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Electrophilic terminal arsinidene iron(0) complexes with a two-coordinated arsenic atom

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Experimental Section

All the manipulations/experiments were carried out under an inert gas (Ar or N_2) atmosphere using standard *Schlenk* techniques/ an MBraun LABmaster Pro glovebox. Solvents for syntheses/NMR such as THF, Toluene, benzene, benzene-d_6, and *n*-hexane were refluxed over NaK, distilled prior to use, and stored over molecular sieve (3 Å). $CDCl_3$ was dried by refluxing over CaH_2 and distilled prior to use. (IPr)C(Ph)$AsCl_2$ (**3**) was synthesized by following to the literature reported methods.[1] DABCO and $AsCl_3$ were purchased from Sigma Aldrich and the latter was distilled prior to use. Melting points were measured using a Büchi B-545 melting point apparatus. NMR spectra were recorded using a Bruker Avance III 500HD NMR spectrometer. Chemical shifts are given in δ ppm and are referenced to the solvent residual peaks.[2] UV-visible spectra were recorded using a Thermo Fisher Evolution 300 spectrophotometer.

Synthesis of (Me–IPr)CPh (2). Compound **2** was synthesized following the literature reported method[1] using (^{Me}IPr)HCl (15.7 g, 34.6 mmol), KO*t*Bu (7.84 g, 69.8 mmol), $PhCH_2Br$ (6.04 g, 35.3 mmol), and THF (120 mL). Yield: 85 % (14.9 g). M.p.: 307 °C. Single crystals were grown by slow evaporation of an saturated *n*-hexane solution of **2** at room temperature. ^{1}H NMR (C_6D_6, 298 K, 500 MHz): δ (ppm) = 7.29 (m, 2H, *p*-C_6H_3), 7.19 (d, *J* = 7.6 Hz, 2H, *m*-C_6H_3), 7.09 (d, *J* = 7.8 Hz, 2H, *m*-C_6H_3), 6.82 – 6.72 (m, 2H, C_6H_5), 6.60 (t, *J* = 6.7 Hz, 1H, *p*-C_6H_3), 6.07 (d, *J* = 7.6 Hz, 2H, C_6H_3), 4.06 (s, 1H, C*H*Ph), 3.28 (m, 2H, C*H*(CH_3)$_2$), 3.20 (m, 2H, C*H*(CH_3)$_2$), 1.52 (s, 3H, C*H*$_3$), 1.51 (s, 3H, C*H*$_3$), 1.39 (d, *J* = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 1.20 (d, *J* = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 1.15 (dd, *J* = 6.8, 5.7 Hz, 12H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 298 K, 125 MHz): δ (ppm) = 149.3, 148.7, 145.6, 139.3, 135.6, 133.0, 129.8, 129.6, 128.4, (*C*$_6$H$_3$), 127.5, 125.6, 124.8, 124.0, 117.2, 117.1 (*C*$_6$H$_5$); 71.1 (C*C*H); 28.9 (*C*H(CH_3)$_2$); 24.8, 24.0, 23.7, 23.5 (CH(*C*H$_3$)$_2$); 10.0, 9.6 (*C*H$_3$).

Synthesis of [(Me–IPr)C(Ph)]$AsCl_2$ (4). Compound **4** was synthesized following the similar method used for IPrC(Ph)$AsCl_2$,[1] using ^{Me}IPrCHPh (5 g, 9.86 mmol), DABCO (1.1 g, 9.86 mmol) and $AsCl_3$ (0.83 mL, 9.86 mmol). Single crystals suitable for X-ray diffraction studies were grown by slow diffusion of *n*-hexane to saturated benzene solution of compound **4**. Yield (2.5 g, 39%); M.p. 221 °C (dec.); Elemental analysis (%), calcd for **4**, $C_{36}H_{45}AsCl_2N_2$ (651.58): C, 66.36; H, 6.96; N, 4.30; found: C, 66.51; H, 6.76; N, 4.49. ^{1}H NMR (C_6D_6, 298 K, 500 MHz): δ (ppm) = 7.18 (br, 5H, *m*-C_6H_3, C_6H_5), 7.11-7.13 (m, 2H, C_6H_5), 7.04 (br, 2H, *p*-C_6H_3, C_6H_5), 7.02 (t, *J* = 3.6 Hz, 2H, C_6H_5), 2.90-3.04 (m, 4H, C*H*(CH_3)$_2$), 1.42 (s, 6H, C*H*$_3$), 1.39 (d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.03 (d, *J* = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 298 K, 125 MHz): δ (ppm) = 152.8 (*C*CAs); 147.5 (N*C*(CH_3)); 135.7, 133.1, 131.1, (C_6H_3), 126.4, 125.8, 121.3 (C_6H_5); 92.4 (C*C*As); 29.0 (*C*H(CH_3)$_2$; 24.6, 23.9 (CH(CH_3)$_2$); 9.9 (*C*H$_3$).

Synthesis of [{(IPr)C(Ph)}As]Fe(CO)$_4$ (5). [IPrCPh]AsCl$_2$ (1 g, 1.60 mmol) and K$_2$Fe(CO)$_4$ (0.41 g, 1.60 mmol) were combined in a 100 mL Schlenk flask and 30 mL of THF was then added. This was stirred for 48 h at room temperature and then the volatiles were removed in vacuo. The red/black residue was extracted with toluene (50 mL) and filtered through a plug of Celite. Removal of toluene from the filtrate in vacuo gave a red solid, which was washed with hexane (10 mL) and dried. X-ray quality crystals were grown by slow diffusion of *n*-hexane to a saturated solution of **5** in benzene. Yield (0.71 g, 61%). M.p. 131 °C (dec.); Elemental analysis (%), calcd for **5**, $C_{38}H_{41}AsFeN_2O_4$ (720.51): C, 63.34; H, 5.74; N, 3.89; found: C, 63.79; H, 6.21; N, 4.27. ^{1}H NMR (C_6D_6, 298 K, 500 MHz): δ (ppm) = 7.19 (d, J = 7.6, 2H, *m*-C_6H_3), 7.08 (t, J = 10.0, 2H, *m*-C_6H_3), 6.96 (t, J = 7.4, 5H, *p*-C_6H_3, C_6H_5), 6.82 (t, J = 7.3 Hz, 1H, C_6H_5), 5.96 (s, 2H, NC*H*), 3.03-3.08 (m, 4H, C*H*(CH$_3$)$_2$), 1.37 (d, J = 6.1 Hz, 12H, CH(C*H*$_3$)$_2$), 1.03 (d, J = 6.7 Hz, 12H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (THF-d_8, 298 K, 125 MHz): δ (ppm) = 217.2 (*C*O); 165.4 (*C*CAs); 155.2, 148.0, 146.6, 133.2, 131.4, 129.1, 127.9, 125.7, 124.7, 124.0 (C_6H_3, C_6H_5); 29.8 (*C*H(CH$_3$)$_2$); 25.9, 22.1 (CH(*C*H$_3$)$_2$). IR (CH$_2$Cl$_2$): ν /cm^{-1} = 1917, 1972, 2011 (CO).

Synthesis of [{(Me–IPr)C(Ph)}As]Fe(CO)$_4$ (6). Compound **6** was synthesized following the similar procedure used for **5** using [^{Me}IPrCPh]AsCl$_2$ (0.8 g, 1.23 mmol), K$_2$Fe(CO)$_4$ (0.3 g, 1.23 mmol) and THF (20 mL). Yield (0.45 g, 48.6%). M.p. 153 °C (dec.); Elemental analysis (%), calcd for **6**, $C_{40}H_{45}AsFeN_2O_4$ (748.56): C, 64.18; H, 6.06; N, 3.74; found: C, 64.71; H, 6.49; N, 4.13. ^{1}H NMR (THF-d_8, 298 K, 500 MHz): δ (ppm) = 7.50 (t, J = 7.78 Hz, 2H, C_6H_3), 7.29 (d, J = 7.78 Hz, 4H, C_6H_3, C_6H_5), 6.68-6.92 (m, 3H, *p*-C_6H_5, C_6H_5), 6.62 (d, J = 7.45 Hz, 2H, C_6H_5), 2.67-2.76 (m, 4H, C*H*(CH$_3$)$_2$), 2.05 (s, 6H, C*H*$_3$), 1.14 (t, J = 6.04 Hz, 24H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (THF-d_8, 298 K, 125 MHz): δ (ppm) = 218.1 (*C*O); 169.2, 155.3, 148.8, 147.4, 132.2, 131.9, 130.2, 128.4, 128.2, 126.6, 126.1 (*C*$_6$H$_3$, *C*$_6$H$_5$); 55.1 (C*C*As); 32.7, 14.6 (*C*H(CH$_3$)$_2$); 30.2, 24.0 (CH(*C*H$_3$)$_2$), 11.0 (*C*H$_3$). IR (CH$_2$Cl$_2$): ν /cm^{-1} = 1915, 1970, 2009 (CO).

Synthesis of [{(IPr)C(Ph)}As(IMe$_4$]Fe(CO)$_4$ (7). To a mixture of **5** (0.2 g, 0.29 mmol) and IMe$_4$ (37 mg, 0.29 mmol), THF (10 mL) was added at room temperature. This was stirred for 1 h and then the volatiles were removed in vacuo. The red residue was washed with hexane (10 mL) and dried. X-ray quality crystals were grown by slow diffusion of *n*-hexane to a saturated solution of **7** in THF. Yield (0.71 g, 61%). M.p. 143 °C (dec.); Elemental analysis (%), calcd for **7**, $C_{45}H_{55}AsFeN_4O_4$ (846.71): C, 63.83; H, 6.55; N, 6.62; found: C, 64.37; H, 6.97; N, 6.73. ^{1}H NMR (THF-d_8, 298 K, 500 MHz): δ (ppm) = 7.30 (bs, 2H, C_6H_3), 7.10-7.12 (m, 4H, C_6H_3), 6.89 (d, J = 7.2, 2H, C_6H_5), 6.66 (t, J = 7.3 Hz, 2H, C_6H_5), 6.51 (t, J = 7.2 Hz, 1H, C_6H_5), 6.20 (s, 2H, NC*H*), 3.43-3.49 (m, 2H, C*H*(CH$_3$)$_2$), 3.30-3.32 (m, 2H, C*H*(CH$_3$)$_2$), 2.81 (s, 6H, NC*H*$_3$), 1.96 (s, 6H, CC*H*$_3$), 1.51 (d, J = 6.3 Hz, 6H, CH(C*H*$_3$)$_2$), 1.22 (d, J = 6.7 Hz, 6H, CH(C*H*$_3$)$_2$), 1.10 (d, J = 5.4 Hz, 6H, CH(C*H*$_3$)$_2$), 1.06 (d, J = 6.7 Hz, 6H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR

(THF-d_8, 298 K, 125 MHz): δ (ppm) = 219.7 (*C*O); 158.6 (*C*CAs); 149.6, 146.6, 144.7, 134.2, 127.1, 127.0, 125.0, 124.1, 124.0 (C_6H_3, C_6H_5); 119.7 (*C*CH_3), 35.7 (N*C*H_3), 29.8, 29.2 (*C*H(CH_3)$_2$); 23.2, 22.0 (CH(*C*H_3)$_2$), 8.6 (C*C*H_3). IR (CH_2Cl_2): ν /cm^{-1} = 1896, 1968, 2001 (CO).

Copies of NMR Spectra

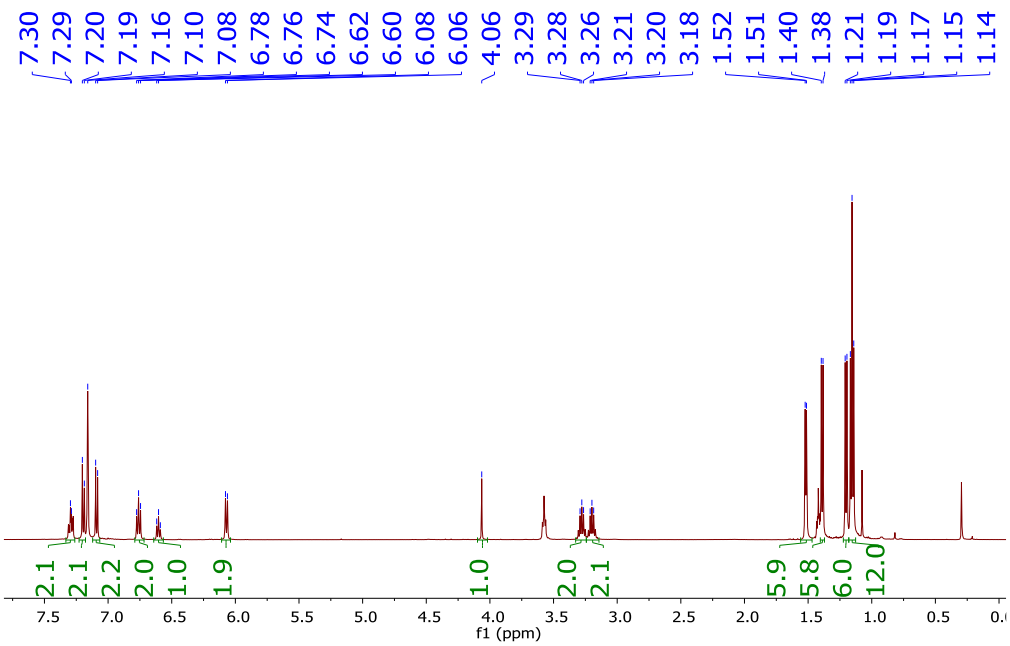


Figure S1. ^{1}H NMR (C_6D_6, 298 K, 500 MHz) spectrum of **2**.

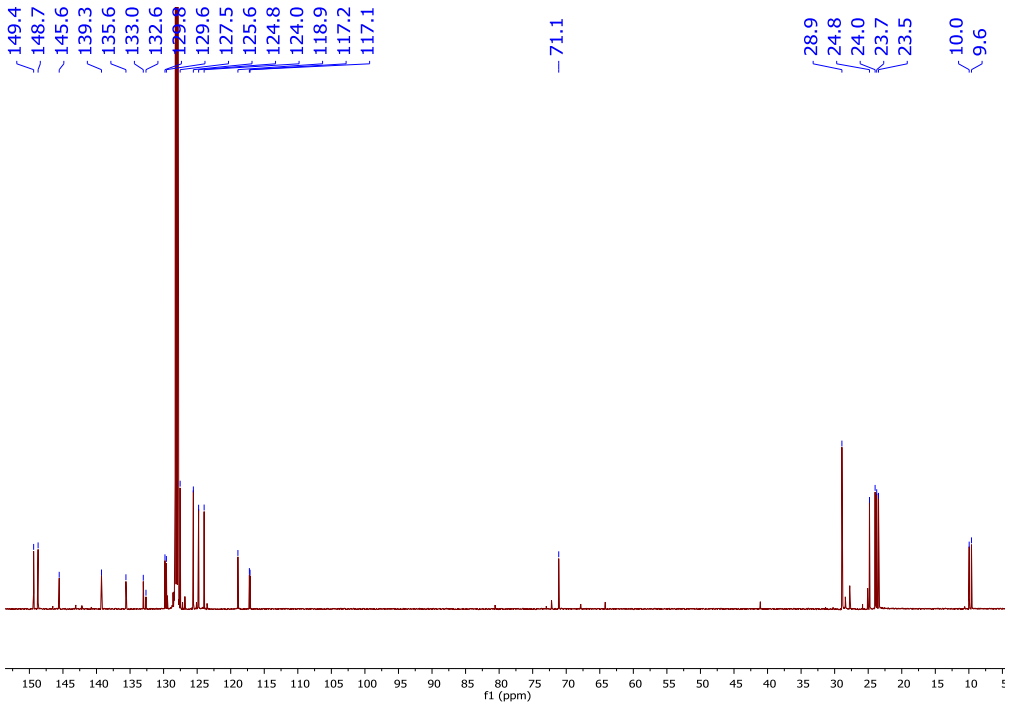


Figure S2. $^{13}C\{^{1}H\}$ NMR (C_6D_6, 298 K, 125 MHz) spectrum of **2**.

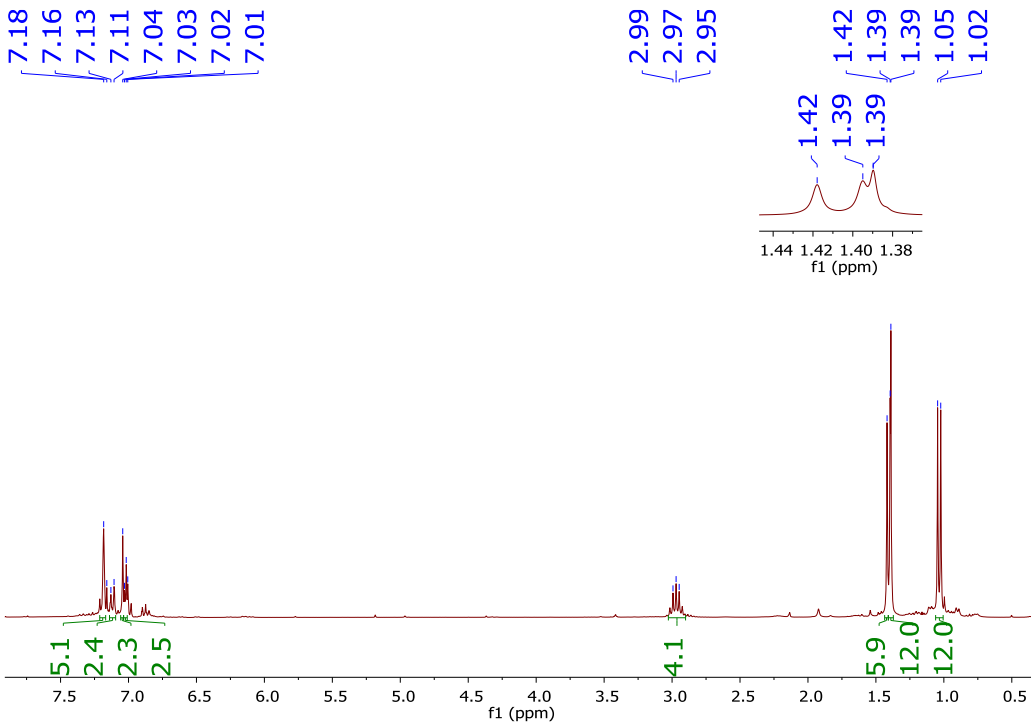


Figure S3. ^{1}H NMR (C_6D_6, 298 K, 500 MHz) spectrum of **4**.

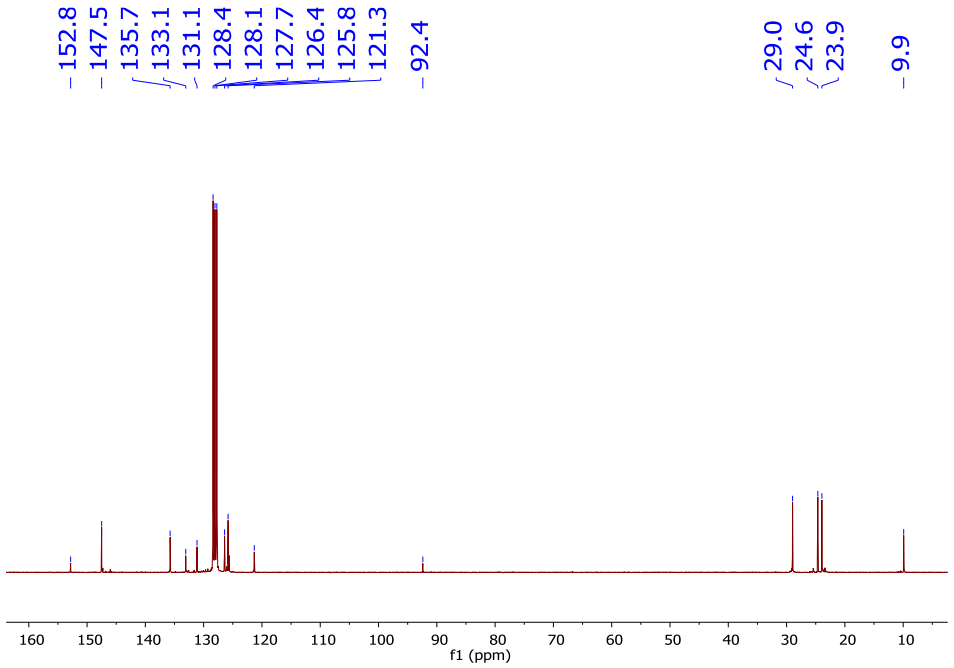


Figure S4. ^{13}C{^{1}H} NMR (C_6D_6, 298 K, 125 MHz) spectrum of **4**.

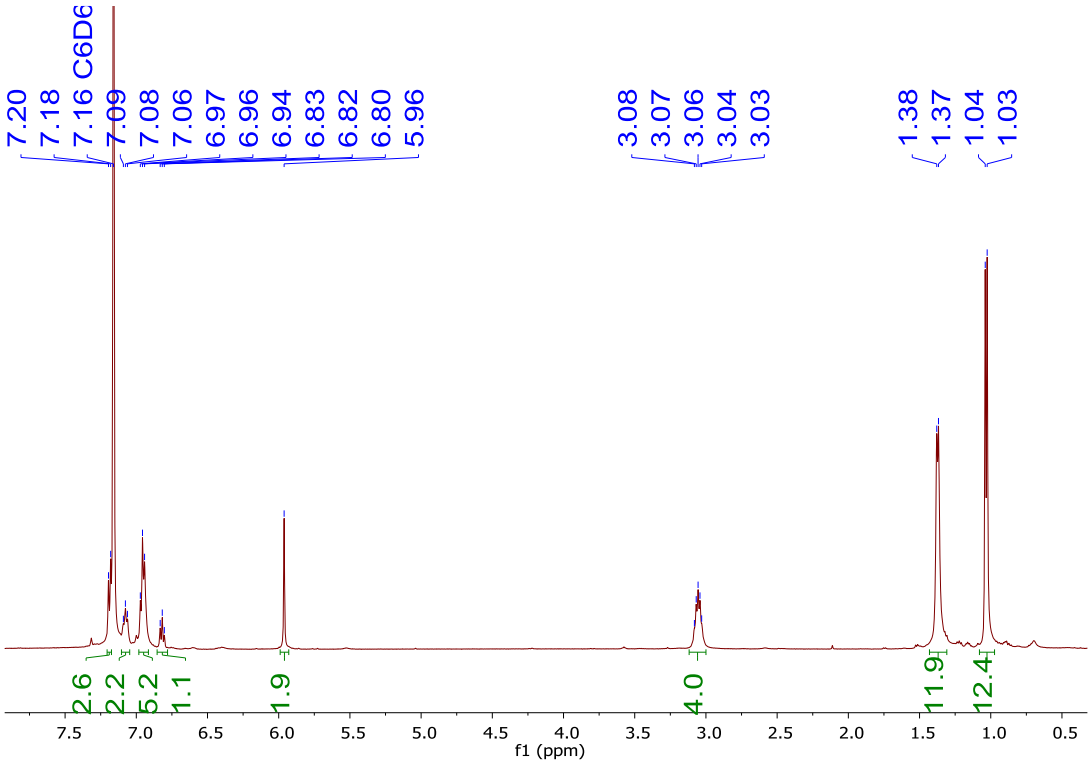


Figure S5. ^{1}H NMR spectrum (C_6D_6, 298 K, 500 MHz) of **5**.

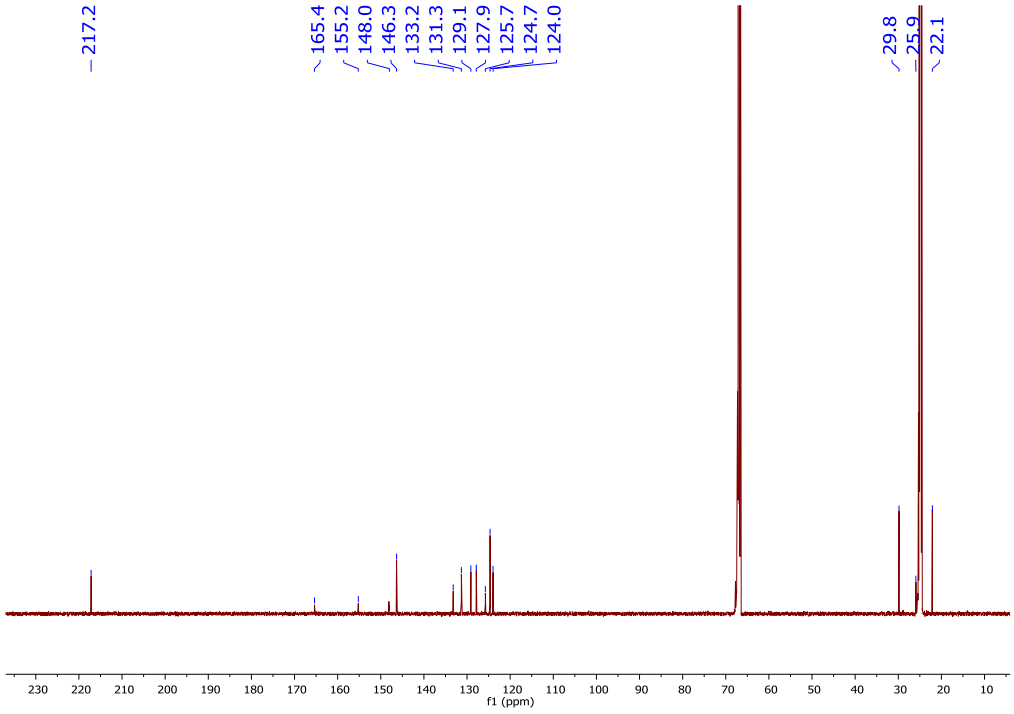


Figure S6. ^{13}C{^{1}H} NMR spectrum (THF-d_8, 298 K, 125 MHz) of **5**.

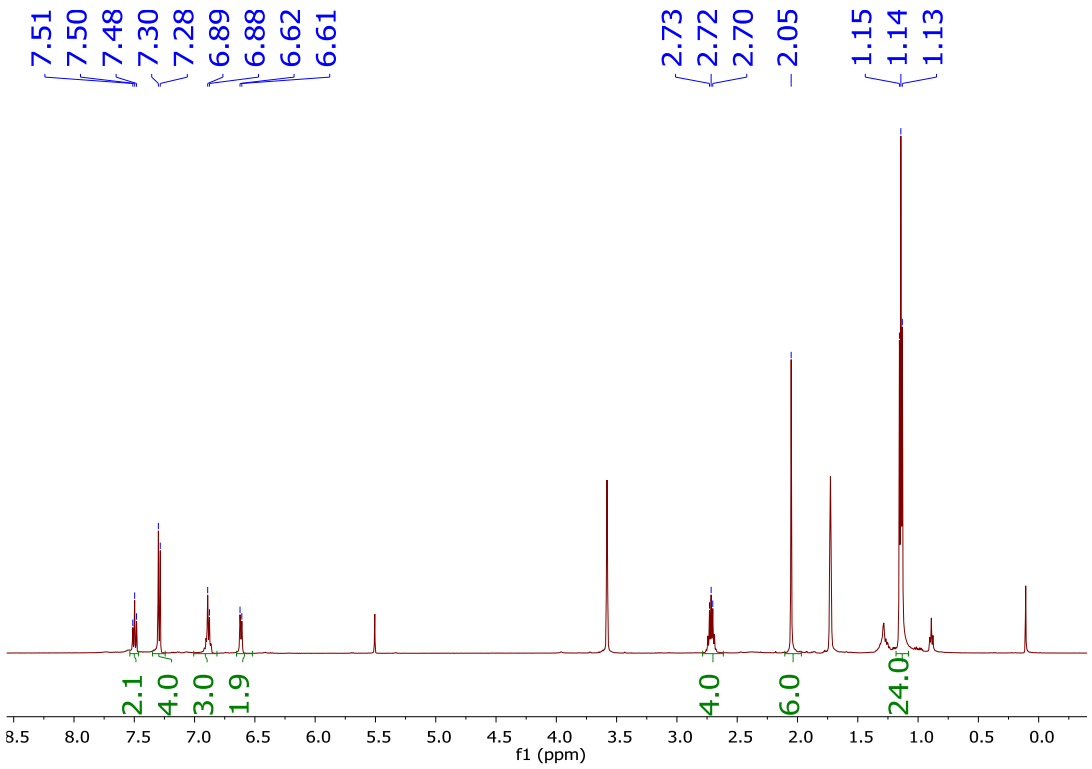


Figure S7. ^{1}H NMR spectrum (THF-d_8, 298 K, 500 MHz) of **6**.

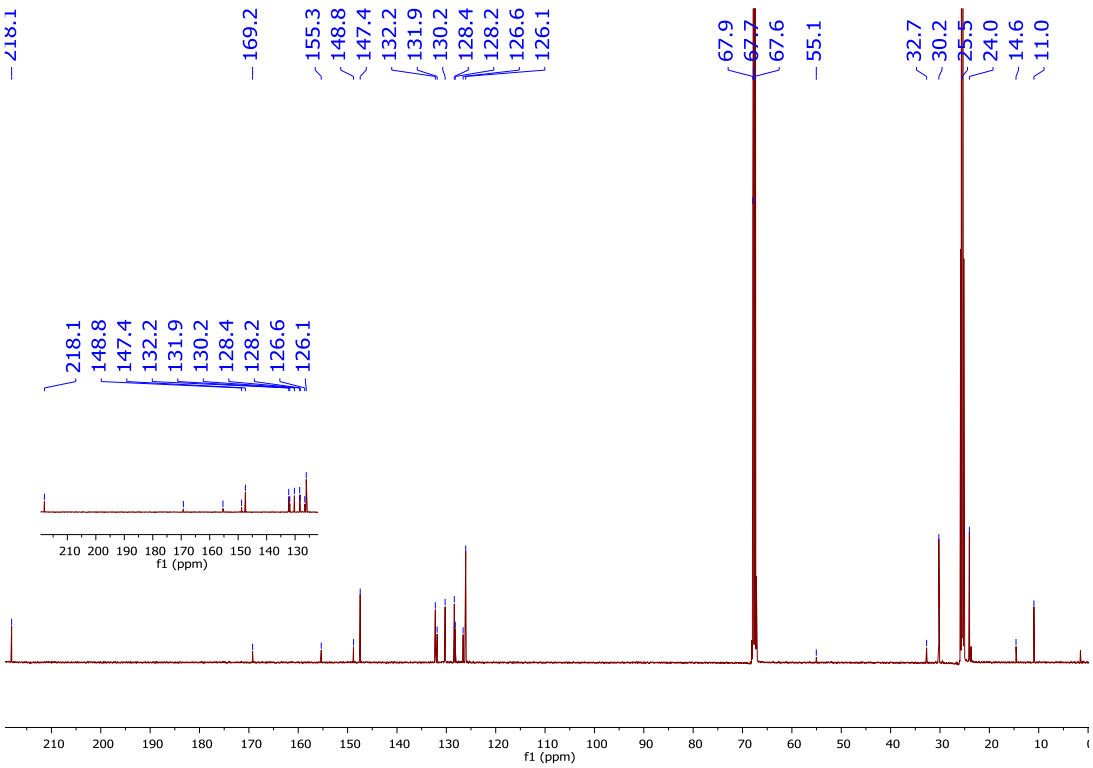


Figure S8. ^{13}C{^{1}H} NMR spectrum (THF-d_8, 298 K, 125 MHz) of **6**.

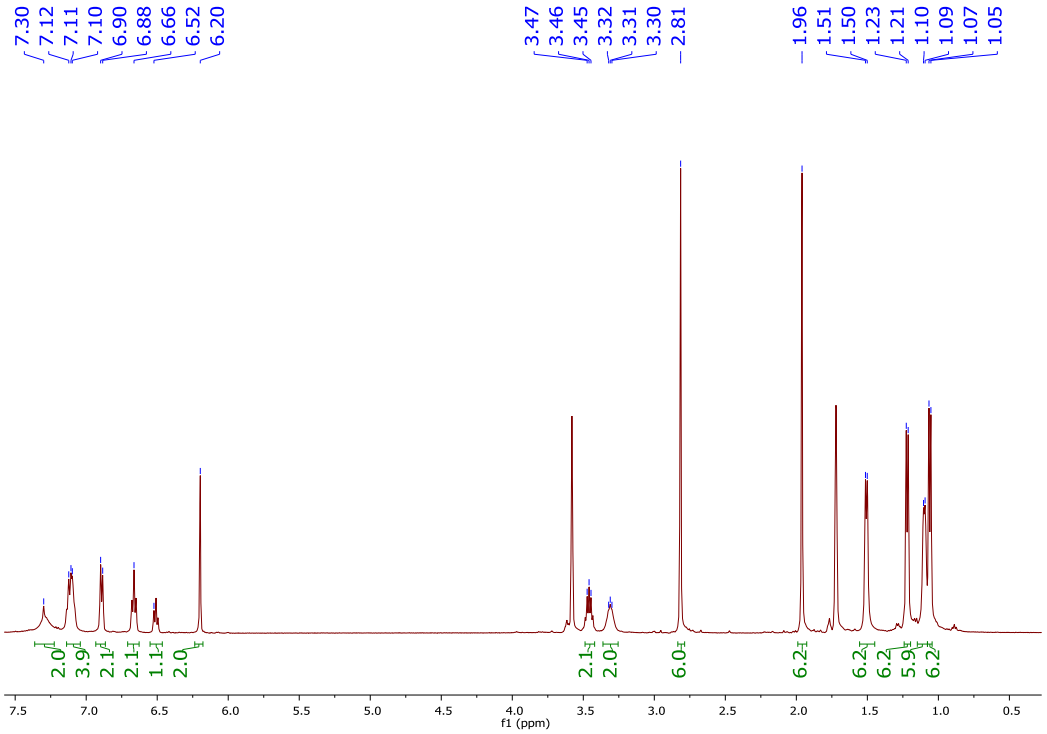


Figure S9. ^{1}H NMR spectrum (THF-d_8, 298 K, 500 MHz) of **7**.

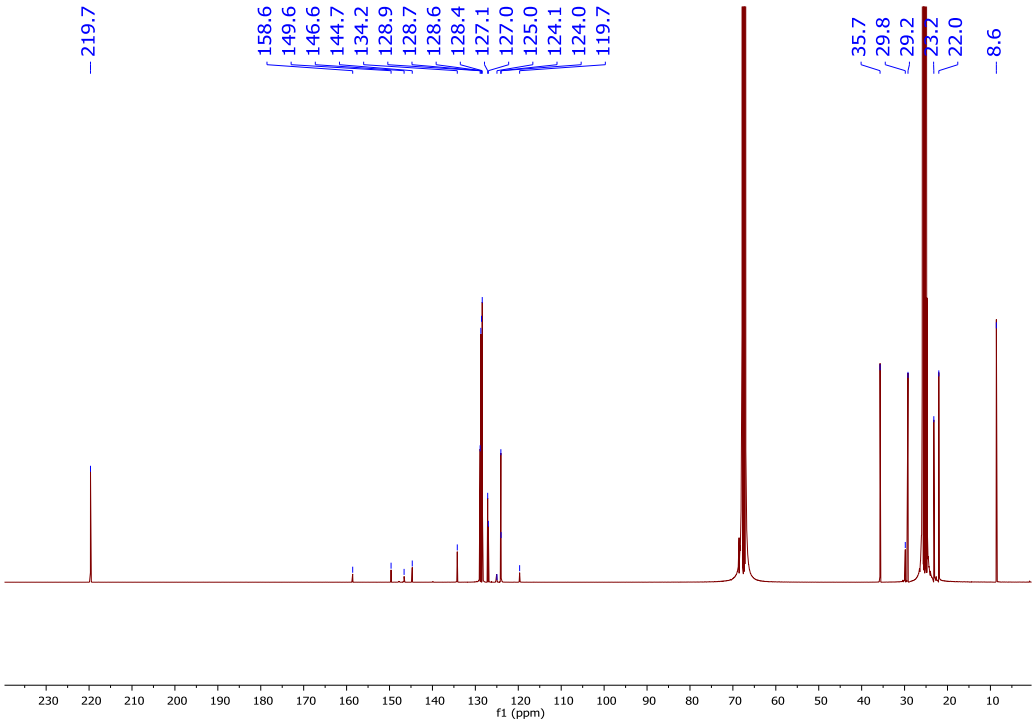


Figure S10. ^{13}C{^{1}H} NMR spectrum (THF-d_8, 298 K, 125 MHz) of **7**.

Copies of IR Spectra

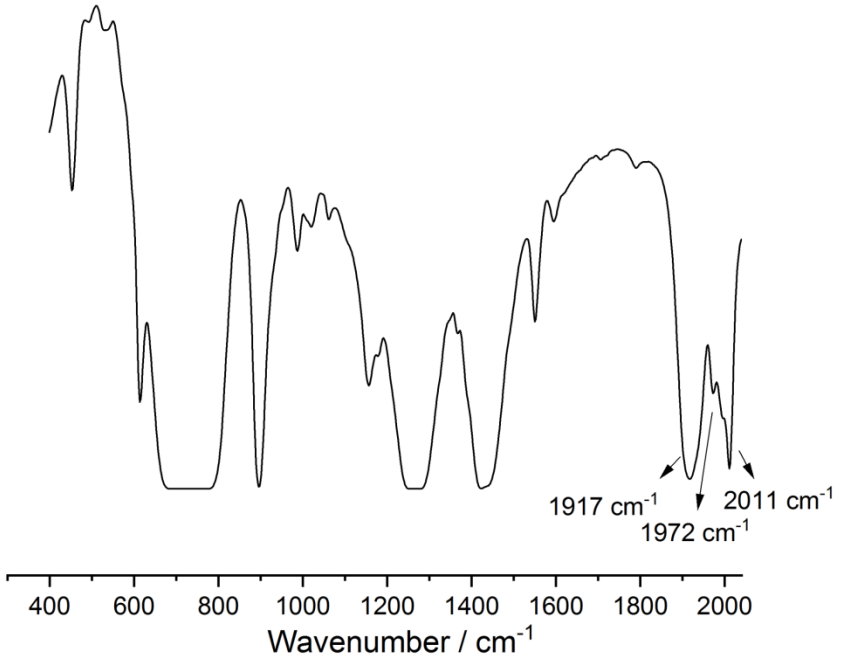


Figure S11. Solution IR spectrum of **5**.

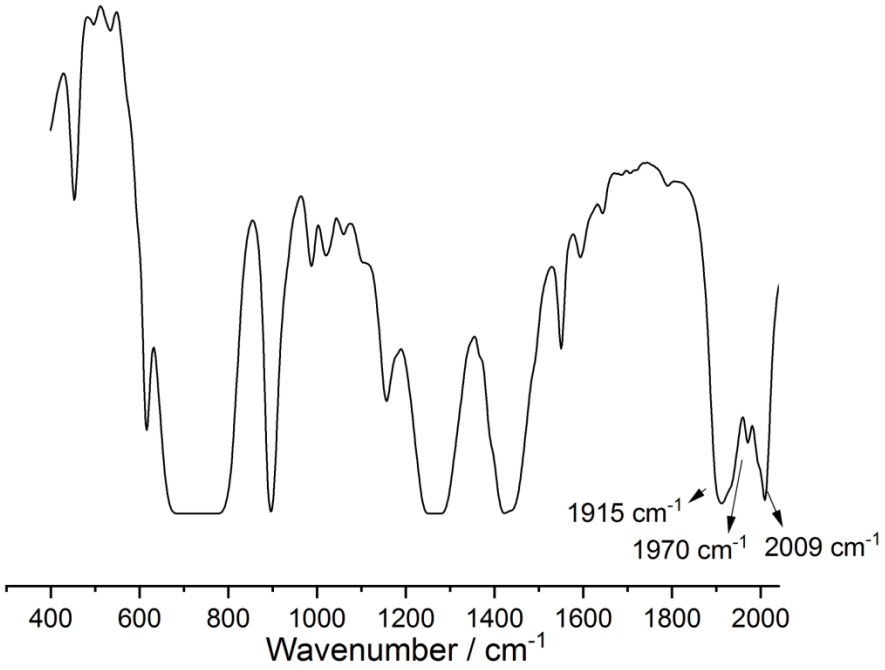


Figure S12. Solution IR spectrum of **6**.

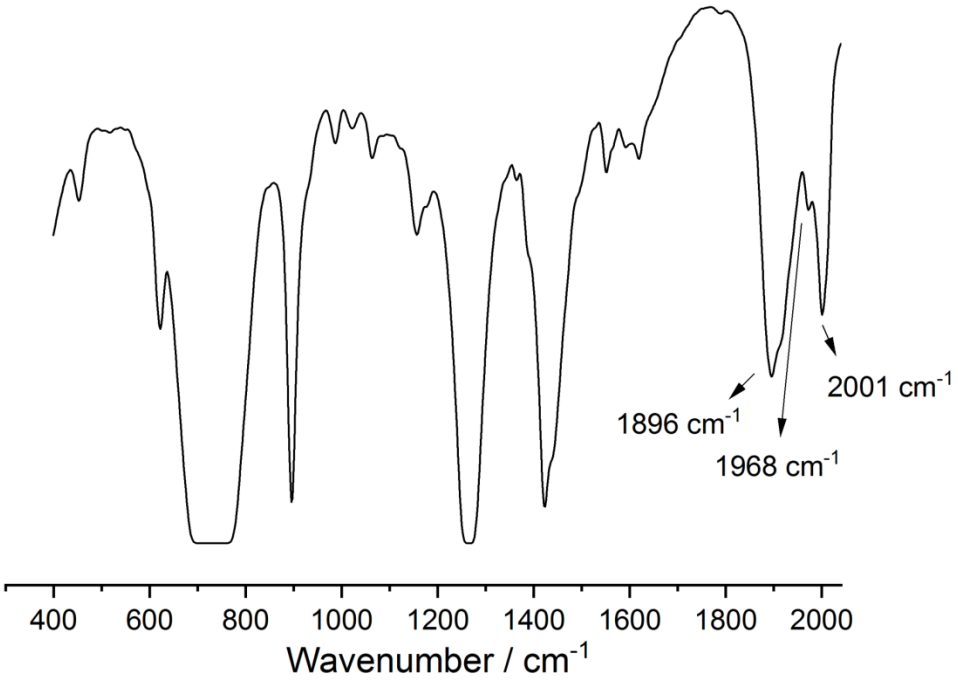


Figure S13. Solution IR spectrum of **7**.

Crystallographic Details

The single crystal data were examined on a Rigaku Supernova diffractometer using either MoKα (λ = 0.71073 Å) or CuKα (λ = 1.54184 Å) radiation. The crystals were kept at 100.0(1) K during data collection. Using Olex2[3], the structures were solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the ShelXL[5] refinement package using Least Squares minimisation. Hydrogen atoms were taken into account using a riding model.

Table T1. Crystal data and structure refinement for compounds **2**, **4** and **5**.

	2	**4**	**5**
Empirical formula	$C_{36}H_{46}N_2$	$C_{39}H_{48}AsCl_2N_2$	$C_{38}H_{41}AsFeN_2O_4$
Formula weight	506.75	690.61	720.50
Temperature/K	100.0(1)	100.0(1)	100.0(1)
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	$P2_1/c$	P-1
a/Å	10.1696(5)	22.4516(5)	10.5768(3)
b/Å	17.3936(8)	9.0396(2)	17.8360(4)
c/Å	18.8594(8)	17.9260(4)	21.1952(4)
α/°	95.703(4)	90	81.8399(16)
β/°	94.597(4)	105.448(2)	87.3548(19)
γ/°	90.041(4)	90	85.871(2)
Volume/Å^3	3308.6(3)	3506.70(14)	3945.04(16)
Z	4	4	4
ρ_{calc}g/cm^3	1.017	1.308	1.213
μ/mm^{-1}	0.437	1.151	4.288
F(000)	1104.0	1452.0	1496.0
Crystal size/mm^3	0.136 × 0.101 × 0.026	0.262 × 0.192 × 0.103	0.229 × 0.145 × 0.088
Radiation/Å	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.724 to 144.252	3.764 to 64.516	5.016 to 154.534
Index ranges	-12 ≤ h ≤ 12, -21 ≤ k ≤ 21, -23 ≤ l ≤ 20	-32 ≤ h ≤ 31, -13 ≤ k ≤ 12, -26 ≤ l ≤ 26	-13 ≤ h ≤ 13, -22 ≤ k ≤ 22, -26 ≤ l ≤ 26
Reflections collected	58682	51545	72562
Independent reflections	13017 [R_{int} = 0.1009, R_{sigma} = 0.0734]	11539 [R_{int} = 0.0537, R_{sigma} = 0.0539]	16360 [R_{int} = 0.0606, R_{sigma} = 0.0423]
Reflections with *I > 2σ(I)*	7705	8523	14713
Data/restraints/parameters	13017/0/705	11539/1/431	16360/0/845
Goodness-of-fit on F^2	1.013	1.029	1.037
Final R indexes [*I > 2σ(I)*]	R_1 = 0.0632, wR_2 = 0.1571	R_1 = 0.0440, wR_2 = 0.0830	R_1 = 0.0356, wR_2 = 0.0911
Final R indexes [all data]	R_1 = 0.1099, wR_2 = 0.1882	R_1 = 0.0718, wR_2 = 0.0934	R_1 = 0.0403, wR_2 = 0.0951
Largest diff. peak/hole/e Å^{-3}	0.22/-0.22	0.89/-0.81	0.61/-0.56
CCDC number	1940136	1940137	1940138

Table T2. Crystal data and structure refinement for compounds **6** and **7**.

	6	**7**
Empirical formula	$AsC_{42}FeH_{49}N_2O_{4.5}$	$C_{45}H_{53}AsFeN_4O_4$
Formula weight	784.60	844.68
Temperature/K	100.0(1)	100.0(1)
Crystal system	monoclinic	monoclinic
Space group	I2/a	$P2_1/n$
a/Å	18.4632(3)	10.33882(14)
b/Å	10.6939(2)	20.3971(3)
c/Å	40.9108(8)	20.0912(2)
α/°	90	90
β/°	101.6009(18)	102.9076(13)
γ/°	90	90
Volume/$Å^3$	7912.6(3)	4129.79(9)
Z	8	4
$\rho_{calc}g/cm^3$	1.317	1.359
μ/mm^{-1}	1.255	4.192
F(000)	3280.0	1768.0
Crystal size/mm^3	0.449 × 0.1 × 0.033	0.365 × 0.174 × 0.033
Radiation/Å	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	3.942 to 64.406	6.256 to 153.27
Index ranges	$-26 \leq h \leq 27$, $-15 \leq k \leq 16$, $-61 \leq l \leq 60$	$-12 \leq h \leq 13$, $-25 \leq k \leq 25$, $-25 \leq l \leq 25$
Reflections collected	92870	79841
Independent reflections	13251 [R_{int} = 0.0538, R_{sigma} = 0.0396]	8652 [R_{int} = 0.0695, R_{sigma} = 0.0315]
Reflections with $I > 2\sigma(I)$	9708	7640
Data/restraints/parameters	13251/0/467	8652/0/508
Goodness-of-fit on F^2	1.036	1.044
Final R indexes [$I > 2\sigma(I)$]	R_1 = 0.0464, wR_2 = 0.1080	R_1 = 0.0328, wR_2 = 0.0822
Final R indexes [all data]	R_1 = 0.0725, wR_2 = 0.1192	R_1 = 0.0393, wR_2 = 0.0866
Largest diff. peak/hole / e $Å^{-3}$	0.64/-0.89	0.46/-0.45
CCDC number	1940139	1955624

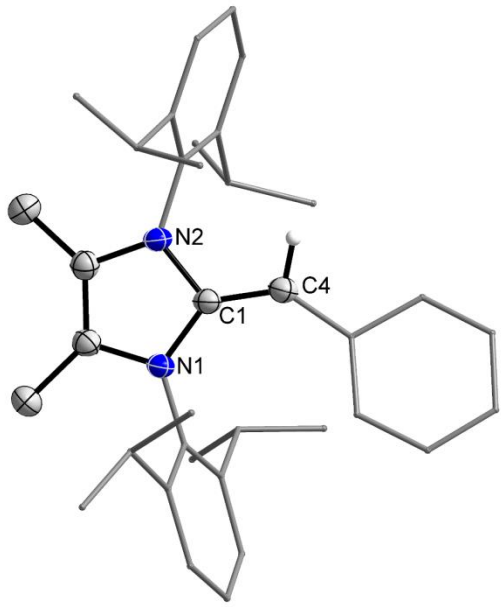


Figure S14. Molecular structure of **2**. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and bond angles (º): C1–C4 1.371(4), N1–C1 1.393(3), N2–C1 1.399(3); C4–C1–N1 135.3(2), C4–C1–N2 121.5(2); N1–C1-N2 103.2(2).

Computational Details

All geometries were optimized without symmetry constraint within the DFT (density functional theory) framework using the M06-2X[6] in combination with the Ahlrichs def2-SVP basis function.[7] For comparison, we also optimized compounds **5-6** using the BP86+D3(BJ)/def2-SVP.[8] These calculations were performed using the Gaussian 16 A.03 software.[9] The stationary points were located with the Berny algorithm[10] using redundant internal coordinates. Analytical Hessians were computed to determine the nature of stationary points (one and zero imaginary frequencies for transition states and minima, respectively)[11] and to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects using the standard statistical-mechanics relationships for an ideal gas. The electronic energies were improved by single point calculations at the M06-2X/def2-TZVPP level of theory.

The Wiberg Bond Indices (WBI)[12] and NPA[13] atomic partial charges have been calculated at the M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory using GENNBO 6.0 programs.[14]

The nature of the chemical bond was investigated by means of an energy decomposition analysis (EDA), which was developed by Morokuma[15] and by Ziegler and Rauk.[16] The EDA focuses on the instantaneous interaction energy ΔE_{int} of a bond A-B between the fragments A and B in the particular electronic reference state at the frozen geometry of the molecule AB.[17] The interaction energy ΔE_{int} is divided into four main components [Eq. (1)].

$$\Delta \mathrm{E_{int}} = \Delta \mathrm{E_{elstat}} + \Delta \mathrm{E_{Pauli}} + \Delta \mathrm{E_{orb}} + \Delta \mathrm{E_{disp}} \qquad (1)$$

The term ΔE_{elstat} corresponds to the quasiclassical electrostatic interaction between the unperturbed charge distributions of the prepared atoms and is usually attractive. The Pauli repulsion ΔE_{Pauli} arises as the energy change associated with the transformation from the superposition of the unperturbed electron densities $\rho^A + \rho^B$ of the isolated fragments to the wavefunction $\Psi^0 = \mathrm{N\hat{A}[\Psi_A \Psi_B]}$, which properly obeys the Pauli principle through explicit antisymmetrization ($\hat{A}$ operator) and renormalization (N = constant) of the product wavefunction. ΔE_{Pauli} comprises the destabilizing interactions between electrons of the same spin on either fragment. The orbital interaction ΔE_{orb} accounts for charge transfer, polarization effects and electron-pair bonding.[18] In the case that the Grimme dispersion corrections [19] are computed the term ΔE_{disp} is added to the equation to count the dispersion interaction between the fragments.

The relaxation of the fragments to their equilibrium geometries at the electronic ground state is termed ΔE_{prep}, because it may be considered as preparation energy for chemical bonding. The addition of ΔE_{prep} to the intrinsic interaction energy ΔE_{int} gives the total energy ΔE, which is - by definition with opposite sign - the bond dissociation energy D_e:

$$\Delta E\,(-D_e) = \Delta E_{int} + \Delta E_{prep} \qquad (2)$$

The EDA–NOCV method combines the EDA with the natural orbitals for chemical valence (NOCV) to decompose the orbital interaction term ΔE_{orb} into pairwise contributions. The NOCVs Ψi are defined as the eigenvector of the valence operator, $\widehat{V}$, given by Equation (3).

$$\widehat{V}\Psi_i = v_i\Psi_i \qquad (3)$$

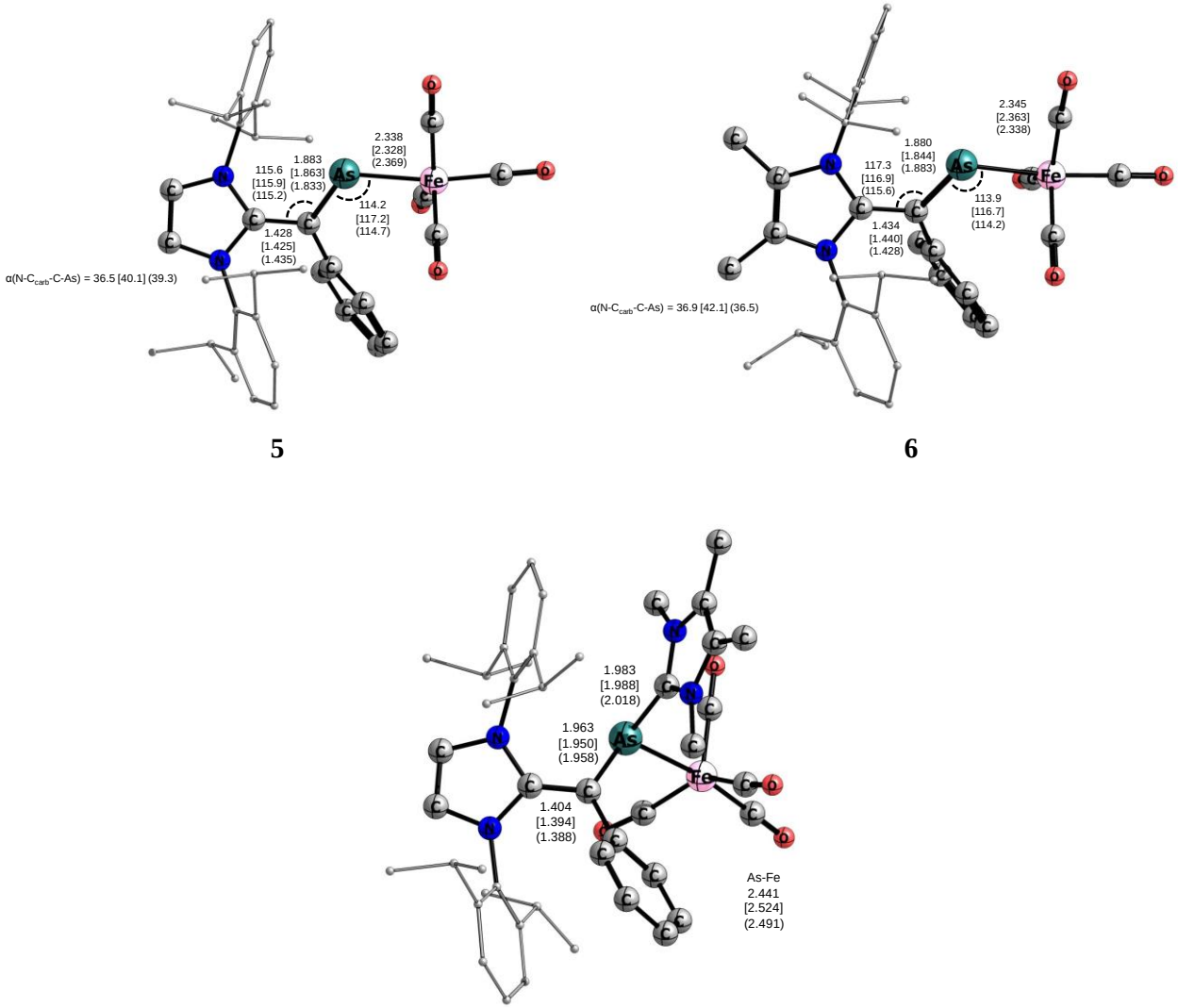
In the EDA–NOCV scheme the orbital interaction term, ΔE_{orb}, is given by Equation (4),

$$\Delta E_{orb} = \sum_k \Delta E_k^{orb} = \sum_{k=1}^{\frac{N}{2}} v_k\left[-F_{-k,-k}^{TS} + F_{k,k}^{TS}\right] \qquad (4)$$

in which $F_{-k,-k}^{TS}$ and $F_{k,k}^{TS}$ are diagonal transition state Kohn–Sham matrix elements corresponding to NOCVs with the eigenvalues –νk and νk, respectively. The ΔE_k^{orb} term for a particular type of bond is assigned by visual inspection of the shape of the deformation density Δρk. The latter term is a measure of the size of the charge deformation and it provides a visual notion of the charge flow that is associated with the pairwise orbital interaction. The EDA–NOCV scheme thus provides both qualitative and quantitative information about the strength of orbital interactions in chemical bonds.

The EDA–NOCV calculations were carried out with program package ADF2018.105[20] using DFT functional BP86[21] with Grimme dispersion corrections D3(BJ) [19] and M06-2X with uncontracted Slater-type orbitals (STOs) [22] with TZ2P quality as basis functions. The latter basis sets for all elements have triple-ζ quality augmented by two sets of polarization functions. An auxiliary set of s, p, d, f, and g STOs was used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle. [23] Scalar relativistic effects have been incorporated by applying the zeroth-order regular approximation (ZORA).[24] The EDA-NOCV calculations at BP86+D3(BJ)/TZ2P and M06-2X/TZ2P level were performed using M06-2X/def2-SVP optimized geometries.

Optimized structures of 5, 6, and 7

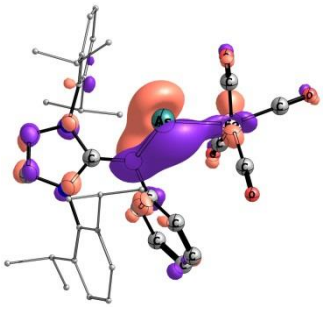


5 **6**

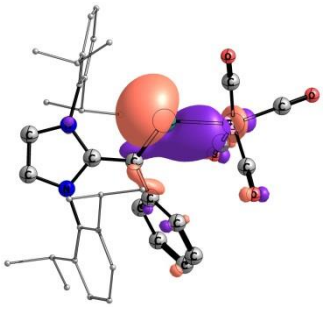
7

Figure S15. Optimized structures of compounds **5**, **6**, and **7** at the BP86+D3(BJ)/def2-SVP [and M06-2X/def2-SVP] level of theory. Selected calculated (experimental in parenthesis) bond length and bond angles are in [Å] and [°], respectively. Hydrogen atoms were omitted for clarity.

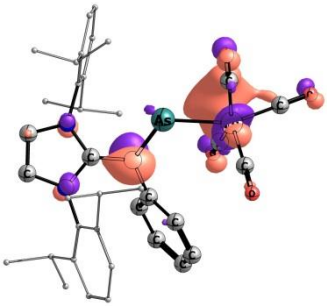
Molecular Orbitals



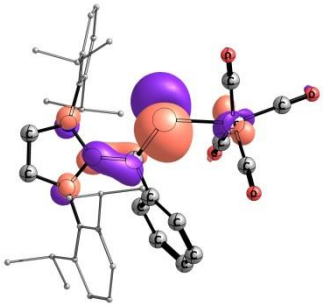
HOMO-2 (ε = -7.18 eV)



HOMO-1 (ε = -6.49 eV)

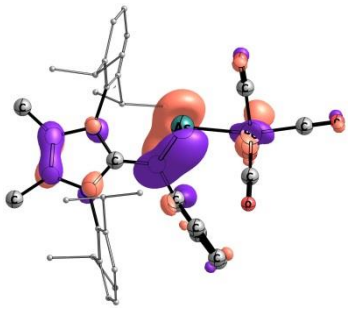


HOMO (ε = -5.65 eV)

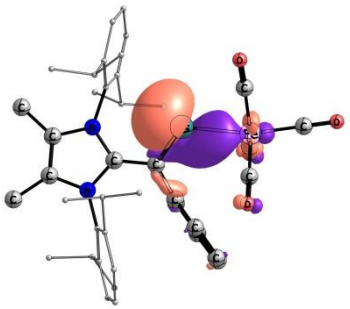


LUMO (ε = -1.15 eV)

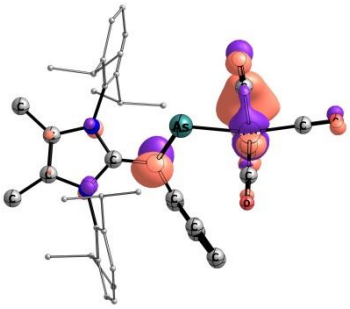
Figure S16. Frontier Molecular Orbitals (isosurface 0.05 a.u.) at M06-2X/def2-TZVPP//M06-2X/def2-SVP of **5**. Hydrogen atoms were omitted for clarity.



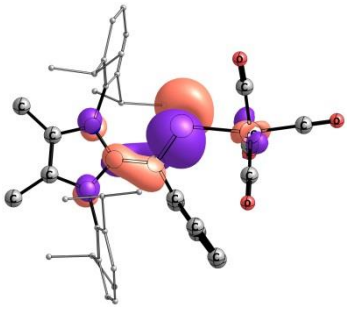
HOMO-2 (ε = -7.05 eV)



HOMO-1 (ε = -6.37 eV)

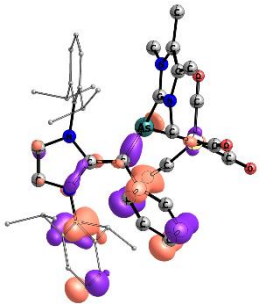


HOMO (ε = -5.80 eV)

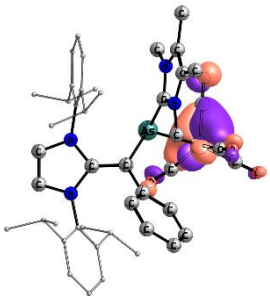


LUMO (ε = -1.11 eV)

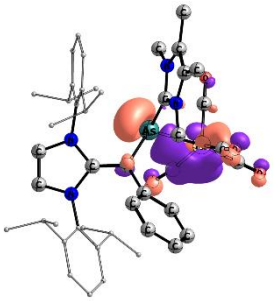
Figure S17. Frontier Molecular Orbitals (isosurface 0.05 a.u.) at M06-2X/def2-TZVPP//M06-2X/def2-SVP of **6**. Hydrogen atoms were omitted for clarity.



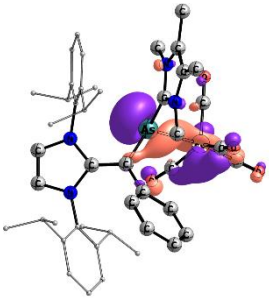
HOMO-4 (ε = -7.43 eV)



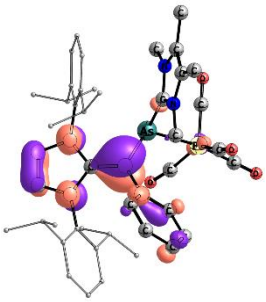
HOMO-3 (ε = -7.05 eV)



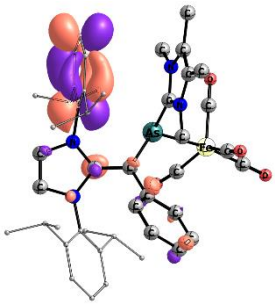
HOMO-2 (ε = -6.23 eV)



HOMO-1 (ε = -5.81 eV)



HOMO (ε = --5.60 eV)

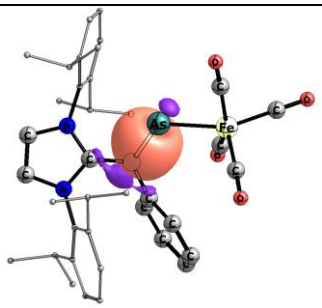
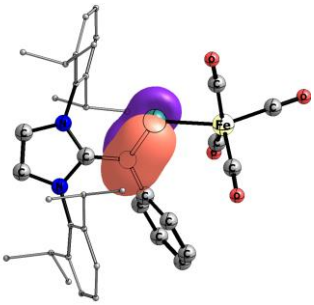
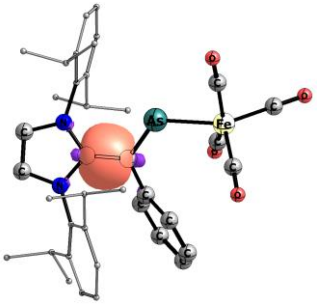
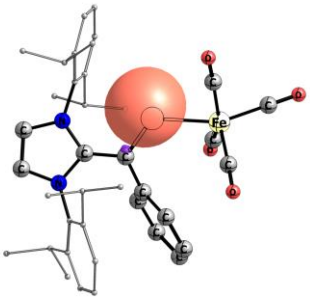
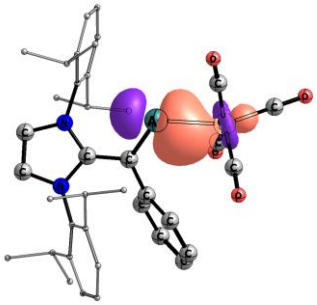


LUMO (ε = 0.01 eV)

Figure S18. Frontier Molecular Orbitals (isosurface 0.05 a.u.) at M06-2X/def2-TZVPP//M06-2X/def2-SVP of **7**. Hydrogen atoms were omitted for clarity.

Table T3. NBO results at the M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory of compounds **5**, **6**, and **7**. Wiberg bond order (P) and partial charges (q).

	5	**6**	**7**
$q(C_{carb})_{IPr}$	+0.48	+0.48	0.44
$q(C_{carb})_{IMe4}$	-	-	0.22
$q(C_{vinyl})$	-0.64	-0.21	-0.59
q(As)	+0.39	+0.42	+0.37
$q(Fe(CO)_4)$	-0.30	-0.40	-0.45
$P(C_{IPr}–C_{vinyl})$	1.24	1.18	1.45
$P(C_{vinyl}–As)$	1.18	1.29	0.89
P(As–Fe)	0.62	0.56	0.37
$P(As–C_{carb\ (IMe4)})$	-	-	0.86

Orbital	Occ.	Contribution from atoms to the orb	Atomic orbitals
	1.94	As (32.12%) - C (67.88%)	As: *s* (16.57%), *p* (82.99%), *d* (0.44%) C: *s* (31.23%), *p* (68.73%), *d* (0.04%)
	1.71	As (29.15%) - C (70.85%)	As: *s* (0.03%), *p* (99.31%), *d* (0.66%) C: *s* (0.06%), *p* (99.93%), *d* (0.01%)
	1.97	C_{carb} (52.30%) –C (47.70%)	C_{carb}: *s* (42.38%), *p* (57.59%), *d* (0.03%) C: *s* (33.72%), *p* (66.20%), *d* (0.08%)
	1.95	LP (As)	*s* (70.80%), *p* (29.17%), *d* (0.03%)
	1.77	As (67.58%) –Fe (32.42%)	As: *s* (13.43%), *p* (86.36%), *d* (0.21%) C: *s* (8.47%), *p* (0.53%), *d* (91.01%)

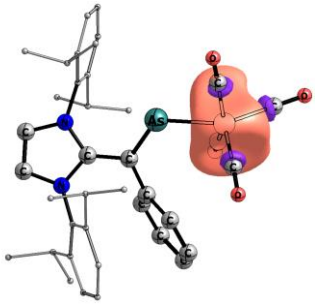
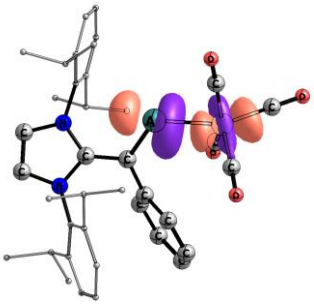
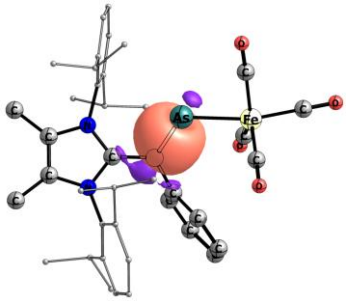
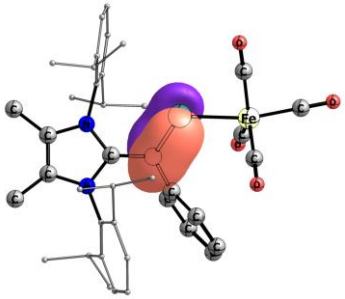
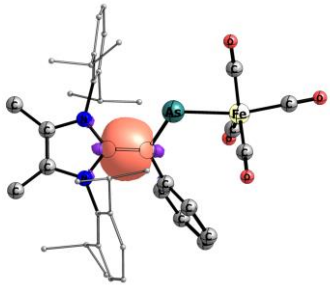
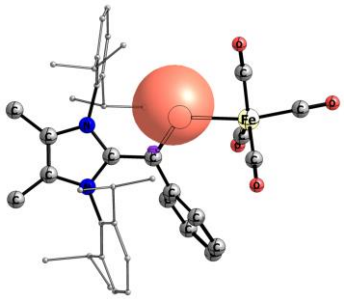
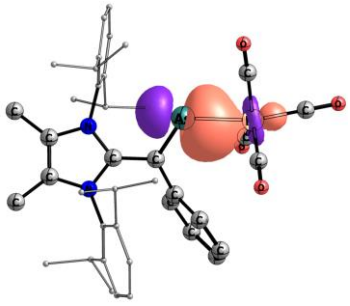
	0.46	LV(Fe)	*s* (90.69%), *p* (0.06%), *d* (9.24%)
	0.51	As (67.58%) –Fe (32.42%)	As: *s* (13.43%), *p* (86.36%), *d* (0.21%) C: *s* (8.47%), *p* (0.53%), *d* (91.01%)

Figure S19. NBO results at the M06-2X/def2-TZVPP//M06-2X/def2-SVP of **5**. Hydrogen atoms were omitted for clarity.

Orbital	Occ.	Contribution from atoms to the orb	Atomic orbitals
	1.94	As (31.69%) - C (68.31%)	As: *s* (17.05%), *p* (82.52%), *d* (0.43%) C: *s* (31.98%), *p* (67.98%), *d* (0.05%)
	1.77	As (30.12%) - C (69.88%)	As: *s* (0.09%), *p* (99.23%), *d* (0.67%) C: *s* (0.11%), *p* (99.88%), *d* (0.01%)
	1.97	C_{carb} (52.33%) –C (47.67%)	C_{carb}: *s* (41.79%), *p* (58.18%), *d* (0.03%) C: *s* (33.13%), *p* (66.79%), *d* (0.08%)
	1.95	LP (As)	*s* (70.52%), *p* (29.45%), *d* (0.02%)
	1.79	As (69.97%) - Fe (30.03%)	As: *s* (13.21%), *p* (86.63%), *d* (0.16%) Fe: s (9.57%), *p* (0.43%), *d* (90.00%)

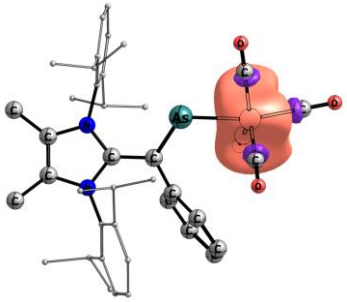
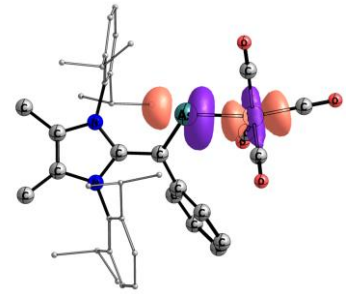
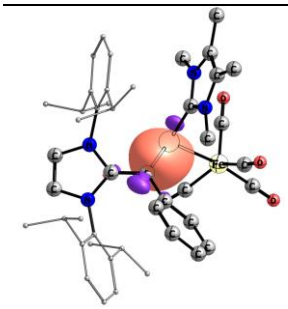
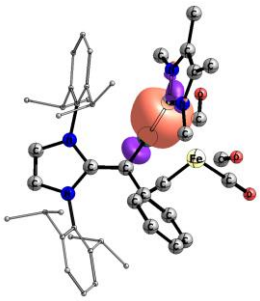
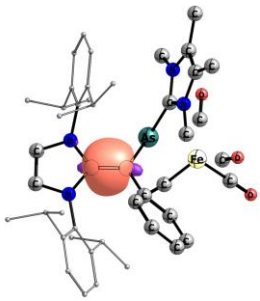
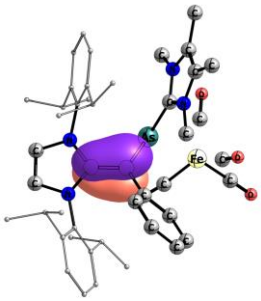
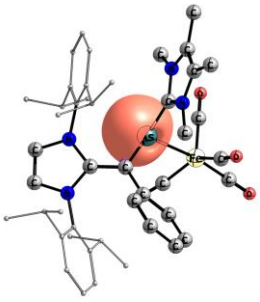
	0.47	LV(Fe)	*s* (90.03%), *p* (0.06%), *d* (9.90%)
	0.45	As (30.03%) –Fe (69.97%)	As: *s* (13.21%), *p* (86.63%), *d* (0.16%) C: *s* (9.57%), *p* (0.43%), *d* (90.00%)

Figure S20. NBO results at the M06-2X/def2-TZVPP//M06-2X/def2-SVP of **6**. Hydrogen atoms were omitted for clarity.

Orbital	Occ.	Contribution from atoms to the orb	Atomic orbitals
	1.93	As (35.93%) - C (64.07%)	As: *s* (21.36%), *p* (78.47%), *d* (0.15%) C: *s* (30.21%), *p* (69.64%), *d* (0.12%)
	1.96	As (29.44%) - C_{carb} (70.56%)	As: *s* (12.55%), *p* (87.19%), *d* (0.25%) C_{carb}: *s (40.00%)*, *p* (59.91%) *d* (0.06%)
	1.97	C_{carb} (52.80%) –C (47.20%)	C_{carb}: *s* (42.74%), *p* (57.15%), *d* (0.04%) C: *s* (34.15%), *p* (65.70%), *d* (0.12%)
	1.87	C_{carb} (35.61%) –C (64.39%)	C_{carb}: *s* (0.48%), *p* (99.40%), *d* (0.06%) C: *s* (0.13%), *p* (99.77%), *d* (0.05%)
	1.89	LP (As)	*s* (58.21%), *p* (41.74%), *d* (0.05%)

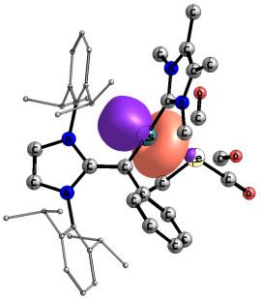
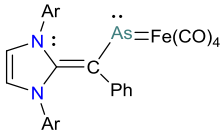
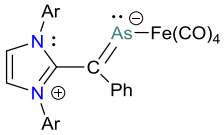
	1.32	LP (As)	*s* (8.07%), *p* (91.75%), *d* (0.17%)

Figure S21. NBO results at the M06-2X/def2-TZVPP//M06-2X/def2-SVP of **7**. Hydrogen atoms were omitted for clarity.



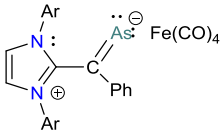
Wgt = 40.4 %

ρNL = 10.1



Wgt = 20.5 %

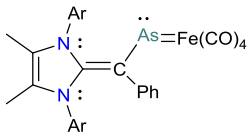
ρNL = 9.9



Wgt = 14.1 %

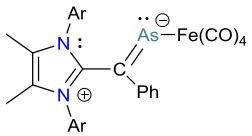
ρNL =10.3

Figure S22. Natural Resonance Theory results weight (Wgt) and Non-Lewis density (ρNL) at M06-2X/def2-SVP of **5**.



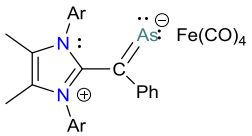
Wgt = 32.2 %

ρNL = 10.1



Wgt = 32.6 %

ρNL = 9.9



Wgt = 22.2 %

ρNL = 10.9

Figure S23. Natural Resonance Theory results weight (Wgt) and Non-Lewis density (ρNL) at M06-2X/def2-SVP of **6**.

Table T4. Energy decomposition analysis (EDA) for **5** and **6** at BP86+D3(BJ)/TZ2P. Energy values are given in kcal/mol.[a]

Compounds	**5**		**6**	
Energy term	(IPr)C(Ph)As$^{(S)}$; Fe(CO)$_4$$^{(S)}$	(IPr)C(Ph)As$^{(T)}$; Fe(CO)$_4$$^{(T)}$	(Me-IPr)C(Ph)As$^{(S)}$; Fe(CO)$_4$$^{(S)}$	(Me-IPr)C(Ph)As$^{(T)}$; Fe(CO)$_4$$^{(T)}$
E_{int}	-90.06	-88.1	-89.61	-94.3
E_{Pauli}	152.26	177.0	138.39	163.5
E_{disp}[b]	-18.1 (8.1 %)	-18.1 (7.3 %)	-18.3 (8.7 %)	-18.3 (7.7 %)
E_{elstat}[b]	-119.6 (53.3 %)	-123.0 (49.8 %)	-109.8 (52.7 %)	-113.8 (47.5 %)
E_{orb}[b]	-104.7 (46.7 %)	-123.9 (50.2 %)	-99.8 (47.6 %)	-125.7 (52.5 %)
$E_{orb\ \sigma\text{-don}}$[c]	-70.1 (67.0 %)		-72.7 (72.8%)	
$E_{orb\ \pi\text{-back don}}$[c]	-20.1 (19.2 %)		-14.6 (14.6 %)	
$E_{orb\ rest}$[c]	-14.5 (20.7 %)		-12.6 (12.6 %)	
$E_{prep\ RAs}$	4.2	5.7	3.9	8.3
$E_{prep\ Fe(CO)4}$	12.6	9.2	11.7	12.0
E_{prep}	16.8	14.9	15.6	20.3
$-D_e = E$	-73.2	-73.2	-74.0	-74.0

[a]S and T stand for singlet and triplet reference states, respectively. [b]The value in parentheses gives the percentage contribution to the total attractive interactions $E_{elstat} + E_{orb} + E_{disp}$. [c]The value in parentheses gives the percentage to the total orbital interaction.

Table T5. Relative Energies (kcal/mol) and Bond lengths (Å) of free arsinidines.[ab]

		(IPr)C(Ph)As	(Me-IPr)C(Ph)As	As-H	As-Ph	As-OH	As-NH$_2$
T	E_{rel}	0.0	0.0	0.0	0.0	0.0	0.0
	R(P-R)	1.908	1.913	1.530	1.928	1.789	1.820
S	E_{rel}	+9.2	+9.9	+34.5	+22.3	+36.2	+7.4
	R(P-R)	1.823	1.818	1.529	1.914	1.765	1.764

[a] S and T stand for singlet and triplet reference states, respectively. [b] All calculations were performed at the M06-2X/def2-SVP level of theory.

Table T6. Energy decomposition analysis (EDA) with different fragmentation schemes for arsinidene iron complexes at the BP86+D3(BJ)/TZ2P. Energy values are given in kcal/mol.[a]

	$HAs=Fe(CO)_4$		$PhAs=Fe(CO)_4$		$HOAs=Fe(CO)_4$		$H_2NAs=Fe(CO)_4$	
	HAs (S); $Fe(CO)_4$ (S)	HAs (T); $Fe(CO)_4$ (T)	PhAs (S); $Fe(CO)_4$ (S)	PhAs (T); $Fe(CO)_4$ (T)	HOAs (S); $Fe(CO)_4$ (S)	HOAs (T); $Fe(CO)_4$ (T)	H_2NAs (S); $Fe(CO)_4$ (S)	H_2NAs (T); $Fe(CO)_4$ (T)
ΔE_{int}	-113.9	-68.8	-111.1	-67.1	-119.6	-73.13	-88.13	-80.4
ΔE_{Pauli}	82.2	179.4	157.7	190.8	90.9	197.44	172.54	189.1
ΔE_{disp}[b]	-6.8 (3.4 %)	-6.8 (2.7 %)	-10.5 (3.9 %)	-10.5 (3.9 %)	-7.4 (3.5 %)	-7.4 (2.7 %)	-8.1 (3.1 %)	-8.1 (3.0 %)
ΔE_{elstat}[b]	-18.1 (9.2 %)	-125.5 (50.6 %)	-123.7 (46.0 %)	-129.9 (46.0 %)	-23.8 (11.3 %)	-138.3 (51.1 %)	-139.0 (35.5 %)	-133.8 (49.7 %)
ΔE_{orb}[b]	-171.2 (87.3 %)	-115.9 (46.7 %)	-134.6 (50.1 %)	-117.5 (50.1 %)	-179.3 (85.2 %)	-124.9 (46.1 %)	-113.6 (43.6 %)	-127.6 (47.3 %)
$\Delta E_{prep\ Fe(CO)4}$	21.9	8.8	20.6	9.8	16.5	8.8	12.1	8.7
$\Delta E_{prep\ RAs}$	32.0	0.0	33.5	0.3	38.8	0.0	5.1	0.8
$\Delta E_{prep\ tot}$	53.9	8.8	54.1	10.1	55.3	8.8	17.2	9.5
$-D_e = E$	-60.0	-60.0	-57.0	-57.0	-64.4	-64.4	-71.0	-71.0

[a] S and T stand for singlet and triplet reference states, respectively.

[b] The value in parentheses gives the percentage contribution to the total attractive interactions $Eelstat + Eorb + Edisp$.

Table T7. NBO results at the M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory of arsinidene iron complexes: Wiberg bond order (P) and partial charges (q).

	$HAs=Fe(CO)_4$	$PhAs=Fe(CO)_4$	$HOAs=Fe(CO)_4$	$H_2NAs=Fe(CO)_4$
q(As)	-0.09	+0.22	+0.56	+0.58
$q(Fe(CO)_4)$	+0.15	+0.16	-0.01	-0.17
P(As-Fe)	0.99	0.96	0.91	0.75
d(As-Fe)	2.277	2.276	2.240	2.269

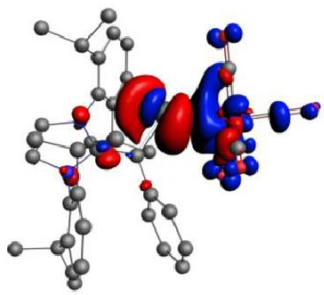
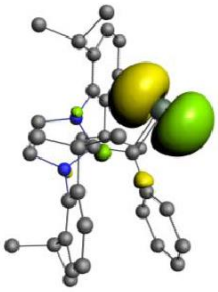
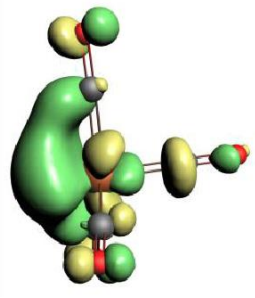
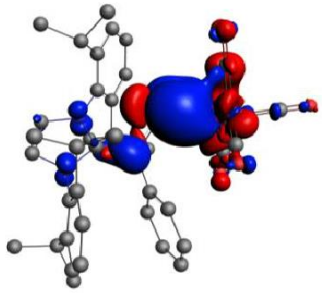
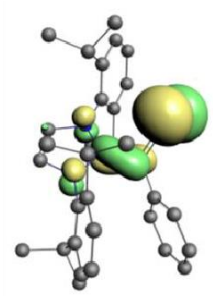
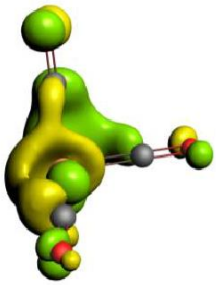
Deformation densities	(NHC)C(Ph)As Molecular Orbitals		Fe(CO)$_4$ Molecular Orbitals
		→	
$E_{orb\ \rho(1)}$ = -70.1 |ν_1| = 1.18	HOMO (ε= -3.03 eV) ν_1 = -0.75		LUMO (ε =-5.30 eV) ν_1 = +0.80
		←	
$\Delta E_{orb\ \rho\ (2)}$= -20.1 |$\nu_2$| = 0.69	LUMO (ε =-2.70 eV) ν_2= +0.27		HOMO (ε =-5.40 eV) ν_2= -0.24

Figure S24. Deformation densities $\Delta\rho$ (isovalue 0.001 a.u.) of the pairwise orbital interactions between (NHC)C(Ph)As and Fe(CO)$_4$ within compound **5**. For the deformation densities the red color shows the charge outflow, whereas blue shows charge density accumulation.

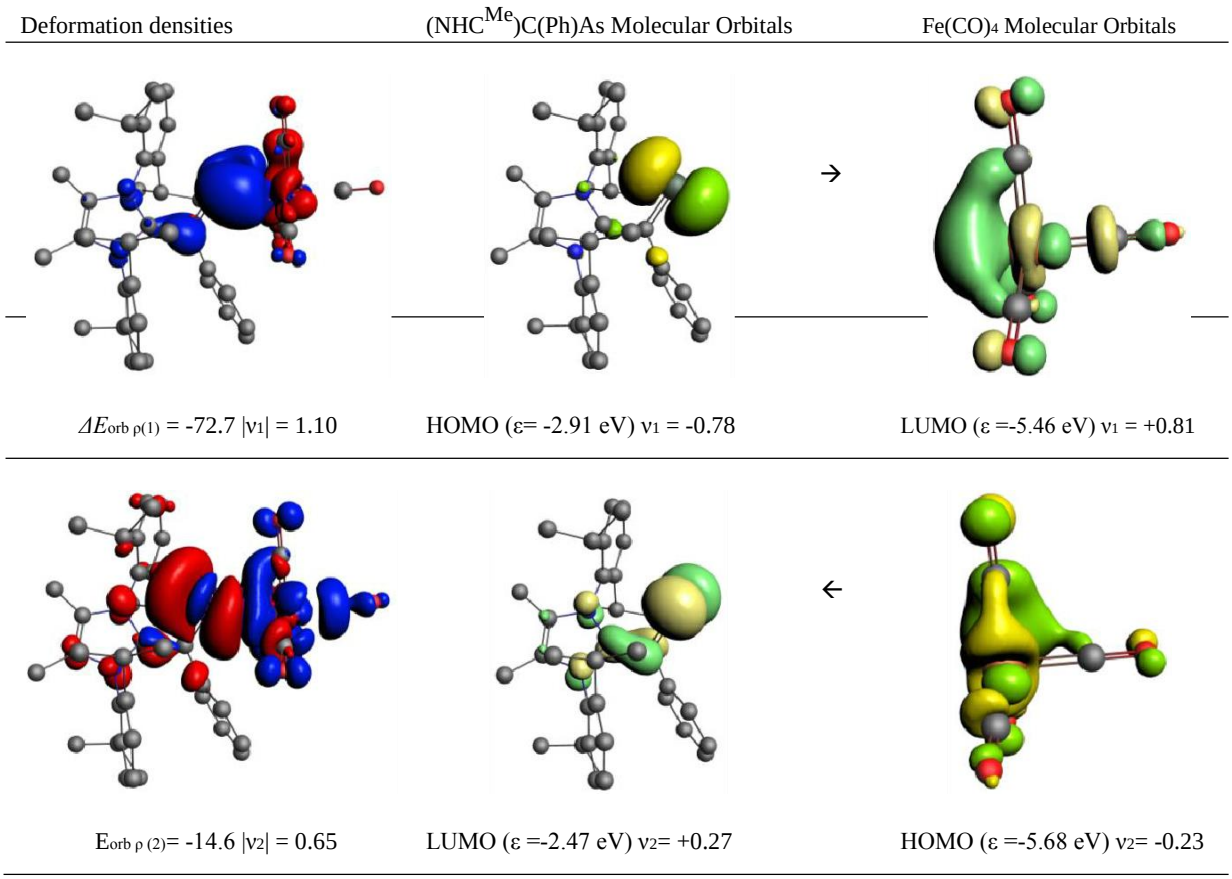


Figure S25. Deformation densities $\Delta\rho$ (isovalue 0.001 a.u.) of the pairwise orbital interactions between (NHC^{Me})C(Ph)As and Fe(CO)$_4$ within compound **6**. For the deformation densities the red color shows the charge outflow, whereas blue shows charge density accumulation.

Table T8. Energy decomposition analysis (EDA) with different fragmentation schemes for **7** complex at the BP86+D3(BJ)/TZ2P. Energy values are given in kcal/mol.[a]

	(IPr)C(Ph)As-Fe(CO)$_4$ (S), IMe$_4$(S)
ΔE_{int}	-61.5
ΔE_{Pauli}	314.7
ΔE_{disp}[b]	-190.0 (8.0 %)
ΔE_{elstat}[b]	-30.1 (50.5 %)
ΔE_{orb}[b]	-156.1 (41.5 %)
$\Delta E_{orb\ \sigma\text{-don}}$[c]	-120.8 (77.4 %)
$\Delta E_{orb\ \pi\text{-back don}}$[c]	-9.2 (5.9 %)
$\Delta E_{orb\ rest}$[c]	-26.1 (16.7 %)
$\Delta E_{prep\ RAsFe(CO)4}$	18.2
$\Delta E_{prep\ IMe4}$	3.3
$\Delta E_{prep\ tot}$	21.5
$-D_e = \Delta E$	-40.0

[a] S and T stand for singlet and triplet reference states, respectively.
[b] The value in parentheses gives the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.
[c] The value in parentheses gives the percentage contribution to the total orbital interactions.

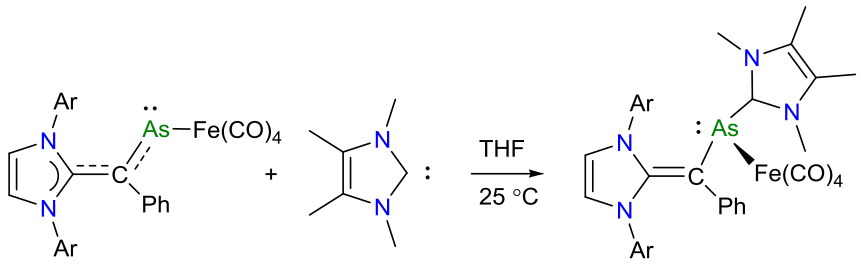


Table T9. Thermodynamic parameters (in kcal/mol) at different level of theory

Method	**ΔE**	**ΔE+ZPE**	**ΔH**	**ΔG**
PCM(THF)-M06-2X/def2-TZVPP//M06-2X/def2-SVP	-28.7	-28.9	-29.5	-11.9
PCM(THF)-B3LYP+D3(BJ)/def2-TZVPP//M06-2X/def2-SVP	-28.7	-28.9	-29.5	-11.9
PCM(THF)-BP86+D3(BJ)/def2-TZVPP//M06-2X/def2-SVP	-33.8	-34.0	-34.6	-17.0

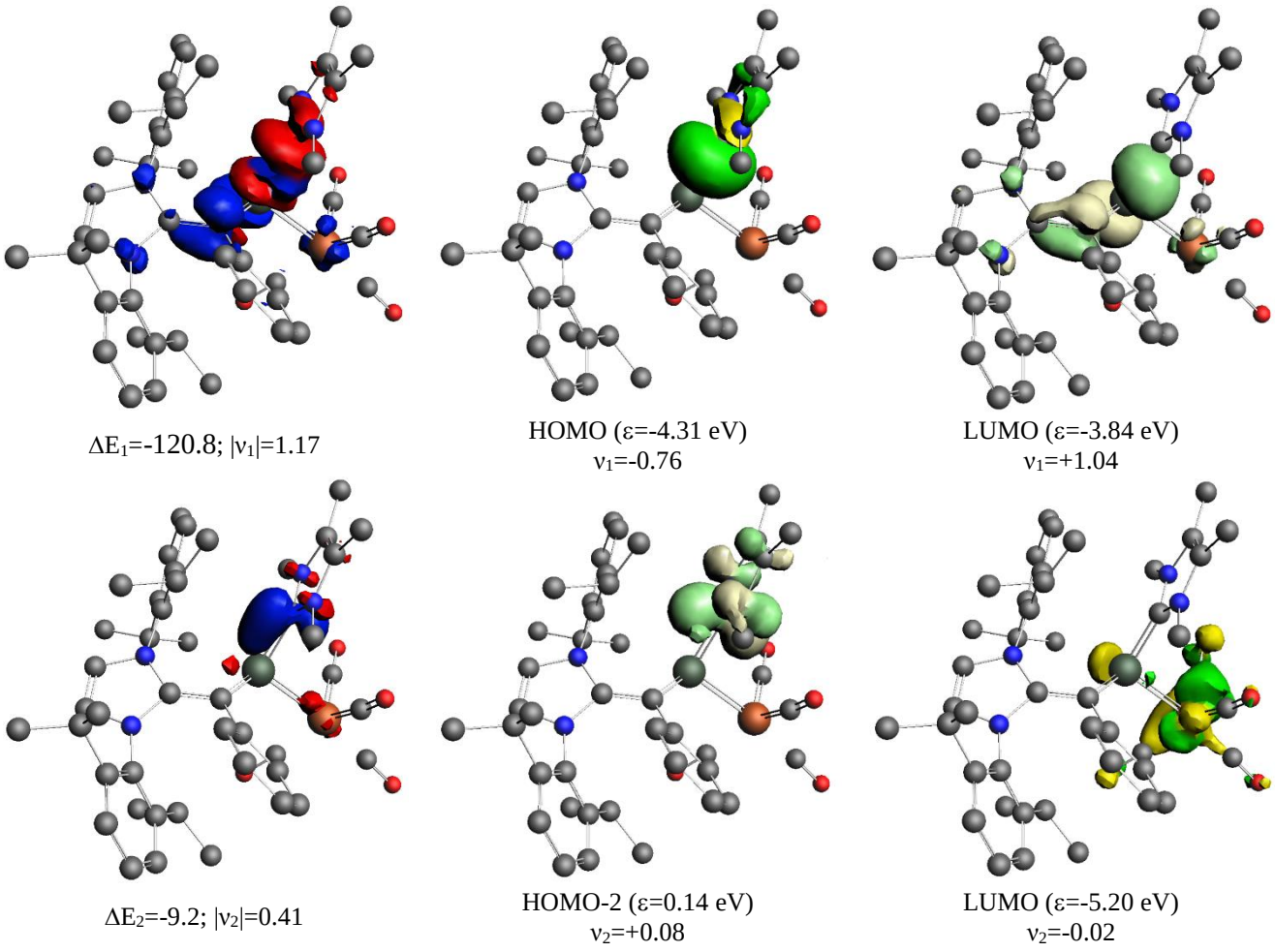


Figure S26. Deformation densities $\Delta\rho$ (isovalue 0.003 a.u.) of the pairwise orbital interactions between IMe_4 and [{(IPr)C(Ph)}AsFe$(CO)_4$] of compound **7** (MOs = molecular orbitals). Associated energies ΔE (in kcal/mol) and eigenvalues ν (in a.u.). The red colour shows the charge outflow, whereas blue shows charge density accumulation. Shape of the most important interacting occupied and vacant orbitals (isovalue 0.05 a.u.) of the fragments.

Cartesian xyz coordinate

5
Energy (M06-2X/def2-SVP)= -5382.60385774

As	1.558768000000	-0.321877000000	0.390510000000
Fe	2.668303000000	-2.305174000000	-0.116563000000
O	4.652800000000	-1.080672000000	1.758150000000
O	4.794895000000	-3.936126000000	-1.394153000000
O	1.253926000000	-2.121734000000	-2.706942000000
O	1.175846000000	-4.255538000000	1.471386000000
N	-0.310978000000	2.358924000000	0.081276000000
N	-2.123138000000	1.232442000000	0.524281000000
C	-0.832559000000	1.093337000000	0.077883000000
C	-1.259211000000	3.260467000000	0.540274000000
H	-1.044413000000	4.321860000000	0.596173000000
C	-2.381270000000	2.561230000000	0.821142000000
H	-3.332197000000	2.879361000000	1.232625000000
C	0.964893000000	2.793201000000	-0.424347000000
C	1.958944000000	3.175963000000	0.495382000000
C	3.158782000000	3.668642000000	-0.020137000000
H	3.951610000000	3.972279000000	0.664795000000
C	3.367859000000	3.756850000000	-1.393730000000
H	4.317004000000	4.135235000000	-1.776372000000
C	2.373855000000	3.356955000000	-2.277860000000
H	2.547842000000	3.423051000000	-3.353583000000
C	1.145800000000	2.873784000000	-1.813726000000
C	1.759067000000	3.059954000000	1.997384000000
H	0.923083000000	2.362477000000	2.162760000000
C	1.394837000000	4.416973000000	2.611526000000
H	0.481418000000	4.840589000000	2.171443000000
H	2.208739000000	5.140748000000	2.451692000000
H	1.235371000000	4.318624000000	3.695512000000

C	2.983839000000	2.469708000000	2.699854000000
H	3.835902000000	3.165680000000	2.679423000000
H	3.289561000000	1.524304000000	2.231454000000
H	2.749242000000	2.273350000000	3.756409000000
C	0.080443000000	2.462492000000	-2.814742000000
H	-0.788316000000	2.079871000000	-2.257448000000
C	-0.395458000000	3.667098000000	-3.633378000000
H	0.425959000000	4.085603000000	-4.234580000000
H	-0.778638000000	4.466088000000	-2.982061000000
H	-1.198142000000	3.368045000000	-4.323377000000
C	0.587611000000	1.335274000000	-3.719109000000
H	0.893046000000	0.458088000000	-3.130159000000
H	1.449885000000	1.666756000000	-4.317379000000
H	-0.200322000000	1.019763000000	-4.419717000000
C	-2.944820000000	0.133979000000	0.958116000000
C	-4.046995000000	-0.254943000000	0.174818000000
C	-4.769407000000	-1.373474000000	0.596094000000
H	-5.617295000000	-1.719697000000	0.004795000000
C	-4.418435000000	-2.060118000000	1.755066000000
H	-4.992505000000	-2.936473000000	2.060067000000
C	-3.346976000000	-1.629696000000	2.528568000000
H	-3.093737000000	-2.165608000000	3.445052000000
C	-2.583452000000	-0.521603000000	2.147083000000
C	-4.476159000000	0.527283000000	-1.055854000000
H	-3.567636000000	0.962686000000	-1.502625000000
C	-5.422012000000	1.673480000000	-0.667976000000
H	-4.965161000000	2.381183000000	0.034562000000
H	-6.327904000000	1.267267000000	-0.192844000000
H	-5.727505000000	2.236270000000	-1.562435000000
C	-5.161614000000	-0.341401000000	-2.111869000000
H	-6.180455000000	-0.615045000000	-1.797820000000

H	-4.599264000000	-1.263003000000	-2.305315000000
H	-5.253528000000	0.218004000000	-3.054064000000
C	-1.456854000000	-0.030585000000	3.044019000000
H	-0.846034000000	0.688643000000	2.480379000000
C	-2.042999000000	0.710188000000	4.252211000000
H	-2.663566000000	0.034174000000	4.860383000000
H	-2.674254000000	1.553700000000	3.935897000000
H	-1.237776000000	1.101700000000	4.891327000000
C	-0.518911000000	-1.153673000000	3.490146000000
H	-0.105420000000	-1.699020000000	2.629246000000
H	-1.029756000000	-1.876527000000	4.144137000000
H	0.325436000000	-0.732966000000	4.055710000000
C	-0.185117000000	-0.135361000000	-0.239010000000
C	-0.997600000000	-1.203527000000	-0.880133000000
C	-1.562151000000	-1.013527000000	-2.149808000000
H	-1.425151000000	-0.054618000000	-2.653650000000
C	-2.237362000000	-2.046221000000	-2.799253000000
H	-2.638278000000	-1.883510000000	-3.801781000000
C	-2.392441000000	-3.284157000000	-2.178571000000
H	-2.917604000000	-4.093963000000	-2.687734000000
C	-1.864178000000	-3.479581000000	-0.901123000000
H	-1.985762000000	-4.439662000000	-0.396193000000
C	-1.171743000000	-2.453837000000	-0.265972000000
H	-0.760914000000	-2.613333000000	0.731580000000
C	3.917207000000	-1.551985000000	1.024283000000
C	3.982242000000	-3.310818000000	-0.903762000000
C	1.772999000000	-2.188783000000	-1.691109000000
C	1.772897000000	-3.510656000000	0.846138000000

6

Energy (M06-2X/def2-SVP)= -5461.22893783

As	-1.661218000000	0.063924000000	-0.436940000000
Fe	-3.348575000000	-1.560828000000	-0.127584000000
O	-4.933310000000	0.494748000000	-1.594817000000
O	-5.817579000000	-3.043346000000	0.585601000000
O	-2.296811000000	-1.843457000000	2.612930000000
O	-2.165741000000	-3.505616000000	-1.960626000000
N	0.937414000000	2.029643000000	0.199422000000
N	2.306958000000	0.423527000000	-0.311930000000
C	1.026325000000	0.674866000000	0.092119000000
C	2.156009000000	2.621434000000	-0.132285000000
C	3.003815000000	1.619916000000	-0.490639000000
C	-0.196757000000	2.831005000000	0.578530000000
C	-0.924576000000	3.479033000000	-0.441186000000
C	-1.921166000000	4.372103000000	-0.045411000000
H	-2.508355000000	4.889105000000	-0.805126000000
C	-2.199776000000	4.592250000000	1.302086000000
H	-2.988682000000	5.289984000000	1.586487000000
C	-1.492309000000	3.908605000000	2.281645000000
H	-1.734690000000	4.066787000000	3.334330000000
C	-0.468358000000	3.016758000000	1.940841000000
C	-0.695633000000	3.192656000000	-1.920757000000
H	-0.210614000000	2.207332000000	-1.981358000000
C	0.215614000000	4.219480000000	-2.606148000000
H	1.252141000000	4.166866000000	-2.248585000000
H	-0.156205000000	5.243512000000	-2.444830000000
H	0.231876000000	4.035351000000	-3.690629000000
C	-2.020526000000	3.084900000000	-2.682037000000
H	-2.495149000000	4.069895000000	-2.808066000000
H	-2.722889000000	2.416092000000	-2.166669000000

H	-1.836670000000	2.682202000000	-3.688969000000
C	0.267266000000	2.266349000000	3.036616000000
H	1.045612000000	1.645919000000	2.565478000000
C	0.963656000000	3.223693000000	4.008517000000
H	0.231847000000	3.848504000000	4.542175000000
H	1.659604000000	3.894979000000	3.484847000000
H	1.530917000000	2.658375000000	4.762126000000
C	-0.697783000000	1.330552000000	3.773828000000
H	-1.176941000000	0.623611000000	3.080960000000
H	-1.488840000000	1.905776000000	4.278318000000
H	-0.164072000000	0.751217000000	4.542490000000
C	2.749064000000	-0.845715000000	-0.825340000000
C	3.571221000000	-1.671088000000	-0.035659000000
C	3.988100000000	-2.880124000000	-0.599769000000
H	4.617016000000	-3.554276000000	-0.018945000000
C	3.592930000000	-3.254090000000	-1.881121000000
H	3.924982000000	-4.207891000000	-2.293779000000
C	2.769384000000	-2.423538000000	-2.631152000000
H	2.458661000000	-2.727721000000	-3.632291000000
C	2.331982000000	-1.197576000000	-2.120621000000
C	3.971777000000	-1.301821000000	1.386573000000
H	3.123888000000	-0.749356000000	1.819379000000
C	5.204624000000	-0.390369000000	1.439251000000
H	5.002334000000	0.607813000000	1.036184000000
H	6.039937000000	-0.832204000000	0.873945000000
H	5.530244000000	-0.264985000000	2.482366000000
C	4.221320000000	-2.534752000000	2.257511000000
H	5.186806000000	-3.004630000000	2.012890000000
H	3.426186000000	-3.281591000000	2.139972000000
H	4.262108000000	-2.238825000000	3.315785000000

C	1.467711000000	-0.289552000000	-2.980665000000
H	1.097371000000	0.533037000000	-2.353778000000
C	2.301389000000	0.333133000000	-4.106413000000
H	2.687734000000	-0.444280000000	-4.783343000000
H	3.162452000000	0.888244000000	-3.706285000000
H	1.688040000000	1.027140000000	-4.700171000000
C	0.241188000000	-1.016190000000	-3.538071000000
H	-0.336094000000	-1.503138000000	-2.738930000000
H	0.525306000000	-1.785878000000	-4.271729000000
H	-0.422299000000	-0.300669000000	-4.046278000000
C	-0.003453000000	-0.315194000000	0.276511000000
C	0.364977000000	-1.595348000000	0.943587000000
C	0.722681000000	-1.615329000000	2.300345000000
H	0.791423000000	-0.670818000000	2.844009000000
C	0.921591000000	-2.817956000000	2.976043000000
H	1.167586000000	-2.807066000000	4.039498000000
C	0.790869000000	-4.029792000000	2.299894000000
H	0.934314000000	-4.973307000000	2.829048000000
C	0.478135000000	-4.026096000000	0.939387000000
H	0.386207000000	-4.966522000000	0.393357000000
C	0.267549000000	-2.822785000000	0.271548000000
H	0.019891000000	-2.826110000000	-0.790921000000
C	-4.346369000000	-0.293179000000	-1.009048000000
C	-4.872912000000	-2.474474000000	0.308830000000
C	-2.693724000000	-1.739515000000	1.544494000000
C	-2.636581000000	-2.755846000000	-1.234718000000
C	2.435572000000	4.074021000000	0.058243000000
H	3.292940000000	4.374524000000	-0.558200000000
H	1.573219000000	4.698009000000	-0.205539000000
H	2.681955000000	4.281918000000	1.111274000000
C	4.376540000000	1.714613000000	-1.076868000000

H	5.073005000000	2.234141000000	-0.404083000000
H	4.782348000000	0.716526000000	-1.284594000000
H	4.345405000000	2.273404000000	-2.023725000000

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Energy (M06-2X/def2-SVP)= -5763.08884624

As	1.253235000000	0.511931000000	0.319462000000
Fe	2.071510000000	2.899070000000	0.263259000000
O	2.598980000000	5.812815000000	0.181997000000
O	0.227821000000	3.101395000000	2.566122000000
O	2.012263000000	2.664945000000	-2.691803000000
O	4.678248000000	2.102360000000	1.349378000000
N	-0.739824000000	-1.748116000000	1.420070000000
N	-2.639167000000	-0.737897000000	0.957914000000
N	3.535946000000	-0.922074000000	-0.841396000000
N	2.109897000000	-0.581113000000	-2.414955000000
C	-1.276170000000	-0.722921000000	0.639200000000
C	-1.725145000000	-2.292096000000	2.244939000000
H	-1.492282000000	-3.087283000000	2.944585000000
C	-2.885617000000	-1.686499000000	1.947738000000
H	-3.879477000000	-1.806202000000	2.364810000000
C	-0.592438000000	0.156313000000	-0.198724000000
C	2.328195000000	-0.372311000000	-1.100141000000
C	4.078083000000	-1.479430000000	-1.987759000000
C	3.173020000000	-1.267753000000	-2.985906000000
C	2.405324000000	4.691143000000	0.219815000000
C	0.896485000000	3.082257000000	1.633785000000
C	1.990524000000	2.808606000000	-1.552791000000
C	3.660015000000	2.397759000000	0.911217000000
C	0.532227000000	-2.403418000000	1.334938000000
C	2.511639000000	-3.177151000000	2.465843000000
H	3.159016000000	-3.186230000000	3.345641000000
C	2.854288000000	-3.932126000000	1.349451000000
H	3.756431000000	-4.547083000000	1.359569000000
C	2.046374000000	-3.900860000000	0.215004000000
H	2.330814000000	-4.490520000000	-0.656779000000
C	0.858274000000	-3.162439000000	0.190147000000
C	1.362305000000	-2.381902000000	2.472682000000
C	1.065060000000	-1.501041000000	3.676639000000
H	0.191005000000	-0.880546000000	3.430729000000
C	2.226234000000	-0.544117000000	3.969332000000
H	3.142424000000	-1.091849000000	4.239374000000
H	1.969340000000	0.111492000000	4.814104000000
H	2.435522000000	0.094565000000	3.099549000000
C	0.736149000000	-2.339366000000	4.916981000000
H	-0.112651000000	-3.016456000000	4.744956000000
H	0.484809000000	-1.686686000000	5.765512000000
H	1.599308000000	-2.956514000000	5.211111000000
C	-0.067608000000	-3.206068000000	-1.016602000000
H	-0.385736000000	-2.167947000000	-1.206170000000
C	0.610201000000	-3.720526000000	-2.285844000000
H	1.555322000000	-3.194578000000	-2.485225000000
H	-0.058460000000	-3.579047000000	-3.148259000000
H	0.828748000000	-4.797561000000	-2.219222000000
C	-1.318504000000	-4.048213000000	-0.729919000000
H	-2.007883000000	-4.010530000000	-1.587840000000
H	-1.861149000000	-3.702049000000	0.159901000000

H	-1.036642000000	-5.099746000000	-0.564944000000
C	-3.724386000000	0.045142000000	0.437935000000
C	-3.806326000000	1.423070000000	0.725106000000
C	-4.892938000000	2.126502000000	0.197946000000
H	-4.974859000000	3.197345000000	0.377729000000
C	-5.881431000000	1.487237000000	-0.545150000000
H	-6.723724000000	2.060574000000	-0.935459000000
C	-5.795057000000	0.123573000000	-0.788187000000
H	-6.572772000000	-0.372212000000	-1.372404000000
C	-4.709705000000	-0.620830000000	-0.317161000000
C	-2.776308000000	2.115503000000	1.604465000000
H	-1.780807000000	1.787161000000	1.268001000000
C	-2.818604000000	3.638373000000	1.493607000000
H	-2.745022000000	3.968654000000	0.447063000000
H	-1.977370000000	4.067871000000	2.052419000000
H	-3.746358000000	4.047581000000	1.923522000000
C	-2.926044000000	1.696483000000	3.073437000000
H	-3.908376000000	2.005075000000	3.464054000000
H	-2.143470000000	2.182112000000	3.674203000000
H	-2.829079000000	0.609615000000	3.206231000000
C	-4.628305000000	-2.102663000000	-0.654846000000
H	-3.621674000000	-2.454650000000	-0.389961000000
C	-4.825783000000	-2.373351000000	-2.150505000000
H	-5.849641000000	-2.131938000000	-2.472488000000
H	-4.658545000000	-3.439585000000	-2.365210000000
H	-4.132076000000	-1.783804000000	-2.765320000000
C	-5.647567000000	-2.914220000000	0.154190000000
H	-5.517893000000	-2.778486000000	1.236347000000
H	-5.553963000000	-3.987384000000	-0.069791000000
H	-6.672648000000	-2.602030000000	-0.098713000000
C	-1.354331000000	0.899561000000	-1.226319000000
C	-1.256808000000	2.292095000000	-1.394240000000
H	-0.604925000000	2.860454000000	-0.730357000000
C	-1.976099000000	2.952433000000	-2.389092000000
H	-1.877011000000	4.035273000000	-2.489253000000
C	-2.824874000000	2.247574000000	-3.241690000000
H	-3.392478000000	2.767761000000	-4.014526000000
C	-2.935724000000	0.864340000000	-3.093160000000
H	-3.595852000000	0.295957000000	-3.752499000000
C	-2.202735000000	0.205428000000	-2.110767000000
H	-2.284715000000	-0.881792000000	-2.005904000000
C	4.211592000000	-0.935227000000	0.444346000000
H	5.001345000000	-0.173918000000	0.474617000000
H	4.636815000000	-1.931300000000	0.615718000000
H	3.473736000000	-0.728639000000	1.229327000000
C	5.401829000000	-2.162098000000	-1.991347000000
H	6.193914000000	-1.499313000000	-1.613616000000
H	5.668940000000	-2.462918000000	-3.011009000000
H	5.388327000000	-3.065291000000	-1.362337000000
C	3.204803000000	-1.644413000000	-4.426774000000
H	2.324714000000	-2.244486000000	-4.702787000000
H	4.100956000000	-2.239460000000	-4.638184000000
H	3.227197000000	-0.756374000000	-5.075854000000

C	0.930249000000	-0.173461000000	-3.157702000000
H	0.164644000000	-0.962611000000	-3.135989000000
H	1.219038000000	0.040092000000	-4.192568000000
H	0.516486000000	0.734835000000	-2.715077000000

PhAs=Fe(CO)$_4$

Energy (M06-2X/def2-SVP)= -4183.26636107

Fe	-1.470998000000	-0.237537000000	-0.000070000000
As	0.209776000000	1.296991000000	0.000143000000
O	0.780915000000	-2.188163000000	-0.000263000000
O	-2.821988000000	-1.458571000000	2.369097000000
O	-2.823433000000	-1.457413000000	-2.369024000000
O	-3.064274000000	2.324518000000	0.000518000000
C	-0.050191000000	-1.415157000000	-0.000251000000
C	-2.345478000000	-1.020677000000	1.443281000000
C	-2.346270000000	-1.020050000000	-1.443293000000
C	-2.479223000000	1.356952000000	0.000295000000
C	1.997439000000	0.489484000000	-0.000129000000
C	2.664553000000	0.234619000000	-1.205465000000
C	2.664645000000	0.234735000000	1.205188000000
C	3.961823000000	-0.276461000000	-1.204784000000
C	3.961901000000	-0.276366000000	1.204506000000
C	4.614548000000	-0.535694000000	-0.000148000000
H	2.165339000000	0.432991000000	-2.157437000000
H	2.165456000000	0.433218000000	2.157169000000
H	4.465460000000	-0.473078000000	-2.153019000000
H	4.465572000000	-0.472859000000	2.152747000000
H	5.629259000000	-0.936292000000	-0.000180000000

HOAs=Fe(CO)$_4$

Energy (M06-2X/def2-SVP)= -4027.63094542

Fe	-0.558458000000	-0.086061000000	-0.000025000000
As	1.531118000000	0.720451000000	-0.001323000000
O	0.816265000000	-2.731286000000	-0.001294000000
O	-2.212226000000	-0.696659000000	2.396911000000
O	-2.227005000000	-0.704911000000	-2.385114000000
O	-1.121923000000	2.854033000000	-0.004639000000
C	0.304898000000	-1.721882000000	-0.001064000000
C	-1.615310000000	-0.475160000000	1.461423000000
C	-1.624022000000	-0.480103000000	-1.454338000000
C	-0.928560000000	1.737030000000	-0.002858000000
O	2.692305000000	-0.668054000000	-0.002257000000
H	3.591650000000	-0.321590000000	-0.003517000000

$H_2NAs=Fe(CO)_4$

Energy (M06-2X/def2-SVP) = -4007.782252

Fe	-0.593950000000	-0.117709000000	0.000114000000
As	1.503701000000	0.748502000000	-0.000194000000
O	0.993493000000	-2.612785000000	-0.001649000000
O	-2.190532000000	-0.784223000000	2.401989000000
O	-2.196406000000	-0.785529000000	-2.397640000000
O	-1.295398000000	2.799637000000	-0.001482000000
C	0.352283000000	-1.666373000000	-0.001007000000
C	-1.595847000000	-0.526484000000	1.471620000000
C	-1.599410000000	-0.527251000000	-1.468903000000
C	-1.050541000000	1.693234000000	-0.000786000000
N	2.866869000000	-0.418721000000	-0.001224000000
H	3.810314000000	-0.051471000000	-0.001752000000
H	2.813992000000	-1.433179000000	-0.001515000000

HAs (Singlet)

Energy (M06-2X/def2-SVP)= -2236.10637504

H 0.000000000000 0.000000000000 -1.484305000000 As 0.000000000000 0.000000000000 0.044979000000

PhAs (Singlet)

Energy (M06-2X/def2-SVP)= -2466.89704178

C	0.000000000000	0.000000000000	-0.036741000000
C	0.000000000000	1.208665000000	-0.755177000000
C	0.000000000000	-1.208665000000	-0.755177000000
C	0.000000000000	1.202167000000	-2.147728000000
C	0.000000000000	-1.202167000000	-2.147728000000

C 0.000000000000 0.000000000000 -2.854433000000

H 0.000000000000 2.169003000000 -0.232514000000

H 0.000000000000 -2.169003000000 -0.232514000000

H 0.000000000000 2.152511000000 -2.684590000000

H 0.000000000000 -2.152511000000 -2.684590000000

H 0.000000000000 0.000000000000 -3.944652000000

As 0.000000000000 0.000000000000 1.877599000000

HOAs (Singlet)

Energy (M06-2X/def2-SVP)= -2311.27381250

As 0.021415000000 -0.386661000000 0.000000000000

O 0.021415000000 1.378535000000 0.000000000000

H -0.878027000000 1.731532000000 0.000000000000

H_2NAs (Singlet)

Energy (M06-2X/def2-SVP)= -2291.44388005

As 0.000024000000 -0.404638000000 0.000000000000

N 0.000024000000 1.359302000000 0.000000000000

H -0.849318000000 1.918163000000 0.000000000000

H 0.848364000000 1.919767000000 0.000000000000

HAs (Triplet)

Energy (M06-2X/def2-SVP)= -2236.16133019

H 0.000000000000 0.000000000000 -1.485325000000 As 0.000000000000 0.000000000000 0.045010000000

PhAs (Triplet)

Energy (M06-2X/def2-SVP)= -2466.95475981

C 0.000000000000 0.000000000000 -0.044542000000

C 0.000000000000 1.208667000000 -0.760982000000

C 0.000000000000 -1.208667000000 -0.760982000000

C	0.000000000000	1.207533000000	-2.153723000000
C	0.000000000000	-1.207533000000	-2.153723000000
C	0.000000000000	0.000000000000	-2.853281000000
H	0.000000000000	2.159080000000	-0.221093000000
H	0.000000000000	-2.159080000000	-0.221093000000
H	0.000000000000	2.154214000000	-2.696452000000
H	0.000000000000	-2.154214000000	-2.696452000000
H	0.000000000000	0.000000000000	-3.944248000000
As	0.000000000000	0.000000000000	1.883114000000

HOAs (Triplet)

Energy (M06-2X/def2-SVP)= -2311.30931506

As	0.021178000000	-0.392315000000	0.000000000000
O	0.021178000000	1.396749000000	0.000000000000
H	-0.868278000000	1.772403000000	0.000000000000

H_2NAs (Triplet)

Energy (M06-2X/def2

As 0.000005000000

N 0.000005000000

H -0.852201000000

H 0.851996000000

NHO(Ph)As(Singlet)

Energy (M06-2X/def2

As -1.052788000000

N -1.318566000000

N 0.772973000000 C

-0.166950000000 C -

1.099122000000 H -

1.895943000000

-SVP)= -
2291.45568643

-0.415935000000	0.000000000000
1.403665000000	0.000000000000
1.949934000000	0.000000000000
1.950268000000	0.000000000000

-SVP)= -
3663.72039067

0.483873000000	-2.272128000000
-0.103745000000	1.069034000000
0.475084000000	1.201043000000
-0.028727000000	0.344990000000
0.357894000000	2.354397000000
0.371831000000	3.089838000000

C	0.200239000000	0.729215000000	2.436202000000
H	0.762625000000	1.178134000000	3.246996000000
C	-2.620419000000	-0.506883000000	0.604861000000
C	-3.582448000000	0.499092000000	0.389500000000
C	-4.859181000000	0.094382000000	-0.001517000000
H	-5.627936000000	0.849110000000	-0.175099000000
C	-5.160513000000	-1.251536000000	-0.193810000000
H	-6.162161000000	-1.545481000000	-0.511254000000
C	-4.187595000000	-2.219929000000	0.016207000000
H	-4.429182000000	-3.273510000000	-0.137658000000
C	-2.897136000000	-1.869461000000	0.429609000000
C	-3.281645000000	1.976862000000	0.582933000000
H	-2.188611000000	2.091161000000	0.632782000000
C	-3.889905000000	2.490755000000	1.893612000000
H	-3.536331000000	1.924693000000	2.767244000000
H	-4.987217000000	2.405321000000	1.867036000000
H	-3.636377000000	3.550263000000	2.047123000000
C	-3.761561000000	2.822998000000	-0.598253000000
H	-4.859820000000	2.834431000000	-0.669806000000
H	-3.341089000000	2.433602000000	-1.535333000000
H	-3.430529000000	3.864636000000	-0.468972000000
C	-1.863769000000	-2.957916000000	0.651689000000
H	-0.947168000000	-2.481926000000	1.030028000000
C	-2.326878000000	-3.958481000000	1.715007000000
H	-3.232549000000	-4.492945000000	1.391129000000
H	-2.553683000000	-3.455295000000	2.666059000000
H	-1.545007000000	-4.710226000000	1.897977000000
C	-1.525873000000	-3.658421000000	-0.668433000000
H	-1.173927000000	-2.934845000000	-1.417907000000
H	-2.412586000000	-4.171820000000	-1.071357000000
H	-0.737898000000	-4.411740000000	-0.518560000000

C	2.061427000000	0.965792000000	0.780957000000
C	3.226786000000	0.259163000000	1.125436000000
C	4.442881000000	0.757242000000	0.648706000000
H	5.366610000000	0.227160000000	0.881296000000
C	4.492646000000	1.910640000000	-0.127323000000
H	5.452345000000	2.274060000000	-0.498254000000
C	3.326241000000	2.606340000000	-0.424728000000
H	3.377740000000	3.520192000000	-1.018291000000
C	2.083983000000	2.154936000000	0.029257000000
C	3.195606000000	-0.964413000000	2.025998000000
H	2.224146000000	-1.459860000000	1.873611000000
C	3.305542000000	-0.552655000000	3.501306000000
H	2.491391000000	0.113034000000	3.814249000000
H	4.255495000000	-0.024726000000	3.675373000000
H	3.284476000000	-1.440981000000	4.149894000000
C	4.301337000000	-1.971438000000	1.703451000000
H	5.280649000000	-1.609352000000	2.052178000000
H	4.365395000000	-2.168876000000	0.626114000000
H	4.105370000000	-2.921268000000	2.222175000000
C	0.834026000000	2.983272000000	-0.217839000000
H	-0.044188000000	2.332947000000	-0.108273000000
C	0.726151000000	4.092984000000	0.835065000000
H	1.580002000000	4.784534000000	0.763731000000
H	0.711886000000	3.678783000000	1.854382000000
H	-0.198373000000	4.671476000000	0.687283000000
C	0.764381000000	3.555272000000	-1.634038000000
H	0.912403000000	2.766197000000	-2.387334000000
H	1.518499000000	4.340227000000	-1.798988000000
H	-0.224869000000	4.005486000000	-1.803184000000
C	0.052218000000	-0.310138000000	-1.058389000000
C	1.262836000000	-1.107301000000	-1.394240000000

C	1.581781000000	-2.277770000000	-0.686410000000
H	0.949819000000	-2.586402000000	0.150042000000
C	2.659091000000	-3.080546000000	-1.060900000000
H	2.865026000000	-4.001112000000	-0.510525000000
C	3.470360000000	-2.709114000000	-2.131110000000
H	4.317417000000	-3.331833000000	-2.423692000000
C	3.184084000000	-1.532129000000	-2.827114000000
H	3.816210000000	-1.226323000000	-3.662829000000
C	2.091651000000	-0.748857000000	-2.470370000000
H	1.847475000000	0.157299000000	-3.027776000000

NHO^{Me}(Ph)As(Singlet)

Energy (M06-2X/def2-SVP)= -3742.25755041

As	0.781413000000	0.049227000000	-2.544742000000
N	1.150100000000	-0.011120000000	0.944908000000
N	-0.928614000000	-0.646976000000	0.847507000000
C	0.038941000000	0.021692000000	0.161999000000
C	0.863470000000	-0.650607000000	2.150841000000
C	-0.431178000000	-1.065535000000	2.085076000000
C	2.504987000000	0.263009000000	0.523182000000
C	3.296789000000	-0.843481000000	0.144215000000
C	4.630684000000	-0.599198000000	-0.186787000000
H	5.266561000000	-1.436104000000	-0.480822000000
C	5.156634000000	0.689657000000	-0.166944000000
H	6.199544000000	0.857464000000	-0.439856000000
C	4.350872000000	1.760430000000	0.193680000000
H	4.762504000000	2.771465000000	0.199259000000
C	3.011517000000	1.569575000000	0.554477000000
C	2.772644000000	-2.272299000000	0.083853000000
H	1.683476000000	-2.240525000000	0.217748000000
C	3.358456000000	-3.145906000000	1.200371000000

H	3.105732000000	-2.773515000000	2.201865000000
H	4.455783000000	-3.193090000000	1.123361000000
H	2.972274000000	-4.172837000000	1.116162000000
C	3.044774000000	-2.914721000000	-1.279866000000
H	4.123074000000	-3.063355000000	-1.444404000000
H	2.636956000000	-2.287499000000	-2.084099000000
H	2.569239000000	-3.907006000000	-1.325941000000
C	2.168549000000	2.769703000000	0.932865000000
H	1.189085000000	2.396538000000	1.254101000000
C	2.774821000000	3.542275000000	2.108241000000
H	3.745851000000	3.984451000000	1.838944000000
H	2.932130000000	2.891182000000	2.980780000000
H	2.107974000000	4.364871000000	2.405434000000
C	1.948434000000	3.680459000000	-0.280232000000
H	1.515967000000	3.119355000000	-1.121105000000
H	2.902583000000	4.121273000000	-0.609702000000
H	1.259234000000	4.499186000000	-0.025816000000
C	-2.166363000000	-1.134771000000	0.277689000000
C	-3.397486000000	-0.559989000000	0.633516000000
C	-4.563124000000	-1.138318000000	0.114453000000
H	-5.530081000000	-0.706046000000	0.377211000000
C	-4.510067000000	-2.236531000000	-0.730130000000
H	-5.430661000000	-2.667633000000	-1.126301000000
C	-3.278752000000	-2.785205000000	-1.074830000000
H	-3.242703000000	-3.646034000000	-1.742410000000
C	-2.085803000000	-2.258052000000	-0.577300000000
C	-3.544185000000	0.653182000000	1.533602000000
H	-2.536552000000	1.009708000000	1.792473000000
C	-4.289422000000	0.306330000000	2.828605000000
H	-3.815698000000	-0.521398000000	3.372904000000
H	-5.325894000000	0.007209000000	2.610925000000

H	-4.328774000000	1.182142000000	3.492868000000
C	-4.279759000000	1.777872000000	0.794167000000
H	-5.336190000000	1.509299000000	0.639879000000
H	-3.826044000000	1.981574000000	-0.185052000000
H	-4.253028000000	2.706286000000	1.382976000000
C	-0.766994000000	-2.931982000000	-0.917304000000
H	0.017747000000	-2.162453000000	-0.918823000000
C	-0.413261000000	-3.995207000000	0.129991000000
H	-1.187892000000	-4.777073000000	0.167419000000
H	-0.313746000000	-3.563527000000	1.137242000000
H	0.544766000000	-4.474416000000	-0.124250000000
C	-0.743898000000	-3.527976000000	-2.324926000000
H	-1.080745000000	-2.792509000000	-3.070013000000
H	-1.373038000000	-4.427629000000	-2.408308000000
H	0.285379000000	-3.817441000000	-2.580465000000
C	-0.131773000000	0.700659000000	-1.114682000000
C	-0.989689000000	1.912701000000	-1.068624000000
C	-1.181016000000	2.637536000000	0.123037000000
H	-0.776049000000	2.252874000000	1.062370000000
C	-1.854982000000	3.857760000000	0.137051000000
H	-1.962541000000	4.404860000000	1.076253000000
C	-2.395636000000	4.372392000000	-1.038568000000
H	-2.927145000000	5.325088000000	-1.033392000000
C	-2.256704000000	3.643762000000	-2.224012000000
H	-2.690240000000	4.025983000000	-3.150167000000
C	-1.564343000000	2.438057000000	-2.240649000000
H	-1.425633000000	1.880998000000	-3.169235000000
C	1.827239000000	-0.682242000000	3.288472000000
H	1.590640000000	-1.509726000000	3.969589000000
H	2.860002000000	-0.796761000000	2.936929000000
H	1.776051000000	0.256702000000	3.861639000000

C	-1.251912000000	-1.797699000000	3.090208000000
H	-1.809425000000	-1.105149000000	3.737879000000
H	-1.978546000000	-2.457670000000	2.595611000000
H	-0.603729000000	-2.410903000000	3.729470000000

NHO(Ph)As(Triplet)

Energy (M06-2X/def2-SVP)= -3663.73501993

As	-1.395840000000	-0.232760000000	-2.308579000000
N	-1.343896000000	0.048843000000	1.098258000000
N	0.855403000000	0.100839000000	1.311541000000
C	-0.166289000000	-0.080130000000	0.370394000000
C	-1.050543000000	0.274785000000	2.442197000000
H	-1.842739000000	0.362160000000	3.178856000000
C	0.287195000000	0.326798000000	2.570890000000
H	0.904572000000	0.536313000000	3.437485000000
C	-2.660742000000	-0.243290000000	0.630715000000
C	-3.452737000000	0.811341000000	0.135179000000
C	-4.749060000000	0.508431000000	-0.282373000000
H	-5.388197000000	1.297677000000	-0.678842000000
C	-5.228549000000	-0.799528000000	-0.228869000000
H	-6.242084000000	-1.018668000000	-0.568478000000
C	-4.416904000000	-1.828014000000	0.234558000000
H	-4.795832000000	-2.852195000000	0.248748000000
C	-3.113622000000	-1.570583000000	0.673935000000
C	-2.879459000000	2.214964000000	0.021428000000
H	-1.804883000000	2.095467000000	-0.189430000000
C	-3.015147000000	2.989787000000	1.336936000000
H	-2.500943000000	2.480826000000	2.164133000000
H	-4.075641000000	3.103943000000	1.609865000000
H	-2.578271000000	3.995133000000	1.235305000000
C	-3.479728000000	3.008294000000	-1.138225000000

H	-4.531005000000	3.274596000000	-0.949795000000
H	-3.425206000000	2.438798000000	-2.077601000000
H	-2.925529000000	3.948405000000	-1.273747000000
C	-2.220292000000	-2.711640000000	1.127424000000
H	-1.250023000000	-2.287636000000	1.424801000000
C	-2.806089000000	-3.431055000000	2.345668000000
H	-3.776718000000	-3.891597000000	2.106052000000
H	-2.959874000000	-2.735250000000	3.183128000000
H	-2.129680000000	-4.230568000000	2.681619000000
C	-1.962539000000	-3.683592000000	-0.028940000000
H	-1.552282000000	-3.152693000000	-0.900861000000
H	-2.893170000000	-4.182126000000	-0.341311000000
H	-1.249137000000	-4.463656000000	0.276624000000
C	2.130165000000	0.657782000000	0.955283000000
C	3.286476000000	-0.143342000000	1.019710000000
C	4.490724000000	0.423345000000	0.595695000000
H	5.402389000000	-0.173762000000	0.611328000000
C	4.543914000000	1.737198000000	0.135541000000
H	5.493351000000	2.155071000000	-0.203151000000
C	3.395796000000	2.519535000000	0.118065000000
H	3.451394000000	3.555474000000	-0.224082000000
C	2.166504000000	1.999364000000	0.536535000000
C	3.227378000000	-1.563202000000	1.558930000000
H	2.279519000000	-1.997020000000	1.203800000000
C	3.205013000000	-1.565030000000	3.093753000000
H	2.326779000000	-1.044908000000	3.495069000000
H	4.106748000000	-1.072225000000	3.488473000000
H	3.185178000000	-2.597103000000	3.474207000000
C	4.376132000000	-2.445207000000	1.071033000000
H	5.327305000000	-2.157237000000	1.545255000000
H	4.498967000000	-2.386054000000	-0.018211000000

H	4.182772000000	-3.493030000000	1.343004000000
C	0.938461000000	2.899692000000	0.555005000000
H	0.089817000000	2.327187000000	0.955388000000
C	1.159068000000	4.085236000000	1.501432000000
H	1.968234000000	4.738998000000	1.141901000000
H	1.425833000000	3.740898000000	2.511076000000
H	0.244219000000	4.691933000000	1.573859000000
C	0.544430000000	3.376411000000	-0.846306000000
H	0.256911000000	2.529552000000	-1.487333000000
H	1.370559000000	3.919586000000	-1.331229000000
H	-0.315803000000	4.061147000000	-0.785130000000
C	-0.024641000000	-0.313807000000	-0.984079000000
C	1.288066000000	-0.740516000000	-1.556783000000
C	1.687323000000	-2.082165000000	-1.457377000000
H	1.042275000000	-2.781871000000	-0.919971000000
C	2.868030000000	-2.526935000000	-2.051291000000
H	3.153408000000	-3.577632000000	-1.969022000000
C	3.680574000000	-1.634482000000	-2.749285000000
H	4.606538000000	-1.980184000000	-3.211926000000
C	3.293404000000	-0.298548000000	-2.863258000000
H	3.919692000000	0.407895000000	-3.410928000000
C	2.104563000000	0.138867000000	-2.285408000000
H	1.801498000000	1.183077000000	-2.383115000000

NHO^{Me}(Ph)As(Triplet)

Energy (M06-2X/def2-SVP)= -3742.27338531

As	1.308649000000	1.459651000000	-2.103975000000
N	1.371063000000	-0.373635000000	0.758407000000
N	-0.797212000000	-0.637195000000	0.993126000000
C	0.155974000000	-0.017673000000	0.183568000000
C	1.167816000000	-1.230356000000	1.853014000000

C	-0.163215000000	-1.408285000000	1.989688000000
C	2.669990000000	0.080717000000	0.383678000000
C	3.527745000000	-0.815628000000	-0.281200000000
C	4.806209000000	-0.361981000000	-0.618228000000
H	5.496392000000	-1.025222000000	-1.140111000000
C	5.208213000000	0.933185000000	-0.307473000000
H	6.206964000000	1.272164000000	-0.587013000000
C	4.344135000000	1.800708000000	0.354282000000
H	4.674383000000	2.814588000000	0.579299000000
C	3.059061000000	1.392529000000	0.719563000000
C	3.052927000000	-2.201297000000	-0.695429000000
H	2.338932000000	-2.557735000000	0.062626000000
C	4.186832000000	-3.223733000000	-0.775155000000
H	4.794912000000	-3.231419000000	0.141746000000
H	4.854979000000	-3.021066000000	-1.625467000000
H	3.772487000000	-4.231114000000	-0.923155000000
C	2.289812000000	-2.132701000000	-2.023921000000
H	2.922168000000	-1.693771000000	-2.811259000000
H	1.385926000000	-1.512137000000	-1.936158000000
H	1.989054000000	-3.142647000000	-2.342187000000
C	2.098856000000	2.328265000000	1.439291000000
H	1.098673000000	2.140951000000	1.020090000000
C	2.041295000000	2.021654000000	2.940904000000
H	3.039463000000	2.117401000000	3.396168000000
H	1.665910000000	1.006307000000	3.132292000000
H	1.365803000000	2.727044000000	3.447752000000
C	2.412592000000	3.803685000000	1.197942000000
H	2.496555000000	4.018674000000	0.122233000000
H	3.347875000000	4.110504000000	1.691042000000
H	1.607179000000	4.427532000000	1.611350000000
C	-2.142531000000	-0.895407000000	0.582790000000

C	-3.173488000000	-0.039360000000	1.016982000000
C	-4.473966000000	-0.332009000000	0.600133000000
H	-5.297066000000	0.316273000000	0.899264000000
C	-4.737685000000	-1.436282000000	-0.208290000000
H	-5.761772000000	-1.645027000000	-0.522114000000
C	-3.704058000000	-2.268933000000	-0.618457000000
H	-3.923456000000	-3.131945000000	-1.251033000000
C	-2.383091000000	-2.013014000000	-0.234392000000
C	-2.869958000000	1.167824000000	1.893598000000
H	-1.958701000000	1.629511000000	1.481494000000
C	-2.567478000000	0.765616000000	3.342449000000
H	-1.640953000000	0.184448000000	3.415495000000
H	-3.392330000000	0.169319000000	3.762912000000
H	-2.445705000000	1.664724000000	3.964768000000
C	-3.981196000000	2.215788000000	1.871474000000
H	-4.874107000000	1.861201000000	2.410043000000
H	-4.272418000000	2.475706000000	0.844895000000
H	-3.638516000000	3.131020000000	2.375425000000
C	-1.269870000000	-2.949575000000	-0.685836000000
H	-0.307574000000	-2.534767000000	-0.350053000000
C	-1.434625000000	-4.328659000000	-0.035762000000
H	-2.361467000000	-4.814821000000	-0.377785000000
H	-1.480172000000	-4.253189000000	1.059592000000
H	-0.591613000000	-4.983385000000	-0.302261000000
C	-1.199667000000	-3.077537000000	-2.210574000000
H	-0.925488000000	-2.122883000000	-2.680849000000
H	-2.159694000000	-3.410944000000	-2.632892000000
H	-0.437218000000	-3.818192000000	-2.492828000000
C	-0.045548000000	0.775947000000	-0.937859000000
C	-1.383613000000	1.322219000000	-1.333958000000
C	-1.737068000000	2.626739000000	-0.949745000000

H	-1.041829000000	3.193711000000	-0.324800000000
C	-2.936364000000	3.205485000000	-1.363043000000
H	-3.183560000000	4.221473000000	-1.048979000000
C	-3.816288000000	2.489300000000	-2.173337000000
H	-4.757770000000	2.937502000000	-2.495131000000
C	-3.472002000000	1.201321000000	-2.584534000000
H	-4.144722000000	0.633650000000	-3.229999000000
C	-2.264975000000	0.634756000000	-2.183131000000
H	-1.998553000000	-0.365828000000	-2.522068000000
C	2.295289000000	-1.732190000000	2.687762000000
H	2.992003000000	-2.358479000000	2.110344000000
H	2.882689000000	-0.898314000000	3.101905000000
H	1.901540000000	-2.326849000000	3.521371000000
C	-0.911740000000	-2.244281000000	2.979798000000
H	-0.932643000000	-1.785508000000	3.979645000000
H	-1.952884000000	-2.387310000000	2.660170000000
H	-0.445972000000	-3.234837000000	3.075131000000

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Energy (M06-2X/def2-SVP)= -7327.55170485

As	-0.658440000000	0.923654000000	-0.160698000000
As	0.658308000000	-0.922920000000	-0.158893000000
N	-3.616913000000	1.943424000000	0.950223000000
N	-4.856829000000	0.409711000000	-0.043667000000
N	4.856863000000	-0.410231000000	-0.044630000000
N	3.617219000000	-1.943718000000	0.949763000000
C	-3.527954000000	0.763902000000	0.215788000000
C	-4.954739000000	2.288931000000	1.136333000000
H	-5.229580000000	3.161490000000	1.719805000000
C	-5.711419000000	1.364976000000	0.518376000000
H	-6.786286000000	1.304297000000	0.388957000000

C	-2.393723000000	0.075673000000	-0.171578000000
C	-2.482555000000	-1.360766000000	-0.553787000000
C	-2.544159000000	-2.344561000000	0.444926000000
H	-2.566261000000	-2.029065000000	1.490795000000
C	-2.547687000000	-3.702176000000	0.120070000000
H	-2.591749000000	-4.448558000000	0.916363000000
C	-2.500072000000	-4.102767000000	-1.213681000000
H	-2.507211000000	-5.163754000000	-1.470850000000
C	-2.426114000000	-3.135681000000	-2.219137000000
H	-2.384202000000	-3.438014000000	-3.267119000000
C	-2.402237000000	-1.783776000000	-1.890807000000
H	-2.332392000000	-1.031267000000	-2.678886000000
C	3.528110000000	-0.764173000000	0.215438000000
C	5.711598000000	-1.365584000000	0.516993000000
H	6.786410000000	-1.305007000000	0.387049000000
C	4.955056000000	-2.289455000000	1.135266000000
H	5.230002000000	-3.162126000000	1.718524000000
C	2.393765000000	-0.075589000000	-0.171136000000
C	2.482561000000	1.360899000000	-0.553244000000
C	2.402585000000	1.784065000000	-1.890220000000
H	2.333218000000	1.031672000000	-2.678450000000
C	2.426158000000	3.136040000000	-2.218346000000
H	2.384490000000	3.438501000000	-3.266299000000
C	2.499478000000	4.102994000000	-1.212731000000
H	2.506383000000	5.164021000000	-1.469743000000
C	2.546785000000	3.702229000000	0.120987000000
H	2.590372000000	4.448507000000	0.917402000000
C	2.543516000000	2.344573000000	0.445639000000
H	2.565284000000	2.028925000000	1.491474000000
C	-2.555593000000	2.550438000000	1.690523000000
C	-2.174230000000	1.975233000000	2.912954000000

C	-1.118054000000	2.572358000000	3.609271000000
H	-0.788808000000	2.142372000000	4.558032000000
C	-0.475953000000	3.697359000000	3.103161000000
H	0.350316000000	4.145755000000	3.658025000000
C	-0.868365000000	4.245005000000	1.883239000000
H	-0.331781000000	5.105543000000	1.482473000000
C	-1.907162000000	3.674947000000	1.146653000000
C	-2.290105000000	4.194871000000	-0.229164000000
H	-2.668746000000	3.327626000000	-0.794734000000
C	-2.847919000000	0.730512000000	3.464645000000
H	-3.565594000000	0.368912000000	2.714136000000
C	-3.632891000000	1.053711000000	4.739888000000
H	-4.395421000000	1.823660000000	4.552921000000
H	-4.137742000000	0.153728000000	5.121205000000
H	-2.962353000000	1.426679000000	5.529571000000
C	-1.830297000000	-0.389703000000	3.701012000000
H	-1.221426000000	-0.573831000000	2.801290000000
H	-1.147680000000	-0.135585000000	4.527188000000
H	-2.344934000000	-1.324228000000	3.974117000000
C	-5.235978000000	-0.338133000000	-1.207892000000
C	-5.762807000000	-1.635893000000	-1.064736000000
C	-6.064867000000	-2.344343000000	-2.230232000000
H	-6.456484000000	-3.359003000000	-2.157879000000
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H	-6.083252000000	-2.359599000000	-4.384630000000
C	-5.363054000000	-0.487429000000	-3.601549000000
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C	-6.013125000000	-2.234463000000	0.309699000000
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C	-7.336584000000	-1.726923000000	0.898588000000

H	-7.518176000000	-2.186662000000	1.881524000000
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H	-6.005983000000	-4.134936000000	1.345733000000
H	-5.136403000000	-4.167844000000	-0.209829000000
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C	-5.636471000000	2.549265000000	-3.333777000000
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C	6.064731000000	2.344415000000	-2.230476000000
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C	5.762645000000	1.635671000000	-1.065171000000
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C	0.476764000000	-3.697572000000	3.103453000000
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H	3.690638000000	-5.582519000000	-1.151389000000
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H	3.089552000000	-6.103795000000	0.443362000000
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C	2.849232000000	-0.731039000000	3.464470000000
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H	4.398440000000	-1.824492000000	4.550017000000
H	4.141024000000	-0.155032000000	5.119799000000
H	2.966475000000	-1.428611000000	5.528731000000
C	7.336304000000	1.726240000000	0.898260000000
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H	7.517790000000	2.185651000000	1.881368000000
H	7.339112000000	0.637836000000	1.033672000000
C	6.013267000000	3.762330000000	0.310955000000
H	6.005418000000	4.134055000000	1.345990000000
H	6.920340000000	4.160503000000	-0.170174000000
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H	-0.267666000000	4.023544000000	-1.021467000000
H	-1.389988000000	4.965164000000	-2.040327000000

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