Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Unexpected Structural Differences between the Phosphorus and Arsenic Derivatives $[(Cp^{BIG}Fe)_2(\mu,\eta^{4:4}\text{-}E_4)]$ (E = P, As)

S. Heinl,[a] A. Y. Timoshkin,[b] J. Müller[a] and M. Scheer[a]

a) Institute of Inorganic Chemistry, University of Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany. E-mail: manfred.scheer@ur.de

b) Institute of Chemistry, St. Petersburg State University, Universitetskii pr. 26, Old Peterhoff, 198504 St. Petersburg, Russia.

1. Experimental Details

1.1 General Remarks:

All experiments were carried out under an atmosphere of dry argon or nitrogen using glovebox and schlenk techniques. Toluene, hexane, 1,3-diisopropylbenzene, *o*-xylene and C_6D_6 were refluxed and distilled over potassium and degassed prior to use. The same procedure was applied for CD_2Cl_2 and CH_3CN but with the use of CaH_2 as drying reagent instead of potassium. P_4 was available and sublimed before use. $[Cp^{BIG}Fe(CO)_2]_2$,[**Fehler! Textmarke nicht definiert.**] $[\{Cp^{BIG}Fe(CO)_2\}_2(\mu,\eta^{1:1}\text{-}P_4)]$, $[\{Cp^{BIG}Fe(CO)_2\}_2(\mu,\eta^{1:1}\text{-}As_4)]$[**Fehler! Textmarke nicht definiert.**] and As_4 solutions[1] were prepared according to literature procedures. The NMR spectra were measured on a Bruker Avance 300, 400 or 600 spectrometer. FD-MS spectra were measured on a Finnigan MAT 95 mass spectrometer. The elemental analyses were determined on a Vario EL III apparatus. The IR spectra were measured on a VARIAN FTS-800 FT-IR spectrometer. For irradiations a TQ150-Z1 Hg lamp from Heraeus was used.

1.2 Synthesis of $[(Cp^{BIG}Fe)_2(\mu,\eta^{4:4}\text{-}P_4)]$ (2a) by UV irradiation:

A solution of **1a** (200 mg, 110 µmol) in 50 mL toluene is irradiated for 30 min. The red solution is dried in vacuum. The residue is dissolved in CH_2Cl_2 and layered with CH_3CN. Complex **2a** is obtained as red crystals after complete diffusion (110 mg, 59%). For analytical data of **2b** see reference **Fehler! Textmarke nicht definiert.**. In one experiment a second very small fraction of crystals of **3** were obtained (yield < 1%).

Analytical Data for **3**:
IR (toluene): ν_{CO} [cm^{-1}] = 2024 (s), 1984 (s).
FD-MS (toluene): *m/z* (%) = 1744.5 (100%, $[M]^+$), 1688.6 (35%, $[M - 2CO]^+$).
$^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ [ppm] = 29.9 (td, $1P^X$), 104.5 (dd, $2P^M$), 173.6 (td, $1P^A$);
$^1J(P^AP^M)$ = 306 Hz, $^2J(P^AP^X)$ = 116 Hz, $^1J(P^MP^X)$ = 349 Hz.

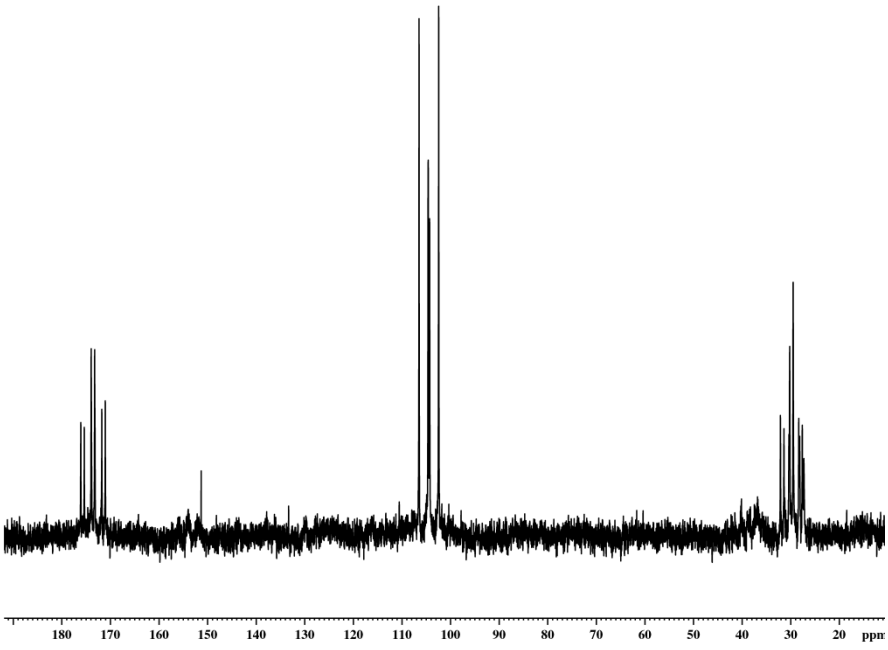

Figure S1. $^{31}P\{^1H\}$ NMR of $[\{Cp^{BIG}Fe\}\{Cp^{BIG}Fe(CO)_2\}(\mu,\eta^{4:1}\text{-}P_4)]$ (**3**) in C_6D_6 at 298 K.

1.3 Synthesis of $[(Cp^{BIG}Fe)_2(\mu,\eta^{4:4}\text{-}As_4)]$ (2b), $[(Cp^{BIG}Fe)_3(\mu^3,\eta^{4:4:4}\text{-}As_6)]$ (4) and $[Cp^{BIG}Fe(\eta^5\text{-}As_5)]$ (5) by thermolysis:

To a freshly prepared solution of As_4 (from ~5 g As_{grey}) in 250 mL 1,3-diisopropylbenzene (DIB) or *o*-xylene a solution of $[Cp^{BIG}Fe(CO)_2]_2$ (500 mg, 149 µmol) in 10 mL DIB is added. An immediate change of color to orange is observed. The mixture is refluxed for 16 h. The brown solution is dried in vacuum. The residue is separated by column chromatography (20x3 cm, silica, hexane/toluene 5:1). The first band yields brown **5** followed by a broad band of a mixture of **2b** and **4**. Once it was possible to obtain an almost clean sample of **4** by fractionalizing the second band into several pieces. The compounds can be crystallized by diffusion of CH_3CN into CH_2Cl_2 solutions. Yield of **5**: 34 mg (6%). (Best yield from 50 mg $[Cp^{BIG}Fe(CO)_2]_2$: 20 mg (34%)). Yield of mixture of **2b** and **4**: 345 mg.

Analytical Data for **2b**:
Elemental analysis: $[C_{110}H_{130}Fe_2As_4]*1/4CH_2Cl_2$ (solvent molecules were found in the crystal structure) calc.: C, 70.26; H, 7.03. Found: C, 69.59; H, 7.04.
FD-MS (toluene): *m/z* (%) = 1937.6 (30%, $[Cp^{BIG}{}_2Fe_2As_5]^+$), 1862.8 (100%, $[M]^+$), 1788.1 (20%, $[Cp^{BIG}{}_2Fe_2As_3]^+$), 725.7 (10%, $[Cp^{BIG}]^+$).
^{1}H NMR (CD_2Cl_2): δ [ppm] = 0.92 (t, $^3J_{HH}$ = 7.3 Hz, 30H, ^{n}Bu), 1.33 (m, 20H, ^{n}Bu), 1.56 (m, 20H, ^{n}Bu), 2.52 (t, $^3J_{HH}$ = 7.7 Hz, 20H, ^{n}Bu), 6.44 (d, $^3J_{HH}$ = 8.4 Hz, 1H, Ph), 6.53 (d, $^3J_{HH}$ = 7.7 Hz, 1H, Ph), 6.64 (d, $^3J_{HH}$ = 7.7 Hz, 1H, Ph), 6.81 (d, $^3J_{HH}$ = 8.1 Hz, 20H, Ph), 7.22 (d, $^3J_{HH}$ = 8.1 Hz, 20H, Ph).
$^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ [ppm] = 14.1 (^{n}Bu), 22.7 (^{n}Bu), 33.6 (^{n}Bu), 35.6 (^{n}Bu), 88.8 (Cp), 127.3 (Ph), 132.8 (Ph), 133.8 (Ph), 141.5 (Ph).

Analytical Data for **4**:
FD-MS (toluene): *m/z* (%) = 2793.9 (100%, $[M]^+$), 726.9 (10%, $[Cp^{BIG}H]^+$).
IR (toluene, cm^{-1}): ν_{CO} 2020 (s), 1980 (s).
^{1}H NMR (C_6D_6): δ [ppm] = 0.74 (m, 45H, ^{n}Bu), 1.09 (m, 30H, ^{n}Bu), 1.22 (m, 30H, ^{n}Bu), 1.65 (m, 30H, ^{n}Bu), 5.71 (s, 30H, Ph), 7.74 (br-s, $\omega_{1/2}$ = 39 Hz, 1H, Ph).
$^{13}C\{^1H\}$ NMR (C_6D_6): δ [ppm] = 12.7 (^{n}Bu), 21.3 (^{n}Bu), 30.2 (^{n}Bu), 35.5 (^{n}Bu), 120.7 (Ph), 129.2 (Ph), 133.4 (Ph), 143.0 (Ph). (Cp signal is not observed).

Analytical Data for **5**:
Elemental analysis: $[C_{55}H_{65}FeAs_5]$ calc.: C, 57.62; H, 4.84. Found: C, 56.89; H, 5.58.
FD-MS (toluene): *m/z* (%) = 1156.3 (100%, $[M]^+$); different settings: 726.7 (20%, $[Cp^{BIG}H]^+$), 299.9 (100%, $[As_4]^+$).
^{1}H NMR (CD_2Cl_2): δ [ppm] = 0.85 (m-br, 15H, ^{n}Bu), 1.21 (m-br, 10H, ^{n}Bu), 1.42 (m-br, 10H, ^{n}Bu), 2.35 (m-br, 10H, ^{n}Bu), 6.81 (d, $^3J_{HH}$ = 8.3 Hz, 10H, Ph), 7.40 (s-br, 10H, Ph).
$^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ [ppm] = 14.1 (^{n}Bu), 22.6 (^{n}Bu), 33.1 (^{n}Bu), 35.5 (^{n}Bu), 89.8 (Cp), 127.4 (Ph), 130.5 (Ph), 134.7 (Ph), 142.2 (Ph).

1.4 Synthesis of $[(Cp^{BIG}Fe)_2(\mu,\eta^{4:4}\text{-}As_4)]$ (2b) by UV irradiation:

A solution of **1b** (210 mg, 110 µmol) in 50 mL toluene is irradiated for 30 min. The brown solution is dried in vacuum. The residue is dissolved in CH_2Cl_2 and CH_3CN is layered above. Complex **2b** is obtained as brown crystals after complete diffusion (110 mg, 54%).

2. Crystallographic Details:

The crystal structure analyses were performed either on an Oxford Diffraction Gemini R Ultra CCD diffractometer (**3**, **4**) or an Oxford Diffraction SuperNova diffractometer (**2b**, **5**). For compound **2b** a Gaussian absorption correction was carried out. For compounds **3**, **4** and **5** an analytical absorption correction was carried out.[2] The structures were solved by direct methods either of the program SIR-92[3] or SUPERFLIP[4] and refined with the least square method on F^2 employing SHELXL-2014[5] (Sheldrick, 2015) with anisotropic displacements for non-H atoms. Hydrogen atoms were located in idealized positions and refined isotropically according to the riding model.

CIF files with comprehensive information on the details of the diffraction experiments and full tables of bond lengths and angles for **2b**, **3**, **4** and **5** are deposited in Cambridge Crystallographic Data Centre under the deposition codes CCDC-1811900 (**2b**), CCDC-1811898 (**3**), CCDC-1811901 (**4**), and CCDC-1811899 (**5**).

	Crystal Data for **2b***0.15 CH_2Cl_2	Crystal Data for **3**
Empirical Formula	$C_{110.15}H_{130.30}As_4Cl_{0.30}Fe_2$	$C_{112}H_{130}Fe_2O_2P_4$
Formula Weight	1876.25	1743.74
Temperature [K]	123.0(1)	123.0(3)
Crystal System	orthorhombic	triclinic
Space Group	*Pbca*	$P\bar{1}$
a [Å]	26.8253(5)	12.4226(3)
b [Å]	24.5770(5)	13.5015(2)
c [Å]	28.7258(5)	16.1699(3)
α [°]	90	106.698(2)
β [°]	90	103.359(2)
γ [°]	90	101.267(2)
Volume [Å^3]	18938.5(6)	2425.67(10)
Z	8	1
ρ_{calc} [mg/mm^3]	1.316	1.194
μ [mm^{-1}]	4.44	3.392
F(000)	7842	930.0
Crystal Size [mm^3]	0.4514 × 0.2874 × 0.2159	0.3415 × 0.2184 × 0.1325
Radiation	Cu-K_α (λ = 1.54178)	Cu-K_α (λ = 1.54178)
2Θ Range	5.76 to 147.56°	7.12 to 133.28°

Index Ranges	$-19 \leq h \leq 32$	$-14 \leq h \leq 14$
	$-28 \leq k \leq 29$	$-15 \leq k \leq 15$
	$-34 \leq l \leq 33$	$-16 \leq l \leq 19$
Reflections Collected	55070	19295
Independent Reflections	18522	8313
	[R_{int} = 0.026, R_{sigma} = 0.0216]	[R_{int} = 0.0185, R_{sigma} = 0.0270]
Data/Restraints/Parameters	18522/15/1207	8313/36/667
Goodness-of-Fit on F^2	1.06	1.072
Final R Indexes [I > 2σ(I)]	R_1 = 0.0589, wR_2 = 0.1751	R_1 = 0.0332, wR_2 = 0.0907
Final R Indexes [All Data]	R_1 = 0.0783, wR_2 = 0.1912	R_1 = 0.0366, wR_2 = 0.0920
Largest Diff. Peak/Hole [e·Å^{-3}]	0.73/-1.01	0.43/-0.23
Flack Parameter	-	-

	Crystal Data for **4***1/2CH_3CN	Crystal Data for **5**
Empirical Formula	$C_{165}H_{195}As_6Fe_3 \cdot (CH_3CN)_{0.50}$	$C_{55}H_{65}As_5Fe$
Formula Weight	2815.80	1156.52
Temperature [K]	122.9(5)	123.00(10)
Crystal System	triclinic	triclinic
Space Group	$P\bar{1}$	$P\bar{1}$
a [Å]	17.9595(4)	13.4626(4)
b [Å]	20.6577(5)	13.7448(3)
c [Å]	23.1771(3)	16.0091(4)
α [°]	98.920(1)	92.777(2)
β [°]	106.184(1)	114.468(3)
γ [°]	114.40(2)	107.131(2)
Volume [Å^3]	7152.4(3)	2526.71(14)
Z	2	2
ρ_{calc} [mg/mm^3]	1.307	1.520

μ [mm^{-1}]	4.331	6.288
F(000)	2944.0	1172.0
Crystal Size [mm^3]	0.4236 × 0.1792 × 0.0551	0.5106 × 0.3445 × 0.1791
Radiation	Cu-K_α (λ = 1.54178)	Cu-K_α (λ = 1.54178)
2Θ Range	5.84 to 133.3°	6.86 to 141.8°
Index Ranges	-20 ≤ h ≤ 21	-15 ≤ h ≤ 14
	-24 ≤ k ≤ 24	-16 ≤ k ≤ 16
	-27 ≤ l ≤ 27	-19 ≤ l ≤ 19
Reflections Collected	63365	34862
Independent Reflections	24535	9516
	[R_{int} = 0.0334, R_{sigma} = 0.0384]	[R_{int} = 0.0259, R_{sigma} = 0.0156]
Data/Restraints/Parameters	24528/324/1741	9516/0/550
Goodness-of-Fit on F^2	1.000	1.078
Final R Indexes [I > 2σ(I)]	R_1 = 0.061, wR_2 = 0.183	R_1 = 0.0292, wR_2 = 0.0786
Final R Indexes [All Data]	R_1 = 0.0776, wR_2 = 0.1995	R_1 = 0.0294, wR_2 = 0.0788
Largest Diff. Peak/Hole [e·Å^{-3}]	1.63/-0.72	1.03/-0.61
Flack Parameter	-	-

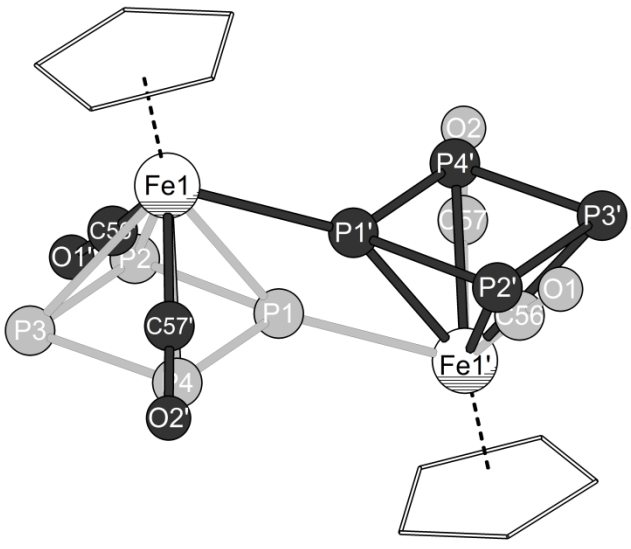

Figure S 2: Disordered central structure of **3** in the crystal. Different parts are colored differently.

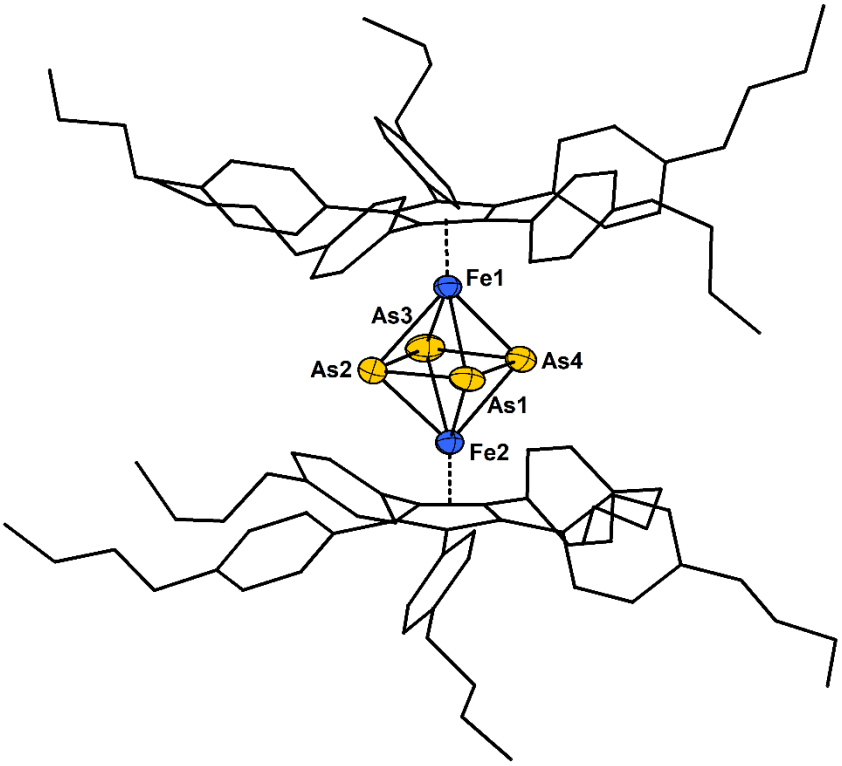

Figure S3: Molecular structure of **2b** in the crystal with selected labels. Ellipsoids are drawn at 50% probability level. For disordered positions only the main part is shown. For clarity reasons the Cp^{BIG} ligands are drawn in 'wire-or-stick' model and solvent molecules are omitted. Selected bond lengths [Å] and angles [°]: As1-As2 2.4331(6), As2-As3 2.3909(7), As3-As4 2.4201(7), As1-As4 2.4558(7), Fe1-As1 2.4144(7), Fs1-As2 2.5012(7), Fe1-As3 2.4902(8), Fe1-As4 2.4619(8), Fe2-As1 2.4432(7), Fe2-As2 2.4631(7), Fe2-As3 2.5130(7), Fe2-As4 2.4388(7), Fe1···Fe2 3.5414(7), As2-As1-As4 89.08(2), As1-As2-As3 90.58(2), As2-As3-As4 90.92(2), As1-As4-As3 89.35(2), Fe1-As1-Fe2 93.61(3), Fe1-As2-Fe2 91.02(3), Fe1-As3-Fe2 90.11(3), Fe1-As4-Fe2 92.54(3), Cp_{plane}(Fe1)-$As_{4,plane}$ 0.6(1), Cp_{plane}(Fe2)-$As_{4,plane}$ 2.5(1), Cpp_{lane}(Fe1)-Cp_{plane}(Fe2) 1.9(2).

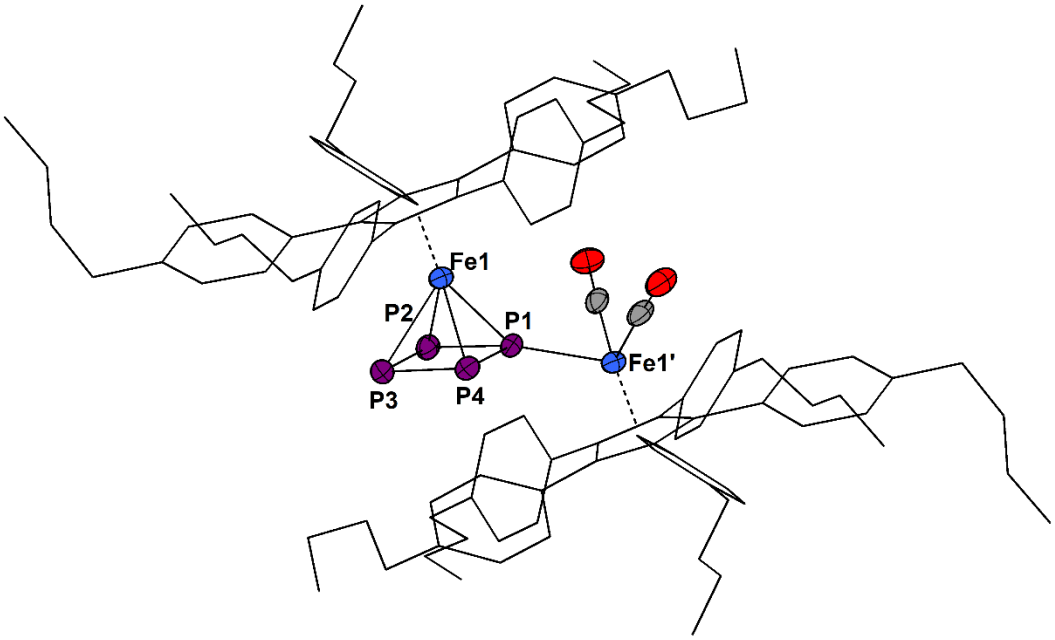

Figure S4: Molecular structure of **3** in the crystal. Ellipsoids are drawn at 50% probability level. For disordered positions only the main part is shown. For clarity the Cp^{BIG} ligands are drawn in 'wire-or-stick' model. Selected bond lengths [Å] and angles [°]: P1-P2 2.140(2), P2-P3 2.159(1), P3-P4 2.164(2), P1-P4 2.133(2), Fe1-P1 2.1756(8), Fe1-P2 2.344(2), Fe1-P3 2.3677(9), Fe1-P4 2.363(2), Fe1'-P1 2.3251(7), P2-P1-P4 96.03(6), P1-P2-P3 84.66(6), P2-P3-P4 94.60(6), P1-P4-P3 84.70(7), P3-P1-Fe1' 159.48(4), Cp_{cent}(Fe1)-Fe1-$P_{4,cent}$ 164.48(3), Cp_{plane}(Fe1)-$P_{4,plane}$ 12.07(6).

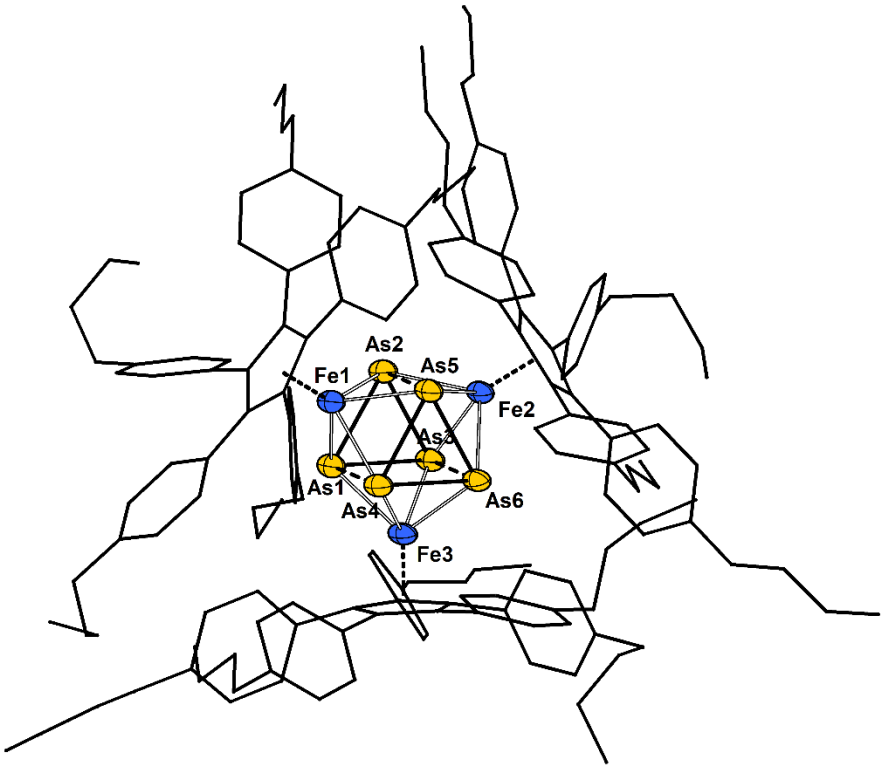

Figure S5: Molecular structure of **4** in the crystal with selected labels. Ellipsoids are drawn at 50% probability level. For disordered positions only the main part is shown. For clarity reasons the Cp^{BIG} ligands are drawn in 'wire-or-stick' model and solvent molecules are omitted. Selected bond lengths [Å] and angles [°]: As1-As2 2.5779(7), As2-As3 2.5589(7) As1-As3 2.5757(6), As4-As5 2.5740(7), As5-As6 2.5821(7), As4-As6 2.5665(6), As1···As4 2.7891(8), As2···As5 2.7343(8), As3···As6 2.7818(8), Fe1-As1 2.3954(9), Fe1-As2 2.4230(8), Fe1-As4 2.3907(9), Fe1-As5 2.4001(9), Fe2-As2 2.4108(9), Fe2-As3 2.4092(9), Fe2-As5 2.3760(8), Fe2-As6 2.4108(8), Fe3-As1 2.4036(9), Fe3-As3 2.4090(8), Fe3-As4 2.3947(8), Fe3-As6 2.3999(9) As2-As1-As3 59.54(2), As1-As2-As3 60.19(2), As1-As3-As2 60.27(2), As5-As4-As6 60.30(2), As4-As5-As6 59.71(2), As4-As6-As5 59.99(2), As4-As1-As2 89.57(3), As1-As2-As5 90.35(3), As2-As5-As4 90.87(2), As1-As4-As5 89.21(2), As3-As2-As5 90.17(2), As2-As3-As6 90.30(2), As3-As6-As5 88.64(2), As2-As5-As6 90.88(2), As3-As1-As4 89.57(2), As1-As3-As6 90.24(2), As3-As6-As4 89.92(2), As1-As4-As6 90.27(2).

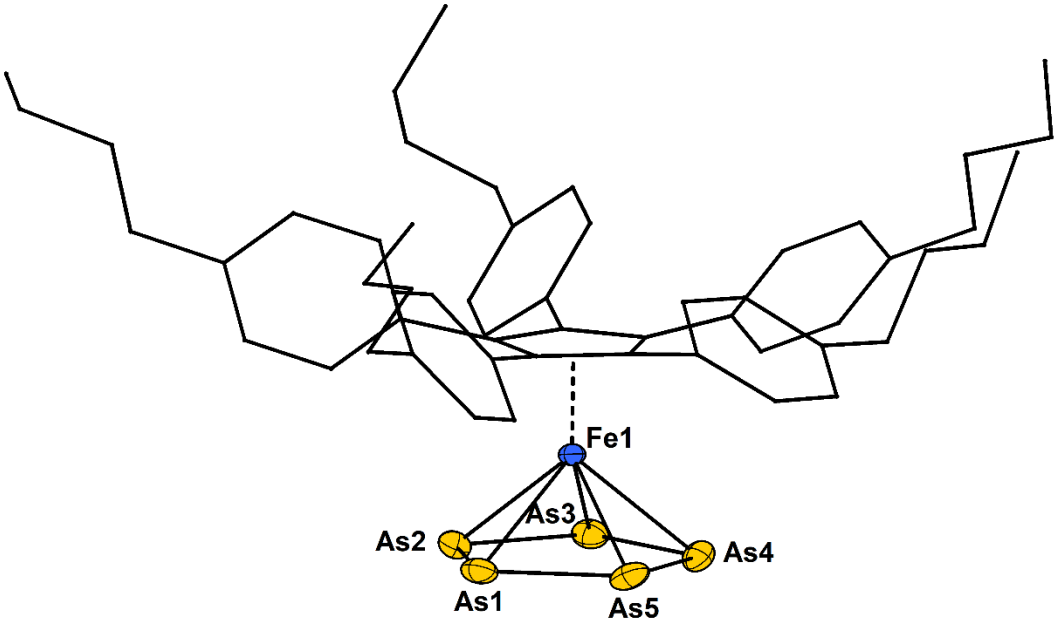

Figure S6: Molecular structure of **5** in the crystal with selected labels. Ellipsoids are drawn at 50% probability level. For clarity reasons the Cp^{BIG} ligand is drawn in 'wire-or-stick' model. Selected bond lengths [Å] and angles [°]: As1-As2 2.3165(4), As2-As3 2.3210(4), As3-As4 2.3202(5), As4-As5 2.3093(4), As1-As5 2.3177(5), Fe1-As1 2.5245(5), Fe1-As2 2.5293(4), Fe1-As3 2.5131(4), Fe1-As4 2.5419(6), Fe1-As5 2.5110(6), As2-As1-As5 107.94(2), As1-As2-As3 107.70(2), As2-As3-As4 108.29(2), As3-As4-As5 107.61(2), As1-As5-As4 108.43(2), Cp_{plane}(Fe1)-$As_{5,plane}$ 0.75(7).

3. Details on DFT calculations

The DFT calculations have been performed by using the standard Gaussian 03 program suite.[6] B3LYP functional [7] has been used together with all electron def2-SVP [8] basis set. Full geometry optimization has been performed both for **2a** and **2b** (*cyclo* and *cisoid* isomers). Due to the large size of the studied molecules, vibrational analysis could not be performed. Both for **2a** and **2b** *cyclo* isomer is predicted to be more stable in the gas phase than *cisoid* isomer. The energy difference in case of the phosphorus analogue is by about 40 kJ mol^{-1} smaller than in the arsenic case (50 vs. 89 kJ mol^{-1}).

Table S1. Relative energies E_{rel} [kJ mol^{-1}] of **2a** and **2b** in different conformations in the gas phase (B3LYP/def2-SVP level of theory).

Compound	E_{rel}	Compound	E_{rel}
2a (cyclo)	0	**2b** (cyclo)	0
2a (cisoid)	49.6	**2b** (cisoid)	89.4

Table S2. Optimized geometries (xyz coordinates in Å) for studied compounds at the B3LYP/def2-SVP level of theory.

2a (*cisoid*)

Atom	x	y	z	Atom	x	y	z
Fe	-0.273698	-0.145189	1.312305	H	-4.96049	-2.107453	-3.465228
P	0.988469	1.520067	0.424853	C	-4.549771	-3.531574	-5.779502
P	-2.371122	0.372003	0.165207	H	-6.647993	-3.522229	4.847298
P	-0.987257	2.128039	0.758394	C	-5.95864	-5.514138	4.348442
C	-2.36527	-2.030827	3.111182	H	-6.827359	-3.940444	3.140058
C	-1.032786	-1.409577	2.872169	C	-7.27	-6.239164	4.664722
C	-0.594274	-0.152766	3.418087	H	-5.270715	-5.601466	5.208954
C	0.1685	-3.442976	1.735935	H	-5.450273	-6.0183	3.506691
C	-1.409323	0.745636	4.283012	H	-7.775188	-5.726727	5.503922
C	0.818155	-0.016306	3.151223	C	-7.081192	-7.7175	5.007949
C	1.70574	1.024999	3.74077	H	-7.954621	-6.144602	3.801994
C	1.249802	-1.187247	2.418621	H	-8.04248	-8.207808	5.230444
C	2.667634	-1.56729	2.159183	H	-6.431111	-7.844359	5.889972
C	0.108511	-2.046232	2.245608	H	-6.613111	-8.266303	4.173496
Fe	-0.41601	0.830547	-1.23592	H	-4.536848	3.782351	6.411578
C	-2.698611	2.293131	-3.12463	H	-3.145336	3.928577	7.489057
C	-1.343288	1.701776	-2.945477	C	-4.544149	2.39015	8.075641
C	-0.966463	0.340785	-3.248012	H	-4.985565	3.10206	8.796846
C	-0.066453	3.916401	-2.470581	H	-3.809407	1.79553	8.648715
C	-1.870356	-0.687201	-3.835502	C	-5.644783	1.464948	7.548514
C	0.469159	0.232495	-3.102719	H	-6.380378	2.065337	6.982086
C	1.301486	-0.919001	-3.553761	C	-6.362253	0.689933	8.654911
C	0.974438	1.524613	-2.721487	H	-5.213498	0.754886	6.821692
C	2.416233	1.88969	-2.676048	H	-6.838016	1.370462	9.381422
C	-0.147186	2.437831	-2.633019	H	-5.659773	0.050768	9.216159
C	-4.848264	-3.312405	3.69171	H	-7.150533	0.03747	8.246231
C	-2.876338	-2.075734	4.422754	H	3.709578	4.842741	5.978823
C	-3.120842	-2.647663	2.099096	C	5.40266	4.471302	4.680021
C	-4.33563	-3.271239	2.386336	H	4.775346	3.548276	6.536791
C	-4.090367	-2.70389	4.703915	H	4.930209	4.892853	3.774472
H	-2.3126	-1.618943	5.237388	H	5.993952	3.604871	4.332565
H	-2.760562	-2.63773	1.070292	C	6.336228	5.512567	5.304596
H	-4.9012	-3.731663	1.570671	H	5.738139	6.374573	5.652837
H	-4.457058	-2.71777	5.734822	C	7.428654	5.999865	4.35169
C	-6.144842	-4.025315	4.003383	H	6.801202	5.085889	6.212274
C	-2.971498	2.357596	6.041336	H	6.996403	6.467537	3.451203
C	-2.65579	1.255345	3.885214	H	8.066797	5.165942	4.013907
C	-0.960306	1.054143	5.580939	H	8.082662	6.745185	4.832063
C	-1.726611	1.843266	6.438938	H	7.202282	-3.184621	2.711989
C	-3.416774	2.04624	4.748223	H	7.492578	-1.743622	1.733238
H	-3.036209	1.034595	2.887663	C	7.184898	-3.550483	0.579753
H	0.001659	0.668937	5.924232	H	6.565746	-4.464108	0.636105
H	-1.343839	2.068911	7.43902	C	8.662683	-3.93763	0.468481
H	-4.378795	2.435276	4.402514	H	6.865998	-3.029257	-0.340879
C	-3.802199	3.196087	6.989637	H	8.974548	-4.447625	1.398375
C	3.382967	2.950827	5.012204	H	9.275138	-3.018998	0.413052
C	1.405196	2.398125	3.691872	C	8.972878	-4.831453	-0.732708
C	2.853279	0.635095	4.456129	H	8.406263	-5.776761	-0.68586
C	3.6719	1.579541	5.077416	H	10.043205	-5.088537	-0.780698
C	2.229931	3.336952	4.311784	H	8.70678	-4.33648	-1.68143
H	0.513015	2.740261	3.167944	H	-0.338459	-8.174211	0.798972
H	3.104276	-0.423031	4.539961	C	1.822613	-8.262603	0.902538
H	4.553358	1.239509	5.629415	H	0.475892	-7.639875	-0.674307
H	1.96637	4.397134	4.251154	H	1.876226	-8.207404	2.00493
C	4.302044	3.976653	5.636163	H	2.686138	-7.681424	0.531376
C	5.421706	-2.276996	1.92768	C	1.954116	-9.721189	0.454577
C	3.581616	-0.727768	1.501965	H	1.086013	-10.29481	0.827781
C	3.159837	-2.772953	2.695261	C	3.247846	-10.38921	0.922523
C	4.506989	-3.11748	2.581188	H	1.891254	-9.769265	-0.648056
C	4.927939	-1.079932	1.388156	H	3.322452	-10.39205	2.022995
H	3.24161	0.223181	1.090552	H	4.134846	-9.860448	0.534862
H	2.481649	-3.441277	3.228539	H	3.309781	-11.43548	0.582704
H	4.85703	-4.054975	3.023992	C	7.044433	3.861859	-1.600627
H	5.61461	-0.394313	0.882712	H	6.926313	3.366557	-3.705817
C	6.878905	-2.658931	1.796466	H	7.268802	1.985015	-2.65897
C	0.382416	-6.151873	0.872861	H	6.767355	3.40365	-0.634108
C	0.829231	-3.775395	0.540366	H	6.434553	4.779765	-1.681127
C	-0.372456	-4.494419	2.49707	C	8.530442	4.231935	-1.586956

C	-0.266939	-5.820061	2.070959	C	8.908901	5.190931	-0.457253
C	0.931849	-5.101254	0.120826	H	8.80204	4.68147	-2.559703
H	1.268441	-2.985519	-0.069893	H	9.133771	3.309092	-1.50615
H	-0.877914	-4.2764	3.438962	H	8.680677	4.756924	0.530726
H	-0.704599	-6.61339	2.684372	H	8.352533	6.140175	-0.534321
H	1.448008	-5.323021	-0.818023	H	9.983597	5.433327	-0.474055
C	0.521471	-7.590395	0.427647	H	3.054256	-5.175066	-5.079075
C	-5.23481	3.507411	-3.587348	C	5.006676	-4.381873	-4.576406
C	-3.318097	3.078093	-2.137662	H	3.730751	-4.092056	-6.299112
C	-3.367827	2.135904	-4.352159	H	4.895911	-4.520458	-3.485802
C	-4.610047	2.731997	-4.575974	H	5.564533	-3.436428	-4.702885
C	-4.560912	3.669138	-2.36692	C	5.819927	-5.539279	-5.163933
H	-2.820299	3.231042	-1.179829	H	5.258732	-6.482124	-5.029504
H	-2.905912	1.547245	-5.146945	C	7.213103	-5.681427	-4.549754
H	-5.101459	2.594848	-5.544027	H	5.910975	-5.400076	-6.25684
H	-5.015179	4.274845	-1.577088	H	7.157145	-5.857042	-3.462622
C	-6.60148	4.113853	-3.813124	H	7.813736	-4.769213	-4.704033
C	0.149798	6.758304	-2.327796	H	7.767901	-6.523084	-4.994484
C	0.667097	4.540551	-1.446848	C	-5.466338	-2.85289	-6.816494
C	-0.680881	4.745943	-3.428474	H	-5.164229	-4.041292	-5.019222
C	-0.572797	6.135231	-3.35681	H	-3.96268	-4.318115	-6.285318
C	0.768548	5.930493	-1.378998	C	-6.386832	-3.812013	-7.584282
H	1.169061	3.935075	-0.691891	H	-4.832757	-2.307613	-7.537382
H	-1.240006	4.297639	-4.251062	H	-6.07444	-2.082262	-6.308571
H	-1.057956	6.747686	-4.122883	H	-6.888472	-3.243839	-8.387267
H	1.347679	6.380938	-0.567264	C	-7.449948	-4.509279	-6.731211
C	0.223988	8.264716	-2.221407	H	-5.769725	-4.572849	-8.096942
C	5.192806	2.53245	-2.746858	H	-8.107425	-5.139566	-7.351387
C	3.362763	1.101504	-1.998793	H	-8.088908	-3.775506	-6.210915
C	2.888255	2.998917	-3.40051	H	-7.003926	-5.161806	-5.963428
C	4.24873	3.311764	-3.431961	C	-7.759695	3.198612	-3.375959
C	4.720205	1.418739	-2.034929	H	-6.723195	4.359674	-4.882416
H	3.03297	0.223189	-1.442818	H	-6.674333	5.069158	-3.264767
H	2.186062	3.619106	-3.959539	C	-9.143701	3.815824	-3.597983
H	4.582782	4.179277	-4.009141	H	-7.634363	2.943857	-2.308099
H	5.429927	0.779811	-1.501229	H	-7.688564	2.240609	-3.922135
C	6.659048	2.901657	-2.74087	C	-10.29378	2.906452	-3.162871
C	2.802474	-3.087119	-4.643502	H	-9.259711	4.072615	-4.666961
C	1.107174	-2.234702	-3.104888	H	-9.204504	4.77531	-3.052429
C	2.26418	-0.709304	-4.560224	H	-11.27326	3.380085	-3.337049
C	2.995868	-1.770946	-5.092178	H	-10.22799	2.662977	-2.089143
C	1.846384	-3.292953	-3.638125	H	-10.28216	1.952643	-3.716715
H	0.356876	-2.437366	-2.340025	C	-0.923958	8.878474	-1.399195
H	2.428358	0.298304	-4.946154	H	0.216091	8.706757	-3.233001
H	3.725588	-1.571948	-5.883018	H	1.18609	8.553689	-1.763798
H	1.660168	-4.307325	-3.272943	H	-0.924608	8.428246	-0.390131
C	3.612073	-4.231944	-5.210079	H	-1.888391	8.590732	-1.855363
C	-3.611302	-2.565068	-5.092404	C	-0.845915	10.403423	-1.281528
C	-3.137823	-0.977922	-3.299339	C	-1.988258	11.010482	-0.465683
C	-1.497591	-1.34807	-5.020784	H	-0.839335	10.846524	-2.294313
C	-2.351811	-2.266246	-5.633351	H	0.122127	10.683516	-0.827133
C	-3.985212	-1.899043	-3.915244	H	-1.999869	10.614834	0.56382
H	-3.468733	-0.47817	-2.389244	H	-2.968506	10.781017	-0.916265
H	-0.529582	-1.136858	-5.476517	H	-1.901182	12.106889	-0.399704
H	-2.027681	-2.7642	-6.552224	P	-1.156718	-1.191747	-0.514789

2a (*cyclo*)

Atom	x	y	z	Atom	x	y	z
Fe	-0.170364	0.694277	-1.457755	H	-4.184122	1.525944	4.111474
P	1.592538	0.119524	0.011613	C	-3.921821	2.382139	6.706134
P	-1.531911	-0.416368	0.201347	H	-7.936969	1.438133	-2.913377
P	0.200343	-1.528164	-0.6674	C	-7.84943	3.579943	-2.601253
P	-0.174692	1.216825	0.884506	H	-7.750313	1.912641	-1.221634
C	-3.097311	1.616319	-2.570493	C	-9.360196	3.807573	-2.495721
C	-1.623293	1.509678	-2.730978	H	-7.509928	3.815905	-3.626143
C	-0.910116	0.428775	-3.373583	H	-7.320573	4.290346	-1.94041
C	-0.984741	3.874876	-1.83087	H	-9.88263	3.089666	-3.154263
C	-1.529654	-0.764148	-4.010847	C	-9.787702	5.232245	-2.851477
C	0.490424	0.788409	-3.423745	H	-9.692917	3.567562	-1.469196
C	1.559973	0.049338	-4.149553	H	-10.87842	5.361651	-2.764419

C	0.638367	2.086335	-2.807283	H	-9.503736	5.489807	-3.885701
C	1.879538	2.908703	-2.798285	H	-9.310891	5.971814	-2.186427
C	-0.667131	2.530211	-2.381829	H	-3.827579	-4.841028	-5.287848
Fe	0.305447	-1.003411	1.656327	H	-2.691993	-4.667997	-6.629242
C	-1.986874	-2.884369	3.009254	C	-4.599632	-3.713763	-6.973321
C	-0.631188	-2.274444	3.032623	H	-4.921744	-4.605571	-7.541297
C	-0.272679	-1.014615	3.644495	H	-4.217007	-2.999066	-7.724911
C	0.687061	-4.263468	1.973181	C	-5.813777	-3.103795	-6.266936
C	-1.194563	-0.112841	4.386905	H	-6.197895	-3.824687	-5.521589
C	1.163281	-0.865493	3.543705	C	-6.938782	-2.714372	-7.227179
C	1.983297	0.195106	4.191665	H	-5.496827	-2.217255	-5.690836
C	1.684908	-2.029742	2.867795	H	-7.302781	-3.585931	-7.797301
C	3.124461	-2.374026	2.708652	H	-6.598433	-1.962666	-7.959263
C	0.576384	-2.897548	2.551694	H	-7.800084	-2.286868	-6.689091
C	-5.921401	1.930194	-2.350567	H	4.370441	-3.095136	-6.55388
C	-3.941671	1.39791	-3.674043	C	6.023579	-1.954856	-5.743254
C	-3.694314	1.994091	-1.355313	H	4.723422	-1.608151	-7.440599
C	-5.076745	2.146386	-1.250355	H	5.945512	-2.372297	-4.723103
C	-5.324715	1.552768	-3.563269	H	6.300288	-0.893217	-5.611172
H	-3.509366	1.108779	-4.633683	C	7.130212	-2.682451	-6.512308
H	-3.066189	2.171048	-0.481293	H	6.843943	-3.741928	-6.644966
H	-5.509987	2.435235	-0.288093	C	8.497597	-2.603922	-5.831773
H	-5.953737	1.374498	-4.44078	H	7.20015	-2.262471	-7.532499
C	-7.414546	2.146128	-2.246752	H	8.469429	-3.050708	-4.823682
C	-2.773452	-2.969358	-5.32333	H	8.829379	-1.558175	-5.71796
C	-2.426224	-1.603778	-3.329514	H	9.269539	-3.13659	-6.410026
C	-1.266959	-1.049582	-5.363695	H	5.430362	6.054142	-3.83631
C	-1.876526	-2.129569	-6.003048	H	6.367579	4.722831	-3.150088
C	-3.032864	-2.682822	-3.974581	C	5.704185	6.178444	-1.691176
H	-2.65472	-1.409305	-2.280426	H	4.820648	6.818096	-1.514021
H	-0.577334	-0.41478	-5.923145	C	6.967352	7.043653	-1.724319
H	-1.644927	-2.32577	-7.054494	H	5.750795	5.487675	-0.829893
H	-3.721538	-3.320545	-3.412926	H	6.913837	7.731946	-2.587727
C	-3.446215	-4.124265	-6.035001	H	7.844765	6.397841	-1.91174
C	3.553453	-1.319372	-5.66074	C	7.189614	7.847849	-0.442562
C	1.829433	-1.312451	-3.932198	H	6.345721	8.530319	-0.245765
C	2.30152	0.710427	-5.146254	H	8.104552	8.458994	-0.501007
C	3.276623	0.037826	-5.884472	H	7.287351	7.185732	0.434167
C	2.807096	-1.978892	-4.671855	H	-2.909872	8.153852	-0.589783
H	1.266224	-1.858234	-3.173778	C	-0.99373	8.982462	-1.166346
H	2.106317	1.764439	-5.352273	H	-1.655154	7.994211	0.643917
H	3.832099	0.580941	-6.655136	H	-1.175483	8.907452	-2.253844
H	2.991216	-3.039681	-4.476341	H	0.07671	8.747111	-1.025248
C	4.645412	-2.033801	-6.425012	C	-1.271453	10.413575	-0.697181
C	4.240137	4.503251	-2.943862	H	-2.344499	10.639663	-0.836562
C	3.114539	2.423604	-2.334673	C	-0.429185	11.465986	-1.419733
C	1.852421	4.205101	-3.345386	H	-1.091613	10.480463	0.391498
C	3.009111	4.983351	-3.415555	H	-0.613744	11.449924	-2.507058
C	4.266512	3.207769	-2.404493	H	0.649001	11.290196	-1.26729
H	3.17536	1.421309	-1.909824	H	-0.654312	12.482585	-1.059413
H	0.913948	4.606696	-3.731931	C	7.65741	-4.22398	1.128813
H	2.952888	5.984926	-3.852685	H	7.630503	-4.086888	3.289867
H	5.211241	2.798204	-2.034085	H	7.971663	-2.556399	2.475104
C	5.484138	5.362193	-2.977982	H	7.370572	-3.598232	0.264323
C	-1.563626	6.508649	-0.906333	H	7.016266	-5.122251	1.073244
C	-0.271047	4.443214	-0.761846	C	9.127452	-4.634146	1.001582
C	-1.990304	4.653943	-2.432506	C	9.437991	-5.394007	-0.288931
C	-2.271098	5.943461	-1.978135	H	9.407461	-5.255335	1.872113
C	-0.558613	5.731081	-0.309701	H	9.763418	-3.732001	1.062053
H	0.514207	3.866237	-0.272994	H	9.206354	-4.784705	-1.178717
H	-2.557586	4.246285	-3.271105	H	8.842925	-6.319867	-0.361132
H	-3.061538	6.521484	-2.466532	H	10.501343	-5.676618	-0.347308
H	0.008934	6.13931	0.531969	H	3.80606	4.122491	6.388832
C	-1.841091	7.92071	-0.441652	C	5.672427	3.547724	5.451087
C	-4.542871	-4.143924	3.043015	H	4.678777	2.845026	7.242596
C	-2.545937	-3.425555	1.838779	H	5.390681	3.895448	4.440767
C	-2.727838	-2.994231	4.199816	H	6.260926	2.625339	5.296297
C	-3.979206	-3.612734	4.213229	C	6.545493	4.605412	6.132937
C	-3.798059	-4.039788	1.857748	H	5.950673	5.524684	6.284991
H	-1.98931	-3.368285	0.902346	C	7.815867	4.941938	5.350734
H	-2.314225	-2.599375	5.129684	H	6.817012	4.254758	7.145551
H	-4.527411	-3.687719	5.157318	H	7.576993	5.33062	4.346501
H	-4.205114	-4.450015	0.928747	H	8.450674	4.05024	5.215035
C	-5.921495	-4.765374	3.051435	H	8.420077	5.704814	5.86741
C	0.96956	-6.924468	0.989428	C	-4.971826	1.551696	7.470317

C	1.443063	-4.536234	0.820218	H	-4.430356	3.092669	6.033843
C	0.083338	-5.351382	2.630344	H	-3.35378	2.990962	7.431127
C	0.224367	-6.653148	2.1472	C	-5.940087	2.37763	8.329186
C	1.576631	-5.838836	0.339318	H	-4.442912	0.828982	8.115575
H	1.931979	-3.717411	0.291817	H	-5.545105	0.943926	6.746537
H	-0.494362	-5.177693	3.539943	H	-6.544832	1.682201	8.937328
H	-0.252184	-7.477081	2.687111	C	-6.879743	3.29411	7.541422
H	2.171676	-6.015641	-0.561669	H	-5.35943	2.979902	9.052213
C	1.080928	-8.3293	0.441264	H	-7.581253	3.816113	8.211859
C	5.885595	-3.069704	2.556177	H	-7.480246	2.720601	6.814782
C	4.063755	-1.498048	2.139084	H	-6.331269	4.067017	6.979368
C	3.597059	-3.600877	3.211548	C	-7.055034	-3.743819	2.845947
C	4.948778	-3.938686	3.13635	H	-6.083042	-5.290371	4.00914
C	5.413925	-1.843419	2.063141	H	-5.984197	-5.533937	2.261753
H	3.733492	-0.537725	1.742582	C	-8.452863	-4.36955	2.854367
H	2.896391	-4.296772	3.676618	H	-6.892462	-3.211875	1.891224
H	5.28267	-4.898457	3.542327	H	-6.990371	-2.971261	3.633323
H	6.118563	-1.138784	1.611038	C	-9.576626	-3.350725	2.658018
C	7.340633	-3.460851	2.427993	H	-8.604344	-4.907582	3.808136
C	3.535531	2.159463	5.556021	H	-8.51074	-5.140619	2.064375
C	1.759315	1.567149	3.9888	H	-10.56742	-3.832626	2.668796
C	2.992957	-0.17456	5.09979	H	-9.474094	-2.821643	1.6957
C	3.750796	0.788967	5.766887	H	-9.568787	-2.587839	3.454545
C	2.52277	2.525913	4.656414	C	-0.069415	-8.712354	-0.507546
H	0.977438	1.88977	3.299585	H	1.108888	-9.049364	1.277795
H	3.181462	-1.232302	5.293163	H	2.039424	-8.439827	-0.094823
H	4.525373	0.466826	6.46957	H	-0.105177	-7.988627	-1.34182
H	2.32306	3.586306	4.474613	H	-1.030024	-8.600029	0.027027
C	4.394803	3.201241	6.236946	C	0.045172	-10.13428	-1.064781
C	-2.964036	1.535965	5.897363	C	-1.103139	-10.51736	-1.999405
C	-2.39698	0.361232	3.833858	H	0.092175	-10.85093	-0.224368
C	-0.897974	0.251402	5.712826	H	1.007084	-10.23826	-1.599513
C	-1.766378	1.058523	6.450332	H	-1.154412	-9.841612	-2.869661
C	-3.260107	1.167795	4.575384	H	-2.076033	-10.46119	-1.482774
H	-2.660639	0.097156	2.808522	H	-0.988864	-11.54423	-2.382182
H	0.025013	-0.103669	6.174753	H	-1.502203	1.327051	7.477714

2b (*cisoid*)

Atom	x	y	z	Atom	x	y	z
Fe	0.396314	0.28034	1.296934	H	4.474629	1.05782	-4.37446
As	-1.453157	-1.125584	0.728158	C	3.833034	2.515563	-6.613874
As	2.311419	-0.892602	0.000867	H	7.709534	1.748413	4.30935
As	0.519643	-2.3033	1.005497	C	7.670689	3.791374	3.590887
C	3.083651	1.553591	2.840065	H	7.917477	1.902012	2.56173
C	1.610877	1.380633	2.692704	C	9.161851	4.076951	3.791979
C	0.810693	0.405402	3.385968	H	7.098441	4.18912	4.448547
C	1.076463	3.605556	1.411164	H	7.304202	4.341684	2.705487
C	1.335901	-0.586158	4.366865	H	9.522298	3.519889	4.676149
C	-0.58347	0.712273	3.149731	C	9.480653	5.563379	3.959193
C	-1.733093	0.087576	3.863575	H	9.727732	3.671874	2.933138
C	-0.637142	1.869661	2.282676	H	10.560122	5.732999	4.100481
C	-1.84385	2.689274	1.966342	H	8.959816	5.989393	4.833213
C	0.713784	2.293848	2.017398	H	9.165675	6.142695	3.075016
Fe	-0.003704	-1.016986	-1.182554	H	3.43713	-4.142117	6.909409
C	1.789813	-2.900935	-3.251919	H	2.111242	-3.700743	7.989103
C	0.562181	-2.126083	-2.915723	C	3.943328	-2.621729	8.371864
C	0.289765	-0.754494	-3.287246	H	4.176332	-3.34253	9.176706
C	-0.855658	-4.134598	-2.058706	H	3.450858	-1.764839	8.867243
C	1.195939	0.115293	-4.090116	C	5.2502	-2.151225	7.726921
C	-1.08815	-0.472296	-2.944927	H	5.742872	-3.012663	7.239245
C	-1.879143	0.721861	-3.363791	C	6.216601	-1.507332	8.72247
C	-1.668775	-1.672468	-2.399478	H	5.02448	-1.436804	6.916308
C	-3.12929	-1.884339	-2.196292	H	6.49044	-2.207772	9.529645
C	-0.643339	-2.693097	-2.371099	H	5.768644	-0.618421	9.198038
C	5.875813	2.015022	3.220338	H	7.149261	-1.186317	8.231337
C	3.657146	1.554941	4.126237	H	-4.694651	-2.565111	6.6562
C	3.937593	1.801222	1.750487	C	-6.22535	-2.04342	5.216296
C	5.301994	2.02311	1.939847	H	-5.387731	-0.956852	6.892578
C	5.022418	1.780953	4.309212	H	-5.874467	-2.741754	4.435146
H	3.025484	1.385435	4.999048	H	-6.571767	-1.142795	4.677847
H	3.534012	1.823549	0.738326	C	-7.397192	-2.670009	5.977684
H	5.936157	2.202135	1.066357	H	-7.041315	-3.566386	6.517952
H	5.432401	1.772374	5.323737	C	-8.575678	-3.049309	5.079725

C	7.34795	2.295532	3.421506
C	2.385924	-2.35686	6.341964
C	2.341691	-1.513277	4.0505
C	0.873336	-0.553878	5.696322
C	1.387469	-1.421681	6.659925
C	2.851057	-2.38086	5.018999
H	2.73333	-1.557382	3.034425
H	0.100108	0.162459	5.980199
H	0.998323	-1.373825	7.681624
H	3.626874	-3.09764	4.734919
C	2.94586	-3.284278	7.399586
C	-3.878094	-1.053364	5.366105
C	-1.820684	-1.301974	4.076843
C	-2.737664	0.892542	4.432428
C	-3.78534	0.331398	5.165642
C	-2.870025	-1.855512	4.809143
H	-1.053924	-1.961414	3.671889
H	-2.695188	1.975342	4.318633
H	-4.543985	0.990665	5.598359
H	-2.902456	-2.939563	4.953659
C	-5.038097	-1.663402	6.11985
C	-4.135599	4.325322	1.517821
C	-2.896284	2.253692	1.149805
C	-1.958228	3.964114	2.554491
C	-3.080888	4.761306	2.336704
C	-4.017729	3.058195	0.929394
H	-2.836023	1.270566	0.682479
H	-1.156149	4.330066	3.199335
H	-3.14107	5.742548	2.817433
H	-4.820839	2.687207	0.285784
C	-5.331582	5.212866	1.254822
C	1.692075	6.195214	0.379312
C	0.465178	4.090928	0.24137
C	1.98967	4.454011	2.063792
C	2.289312	5.719625	1.555996
C	0.770761	5.354213	-0.263784
H	-0.264396	3.470876	-0.278988
H	2.469088	4.125969	2.986592
H	3.008205	6.349799	2.088318
H	0.284739	5.691266	-1.184269
C	1.99061	7.579699	-0.150248
C	4.03542	-4.485494	-4.012224
C	2.461117	-3.706525	-2.316453
C	2.256693	-2.915109	-4.579163
C	3.357208	-3.690404	-4.948474
C	3.561024	-4.478751	-2.691304
H	2.113281	-3.735603	-1.283799
H	1.744384	-2.319675	-5.337056
H	3.690814	-3.681816	-5.990585
H	4.059075	-5.095855	-1.937424
C	5.253902	-5.291828	-4.40204
C	-1.360604	-6.907287	-1.604929
C	-1.501191	-4.576781	-0.890565
C	-0.480635	-5.110662	-3.001964
C	-0.728907	-6.465525	-2.777565
C	-1.743118	-5.933299	-0.670373
H	-1.826276	-3.852562	-0.143661
H	-0.001037	-4.805392	-3.932943
H	-0.429637	-7.194826	-3.536478
H	-2.247369	-6.239921	0.250953
C	-1.585804	-8.379034	-1.341404
C	-5.951646	-2.262222	-1.990054
C	-3.948284	-0.940089	-1.552303
C	-3.758617	-3.012909	-2.754038
C	-5.138503	-3.195379	-2.650435
C	-5.326334	-1.128855	-1.448297
H	-3.501065	-0.037468	-1.136425
H	-3.165301	-3.753224	-3.291493
H	-5.592926	-4.082601	-3.101689
H	-5.930414	-0.373292	-0.937173
C	-7.438863	-2.487399	-1.838131
C	-3.395054	2.933457	-4.33476
C	-1.660108	2.018812	-2.879486
C	-2.876674	0.550756	-4.343563
C	-3.614581	1.633479	-4.819348
H	-7.740305	-1.967569	6.759377
H	-8.27548	-3.783187	4.31305
H	-8.97737	-2.168051	4.551871
H	-9.400501	-3.493576	5.659634
H	-5.614642	5.731635	2.18774
H	-6.197554	4.59021	0.971976
C	-5.087965	6.265194	0.158209
H	-4.205607	6.872162	0.430518
C	-6.287379	7.186361	-0.083978
H	-4.818543	5.750334	-0.781829
H	-6.561537	7.681448	0.865525
H	-7.164569	6.575144	-0.365443
C	-6.036061	8.245725	-1.157939
H	-5.186575	8.895511	-0.888476
H	-6.916338	8.892131	-1.302975
H	-5.800261	7.782804	-2.130856
H	3.02521	7.859788	0.113364
C	1.03006	8.660216	0.379062
H	1.944033	7.569299	-1.253122
H	1.074848	8.673509	1.483141
H	-0.007214	8.37561	0.125458
C	1.325509	10.061259	-0.164143
H	2.365262	10.337633	0.089978
C	0.368915	11.132789	0.360966
H	1.284605	10.038192	-1.268562
H	0.413047	11.205389	1.460698
H	-0.675649	10.905818	0.088765
H	0.610204	12.127154	-0.047671
C	-7.813378	-3.296606	-0.58299
H	-7.824001	-3.012566	-2.729618
H	-7.957067	-1.513386	-1.803903
H	-7.423735	-2.777182	0.310966
H	-7.292807	-4.270808	-0.613357
C	-9.320356	-3.523587	-0.430529
C	-9.691979	-4.33385	0.812177
H	-9.703656	-4.034478	-1.332854
H	-9.833713	-2.544954	-0.401274
H	-9.354413	-3.831594	1.734249
H	-9.22547	-5.333103	0.792726
H	-10.78152	-4.477319	0.891703
H	-3.665524	5.037707	-4.677531
C	-5.600611	4.210587	-4.158177
H	-4.368174	4.001699	-5.923696
H	-5.460012	4.320512	-3.067545
H	-6.148729	3.260995	-4.295203
C	-6.447712	5.371035	-4.688411
H	-5.898582	6.319191	-4.541207
C	-7.825605	5.470149	-4.032153
H	-6.566992	5.262628	-5.781994
H	-7.740997	5.621293	-2.94289
H	-8.412192	4.549907	-4.191827
H	-8.408867	6.311361	-4.439527
C	4.443421	1.704619	-7.773928
H	4.639993	2.944072	-5.996882
H	3.274244	3.370138	-7.034034
C	5.341563	2.515989	-8.718583
H	3.620393	1.254937	-8.356021
H	5.015566	0.855535	-7.357545
H	5.599174	1.881009	-9.584441
C	6.63353	3.04173	-8.087525
H	4.761987	3.36268	-9.130563
H	7.253344	3.569317	-8.830226
H	7.240148	2.217546	-7.675062
H	6.436927	3.749769	-7.266361
C	6.580874	-4.535763	-4.207897
H	5.168624	-5.599933	-5.458583
H	5.283029	-6.222616	-3.809057
C	7.814411	-5.35565	-4.597577
H	6.664919	-4.219175	-3.152594
H	6.554214	-3.602356	-4.79884
C	9.132246	-4.604364	-4.403137
H	7.721636	-5.672399	-5.652643
H	7.830943	-6.289476	-4.006171
H	9.997495	-5.222344	-4.692097
H	9.272452	-4.306951	-3.350347

C	-2.406573	3.100791	-3.35459	H	9.162776	-3.684307	-5.010725
H	-0.892019	2.183931	-2.123532	C	-0.403018	-9.06434	-0.632965
H	-3.067229	-0.446856	-4.745223	H	-1.780504	-8.89859	-2.29585
H	-4.374384	1.465315	-5.588739	H	-2.493989	-8.507432	-0.727249
H	-2.208474	4.099902	-2.955372	H	-0.200152	-8.540969	0.318767
C	-4.221871	4.097596	-4.833252	H	0.507926	-8.935437	-1.245053
C	2.916168	1.699796	-5.730421	C	-0.632765	-10.55397	-0.361208
C	2.574831	0.217489	-3.821691	C	0.543907	-11.23366	0.34062
C	0.702402	0.813325	-5.208184	H	-0.841675	-11.06962	-1.316497
C	1.546139	1.587104	-6.007678	H	-1.546587	-10.67484	0.248988
C	3.411038	0.993818	-4.623023	H	0.75459	-10.7632	1.315687
H	3.002297	-0.315578	-2.973161	H	1.464706	-11.16461	-0.262651
H	-0.35415	0.747531	-5.466445	H	0.345096	-12.30199	0.522753
H	1.124075	2.119679	-6.865417	As	1.252214	0.98882	-0.830314

2b (*cyclo*)

Atom	x	y	z	Atom	x	y	z
Fe	-0.050922	0.609581	-1.605981	H	-3.339562	1.003804	7.113986
As	1.70998	0.128732	0.015252	H	-5.236728	0.960502	3.245605
As	-1.713712	-0.31195	-0.097298	C	-5.672623	1.719523	5.850771
As	0.230375	-1.764075	-0.483434	H	-7.175163	3.849426	-2.896828
As	-0.219417	1.363991	0.908552	C	-6.399432	5.839775	-2.539263
C	-2.544318	2.41296	-2.665355	H	-6.814269	4.188303	-1.201209
C	-1.202133	1.800704	-2.864233	C	-7.755871	6.533009	-2.381396
C	-0.938984	0.528957	-3.498069	H	-6.025683	5.986865	-3.568816
C	0.260725	3.822133	-2.089839	H	-5.656598	6.323563	-1.879524
C	-1.950605	-0.367892	-4.124538	H	-8.494636	6.039109	-3.038878
C	0.493048	0.38806	-3.633055	C	-7.715331	8.03003	-2.691722
C	1.182784	-0.697536	-4.38305	H	-8.124046	6.379103	-1.350552
C	1.11567	1.573668	-3.097933	H	-8.705948	8.496631	-2.569276
C	2.561148	1.914088	-3.196631	H	-7.385951	8.2157	-3.727935
C	0.070063	2.441859	-2.611734	H	-7.013821	8.558776	-2.024704
Fe	0.015839	-0.891168	1.784366	H	-5.505025	-3.407184	-5.428837
C	-2.196694	-3.07932	2.741534	H	-4.420751	-3.549924	-6.815509
C	-0.981169	-2.257879	2.995405	C	-5.920718	-2.010924	-7.036979
C	-0.967248	-0.952453	3.620698	H	-6.533352	-2.721142	-7.621798
C	0.838881	-4.026973	2.36231	H	-5.349568	-1.422833	-7.778587
C	-2.157475	-0.226427	4.14514	C	-6.84732	-1.076219	-6.25452
C	0.409911	-0.575848	3.835642	H	-7.421125	-1.669318	-5.518506
C	0.878356	0.586852	4.639628	C	-7.814901	-0.29828	-7.14796
C	1.243926	-1.642935	3.335744	H	-6.241934	-0.368098	-5.662562
C	2.722533	-1.722683	3.486816	H	-8.461884	-0.976731	-7.729506
C	0.38828	-2.688091	2.828612	H	-7.272303	0.335876	-7.869365
C	-5.099696	3.647571	-2.376749	H	-8.471489	0.359874	-6.556435
C	-3.443374	2.489703	-3.744644	H	2.492889	-4.684364	-6.823508
C	-2.947306	2.975594	-1.441687	C	4.500846	-4.214273	-6.16161
C	-4.198116	3.577737	-1.303115	H	3.297298	-3.440768	-7.786858
C	-4.693693	3.094594	-3.600495	H	4.350591	-4.563782	-5.124109
H	-3.159376	2.07239	-4.712292	H	5.151808	-3.324504	-6.085919
H	-2.271688	2.942806	-0.585617	C	5.210585	-5.302289	-6.972721
H	-4.48234	3.997181	-0.333258	H	4.552847	-6.187745	-7.045808
H	-5.370308	3.132565	-4.459744	C	6.56164	-5.71574	-6.387197
C	-6.440082	4.332214	-2.229774	H	5.350469	-4.948306	-8.010592
C	-3.897303	-1.981646	-5.450994	H	6.451105	-6.108953	-5.362609
C	-3.057087	-0.88859	-3.435429	H	7.255372	-4.859697	-6.336934
C	-1.841104	-0.668166	-5.496417	H	7.043714	-6.499096	-6.993783
C	-2.792991	-1.457015	-6.141991	H	6.899077	3.632952	-4.543886
C	-4.006462	-1.680104	-4.085647	H	7.359135	2.039967	-3.934115
H	-3.18046	-0.67545	-2.372967	C	7.371901	3.598651	-2.43079
H	-0.997204	-0.275203	-6.066205	H	6.786847	4.502501	-2.18196
H	-2.670113	-1.674165	-7.207542	C	8.851126	3.968106	-2.57589
H	-4.850774	-2.075327	-3.513379	H	7.243657	2.914059	-1.572854
C	-4.934942	-2.819006	-6.168262	H	8.972525	4.649654	-3.43775
C	2.440385	-2.720919	-5.952349	H	9.428786	3.060443	-2.829917
C	0.931746	-2.060455	-4.149938	C	9.442796	4.616931	-1.323744
C	2.064988	-0.367721	-5.429168	H	8.910906	5.548006	-1.065366
C	2.678988	-1.359533	-6.195333	H	10.506456	4.869059	-1.461762
C	1.552083	-3.048046	-4.916251	H	9.37039	3.945108	-0.451959
H	0.242352	-2.353585	-3.357636	H	-0.045938	8.505693	-0.857329
H	2.264813	0.681372	-5.654173	C	1.997632	8.647922	-1.560001
H	3.354338	-1.066691	-7.005019	H	1.157423	7.94388	0.307945
H	1.333902	-4.099533	-4.706205	H	1.737218	8.630833	-2.633842
C	3.142462	-3.794699	-6.752667	H	2.937206	8.073187	-1.47082

C	5.314993	2.577421	-3.547168	C	2.235417	10.093378	-1.11271
C	3.580049	1.00766	-2.852823	H	1.290618	10.660338	-1.20116
C	2.951346	3.155074	-3.733338	C	3.334231	10.803667	-1.904528
C	4.299169	3.477065	-3.903139	H	2.489736	10.103318	-0.036964
C	4.925164	1.335421	-3.021852	H	3.091855	10.843378	-2.979838
H	3.317505	0.026813	-2.455292	H	4.301043	10.282137	-1.805087
H	2.189148	3.874462	-4.036722	H	3.478381	11.839577	-1.557981
H	4.565433	4.448959	-4.329652	C	7.753662	-2.648204	2.916624
H	5.69014	0.604183	-2.74377	H	7.250922	-2.572139	5.02162
C	6.774916	2.944439	-3.690077	H	7.45674	-0.985308	4.272014
C	0.655685	6.505025	-1.207154	H	7.531206	-2.073239	1.9995
C	1.187209	4.126772	-1.077389	H	7.329312	-3.654613	2.748857
C	-0.458707	4.889784	-2.656986	C	9.270306	-2.754722	3.101128
C	-0.263384	6.20217	-2.222915	C	9.9837	-3.408977	1.917039
C	1.377455	5.439523	-0.646233	H	9.484815	-3.325734	4.02308
H	1.768048	3.32408	-0.621646	H	9.6871	-1.745201	3.271933
H	-1.178844	4.690851	-3.45246	H	9.818776	-2.840884	0.986091
H	-0.843488	7.0082	-2.682471	H	9.61646	-4.434678	1.744908
H	2.099366	5.639438	0.151288	H	11.071505	-3.468661	2.08176
C	0.892071	7.931385	-0.763466	H	1.36143	4.624509	7.291761
C	-4.502182	-4.717169	2.36564	C	3.441753	4.569	6.693928
C	-2.451514	-3.706955	1.51042	H	2.351379	3.501997	8.230464
C	-3.114938	-3.298446	3.785237	H	3.260863	4.943995	5.670293
C	-4.241824	-4.100458	3.598955	H	4.24846	3.819667	6.600007
C	-3.580623	-4.50635	1.328438	C	3.911638	5.720144	7.587826
H	-1.75436	-3.572877	0.682292	H	3.09727	6.461578	7.683388
H	-2.9389	-2.840629	4.760252	C	5.176072	6.412697	7.077148
H	-4.932115	-4.252745	4.434277	H	4.087439	5.337146	8.609781
H	-3.747852	-4.978423	0.355623	H	5.020633	6.841261	6.072746
C	-5.752733	-5.539721	2.1509	H	6.019307	5.705311	7.004989
C	1.749478	-6.621074	1.601308	H	5.486666	7.233036	7.74397
C	1.891577	-4.190063	1.444065	C	-6.688772	0.704524	6.410764
C	0.256995	-5.190209	2.89794	H	-6.158003	2.344412	5.083232
C	0.704148	-6.458702	2.522536	H	-5.369279	2.402787	6.663429
C	2.334069	-5.459261	1.072464	C	-7.920885	1.332055	7.077752
H	2.377101	-3.309178	1.021941	H	-6.1711	0.061533	7.143593
H	-0.548884	-5.102096	3.628397	H	-7.010222	0.031151	5.595353
H	0.232753	-7.342218	2.963627	H	-8.501808	0.52711	7.561273
H	3.158155	-5.548272	0.35813	C	-8.841505	2.109918	6.133793
C	2.206167	-7.995241	1.166156	H	-7.589434	1.995646	7.897806
C	5.536311	-1.884706	3.923282	H	-9.731631	2.48387	6.66475
C	3.578599	-0.672669	3.113497	H	-9.193409	1.472749	5.304539
C	3.302446	-2.850522	4.09717	H	-8.337987	2.983112	5.688512
C	4.679724	-2.92696	4.309695	C	-6.971192	-4.701004	1.723632
C	4.955181	-0.756057	3.324613	H	-6.000877	-6.082139	3.079988
H	3.16086	0.222003	2.651477	H	-5.560758	-6.309867	1.383945
H	2.664724	-3.675143	4.420461	C	-8.241186	-5.529862	1.510423
H	5.09645	-3.815998	4.79281	H	-6.724873	-4.153783	0.795748
H	5.592156	0.079864	3.02001	H	-7.159328	-3.924409	2.486905
C	7.033206	-1.991449	4.108324	C	-9.451783	-4.692894	1.094381
C	1.702295	2.731888	6.333316	H	-8.47506	-6.081179	2.43968
C	0.415739	1.897806	4.433927	H	-8.046131	-6.30397	0.745699
C	1.756092	0.37106	5.719234	H	-10.34709	-5.318651	0.949968
C	2.157603	1.421766	6.545326	H	-9.263468	-4.157862	0.14843
C	0.822594	2.945422	5.261002	H	-9.695201	-3.934496	1.857318
H	-0.277374	2.102685	3.61793	C	1.469652	-8.526187	-0.077277
H	2.118625	-0.637359	5.924896	H	2.06582	-8.708905	1.99655
H	2.834101	1.215094	7.380261	H	3.289922	-7.972852	0.956793
H	0.439055	3.952503	5.071289	H	1.603102	-7.810845	-0.908928
C	2.16727	3.874646	7.207762	H	0.384037	-8.547091	0.127675
C	-4.444749	1.067428	5.255206	C	1.937327	-9.917098	-0.515433
C	-3.272267	0.088632	3.350414	C	1.207135	-10.44554	-1.751015
C	-2.212932	0.114788	5.509471	H	1.804992	-10.62544	0.322873
C	-3.333164	0.747876	6.050025	H	3.024645	-9.888647	-0.712805
C	-4.389401	0.723025	3.895999	H	1.351101	-9.77845	-2.617531
H	-3.265549	-0.162666	2.288893	H	0.121314	-10.52215	-1.572957
H	-1.366432	-0.120009	6.157467	H	1.568216	-11.44613	-2.03819

4. References for Supplementary Information

[1] O. J. Scherer, H. Sitzmann, G. Wolmershäuser, *J. Organomet. Chem.,* 1986, **309**, 77-86.

[2] R. C. Clark, J. S. Reid, *Acta Cryst.* 1995, **A51**, 887-897.

[3] A. Altomare, M. C. Burla, M. Camalli, G.L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* 1999, **32**, 115-119.

[4] L. Palatinus, G. Chapuis, *J. Appl. Cryst.* 2007, **40**, 786-790.

[5] G. M. Sheldrick, *Acta Cryst.* 2015, **C27**, 3-8.

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03 (Revision D.01): Gaussian, Inc., Wallingford CT, 2004.

[7] a) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*., 1988, **37**, 785.

[8] F. Weigend, R. Ahlrichs, *Phys.Chem.Chem.Phys.*, 2005, **7**, 3297-3305.