876975000 |
| C | -4.675537000 | -3.379547000 | -0.442131000 |
| H | -4.938736000 | -4.427788000 | -0.244512000 |
| H | -3.768349000 | -3.346593000 | -1.048564000 |
| H | -5.494686000 | -2.920004000 | -1.008198000 |

Scan-3d-3d'-CBiC-136.453

| | | | |
|---|---|---|---|
| Bi | -0.000058000 | -1.183341000 | -1.265520000 |
| O | 2.145646000 | -1.833373000 | -0.594556000 |
| O | -2.145289000 | -1.833402000 | -0.594226000 |
| N | 1.323139000 | 0.645490000 | -0.985303000 |
| N | -1.323256000 | 0.645473000 | -0.985412000 |
| C | 2.933684000 | -0.879177000 | -0.133968000 |
| C | 4.125676000 | -1.157333000 | 0.592299000 |
| C | 4.893746000 | -0.084784000 | 1.044569000 |
| H | 5.819181000 | -0.291492000 | 1.573189000 |
| C | 4.513951000 | 1.256286000 | 0.862358000 |
| C | 3.339058000 | 1.524167000 | 0.166135000 |
| H | 2.992678000 | 2.543307000 | 0.064023000 |
| C | 2.549790000 | 0.484436000 | -0.362063000 |
| C | 5.392085000 | 2.371012000 | 1.444316000 |
| C | 5.503694000 | 2.199839000 | 2.975631000 |
| H | 4.513718000 | 2.264441000 | 3.439818000 |
| H | 6.143379000 | 2.982033000 | 3.406543000 |
| H | 5.932484000 | 1.225948000 | 3.232726000 |
| C | 4.825368000 | 3.770996000 | 1.159002000 |
| H | 4.746779000 | 3.958697000 | 0.082503000 |
| H | 5.488844000 | 4.531437000 | 1.589167000 |

| | | | |
|---|---|---|---|
| H | 3.831261000 | 3.899074000 | 1.600436000 |
| C | 6.806042000 | 2.290711000 | 0.826677000 |
| H | 7.268982000 | 1.319002000 | 1.026568000 |
| H | 7.454803000 | 3.072882000 | 1.243942000 |
| H | 6.756140000 | 2.422583000 | -0.259736000 |
| C | 4.539383000 | -2.610638000 | 0.855611000 |
| C | 4.730477000 | -3.357459000 | -0.484010000 |
| H | 3.807756000 | -3.333933000 | -1.066976000 |
| H | 5.010742000 | -4.402898000 | -0.295234000 |
| H | 5.529587000 | -2.887441000 | -1.069763000 |
| C | 5.860665000 | -2.707618000 | 1.637366000 |
| H | 6.692087000 | -2.250526000 | 1.087819000 |
| H | 6.103950000 | -3.764841000 | 1.799548000 |
| H | 5.787771000 | -2.224035000 | 2.618459000 |
| C | 3.446163000 | -3.317329000 | 1.689277000 |
| H | 3.332552000 | -2.823461000 | 2.661428000 |
| H | 3.725097000 | -4.365267000 | 1.865220000 |
| H | 2.488818000 | -3.285682000 | 1.165754000 |
| C | 0.720611000 | 1.844924000 | -1.306997000 |
| C | 1.394962000 | 3.006017000 | -1.729746000 |
| H | 2.476130000 | 2.985111000 | -1.806037000 |
| C | 0.699083000 | 4.145063000 | -2.124164000 |
| H | 1.249492000 | 5.019864000 | -2.462094000 |
| C | -0.699186000 | 4.145052000 | -2.124243000 |
| H | -1.249573000 | 5.019849000 | -2.462220000 |
| C | -1.395071000 | 3.005980000 | -1.729905000 |
| H | -2.476230000 | 2.985031000 | -1.806313000 |
| C | -0.720727000 | 1.844924000 | -1.307075000 |
| C | -2.549874000 | 0.484360000 | -0.362167000 |
| C | -2.933552000 | -0.879271000 | -0.133779000 |
| C | -4.125434000 | -1.157544000 | 0.592539000 |
| C | -4.893752000 | -0.085054000 | 1.044576000 |
| H | -5.819125000 | -0.291861000 | 1.573265000 |
| C | -4.514252000 | 1.256038000 | 0.862025000 |
| C | -3.339404000 | 1.524034000 | 0.165754000 |
| H | -2.993301000 | 2.543243000 | 0.063393000 |
| C | -5.392519000 | 2.370726000 | 1.443860000 |
| C | -6.806687000 | 2.289849000 | 0.826799000 |
| H | -6.757259000 | 2.421368000 | -0.259680000 |
| H | -7.455468000 | 3.072007000 | 1.244056000 |
| H | -7.269352000 | 1.318115000 | 1.027199000 |
| C | -5.503462000 | 2.200050000 | 2.975288000 |
| H | -5.931871000 | 1.226116000 | 3.232854000 |
| H | -6.143186000 | 2.982212000 | 3.406207000 |
| H | -4.513313000 | 2.265076000 | 3.439043000 |
| C | -4.826291000 | 3.770753000 | 1.157801000 |
| H | -3.832110000 | 3.899332000 | 1.598924000 |
| H | -5.489882000 | 4.531177000 | 1.587815000 |
| H | -4.748040000 | 3.958001000 | 0.081198000 |
| C | -4.538814000 | -2.610871000 | 0.856180000 |
| C | -3.445401000 | -3.317120000 | 1.689965000 |
| H | -3.724056000 | -4.365097000 | 1.866110000 |

| | | | |
|---|---|---|---|
| H | -3.331905000 | -2.823038000 | 2.662019000 |
| H | -2.488070000 | -3.285322000 | 1.166425000 |
| C | -5.860058000 | -2.707939000 | 1.637989000 |
| H | -6.691593000 | -2.251161000 | 1.088352000 |
| H | -5.787253000 | -2.224105000 | 2.618967000 |
| H | -6.103108000 | -3.765176000 | 1.800430000 |
| C | -4.729768000 | -3.358015000 | -0.483279000 |
| H | -5.009768000 | -4.403483000 | -0.294273000 |
| H | -3.807079000 | -3.334387000 | -1.066294000 |
| H | -5.529013000 | -2.888319000 | -1.069104000 |

Scan-3d-3d'-CBiC-138.953

| | | | |
|---|---|---|---|
| Bi | 0.000093000 | -1.204876000 | -1.190769000 |
| O | 2.173235000 | -1.839516000 | -0.568265000 |
| O | -2.173405000 | -1.839622000 | -0.568293000 |
| N | 1.323362000 | 0.632030000 | -0.946020000 |
| N | -1.323327000 | 0.631983000 | -0.945945000 |
| C | 2.964363000 | -0.880071000 | -0.129639000 |
| C | 4.177819000 | -1.146975000 | 0.566376000 |
| C | 4.944931000 | -0.067687000 | 1.002520000 |
| H | 5.884416000 | -0.265807000 | 1.509276000 |
| C | 4.547099000 | 1.270275000 | 0.832988000 |
| C | 3.354420000 | 1.527465000 | 0.164114000 |
| H | 2.994771000 | 2.543120000 | 0.073174000 |
| C | 2.564033000 | 0.480687000 | -0.348825000 |
| C | 5.426074000 | 2.392290000 | 1.399340000 |
| C | 5.573910000 | 2.216829000 | 2.927125000 |
| H | 4.593959000 | 2.268750000 | 3.413639000 |
| H | 6.214424000 | 3.004521000 | 3.346619000 |
| H | 6.019114000 | 1.246864000 | 3.170807000 |
| C | 4.838042000 | 3.787043000 | 1.132191000 |
| H | 4.733003000 | 3.977792000 | 0.058496000 |
| H | 5.502860000 | 4.553091000 | 1.550149000 |
| H | 3.852878000 | 3.902847000 | 1.596505000 |
| C | 6.826554000 | 2.329460000 | 0.749815000 |
| H | 7.304094000 | 1.361933000 | 0.935140000 |
| H | 7.476273000 | 3.116764000 | 1.155749000 |
| H | 6.750852000 | 2.465176000 | -0.334624000 |
| C | 4.612518000 | -2.596401000 | 0.816412000 |
| C | 4.775035000 | -3.339290000 | -0.529186000 |
| H | 3.836961000 | -3.323553000 | -1.087326000 |
| H | 5.070029000 | -4.382327000 | -0.349811000 |
| H | 5.553876000 | -2.860827000 | -1.135050000 |
| C | 5.955041000 | -2.681477000 | 1.562426000 |
| H | 6.766619000 | -2.214152000 | 0.992202000 |
| H | 6.213651000 | -3.736475000 | 1.715030000 |
| H | 5.903240000 | -2.201246000 | 2.546517000 |
| C | 3.548711000 | -3.315072000 | 1.677508000 |
| H | 3.456066000 | -2.823757000 | 2.653201000 |
| H | 3.842570000 | -4.360439000 | 1.844245000 |
| H | 2.577683000 | -3.291983000 | 1.179336000 |
| C | 0.720779000 | 1.825764000 | -1.283901000 |

| | | | |
|---|---|---|---|
| C | 1.395051000 | 2.980443000 | -1.725980000 |
| H | 2.476011000 | 2.957676000 | -1.803596000 |
| C | 0.699350000 | 4.112305000 | -2.138723000 |
| H | 1.249521000 | 4.981130000 | -2.492093000 |
| C | -0.699450000 | 4.112291000 | -2.138628000 |
| H | -1.249684000 | 4.981107000 | -2.491932000 |
| C | -1.395118000 | 2.980443000 | -1.725804000 |
| H | -2.476088000 | 2.957726000 | -1.803302000 |
| C | -0.720815000 | 1.825726000 | -1.283827000 |
| C | -2.564004000 | 0.480620000 | -0.348704000 |
| C | -2.964377000 | -0.880115000 | -0.129627000 |
| C | -4.177903000 | -1.146941000 | 0.566391000 |
| C | -4.944903000 | -0.067639000 | 1.002636000 |
| H | -5.884441000 | -0.265703000 | 1.509321000 |
| C | -4.546930000 | 1.270319000 | 0.833273000 |
| C | -3.354254000 | 1.527433000 | 0.164383000 |
| H | -2.994438000 | 2.543043000 | 0.073566000 |
| C | -5.425981000 | 2.392362000 | 1.399408000 |
| C | -6.825946000 | 2.330051000 | 0.748665000 |
| H | -6.749262000 | 2.466169000 | -0.335650000 |
| H | -7.475913000 | 3.117284000 | 1.154345000 |
| H | -7.303710000 | 1.362484000 | 0.933214000 |
| C | -5.575148000 | 2.216525000 | 2.927000000 |
| H | -6.020725000 | 1.246597000 | 3.170142000 |
| H | -6.215916000 | 3.004219000 | 3.346098000 |
| H | -4.595623000 | 2.268206000 | 3.414402000 |
| C | -4.837311000 | 3.787033000 | 1.133226000 |
| H | -3.852384000 | 3.902252000 | 1.598192000 |
| H | -5.502122000 | 4.553126000 | 1.551112000 |
| H | -4.731540000 | 3.978261000 | 0.059688000 |
| C | -4.612734000 | -2.596346000 | 0.816281000 |
| C | -3.548999000 | -3.315209000 | 1.677303000 |
| H | -3.842971000 | -4.360562000 | 1.843937000 |
| H | -3.456305000 | -2.823998000 | 2.653044000 |
| H | -2.577969000 | -3.292167000 | 1.179132000 |
| C | -5.955267000 | -2.681370000 | 1.562299000 |
| H | -6.766810000 | -2.213931000 | 0.992119000 |
| H | -5.903418000 | -2.201222000 | 2.546429000 |
| H | -6.213960000 | -3.736360000 | 1.714814000 |
| C | -4.775325000 | -3.339087000 | -0.529391000 |
| H | -5.070386000 | -4.382122000 | -0.350110000 |
| H | -3.837260000 | -3.323355000 | -1.087545000 |
| H | -5.554149000 | -2.860513000 | -1.135188000 |

Scan-3d-3d'-CBiC-141.453

| | | | |
|---|---|---|---|
| Bi | -0.000028000 | -1.222548000 | -1.114833000 |
| O | 2.198089000 | -1.844738000 | -0.541804000 |
| O | -2.197881000 | -1.844776000 | -0.541561000 |
| N | 1.323643000 | 0.621136000 | -0.904550000 |
| N | -1.323674000 | 0.621106000 | -0.904631000 |
| C | 2.993066000 | -0.880773000 | -0.125641000 |
| C | 4.227699000 | -1.137930000 | 0.537825000 |

| | | | |
|---|---|---|---|
| C | 4.994747000 | -0.053067000 | 0.958495000 |
| H | 5.948122000 | -0.243794000 | 1.441712000 |
| C | 4.580171000 | 1.282110000 | 0.804321000 |
| C | 3.370119000 | 1.530083000 | 0.164380000 |
| H | 2.998133000 | 2.542431000 | 0.086346000 |
| C | 2.577768000 | 0.477525000 | -0.334021000 |
| C | 5.461282000 | 2.410051000 | 1.355098000 |
| C | 5.649102000 | 2.228042000 | 2.877749000 |
| H | 4.681133000 | 2.267000000 | 3.388845000 |
| H | 6.291586000 | 3.020297000 | 3.285436000 |
| H | 6.110479000 | 1.261666000 | 3.105039000 |
| C | 4.852056000 | 3.799931000 | 1.110828000 |
| H | 4.718379000 | 3.995852000 | 0.041266000 |
| H | 5.518833000 | 4.570666000 | 1.516860000 |
| H | 3.877516000 | 3.902423000 | 1.600054000 |
| C | 6.845567000 | 2.365457000 | 0.670372000 |
| H | 7.337264000 | 1.401744000 | 0.837720000 |
| H | 7.497345000 | 3.156925000 | 1.064716000 |
| H | 6.741202000 | 2.506817000 | -0.410950000 |
| C | 4.682037000 | -2.583900000 | 0.771887000 |
| C | 4.813289000 | -3.321958000 | -0.579789000 |
| H | 3.859931000 | -3.312897000 | -1.111494000 |
| H | 5.122034000 | -4.362860000 | -0.411549000 |
| H | 5.570883000 | -2.835348000 | -1.205771000 |
| C | 6.045653000 | -2.658743000 | 1.479682000 |
| H | 6.836292000 | -2.181291000 | 0.888803000 |
| H | 6.318615000 | -3.711730000 | 1.620675000 |
| H | 6.016842000 | -2.182804000 | 2.466809000 |
| C | 3.649049000 | -3.314215000 | 1.660317000 |
| H | 3.579029000 | -2.825933000 | 2.639442000 |
| H | 3.956946000 | -4.357216000 | 1.816263000 |
| H | 2.664522000 | -3.298764000 | 1.189037000 |
| C | 0.720907000 | 1.809396000 | -1.256923000 |
| C | 1.395102000 | 2.958073000 | -1.716588000 |
| H | 2.475872000 | 2.933691000 | -1.795250000 |
| C | 0.699635000 | 4.083019000 | -2.146127000 |
| H | 1.249733000 | 4.946084000 | -2.513445000 |
| C | -0.699698000 | 4.082993000 | -2.146214000 |
| H | -1.249783000 | 4.946029000 | -2.513615000 |
| C | -1.395148000 | 2.958006000 | -1.716746000 |
| H | -2.475907000 | 2.933534000 | -1.795535000 |
| C | -0.720933000 | 1.809390000 | -1.256991000 |
| C | -2.577795000 | 0.477483000 | -0.334111000 |
| C | -2.992995000 | -0.880825000 | -0.125561000 |
| C | -4.227581000 | -1.138026000 | 0.537933000 |
| C | -4.994748000 | -0.053172000 | 0.958441000 |
| H | -5.948094000 | -0.243929000 | 1.441699000 |
| C | -4.580322000 | 1.282020000 | 0.804057000 |
| C | -3.370269000 | 1.530026000 | 0.164118000 |
| H | -2.998406000 | 2.542404000 | 0.085934000 |
| C | -5.461476000 | 2.409944000 | 1.354840000 |
| C | -6.845984000 | 2.365023000 | 0.670614000 |

| | | | |
|---|---|---|---|
| H | -6.742036000 | 2.506199000 | -0.410774000 |
| H | -7.497716000 | 3.156484000 | 1.065045000 |
| H | -7.337527000 | 1.401292000 | 0.838309000 |
| C | -5.648752000 | 2.228170000 | 2.877595000 |
| H | -6.109933000 | 1.261765000 | 3.105153000 |
| H | -6.291180000 | 3.020412000 | 3.285401000 |
| H | -4.680602000 | 2.267303000 | 3.388333000 |
| C | -4.852599000 | 3.799892000 | 1.110093000 |
| H | -3.877940000 | 3.902706000 | 1.599011000 |
| H | -5.519411000 | 4.570585000 | 1.516147000 |
| H | -4.719278000 | 3.995579000 | 0.040444000 |
| C | -4.681788000 | -2.584011000 | 0.772186000 |
| C | -3.648750000 | -3.314112000 | 1.660734000 |
| H | -3.956582000 | -4.357105000 | 1.816862000 |
| H | -3.578753000 | -2.825656000 | 2.639774000 |
| H | -2.664227000 | -3.298689000 | 1.189447000 |
| C | -6.045406000 | -2.658890000 | 1.479965000 |
| H | -6.836075000 | -2.181573000 | 0.889016000 |
| H | -6.016654000 | -2.182836000 | 2.467038000 |
| H | -6.318284000 | -3.711882000 | 1.621078000 |
| C | -4.812949000 | -3.322267000 | -0.579392000 |
| H | -5.121624000 | -4.363167000 | -0.411013000 |
| H | -3.859576000 | -3.313218000 | -1.111069000 |
| H | -5.570559000 | -2.835799000 | -1.205464000 |

Scan-3d-3d'-CBiC-143.953

| | | | |
|---|---|---|---|
| Bi | 0.000046000 | -1.237242000 | -1.036582000 |
| O | 2.220088000 | -1.849330000 | -0.513067000 |
| O | -2.220115000 | -1.849306000 | -0.513207000 |
| N | 1.323988000 | 0.612040000 | -0.860109000 |
| N | -1.324076000 | 0.612059000 | -0.860159000 |
| C | 3.019918000 | -0.881433000 | -0.120621000 |
| C | 4.275622000 | -1.130079000 | 0.507333000 |
| C | 5.043765000 | -0.040519000 | 0.912204000 |
| H | 6.010908000 | -0.224884000 | 1.369957000 |
| C | 4.613879000 | 1.292080000 | 0.775378000 |
| C | 3.386576000 | 1.532061000 | 0.166504000 |
| H | 3.003585000 | 2.541358000 | 0.102537000 |
| C | 2.591068000 | 0.474745000 | -0.316958000 |
| C | 5.498678000 | 2.424949000 | 1.309667000 |
| C | 5.729656000 | 2.235473000 | 2.825441000 |
| H | 4.775619000 | 2.261703000 | 3.362889000 |
| H | 6.375208000 | 3.031593000 | 3.220537000 |
| H | 6.206548000 | 1.272435000 | 3.034104000 |
| C | 4.869654000 | 3.810286000 | 1.091080000 |
| H | 4.705842000 | 4.012106000 | 0.026827000 |
| H | 5.539304000 | 4.584928000 | 1.484741000 |
| H | 3.907409000 | 3.899762000 | 1.606530000 |
| C | 6.864142000 | 2.398161000 | 0.587231000 |
| H | 7.369296000 | 1.438170000 | 0.734726000 |
| H | 7.518910000 | 3.193344000 | 0.968924000 |
| H | 6.728876000 | 2.545422000 | -0.489862000 |

| | | | |
|---|---|---|---|
| C | 4.748557000 | -2.572919000 | 0.722631000 |
| C | 4.845222000 | -3.305030000 | -0.635222000 |
| H | 3.876442000 | -3.301466000 | -1.138334000 |
| H | 5.166763000 | -4.344096000 | -0.480201000 |
| H | 5.580207000 | -2.810322000 | -1.281472000 |
| C | 6.133352000 | -2.638914000 | 1.388892000 |
| H | 6.901551000 | -2.151322000 | 0.777063000 |
| H | 6.419842000 | -3.690055000 | 1.516149000 |
| H | 6.130022000 | -2.168221000 | 2.378967000 |
| C | 3.748561000 | -3.314954000 | 1.638641000 |
| H | 3.703441000 | -2.830496000 | 2.621153000 |
| H | 4.069739000 | -4.355803000 | 1.781693000 |
| H | 2.750547000 | -3.306134000 | 1.196471000 |
| C | 0.721010000 | 1.795089000 | -1.225897000 |
| C | 1.395135000 | 2.937757000 | -1.702277000 |
| H | 2.475687000 | 2.911729000 | -1.782183000 |
| C | 0.699916000 | 4.056080000 | -2.147292000 |
| H | 1.249917000 | 4.913491000 | -2.527750000 |
| C | -0.699905000 | 4.056115000 | -2.147233000 |
| H | -1.249895000 | 4.913575000 | -2.527599000 |
| C | -1.395165000 | 2.937837000 | -1.702175000 |
| H | -2.475726000 | 2.911896000 | -1.782016000 |
| C | -0.721085000 | 1.795090000 | -1.225884000 |
| C | -2.591134000 | 0.474736000 | -0.317014000 |
| C | -3.019944000 | -0.881469000 | -0.120668000 |
| C | -4.275578000 | -1.130152000 | 0.507395000 |
| C | -5.043749000 | -0.040625000 | 0.912299000 |
| H | -6.010849000 | -0.225028000 | 1.370134000 |
| C | -4.613946000 | 1.291986000 | 0.775381000 |
| C | -3.386681000 | 1.532025000 | 0.166443000 |
| H | -3.003740000 | 2.541340000 | 0.102462000 |
| C | -5.498884000 | 2.424819000 | 1.309487000 |
| C | -6.864104000 | 2.397995000 | 0.586568000 |
| H | -6.728457000 | 2.545296000 | -0.490471000 |
| H | -7.519050000 | 3.193128000 | 0.968061000 |
| H | -7.369237000 | 1.437957000 | 0.733856000 |
| C | -5.730384000 | 2.235278000 | 2.825160000 |
| H | -6.207281000 | 1.272208000 | 3.033668000 |
| H | -6.376145000 | 3.031340000 | 3.220023000 |
| H | -4.776548000 | 2.261591000 | 3.362965000 |
| C | -4.869786000 | 3.810173000 | 1.091170000 |
| H | -3.907641000 | 3.899572000 | 1.606822000 |
| H | -5.539508000 | 4.584780000 | 1.484776000 |
| H | -4.705760000 | 4.012120000 | 0.026974000 |
| C | -4.748380000 | -2.573005000 | 0.722830000 |
| C | -3.748205000 | -3.314871000 | 1.638786000 |
| H | -4.069204000 | -4.355771000 | 1.781881000 |
| H | -3.703090000 | -2.830387000 | 2.621283000 |
| H | -2.750225000 | -3.305902000 | 1.196541000 |
| C | -6.133100000 | -2.639043000 | 1.389241000 |
| H | -6.901398000 | -2.151566000 | 0.777445000 |
| H | -6.129708000 | -2.168257000 | 2.379273000 |

| | | | |
|---|---|---|---|
| H | -6.419496000 | -3.690194000 | 1.516623000 |
| C | -4.845107000 | -3.305214000 | -0.634961000 |
| H | -5.166539000 | -4.344297000 | -0.479835000 |
| H | -3.876376000 | -3.301595000 | -1.138169000 |
| H | -5.580197000 | -2.810619000 | -1.281179000 |

Scan-3d-3d'-CBiC-146.453

| | | | |
|---|---|---|---|
| Bi | 0.000063000 | -1.248400000 | -0.957637000 |
| O | 2.239666000 | -1.852891000 | -0.485015000 |
| O | -2.239581000 | -1.852933000 | -0.484866000 |
| N | 1.324511000 | 0.605390000 | -0.814175000 |
| N | -1.324567000 | 0.605363000 | -0.814171000 |
| C | 3.044776000 | -0.881866000 | -0.116295000 |
| C | 4.320436000 | -1.123561000 | 0.474732000 |
| C | 5.090647000 | -0.030457000 | 0.864536000 |
| H | 6.070688000 | -0.209774000 | 1.296195000 |
| C | 4.647402000 | 1.299892000 | 0.746631000 |
| C | 3.403663000 | 1.533490000 | 0.169953000 |
| H | 3.011231000 | 2.540086000 | 0.121294000 |
| C | 2.603928000 | 0.472678000 | -0.298969000 |
| C | 5.537069000 | 2.436358000 | 1.264734000 |
| C | 5.810479000 | 2.239165000 | 2.772407000 |
| H | 4.871178000 | 2.254291000 | 3.335641000 |
| H | 6.460158000 | 3.037985000 | 3.155059000 |
| H | 6.300552000 | 1.278781000 | 2.961888000 |
| C | 4.891427000 | 3.817886000 | 1.072203000 |
| H | 4.698096000 | 4.025469000 | 0.014038000 |
| H | 5.564924000 | 4.595390000 | 1.453439000 |
| H | 3.942373000 | 3.896014000 | 1.613342000 |
| C | 6.882745000 | 2.425195000 | 0.505583000 |
| H | 7.399302000 | 1.468421000 | 0.633207000 |
| H | 7.541260000 | 3.223244000 | 0.874632000 |
| H | 6.717308000 | 2.578055000 | -0.566503000 |
| C | 4.809663000 | -2.563802000 | 0.669561000 |
| C | 4.869960000 | -3.289331000 | -0.693931000 |
| H | 3.886467000 | -3.289640000 | -1.167722000 |
| H | 5.202389000 | -4.327016000 | -0.553377000 |
| H | 5.582214000 | -2.787206000 | -1.359618000 |
| C | 6.214514000 | -2.622789000 | 1.293092000 |
| H | 6.960003000 | -2.125938000 | 0.660952000 |
| H | 6.512690000 | -3.672362000 | 1.405636000 |
| H | 6.237949000 | -2.157636000 | 2.285531000 |
| C | 3.843041000 | -3.316756000 | 1.612145000 |
| H | 3.824471000 | -2.836846000 | 2.597766000 |
| H | 4.175585000 | -4.355933000 | 1.740650000 |
| H | 2.832117000 | -3.312773000 | 1.200298000 |
| C | 0.721163000 | 1.783554000 | -1.191726000 |
| C | 1.395092000 | 2.920729000 | -1.683180000 |
| H | 2.475425000 | 2.893283000 | -1.764288000 |
| C | 0.700076000 | 4.032840000 | -2.142018000 |
| H | 1.249945000 | 4.885051000 | -2.534167000 |
| C | -0.700205000 | 4.032835000 | -2.141984000 |

| | | | |
|---|---|---|---|
| H | -1.250097000 | 4.885051000 | -2.534094000 |
| C | -1.395201000 | 2.920726000 | -1.683114000 |
| H | -2.475537000 | 2.893284000 | -1.764174000 |
| C | -0.721249000 | 1.783536000 | -1.191711000 |
| C | -2.603973000 | 0.472623000 | -0.298986000 |
| C | -3.044741000 | -0.881949000 | -0.116205000 |
| C | -4.320370000 | -1.123671000 | 0.474876000 |
| C | -5.090659000 | -0.030586000 | 0.864577000 |
| H | -6.070686000 | -0.209931000 | 1.296259000 |
| C | -4.647515000 | 1.299781000 | 0.746528000 |
| C | -3.403794000 | 1.533420000 | 0.169819000 |
| H | -3.011453000 | 2.540047000 | 0.121047000 |
| C | -5.537305000 | 2.436233000 | 1.264426000 |
| C | -6.882880000 | 2.424886000 | 0.505092000 |
| H | -6.717311000 | 2.577714000 | -0.566977000 |
| H | -7.541538000 | 3.222874000 | 0.874015000 |
| H | -7.399336000 | 1.468051000 | 0.632692000 |
| C | -5.810901000 | 2.239176000 | 2.772079000 |
| H | -6.300873000 | 1.278750000 | 2.961617000 |
| H | -6.460748000 | 3.037952000 | 3.154537000 |
| H | -4.871687000 | 2.254504000 | 3.335454000 |
| C | -4.891710000 | 3.817778000 | 1.071830000 |
| H | -3.942717000 | 3.896006000 | 1.613061000 |
| H | -5.565291000 | 4.595280000 | 1.452921000 |
| H | -4.698277000 | 4.025276000 | 0.013666000 |
| C | -4.809485000 | -2.563923000 | 0.669871000 |
| C | -3.842767000 | -3.316701000 | 1.612499000 |
| H | -4.175224000 | -4.355890000 | 1.741132000 |
| H | -3.824192000 | -2.836681000 | 2.598066000 |
| H | -2.831861000 | -3.312688000 | 1.200609000 |
| C | -6.214309000 | -2.622932000 | 1.293459000 |
| H | -6.959859000 | -2.126220000 | 0.661280000 |
| H | -6.237746000 | -2.157648000 | 2.285836000 |
| H | -6.512403000 | -3.672512000 | 1.406153000 |
| C | -4.869772000 | -3.289600000 | -0.693541000 |
| H | -5.202115000 | -4.327294000 | -0.552863000 |
| H | -3.886294000 | -3.289882000 | -1.167365000 |
| H | -5.582088000 | -2.787604000 | -1.359261000 |

Scan-3d-3d'-CBiC-148.953

| | | | |
|---|---|---|---|
| Bi | -0.000238000 | -1.256259000 | -0.878717000 |
| O | 2.256688000 | -1.856128000 | -0.457157000 |
| O | -2.257009000 | -1.856063000 | -0.457933000 |
| N | 1.325248000 | 0.600500000 | -0.768210000 |
| N | -1.325115000 | 0.600551000 | -0.768351000 |
| C | 3.067435000 | -0.882527000 | -0.112853000 |
| C | 4.361671000 | -1.118475000 | 0.440617000 |
| C | 5.134766000 | -0.022705000 | 0.815687000 |
| H | 6.126589000 | -0.198030000 | 1.221398000 |
| C | 4.680300000 | 1.305709000 | 0.717212000 |
| C | 3.421221000 | 1.534184000 | 0.173102000 |
| H | 3.020954000 | 2.538411000 | 0.140182000 |

| | | | |
|---|---|---|---|
| C | 2.616344000 | 0.470852000 | -0.281242000 |
| C | 5.575109000 | 2.444609000 | 1.220608000 |
| C | 5.884692000 | 2.240903000 | 2.720420000 |
| H | 4.958700000 | 2.247741000 | 3.305443000 |
| H | 6.538749000 | 3.041243000 | 3.092275000 |
| H | 6.384269000 | 1.282224000 | 2.893061000 |
| C | 4.917175000 | 3.823257000 | 1.050484000 |
| H | 4.697719000 | 4.035004000 | -0.001745000 |
| H | 5.594949000 | 4.602806000 | 1.419754000 |
| H | 3.980747000 | 3.893079000 | 1.614286000 |
| C | 6.902872000 | 2.445490000 | 0.430446000 |
| H | 7.427934000 | 1.491200000 | 0.540791000 |
| H | 7.565064000 | 3.245442000 | 0.788599000 |
| H | 6.711829000 | 2.603123000 | -0.636677000 |
| C | 4.864725000 | -2.556539000 | 0.614733000 |
| C | 4.887664000 | -3.275895000 | -0.753171000 |
| H | 3.890355000 | -3.279051000 | -1.197244000 |
| H | 5.229260000 | -4.312468000 | -0.627248000 |
| H | 5.577196000 | -2.767317000 | -1.437619000 |
| C | 6.288172000 | -2.609800000 | 1.195130000 |
| H | 7.010989000 | -2.104790000 | 0.543412000 |
| H | 6.596244000 | -3.657993000 | 1.292899000 |
| H | 6.338879000 | -2.149831000 | 2.188980000 |
| C | 3.931424000 | -3.319131000 | 1.582860000 |
| H | 3.940001000 | -2.843533000 | 2.570732000 |
| H | 4.273734000 | -4.356860000 | 1.696631000 |
| H | 2.908517000 | -3.319170000 | 1.201732000 |
| C | 0.721515000 | 1.774085000 | -1.156511000 |
| C | 1.395220000 | 2.906004000 | -1.662041000 |
| H | 2.475315000 | 2.877240000 | -1.744432000 |
| C | 0.700441000 | 4.012286000 | -2.133445000 |
| H | 1.250277000 | 4.859486000 | -2.536357000 |
| C | -0.700249000 | 4.012370000 | -2.133307000 |
| H | -1.250077000 | 4.859650000 | -2.536058000 |
| C | -1.395028000 | 2.906126000 | -1.661799000 |
| H | -2.475147000 | 2.877424000 | -1.743918000 |
| C | -0.721293000 | 1.774157000 | -1.156467000 |
| C | -2.616229000 | 0.470936000 | -0.281229000 |
| C | -3.067570000 | -0.882331000 | -0.113274000 |
| C | -4.361809000 | -1.118178000 | 0.440191000 |
| C | -5.134604000 | -0.022357000 | 0.815741000 |
| H | -6.126425000 | -0.197583000 | 1.221490000 |
| C | -4.679804000 | 1.305991000 | 0.717781000 |
| C | -3.420731000 | 1.534334000 | 0.173603000 |
| H | -3.020130000 | 2.538445000 | 0.140972000 |
| C | -5.574327000 | 2.444953000 | 1.221594000 |
| C | -6.902032000 | 2.446534000 | 0.431316000 |
| H | -6.710850000 | 2.604398000 | -0.635747000 |
| H | -7.563989000 | 3.246605000 | 0.789635000 |
| H | -7.427404000 | 1.492382000 | 0.541360000 |
| C | -5.884093000 | 2.240861000 | 2.721309000 |
| H | -6.384157000 | 1.282375000 | 2.893584000 |

| | | | |
|---|---|---|---|
| H | -6.537786000 | 3.041387000 | 3.093409000 |
| H | -4.958143000 | 2.247037000 | 3.306407000 |
| C | -4.915975000 | 3.823462000 | 1.052022000 |
| H | -3.979595000 | 3.892799000 | 1.615960000 |
| H | -5.593564000 | 4.603086000 | 1.421474000 |
| H | -4.696326000 | 4.035486000 | -0.000109000 |
| C | -4.865179000 | -2.556185000 | 0.613845000 |
| C | -3.932026000 | -3.319275000 | 1.581723000 |
| H | -4.274515000 | -4.356987000 | 1.695126000 |
| H | -3.940539000 | -2.844017000 | 2.569756000 |
| H | -2.909111000 | -3.319358000 | 1.200623000 |
| C | -6.288630000 | -2.609305000 | 1.194250000 |
| H | -7.011324000 | -2.103880000 | 0.542719000 |
| H | -6.339219000 | -2.149684000 | 2.188268000 |
| H | -6.596953000 | -3.657457000 | 1.291646000 |
| C | -4.888292000 | -3.275102000 | -0.754282000 |
| H | -5.230034000 | -4.311663000 | -0.628655000 |
| H | -3.891015000 | -3.278275000 | -1.198422000 |
| H | -5.577791000 | -2.766215000 | -1.438530000 |

Scan-3d-3d'-CBiC-151.453

| | | | |
|---|---|---|---|
| Bi | -0.000010000 | -1.261441000 | -0.798892000 |
| O | 2.271611000 | -1.858363000 | -0.430331000 |
| O | -2.271608000 | -1.858479000 | -0.430291000 |
| N | 1.325954000 | 0.597550000 | -0.721604000 |
| N | -1.325825000 | 0.597514000 | -0.721379000 |
| C | 3.088253000 | -0.882765000 | -0.110517000 |
| C | 4.399872000 | -1.114053000 | 0.404389000 |
| C | 5.176252000 | -0.016360000 | 0.765614000 |
| H | 6.178965000 | -0.188489000 | 1.145173000 |
| C | 4.712036000 | 1.310316000 | 0.687984000 |
| C | 3.438565000 | 1.534713000 | 0.177144000 |
| H | 3.031632000 | 2.536753000 | 0.160801000 |
| C | 2.628077000 | 0.469699000 | -0.263148000 |
| C | 5.612188000 | 2.450720000 | 1.178082000 |
| C | 5.955085000 | 2.239985000 | 2.669688000 |
| H | 5.042007000 | 2.239609000 | 3.274716000 |
| H | 6.613824000 | 3.040898000 | 3.031932000 |
| H | 6.462106000 | 1.282364000 | 2.825746000 |
| C | 4.944304000 | 3.827017000 | 1.029764000 |
| H | 4.700389000 | 4.042883000 | -0.016223000 |
| H | 5.626478000 | 4.607948000 | 1.387810000 |
| H | 4.020412000 | 3.889643000 | 1.614709000 |
| C | 6.922689000 | 2.462447000 | 0.359630000 |
| H | 7.454664000 | 1.510196000 | 0.453177000 |
| H | 7.588583000 | 3.263552000 | 0.708168000 |
| H | 6.708148000 | 2.625189000 | -0.702247000 |
| C | 4.915240000 | -2.550221000 | 0.556263000 |
| C | 4.900106000 | -3.262674000 | -0.815389000 |
| H | 3.889753000 | -3.268651000 | -1.228922000 |
| H | 5.250482000 | -4.298092000 | -0.705109000 |
| H | 5.566075000 | -2.747228000 | -1.517781000 |

| | | | |
|---|---|---|---|
| C | 6.355978000 | -2.598740000 | 1.092695000 |
| H | 7.055666000 | -2.085568000 | 0.422361000 |
| H | 6.672856000 | -3.645670000 | 1.174607000 |
| H | 6.434584000 | -2.144606000 | 2.087432000 |
| C | 4.015861000 | -3.322603000 | 1.548481000 |
| H | 4.051434000 | -2.851346000 | 2.537848000 |
| H | 4.367446000 | -4.358790000 | 1.647091000 |
| H | 2.982032000 | -3.326805000 | 1.198132000 |
| C | 0.721582000 | 1.766718000 | -1.119751000 |
| C | 1.395016000 | 2.893480000 | -1.638614000 |
| H | 2.474865000 | 2.863483000 | -1.722251000 |
| C | 0.700416000 | 3.994110000 | -2.121810000 |
| H | 1.250090000 | 4.836570000 | -2.534758000 |
| C | -0.700658000 | 3.994079000 | -2.121703000 |
| H | -1.250433000 | 4.836503000 | -2.534590000 |
| C | -1.395133000 | 2.893422000 | -1.638389000 |
| H | -2.474997000 | 2.863377000 | -1.721846000 |
| C | -0.721562000 | 1.766708000 | -1.119613000 |
| C | -2.627992000 | 0.469620000 | -0.262959000 |
| C | -3.088185000 | -0.882812000 | -0.110459000 |
| C | -4.399869000 | -1.114068000 | 0.404301000 |
| C | -5.176221000 | -0.016400000 | 0.765624000 |
| H | -6.178965000 | -0.188562000 | 1.145094000 |
| C | -4.711954000 | 1.310278000 | 0.688186000 |
| C | -3.438451000 | 1.534638000 | 0.177399000 |
| H | -3.031437000 | 2.536642000 | 0.161158000 |
| C | -5.612111000 | 2.450698000 | 1.178324000 |
| C | -6.922380000 | 2.462795000 | 0.359489000 |
| H | -6.707466000 | 2.625458000 | -0.702323000 |
| H | -7.588158000 | 3.264092000 | 0.707815000 |
| H | -7.454628000 | 1.510689000 | 0.452901000 |
| C | -5.955477000 | 2.239756000 | 2.669785000 |
| H | -6.462908000 | 1.282302000 | 2.825499000 |
| H | -6.614000000 | 3.040836000 | 3.032058000 |
| H | -5.042559000 | 2.238884000 | 3.275057000 |
| C | -4.944062000 | 3.826954000 | 1.030521000 |
| H | -4.020305000 | 3.889317000 | 1.615708000 |
| H | -5.626231000 | 4.607877000 | 1.388605000 |
| H | -4.699876000 | 4.043067000 | -0.015348000 |
| C | -4.915293000 | -2.550200000 | 0.555965000 |
| C | -4.016014000 | -3.322724000 | 1.548158000 |
| H | -4.367492000 | -4.358980000 | 1.646419000 |
| H | -4.051848000 | -2.851734000 | 2.537642000 |
| H | -2.982107000 | -3.326687000 | 1.198033000 |
| C | -6.356089000 | -2.598643000 | 1.092274000 |
| H | -7.055677000 | -2.085317000 | 0.421953000 |
| H | -6.434746000 | -2.144638000 | 2.087069000 |
| H | -6.673061000 | -3.645555000 | 1.174008000 |
| C | -4.900023000 | -3.262451000 | -0.815794000 |
| H | -5.250247000 | -4.297934000 | -0.705668000 |
| H | -3.889663000 | -3.268220000 | -1.229326000 |
| H | -5.566062000 | -2.747001000 | -1.518115000 |

**TS-3d-3d'**

| | | | |
|---|---|---|---|
| Bi | 0.000000000 | -0.884925000 | -1.784087000 |
| O | 1.837380000 | -1.738204000 | -0.795933000 |
| O | -1.837383000 | -1.738202000 | -0.795936000 |
| N | 1.328608000 | 0.837532000 | -1.206121000 |
| N | -1.328608000 | 0.837533000 | -1.206122000 |
| C | 2.646041000 | -0.859525000 | -0.188470000 |
| C | 3.673576000 | -1.281839000 | 0.688056000 |
| C | 4.485163000 | -0.306727000 | 1.278763000 |
| H | 5.297631000 | -0.625280000 | 1.923916000 |
| C | 4.284124000 | 1.065815000 | 1.081447000 |
| C | 3.248628000 | 1.472544000 | 0.239990000 |
| H | 3.039626000 | 2.525177000 | 0.110590000 |
| C | 2.430868000 | 0.536756000 | -0.416123000 |
| C | 5.194288000 | 2.071405000 | 1.798917000 |
| C | 5.077844000 | 1.878500000 | 3.327207000 |
| H | 4.047026000 | 2.049332000 | 3.655585000 |
| H | 5.734743000 | 2.581777000 | 3.857164000 |
| H | 5.358627000 | 0.861049000 | 3.617575000 |
| C | 4.829355000 | 3.528379000 | 1.471744000 |
| H | 4.921120000 | 3.731686000 | 0.399034000 |
| H | 5.507072000 | 4.206312000 | 2.005426000 |
| H | 3.804064000 | 3.763414000 | 1.776633000 |
| C | 6.661137000 | 1.837449000 | 1.374401000 |
| H | 6.982681000 | 0.818909000 | 1.614404000 |
| H | 7.329940000 | 2.540075000 | 1.890253000 |
| H | 6.773162000 | 1.979660000 | 0.293886000 |
| C | 3.876310000 | -2.775871000 | 0.975879000 |
| C | 4.184434000 | -3.534905000 | -0.334538000 |
| H | 3.370168000 | -3.407704000 | -1.050347000 |
| H | 4.315867000 | -4.605789000 | -0.126993000 |
| H | 5.110111000 | -3.155408000 | -0.783773000 |
| C | 5.045019000 | -3.027972000 | 1.944302000 |
| H | 5.996700000 | -2.669384000 | 1.534582000 |
| H | 5.137840000 | -4.106845000 | 2.119456000 |
| H | 4.880653000 | -2.541902000 | 2.912837000 |
| C | 2.598100000 | -3.356196000 | 1.623847000 |
| H | 2.397853000 | -2.856497000 | 2.578641000 |
| H | 2.727767000 | -4.429866000 | 1.816940000 |
| H | 1.736507000 | -3.214513000 | 0.968845000 |
| C | 0.720450000 | 2.079562000 | -1.342006000 |
| C | 1.394285000 | 3.291198000 | -1.559457000 |
| H | 2.476830000 | 3.287016000 | -1.624696000 |
| C | 0.697038000 | 4.486193000 | -1.750162000 |
| H | 1.248630000 | 5.407335000 | -1.922802000 |
| C | -0.697037000 | 4.486193000 | -1.750163000 |
| H | -1.248628000 | 5.407336000 | -1.922804000 |
| C | -1.394284000 | 3.291198000 | -1.559459000 |
| H | -2.476829000 | 3.287016000 | -1.624699000 |
| C | -0.720450000 | 2.079563000 | -1.342007000 |
| C | -2.430868000 | 0.536757000 | -0.416124000 |

| | | | |
|---|---|---|---|
| C | -2.646043000 | -0.859523000 | -0.188472000 |
| C | -3.673578000 | -1.281837000 | 0.688054000 |
| C | -4.485163000 | -0.306724000 | 1.278763000 |
| H | -5.297631000 | -0.625276000 | 1.923916000 |
| C | -4.284123000 | 1.065818000 | 1.081448000 |
| C | -3.248626000 | 1.472546000 | 0.239990000 |
| H | -3.039622000 | 2.525178000 | 0.110592000 |
| C | -5.194283000 | 2.071408000 | 1.798921000 |
| C | -6.661134000 | 1.837453000 | 1.374412000 |
| H | -6.773163000 | 1.979664000 | 0.293897000 |
| H | -7.329933000 | 2.540080000 | 1.890267000 |
| H | -6.982677000 | 0.818914000 | 1.614417000 |
| C | -5.077832000 | 1.878503000 | 3.327211000 |
| H | -5.358614000 | 0.861052000 | 3.617580000 |
| H | -5.734728000 | 2.581781000 | 3.857171000 |
| H | -4.047013000 | 2.049335000 | 3.655584000 |
| C | -4.829350000 | 3.528382000 | 1.471747000 |
| H | -3.804057000 | 3.763417000 | 1.776632000 |
| H | -5.507064000 | 4.206316000 | 2.005431000 |
| H | -4.921119000 | 3.731689000 | 0.399037000 |
| C | -3.876315000 | -2.775869000 | 0.975875000 |
| C | -2.598105000 | -3.356197000 | 1.623842000 |
| H | -2.727774000 | -4.429867000 | 1.816934000 |
| H | -2.397857000 | -2.856499000 | 2.578637000 |
| H | -1.736512000 | -3.214515000 | 0.968840000 |
| C | -5.045023000 | -3.027970000 | 1.944298000 |
| H | -5.996704000 | -2.669379000 | 1.534579000 |
| H | -4.880657000 | -2.541901000 | 2.912833000 |
| H | -5.137847000 | -4.106842000 | 2.119451000 |
| C | -4.184441000 | -3.534901000 | -0.334542000 |
| H | -4.315875000 | -4.605785000 | -0.126999000 |
| H | -3.370174000 | -3.407701000 | -1.050351000 |
| H | -5.110116000 | -3.155402000 | -0.783777000 |

## References


1 P. Chaudhuri, M. Hess, J. Müller, K. Hildenbrand, E. Bill, T. Weyhermüller and K. Wieghardt, *J. Am. Chem. Soc.*, 1999, **121**, 9599.

2 C. J. Carmalt, N. A. Compton, R. J. Errington, G. A. Fisher, I. Moenandar, N. C. Norman and K. H. Whitmire, in *Inorganic Syntheses*, ed. A. H. Cowley, Wiley, 1996, vol. 31, pp. 98–101.

3 S. B. H. Karnbrock, C. Golz, R. A. Mata and M. Alcarazo, *Angew. Chem. Int. Ed.*, 2022, **61**, e202207450.

4 S. B. H. Karnbrock, J. F. Köster, C. Golz, R. A. Mata and M. Alcarazo, *Angew. Chem. Int. Ed.*, 2025, e202501439.

5 R. B. King, F. G. A. Stone, W. L. Jolly, G. Austin, W. Covey, D. Rabinovich, H. Steinberg and R. Tsugawa, in *Inorganic syntheses*, ed. J. Kleinberg and L. F. Audrieth, McGraw Hill, New York, 1963, pp. 99–115.

6 D. L. Reger and C. Coleman, *J. Organomet. Chem.*, 1977, **131**, 153.

7 G. M. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112.

8 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339.

9 D. Kratzert, FinalCif (V96), Kratzert, D.

10 a) S. K. Chopra and J. C. Martin, *Heteroat. Chem.*, 1991, **2**, 71; b) Y. Yamamoto, K. Toyota, Y. Wakisaka and K. Akiba, *Heteroat. Chem.*, 2000, **11**, 42; c) Y. Yamamoto, M. Okazaki, Y. Wakisaka and K. Akiba, *Organometallics*, 1995, **14**, 3364; d) H. Nakazawa, K. Kubo and K. Miyoshi, *J. Am. Chem. Soc.*, 1993, **115**, 5863; e) J. Ramler, F. Geist, C. Mihm, L. Lubczyk, S. Reith, C. Herok, F. Fantuzzi and C. Lichtenberg, *Chem. Eur. J.*, 2025, **31**, e202403253; f) H. Schumann and L. Eguren, *J. Organomet. Chem.*, 1991, **403**, 183; g) I. Vránová, V. Kremláček, M. Erben, J. Turek, R. Jambor, A. Růžička, M. Alonso and L. Dostál, *Dalton Trans.*, 2017, **46**, 3556; h) M. Wieber, D. Wirth and C. Burschka, *Z. Naturforsch. B*, 1985, **40**, 258;

11 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16 Rev. A.03, Wallingford, CT, 2016.

12 J. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett.*, 2003, **91**, 146401.

13 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.

14 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158.

15 G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2010, **132**, 114110.

16 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456.

17 R. F. W. Bader, *Atoms in molecules. A quantum theory*, Clarendon Press, Oxford, 2003, vol. 22.

18 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580.

19 E. Ramos-Cordoba, P. Salvador and I. Mayer, *J. Chem. Phys.*, 2013, **138**, 214107.

20 E. Ramos-Cordoba, V. Postils and P. Salvador, *J. Chem. Theory Comput.*, 2015, **11**, 1501.

21 P. Salvador, E. Ramos-Cordoba, M. Montilla, L. Pujal and M. Gimferrer, *J. Chem. Phys.*, 2024, **160**, 172502.
22 P. Salvador and E. Ramos-Cordoba, *J. Chem. Phys.*, 2013, **139**, 71103.
23 T. J. Hannah, T. Z. Kirsch and S. S. Chitnis, *Chem. Eur. J.*, 2024, **30**.