Supporting Information for

H–H and Si–H Bond Addition to Fe≡NNR$_2$ Intermediates Derived from N$_2$

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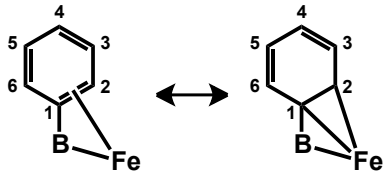
Table S1. Structural correlations between Fe–BCC and C–C bond lengths.



	Fe-B	Fe-C1	Fe-C2	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C1
3a	2.3234(11)	2.2608(9)	2.5486(11)	1.4191(14)	1.3891(18)	1.3977(15)	1.3935(18)	1.3880(16)	1.4212(15)
3b	2.330(4)	2.193(3)	2.692(4)	1.402(5)	1.384(5)	1.369(5)	1.377(5)	1.379(5)	1.422(5)
4[a]	*2.3740(7)*	*2.2517(6)*	*2.2715(7)*	*1.4211(10)*	*1.4185(10)*	*1.3711(12)*	*1.4124(12)*	*1.3785(10)*	*1.4303(10)*
	2.3134(7)	2.2134(6)	2.6645(7)	1.4167(10)	1.3987(11)	1.3839(14)	1.3944(15)	1.3890(12)	1.4184(10
6a[b]	*2.3768(6)*	*2.1493(5)*	*2.3405(6)*	*1.4231(7)*	*1.4238(8)*	*1.3681(9)*	*1.4196(10)*	*1.3690(8)*	*1.4324(7)*
	2.4288(7)	*2.1440(6)*	*2.2266(6)*	*1.4285(9)*	*1.4357(9)*	*1.3645(13)*	*1.4223(13)*	*1.3648(9)*	*1.4372(9)*
6b	*2.4242(10)*	*2.1542(9)*	*2.2041(9)*	*1.4356(13)*	*1.4342(13)*	*1.3641(16)*	*1.4218(17)*	*1.3680(14)*	*1.4365(13)*

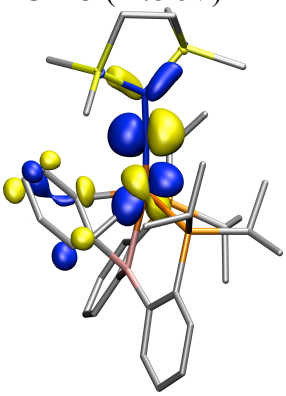
Italicized entries display alternating C–C bonds. (a) two Fe centers per molecule. (b) two molecules per asymmetric unit.

Chart S1. DFT study of **6a**: molecular orbital analysis

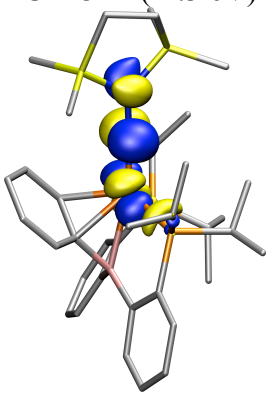
Geometry optimized using Gaussian09 Revision B.01[1] at the M06L/6-31g(d) level. Initial atomic coordinates were taken from one of the two unique molecules in the XRD structure. Molecular orbitals shown with 0.05 isosurfaces.

Frontier molecular orbitals

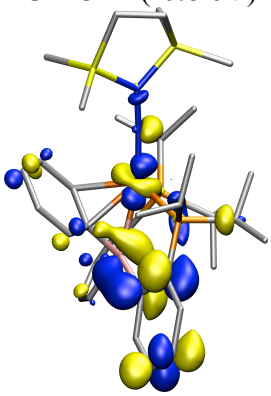
LUMO (-1.8 eV)



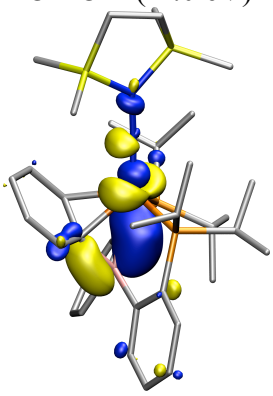
LUMO+1 (-1.3 eV)



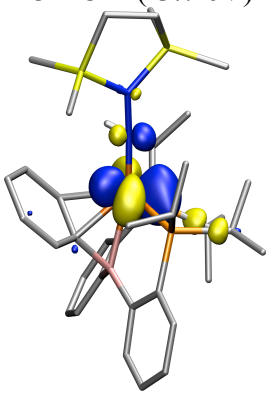
LUMO+2 (-0.8 eV)



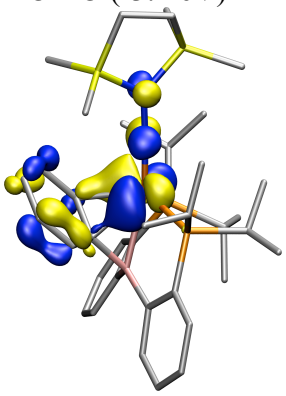
HOMO-2 (-4.0 eV)



HOMO-1 (-3.7 eV)

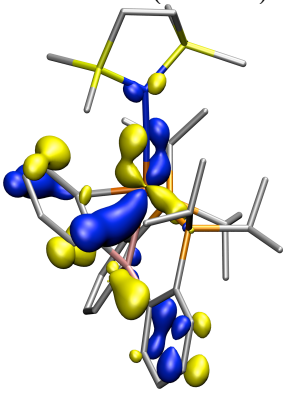


HOMO (-3.4 eV)



Orbitals with Fe-aryl bonding character

HOMO-10 (-6.2 eV)



HOMO-9 (-5.9 eV)

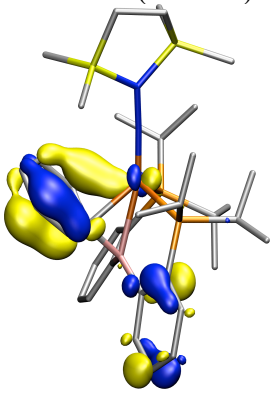


Table S2. Comparison of selected experimental and DFT-optimized bond lengths in **6a** (Å)

	XRD	Calc
Fe-P (avg.)	2.246	2.222
Fe-B	2.4288(7)	2.382
Fe-Cipso	2.1440(6)	2.119
Fe-Cortho	2.2266(6)	2.197
Fe-N	1.6658(5)	1.647
N-N	1.3242(7)	1.327

Table S3. Atomic coordinates of DFT-optimized **6a**

Atom	x	y	z
Fe1	0.0127	-0.0812	0.2109
P2	1.1256	-1.7899	-0.6322
P3	0.626	1.7803	-0.8701
Si4	-4.0082	-0.7725	-1.2819
Si5	-3.9552	0.344	1.4818
N6	-1.6282	-0.159	0.0948
N7	-2.9549	-0.1795	0.0627
C8	3.0348	-1.2199	1.0863
C9	2.4588	-2.342	0.463
C10	2.0608	-1.758	-2.2712
C11	-0.71	-0.6876	3.2645
C12	1.1147	0.3625	1.9654
C13	4.1682	-1.4467	1.8813
C14	2.2352	2.4185	-0.3125
C15	2.9857	1.4775	0.4245
C16	0.812	1.5796	2.6519
C17	4.3105	1.8261	0.7383
C18	-0.1555	1.6421	3.6211
C19	0.0397	-3.2885	-0.8458
C20	2.9644	-3.6326	0.6352
C21	-0.4719	3.2919	-0.8029
B22	2.2663	0.1682	0.942
C23	4.8375	3.0704	0.4094
C24	0.9002	1.558	-2.7207
C25	3.3626	-0.9719	-2.1377
C26	0.3097	-0.7859	2.27
C27	4.0888	-3.8256	1.4328
C28	4.0496	4.0168	-0.2449
C29	-0.9318	0.4906	3.927
C30	-0.9572	-3.0414	-1.9658

C31	1.1355	2.8316	-3.52
C32	-0.5087	3.8766	0.6002
C33	4.6906	-2.7277	2.0469
C34	2.7483	3.6863	-0.6091
C35	-1.8724	2.9913	-1.3214
C36	-0.6727	-3.6389	0.454
C37	-5.6489	0.3357	0.627
C38	2.3779	-3.1408	-2.8327
C39	-0.1809	0.7053	-3.3729
C40	-3.3627	-0.4532	-3.0046
C41	-5.4624	0.3553	-0.8983
C42	-3.4316	2.0388	2.0557
C43	-4.4549	-2.5711	-0.9805
C44	-3.9617	-0.9502	2.8461
H45	1.3996	-1.2339	-2.9759
H46	0.6986	-4.126	-1.122
H47	-0.0079	4.0366	-1.4703
H48	1.8335	0.98	-2.7296
H49	3.7818	-0.7653	-3.1315
H50	4.1085	-1.5491	-1.5761
H51	3.2405	-0.0178	-1.6134
H52	-1.6085	-3.9111	-2.129
H53	-0.4763	-2.8004	-2.9237
H54	-1.5919	-2.1884	-1.6961
H55	1.4061	2.5817	-4.5548
H56	1.9493	3.438	-3.1076
H57	0.232	3.4543	-3.5694
H58	-0.9027	3.1538	1.3226
H59	0.4905	4.1696	0.9433
H60	-1.1527	4.7663	0.6276
H61	-2.3261	2.1585	-0.7691
H62	-1.8706	2.7242	-2.3851
H63	-2.5233	3.8691	-1.2051
H64	-1.2971	-4.5338	0.3253
H65	0.0393	-3.8394	1.265
H66	-1.321	-2.811	0.7757
H67	-6.1906	-0.5746	0.9211
H68	-6.27	1.174	0.9739
H69	3.0029	-3.0428	-3.7304
H70	2.9504	-3.7349	-2.1071
H71	1.4889	-3.7147	-3.116
H72	0.1786	0.2773	-4.3193
H73	-0.5002	-0.119	-2.72

H74	-1.0704	1.2987	-3.6135
H75	-3.089	0.6011	-3.1211
H76	-2.5057	-1.0599	-3.3088
H77	-4.1771	-0.657	-3.7126
H78	-6.386	0.0936	-1.4328
H79	-5.1888	1.3683	-1.232
H80	-2.3606	2.0603	2.2847
H81	-3.9673	2.3259	2.9695
H82	-3.6322	2.8018	1.2939
H83	-5.1296	-2.9599	-1.7538
H84	-3.5722	-3.2191	-0.9557
H85	-4.9634	-2.6845	-0.0145
H86	-3.4274	-1.8553	2.5335
H87	-3.4909	-0.5985	3.7689
H88	-4.9922	-1.2434	3.0833
H89	4.6319	-0.6188	2.4189
H90	5.5655	-2.8771	2.6793
H91	4.494	-4.8261	1.5782
H92	2.4836	-4.4864	0.1531
H93	4.9406	1.1119	1.2686
H94	5.8653	3.3129	0.6779
H95	4.4528	4.9997	-0.4844
H96	2.1351	4.4214	-1.1329
H97	1.4128	2.4617	2.4222
H98	-0.3281	2.5699	4.1671
H99	-1.6872	0.5481	4.7123
H100	-1.2701	-1.5832	3.5351
H101	0.7153	-1.7819	2.0941

*General Considerations***.** All manipulations were carried out using standard Schlenk or glovebox techniques under an atmosphere of dinitrogen. Solvents were degassed and dried by sparging with N_2 gas and passage through an activated alumina column. Deuterated solvents were purchased from Cambridge Isotopes Laboratories, Inc. and were degassed and stored over activated 3 Å molecular sieves prior to use. Reagents were purchased from commercial vendors and used without further purification unless otherwise noted. ($^{i\text{Pr}}$TPB)FeNNSi$_2$ (**1**)[2], $^{i\text{Pr}}$DPB (**2a**)[3], and $^{\text{Ph}}$DPB (**2b**)[4] were synthesized according to literature procedures. Elemental analyses were performed by Midwest Microlab (Indianapolis, IN) or Robertson Microlit Laboratories (Ledgewood, NJ). Combustion analysis on samples of **6a** and **7** revealed low values for N. Based on NMR, IR, and UV/vis spectroscopic data, we are confident in the purity of these samples. It is possible that these samples partially decomposed and released N_2 during their shipping and/or handling.

Spectroscopic measurements. ^{1}H, ^{13}C, ^{31}P, and ^{11}B NMR spectra were collected at room temperature on a Varian 400 MHz spectrometer. ^{1}H and ^{13}C spectra were referenced to residual solvent resonances. ^{31}P spectra were referenced to external 85% phosphoric acid (δ = 0 ppm). ^{11}B spectra were referenced to BF_3•Et_2O (0 ppm). UV-vis measurements were performed with a Cary 50 instrument with Cary WinUV software. IR measurements were obtained as thin films formed by evaporation or as a solution using a cell with KBr windows using a Bruker Alpha Platinum ATR spectrometer with OPUS software.

X-ray Crystallography. X-ray diffraction studies for **3a**, **3b**, **4**, **5**, **6a**, **6b**, and **8** were carried out at the Caltech Division of Chemistry and Chemical Engineering X-ray Crystallography Facility on a Bruker three-circle SMART diffractometer with a SMART 1K CCD detector or APEX CCD detector. Data were collected at 100K using Mo Kα radiation (λ = 0.71073 Å). Structures were solved by direct or Patterson methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-97.[5] Data for complex **7** were collected with synchrotron radiation at the Stanford Synchrotron Radiation Laboratory (SSRL) beam line 12-2 at 17 keV using a single phi axis and recorded on a Dectris Pilatus 6M. The images were processed using XDS[6] and further workup of the data was analogous to the other datasets. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 (1.5 for methyl groups) times the Ueq of the atoms to which they are bonded.

($^{i\text{Pr}}$DPB)FeBr (3a) A solution of $^{i\text{Pr}}$DPB (**2a**, 1.318 g, 2.778 mmol) and $FeBr_2$ (0.599 g, 2.778 mmol) in THF (50 ml) was stirred at RT until all of the solids dissolved. The solvent was removed in vacuo and Et_2O (100ml) was added. The suspension was stirred vigorously to give a bright yellow precipitate. The solvent was removed in vacuo and benzene (100 ml) was added with a freshly-prepared 1% Na/Hg amalgam (Na: 63.9 mg, 2.778 mmol). The reaction was stirred vigorously for 18 hr to give a dark brown mixture. The mixture was decanted from the Hg and solvent was removed in vacuo. Et_2O (20 ml) was added and subsequently removed in vacuo. The dark solids were then dissolved by adding pentane (200 ml) and Et_2O (50 ml) and filtered through a pad of Celite. To the brown solids were added pentane (5 ml) and HMDSO (5 ml). The washings were removed and the solids were dried in vacuo. Lyophilization from benzene (10 ml) furnished brown microcrystals (1.423 g, 2.332 mmol, 84%). Single crystals suitable for X-ray diffraction may be obtained by concentration of an Et_2O solution. ^{1}H NMR (300 MHz, C_6D_6) δ 184.72, 78.42, 39.48, 33.44, 27.94, 25.39, 8.58, 0.91, -1.71, -5.56, -9.89, -11.76, -58.05. UV/vis

(toluene, nm {M^{-1} cm^{-1}}): 461 {1400, sh}, 581 {550}, 715 {250}, 992 {590}. μ_{eff} (C_6D_6, 298 K) = 3.8 μ_B. Elemental analysis for $C_{30}H_{41}BBrFeP_2$: calc. C 59.05, H 6.77; found C 58.97, H 6.98.

(^{Ph}DPB)FeBr (3b)
A solution of ^{Ph}DPB (**2b**, 1.398 g, 2.290 mmol) and $FeBr_2$ (0.494 g, 2.29 mmol) in THF (60 ml) was stirred at RT until all of the solids dissolved. The solvent was removed in vacuo and Et_2O (100ml) was added. The suspension was stirred vigorously to give a bright yellow precipitate in a yellow solution. The solvent was removed in vacuo and benzene (60 ml) was added with a freshly-prepared 1% Na/Hg amalgam (Na: 52.7 mg, 2.29 mmol). The reaction was stirred vigorously for 18 hr to give a dark brown mixture. The mixture was decanted from the Hg, filtered through Celite, and dried in vacuo. The solids were washed with Et_2O (3 x 20 ml). The dark, microcrystalline solids were dried in vacuo. Lyophilization from benzene (10 ml) furnished brown microcrystals (1.095 g, 1.467 mmol, 64%). Single crystals suitable for X-ray diffraction may be obtained by diffusion of n-pentane into a concentrated benzene solution. ^{1}H NMR (400 MHz, C_6D_6) δ 82.99, 32.99, 31.22, 22.92, 10.53, 9.41, 5.50, 3.24, 1.83, -0.53, -4.50, -10.18, -72.92. UV/vis (toluene, nm {M^{-1} cm^{-1}}): 474 {1600, sh}, 581 {530}, 717 {260}, 1003 {600}. μ_{eff} (C_6D_6, 298 K) = 3.6 μ_B. Elemental analysis for $C_{42}H_{33}BBrFeP_2$: calc. C 67.60, H 4.46; found C 67.59 H 4.49.

[(^{iPr}DPB)Fe]N_2 (4)
A solution of ^{iPr}DPB (**3a**, 0.942 g, 1.98 mmol) and $FeBr_2$ (0.428 g, 1.98 mmol) in THF (40 ml) was stirred at RT until all of the solids dissolved. The solvent was removed in vacuo and Et_2O (80ml) was added. The suspension was stirred vigorously to give a bright yellow precipitate. The solvent was removed in vacuo and benzene (80 ml) was added with a freshly-prepared 1% Na/Hg amalgam (Na: 95.9 mg, 4.17 mmol). The reaction was stirred vigorously for 18 hr to give a dark red-brown mixture. The mixture was decanted from the Hg and filtered through Celite. The solvent was removed in vacuo to give a brown residue. Addition of pentane (5 ml) induced precipitation of dark crystals. The solvent was decanted and the solids were washed with cold Et_2O (3 x 5 ml) and dried in vacuo (0.762 g, 0.700 mmol, 71%). Single crystals suitable for X-ray diffraction may be obtained by concentration of an Et_2O solution. Alternative synthesis of **7**: a 2 ml THF solution of **6a** (53.1 mg, 0.0870 mmol) was stirred over a freshly-prepared 1% Na/Hg (Na: 2.2 mg, 0.095 mmol) for 18 hr. The mixture was decanted from the Hg, concentrated in vacuo, and extracted with 5 ml benzene. The dark benzene solution was filtered through Celite, lyophilized, and recrystallized by concentration of an n-pentane solution to give crystals of **7** (31 mg, 0.028 mmol, 66%). ^{1}H NMR (400 MHz, C_6D_6) δ 171.85, 133.26, 43.95, 34.57, 28.15, 26.17, 7.42, 0.33, -1.50, -2.29, -6.28, -9.12, -76.00. UV/vis (toluene, nm {M^{-1} cm^{-1}}): 405 {15000}, 501 {8300, sh}, 990 {8300}. μ_{eff} (C_6D_6, 298 K) = 4.6 μ_B. Elemental analysis for $C_{60}H_{82}B_2Fe_2N_2P_4$: calc. C 66.20, H 7.59, N 2.57; found C 65.85 H 7.86 N 2.23.

(^{Ph}DPB)Fe (5)
A 3 ml THF solution of **3b** (77.9 mg, 0.1044 mmol) was stirred over freshly-prepared 1% Na/Hg amalgam (Na: 2.5 mg, 0.11 mmol) for 10 hr. The red-brown solution was decanted from the Hg and solvent was removed in vacuo. The solids were extracted into benzene (5 ml) and filtered through Celite. The solvent was removed in vacuo. The solids were washed with Et_2O (2 x 2 ml) and dissolved in benzene (2 ml). Layering the solution with pentane furnished brown single crystals of the title compound (78.0 mg, 0.0948 mmol, 90.8% for **5**•$2C_6H_6$). XRD studies

revealed that the compound crystallizes with two molecules of C_6H_6. The compound exhibits a degree of paramagnetic speciation in C_6D_6 under N_2 or Ar but is fully diamagnetic in THF-d_8; as such, ^{1}H NMR data are reported in both solvents. ^{1}H NMR (400 MHz, C_6D_6) δ 8.80 (d, *J* = 7.2 Hz, 2H), 7.64 (s, 4H), 7.37 (t, *J* = 6.8 Hz, 2H), 7.16 (s, 4H), 7.06 - 6.83 (m, 12H), 6.48 (t, *J* = 7.0 Hz, 4H), 6.29 (t, *J* = 6.2 Hz, 1H), 3.63 (br s, 2H), 3.23 (br s, 2H). ^{1}H NMR (400 MHz, THF-d_8) δ 8.58 (d, *J* = 7.5 Hz, 2H), 7.56 (m, 4H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 7.0 Hz, 6H), 7.07 (m, 6H), 6.97 - 6.82 (m, 2H), 6.73 (t, *J* = 7.4 Hz, 2H), 6.57 (m, 4H), 3.32 - 3.17 (br s, 2H), 3.07 (br s, 2H). ^{13}C NMR (101 MHz, C_6D_6) δ 161.76, 146.25-145.37 (m), 143.47 (t, *J* = 13.8 Hz), 134.07 (t, *J* = 15.8 Hz), 132.61, 131.42, 130.93, 128.26, 127.12, 126.97, 124.44, 106.77, 99.41, 86.36, 78.73. ^{11}B NMR (128 MHz, C_6D_6) δ 36.44. ^{31}P NMR (162 MHz, C_6D_6) δ 77.51. Elemental analysis for $C_{42}H_{33}BFeP_2$•$0.5C_6H_6$: calc. C 76.62, H 5.14, N 0; found C 76.55, H 5.60, N <0.02.

(^{iPr}DPB)FeNNSi$_2$ (6a)

A mixture of **3a** (0.233 g, 0.381 mmol), 1,2-bis(chlorodimethylsilyl)ethane (0.0905 g, 0.420 mmol), and freshly-prepared 1% Na/Hg (Na: 0.0272 g, 1.18 mmol) was rapidly stirred in 5 ml THF under 1 atm N_2. The solution turned deep green within 15 min. and was decanted from the Hg. Solvent was removed in vacuo, benzene (3 ml) was added to the solids, and the solution was filtered through Celite. Solvent was removed in vacuo to give green solids which were dissolved in 5 ml pentane. Upon stand for 10 min., dark green crystals formed. The remaining solution was again filtered and allowed to evaporate into HMDSO thereby furnishing more dark green crystals. The combined crystals were washed with pentane (3 x 0.5 ml) and lyophilized from benzene to give the title compound (0.202 mg, 0.287 mmol, 75.5%). ^{1}H NMR (400 MHz, C_6D_6) δ 8.56 (d, *J* = 7.4 Hz, 2H), 7.52 (td, *J* = 7.3, 1.2 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 2H), 6.97 (td, *J* = 7.3, 1.2 Hz, 2H), 6.49 (t, *J* = 7.2 Hz, 1H), 5.11 (d, *J* = 6.5 Hz, 2H), 4.75 (t, *J* = 6.9 Hz, 2H), 2.31 (m, 2H), 1.54 (m, 2H), 1.19 - 1.06 (m, 6H), 1.06 - 0.94 (m, 6H), 0.81 (s, 4H), 0.73 - 0.55 (m, 12H), 0.27 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 176.07, 140.35, 140.21, 137.17, 133.00, 130.09, 126.34, 124.92, 122.67, 113.68, 29.82, 21.14, 19.25, 18.54, 18.46, 15.15, 10.28, -5.53. ^{31}P NMR (162 MHz, C_6D_6) δ 29.43. ^{11}B NMR (128 MHz, C_6D_6) δ -28.16. UV/vis (toluene, nm {M^{-1} cm^{-1}}): 651 {1100}, 988 {1600}. Elemental analysis for $C_{36}H_{57}BFeN_2P_2Si_2$: calc. C 61.54, H 8.18, N 3.99; found C 61.82, H 7.93, N 3.35.

(^{Ph}DPB)FeNNSi$_2$ (6b)

A mixture of **3b** (0.195 g, 0.262 mmol), 1,2-bis(chlorodimethylsilyl)ethane (0.0621 g, 0.288 mmol), and freshly-prepared 1% Na/Hg (Na: 0.0187 g, 0.813 mmol) was rapidly stirred in 5 ml THF under 1 atm N_2. The solution turned deep green within 90 min. and was decanted from the Hg. Solvent was removed in vacuo, benzene (5 ml) was added to the solids, and the solution was filtered through Celite after standing at RT for 2 hr. Solvent was removed in vacuo to give green solids which were washed with pentane (3 x 1 ml) and redissolved in a minimal amount of benzene. The solution was again filtered and layer with pentane to provide dichroic green/brown crystals. The crystals were washed with pentane (3 x 0.5 ml) to give the title compound (0.188 g, 0.2242 mmol, 85.6%). ^{1}H NMR (400 MHz, C_6D_6) δ 8.08 (m, 4H), 7.95 (m, 2H), 7.36 - 6.90 (m, 15H), 6.75 (m, 8H), 6.53 (m, 4H), 0.34 (s, 4H), -0.22 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 159.64 , 143.47 - 142.65 (m), 139.85 (t, *J* = 15.3 Hz), 139.28 - 138.72 (m), 134.58 , 132.15 , 130.32 , 130.10 , 128.57 , 126.33 , 125.81 , 115.89 , 97.93 , 7.93 , -1.82 . ^{31}P NMR (162 MHz, C_6D_6) δ 88.02. ^{11}B NMR (128 MHz, C_6D_6) δ 32.67. UV/vis (toluene, nm {M^{-1} cm^{-1}}): 653

{850}. Elemental analysis for $C_{48}H_{49}BFeN_2P_2Si_2$: calc. C 68.74, H 5.89, N 3.34; found C 68.48, H 5.67, N 3.07.

(^{iPr}DPB-H)FeNSiNSi$_2$ (7)
A solution of **6a** (82.5 mg, 0.117 mmol) and $PhSiH_3$ (14.0 mg, 0.129 mmol) was allowed to stand in 2 ml benzene until the solution turned from green to deep orange (1 hr.). The benzene was lyophilized and the solids were extracted into TMS (5 ml) and filtered through Celite. Small orange crystals of the product formed upon concentration of the solution into HMDSO (41.0 mg, 0.0506 mmol, 43.2%). The reaction is quantitative by NMR, though the isolated yield of solids suffers due to the high solubility of the product. ^{1}H NMR (400 MHz, C_6D_6) δ 113.98, 52.22, 32.54, 25.37, 24.56, 18.16, 17.55, 12.78, 11.51, -1.09, -9.62, -10.32, -18.45, -25.52, -29.85, -33.94. IR (thin film from C_6D_6, cm^{-1}): 2090 (s, Si–H), 2000 (s and br, B–H–Fe). μ_{eff} (C_6D_6, 298 K) = 5.0 μ_B. Elemental analysis for $C_{42}H_{65}BFeN_2P_2Si_3$: calc. C 62.21, H 8.08, N 3.45; found C 61.92 H 7.81 N 1.95.

*Synthesis of 7 from **3a***
A 2 ml THF solution of **3a** (48.8 mg, 0.0800 mmol), 1,2-bis-(chlorodimethylsilyl)ethane (19.0 mg, 0.0881 mmol) and 1% Na/Hg (5.7 mg Na, 0.25 mmol) was vigorously stirred for 5 min. to give a green solution which was then added to neat $PhSiH_3$ (9.5 mg, 0.088 mmol). The solution deep orange within 10 min. The volatiles were removed in vacuo and the solids were dissolved in pentane and filtered through a plug of Celite. The volatiles were removed in vacuo to give an orange foam (57.7 mg) that was identified as **8** (>95% purity by ^{1}H NMR).

*Synthesis of 7 from **4***
A 2 ml THF solution of **4** (20.8 mg, 0.0191 mmol), 1,2-bis-(chlorodimethylsilyl)ethane (8.6 mg, 0.040 mmol) and 1% Na/Hg (1.8 mg Na, 0.078 mmol) was vigorously stirred for 5 min. to give a green solution which was then added to neat $PhSiH_3$ (4.3 mg, 0.040 mmol). The solution turned deep orange within 10 min. The volatiles were removed in vacuo and the solids were dissolved in pentane and filtered through a plug of Celite. The volatiles were removed in vacuo to give an orange foam (25.1 mg) that was identified as **8** (>95% purity by ^{1}H NMR).

(^{Ph}DPB-H)*FeNHSiNSi (8)
A solution of **6b** (45.0 mg, 0.0537 mmol) in benzene (5 ml) was stirred under 1 atm H_2 at 50 ˚C for three hours. The solution changed from dark green to light brown. Solvent was removed in vacuo to give a tan solid. The solids were washed with pentane (2 x 5 ml) and dissolved in minimal Et_2O (~10 ml). The solution was allowed to evaporate into HMDSO to give white solids (28.7 mg, 0.0341 mmol, 63.6%). Single crystals suitable for XRD were grown by vapor diffusion of n-pentane into a concentrated THF solution. ^{1}H NMR (400 MHz, C_6D_6) δ 188.54, 26.16, 25.70, 20.47, 16.37, 14.59, 12.01, 5.79, 4.77, 3.85, 3.23, 2.25, 1.97, 1.21, 0.84, 0.25, -0.04, -1.89, -7.20, -9.74. IR (thin film from C_6D_6, cm^{-1}): 3343 (w, N–H), ~2100 (s and br, B–H–Fe). μ_{eff} (C_6D_6, 298 K) = 4.8 μ_B. Satisfactory combustion analysis data were not obtained for **11**, though we are confident in our assignment of the product based on NMR and IR spectra of bulk samples as well as XRD analysis of single crystalline samples. (^{Ph}DPB-D)*FeNDSiNSi **(11-D$_2$).** The D-labeled compound was generated in a procedure that is identical to that for **11** using D_2 instead of H_2. ^{1}H NMR data are the same between **11** and **11-D$_2$**. IR (thin film from C_6D_6, cm^{-1}): 2476 (w, N–D), ~1550 (s and br, B–D–Fe).

*Attempted reaction of **1** with H_2*

To a J. Young tube was added a C_6D_6 solution of **1**. The green solution as subjected to three freeze-pump-thaw cycles and 1 atm H_2 was added. No reaction occurred at RT after 15 min. by ^{1}H NMR analysis. After heating the solution to 50 ˚C for 2 hr., the ^{1}H NMR spectrum showed a mixture of **1**, the previously-characterized (TPB)Fe(N_2) complex,[7] and other unidentified diamagnetic and paramagnetic species.

*Attempted reaction of **1** with $PhSiH_3$*

To a J. Young tube was added a C_6D_6 solution of **1** (9.5 mg, 0.0116 mmol) with $PhSiH_3$ (1.4 mg, 0.013 mmol). No reaction occurred at RT after 15 min. by ^{1}H NMR analysis. After heating the solution to 50 ˚C for 6 hr., the ^{1}H NMR spectrum showed mostly **1** and small amounts of unidentified diamagnetic and paramagnetic species.

NMR spectra

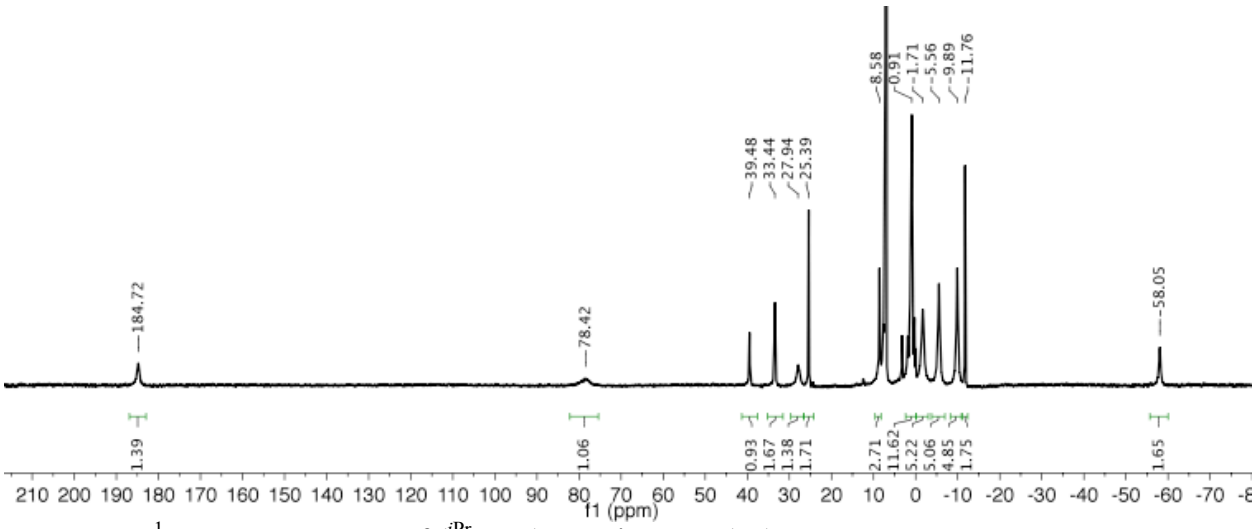


Figure S1. ^{1}H NMR spectrum of ($^{i\mathrm{Pr}}$DPB)FeBr in C_6D_6 (**3a**)

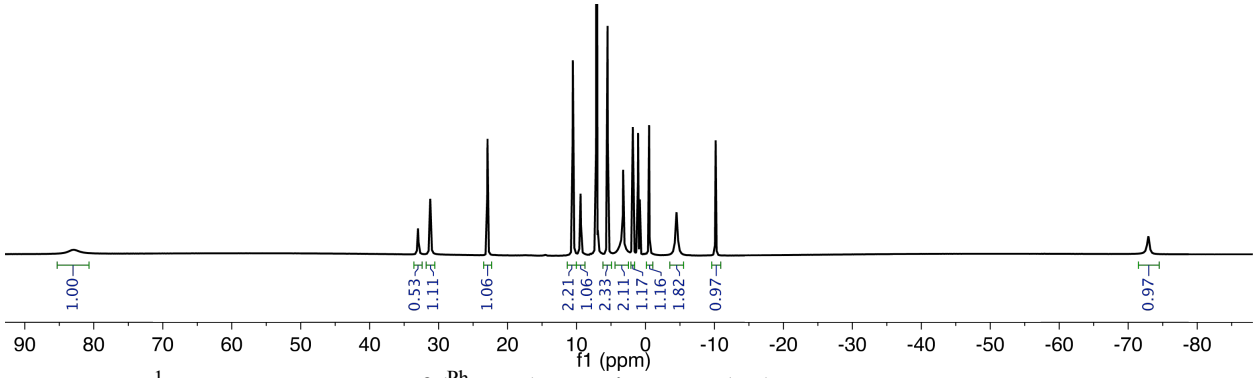


Figure S2. ^{1}H NMR spectrum of ($^{\mathrm{Ph}}$DPB)FeBr in C_6D_6 (**3b**)

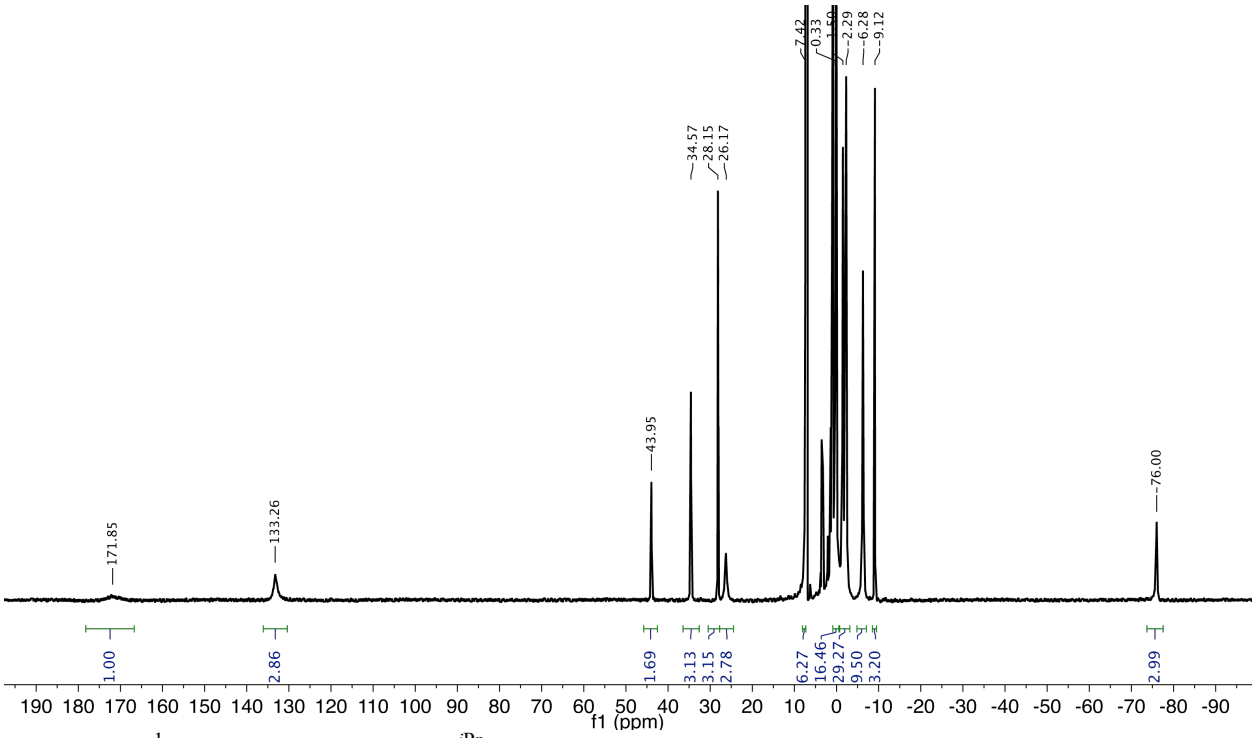


Figure S3. ^{1}H NMR spectrum of [($^{i\text{Pr}}$DPB)Fe]$_2$(μ-1,2-N$_2$) in C_6D_6 (**4**)

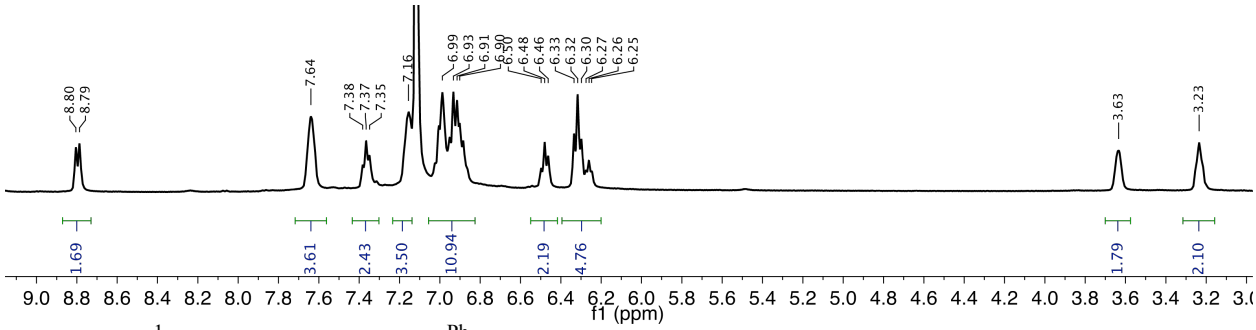


Figure S4. ^{1}H NMR spectrum of ($^{\text{Ph}}$DPB)Fe in C_6D_6 (**5**)

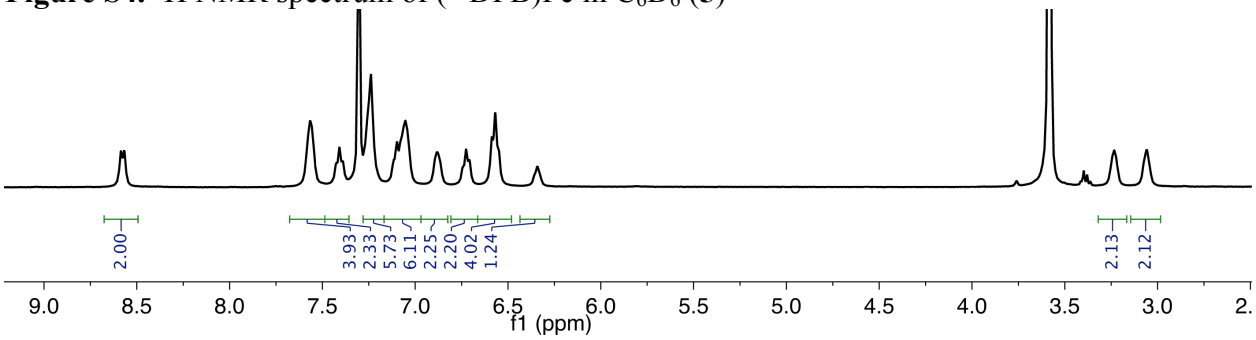


Figure S5. ^{1}H NMR spectrum of ($^{\text{Ph}}$DPB)Fe in d_8-THF (**5**)

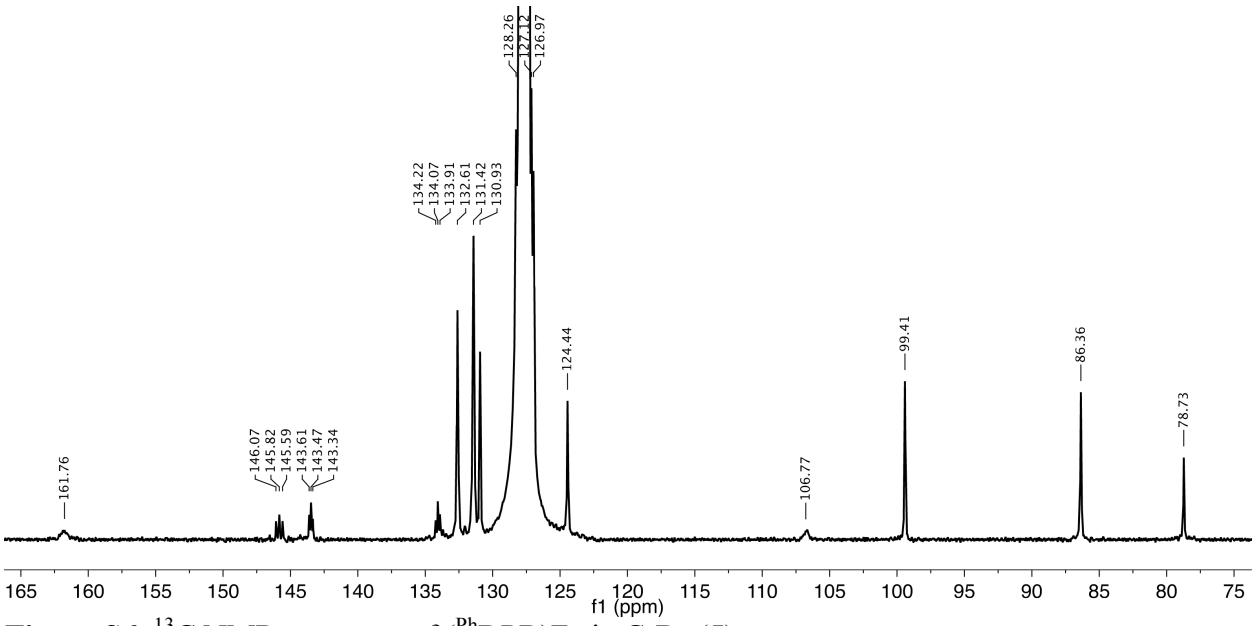


Figure S6. ^{13}C NMR spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

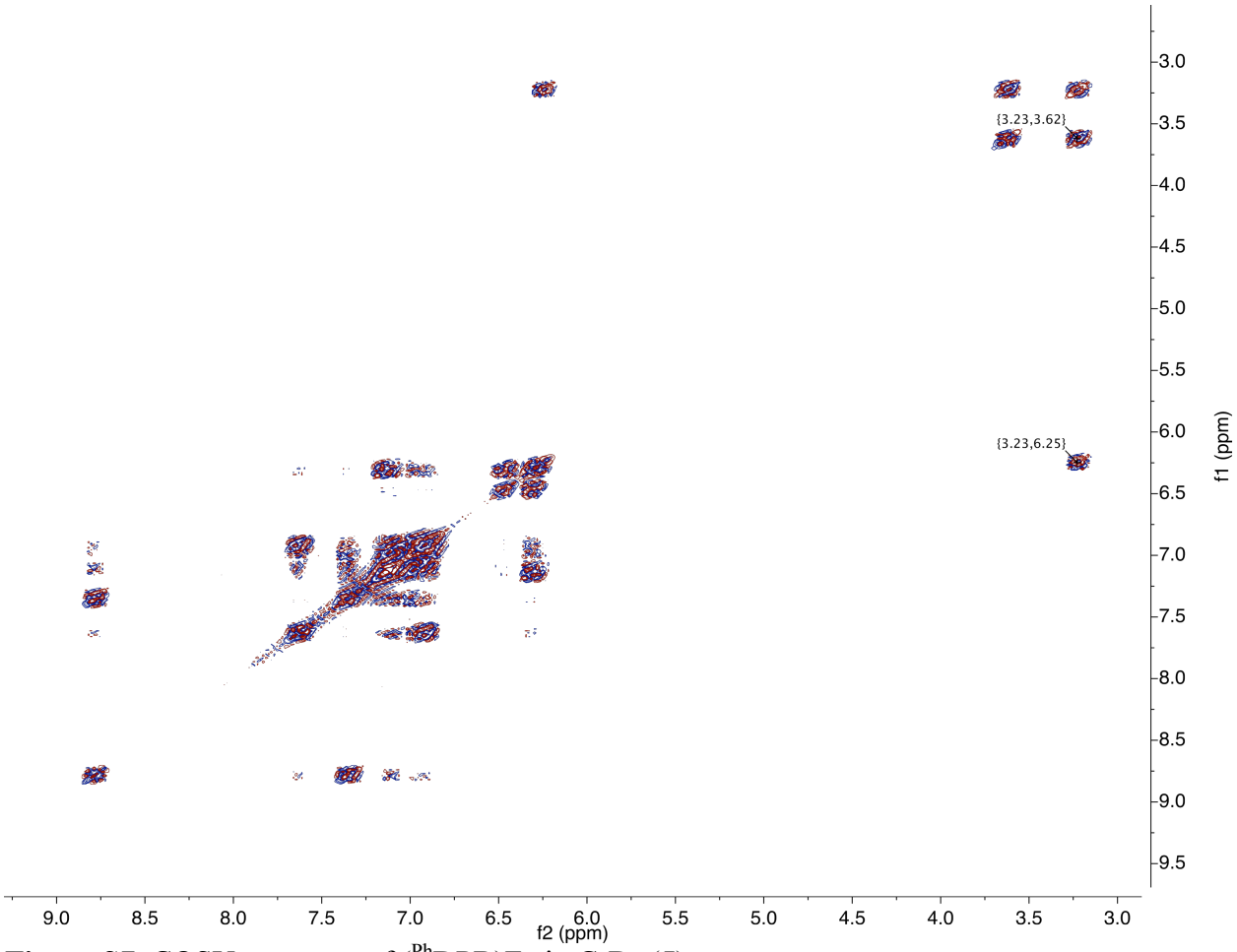


Figure S7. COSY spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

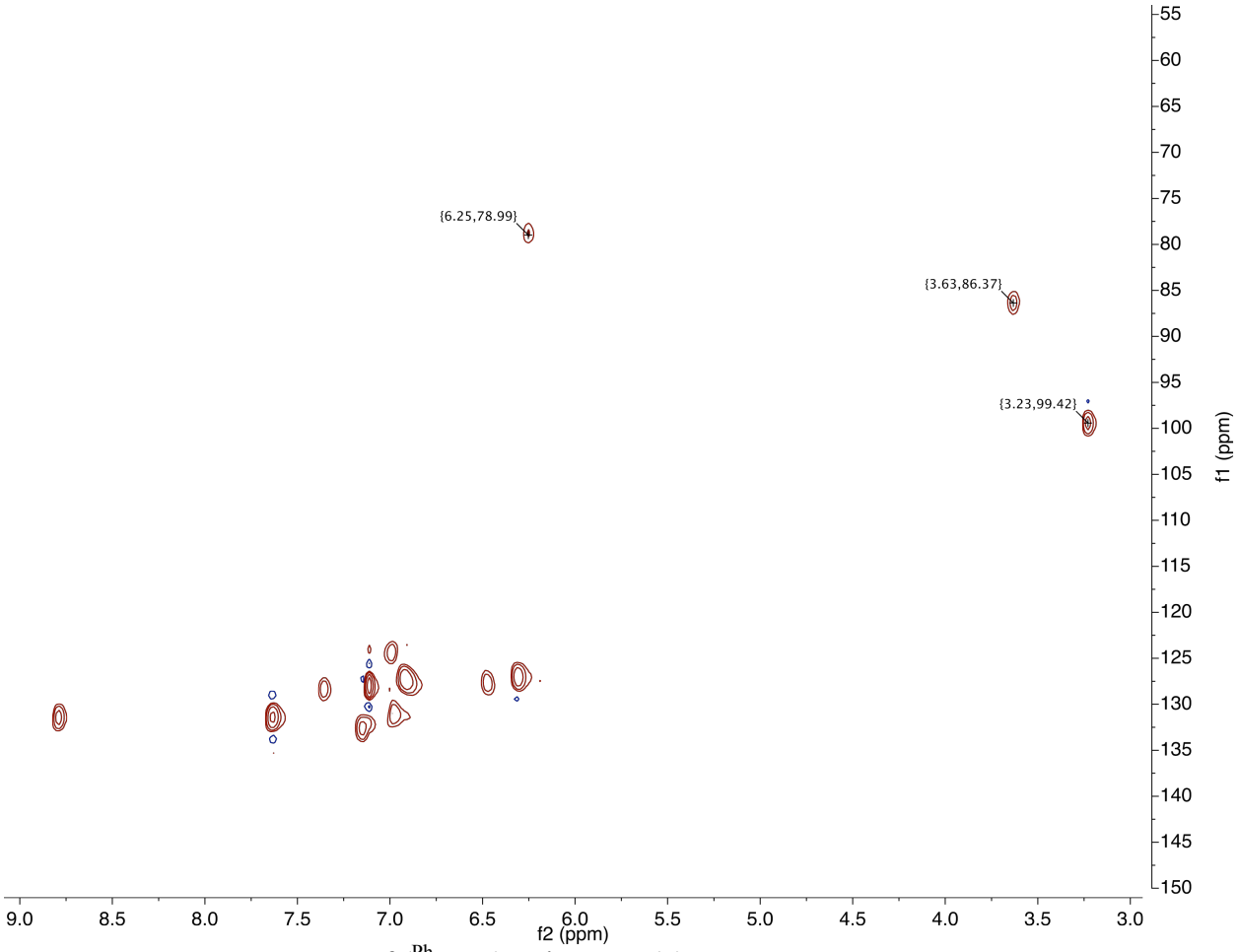


Figure S8. HSQC spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

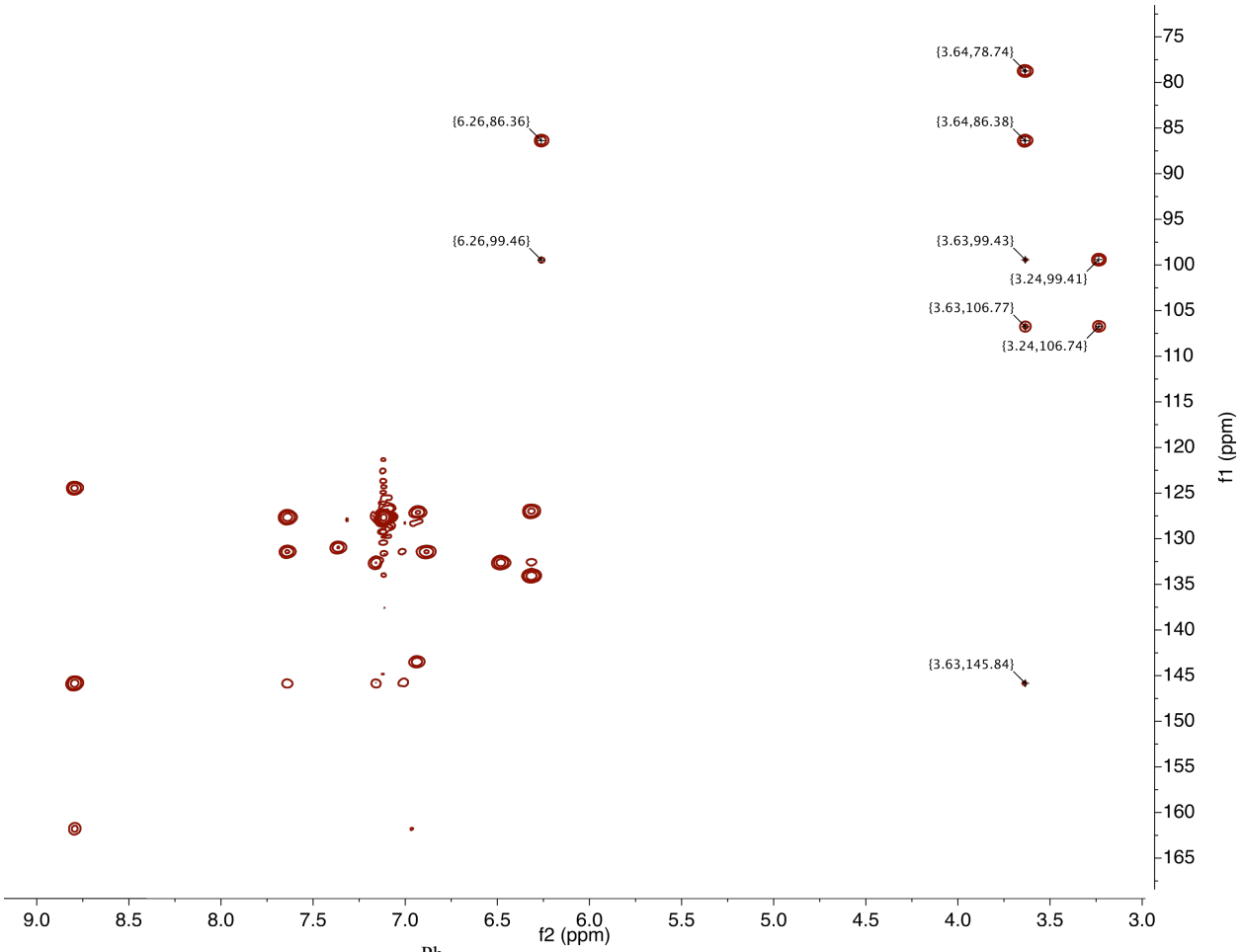


Figure S9. HMBC spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

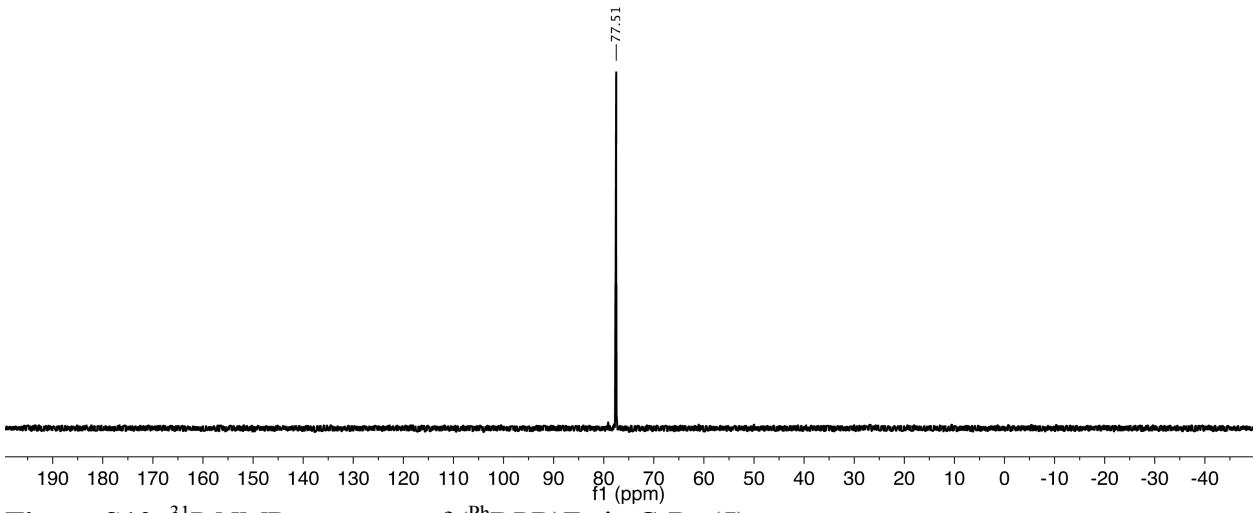


Figure S10. ^{31}P NMR spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

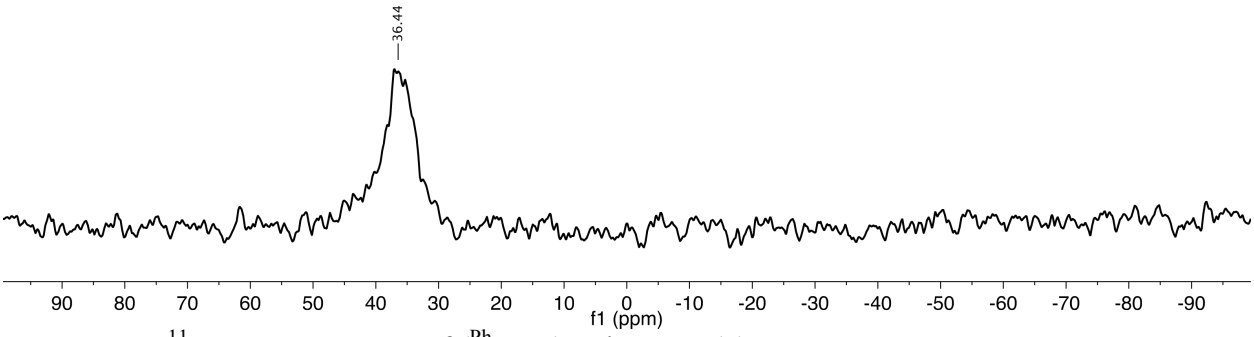


Figure S11. ^{11}B NMR spectrum of (^{Ph}DPB)Fe in C_6D_6 (**5**)

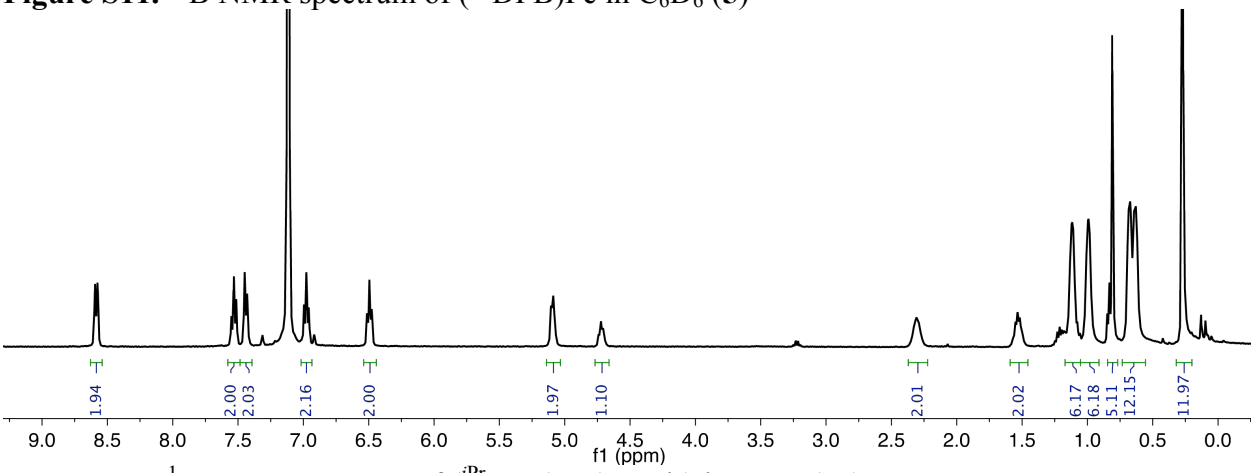


Figure S12. ^{1}H NMR spectrum of (^{iPr}DPB)Fe($NNSi_2$) in C_6D_6 (**6a**)

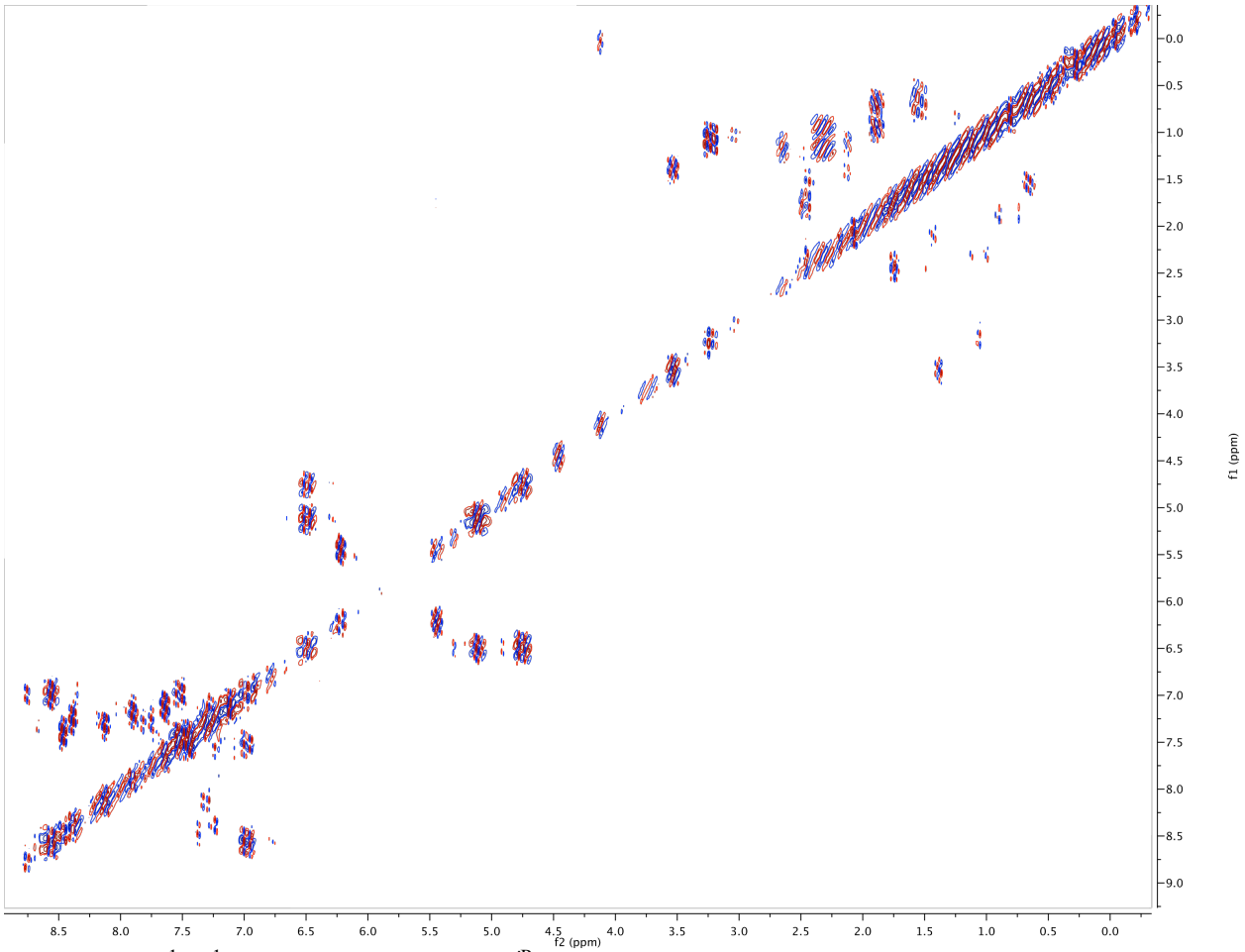


Figure S13. ^{1}H-^{1}H COSY spectrum of ($^{i\text{Pr}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6a**)

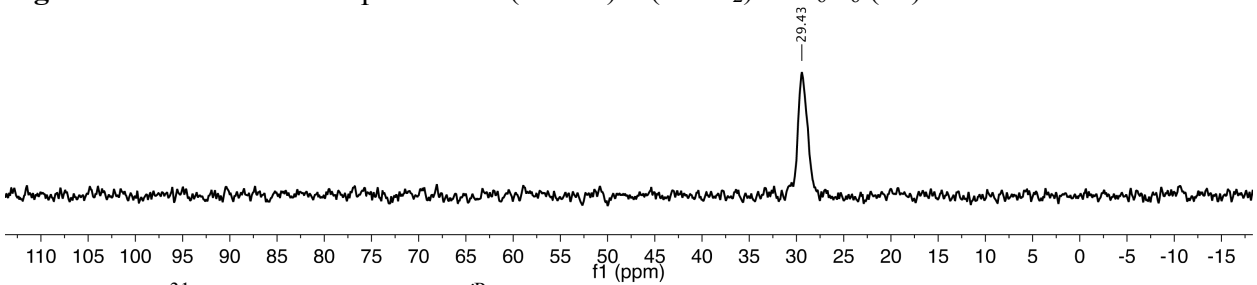


Figure S14. ^{31}P NMR spectrum of ($^{i\text{Pr}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6a**)

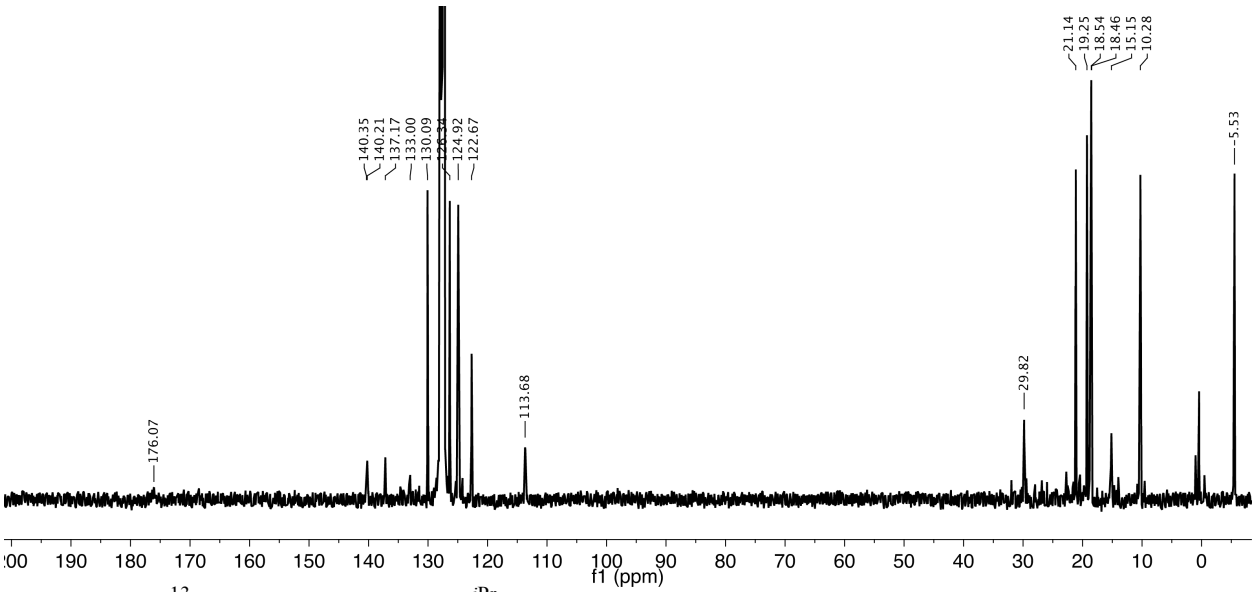


Figure S15. ^{13}C NMR spectrum of ($^{i\text{Pr}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6a**)

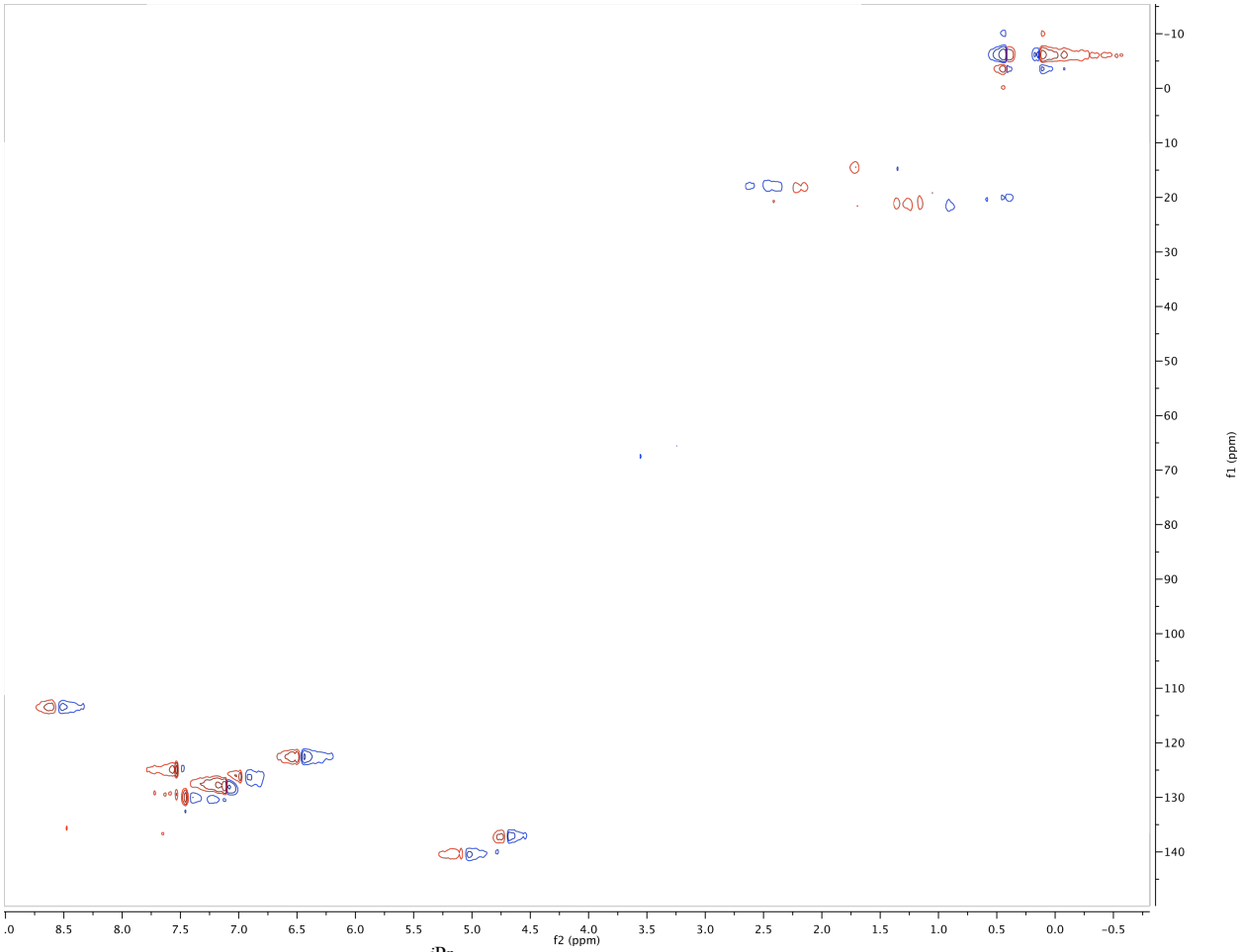


Figure S16. HSQC spectrum of ($^{i\text{Pr}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6a**)

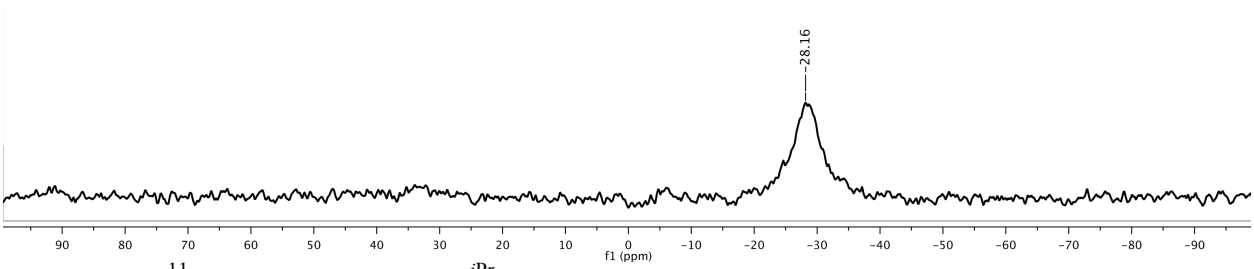


Figure S17. ^{11}B NMR spectrum of ($^{i\text{Pr}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6a**)

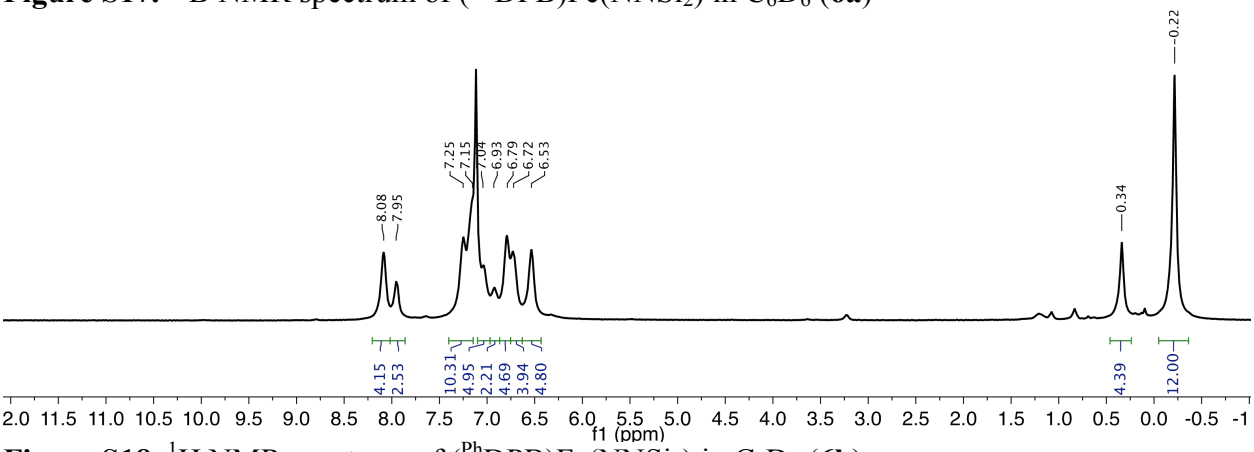


Figure S18. ^{1}H NMR spectrum of ($^{\text{Ph}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6b**)

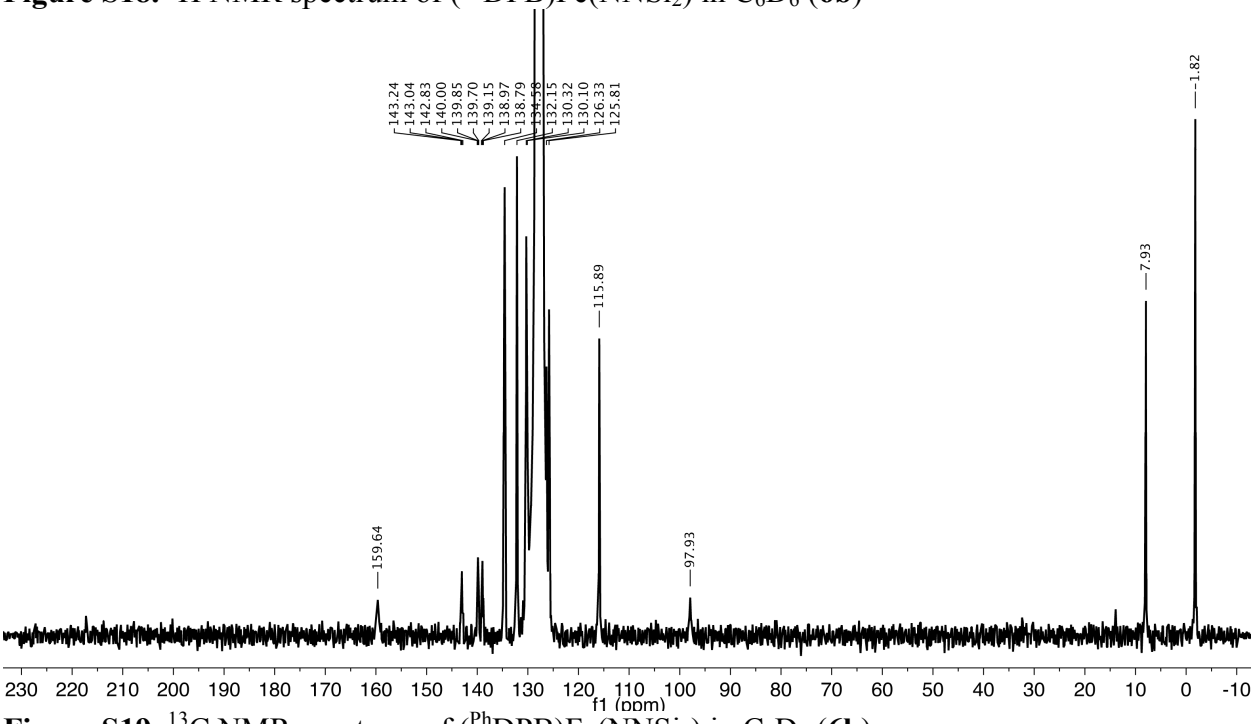


Figure S19. ^{13}C NMR spectrum of ($^{\text{Ph}}$DPB)Fe(NNSi$_2$) in C_6D_6 (**6b**)

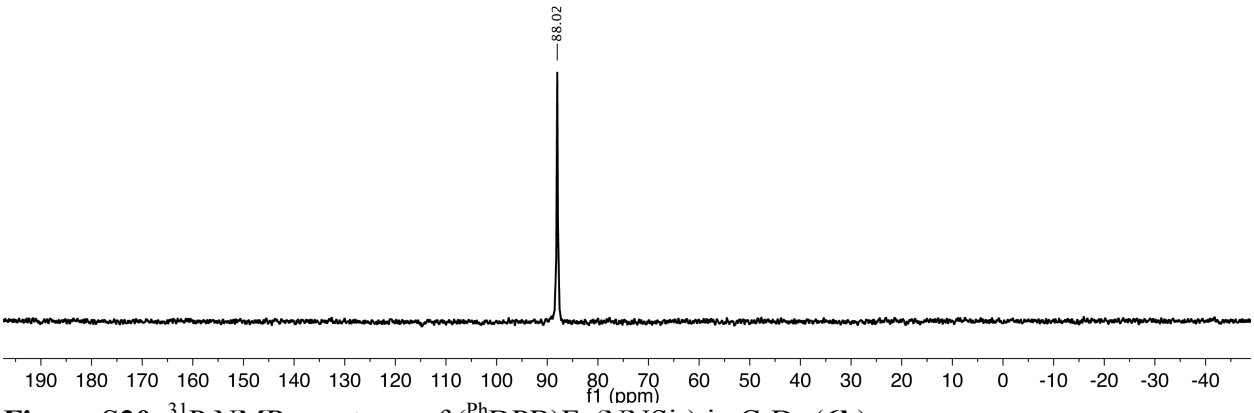


Figure S20. ^{31}P NMR spectrum of (^{Ph}DPB)Fe(NNSi$_2$) in C_6D_6 (**6b**)

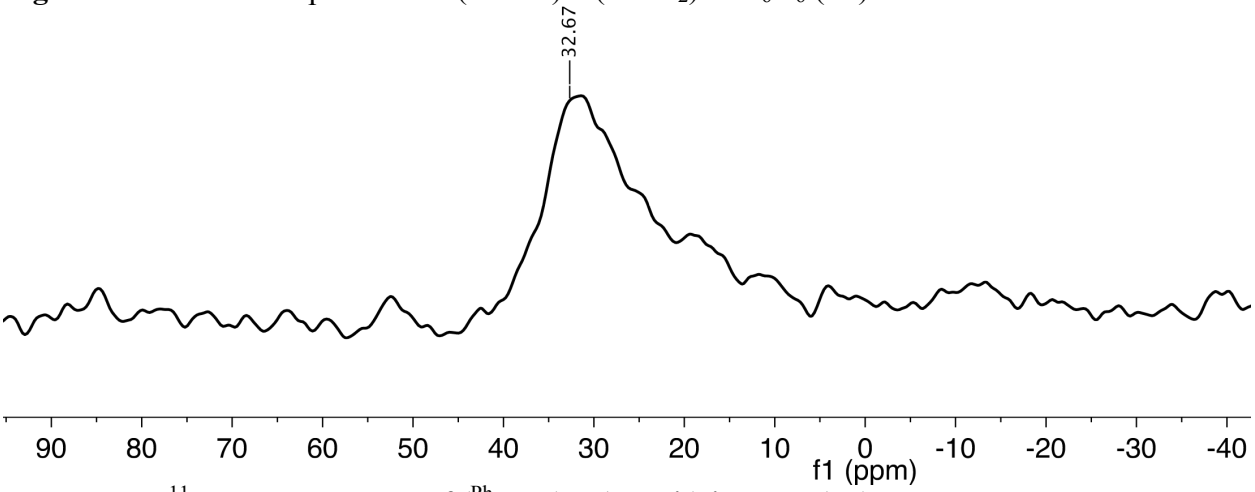


Figure S21. ^{11}B NMR spectrum of (^{Ph}DPB)Fe(NNSi$_2$) in C_6D_6 (**6b**)

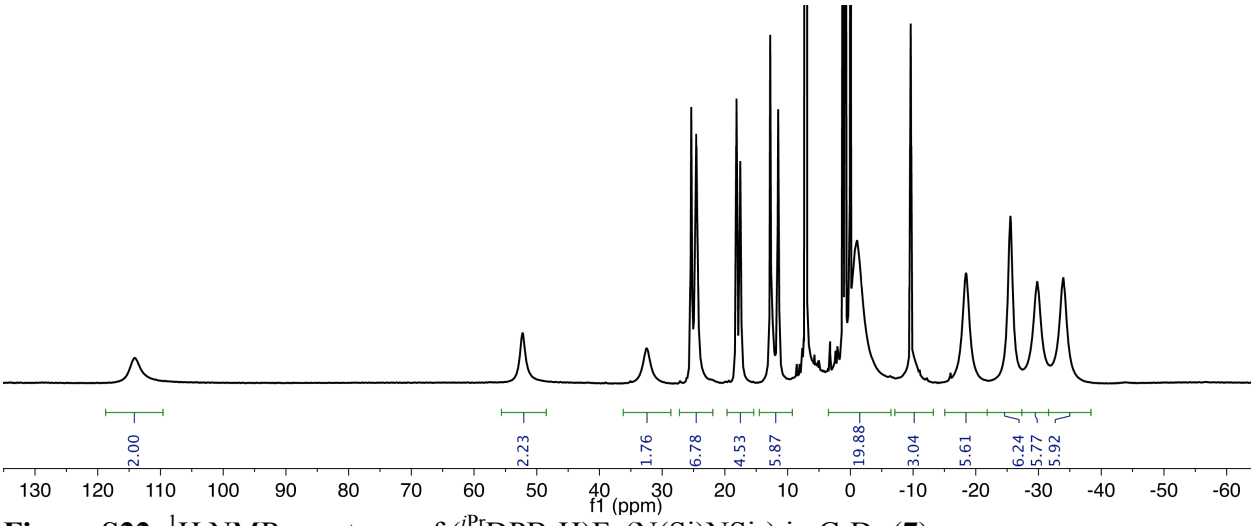


Figure S22. ^{1}H NMR spectrum of ($^{i\text{Pr}}$DPB-H)Fe(N(Si)NSi$_2$) in C_6D_6 (**7**)

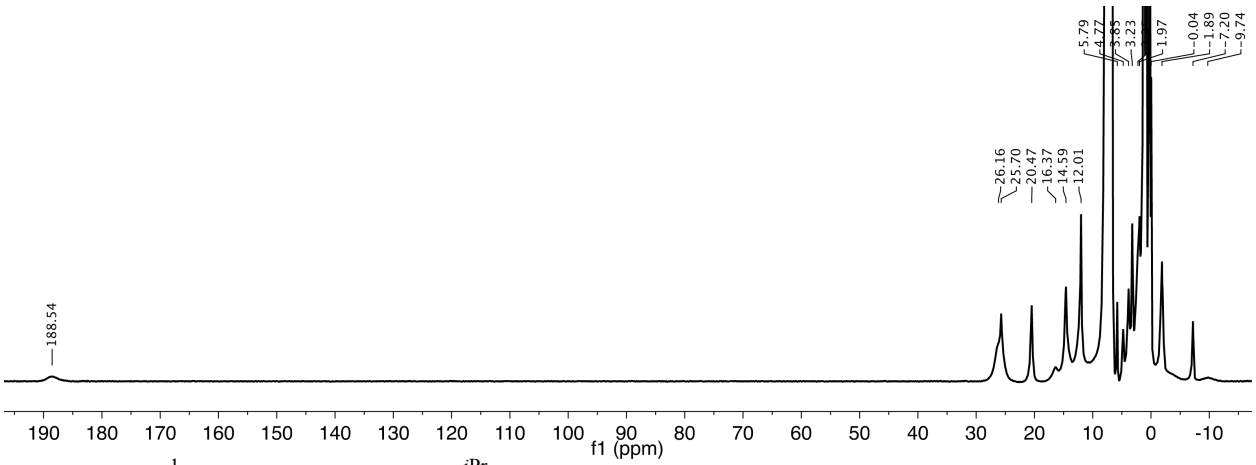


Figure S23. ^{1}H NMR spectrum of ($^{i\text{Pr}}$DPB-H)*Fe(N(Si)NSi$_2$) in C_6D_6 (**8**)

UV/vis spectra

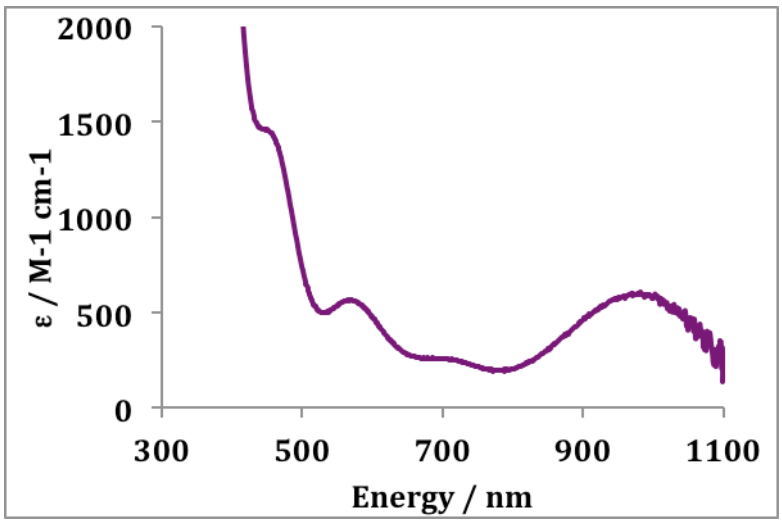


Figure S24. UV/vis spectrum of ($^{i\text{Pr}}$DPB)FeBr (**3a**) in toluene.

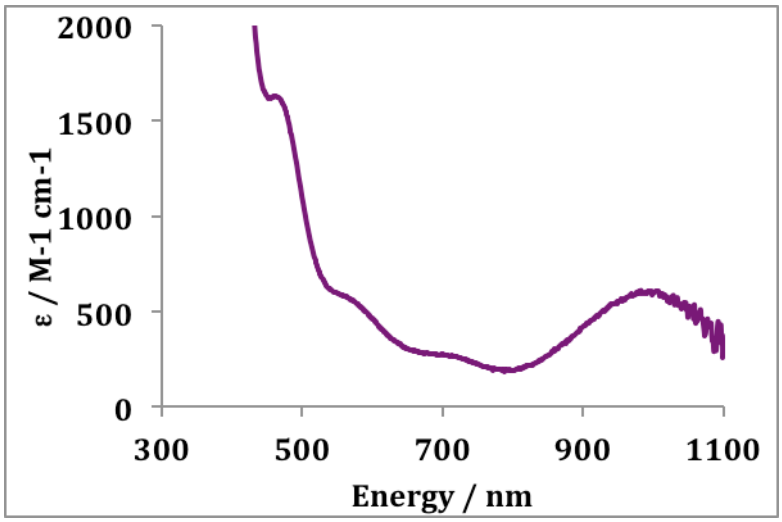


Figure S25. UV/vis spectrum of ($^{\text{Ph}}$DPB)FeBr (**3b**) in toluene.

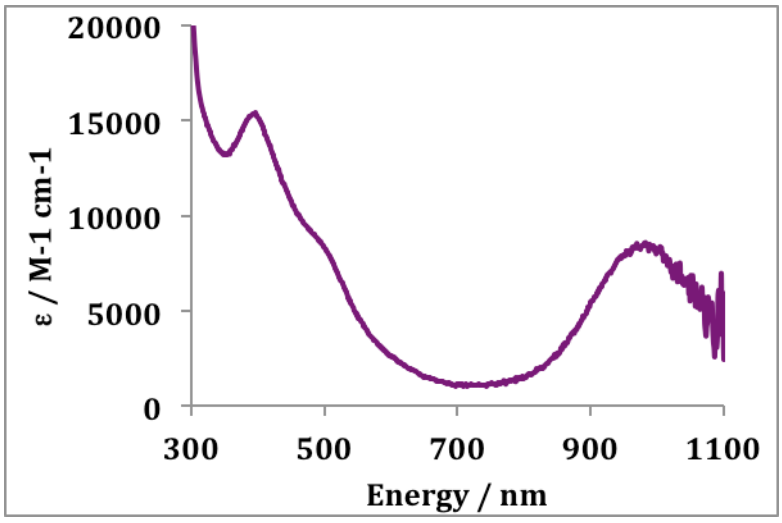


Figure S26. UV/vis spectrum of [($^{i\text{Pr}}$DPB)Fe]$_2$(μ-1,2-N_2) (**4**) in toluene.

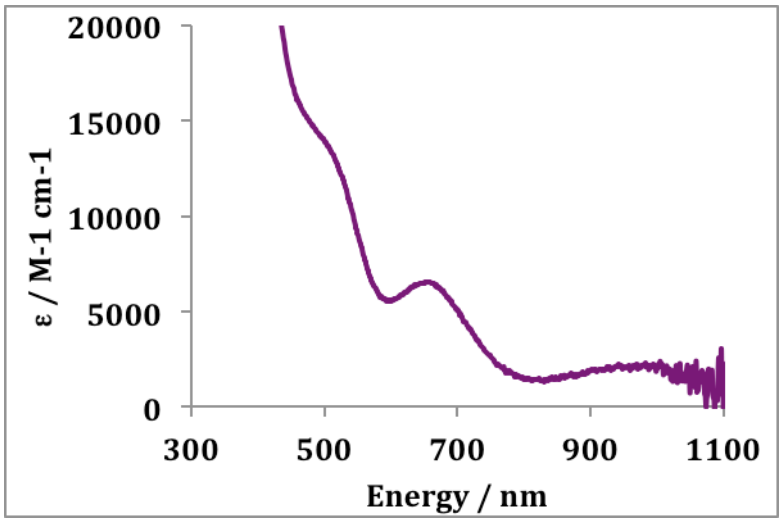


Figure S27. UV/vis spectrum of ($^{\text{Ph}}$DPB)Fe (**5**) in toluene.

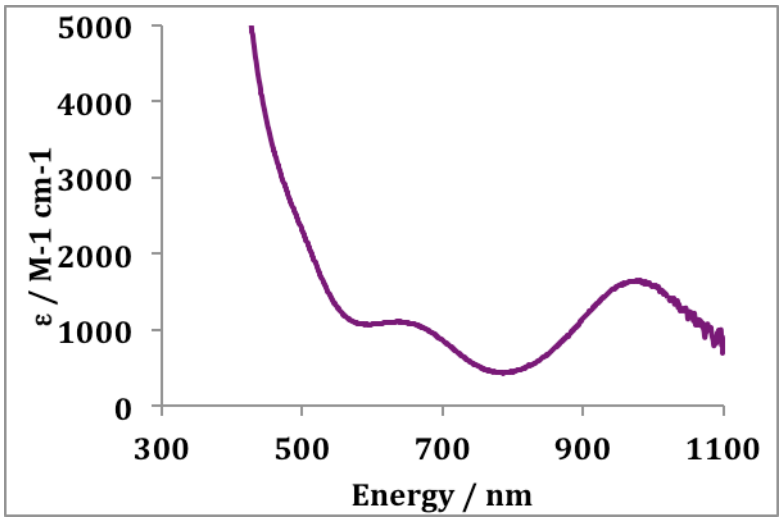


Figure S28. UV/vis spectrum of ($^{i\text{Pr}}$DPB)FeNNSi$_2$ (**6a**) in toluene.

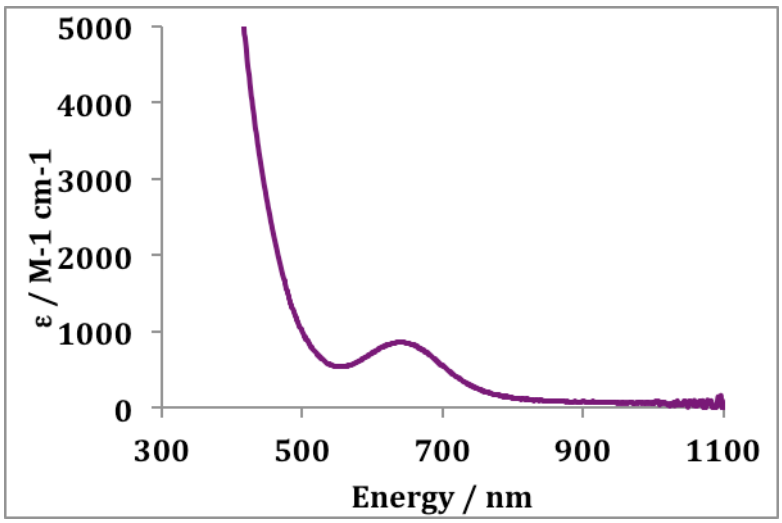


Figure S29. UV/vis spectrum of ($^{\text{Ph}}$DPB)FeNNSi$_2$ (**6b**) in toluene.

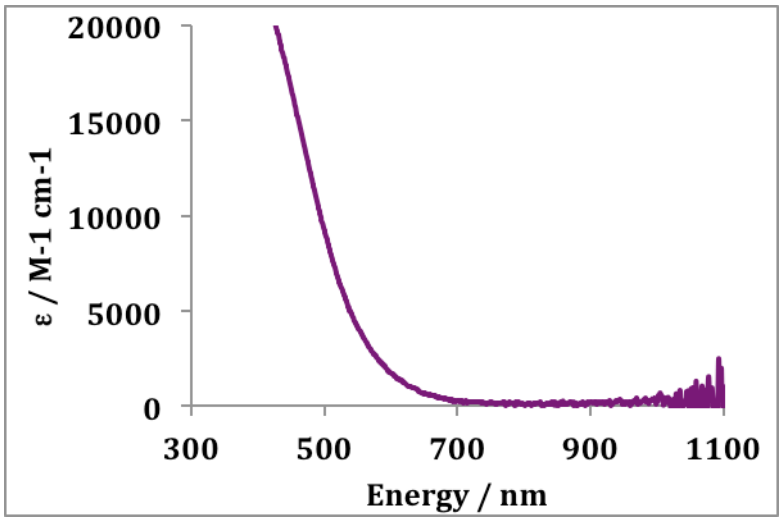


Figure S30. UV/vis spectrum of ($^{i\text{Pr}}$DPB-H)Fe(N(Si)NSi$_2$) (**7**) in toluene.

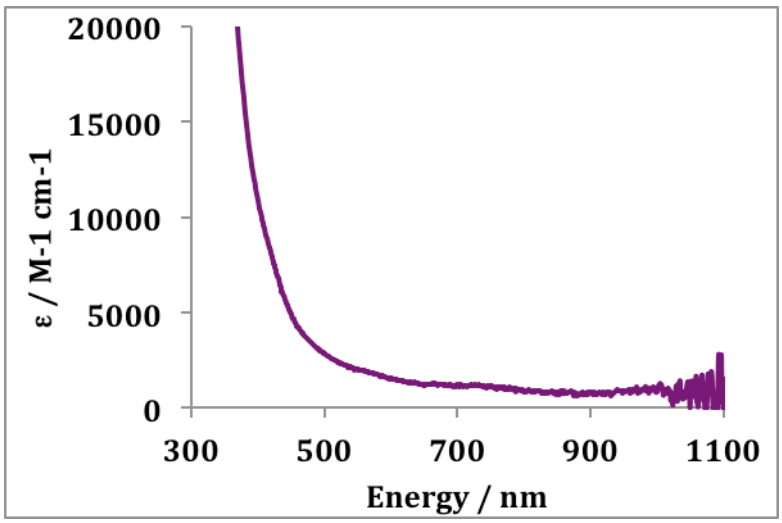


Figure S31. UV/vis spectrum of ($^{\text{Ph}}$DPB-H)*Fe(N(H)NSi$_2$) (**8**) in toluene.

IR spectra

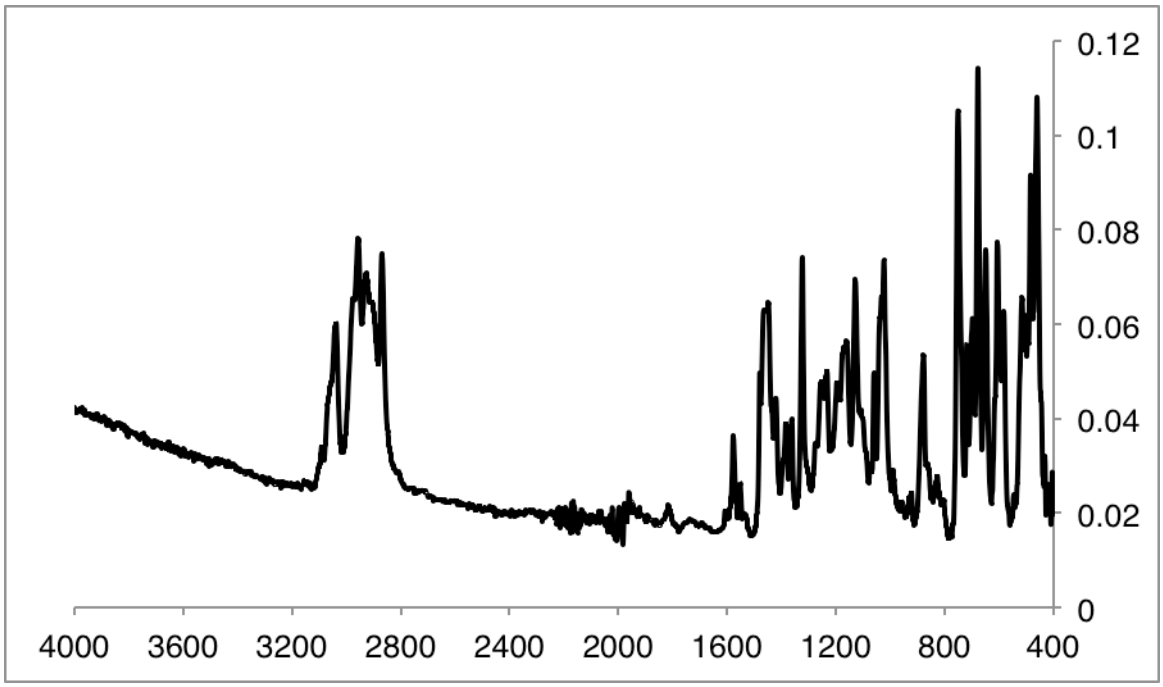


Figure S32. Thin film (C_6D_6) IR spectrum of [($^{i\text{Pr}}$DPB)Fe]$_2$(μ-1,2-N_2) (**4**)

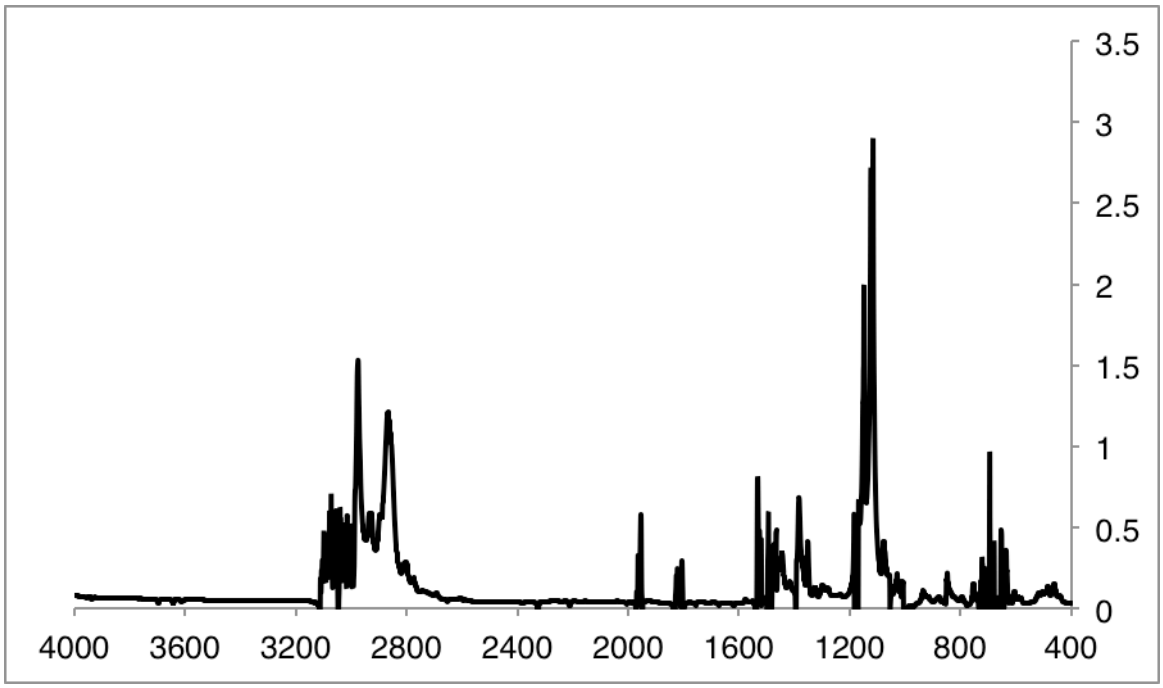


Figure S33. Solution IR spectrum (benzene) of [($^{i\text{Pr}}$DPB)Fe]$_2$(μ-1,2-N_2) (**4**). The small, sharp features at ~1960 and ~1820 cm^{-1} arise from imperfect subtraction of solvent.

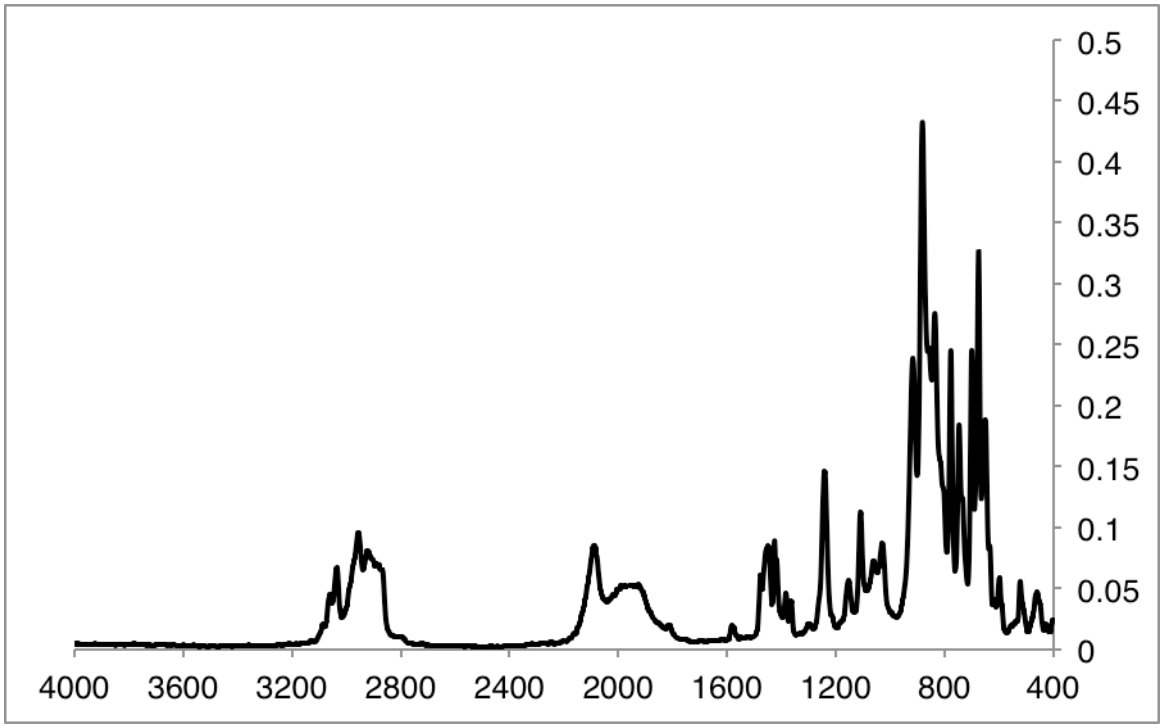


Figure S34. Thin film (C_6D_6) IR spectrum of ($^{i\text{Pr}}$DPB-H)Fe(N(Si)NSi$_2$) (**7**).

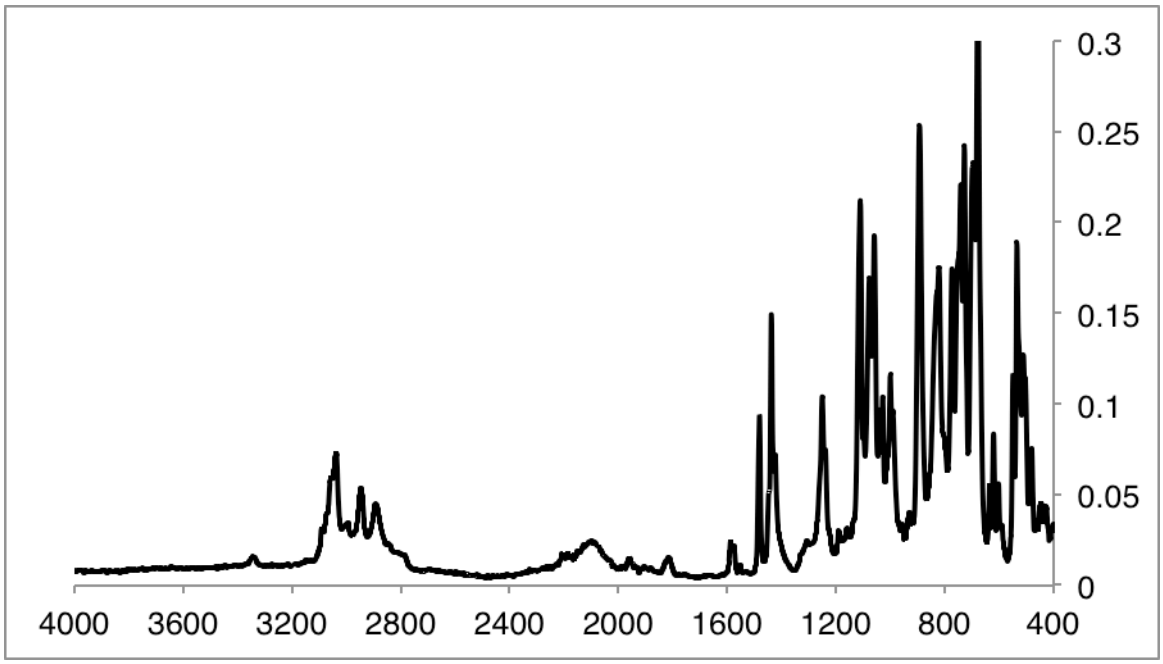


Figure S35. Thin film (C_6D_6) IR spectrum of ($^{\text{Ph}}$DPB*-H)Fe(N(H)NSi$_2$) (**8**).

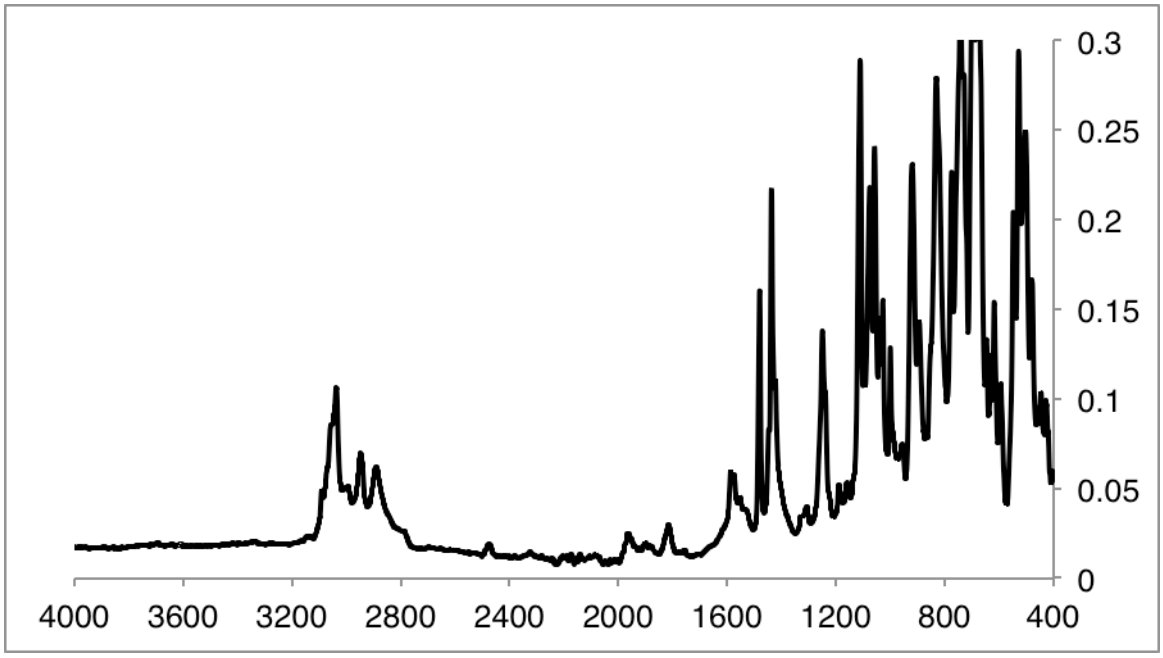


Figure S36. Thin film (C_6D_6) IR spectrum of (^{Ph}DPB*-D)Fe(N(D)NSi$_2$) (**8**-D$_2$).

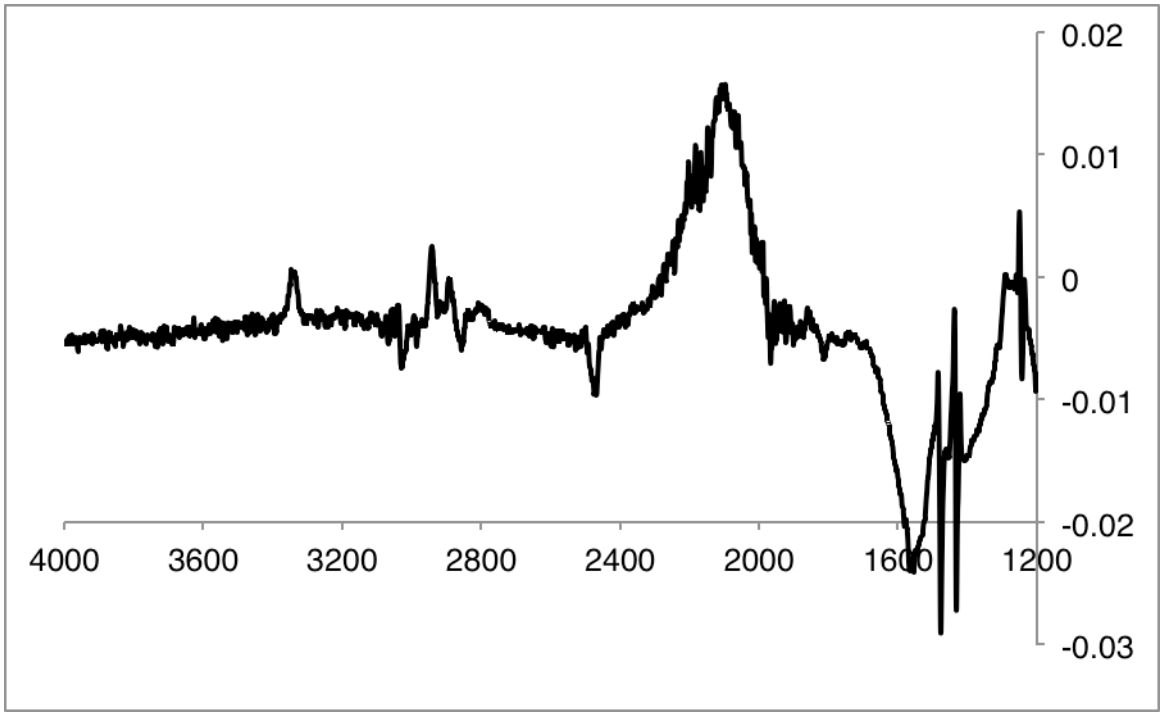


Figure S37. Thin film (C_6D_6) subtraction IR spectrum of **8** - **8**-D$_2$. The features at ca. 2900 and ca. 1480 cm^{-1} correspond to imperfect subtraction of the intense C–H stretching modes and aryl breathing modes, respectively.

X-ray diffraction Tables

Table S4. Crystal data and structure refinement for **3a**.

Identification code	**3a**	
Empirical formula	C30 H41 B Br Fe P2	
Formula weight	610.14	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.921(3) Å	α = 90°.
	b = 9.9768(12) Å	β = 104.872(8)°.
	c = 31.705(4) Å	γ = 90°.
Volume	5784.4(13) $Å^3$	
Z	8	
Density (calculated)	1.401 Mg/m^3	
Absorption coefficient	2.031 mm^{-1}	
F(000)	2536	
Crystal size	0.388 x 0.312 x 0.298 mm^3	
Theta range for data collection	2.23 to 44.08°.	
Index ranges	-36<=h<=36, -19<=k<=19, -59<=l<=62	
Reflections collected	130537	
Independent reflections	22550 [R(int) = 0.0437]	
Completeness to theta = 44.08°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	22550 / 0 / 344	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0929	
R indices (all data)	R1 = 0.0675, wR2 = 0.1012	
Largest diff. peak and hole	0.987 and -1.739 $e.Å^{-3}$	

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6363(1)	2789(1)	6064(1)	10(1)
Br(1)	5830(1)	4941(1)	5865(1)	21(1)
P(2)	6150(1)	2174(1)	6746(1)	11(1)
P(1)	7650(1)	2649(1)	6151(1)	11(1)
C(8)	7264(1)	163(1)	5842(1)	12(1)
C(7)	7803(1)	1153(1)	5861(1)	13(1)
C(16)	8327(1)	2389(1)	6691(1)	13(1)
C(1)	5872(1)	1034(1)	5638(1)	11(1)
C(28)	5278(1)	2656(1)	6878(1)	15(1)
C(25)	6879(1)	2687(1)	7239(1)	13(1)
C(27)	7110(1)	4152(1)	7200(1)	16(1)
C(19)	6147(1)	341(1)	6750(1)	12(1)
C(6)	5135(1)	819(1)	5650(1)	16(1)
C(20)	6372(1)	-301(1)	6407(1)	12(1)
C(2)	5977(1)	1847(1)	5292(1)	15(1)
C(4)	4677(1)	2140(1)	5000(1)	20(1)
C(30)	4620(1)	2158(1)	6524(1)	22(1)
C(13)	8026(1)	4091(1)	5911(1)	16(1)
C(29)	5216(1)	4176(1)	6934(1)	19(1)
B(1)	6544(1)	499(1)	6005(1)	11(1)
C(26)	6715(1)	2433(1)	7682(1)	19(1)
C(18)	8278(1)	937(1)	6846(1)	16(1)
C(24)	5940(1)	-412(1)	7075(1)	16(1)
C(3)	5389(1)	2407(1)	4982(1)	20(1)
C(21)	6400(1)	-1714(1)	6417(1)	17(1)
C(23)	5975(1)	-1808(1)	7072(1)	17(1)
C(10)	8004(1)	-1324(1)	5511(1)	19(1)
C(12)	8428(1)	917(1)	5708(1)	17(1)
C(17)	9124(1)	2698(1)	6696(1)	21(1)
C(9)	7380(1)	-1082(1)	5658(1)	16(1)
C(11)	8532(1)	-330(1)	5536(1)	20(1)

C(22)	6204(1)	-2456(1)	6742(1)	18(1)
C(15)	7614(1)	4265(1)	5432(1)	21(1)
C(5)	4552(1)	1330(1)	5331(1)	20(1)
C(14)	7963(1)	5362(1)	6172(1)	22(1)

Table S6. Bond lengths [Å] and angles [°] for **3a**.

Fe(1)-C(1)	2.2608(9)
Fe(1)-B(1)	2.3243(11)
Fe(1)-P(2)	2.3785(4)
Fe(1)-P(1)	2.3835(5)
Fe(1)-Br(1)	2.3870(3)
Fe(1)-C(2)	2.5486(11)
Fe(1)-C(6)	3.0692(12)
P(2)-C(19)	1.8286(10)
P(2)-C(28)	1.8666(11)
P(2)-C(25)	1.8711(10)
P(1)-C(7)	1.8155(10)
P(1)-C(13)	1.8532(11)
P(1)-C(16)	1.8737(10)
C(8)-C(7)	1.4105(14)
C(8)-C(9)	1.4124(14)
C(8)-B(1)	1.6136(15)
C(7)-C(12)	1.4074(15)
C(16)-C(17)	1.5346(15)
C(16)-C(18)	1.5395(15)
C(16)-H(16)	1.0000
C(1)-C(2)	1.4191(14)
C(1)-C(6)	1.4212(15)
C(1)-B(1)	1.5789(14)
C(28)-C(30)	1.5307(16)
C(28)-C(29)	1.5353(16)
C(28)-H(28)	1.0000
C(25)-C(26)	1.5349(15)
C(25)-C(27)	1.5400(15)
C(25)-H(25)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(19)-C(24)	1.4073(14)
C(19)-C(20)	1.4195(14)

C(6)-C(5)	1.3880(16)
C(6)-H(6)	0.92(2)
C(20)-C(21)	1.4101(14)
C(20)-B(1)	1.6057(15)
C(2)-C(3)	1.3977(15)
C(2)-H(2)	0.921(19)
C(4)-C(3)	1.3891(18)
C(4)-C(5)	1.3935(18)
C(4)-H(4)	0.918(19)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(13)-C(15)	1.5292(15)
C(13)-C(14)	1.5363(17)
C(13)-H(13)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(24)-C(23)	1.3939(16)
C(24)-H(24)	0.9500
C(3)-H(3)	0.962(19)
C(21)-C(22)	1.3939(16)
C(21)-H(21)	0.9500
C(23)-C(22)	1.3896(18)
C(23)-H(23)	0.9500
C(10)-C(11)	1.3952(19)
C(10)-C(9)	1.3976(16)
C(10)-H(10)	0.9500
C(12)-C(11)	1.3930(17)
C(12)-H(12)	0.9500

C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(9)-H(9)	0.9500
C(11)-H(11)	0.9500
C(22)-H(22)	0.9500
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(5)-H(5)	1.00(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

C(1)-Fe(1)-B(1)	40.25(4)
C(1)-Fe(1)-P(2)	101.74(3)
B(1)-Fe(1)-P(2)	83.23(3)
C(1)-Fe(1)-P(1)	105.95(3)
B(1)-Fe(1)-P(1)	77.58(3)
P(2)-Fe(1)-P(1)	106.609(12)
C(1)-Fe(1)-Br(1)	117.23(3)
B(1)-Fe(1)-Br(1)	157.42(3)
P(2)-Fe(1)-Br(1)	108.270(9)
P(1)-Fe(1)-Br(1)	115.703(10)
C(1)-Fe(1)-C(2)	33.65(3)
B(1)-Fe(1)-C(2)	64.64(4)
P(2)-Fe(1)-C(2)	134.75(3)
P(1)-Fe(1)-C(2)	97.02(3)
Br(1)-Fe(1)-C(2)	94.61(3)
C(1)-Fe(1)-C(6)	25.64(3)
B(1)-Fe(1)-C(6)	56.41(4)
P(2)-Fe(1)-C(6)	86.38(2)
P(1)-Fe(1)-C(6)	130.61(2)
Br(1)-Fe(1)-C(6)	103.91(2)
C(2)-Fe(1)-C(6)	49.76(3)
C(19)-P(2)-C(28)	104.54(5)

C(19)-P(2)-C(25)	105.72(4)
C(28)-P(2)-C(25)	104.27(5)
C(19)-P(2)-Fe(1)	105.47(3)
C(28)-P(2)-Fe(1)	120.18(4)
C(25)-P(2)-Fe(1)	115.35(4)
C(7)-P(1)-C(13)	107.52(5)
C(7)-P(1)-C(16)	100.89(5)
C(13)-P(1)-C(16)	103.81(5)
C(7)-P(1)-Fe(1)	106.31(3)
C(13)-P(1)-Fe(1)	113.28(4)
C(16)-P(1)-Fe(1)	123.55(3)
C(7)-C(8)-C(9)	116.53(9)
C(7)-C(8)-B(1)	120.12(9)
C(9)-C(8)-B(1)	123.28(9)
C(12)-C(7)-C(8)	122.01(10)
C(12)-C(7)-P(1)	124.72(8)
C(8)-C(7)-P(1)	112.94(7)
C(17)-C(16)-C(18)	108.96(9)
C(17)-C(16)-P(1)	114.84(7)
C(18)-C(16)-P(1)	109.75(7)
C(17)-C(16)-H(16)	107.7
C(18)-C(16)-H(16)	107.7
P(1)-C(16)-H(16)	107.7
C(2)-C(1)-C(6)	116.12(9)
C(2)-C(1)-B(1)	121.14(9)
C(6)-C(1)-B(1)	122.59(9)
C(2)-C(1)-Fe(1)	84.37(6)
C(6)-C(1)-Fe(1)	110.87(7)
B(1)-C(1)-Fe(1)	72.04(5)
C(30)-C(28)-C(29)	109.47(9)
C(30)-C(28)-P(2)	110.59(8)
C(29)-C(28)-P(2)	112.25(7)
C(30)-C(28)-H(28)	108.1
C(29)-C(28)-H(28)	108.1
P(2)-C(28)-H(28)	108.1
C(26)-C(25)-C(27)	111.00(9)

C(26)-C(25)-P(2)	116.11(8)
C(27)-C(25)-P(2)	110.87(7)
C(26)-C(25)-H(25)	106.0
C(27)-C(25)-H(25)	106.0
P(2)-C(25)-H(25)	106.0
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(19)-C(20)	120.90(9)
C(24)-C(19)-P(2)	122.79(8)
C(20)-C(19)-P(2)	116.31(7)
C(5)-C(6)-C(1)	121.73(10)
C(5)-C(6)-Fe(1)	116.66(8)
C(1)-C(6)-Fe(1)	43.49(5)
C(5)-C(6)-H(6)	120.9(13)
C(1)-C(6)-H(6)	117.2(13)
Fe(1)-C(6)-H(6)	107.6(13)
C(21)-C(20)-C(19)	116.77(9)
C(21)-C(20)-B(1)	120.09(9)
C(19)-C(20)-B(1)	123.04(8)
C(3)-C(2)-C(1)	121.90(10)
C(3)-C(2)-Fe(1)	120.53(8)
C(1)-C(2)-Fe(1)	61.98(5)
C(3)-C(2)-H(2)	120.4(12)
C(1)-C(2)-H(2)	117.5(12)
Fe(1)-C(2)-H(2)	89.8(12)
C(3)-C(4)-C(5)	119.64(10)
C(3)-C(4)-H(4)	118.2(12)
C(5)-C(4)-H(4)	122.2(12)
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5

H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(15)-C(13)-C(14)	110.59(10)
C(15)-C(13)-P(1)	110.22(8)
C(14)-C(13)-P(1)	109.11(8)
C(15)-C(13)-H(13)	109.0
C(14)-C(13)-H(13)	109.0
P(1)-C(13)-H(13)	109.0
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(1)-B(1)-C(20)	117.69(9)
C(1)-B(1)-C(8)	114.86(8)
C(20)-B(1)-C(8)	120.67(8)
C(1)-B(1)-Fe(1)	67.71(5)
C(20)-B(1)-Fe(1)	111.19(6)
C(8)-B(1)-Fe(1)	112.60(7)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(23)-C(24)-C(19)	120.41(10)
C(23)-C(24)-H(24)	119.8
C(19)-C(24)-H(24)	119.8
C(4)-C(3)-C(2)	120.04(11)

C(4)-C(3)-H(3)	118.7(12)
C(2)-C(3)-H(3)	121.3(12)
C(22)-C(21)-C(20)	122.16(10)
C(22)-C(21)-H(21)	118.9
C(20)-C(21)-H(21)	118.9
C(22)-C(23)-C(24)	119.61(10)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(11)-C(10)-C(9)	120.80(10)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(11)-C(12)-C(7)	119.99(11)
C(11)-C(12)-H(12)	120.0
C(7)-C(12)-H(12)	120.0
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(10)-C(9)-C(8)	121.56(11)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(12)-C(11)-C(10)	119.09(10)
C(12)-C(11)-H(11)	120.5
C(10)-C(11)-H(11)	120.5
C(23)-C(22)-C(21)	120.13(10)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(6)-C(5)-C(4)	120.47(11)

C(6)-C(5)-H(5)	121.7(12)
C(4)-C(5)-H(5)	117.8(12)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S7. Crystal data and structure refinement for **3b**.

Identification code	**3b**	
Empirical formula	C42 H33 B Br Fe P2	
Formula weight	373.10	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.6143(6) Å	α = 87.525(3)°.
	b = 9.7710(5) Å	β = 88.376(4)°.
	c = 19.9222(14) Å	γ = 68.912(2)°.
Volume	1744.39(19) $Å^3$	
Z	2	
Density (calculated)	1.421 Mg/m^3	
Absorption coefficient	1.699 mm^{-1}	
F(000)	762	
Crystal size	0.18 x 0.16 x 0.08 mm^3	
Theta range for data collection	2.05 to 27.11°.	
Index ranges	-12<=h<=12, -12<=k<=12, -25<=l<=25	
Reflections collected	66744	
Independent reflections	7693 [R(int) = 0.0822]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7693 / 434 / 444	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1122	
R indices (all data)	R1 = 0.0774, wR2 = 0.1196	
Largest diff. peak and hole	0.545 and -0.474 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-2836(1)	759(1)	2486(1)	30(1)
Fe(1)	-789(1)	1515(1)	2502(1)	18(1)
P(1)	-873(1)	2928(1)	1512(1)	18(1)
P(2)	-1099(1)	2964(1)	3446(1)	21(1)
C(13)	-1914(4)	4892(4)	1506(2)	21(1)
C(31)	-2217(4)	4913(4)	3380(2)	26(1)
C(1)	1554(3)	62(4)	2571(2)	22(1)
C(7)	1027(4)	2724(4)	1282(2)	21(1)
C(25)	736(4)	2851(4)	3700(2)	23(1)
C(8)	2050(4)	2208(4)	1808(2)	23(1)
C(27)	3283(4)	2301(4)	3378(2)	28(1)
C(18)	-1205(4)	5898(4)	1468(2)	35(1)
C(30)	1035(4)	3263(4)	4327(2)	29(1)
C(14)	-3456(4)	5381(4)	1557(2)	30(1)
C(32)	-1625(4)	5988(4)	3477(2)	34(1)
C(26)	1867(4)	2327(4)	3208(2)	21(1)
C(38)	-1868(4)	939(4)	4248(2)	33(1)
C(15)	-4279(4)	6889(4)	1550(2)	33(1)
C(20)	-1507(4)	900(4)	757(2)	28(1)
C(12)	1460(4)	3048(4)	633(2)	27(1)
C(5)	1407(4)	-2077(4)	2026(2)	30(1)
C(9)	3522(4)	2066(4)	1652(2)	32(1)
C(6)	1535(4)	-715(4)	1986(2)	26(1)
C(28)	3577(4)	2709(4)	3998(2)	35(1)
C(10)	3964(4)	2392(4)	1014(2)	34(1)
C(19)	-1635(4)	2359(4)	785(2)	22(1)
C(2)	1354(4)	-623(4)	3180(2)	26(1)
C(17)	-2054(5)	7398(4)	1481(2)	45(1)
C(42)	-2776(4)	3368(4)	4671(2)	29(1)
C(36)	-3726(4)	5312(4)	3235(2)	34(1)
C(3)	1223(4)	-1990(4)	3210(2)	29(1)

C(24)	-2396(4)	3329(4)	274(2)	32(1)
C(16)	-3578(5)	7887(4)	1515(2)	36(1)
C(41)	-3424(4)	2886(4)	5205(2)	33(1)
C(37)	-1963(4)	2387(4)	4181(2)	22(1)
C(4)	1252(4)	-2724(4)	2637(2)	31(1)
C(29)	2449(4)	3193(4)	4475(2)	33(1)
C(22)	-2906(4)	1420(5)	-254(2)	37(1)
C(23)	-3024(5)	2859(5)	-238(2)	41(1)
C(34)	-4039(5)	7857(4)	3291(2)	43(1)
C(11)	2929(4)	2869(4)	499(2)	32(1)
C(40)	-3330(4)	1452(4)	5270(2)	35(1)
C(21)	-2128(4)	429(4)	234(2)	34(1)
C(39)	-2551(5)	477(4)	4796(2)	40(1)
C(35)	-4611(4)	6789(4)	3195(2)	40(1)
B(1)	1571(4)	1670(4)	2523(2)	21(1)
C(33)	-2553(5)	7467(4)	3430(2)	45(1)

Table S9. Bond lengths [Å] and angles [°] for **3b**.

Br(1)-Fe(1)	2.3388(6)
Fe(1)-C(1)	2.193(3)
Fe(1)-B(1)	2.330(4)
Fe(1)-P(1)	2.3460(10)
Fe(1)-P(2)	2.3499(10)
Fe(1)-C(2)	2.692(4)
Fe(1)-C(6)	2.712(3)
P(1)-C(7)	1.812(3)
P(1)-C(13)	1.817(3)
P(1)-C(19)	1.834(3)
P(2)-C(25)	1.813(4)
P(2)-C(31)	1.820(4)
P(2)-C(37)	1.830(3)
C(13)-C(18)	1.382(5)
C(13)-C(14)	1.387(5)
C(31)-C(32)	1.385(5)
C(31)-C(36)	1.396(5)
C(1)-C(2)	1.402(5)
C(1)-C(6)	1.421(5)
C(1)-B(1)	1.576(5)
C(7)-C(12)	1.405(5)
C(7)-C(8)	1.407(5)
C(25)-C(30)	1.398(5)
C(25)-C(26)	1.410(4)
C(8)-C(9)	1.399(5)
C(8)-B(1)	1.610(5)
C(27)-C(28)	1.383(5)
C(27)-C(26)	1.403(5)
C(27)-H(27)	0.9500
C(18)-C(17)	1.399(5)
C(18)-H(18)	0.9500
C(30)-C(29)	1.376(5)
C(30)-H(30)	0.9500
C(14)-C(15)	1.399(5)

C(14)-H(14)	0.9500
C(32)-C(33)	1.399(5)
C(32)-H(32)	0.9500
C(26)-B(1)	1.607(5)
C(38)-C(37)	1.386(5)
C(38)-C(39)	1.398(5)
C(38)-H(38)	0.9500
C(15)-C(16)	1.370(5)
C(15)-H(15)	0.9500
C(20)-C(21)	1.389(5)
C(20)-C(19)	1.389(5)
C(20)-H(20)	0.9500
C(12)-C(11)	1.379(5)
C(12)-H(12)	0.9500
C(5)-C(4)	1.377(5)
C(5)-C(6)	1.379(5)
C(5)-H(5)	1.00(3)
C(9)-C(10)	1.389(5)
C(9)-H(9)	0.9500
C(6)-H(6)	0.99(3)
C(28)-C(29)	1.383(5)
C(28)-H(28)	0.9500
C(10)-C(11)	1.394(5)
C(10)-H(10)	0.9500
C(19)-C(24)	1.390(5)
C(2)-C(3)	1.384(5)
C(2)-H(2)	0.87(3)
C(17)-C(16)	1.369(6)
C(17)-H(17)	0.9500
C(42)-C(41)	1.369(5)
C(42)-C(37)	1.408(4)
C(42)-H(42)	0.9500
C(36)-C(35)	1.387(5)
C(36)-H(36)	0.9500
C(3)-C(4)	1.369(5)
C(3)-H(3)	0.76(4)

C(24)-C(23)	1.374(5)
C(24)-H(24)	0.9500
C(16)-H(16)	0.9500
C(41)-C(40)	1.371(5)
C(41)-H(41)	0.9500
C(4)-H(4)	0.95(4)
C(29)-H(29)	0.9500
C(22)-C(23)	1.371(6)
C(22)-C(21)	1.372(5)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(34)-C(35)	1.365(6)
C(34)-C(33)	1.374(6)
C(34)-H(34)	0.9500
C(11)-H(11)	0.9500
C(40)-C(39)	1.373(5)
C(40)-H(40)	0.9500
C(21)-H(21)	0.9500
C(39)-H(39)	0.9500
C(35)-H(35)	0.9500
C(33)-H(33)	0.9500

C(1)-Fe(1)-B(1)	40.64(13)
C(1)-Fe(1)-Br(1)	125.74(9)
B(1)-Fe(1)-Br(1)	166.36(10)
C(1)-Fe(1)-P(1)	104.04(9)
B(1)-Fe(1)-P(1)	80.20(10)
Br(1)-Fe(1)-P(1)	106.78(3)
C(1)-Fe(1)-P(2)	102.46(9)
B(1)-Fe(1)-P(2)	80.60(9)
Br(1)-Fe(1)-P(2)	107.03(3)
P(1)-Fe(1)-P(2)	110.33(4)
C(1)-Fe(1)-C(2)	31.28(11)
B(1)-Fe(1)-C(2)	62.28(13)
Br(1)-Fe(1)-C(2)	106.06(8)
P(1)-Fe(1)-C(2)	135.30(8)

P(2)-Fe(1)-C(2)	87.74(9)
C(1)-Fe(1)-C(6)	31.48(11)
B(1)-Fe(1)-C(6)	62.00(12)
Br(1)-Fe(1)-C(6)	105.70(8)
P(1)-Fe(1)-C(6)	89.85(8)
P(2)-Fe(1)-C(6)	133.94(8)
C(2)-Fe(1)-C(6)	52.31(11)
C(7)-P(1)-C(13)	105.81(16)
C(7)-P(1)-C(19)	106.05(14)
C(13)-P(1)-C(19)	102.14(15)
C(7)-P(1)-Fe(1)	107.58(11)
C(13)-P(1)-Fe(1)	119.41(11)
C(19)-P(1)-Fe(1)	114.82(11)
C(25)-P(2)-C(31)	105.85(16)
C(25)-P(2)-C(37)	106.53(15)
C(31)-P(2)-C(37)	101.08(15)
C(25)-P(2)-Fe(1)	107.66(11)
C(31)-P(2)-Fe(1)	119.58(11)
C(37)-P(2)-Fe(1)	115.12(11)
C(18)-C(13)-C(14)	119.6(3)
C(18)-C(13)-P(1)	121.7(3)
C(14)-C(13)-P(1)	118.7(3)
C(32)-C(31)-C(36)	119.8(3)
C(32)-C(31)-P(2)	122.4(3)
C(36)-C(31)-P(2)	117.8(3)
C(2)-C(1)-C(6)	115.1(3)
C(2)-C(1)-B(1)	122.8(3)
C(6)-C(1)-B(1)	121.6(3)
C(2)-C(1)-Fe(1)	94.4(2)
C(6)-C(1)-Fe(1)	94.9(2)
B(1)-C(1)-Fe(1)	74.36(18)
C(12)-C(7)-C(8)	122.1(3)
C(12)-C(7)-P(1)	123.4(3)
C(8)-C(7)-P(1)	114.5(2)
C(30)-C(25)-C(26)	121.4(3)
C(30)-C(25)-P(2)	123.8(3)

C(26)-C(25)-P(2)	114.8(2)
C(9)-C(8)-C(7)	116.0(3)
C(9)-C(8)-B(1)	122.4(3)
C(7)-C(8)-B(1)	121.3(3)
C(28)-C(27)-C(26)	122.4(3)
C(28)-C(27)-H(27)	118.8
C(26)-C(27)-H(27)	118.8
C(13)-C(18)-C(17)	119.5(4)
C(13)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(29)-C(30)-C(25)	120.4(3)
C(29)-C(30)-H(30)	119.8
C(25)-C(30)-H(30)	119.8
C(13)-C(14)-C(15)	119.6(3)
C(13)-C(14)-H(14)	120.2
C(15)-C(14)-H(14)	120.2
C(31)-C(32)-C(33)	119.5(4)
C(31)-C(32)-H(32)	120.3
C(33)-C(32)-H(32)	120.3
C(27)-C(26)-C(25)	116.0(3)
C(27)-C(26)-B(1)	122.4(3)
C(25)-C(26)-B(1)	121.4(3)
C(37)-C(38)-C(39)	120.3(3)
C(37)-C(38)-H(38)	119.9
C(39)-C(38)-H(38)	119.9
C(16)-C(15)-C(14)	120.8(4)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(21)-C(20)-C(19)	120.8(4)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(11)-C(12)-C(7)	119.9(3)
C(11)-C(12)-H(12)	120.1
C(7)-C(12)-H(12)	120.1
C(4)-C(5)-C(6)	121.0(4)
C(4)-C(5)-H(5)	125.2(17)

C(6)-C(5)-H(5)	113.8(17)
C(10)-C(9)-C(8)	122.5(3)
C(10)-C(9)-H(9)	118.8
C(8)-C(9)-H(9)	118.8
C(5)-C(6)-C(1)	121.7(3)
C(5)-C(6)-Fe(1)	115.8(2)
C(1)-C(6)-Fe(1)	53.66(16)
C(5)-C(6)-H(6)	116.2(18)
C(1)-C(6)-H(6)	122.0(18)
Fe(1)-C(6)-H(6)	98.7(18)
C(27)-C(28)-C(29)	120.2(4)
C(27)-C(28)-H(28)	119.9
C(29)-C(28)-H(28)	119.9
C(9)-C(10)-C(11)	120.1(3)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(20)-C(19)-C(24)	118.1(3)
C(20)-C(19)-P(1)	118.6(3)
C(24)-C(19)-P(1)	123.2(3)
C(3)-C(2)-C(1)	122.4(4)
C(3)-C(2)-Fe(1)	116.0(3)
C(1)-C(2)-Fe(1)	54.31(17)
C(3)-C(2)-H(2)	117(2)
C(1)-C(2)-H(2)	120(2)
Fe(1)-C(2)-H(2)	106(2)
C(16)-C(17)-C(18)	121.0(4)
C(16)-C(17)-H(17)	119.5
C(18)-C(17)-H(17)	119.5
C(41)-C(42)-C(37)	120.5(4)
C(41)-C(42)-H(42)	119.8
C(37)-C(42)-H(42)	119.8
C(35)-C(36)-C(31)	119.0(4)
C(35)-C(36)-H(36)	120.5
C(31)-C(36)-H(36)	120.5
C(4)-C(3)-C(2)	120.8(4)
C(4)-C(3)-H(3)	120(3)

C(2)-C(3)-H(3)	118(3)
C(23)-C(24)-C(19)	120.8(4)
C(23)-C(24)-H(24)	119.6
C(19)-C(24)-H(24)	119.6
C(17)-C(16)-C(15)	119.4(4)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(42)-C(41)-C(40)	121.2(3)
C(42)-C(41)-H(41)	119.4
C(40)-C(41)-H(41)	119.4
C(38)-C(37)-C(42)	118.2(3)
C(38)-C(37)-P(2)	119.0(2)
C(42)-C(37)-P(2)	122.8(3)
C(3)-C(4)-C(5)	118.9(4)
C(3)-C(4)-H(4)	117(2)
C(5)-C(4)-H(4)	124(2)
C(30)-C(29)-C(28)	119.5(3)
C(30)-C(29)-H(29)	120.3
C(28)-C(29)-H(29)	120.3
C(23)-C(22)-C(21)	120.0(4)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	120.5(4)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(35)-C(34)-C(33)	119.5(4)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(12)-C(11)-C(10)	119.4(3)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3
C(41)-C(40)-C(39)	119.5(3)
C(41)-C(40)-H(40)	120.3
C(39)-C(40)-H(40)	120.3
C(22)-C(21)-C(20)	119.8(4)
C(22)-C(21)-H(21)	120.1

C(20)-C(21)-H(21)	120.1
C(40)-C(39)-C(38)	120.5(4)
C(40)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(34)-C(35)-C(36)	121.6(4)
C(34)-C(35)-H(35)	119.2
C(36)-C(35)-H(35)	119.2
C(1)-B(1)-C(26)	116.7(3)
C(1)-B(1)-C(8)	116.5(3)
C(26)-B(1)-C(8)	120.6(3)
C(1)-B(1)-Fe(1)	65.00(17)
C(26)-B(1)-Fe(1)	112.6(2)
C(8)-B(1)-Fe(1)	112.3(2)
C(34)-C(33)-C(32)	120.5(4)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7

Symmetry transformations used to generate equivalent atoms:

Table S10. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C60 H82 B2 Fe2 N2 P4	
Formula weight	544.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.6080(5) Å	α = 90°.
	b = 22.6752(7) Å	β = 103.3660(10)°.
	c = 18.8057(7) Å	γ = 90°.
Volume	5645.6(3) $Å^3$	
Z	4	
Density (calculated)	1.281 Mg/m^3	
Absorption coefficient	0.667 mm^{-1}	
F(000)	2312	
Crystal size	0.46 x 0.38 x 0.25 mm^3	
Theta range for data collection	1.43 to 46.11°.	
Index ranges	-27<=h<=27, -45<=k<=45, -37<=l<=37	
Reflections collected	485190	
Independent reflections	48836 [R(int) = 0.0684]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	48836 / 0 / 687	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0794	
R indices (all data)	R1 = 0.0667, wR2 = 0.0915	
Largest diff. peak and hole	0.967 and -0.335 $e.Å^{-3}$	

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4265(1)	2838(1)	3966(1)	10(1)
Fe(2)	1328(1)	3925(1)	2699(1)	10(1)
P(3)	1296(1)	4919(1)	3035(1)	11(1)
P(1)	5731(1)	3206(1)	3704(1)	11(1)
P(2)	4201(1)	1821(1)	3655(1)	12(1)
P(4)	1210(1)	3895(1)	1439(1)	11(1)
N(2)	2484(1)	3531(1)	3154(1)	12(1)
N(1)	3184(1)	3250(1)	3443(1)	11(1)
C(1)	4818(1)	2886(1)	5189(1)	13(1)
C(101)	-170(1)	3593(1)	2784(1)	13(1)
C(120)	-772(1)	4107(1)	1448(1)	13(1)
C(6)	5188(1)	3425(1)	5546(1)	16(1)
C(16)	6109(1)	2853(1)	2908(1)	14(1)
C(2)	3754(1)	2804(1)	5033(1)	14(1)
C(119)	-128(1)	3938(1)	991(1)	14(1)
C(20)	5242(1)	1748(1)	5058(1)	13(1)
C(7)	6814(1)	3064(1)	4464(1)	13(1)
C(11)	8524(1)	3223(1)	5162(1)	20(1)
C(28)	5045(1)	1444(1)	3132(1)	15(1)
C(19)	4541(1)	1435(1)	4523(1)	14(1)
C(107)	49(1)	5073(1)	3185(1)	13(1)
C(125)	1791(1)	4527(1)	1048(1)	16(1)
C(30)	6124(1)	1390(1)	3603(1)	18(1)
C(121)	-1806(1)	4167(1)	1109(1)	16(1)
C(18)	5209(1)	2792(1)	2249(1)	17(1)
C(5)	4561(1)	3817(1)	5787(1)	20(1)
C(17)	7027(1)	3122(1)	2684(1)	22(1)
C(23)	4594(1)	596(1)	5324(1)	21(1)
C(109)	-1702(1)	4810(1)	2820(1)	18(1)
C(3)	3110(1)	3224(1)	5251(1)	19(1)
C(108)	-702(1)	4714(1)	2758(1)	13(1)

C(122)	-2185(1)	4046(1)	372(1)	18(1)
C(10)	8370(1)	2807(1)	5667(1)	20(1)
C(8)	6636(1)	2647(1)	4977(1)	13(1)
B(2)	-359(1)	4176(1)	2313(1)	13(1)
C(116)	2180(1)	5115(1)	3910(1)	16(1)
C(130)	1068(1)	2687(1)	1101(1)	20(1)
C(15)	5015(1)	4217(1)	2892(1)	20(1)
C(129)	2803(1)	3152(1)	1322(1)	18(1)
C(128)	1669(1)	3242(1)	1007(1)	14(1)
C(9)	7448(1)	2517(1)	5571(1)	18(1)
C(14)	5775(1)	4353(1)	4233(1)	22(1)
C(24)	4209(1)	868(1)	4654(1)	18(1)
C(102)	113(1)	3607(1)	3558(1)	18(1)
C(124)	-514(1)	3807(1)	250(1)	18(1)
C(106)	-230(1)	3026(1)	2460(1)	18(1)
C(113)	1438(1)	5548(1)	2411(1)	17(1)
C(4)	3509(1)	3716(1)	5635(1)	20(1)
B(1)	5512(1)	2422(1)	4930(1)	13(1)
C(12)	7750(1)	3350(1)	4557(1)	18(1)
C(13)	5838(1)	4011(1)	3545(1)	16(1)
C(112)	-178(1)	5507(1)	3654(1)	18(1)
C(25)	2930(1)	1539(1)	3213(1)	20(1)
C(123)	-1540(1)	3858(1)	-60(1)	19(1)
C(127)	2868(1)	4654(1)	1491(1)	20(1)
C(110)	-1933(1)	5238(1)	3286(1)	21(1)
C(104)	128(1)	2544(1)	3636(1)	27(1)
C(126)	1766(1)	4484(1)	232(1)	25(1)
C(118)	3265(1)	5016(1)	3836(1)	26(1)
C(111)	-1174(1)	5589(1)	3705(1)	21(1)
C(117)	1963(1)	4742(1)	4534(1)	24(1)
C(27)	2596(1)	1805(1)	2447(1)	28(1)
C(21)	5629(1)	1453(1)	5723(1)	17(1)
C(115)	454(1)	5639(1)	1828(1)	22(1)
C(105)	-101(1)	2513(1)	2875(1)	26(1)
C(103)	254(1)	3090(1)	3974(1)	23(1)
C(29)	4692(1)	831(1)	2836(1)	23(1)

C(114)	1765(1)	6136(1)	2798(1)	27(1)
C(22)	5315(1)	887(1)	5852(1)	21(1)
C(26)	2178(1)	1699(1)	3675(1)	28(1)

Table S12. Bond lengths [Å] and angles [°] for **4**.

Fe(1)-N(1)	1.8261(5)
Fe(1)-C(1)	2.2517(6)
Fe(1)-C(2)	2.2715(7)
Fe(1)-P(1)	2.3182(2)
Fe(1)-B(1)	2.3740(7)
Fe(1)-P(2)	2.3749(2)
Fe(2)-N(2)	1.8382(6)
Fe(2)-C(101)	2.2134(6)
Fe(2)-B(2)	2.3134(7)
Fe(2)-P(4)	2.3381(2)
Fe(2)-P(3)	2.3439(2)
Fe(2)-C(102)	2.6645(7)
P(3)-C(107)	1.8175(7)
P(3)-C(116)	1.8549(7)
P(3)-C(113)	1.8859(7)
P(1)-C(7)	1.8282(7)
P(1)-C(13)	1.8608(7)
P(1)-C(16)	1.8714(7)
P(2)-C(19)	1.8151(7)
P(2)-C(25)	1.8503(8)
P(2)-C(28)	1.8819(7)
P(4)-C(119)	1.8238(7)
P(4)-C(128)	1.8650(7)
P(4)-C(125)	1.8676(7)
N(2)-N(1)	1.1705(8)
C(1)-C(2)	1.4211(10)
C(1)-C(6)	1.4303(10)
C(1)-B(1)	1.5627(9)
C(101)-C(106)	1.4167(10)
C(101)-C(102)	1.4184(10)
C(101)-B(2)	1.5789(10)
C(120)-C(121)	1.4103(9)
C(120)-C(119)	1.4141(9)
C(120)-B(2)	1.6022(10)

C(6)-C(5)	1.3785(10)
C(6)-H(6)	0.952(13)
C(16)-C(17)	1.5330(10)
C(16)-C(18)	1.5340(10)
C(16)-H(16)	1.0000
C(2)-C(3)	1.4185(10)
C(2)-H(2)	0.937(13)
C(119)-C(124)	1.4040(10)
C(20)-C(19)	1.4068(10)
C(20)-C(21)	1.4081(9)
C(20)-B(1)	1.6039(10)
C(7)-C(12)	1.4045(10)
C(7)-C(8)	1.4103(10)
C(11)-C(10)	1.3883(13)
C(11)-C(12)	1.3905(11)
C(11)-H(11)	0.9500
C(28)-C(29)	1.5319(10)
C(28)-C(30)	1.5342(10)
C(28)-H(28)	1.0000
C(19)-C(24)	1.4034(10)
C(107)-C(112)	1.4017(9)
C(107)-C(108)	1.4063(10)
C(125)-C(126)	1.5303(11)
C(125)-C(127)	1.5368(11)
C(125)-H(125)	1.0000
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(121)-C(122)	1.3899(10)
C(121)-H(121)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(5)-C(4)	1.4124(12)
C(5)-H(5)	0.948(14)
C(17)-H(17A)	0.9800

C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(23)-C(22)	1.3894(13)
C(23)-C(24)	1.3924(11)
C(23)-H(23)	0.9500
C(109)-C(110)	1.3922(11)
C(109)-C(108)	1.4088(9)
C(109)-H(109)	0.9500
C(3)-C(4)	1.3711(12)
C(3)-H(3)	0.984(13)
C(108)-B(2)	1.6071(10)
C(122)-C(123)	1.3947(11)
C(122)-H(122)	0.9500
C(10)-C(9)	1.3909(11)
C(10)-H(10)	0.9500
C(8)-C(9)	1.4090(10)
C(8)-B(1)	1.5960(10)
C(116)-C(117)	1.5295(12)
C(116)-C(118)	1.5312(11)
C(116)-H(116)	1.0000
C(130)-C(128)	1.5319(10)
C(130)-H(13A)	0.9800
C(130)-H(13B)	0.9800
C(130)-H(13C)	0.9800
C(15)-C(13)	1.5320(11)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(129)-C(128)	1.5335(10)
C(129)-H(12A)	0.9800
C(129)-H(12B)	0.9800
C(129)-H(12C)	0.9800
C(128)-H(128)	1.0000
C(9)-H(9)	0.9500
C(14)-C(13)	1.5278(11)
C(14)-H(14A)	0.9800

C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(24)-H(24)	0.9500
C(102)-C(103)	1.3987(11)
C(102)-H(102)	0.959(12)
C(124)-C(123)	1.3878(10)
C(124)-H(124)	0.9500
C(106)-C(105)	1.3890(12)
C(106)-H(106)	0.952(13)
C(113)-C(114)	1.5355(11)
C(113)-C(115)	1.5365(12)
C(113)-H(113)	1.0000
C(4)-H(4)	0.958(13)
C(12)-H(12)	0.9500
C(13)-H(13)	1.0000
C(112)-C(111)	1.3920(11)
C(112)-H(112)	0.9500
C(25)-C(27)	1.5299(12)
C(25)-C(26)	1.5304(13)
C(25)-H(25)	1.0000
C(123)-H(123)	0.9500
C(127)-H(12D)	0.9800
C(127)-H(12E)	0.9800
C(127)-H(12F)	0.9800
C(110)-C(111)	1.3934(12)
C(110)-H(110)	0.9500
C(104)-C(103)	1.3839(14)
C(104)-C(105)	1.3944(15)
C(104)-H(104)	0.948(15)
C(126)-H(12G)	0.9800
C(126)-H(12H)	0.9800
C(126)-H(12I)	0.9800
C(118)-H(11A)	0.9800
C(118)-H(11B)	0.9800
C(118)-H(11C)	0.9800
C(111)-H(111)	0.9500

C(117)-H(11D)	0.9800
C(117)-H(11E)	0.9800
C(117)-H(11F)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(21)-C(22)	1.3932(11)
C(21)-H(21)	0.9500
C(115)-H(11G)	0.9800
C(115)-H(11H)	0.9800
C(115)-H(11I)	0.9800
C(105)-H(105)	0.960(15)
C(103)-H(103)	0.946(14)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(114)-H(11J)	0.9800
C(114)-H(11K)	0.9800
C(114)-H(11L)	0.9800
C(22)-H(22)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

N(1)-Fe(1)-C(1)	124.27(2)
N(1)-Fe(1)-C(2)	96.92(2)
C(1)-Fe(1)-C(2)	36.62(2)
N(1)-Fe(1)-P(1)	109.090(18)
C(1)-Fe(1)-P(1)	95.653(18)
C(2)-Fe(1)-P(1)	130.817(19)
N(1)-Fe(1)-B(1)	163.55(2)
C(1)-Fe(1)-B(1)	39.38(2)
C(2)-Fe(1)-B(1)	67.78(2)
P(1)-Fe(1)-B(1)	78.862(19)
N(1)-Fe(1)-P(2)	112.661(18)
C(1)-Fe(1)-P(2)	106.409(17)

C(2)-Fe(1)-P(2)	100.549(18)
P(1)-Fe(1)-P(2)	106.358(7)
B(1)-Fe(1)-P(2)	77.396(18)
N(2)-Fe(2)-C(101)	120.30(2)
N(2)-Fe(2)-B(2)	161.03(3)
C(101)-Fe(2)-B(2)	40.75(3)
N(2)-Fe(2)-P(4)	107.994(18)
C(101)-Fe(2)-P(4)	102.389(18)
B(2)-Fe(2)-P(4)	81.894(19)
N(2)-Fe(2)-P(3)	114.095(18)
C(101)-Fe(2)-P(3)	103.441(18)
B(2)-Fe(2)-P(3)	76.606(19)
P(4)-Fe(2)-P(3)	107.461(7)
N(2)-Fe(2)-C(102)	99.82(2)
C(101)-Fe(2)-C(102)	32.15(2)
B(2)-Fe(2)-C(102)	63.03(2)
P(4)-Fe(2)-C(102)	134.419(18)
P(3)-Fe(2)-C(102)	92.452(18)
C(107)-P(3)-C(116)	104.68(3)
C(107)-P(3)-C(113)	100.64(3)
C(116)-P(3)-C(113)	103.42(3)
C(107)-P(3)-Fe(2)	107.71(2)
C(116)-P(3)-Fe(2)	114.92(2)
C(113)-P(3)-Fe(2)	123.23(2)
C(7)-P(1)-C(13)	102.70(3)
C(7)-P(1)-C(16)	103.28(3)
C(13)-P(1)-C(16)	104.16(3)
C(7)-P(1)-Fe(1)	110.39(2)
C(13)-P(1)-Fe(1)	119.32(2)
C(16)-P(1)-Fe(1)	115.16(2)
C(19)-P(2)-C(25)	104.80(4)
C(19)-P(2)-C(28)	100.97(3)
C(25)-P(2)-C(28)	103.19(4)
C(19)-P(2)-Fe(1)	105.03(2)
C(25)-P(2)-Fe(1)	115.04(3)
C(28)-P(2)-Fe(1)	125.31(2)

C(119)-P(4)-C(128)	103.90(3)
C(119)-P(4)-C(125)	104.20(3)
C(128)-P(4)-C(125)	102.92(3)
C(119)-P(4)-Fe(2)	107.06(2)
C(128)-P(4)-Fe(2)	120.85(2)
C(125)-P(4)-Fe(2)	116.15(2)
N(1)-N(2)-Fe(2)	175.85(5)
N(2)-N(1)-Fe(1)	175.21(5)
C(2)-C(1)-C(6)	116.07(6)
C(2)-C(1)-B(1)	120.51(6)
C(6)-C(1)-B(1)	123.29(6)
C(2)-C(1)-Fe(1)	72.45(4)
C(6)-C(1)-Fe(1)	121.29(5)
B(1)-C(1)-Fe(1)	74.54(4)
C(106)-C(101)-C(102)	115.94(6)
C(106)-C(101)-B(2)	122.29(6)
C(102)-C(101)-B(2)	121.71(6)
C(106)-C(101)-Fe(2)	103.90(5)
C(102)-C(101)-Fe(2)	91.72(4)
B(2)-C(101)-Fe(2)	73.03(4)
C(121)-C(120)-C(119)	116.48(6)
C(121)-C(120)-B(2)	121.90(6)
C(119)-C(120)-B(2)	121.45(6)
C(5)-C(6)-C(1)	121.90(7)
C(5)-C(6)-H(6)	120.0(8)
C(1)-C(6)-H(6)	118.0(8)
C(17)-C(16)-C(18)	111.33(6)
C(17)-C(16)-P(1)	116.19(5)
C(18)-C(16)-P(1)	111.68(5)
C(17)-C(16)-H(16)	105.6
C(18)-C(16)-H(16)	105.6
P(1)-C(16)-H(16)	105.6
C(3)-C(2)-C(1)	121.42(7)
C(3)-C(2)-Fe(1)	124.66(5)
C(1)-C(2)-Fe(1)	70.93(4)
C(3)-C(2)-H(2)	118.3(8)

C(1)-C(2)-H(2)	119.3(8)
Fe(1)-C(2)-H(2)	84.6(8)
C(124)-C(119)-C(120)	121.25(6)
C(124)-C(119)-P(4)	123.44(5)
C(120)-C(119)-P(4)	115.30(5)
C(19)-C(20)-C(21)	116.73(6)
C(19)-C(20)-B(1)	120.89(6)
C(21)-C(20)-B(1)	122.21(6)
C(12)-C(7)-C(8)	121.24(6)
C(12)-C(7)-P(1)	124.04(5)
C(8)-C(7)-P(1)	114.70(5)
C(10)-C(11)-C(12)	119.71(7)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(29)-C(28)-C(30)	108.46(6)
C(29)-C(28)-P(2)	115.13(6)
C(30)-C(28)-P(2)	110.68(5)
C(29)-C(28)-H(28)	107.4
C(30)-C(28)-H(28)	107.4
P(2)-C(28)-H(28)	107.4
C(24)-C(19)-C(20)	121.87(6)
C(24)-C(19)-P(2)	125.00(6)
C(20)-C(19)-P(2)	113.01(5)
C(112)-C(107)-C(108)	121.98(6)
C(112)-C(107)-P(3)	125.64(5)
C(108)-C(107)-P(3)	112.36(5)
C(126)-C(125)-C(127)	110.66(6)
C(126)-C(125)-P(4)	115.64(5)
C(127)-C(125)-P(4)	111.55(5)
C(126)-C(125)-H(125)	106.1
C(127)-C(125)-H(125)	106.1
P(4)-C(125)-H(125)	106.1
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5

H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(122)-C(121)-C(120)	122.13(6)
C(122)-C(121)-H(121)	118.9
C(120)-C(121)-H(121)	118.9
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(6)-C(5)-C(4)	120.29(7)
C(6)-C(5)-H(5)	120.2(8)
C(4)-C(5)-H(5)	119.5(8)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(22)-C(23)-C(24)	119.49(7)
C(22)-C(23)-H(23)	120.3
C(24)-C(23)-H(23)	120.3
C(110)-C(109)-C(108)	121.54(7)
C(110)-C(109)-H(109)	119.2
C(108)-C(109)-H(109)	119.2
C(4)-C(3)-C(2)	120.16(7)
C(4)-C(3)-H(3)	121.3(8)
C(2)-C(3)-H(3)	118.5(8)
C(107)-C(108)-C(109)	116.80(6)
C(107)-C(108)-B(2)	118.48(5)
C(109)-C(108)-B(2)	124.28(6)
C(121)-C(122)-C(123)	120.29(7)
C(121)-C(122)-H(122)	119.9
C(123)-C(122)-H(122)	119.9
C(11)-C(10)-C(9)	120.42(7)

C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(9)-C(8)-C(7)	117.11(6)
C(9)-C(8)-B(1)	122.84(6)
C(7)-C(8)-B(1)	119.39(6)
C(101)-B(2)-C(120)	117.41(6)
C(101)-B(2)-C(108)	111.94(5)
C(120)-B(2)-C(108)	121.76(6)
C(101)-B(2)-Fe(2)	66.22(3)
C(120)-B(2)-Fe(2)	112.59(4)
C(108)-B(2)-Fe(2)	114.26(4)
C(117)-C(116)-C(118)	110.52(7)
C(117)-C(116)-P(3)	110.33(5)
C(118)-C(116)-P(3)	108.98(5)
C(117)-C(116)-H(116)	109.0
C(118)-C(116)-H(116)	109.0
P(3)-C(116)-H(116)	109.0
C(128)-C(130)-H(13A)	109.5
C(128)-C(130)-H(13B)	109.5
H(13A)-C(130)-H(13B)	109.5
C(128)-C(130)-H(13C)	109.5
H(13A)-C(130)-H(13C)	109.5
H(13B)-C(130)-H(13C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(128)-C(129)-H(12A)	109.5
C(128)-C(129)-H(12B)	109.5
H(12A)-C(129)-H(12B)	109.5
C(128)-C(129)-H(12C)	109.5
H(12A)-C(129)-H(12C)	109.5
H(12B)-C(129)-H(12C)	109.5
C(130)-C(128)-C(129)	111.26(6)

C(130)-C(128)-P(4)	111.12(5)
C(129)-C(128)-P(4)	110.22(5)
C(130)-C(128)-H(128)	108.0
C(129)-C(128)-H(128)	108.0
P(4)-C(128)-H(128)	108.0
C(10)-C(9)-C(8)	121.50(7)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(23)-C(24)-C(19)	119.72(8)
C(23)-C(24)-H(24)	120.1
C(19)-C(24)-H(24)	120.1
C(103)-C(102)-C(101)	121.64(8)
C(103)-C(102)-Fe(2)	122.86(5)
C(101)-C(102)-Fe(2)	56.13(4)
C(103)-C(102)-H(102)	118.1(8)
C(101)-C(102)-H(102)	120.2(8)
Fe(2)-C(102)-H(102)	94.0(8)
C(123)-C(124)-C(119)	120.55(7)
C(123)-C(124)-H(124)	119.7
C(119)-C(124)-H(124)	119.7
C(105)-C(106)-C(101)	122.10(8)
C(105)-C(106)-H(106)	119.8(8)
C(101)-C(106)-H(106)	117.9(8)
C(114)-C(113)-C(115)	109.28(7)
C(114)-C(113)-P(3)	114.92(6)
C(115)-C(113)-P(3)	110.36(5)
C(114)-C(113)-H(113)	107.3
C(115)-C(113)-H(113)	107.3
P(3)-C(113)-H(113)	107.3
C(3)-C(4)-C(5)	119.89(7)

C(3)-C(4)-H(4)	121.0(8)
C(5)-C(4)-H(4)	119.1(8)
C(1)-B(1)-C(8)	114.09(6)
C(1)-B(1)-C(20)	114.80(6)
C(8)-B(1)-C(20)	123.10(6)
C(1)-B(1)-Fe(1)	66.09(3)
C(8)-B(1)-Fe(1)	114.93(4)
C(20)-B(1)-Fe(1)	110.20(5)
C(11)-C(12)-C(7)	119.96(7)
C(11)-C(12)-H(12)	120.0
C(7)-C(12)-H(12)	120.0
C(14)-C(13)-C(15)	110.53(6)
C(14)-C(13)-P(1)	109.96(5)
C(15)-C(13)-P(1)	111.03(5)
C(14)-C(13)-H(13)	108.4
C(15)-C(13)-H(13)	108.4
P(1)-C(13)-H(13)	108.4
C(111)-C(112)-C(107)	119.73(7)
C(111)-C(112)-H(112)	120.1
C(107)-C(112)-H(112)	120.1
C(27)-C(25)-C(26)	110.42(8)
C(27)-C(25)-P(2)	109.26(6)
C(26)-C(25)-P(2)	109.95(6)
C(27)-C(25)-H(25)	109.1
C(26)-C(25)-H(25)	109.1
P(2)-C(25)-H(25)	109.1
C(124)-C(123)-C(122)	119.21(7)
C(124)-C(123)-H(123)	120.4
C(122)-C(123)-H(123)	120.4
C(125)-C(127)-H(12D)	109.5
C(125)-C(127)-H(12E)	109.5
H(12D)-C(127)-H(12E)	109.5
C(125)-C(127)-H(12F)	109.5
H(12D)-C(127)-H(12F)	109.5
H(12E)-C(127)-H(12F)	109.5
C(109)-C(110)-C(111)	120.53(7)

C(109)-C(110)-H(110)	119.7
C(111)-C(110)-H(110)	119.7
C(103)-C(104)-C(105)	119.52(8)
C(103)-C(104)-H(104)	119.4(9)
C(105)-C(104)-H(104)	121.0(9)
C(125)-C(126)-H(12G)	109.5
C(125)-C(126)-H(12H)	109.5
H(12G)-C(126)-H(12H)	109.5
C(125)-C(126)-H(12I)	109.5
H(12G)-C(126)-H(12I)	109.5
H(12H)-C(126)-H(12I)	109.5
C(116)-C(118)-H(11A)	109.5
C(116)-C(118)-H(11B)	109.5
H(11A)-C(118)-H(11B)	109.5
C(116)-C(118)-H(11C)	109.5
H(11A)-C(118)-H(11C)	109.5
H(11B)-C(118)-H(11C)	109.5
C(112)-C(111)-C(110)	119.43(7)
C(112)-C(111)-H(111)	120.3
C(110)-C(111)-H(111)	120.3
C(116)-C(117)-H(11D)	109.5
C(116)-C(117)-H(11E)	109.5
H(11D)-C(117)-H(11E)	109.5
C(116)-C(117)-H(11F)	109.5
H(11D)-C(117)-H(11F)	109.5
H(11E)-C(117)-H(11F)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(22)-C(21)-C(20)	121.62(7)
C(22)-C(21)-H(21)	119.2
C(20)-C(21)-H(21)	119.2
C(113)-C(115)-H(11G)	109.5

C(113)-C(115)-H(11H)	109.5
H(11G)-C(115)-H(11H)	109.5
C(113)-C(115)-H(11I)	109.5
H(11G)-C(115)-H(11I)	109.5
H(11H)-C(115)-H(11I)	109.5
C(106)-C(105)-C(104)	120.18(8)
C(106)-C(105)-H(105)	119.4(9)
C(104)-C(105)-H(105)	120.3(9)
C(104)-C(103)-C(102)	120.40(8)
C(104)-C(103)-H(103)	118.6(9)
C(102)-C(103)-H(103)	120.8(9)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(113)-C(114)-H(11J)	109.5
C(113)-C(114)-H(11K)	109.5
H(11J)-C(114)-H(11K)	109.5
C(113)-C(114)-H(11L)	109.5
H(11J)-C(114)-H(11L)	109.5
H(11K)-C(114)-H(11L)	109.5
C(23)-C(22)-C(21)	120.50(7)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S13. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	C108 H90 B2 Fe2 P4	
Formula weight	1645.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8333(19) Å	α = 78.661(7)°.
	b = 11.167(3) Å	β = 76.780(5)°.
	c = 19.774(3) Å	γ = 88.148(8)°.
Volume	2072.3(7) $Å^3$	
Z	1	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.479 mm^{-1}	
F(000)	860	
Crystal size	0.32 x 0.30 x 0.19 mm^3	
Theta range for data collection	1.08 to 41.29°.	
Index ranges	-18<=h<=18, -20<=k<=20, -36<=l<=36	
Reflections collected	88753	
Independent reflections	25823 [R(int) = 0.0617]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25823 / 0 / 543	
Goodness-of-fit on F^2	0.987	
Final R indices [I>2sigma(I)]	R1 = 0.0505, wR2 = 0.1162	
R indices (all data)	R1 = 0.0929, wR2 = 0.1311	
Largest diff. peak and hole	1.331 and -0.473 e.$Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6220(1)	-43(1)	7986(1)	8(1)
P(1)	6735(1)	142(1)	6836(1)	8(1)
P(2)	5850(1)	-2009(1)	8337(1)	9(1)
C(27)	9975(1)	-2322(1)	8369(1)	12(1)
C(26)	8682(1)	-1866(1)	8250(1)	10(1)
C(44)	1071(2)	1959(2)	8379(1)	25(1)
C(25)	7526(1)	-2689(1)	8470(1)	10(1)
C(24)	4541(1)	1653(1)	6568(1)	14(1)
C(5)	5334(1)	368(1)	9023(1)	12(1)
C(35)	4484(2)	-4804(1)	7537(1)	22(1)
C(51)	10430(2)	-3580(1)	6334(1)	28(1)
C(48)	1681(2)	3224(1)	9123(1)	23(1)
C(52)	9759(2)	-4278(1)	6976(1)	24(1)
C(46)	1334(1)	1064(1)	9550(1)	20(1)
C(19)	6002(1)	1558(1)	6419(1)	11(1)
C(8)	9379(1)	-24(1)	7079(1)	10(1)
C(7)	8642(1)	306(1)	6539(1)	10(1)
B(1)	8519(1)	-476(1)	7881(1)	10(1)
C(37)	4650(1)	-2444(1)	9219(1)	11(1)
C(14)	5545(1)	-813(1)	5851(1)	13(1)
C(28)	10123(1)	-3519(1)	8707(1)	15(1)
C(11)	10792(1)	724(1)	5639(1)	16(1)
C(13)	6445(1)	-981(1)	6313(1)	10(1)
C(42)	5096(1)	-2888(1)	9839(1)	14(1)
C(47)	1630(1)	2207(1)	9657(1)	19(1)
C(1)	7798(1)	485(1)	8319(1)	10(1)
C(54)	10097(2)	-6091(2)	6473(1)	26(1)
C(53)	9589(2)	-5525(1)	7048(1)	24(1)
C(4)	4903(1)	1279(1)	8514(1)	13(1)
C(6)	6746(1)	4(1)	8944(1)	11(1)
C(17)	7010(1)	-2986(1)	6033(1)	17(1)

C(3)	5955(1)	1902(1)	7961(1)	12(1)
C(12)	9341(1)	662(1)	5826(1)	13(1)
C(50)	10926(2)	-4144(2)	5764(1)	38(1)
C(34)	3460(1)	-4225(1)	7218(1)	18(1)
C(38)	3225(1)	-2208(1)	9270(1)	16(1)
C(18)	7187(1)	-2072(1)	6397(1)	13(1)
C(49)	10756(2)	-5394(2)	5834(1)	36(1)
C(2)	7368(1)	1560(1)	7878(1)	11(1)
C(30)	7678(1)	-3897(1)	8819(1)	13(1)
C(22)	4700(2)	3763(1)	5982(1)	18(1)
C(36)	5268(1)	-4169(1)	7857(1)	17(1)
C(41)	4149(2)	-3082(1)	10495(1)	18(1)
C(21)	6144(2)	3696(1)	5843(1)	18(1)
C(29)	8970(1)	-4306(1)	8938(1)	16(1)
C(23)	3894(1)	2735(1)	6346(1)	17(1)
C(9)	10850(1)	34(1)	6870(1)	14(1)
C(15)	5373(1)	-1729(1)	5489(1)	17(1)
C(39)	2281(1)	-2404(1)	9921(1)	21(1)
C(45)	1042(2)	941(1)	8911(1)	23(1)
C(31)	5028(1)	-2926(1)	7861(1)	11(1)
C(16)	6107(2)	-2812(1)	5579(1)	18(1)
C(43)	1404(2)	3100(1)	8483(1)	26(1)
C(33)	3219(1)	-2988(1)	7212(1)	14(1)
C(40)	2744(2)	-2830(1)	10538(1)	21(1)
C(32)	4001(1)	-2352(1)	7531(1)	12(1)
C(10)	11539(1)	407(1)	6163(1)	17(1)
C(20)	6799(1)	2600(1)	6053(1)	14(1)

Table S15. Bond lengths [Å] and angles [°] for **5**.

Fe(1)-C(1)	1.9667(11)
Fe(1)-C(6)	2.0838(12)
Fe(1)-C(2)	2.0962(12)
Fe(1)-C(5)	2.1676(11)
Fe(1)-C(3)	2.1705(12)
Fe(1)-P(1)	2.1827(5)
Fe(1)-P(2)	2.1840(6)
Fe(1)-C(4)	2.1934(11)
Fe(1)-B(1)	2.2668(13)
P(1)-C(7)	1.8368(12)
P(1)-C(19)	1.8408(12)
P(1)-C(13)	1.8417(11)
P(2)-C(31)	1.8354(12)
P(2)-C(25)	1.8441(11)
P(2)-C(37)	1.8533(12)
C(27)-C(28)	1.3916(16)
C(27)-C(26)	1.4071(15)
C(27)-H(27)	0.9500
C(26)-C(25)	1.4181(16)
C(26)-B(1)	1.5999(17)
C(44)-C(45)	1.385(2)
C(44)-C(43)	1.391(2)
C(44)-H(44)	0.9500
C(25)-C(30)	1.4096(16)
C(24)-C(23)	1.3888(16)
C(24)-C(19)	1.4037(16)
C(24)-H(24)	0.9500
C(5)-C(4)	1.4106(17)
C(5)-C(6)	1.4171(16)
C(5)-H(5)	0.907(15)
C(35)-C(34)	1.3854(19)
C(35)-C(36)	1.3898(19)
C(35)-H(35)	0.9500
C(51)-C(50)	1.382(2)

C(51)-C(52)	1.384(2)
C(51)-H(51)	0.9500
C(48)-C(47)	1.384(2)
C(48)-C(43)	1.387(2)
C(48)-H(48)	0.9500
C(52)-C(53)	1.384(2)
C(52)-H(52)	0.9500
C(46)-C(47)	1.3844(19)
C(46)-C(45)	1.391(2)
C(46)-H(46)	0.9500
C(19)-C(20)	1.3996(17)
C(8)-C(7)	1.4087(16)
C(8)-C(9)	1.4108(16)
C(8)-B(1)	1.6070(17)
C(7)-C(12)	1.4037(16)
B(1)-C(1)	1.5625(16)
C(37)-C(42)	1.3904(17)
C(37)-C(38)	1.4024(16)
C(14)-C(13)	1.3933(16)
C(14)-C(15)	1.3944(17)
C(14)-H(14)	0.9500
C(28)-C(29)	1.3909(18)
C(28)-H(28)	0.9500
C(11)-C(10)	1.3874(19)
C(11)-C(12)	1.3893(17)
C(11)-H(11)	0.9500
C(13)-C(18)	1.4013(16)
C(42)-C(41)	1.3951(17)
C(42)-H(42)	0.9500
C(47)-H(47)	0.9500
C(1)-C(6)	1.4403(16)
C(1)-C(2)	1.4513(16)
C(1)-C(4)	2.9169(17)
C(54)-C(49)	1.375(2)
C(54)-C(53)	1.394(2)
C(54)-H(54)	0.9500

C(53)-H(53)	0.9500
C(4)-C(3)	1.4074(17)
C(4)-H(4)	0.925(17)
C(6)-H(6)	1.005(15)
C(17)-C(16)	1.3838(19)
C(17)-C(18)	1.3948(16)
C(17)-H(17)	0.9500
C(3)-C(2)	1.4102(17)
C(3)-H(3)	0.956(16)
C(12)-H(12)	0.9500
C(50)-C(49)	1.388(3)
C(50)-H(50)	0.9500
C(34)-C(33)	1.3915(17)
C(34)-H(34)	0.9500
C(38)-C(39)	1.3876(17)
C(38)-H(38)	0.9500
C(18)-H(18)	0.9500
C(49)-H(49)	0.9500
C(2)-H(2)	0.899(17)
C(30)-C(29)	1.3911(17)
C(30)-H(30)	0.9500
C(22)-C(21)	1.3857(19)
C(22)-C(23)	1.3919(19)
C(22)-H(22)	0.9500
C(36)-C(31)	1.4012(16)
C(36)-H(36)	0.9500
C(41)-C(40)	1.388(2)
C(41)-H(41)	0.9500
C(21)-C(20)	1.3982(17)
C(21)-H(21)	0.9500
C(29)-H(29)	0.9500
C(23)-H(23)	0.9500
C(9)-C(10)	1.3943(17)
C(9)-H(9)	0.9500
C(15)-C(16)	1.3900(18)
C(15)-H(15)	0.9500

C(39)-C(40)	1.389(2)
C(39)-H(39)	0.9500
C(45)-H(45)	0.9500
C(31)-C(32)	1.3978(16)
C(16)-H(16)	0.9500
C(43)-H(43)	0.9500
C(33)-C(32)	1.3875(17)
C(33)-H(33)	0.9500
C(40)-H(40)	0.9500
C(32)-H(32)	0.9500
C(10)-H(10)	0.9500
C(20)-H(20)	0.9500

C(1)-Fe(1)-C(6)	41.53(5)
C(1)-Fe(1)-C(2)	41.71(5)
C(6)-Fe(1)-C(2)	70.88(5)
C(1)-Fe(1)-C(5)	74.12(5)
C(6)-Fe(1)-C(5)	38.88(4)
C(2)-Fe(1)-C(5)	81.92(5)
C(1)-Fe(1)-C(3)	74.18(5)
C(6)-Fe(1)-C(3)	82.29(4)
C(2)-Fe(1)-C(3)	38.55(5)
C(5)-Fe(1)-C(3)	67.34(5)
C(1)-Fe(1)-P(1)	111.01(4)
C(6)-Fe(1)-P(1)	152.23(3)
C(2)-Fe(1)-P(1)	89.47(3)
C(5)-Fe(1)-P(1)	159.67(3)
C(3)-Fe(1)-P(1)	94.58(3)
C(1)-Fe(1)-P(2)	110.90(4)
C(6)-Fe(1)-P(2)	88.91(3)
C(2)-Fe(1)-P(2)	152.40(4)
C(5)-Fe(1)-P(2)	94.16(4)
C(3)-Fe(1)-P(2)	159.26(3)
P(1)-Fe(1)-P(2)	101.757(15)
C(1)-Fe(1)-C(4)	88.87(5)
C(6)-Fe(1)-C(4)	70.45(5)

C(2)-Fe(1)-C(4)	69.97(5)
C(5)-Fe(1)-C(4)	37.74(5)
C(3)-Fe(1)-C(4)	37.63(5)
P(1)-Fe(1)-C(4)	121.94(4)
P(2)-Fe(1)-C(4)	121.64(4)
C(1)-Fe(1)-B(1)	42.58(4)
C(6)-Fe(1)-B(1)	71.29(5)
C(2)-Fe(1)-B(1)	70.00(5)
C(5)-Fe(1)-B(1)	110.07(5)
C(3)-Fe(1)-B(1)	108.53(5)
P(1)-Fe(1)-B(1)	83.80(3)
P(2)-Fe(1)-B(1)	86.07(3)
C(4)-Fe(1)-B(1)	131.42(5)
C(7)-P(1)-C(19)	106.36(5)
C(7)-P(1)-C(13)	99.04(5)
C(19)-P(1)-C(13)	103.69(5)
C(7)-P(1)-Fe(1)	107.29(4)
C(19)-P(1)-Fe(1)	110.36(4)
C(13)-P(1)-Fe(1)	128.02(4)
C(31)-P(2)-C(25)	109.88(5)
C(31)-P(2)-C(37)	97.93(5)
C(25)-P(2)-C(37)	103.74(5)
C(31)-P(2)-Fe(1)	122.91(4)
C(25)-P(2)-Fe(1)	106.81(4)
C(37)-P(2)-Fe(1)	113.95(4)
C(28)-C(27)-C(26)	122.09(11)
C(28)-C(27)-H(27)	119.0
C(26)-C(27)-H(27)	119.0
C(27)-C(26)-C(25)	117.27(10)
C(27)-C(26)-B(1)	121.51(10)
C(25)-C(26)-B(1)	121.22(10)
C(45)-C(44)-C(43)	119.85(14)
C(45)-C(44)-H(44)	120.1
C(43)-C(44)-H(44)	120.1
C(30)-C(25)-C(26)	120.38(10)
C(30)-C(25)-P(2)	124.55(9)

C(26)-C(25)-P(2)	114.82(8)
C(23)-C(24)-C(19)	121.45(11)
C(23)-C(24)-H(24)	119.3
C(19)-C(24)-H(24)	119.3
C(4)-C(5)-C(6)	121.63(11)
C(4)-C(5)-Fe(1)	72.12(7)
C(6)-C(5)-Fe(1)	67.37(6)
C(4)-C(5)-H(5)	120.1(10)
C(6)-C(5)-H(5)	118.0(10)
Fe(1)-C(5)-H(5)	130.5(9)
C(34)-C(35)-C(36)	120.91(12)
C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5
C(50)-C(51)-C(52)	119.26(15)
C(50)-C(51)-H(51)	120.4
C(52)-C(51)-H(51)	120.4
C(47)-C(48)-C(43)	119.77(13)
C(47)-C(48)-H(48)	120.1
C(43)-C(48)-H(48)	120.1
C(53)-C(52)-C(51)	120.35(14)
C(53)-C(52)-H(52)	119.8
C(51)-C(52)-H(52)	119.8
C(47)-C(46)-C(45)	119.88(13)
C(47)-C(46)-H(46)	120.1
C(45)-C(46)-H(46)	120.1
C(20)-C(19)-C(24)	118.07(10)
C(20)-C(19)-P(1)	124.07(9)
C(24)-C(19)-P(1)	117.16(9)
C(7)-C(8)-C(9)	116.81(10)
C(7)-C(8)-B(1)	119.09(10)
C(9)-C(8)-B(1)	124.08(10)
C(12)-C(7)-C(8)	121.49(10)
C(12)-C(7)-P(1)	123.60(9)
C(8)-C(7)-P(1)	114.81(8)
C(1)-B(1)-C(26)	121.37(10)
C(1)-B(1)-C(8)	119.56(10)

C(26)-B(1)-C(8)	117.97(9)
C(1)-B(1)-Fe(1)	58.40(6)
C(26)-B(1)-Fe(1)	109.47(8)
C(8)-B(1)-Fe(1)	110.78(8)
C(42)-C(37)-C(38)	118.33(11)
C(42)-C(37)-P(2)	123.77(9)
C(38)-C(37)-P(2)	117.66(9)
C(13)-C(14)-C(15)	120.25(11)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(29)-C(28)-C(27)	119.93(11)
C(29)-C(28)-H(28)	120.0
C(27)-C(28)-H(28)	120.0
C(10)-C(11)-C(12)	119.27(11)
C(10)-C(11)-H(11)	120.4
C(12)-C(11)-H(11)	120.4
C(14)-C(13)-C(18)	118.98(10)
C(14)-C(13)-P(1)	124.48(8)
C(18)-C(13)-P(1)	116.54(9)
C(37)-C(42)-C(41)	120.79(12)
C(37)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(48)-C(47)-C(46)	120.35(13)
C(48)-C(47)-H(47)	119.8
C(46)-C(47)-H(47)	119.8
C(6)-C(1)-C(2)	113.91(10)
C(6)-C(1)-B(1)	115.46(10)
C(2)-C(1)-B(1)	112.48(10)
C(6)-C(1)-Fe(1)	73.60(7)
C(2)-C(1)-Fe(1)	73.93(7)
B(1)-C(1)-Fe(1)	79.02(7)
C(6)-C(1)-C(4)	57.71(6)
C(2)-C(1)-C(4)	57.42(6)
B(1)-C(1)-C(4)	127.73(8)
Fe(1)-C(1)-C(4)	48.75(3)
C(49)-C(54)-C(53)	119.25(15)

C(49)-C(54)-H(54)	120.4
C(53)-C(54)-H(54)	120.4
C(52)-C(53)-C(54)	120.22(14)
C(52)-C(53)-H(53)	119.9
C(54)-C(53)-H(53)	119.9
C(3)-C(4)-C(5)	117.17(11)
C(3)-C(4)-Fe(1)	70.30(6)
C(5)-C(4)-Fe(1)	70.14(6)
C(3)-C(4)-C(1)	58.93(7)
C(5)-C(4)-C(1)	58.78(7)
Fe(1)-C(4)-C(1)	42.38(3)
C(3)-C(4)-H(4)	119.5(10)
C(5)-C(4)-H(4)	123.2(10)
Fe(1)-C(4)-H(4)	127.7(10)
C(1)-C(4)-H(4)	170.0(10)
C(5)-C(6)-C(1)	121.79(11)
C(5)-C(6)-Fe(1)	73.76(7)
C(1)-C(6)-Fe(1)	64.87(6)
C(5)-C(6)-H(6)	118.7(9)
C(1)-C(6)-H(6)	118.1(9)
Fe(1)-C(6)-H(6)	124.1(9)
C(16)-C(17)-C(18)	119.93(11)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(4)-C(3)-C(2)	121.69(11)
C(4)-C(3)-Fe(1)	72.07(7)
C(2)-C(3)-Fe(1)	67.88(6)
C(4)-C(3)-H(3)	120.4(10)
C(2)-C(3)-H(3)	117.7(10)
Fe(1)-C(3)-H(3)	129.9(9)
C(11)-C(12)-C(7)	120.24(11)
C(11)-C(12)-H(12)	119.9
C(7)-C(12)-H(12)	119.9
C(51)-C(50)-C(49)	120.48(16)
C(51)-C(50)-H(50)	119.8
C(49)-C(50)-H(50)	119.8

C(35)-C(34)-C(33)	119.60(12)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(39)-C(38)-C(37)	120.98(12)
C(39)-C(38)-H(38)	119.5
C(37)-C(38)-H(38)	119.5
C(17)-C(18)-C(13)	120.54(11)
C(17)-C(18)-H(18)	119.7
C(13)-C(18)-H(18)	119.7
C(54)-C(49)-C(50)	120.44(15)
C(54)-C(49)-H(49)	119.8
C(50)-C(49)-H(49)	119.8
C(3)-C(2)-C(1)	121.79(11)
C(3)-C(2)-Fe(1)	73.57(7)
C(1)-C(2)-Fe(1)	64.36(6)
C(3)-C(2)-H(2)	118.8(10)
C(1)-C(2)-H(2)	117.9(10)
Fe(1)-C(2)-H(2)	124.5(10)
C(29)-C(30)-C(25)	120.50(11)
C(29)-C(30)-H(30)	119.8
C(25)-C(30)-H(30)	119.8
C(21)-C(22)-C(23)	119.64(11)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(35)-C(36)-C(31)	120.11(12)
C(35)-C(36)-H(36)	119.9
C(31)-C(36)-H(36)	119.9
C(40)-C(41)-C(42)	120.22(13)
C(40)-C(41)-H(41)	119.9
C(42)-C(41)-H(41)	119.9
C(22)-C(21)-C(20)	120.67(12)
C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(28)-C(29)-C(30)	119.79(11)
C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1

C(24)-C(23)-C(22)	119.78(12)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(10)-C(9)-C(8)	121.46(11)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.3
C(16)-C(15)-C(14)	120.29(12)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(38)-C(39)-C(40)	120.07(13)
C(38)-C(39)-H(39)	120.0
C(40)-C(39)-H(39)	120.0
C(44)-C(45)-C(46)	119.96(13)
C(44)-C(45)-H(45)	120.0
C(46)-C(45)-H(45)	120.0
C(32)-C(31)-C(36)	118.30(11)
C(32)-C(31)-P(2)	116.43(8)
C(36)-C(31)-P(2)	125.03(9)
C(17)-C(16)-C(15)	120.01(11)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(48)-C(43)-C(44)	120.15(14)
C(48)-C(43)-H(43)	119.9
C(44)-C(43)-H(43)	119.9
C(32)-C(33)-C(34)	119.61(12)
C(32)-C(33)-H(33)	120.2
C(34)-C(33)-H(33)	120.2
C(41)-C(40)-C(39)	119.60(12)
C(41)-C(40)-H(40)	120.2
C(39)-C(40)-H(40)	120.2
C(33)-C(32)-C(31)	121.47(11)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(11)-C(10)-C(9)	120.72(11)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6

C(21)-C(20)-C(19)	120.36(12)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8

Symmetry transformations used to generate equivalent atoms:

Table S16. Crystal data and structure refinement for **6a**.

Identification code	**6a**	
Empirical formula	C36 H57 B Fe N2 P2 Si2	
Formula weight	702.62	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5707(8) Å	α = 118.196(3)°.
	b = 19.9433(14) Å	β = 97.760(4)°.
	c = 20.5612(15) Å	γ = 92.754(3)°.
Volume	3754.1(5) $Å^3$	
Z	4	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.578 mm^{-1}	
F(000)	1504	
Crystal size	0.38 x 0.38 x 0.31 mm^3	
Theta range for data collection	1.96 to 50.11°.	
Index ranges	-22<=h<=22, -42<=k<=43, -43<=l<=44	
Reflections collected	501556	
Independent reflections	77845 [R(int) = 0.0593]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8411 and 0.8102	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	77845 / 0 / 857	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0824	
R indices (all data)	R1 = 0.0690, wR2 = 0.0937	
Largest diff. peak and hole	0.858 and -0.431 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	9303(1)	6947(1)	2615(1)	7(1)
Fe(2)	5306(1)	8228(1)	7590(1)	9(1)
P(1)	9536(1)	7954(1)	3762(1)	8(1)
P(11)	5032(1)	7256(1)	6397(1)	10(1)
P(2)	9411(1)	5859(1)	2701(1)	9(1)
P(12)	5514(1)	7682(1)	8319(1)	11(1)
Si(11)	7073(1)	10143(1)	7524(1)	14(1)
Si(12)	9087(1)	9443(1)	8043(1)	17(1)
Si(1)	5252(1)	6701(1)	1672(1)	13(1)
Si(2)	7029(1)	6604(1)	645(1)	13(1)
N(11)	6501(1)	8854(1)	7670(1)	11(1)
N(1)	7943(1)	6830(1)	2043(1)	9(1)
N(2)	6897(1)	6724(1)	1551(1)	12(1)
C(119)	4063(1)	7659(1)	8694(1)	14(1)
C(8)	12038(1)	7982(1)	3746(1)	9(1)
C(7)	11128(1)	8489(1)	4031(1)	10(1)
C(13)	9437(1)	7912(1)	4650(1)	12(1)
C(3)	10572(1)	7531(1)	1514(1)	15(1)
C(1)	11186(1)	6965(1)	2334(1)	9(1)
N(12)	7396(1)	9366(1)	7709(1)	13(1)
C(107)	3388(1)	6756(1)	6068(1)	13(1)
C(9)	13330(1)	8301(1)	3927(1)	12(1)
C(19)	11065(1)	5735(1)	2963(1)	11(1)
C(20)	11937(1)	6409(1)	3261(1)	9(1)
C(6)	11400(1)	6302(1)	1676(1)	11(1)
C(21)	13195(1)	6398(1)	3578(1)	11(1)
C(5)	11257(1)	6272(1)	991(1)	14(1)
C(16)	8383(1)	8646(1)	3813(1)	12(1)
C(12)	11483(1)	9280(1)	4464(1)	14(1)
C(120)	2966(1)	7538(1)	8164(1)	13(1)
C(25)	8746(1)	4907(1)	1878(1)	13(1)

B(1)	11505(1)	7105(1)	3154(1)	9(1)
C(116)	5239(1)	7486(1)	5634(1)	14(1)
C(113)	6097(1)	6478(1)	6212(1)	14(1)
C(22)	13595(1)	5732(1)	3548(1)	14(1)
C(28)	8677(1)	5852(1)	3480(1)	12(1)
C(15)	10622(1)	7614(1)	4890(1)	15(1)
C(110)	827(1)	6092(1)	5642(1)	20(1)
C(128)	5808(1)	6654(1)	7978(1)	14(1)
C(109)	1320(1)	6622(1)	6385(1)	17(1)
C(101)	3347(1)	8461(1)	7586(1)	13(1)
C(2)	10717(1)	7572(1)	2231(1)	11(1)
C(11)	12771(1)	9581(1)	4632(1)	17(1)
C(23)	12739(1)	5058(1)	3209(1)	16(1)
C(106)	2774(1)	8698(1)	7065(1)	16(1)
C(108)	2606(1)	6972(1)	6619(1)	12(1)
C(4)	10857(1)	6902(1)	910(1)	16(1)
C(18)	7025(1)	8303(1)	3762(1)	16(1)
C(121)	1766(1)	7399(1)	8330(1)	19(1)
C(102)	4060(1)	9045(1)	8288(1)	16(1)
C(30)	8622(1)	5104(1)	3519(1)	18(1)
C(27)	9515(1)	4676(1)	1244(1)	20(1)
C(115)	7477(1)	6809(1)	6637(1)	17(1)
C(10)	13692(1)	9089(1)	4368(1)	15(1)
C(125)	6806(1)	8193(1)	9157(1)	18(1)
C(24)	11474(1)	5059(1)	2920(1)	14(1)
C(26)	7330(1)	4882(1)	1580(1)	19(1)
C(122)	1670(1)	7395(1)	8998(1)	23(1)
C(130)	4597(1)	6102(1)	7480(1)	16(1)
C(17)	8413(1)	8872(1)	3200(1)	19(1)
C(34)	5278(1)	6320(1)	204(1)	18(1)
C(14)	9293(1)	8680(1)	5321(1)	16(1)
C(112)	2887(1)	6226(1)	5318(1)	17(1)
B(11)	3159(1)	7629(1)	7450(1)	12(1)
C(118)	4220(1)	7967(1)	5552(1)	19(1)
C(29)	7356(1)	6135(1)	3521(1)	16(1)
C(103)	4170(1)	9830(1)	8444(1)	22(1)

C(117)	6590(1)	7878(1)	5746(1)	18(1)
C(124)	3968(1)	7674(1)	9374(1)	19(1)
C(31)	4918(1)	6311(1)	2292(1)	22(1)
C(33)	4562(1)	6050(1)	662(1)	17(1)
C(111)	1611(1)	5891(1)	5105(1)	20(1)
C(114)	6126(1)	5911(1)	5389(1)	21(1)
C(35)	7981(1)	5812(1)	171(1)	20(1)
C(131)	5685(1)	9931(1)	6777(1)	22(1)
C(32)	4699(1)	7659(1)	1984(1)	25(1)
C(104)	3555(1)	10028(1)	7944(1)	25(1)
C(135)	9712(1)	8515(1)	7533(1)	23(1)
C(129)	6267(1)	6447(1)	8592(1)	23(1)
C(132)	6964(1)	10991(1)	8436(1)	22(1)
C(123)	2766(1)	7541(1)	9525(1)	23(1)
C(105)	2834(1)	9452(1)	7246(1)	22(1)
C(133)	8641(1)	10257(1)	7246(1)	20(1)
C(134)	9693(1)	10185(1)	7801(1)	24(1)
C(36)	7629(1)	7545(1)	734(1)	22(1)
C(127)	8128(1)	8077(1)	8930(1)	24(1)
C(126)	6657(1)	9046(1)	9590(1)	26(1)
C(136)	9491(1)	9844(1)	9077(1)	32(1)

Table S18. Bond lengths [Å] and angles [°] for **6a**.

Fe(1)-N(1)	1.6605(5)
Fe(1)-C(1)	2.1493(5)
Fe(1)-P(1)	2.2312(2)
Fe(1)-P(2)	2.2660(2)
Fe(1)-C(2)	2.3405(6)
Fe(1)-B(1)	2.3768(6)
Fe(2)-N(11)	1.6658(5)
Fe(2)-C(101)	2.1440(6)
Fe(2)-C(102)	2.2266(6)
Fe(2)-P(12)	2.2287(2)
Fe(2)-P(11)	2.2632(2)
Fe(2)-B(11)	2.4288(7)
P(1)-C(7)	1.8148(5)
P(1)-C(16)	1.8596(6)
P(1)-C(13)	1.8835(6)
P(11)-C(107)	1.8311(6)
P(11)-C(116)	1.8656(6)
P(11)-C(113)	1.8830(6)
P(2)-C(19)	1.8226(6)
P(2)-C(25)	1.8653(6)
P(2)-C(28)	1.8771(6)
P(12)-C(119)	1.8155(6)
P(12)-C(125)	1.8549(7)
P(12)-C(128)	1.8833(6)
Si(11)-N(12)	1.7991(5)
Si(11)-C(131)	1.8460(8)
Si(11)-C(133)	1.8616(7)
Si(11)-C(132)	1.8630(8)
Si(12)-N(12)	1.7983(6)
Si(12)-C(135)	1.8519(8)
Si(12)-C(136)	1.8594(10)
Si(12)-C(134)	1.8802(8)
Si(1)-N(2)	1.7908(5)
Si(1)-C(31)	1.8409(7)

Si(1)-C(32)	1.8578(8)
Si(1)-C(33)	1.8656(7)
Si(2)-N(2)	1.7885(5)
Si(2)-C(35)	1.8491(8)
Si(2)-C(36)	1.8667(7)
Si(2)-C(34)	1.8790(7)
N(11)-N(12)	1.3242(7)
N(1)-N(2)	1.3282(6)
C(119)-C(124)	1.4004(9)
C(119)-C(120)	1.4055(9)
C(8)-C(9)	1.4021(8)
C(8)-C(7)	1.4053(7)
C(8)-B(1)	1.6016(8)
C(7)-C(12)	1.3967(7)
C(13)-C(15)	1.5325(9)
C(13)-C(14)	1.5348(8)
C(13)-H(13)	1.0000
C(3)-C(4)	1.3681(9)
C(3)-C(2)	1.4238(8)
C(3)-H(3)	0.988(12)
C(1)-C(2)	1.4231(7)
C(1)-C(6)	1.4324(7)
C(1)-B(1)	1.5574(8)
C(107)-C(112)	1.4000(9)
C(107)-C(108)	1.4069(9)
C(9)-C(10)	1.3928(8)
C(9)-H(9)	0.9500
C(19)-C(24)	1.4011(7)
C(19)-C(20)	1.4077(7)
C(20)-C(21)	1.4047(8)
C(20)-B(1)	1.5843(8)
C(6)-C(5)	1.3690(8)
C(6)-H(6)	0.971(11)
C(21)-C(22)	1.3894(8)
C(21)-H(21)	0.9500
C(5)-C(4)	1.4196(10)

C(5)-H(5)	0.955(11)
C(16)-C(18)	1.5284(9)
C(16)-C(17)	1.5295(9)
C(16)-H(16)	1.0000
C(12)-C(11)	1.3896(9)
C(12)-H(12)	0.9500
C(120)-C(121)	1.4055(9)
C(120)-B(11)	1.5994(9)
C(25)-C(27)	1.5263(10)
C(25)-C(26)	1.5276(9)
C(25)-H(25)	1.0000
C(116)-C(118)	1.5215(9)
C(116)-C(117)	1.5288(9)
C(116)-H(116)	1.0000
C(113)-C(115)	1.5318(9)
C(113)-C(114)	1.5333(9)
C(113)-H(113)	1.0000
C(22)-C(23)	1.3919(9)
C(22)-H(22)	0.9500
C(28)-C(29)	1.5284(9)
C(28)-C(30)	1.5302(8)
C(28)-H(28)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(110)-C(109)	1.3886(10)
C(110)-C(111)	1.3890(12)
C(110)-H(110)	0.9500
C(128)-C(130)	1.5312(9)
C(128)-C(129)	1.5326(9)
C(128)-H(128)	1.0000
C(109)-C(108)	1.4080(8)
C(109)-H(109)	0.9500
C(101)-C(102)	1.4285(9)
C(101)-C(106)	1.4372(9)
C(101)-B(11)	1.5443(9)

C(2)-H(2)	0.919(11)
C(11)-C(10)	1.3917(9)
C(11)-H(11)	0.9500
C(23)-C(24)	1.3887(9)
C(23)-H(23)	0.9500
C(106)-C(105)	1.3648(9)
C(106)-H(106)	0.965(12)
C(108)-B(11)	1.5878(9)
C(4)-H(4)	0.964(12)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(121)-C(122)	1.3953(10)
C(121)-H(121)	0.9500
C(102)-C(103)	1.4357(9)
C(102)-H(102)	0.931(12)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(115)-H(11A)	0.9800
C(115)-H(11B)	0.9800
C(115)-H(11C)	0.9800
C(10)-H(10)	0.9500
C(125)-C(127)	1.5262(11)
C(125)-C(126)	1.5305(12)
C(125)-H(125)	1.0000
C(24)-H(24)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(122)-C(123)	1.3892(12)
C(122)-H(122)	0.9500
C(130)-H(13A)	0.9800

C(130)-H(13B)	0.9800
C(130)-H(13C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(34)-C(33)	1.5445(10)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(112)-C(111)	1.3911(10)
C(112)-H(112)	0.9500
C(118)-H(11D)	0.9800
C(118)-H(11E)	0.9800
C(118)-H(11F)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(103)-C(104)	1.3645(13)
C(103)-H(103)	0.942(13)
C(117)-H(11G)	0.9800
C(117)-H(11H)	0.9800
C(117)-H(11I)	0.9800
C(124)-C(123)	1.3908(11)
C(124)-H(124)	0.9500
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(111)-H(111)	0.9500
C(114)-H(11J)	0.9800
C(114)-H(11K)	0.9800
C(114)-H(11L)	0.9800
C(35)-H(35A)	0.9800

C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(131)-H(13D)	0.9800
C(131)-H(13E)	0.9800
C(131)-H(13F)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(104)-C(105)	1.4223(13)
C(104)-H(104)	0.955(14)
C(135)-H(13G)	0.9800
C(135)-H(13H)	0.9800
C(135)-H(13I)	0.9800
C(129)-H(12A)	0.9800
C(129)-H(12B)	0.9800
C(129)-H(12C)	0.9800
C(132)-H(13J)	0.9800
C(132)-H(13K)	0.9800
C(132)-H(13L)	0.9800
C(123)-H(123)	0.9500
C(105)-H(105)	0.960(13)
C(133)-C(134)	1.5454(12)
C(133)-H(13M)	0.9900
C(133)-H(13N)	0.9900
C(134)-H(13O)	0.9900
C(134)-H(13P)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(127)-H(12D)	0.9800
C(127)-H(12E)	0.9800
C(127)-H(12F)	0.9800
C(126)-H(12G)	0.9800
C(126)-H(12H)	0.9800
C(126)-H(12I)	0.9800
C(136)-H(13Q)	0.9800

C(136)-H(13R)	0.9800
C(136)-H(13S)	0.9800

N(1)-Fe(1)-C(1)	124.23(2)
N(1)-Fe(1)-P(1)	115.257(18)
C(1)-Fe(1)-P(1)	103.259(15)
N(1)-Fe(1)-P(2)	107.771(17)
C(1)-Fe(1)-P(2)	94.473(14)
P(1)-Fe(1)-P(2)	109.521(8)
N(1)-Fe(1)-C(2)	100.68(2)
C(1)-Fe(1)-C(2)	36.646(19)
P(1)-Fe(1)-C(2)	92.649(15)
P(2)-Fe(1)-C(2)	130.728(15)
N(1)-Fe(1)-B(1)	164.05(2)
C(1)-Fe(1)-B(1)	39.85(2)
P(1)-Fe(1)-B(1)	74.585(15)
P(2)-Fe(1)-B(1)	78.689(15)
C(2)-Fe(1)-B(1)	65.30(2)
N(11)-Fe(2)-C(101)	122.67(2)
N(11)-Fe(2)-C(102)	99.39(2)
C(101)-Fe(2)-C(102)	38.09(2)
N(11)-Fe(2)-P(12)	119.708(19)
C(101)-Fe(2)-P(12)	102.087(17)
C(102)-Fe(2)-P(12)	92.211(19)
N(11)-Fe(2)-P(11)	105.884(18)
C(101)-Fe(2)-P(11)	97.394(18)
C(102)-Fe(2)-P(11)	135.216(19)
P(12)-Fe(2)-P(11)	105.878(10)
N(11)-Fe(2)-B(11)	161.34(2)
C(101)-Fe(2)-B(11)	38.85(2)
C(102)-Fe(2)-B(11)	66.53(2)
P(12)-Fe(2)-B(11)	74.645(17)
P(11)-Fe(2)-B(11)	79.103(18)
C(7)-P(1)-C(16)	105.78(3)
C(7)-P(1)-C(13)	99.26(3)
C(16)-P(1)-C(13)	101.20(3)

C(7)-P(1)-Fe(1)	110.465(18)
C(16)-P(1)-Fe(1)	112.20(2)
C(13)-P(1)-Fe(1)	125.759(19)
C(107)-P(11)-C(116)	101.28(3)
C(107)-P(11)-C(113)	104.92(3)
C(116)-P(11)-C(113)	101.43(3)
C(107)-P(11)-Fe(2)	111.85(2)
C(116)-P(11)-Fe(2)	118.70(2)
C(113)-P(11)-Fe(2)	116.66(2)
C(19)-P(2)-C(25)	103.31(3)
C(19)-P(2)-C(28)	100.65(3)
C(25)-P(2)-C(28)	103.35(3)
C(19)-P(2)-Fe(1)	111.878(18)
C(25)-P(2)-Fe(1)	120.49(2)
C(28)-P(2)-Fe(1)	114.763(19)
C(119)-P(12)-C(125)	104.70(3)
C(119)-P(12)-C(128)	98.75(3)
C(125)-P(12)-C(128)	101.43(3)
C(119)-P(12)-Fe(2)	111.84(2)
C(125)-P(12)-Fe(2)	113.80(2)
C(128)-P(12)-Fe(2)	123.84(2)
N(12)-Si(11)-C(131)	115.60(3)
N(12)-Si(11)-C(133)	96.95(3)
C(131)-Si(11)-C(133)	112.60(4)
N(12)-Si(11)-C(132)	107.24(3)
C(131)-Si(11)-C(132)	113.24(4)
C(133)-Si(11)-C(132)	109.97(4)
N(12)-Si(12)-C(135)	111.09(3)
N(12)-Si(12)-C(136)	112.99(4)
C(135)-Si(12)-C(136)	111.95(5)
N(12)-Si(12)-C(134)	98.81(3)
C(135)-Si(12)-C(134)	112.87(4)
C(136)-Si(12)-C(134)	108.46(4)
N(2)-Si(1)-C(31)	113.82(3)
N(2)-Si(1)-C(32)	111.27(3)
C(31)-Si(1)-C(32)	111.14(4)

N(2)-Si(1)-C(33)	95.98(3)
C(31)-Si(1)-C(33)	113.74(4)
C(32)-Si(1)-C(33)	110.02(4)
N(2)-Si(2)-C(35)	109.88(3)
N(2)-Si(2)-C(36)	109.61(3)
C(35)-Si(2)-C(36)	115.53(4)
N(2)-Si(2)-C(34)	98.59(3)
C(35)-Si(2)-C(34)	111.17(3)
C(36)-Si(2)-C(34)	110.75(3)
N(12)-N(11)-Fe(2)	176.17(5)
N(2)-N(1)-Fe(1)	176.35(4)
N(1)-N(2)-Si(2)	120.68(4)
N(1)-N(2)-Si(1)	127.93(4)
Si(2)-N(2)-Si(1)	111.37(3)
C(124)-C(119)-C(120)	121.76(6)
C(124)-C(119)-P(12)	127.56(5)
C(120)-C(119)-P(12)	110.36(4)
C(9)-C(8)-C(7)	117.32(5)
C(9)-C(8)-B(1)	124.59(5)
C(7)-C(8)-B(1)	117.55(5)
C(12)-C(7)-C(8)	121.80(5)
C(12)-C(7)-P(1)	128.24(4)
C(8)-C(7)-P(1)	109.96(4)
C(15)-C(13)-C(14)	107.59(5)
C(15)-C(13)-P(1)	111.40(4)
C(14)-C(13)-P(1)	114.52(4)
C(15)-C(13)-H(13)	107.7
C(14)-C(13)-H(13)	107.7
P(1)-C(13)-H(13)	107.7
C(4)-C(3)-C(2)	120.57(6)
C(4)-C(3)-H(3)	120.0(7)
C(2)-C(3)-H(3)	119.3(7)
C(2)-C(1)-C(6)	116.60(5)
C(2)-C(1)-B(1)	117.21(5)
C(6)-C(1)-B(1)	126.06(5)
C(2)-C(1)-Fe(1)	79.00(3)

C(6)-C(1)-Fe(1)	116.08(4)
B(1)-C(1)-Fe(1)	77.97(3)
N(11)-N(12)-Si(12)	124.97(4)
N(11)-N(12)-Si(11)	124.64(4)
Si(12)-N(12)-Si(11)	110.12(3)
C(112)-C(107)-C(108)	120.77(6)
C(112)-C(107)-P(11)	123.86(5)
C(108)-C(107)-P(11)	115.27(4)
C(10)-C(9)-C(8)	121.10(5)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(24)-C(19)-C(20)	120.91(5)
C(24)-C(19)-P(2)	125.47(4)
C(20)-C(19)-P(2)	113.54(4)
C(21)-C(20)-C(19)	117.47(5)
C(21)-C(20)-B(1)	123.23(5)
C(19)-C(20)-B(1)	119.00(5)
C(5)-C(6)-C(1)	122.03(5)
C(5)-C(6)-H(6)	119.6(7)
C(1)-C(6)-H(6)	118.3(7)
C(22)-C(21)-C(20)	121.45(5)
C(22)-C(21)-H(21)	119.3
C(20)-C(21)-H(21)	119.3
C(6)-C(5)-C(4)	120.20(5)
C(6)-C(5)-H(5)	119.6(7)
C(4)-C(5)-H(5)	120.2(7)
C(18)-C(16)-C(17)	110.49(5)
C(18)-C(16)-P(1)	109.60(4)
C(17)-C(16)-P(1)	112.01(4)
C(18)-C(16)-H(16)	108.2
C(17)-C(16)-H(16)	108.2
P(1)-C(16)-H(16)	108.2
C(11)-C(12)-C(7)	119.64(5)
C(11)-C(12)-H(12)	120.2
C(7)-C(12)-H(12)	120.2
C(119)-C(120)-C(121)	117.03(6)

C(119)-C(120)-B(11)	118.11(5)
C(121)-C(120)-B(11)	124.69(6)
C(27)-C(25)-C(26)	109.74(6)
C(27)-C(25)-P(2)	112.57(4)
C(26)-C(25)-P(2)	111.76(4)
C(27)-C(25)-H(25)	107.5
C(26)-C(25)-H(25)	107.5
P(2)-C(25)-H(25)	107.5
C(1)-B(1)-C(20)	116.95(4)
C(1)-B(1)-C(8)	112.57(4)
C(20)-B(1)-C(8)	122.93(5)
C(1)-B(1)-Fe(1)	62.18(3)
C(20)-B(1)-Fe(1)	114.72(4)
C(8)-B(1)-Fe(1)	112.26(4)
C(118)-C(116)-C(117)	110.87(5)
C(118)-C(116)-P(11)	110.77(5)
C(117)-C(116)-P(11)	112.54(4)
C(118)-C(116)-H(116)	107.5
C(117)-C(116)-H(116)	107.5
P(11)-C(116)-H(116)	107.5
C(115)-C(113)-C(114)	109.36(6)
C(115)-C(113)-P(11)	111.48(4)
C(114)-C(113)-P(11)	116.98(5)
C(115)-C(113)-H(113)	106.1
C(114)-C(113)-H(113)	106.1
P(11)-C(113)-H(113)	106.1
C(21)-C(22)-C(23)	120.10(5)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(29)-C(28)-C(30)	109.96(5)
C(29)-C(28)-P(2)	112.85(4)
C(30)-C(28)-P(2)	116.66(5)
C(29)-C(28)-H(28)	105.5
C(30)-C(28)-H(28)	105.5
P(2)-C(28)-H(28)	105.5
C(13)-C(15)-H(15A)	109.5

C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(109)-C(110)-C(111)	120.00(6)
C(109)-C(110)-H(110)	120.0
C(111)-C(110)-H(110)	120.0
C(130)-C(128)-C(129)	107.80(5)
C(130)-C(128)-P(12)	110.98(4)
C(129)-C(128)-P(12)	115.58(5)
C(130)-C(128)-H(128)	107.4
C(129)-C(128)-H(128)	107.4
P(12)-C(128)-H(128)	107.4
C(110)-C(109)-C(108)	121.97(7)
C(110)-C(109)-H(109)	119.0
C(108)-C(109)-H(109)	119.0
C(102)-C(101)-C(106)	117.26(6)
C(102)-C(101)-B(11)	118.78(5)
C(106)-C(101)-B(11)	123.83(6)
C(102)-C(101)-Fe(2)	74.09(4)
C(106)-C(101)-Fe(2)	118.68(4)
B(11)-C(101)-Fe(2)	80.59(3)
C(1)-C(2)-C(3)	120.52(5)
C(1)-C(2)-Fe(1)	64.35(3)
C(3)-C(2)-Fe(1)	126.15(4)
C(1)-C(2)-H(2)	119.3(7)
C(3)-C(2)-H(2)	117.4(7)
Fe(1)-C(2)-H(2)	94.9(7)
C(12)-C(11)-C(10)	119.57(5)
C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
C(24)-C(23)-C(22)	119.77(5)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(105)-C(106)-C(101)	121.82(7)

C(105)-C(106)-H(106)	119.8(7)
C(101)-C(106)-H(106)	118.1(7)
C(107)-C(108)-C(109)	117.19(6)
C(107)-C(108)-B(11)	119.78(5)
C(109)-C(108)-B(11)	122.90(6)
C(3)-C(4)-C(5)	119.87(6)
C(3)-C(4)-H(4)	119.0(7)
C(5)-C(4)-H(4)	121.1(7)
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(122)-C(121)-C(120)	121.34(7)
C(122)-C(121)-H(121)	119.3
C(120)-C(121)-H(121)	119.3
C(101)-C(102)-C(103)	119.55(6)
C(101)-C(102)-Fe(2)	67.82(3)
C(103)-C(102)-Fe(2)	121.51(5)
C(101)-C(102)-H(102)	120.2(7)
C(103)-C(102)-H(102)	116.7(7)
Fe(2)-C(102)-H(102)	98.7(7)
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(113)-C(115)-H(11A)	109.5

C(113)-C(115)-H(11B)	109.5
H(11A)-C(115)-H(11B)	109.5
C(113)-C(115)-H(11C)	109.5
H(11A)-C(115)-H(11C)	109.5
H(11B)-C(115)-H(11C)	109.5
C(11)-C(10)-C(9)	120.55(5)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(127)-C(125)-C(126)	111.37(6)
C(127)-C(125)-P(12)	110.48(5)
C(126)-C(125)-P(12)	110.83(5)
C(127)-C(125)-H(125)	108.0
C(126)-C(125)-H(125)	108.0
P(12)-C(125)-H(125)	108.0
C(23)-C(24)-C(19)	120.05(5)
C(23)-C(24)-H(24)	120.0
C(19)-C(24)-H(24)	120.0
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(123)-C(122)-C(121)	120.53(7)
C(123)-C(122)-H(122)	119.7
C(121)-C(122)-H(122)	119.7
C(128)-C(130)-H(13A)	109.5
C(128)-C(130)-H(13B)	109.5
H(13A)-C(130)-H(13B)	109.5
C(128)-C(130)-H(13C)	109.5
H(13A)-C(130)-H(13C)	109.5
H(13B)-C(130)-H(13C)	109.5
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5

H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(33)-C(34)-Si(2)	109.03(4)
C(33)-C(34)-H(34A)	109.9
Si(2)-C(34)-H(34A)	109.9
C(33)-C(34)-H(34B)	109.9
Si(2)-C(34)-H(34B)	109.9
H(34A)-C(34)-H(34B)	108.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(111)-C(112)-C(107)	120.63(7)
C(111)-C(112)-H(112)	119.7
C(107)-C(112)-H(112)	119.7
C(101)-B(11)-C(108)	117.39(5)
C(101)-B(11)-C(120)	115.75(5)
C(108)-B(11)-C(120)	121.77(5)
C(101)-B(11)-Fe(2)	60.56(3)
C(108)-B(11)-Fe(2)	113.20(4)
C(120)-B(11)-Fe(2)	112.30(4)
C(116)-C(118)-H(11D)	109.5
C(116)-C(118)-H(11E)	109.5
H(11D)-C(118)-H(11E)	109.5
C(116)-C(118)-H(11F)	109.5
H(11D)-C(118)-H(11F)	109.5
H(11E)-C(118)-H(11F)	109.5
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(104)-C(103)-C(102)	120.80(7)

C(104)-C(103)-H(103)	120.4(8)
C(102)-C(103)-H(103)	118.7(8)
C(116)-C(117)-H(11G)	109.5
C(116)-C(117)-H(11H)	109.5
H(11G)-C(117)-H(11H)	109.5
C(116)-C(117)-H(11I)	109.5
H(11G)-C(117)-H(11I)	109.5
H(11H)-C(117)-H(11I)	109.5
C(123)-C(124)-C(119)	119.81(7)
C(123)-C(124)-H(124)	120.1
C(119)-C(124)-H(124)	120.1
Si(1)-C(31)-H(31A)	109.5
Si(1)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(1)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(34)-C(33)-Si(1)	106.97(4)
C(34)-C(33)-H(33A)	110.3
Si(1)-C(33)-H(33A)	110.3
C(34)-C(33)-H(33B)	110.3
Si(1)-C(33)-H(33B)	110.3
H(33A)-C(33)-H(33B)	108.6
C(110)-C(111)-C(112)	119.44(6)
C(110)-C(111)-H(111)	120.3
C(112)-C(111)-H(111)	120.3
C(113)-C(114)-H(11J)	109.5
C(113)-C(114)-H(11K)	109.5
H(11J)-C(114)-H(11K)	109.5
C(113)-C(114)-H(11L)	109.5
H(11J)-C(114)-H(11L)	109.5
H(11K)-C(114)-H(11L)	109.5
Si(2)-C(35)-H(35A)	109.5
Si(2)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
Si(2)-C(35)-H(35C)	109.5

H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
Si(11)-C(131)-H(13D)	109.5
Si(11)-C(131)-H(13E)	109.5
H(13D)-C(131)-H(13E)	109.5
Si(11)-C(131)-H(13F)	109.5
H(13D)-C(131)-H(13F)	109.5
H(13E)-C(131)-H(13F)	109.5
Si(1)-C(32)-H(32A)	109.5
Si(1)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si(1)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(103)-C(104)-C(105)	120.15(6)
C(103)-C(104)-H(104)	120.3(8)
C(105)-C(104)-H(104)	119.6(8)
Si(12)-C(135)-H(13G)	109.5
Si(12)-C(135)-H(13H)	109.5
H(13G)-C(135)-H(13H)	109.5
Si(12)-C(135)-H(13I)	109.5
H(13G)-C(135)-H(13I)	109.5
H(13H)-C(135)-H(13I)	109.5
C(128)-C(129)-H(12A)	109.5
C(128)-C(129)-H(12B)	109.5
H(12A)-C(129)-H(12B)	109.5
C(128)-C(129)-H(12C)	109.5
H(12A)-C(129)-H(12C)	109.5
H(12B)-C(129)-H(12C)	109.5
Si(11)-C(132)-H(13J)	109.5
Si(11)-C(132)-H(13K)	109.5
H(13J)-C(132)-H(13K)	109.5
Si(11)-C(132)-H(13L)	109.5
H(13J)-C(132)-H(13L)	109.5
H(13K)-C(132)-H(13L)	109.5
C(122)-C(123)-C(124)	119.47(7)

C(122)-C(123)-H(123)	120.3
C(124)-C(123)-H(123)	120.3
C(106)-C(105)-C(104)	120.23(7)
C(106)-C(105)-H(105)	119.5(8)
C(104)-C(105)-H(105)	120.3(8)
C(134)-C(133)-Si(11)	106.69(5)
C(134)-C(133)-H(13M)	110.4
Si(11)-C(133)-H(13M)	110.4
C(134)-C(133)-H(13N)	110.4
Si(11)-C(133)-H(13N)	110.4
H(13M)-C(133)-H(13N)	108.6
C(133)-C(134)-Si(12)	110.09(5)
C(133)-C(134)-H(13O)	109.6
Si(12)-C(134)-H(13O)	109.6
C(133)-C(134)-H(13P)	109.6
Si(12)-C(134)-H(13P)	109.6
H(13O)-C(134)-H(13P)	108.2
Si(2)-C(36)-H(36A)	109.5
Si(2)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
Si(2)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(125)-C(127)-H(12D)	109.5
C(125)-C(127)-H(12E)	109.5
H(12D)-C(127)-H(12E)	109.5
C(125)-C(127)-H(12F)	109.5
H(12D)-C(127)-H(12F)	109.5
H(12E)-C(127)-H(12F)	109.5
C(125)-C(126)-H(12G)	109.5
C(125)-C(126)-H(12H)	109.5
H(12G)-C(126)-H(12H)	109.5
C(125)-C(126)-H(12I)	109.5
H(12G)-C(126)-H(12I)	109.5
H(12H)-C(126)-H(12I)	109.5
Si(12)-C(136)-H(13Q)	109.5

Si(12)-C(136)-H(13R)	109.5
H(13Q)-C(136)-H(13R)	109.5
Si(12)-C(136)-H(13S)	109.5
H(13Q)-C(136)-H(13S)	109.5
H(13R)-C(136)-H(13S)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S19. Crystal data and structure refinement for **6b**.

Identification code	**6b**	
Empirical formula	C48 H49 B Fe N2 P2 Si2	
Formula weight	838.67	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.7196(6) Å	α = 90°.
	b = 18.1906(11) Å	β = 92.637(2)°.
	c = 21.7101(10) Å	γ = 90°.
Volume	4228.9(4) $Å^3$	
Z	4	
Density (calculated)	1.317 Mg/m^3	
Absorption coefficient	0.526 mm^{-1}	
F(000)	1760	
Crystal size	0.37 x 0.16 x 0.08 mm^3	
Theta range for data collection	1.88 to 41.63°.	
Index ranges	-19<=h<=19, -33<=k<=33, -39<=l<=40	
Reflections collected	196104	
Independent reflections	28150 [R(int) = 0.0667]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9285	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28150 / 0 / 529	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0901	
R indices (all data)	R1 = 0.0750, wR2 = 0.1024	
Largest diff. peak and hole	0.789 and -0.378 $e.Å^{-3}$	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5380(1)	2224(1)	8265(1)	8(1)
P(1)	6191(1)	2067(1)	9207(1)	8(1)
P(2)	4537(1)	3342(1)	8294(1)	9(1)
Si(1)	6747(1)	2697(1)	6503(1)	13(1)
Si(2)	8832(1)	2245(1)	7385(1)	12(1)
N(1)	6366(1)	2285(1)	7699(1)	10(1)
N(2)	7175(1)	2382(1)	7266(1)	12(1)
C(19)	6575(1)	2845(1)	9720(1)	10(1)
C(11)	4778(1)	670(1)	10520(1)	16(1)
C(9)	3140(1)	1063(1)	9793(1)	14(1)
C(7)	5232(1)	1498(1)	9692(1)	10(1)
C(40)	7355(1)	5143(1)	8949(1)	23(1)
C(38)	6720(1)	4138(1)	8283(1)	16(1)
C(23)	6118(1)	3601(1)	10598(1)	17(1)
C(26)	2821(1)	2720(1)	9014(1)	11(1)
C(2)	4627(1)	1100(1)	8179(1)	12(1)
C(5)	2893(1)	1364(1)	7194(1)	18(1)
C(3)	4733(1)	732(1)	7600(1)	17(1)
C(8)	3981(1)	1504(1)	9480(1)	10(1)
C(37)	5602(1)	4066(1)	8586(1)	12(1)
C(24)	5810(1)	3019(1)	10202(1)	14(1)
C(41)	6257(1)	5069(1)	9257(1)	20(1)
C(32)	3464(1)	3330(1)	7094(1)	15(1)
C(29)	1393(1)	4012(1)	9169(1)	18(1)
C(36)	3908(1)	4540(1)	7491(1)	14(1)
C(10)	3532(1)	648(1)	10305(1)	16(1)
C(31)	3960(1)	3777(1)	7568(1)	11(1)
C(1)	3646(1)	1625(1)	8256(1)	11(1)
C(25)	3137(1)	3388(1)	8736(1)	11(1)
C(42)	5379(1)	4535(1)	9077(1)	15(1)
C(35)	3361(1)	4847(1)	6958(1)	16(1)

C(34)	2860(1)	4396(1)	6492(1)	18(1)
C(48)	9211(1)	1250(1)	7332(1)	18(1)
C(39)	7586(1)	4677(1)	8461(1)	22(1)
C(22)	7180(1)	4015(1)	10516(1)	17(1)
C(47)	9398(1)	2676(1)	8118(1)	20(1)
C(12)	5632(1)	1087(1)	10210(1)	14(1)
C(21)	7937(1)	3854(1)	10030(1)	16(1)
C(27)	1799(1)	2734(1)	9400(1)	15(1)
C(30)	2408(1)	4022(1)	8793(1)	16(1)
C(6)	2795(1)	1741(1)	7735(1)	14(1)
C(44)	6443(1)	3704(1)	6516(1)	18(1)
C(15)	8933(1)	584(1)	8829(1)	15(1)
C(13)	7663(1)	1545(1)	9255(1)	10(1)
C(17)	9528(1)	1108(1)	9814(1)	18(1)
C(20)	7635(1)	3275(1)	9633(1)	13(1)
C(4)	3891(1)	860(1)	7122(1)	20(1)
C(33)	2914(1)	3636(1)	6562(1)	19(1)
C(18)	8499(1)	1573(1)	9770(1)	14(1)
C(16)	9745(1)	611(1)	9344(1)	17(1)
C(28)	1109(1)	3368(1)	9481(1)	18(1)
C(43)	5414(1)	2164(1)	6158(1)	20(1)
C(14)	7895(1)	1047(1)	8785(1)	12(1)
C(46)	9308(1)	2714(1)	6665(1)	18(1)
C(45)	8287(1)	2526(1)	6158(1)	17(1)
B(1)	3609(1)	1998(1)	8894(1)	10(1)

Table S21. Bond lengths [Å] and angles [°] for **6b**.

Fe(1)-N(1)	1.6610(7)
Fe(1)-C(1)	2.1542(9)
Fe(1)-P(1)	2.2026(3)
Fe(1)-C(2)	2.2041(9)
Fe(1)-P(2)	2.2264(3)
Fe(1)-B(1)	2.4242(10)
P(1)-C(7)	1.8265(9)
P(1)-C(19)	1.8356(9)
P(1)-C(13)	1.8409(9)
P(2)-C(25)	1.8208(9)
P(2)-C(37)	1.8363(10)
P(2)-C(31)	1.8442(9)
Si(1)-N(2)	1.7933(8)
Si(1)-C(43)	1.8556(12)
Si(1)-C(44)	1.8608(11)
Si(1)-C(45)	1.8702(10)
Si(2)-N(2)	1.8001(8)
Si(2)-C(47)	1.8512(11)
Si(2)-C(48)	1.8593(11)
Si(2)-C(46)	1.8718(10)
N(1)-N(2)	1.3193(10)
C(19)-C(24)	1.3947(12)
C(19)-C(20)	1.3999(13)
C(11)-C(12)	1.3866(14)
C(11)-C(10)	1.3950(15)
C(11)-H(11)	0.9500
C(9)-C(10)	1.3930(14)
C(9)-C(8)	1.4047(12)
C(9)-H(9)	0.9500
C(7)-C(8)	1.3980(12)
C(7)-C(12)	1.4009(12)
C(40)-C(41)	1.3860(17)
C(40)-C(39)	1.3883(17)
C(40)-H(40)	0.9500

C(38)-C(39)	1.3923(15)
C(38)-C(37)	1.4000(13)
C(38)-H(38)	0.9500
C(23)-C(22)	1.3836(15)
C(23)-C(24)	1.3936(14)
C(23)-H(23)	0.9500
C(26)-C(25)	1.4059(13)
C(26)-C(27)	1.4086(12)
C(26)-B(1)	1.5895(14)
C(2)-C(3)	1.4342(13)
C(2)-C(1)	1.4356(13)
C(2)-H(2)	0.951(14)
C(5)-C(6)	1.3680(14)
C(5)-C(4)	1.4218(17)
C(5)-H(5)	0.974(17)
C(3)-C(4)	1.3641(16)
C(3)-H(3)	0.942(17)
C(8)-B(1)	1.5927(13)
C(37)-C(42)	1.3942(13)
C(24)-H(24)	0.9500
C(41)-C(42)	1.3967(15)
C(41)-H(41)	0.9500
C(32)-C(33)	1.3886(14)
C(32)-C(31)	1.3986(13)
C(32)-H(32)	0.9500
C(29)-C(30)	1.3895(13)
C(29)-C(28)	1.3940(16)
C(29)-H(29)	0.9500
C(36)-C(35)	1.3914(13)
C(36)-C(31)	1.3985(13)
C(36)-H(36)	0.9500
C(10)-H(10)	0.9500
C(1)-C(6)	1.4365(13)
C(1)-B(1)	1.5450(13)
C(25)-C(30)	1.4015(13)
C(42)-H(42)	0.9500

C(35)-C(34)	1.3906(14)
C(35)-H(35)	0.9500
C(34)-C(33)	1.3916(15)
C(34)-H(34)	0.9500
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(39)-H(39)	0.9500
C(22)-C(21)	1.3911(14)
C(22)-H(22)	0.9500
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(12)-H(12)	0.9500
C(21)-C(20)	1.3888(13)
C(21)-H(21)	0.9500
C(27)-C(28)	1.3870(14)
C(27)-H(27)	0.9500
C(30)-H(30)	0.9500
C(6)-H(6)	0.944(14)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(15)-C(16)	1.3853(14)
C(15)-C(14)	1.3952(13)
C(15)-H(15)	0.9500
C(13)-C(14)	1.3956(13)
C(13)-C(18)	1.4021(13)
C(17)-C(18)	1.3901(14)
C(17)-C(16)	1.3920(15)
C(17)-H(17)	0.9500
C(20)-H(20)	0.9500
C(4)-H(4)	0.945(16)
C(33)-H(33)	0.9500
C(18)-H(18)	0.9500
C(16)-H(16)	0.9500

C(28)-H(28)	0.9500
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(14)-H(14)	0.9500
C(46)-C(45)	1.5545(15)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900

N(1)-Fe(1)-C(1)	127.17(4)
N(1)-Fe(1)-P(1)	117.30(3)
C(1)-Fe(1)-P(1)	104.26(2)
N(1)-Fe(1)-C(2)	103.97(4)
C(1)-Fe(1)-C(2)	38.44(3)
P(1)-Fe(1)-C(2)	94.92(3)
N(1)-Fe(1)-P(2)	103.46(3)
C(1)-Fe(1)-P(2)	96.38(3)
P(1)-Fe(1)-P(2)	103.657(10)
C(2)-Fe(1)-P(2)	134.58(3)
N(1)-Fe(1)-B(1)	165.75(4)
C(1)-Fe(1)-B(1)	38.88(3)
P(1)-Fe(1)-B(1)	74.99(2)
C(2)-Fe(1)-B(1)	66.23(3)
P(2)-Fe(1)-B(1)	79.03(3)
C(7)-P(1)-C(19)	101.75(4)
C(7)-P(1)-C(13)	100.32(4)
C(19)-P(1)-C(13)	101.29(4)
C(7)-P(1)-Fe(1)	113.59(3)
C(19)-P(1)-Fe(1)	122.04(3)
C(13)-P(1)-Fe(1)	114.82(3)
C(25)-P(2)-C(37)	107.38(4)
C(25)-P(2)-C(31)	100.25(4)
C(37)-P(2)-C(31)	99.51(4)
C(25)-P(2)-Fe(1)	113.75(3)

C(37)-P(2)-Fe(1)	114.71(3)
C(31)-P(2)-Fe(1)	119.29(3)
N(2)-Si(1)-C(43)	111.39(5)
N(2)-Si(1)-C(44)	109.80(4)
C(43)-Si(1)-C(44)	112.84(5)
N(2)-Si(1)-C(45)	97.13(4)
C(43)-Si(1)-C(45)	115.37(5)
C(44)-Si(1)-C(45)	109.20(5)
N(2)-Si(2)-C(47)	110.28(4)
N(2)-Si(2)-C(48)	110.06(5)
C(47)-Si(2)-C(48)	113.63(5)
N(2)-Si(2)-C(46)	97.07(4)
C(47)-Si(2)-C(46)	115.68(5)
C(48)-Si(2)-C(46)	108.88(5)
N(2)-N(1)-Fe(1)	175.62(7)
N(1)-N(2)-Si(1)	123.53(6)
N(1)-N(2)-Si(2)	123.82(6)
Si(1)-N(2)-Si(2)	112.62(4)
C(24)-C(19)-C(20)	118.85(8)
C(24)-C(19)-P(1)	120.46(7)
C(20)-C(19)-P(1)	120.69(6)
C(12)-C(11)-C(10)	119.77(9)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(10)-C(9)-C(8)	121.28(9)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(8)-C(7)-C(12)	121.46(8)
C(8)-C(7)-P(1)	111.26(6)
C(12)-C(7)-P(1)	127.28(7)
C(41)-C(40)-C(39)	119.64(10)
C(41)-C(40)-H(40)	120.2
C(39)-C(40)-H(40)	120.2
C(39)-C(38)-C(37)	120.71(10)
C(39)-C(38)-H(38)	119.6
C(37)-C(38)-H(38)	119.6

C(22)-C(23)-C(24)	120.47(9)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(25)-C(26)-C(27)	116.69(8)
C(25)-C(26)-B(1)	120.22(7)
C(27)-C(26)-B(1)	123.09(8)
C(3)-C(2)-C(1)	120.06(9)
C(3)-C(2)-Fe(1)	117.65(7)
C(1)-C(2)-Fe(1)	68.89(5)
C(3)-C(2)-H(2)	118.8(8)
C(1)-C(2)-H(2)	117.6(8)
Fe(1)-C(2)-H(2)	100.5(9)
C(6)-C(5)-C(4)	120.36(9)
C(6)-C(5)-H(5)	120.4(10)
C(4)-C(5)-H(5)	119.3(10)
C(4)-C(3)-C(2)	120.70(10)
C(4)-C(3)-H(3)	121.3(10)
C(2)-C(3)-H(3)	117.8(10)
C(7)-C(8)-C(9)	117.60(8)
C(7)-C(8)-B(1)	117.92(7)
C(9)-C(8)-B(1)	124.48(8)
C(42)-C(37)-C(38)	118.76(9)
C(42)-C(37)-P(2)	125.29(7)
C(38)-C(37)-P(2)	115.95(7)
C(23)-C(24)-C(19)	120.32(9)
C(23)-C(24)-H(24)	119.8
C(19)-C(24)-H(24)	119.8
C(40)-C(41)-C(42)	120.53(10)
C(40)-C(41)-H(41)	119.7
C(42)-C(41)-H(41)	119.7
C(33)-C(32)-C(31)	120.82(9)
C(33)-C(32)-H(32)	119.6
C(31)-C(32)-H(32)	119.6
C(30)-C(29)-C(28)	119.34(9)
C(30)-C(29)-H(29)	120.3
C(28)-C(29)-H(29)	120.3

C(35)-C(36)-C(31)	120.73(9)
C(35)-C(36)-H(36)	119.6
C(31)-C(36)-H(36)	119.6
C(9)-C(10)-C(11)	120.01(9)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(36)-C(31)-C(32)	118.48(8)
C(36)-C(31)-P(2)	122.58(7)
C(32)-C(31)-P(2)	118.74(7)
C(2)-C(1)-C(6)	116.60(8)
C(2)-C(1)-B(1)	116.49(8)
C(6)-C(1)-B(1)	126.90(8)
C(2)-C(1)-Fe(1)	72.66(5)
C(6)-C(1)-Fe(1)	116.76(6)
B(1)-C(1)-Fe(1)	80.05(5)
C(30)-C(25)-C(26)	121.76(8)
C(30)-C(25)-P(2)	124.20(7)
C(26)-C(25)-P(2)	114.03(7)
C(37)-C(42)-C(41)	120.26(10)
C(37)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(34)-C(35)-C(36)	120.18(9)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(35)-C(34)-C(33)	119.58(9)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
Si(2)-C(48)-H(48A)	109.5
Si(2)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
Si(2)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(40)-C(39)-C(38)	120.09(10)
C(40)-C(39)-H(39)	120.0
C(38)-C(39)-H(39)	120.0

C(23)-C(22)-C(21)	119.62(9)
C(23)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
Si(2)-C(47)-H(47A)	109.5
Si(2)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
Si(2)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(11)-C(12)-C(7)	119.83(9)
C(11)-C(12)-H(12)	120.1
C(7)-C(12)-H(12)	120.1
C(20)-C(21)-C(22)	120.22(9)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(28)-C(27)-C(26)	121.64(9)
C(28)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(29)-C(30)-C(25)	119.81(9)
C(29)-C(30)-H(30)	120.1
C(25)-C(30)-H(30)	120.1
C(5)-C(6)-C(1)	122.11(9)
C(5)-C(6)-H(6)	120.4(9)
C(1)-C(6)-H(6)	117.4(9)
Si(1)-C(44)-H(44A)	109.5
Si(1)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
Si(1)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(16)-C(15)-C(14)	120.27(9)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(14)-C(13)-C(18)	118.60(8)
C(14)-C(13)-P(1)	118.33(7)
C(18)-C(13)-P(1)	122.76(7)

C(18)-C(17)-C(16)	120.23(9)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(21)-C(20)-C(19)	120.50(8)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(3)-C(4)-C(5)	120.10(9)
C(3)-C(4)-H(4)	118.1(10)
C(5)-C(4)-H(4)	121.8(10)
C(32)-C(33)-C(34)	120.21(9)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(17)-C(18)-C(13)	120.60(9)
C(17)-C(18)-H(18)	119.7
C(13)-C(18)-H(18)	119.7
C(15)-C(16)-C(17)	119.67(9)
C(15)-C(16)-H(16)	120.2
C(17)-C(16)-H(16)	120.2
C(27)-C(28)-C(29)	120.51(9)
C(27)-C(28)-H(28)	119.7
C(29)-C(28)-H(28)	119.7
Si(1)-C(43)-H(43A)	109.5
Si(1)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
Si(1)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(15)-C(14)-C(13)	120.63(8)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(45)-C(46)-Si(2)	106.28(7)
C(45)-C(46)-H(46A)	110.5
Si(2)-C(46)-H(46A)	110.5
C(45)-C(46)-H(46B)	110.5
Si(2)-C(46)-H(46B)	110.5
H(46A)-C(46)-H(46B)	108.7

C(46)-C(45)-Si(1)	106.54(6)
C(46)-C(45)-H(45A)	110.4
Si(1)-C(45)-H(45A)	110.4
C(46)-C(45)-H(45B)	110.4
Si(1)-C(45)-H(45B)	110.4
H(45A)-C(45)-H(45B)	108.6
C(1)-B(1)-C(26)	123.09(8)
C(1)-B(1)-C(8)	116.86(8)
C(26)-B(1)-C(8)	116.79(7)
C(1)-B(1)-Fe(1)	61.07(4)
C(26)-B(1)-Fe(1)	112.86(6)
C(8)-B(1)-Fe(1)	111.82(6)

Symmetry transformations used to generate equivalent atoms:

Table S22. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	C42 H65 B Fe N2 P2 Si3	
Formula weight	810.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.167(15) Å	α = 99.79(5)°.
	b = 12.843(12) Å	β = 95.23(5)°.
	c = 18.21(3) Å	γ = 101.42(5)°.
Volume	2277(5) $Å^3$	
Z	2	
Density (calculated)	1.183 Mg/m^3	
Absorption coefficient	0.510 mm^{-1}	
F(000)	868	
Crystal size	0.05 x 0.05 x 0.04 mm^3	
Theta range for data collection	1.65 to 24.55°.	
Index ranges	-11<=h<=11, -14<=k<=14, -20<=l<=21	
Reflections collected	11316	
Independent reflections	5912 [R(int) = 0.0330]	
Completeness to theta = 24.55°	77.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5912 / 0 / 485	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1547	
R indices (all data)	R1 = 0.0648, wR2 = 0.1615	
Largest diff. peak and hole	0.778 and -0.295 $e.Å^{-3}$	

Table S23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2867(1)	1679(1)	2298(1)	37(1)
P(2)	2832(1)	-308(1)	1958(1)	38(1)
P(1)	1389(1)	2042(1)	3238(1)	42(1)
Si(3)	2940(1)	4652(1)	1522(1)	46(1)
Si(2)	2068(1)	2651(1)	393(1)	46(1)
Si(1)	5416(1)	2811(1)	1638(1)	47(1)
N(2)	2976(3)	3288(2)	1262(2)	43(1)
C(20)	4923(3)	169(3)	3166(2)	37(1)
C(10)	1645(4)	-890(3)	4381(2)	47(1)
C(13)	1795(4)	3300(3)	3979(3)	52(1)
N(1)	3713(3)	2662(2)	1710(2)	41(1)
C(7)	1527(3)	917(3)	3727(2)	40(1)
C(30)	3900(5)	-136(4)	640(3)	61(1)
C(9)	2793(4)	-293(3)	4176(2)	44(1)
C(27)	130(4)	-1521(3)	1710(2)	48(1)
C(28)	2733(4)	-803(3)	924(2)	45(1)
C(21)	6061(4)	-81(3)	3556(2)	46(1)
C(29)	2571(4)	-2011(3)	601(2)	52(1)
C(22)	6640(4)	-934(3)	3255(3)	50(1)
C(19)	4413(3)	-494(3)	2453(2)	38(1)
C(8)	2803(3)	606(3)	3827(2)	38(1)
C(6)	5129(4)	2005(3)	5014(3)	55(1)
C(25)	1453(3)	-1273(3)	2263(2)	43(1)
C(38)	2827(5)	5052(4)	2536(3)	62(1)
C(24)	5025(4)	-1322(3)	2152(3)	47(1)
C(12)	369(4)	330(3)	3942(2)	46(1)
C(23)	6131(4)	-1543(3)	2553(3)	49(1)
C(5)	6032(6)	2739(4)	5596(3)	68(2)
C(16)	-448(4)	1924(3)	2928(3)	53(1)
C(37)	4376(4)	5602(4)	1257(3)	64(1)
C(36)	7521(4)	4684(4)	1737(3)	56(1)

C(11)	414(4)	-595(3)	4250(2)	49(1)
C(4)	7128(5)	3418(4)	5405(3)	71(2)
C(35)	8359(5)	5677(4)	2085(3)	67(1)
C(15)	1063(5)	3169(4)	4663(3)	76(1)
C(33)	7211(5)	5643(4)	3171(3)	67(1)
C(34)	8196(5)	6140(4)	2794(3)	72(2)
C(26)	1836(4)	-2303(3)	2447(2)	50(1)
C(2)	6418(4)	2647(3)	4097(3)	52(1)
C(18)	-1040(4)	887(4)	2349(3)	56(1)
C(17)	-634(5)	2905(4)	2576(3)	66(1)
C(42)	3116(4)	2169(4)	-326(3)	58(1)
C(14)	3293(4)	3725(3)	4221(3)	57(1)
C(41)	722(4)	1492(3)	510(3)	56(1)
C(1)	5281(4)	1946(3)	4260(2)	44(1)
C(40)	1371(4)	3833(3)	141(3)	54(1)
C(39)	1348(4)	4618(3)	886(2)	52(1)
C(31)	6511(4)	4155(3)	2106(3)	51(1)
B(1)	4241(4)	1134(3)	3573(2)	37(1)
C(3)	7323(5)	3395(3)	4672(3)	65(1)
C(32)	6380(4)	4641(4)	2821(3)	54(1)

Table S24. Bond lengths [Å] and angles [°] for **7**.

Fe(1)-N(1)	1.918(4)
Fe(1)-P(1)	2.424(3)
Fe(1)-P(2)	2.514(3)
Fe(1)-B(1)	2.859(5)
Fe(1)-H(103)	1.77(4)
P(2)-C(19)	1.846(4)
P(2)-C(28)	1.869(5)
P(2)-C(25)	1.870(4)
P(1)-C(7)	1.842(4)
P(1)-C(13)	1.870(5)
P(1)-C(16)	1.871(5)
Si(3)-N(2)	1.743(4)
Si(3)-C(38)	1.851(6)
Si(3)-C(37)	1.865(5)
Si(3)-C(39)	1.892(4)
Si(2)-N(2)	1.737(4)
Si(2)-C(42)	1.864(5)
Si(2)-C(41)	1.868(5)
Si(2)-C(40)	1.903(4)
Si(1)-N(1)	1.723(4)
Si(1)-C(31)	1.874(5)
Si(1)-H(101)	1.33(3)
Si(1)-H(102)	1.47(6)
N(2)-N(1)	1.492(4)
C(20)-C(19)	1.416(6)
C(20)-C(21)	1.422(5)
C(20)-B(1)	1.640(5)
C(10)-C(9)	1.383(6)
C(10)-C(11)	1.390(6)
C(10)-H(10)	0.9500
C(13)-C(14)	1.510(6)
C(13)-C(15)	1.523(7)
C(13)-H(13)	1.0000
C(7)-C(12)	1.394(6)

C(7)-C(8)	1.437(5)
C(30)-C(28)	1.507(6)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(9)-C(8)	1.407(5)
C(9)-H(9)	0.9500
C(27)-C(25)	1.549(5)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.533(6)
C(28)-H(28)	1.0000
C(21)-C(22)	1.399(6)
C(21)-H(21)	0.9500
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(22)-C(23)	1.375(6)
C(22)-H(22)	0.9500
C(19)-C(24)	1.395(5)
C(8)-B(1)	1.627(6)
C(6)-C(1)	1.387(7)
C(6)-C(5)	1.413(6)
C(6)-H(6)	0.9500
C(25)-C(26)	1.531(5)
C(25)-H(25)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(24)-C(23)	1.388(5)
C(24)-H(24)	0.9500
C(12)-C(11)	1.404(6)
C(12)-H(12)	0.9500
C(23)-H(23)	0.9500
C(5)-C(4)	1.384(8)

C(5)-H(5)	0.9500
C(16)-C(18)	1.528(6)
C(16)-C(17)	1.543(6)
C(16)-H(16)	1.0000
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(36)-C(35)	1.397(7)
C(36)-C(31)	1.405(6)
C(36)-H(36)	0.9500
C(11)-H(11)	0.9500
C(4)-C(3)	1.363(8)
C(4)-H(4)	0.9500
C(35)-C(34)	1.365(8)
C(35)-H(35)	0.9500
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(33)-C(34)	1.380(8)
C(33)-C(32)	1.403(7)
C(33)-H(33)	0.9500
C(34)-H(34)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(2)-C(1)	1.407(6)
C(2)-C(3)	1.413(6)
C(2)-H(2)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800

C(42)-H(42C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(1)-B(1)	1.628(6)
C(40)-C(39)	1.551(7)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(31)-C(32)	1.374(7)
B(1)-H(103)	1.20(4)
C(3)-H(3)	0.9500
C(32)-H(32)	0.9500

N(1)-Fe(1)-P(1)	127.08(11)
N(1)-Fe(1)-P(2)	120.31(12)
P(1)-Fe(1)-P(2)	111.54(6)
N(1)-Fe(1)-B(1)	124.03(14)
P(1)-Fe(1)-B(1)	78.95(14)
P(2)-Fe(1)-B(1)	73.66(11)
N(1)-Fe(1)-H(103)	111.7(13)
P(1)-Fe(1)-H(103)	83.0(12)
P(2)-Fe(1)-H(103)	83.3(13)
B(1)-Fe(1)-H(103)	13.1(13)
C(19)-P(2)-C(28)	110.42(18)
C(19)-P(2)-C(25)	104.86(18)
C(28)-P(2)-C(25)	104.70(19)
C(19)-P(2)-Fe(1)	105.81(13)
C(28)-P(2)-Fe(1)	113.04(13)
C(25)-P(2)-Fe(1)	117.70(14)
C(7)-P(1)-C(13)	106.3(2)
C(7)-P(1)-C(16)	107.42(19)

C(13)-P(1)-C(16)	101.97(19)
C(7)-P(1)-Fe(1)	98.34(14)
C(13)-P(1)-Fe(1)	122.41(16)
C(16)-P(1)-Fe(1)	119.05(18)
N(2)-Si(3)-C(38)	112.67(19)
N(2)-Si(3)-C(37)	114.3(2)
C(38)-Si(3)-C(37)	109.4(2)
N(2)-Si(3)-C(39)	97.15(17)
C(38)-Si(3)-C(39)	114.2(2)
C(37)-Si(3)-C(39)	108.7(2)
N(2)-Si(2)-C(42)	114.6(2)
N(2)-Si(2)-C(41)	109.8(2)
C(42)-Si(2)-C(41)	109.6(2)
N(2)-Si(2)-C(40)	98.72(18)
C(42)-Si(2)-C(40)	110.7(2)
C(41)-Si(2)-C(40)	113.2(2)
N(1)-Si(1)-C(31)	115.76(18)
N(1)-Si(1)-H(101)	104.6(15)
C(31)-Si(1)-H(101)	104.8(16)
N(1)-Si(1)-H(102)	119(2)
C(31)-Si(1)-H(102)	96(2)
H(101)-Si(1)-H(102)	116(3)
N(1)-N(2)-Si(2)	119.5(2)
N(1)-N(2)-Si(3)	125.8(2)
Si(2)-N(2)-Si(3)	114.69(17)
C(19)-C(20)-C(21)	116.1(3)
C(19)-C(20)-B(1)	124.4(3)
C(21)-C(20)-B(1)	119.4(3)
C(9)-C(10)-C(11)	119.3(4)
C(9)-C(10)-H(10)	120.3
C(11)-C(10)-H(10)	120.3
C(14)-C(13)-C(15)	110.2(4)
C(14)-C(13)-P(1)	113.4(3)
C(15)-C(13)-P(1)	112.6(3)
C(14)-C(13)-H(13)	106.7
C(15)-C(13)-H(13)	106.7

P(1)-C(13)-H(13)	106.7
N(2)-N(1)-Si(1)	115.8(2)
N(2)-N(1)-Fe(1)	124.2(2)
Si(1)-N(1)-Fe(1)	119.91(16)
C(12)-C(7)-C(8)	121.0(3)
C(12)-C(7)-P(1)	119.4(3)
C(8)-C(7)-P(1)	119.5(3)
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(10)-C(9)-C(8)	124.0(3)
C(10)-C(9)-H(9)	118.0
C(8)-C(9)-H(9)	118.0
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(30)-C(28)-C(29)	110.8(3)
C(30)-C(28)-P(2)	108.5(3)
C(29)-C(28)-P(2)	120.8(3)
C(30)-C(28)-H(28)	105.2
C(29)-C(28)-H(28)	105.2
P(2)-C(28)-H(28)	105.2
C(22)-C(21)-C(20)	122.0(4)
C(22)-C(21)-H(21)	119.0
C(20)-C(21)-H(21)	119.0
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5

H(29B)-C(29)-H(29C)	109.5
C(23)-C(22)-C(21)	120.1(3)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(24)-C(19)-C(20)	121.2(3)
C(24)-C(19)-P(2)	120.3(3)
C(20)-C(19)-P(2)	118.4(3)
C(9)-C(8)-C(7)	115.3(3)
C(9)-C(8)-B(1)	116.0(3)
C(7)-C(8)-B(1)	128.6(3)
C(1)-C(6)-C(5)	123.0(5)
C(1)-C(6)-H(6)	118.5
C(5)-C(6)-H(6)	118.5
C(26)-C(25)-C(27)	112.3(3)
C(26)-C(25)-P(2)	115.3(3)
C(27)-C(25)-P(2)	111.5(3)
C(26)-C(25)-H(25)	105.6
C(27)-C(25)-H(25)	105.6
P(2)-C(25)-H(25)	105.6
Si(3)-C(38)-H(38A)	109.5
Si(3)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
Si(3)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(23)-C(24)-C(19)	120.9(4)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
C(7)-C(12)-C(11)	120.8(3)
C(7)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(22)-C(23)-C(24)	119.8(4)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(4)-C(5)-C(6)	118.4(5)
C(4)-C(5)-H(5)	120.8

C(6)-C(5)-H(5)	120.8
C(18)-C(16)-C(17)	108.9(4)
C(18)-C(16)-P(1)	111.4(3)
C(17)-C(16)-P(1)	109.6(3)
C(18)-C(16)-H(16)	109.0
C(17)-C(16)-H(16)	109.0
P(1)-C(16)-H(16)	109.0
Si(3)-C(37)-H(37A)	109.5
Si(3)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
Si(3)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(35)-C(36)-C(31)	120.9(5)
C(35)-C(36)-H(36)	119.5
C(31)-C(36)-H(36)	119.5
C(10)-C(11)-C(12)	119.4(4)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(3)-C(4)-C(5)	120.9(4)
C(3)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(34)-C(35)-C(36)	119.6(5)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(34)-C(33)-C(32)	119.2(5)
C(34)-C(33)-H(33)	120.4
C(32)-C(33)-H(33)	120.4
C(35)-C(34)-C(33)	120.9(5)
C(35)-C(34)-H(34)	119.5

C(33)-C(34)-H(34)	119.5
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(1)-C(2)-C(3)	121.4(5)
C(1)-C(2)-H(2)	119.3
C(3)-C(2)-H(2)	119.3
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(2)-C(42)-H(42A)	109.5
Si(2)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
Si(2)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(2)-C(41)-H(41A)	109.5
Si(2)-C(41)-H(41B)	109.5

H(41A)-C(41)-H(41B)	109.5
Si(2)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(6)-C(1)-C(2)	116.3(4)
C(6)-C(1)-B(1)	124.4(4)
C(2)-C(1)-B(1)	119.3(4)
C(39)-C(40)-Si(2)	107.6(3)
C(39)-C(40)-H(40A)	110.2
Si(2)-C(40)-H(40A)	110.2
C(39)-C(40)-H(40B)	110.2
Si(2)-C(40)-H(40B)	110.2
H(40A)-C(40)-H(40B)	108.5
C(40)-C(39)-Si(3)	106.7(3)
C(40)-C(39)-H(39A)	110.4
Si(3)-C(39)-H(39A)	110.4
C(40)-C(39)-H(39B)	110.4
Si(3)-C(39)-H(39B)	110.4
H(39A)-C(39)-H(39B)	108.6
C(32)-C(31)-C(36)	118.0(4)
C(32)-C(31)-Si(1)	121.7(3)
C(36)-C(31)-Si(1)	120.4(4)
C(8)-B(1)-C(1)	113.2(3)
C(8)-B(1)-C(20)	109.7(3)
C(1)-B(1)-C(20)	111.6(3)
C(8)-B(1)-Fe(1)	90.8(2)
C(1)-B(1)-Fe(1)	128.0(3)
C(20)-B(1)-Fe(1)	101.1(2)
C(8)-B(1)-H(103)	106.7(18)
C(1)-B(1)-H(103)	110(2)
C(20)-B(1)-H(103)	105.4(19)
Fe(1)-B(1)-H(103)	19.5(19)
C(4)-C(3)-C(2)	119.9(5)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(31)-C(32)-C(33)	121.4(5)

C(31)-C(32)-H(32)	119.3
C(33)-C(32)-H(32)	119.3

Symmetry transformations used to generate equivalent atoms:

Table S25. Crystal data and structure refinement for **8**.

Identification code	**8**	
Empirical formula	C56 H67 B Fe N2 O2 P2 Si2	
Formula weight	984.90	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.2122(7) Å	α = 88.967(3)°.
	b = 13.2685(8) Å	β = 80.813(3)°.
	c = 16.1433(12) Å	γ = 84.376(2)°.
Volume	2569.8(3) $Å^3$	
Z	2	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.446 mm^{-1}	
F(000)	1044	
Crystal size	0.3 x 0.22 x 0.2 mm^3	
Theta range for data collection	1.96 to 44.14°.	
Index ranges	-23<=h<=23, -25<=k<=25, -31<=l<=31	
Reflections collected	310067	
Independent reflections	40098 [R(int) = 0.0425]	
Completeness to theta = 44.14°	99.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	40098 / 585 / 627	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.1070	
R indices (all data)	R1 = 0.0607, wR2 = 0.1162	
Largest diff. peak and hole	1.304 and -0.835 e.$Å^{-3}$	

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3204(1)	1775(1)	1982(1)	10(1)
P(2)	1734(1)	52(1)	2541(1)	10(1)
P(1)	5031(1)	1497(1)	2400(1)	11(1)
Si(2)	2609(1)	269(1)	673(1)	11(1)
Si(1)	2586(1)	3472(1)	599(1)	17(1)
C(7)	4878(1)	2222(1)	3368(1)	11(1)
C(8)	3857(1)	2218(1)	3930(1)	10(1)
C(6)	1229(1)	1724(1)	5130(1)	16(1)
C(37)	545(1)	877(1)	2998(1)	14(1)
N(2)	2472(1)	533(1)	1747(1)	11(1)
N(1)	2912(1)	3098(1)	1548(1)	17(1)
C(1)	1674(1)	2134(1)	4359(1)	12(1)
C(9)	3785(1)	2786(1)	4669(1)	13(1)
C(28)	3791(1)	-1014(1)	4609(1)	15(1)
C(30)	2639(1)	-1354(1)	3593(1)	13(1)
C(42)	-47(1)	599(1)	3771(1)	18(1)
C(25)	2502(1)	-320(1)	3392(1)	11(1)
C(3)	295(1)	3601(1)	4674(1)	24(1)
C(27)	3619(1)	15(1)	4431(1)	13(1)
C(40)	-1360(1)	2057(1)	3716(1)	28(1)
C(19)	5586(1)	219(1)	2641(1)	13(1)
C(48)	1271(1)	5(1)	337(1)	18(1)
C(13)	6186(1)	2014(1)	1718(1)	13(1)
C(26)	2974(1)	409(1)	3829(1)	11(1)
C(41)	-1003(1)	1187(1)	4126(1)	24(1)
C(38)	182(1)	1745(1)	2584(1)	18(1)
C(31)	1142(1)	-1042(1)	2201(1)	14(1)
C(5)	352(1)	2244(1)	5671(1)	24(1)
C(2)	1172(1)	3081(1)	4144(1)	17(1)
C(12)	5722(1)	2800(1)	3525(1)	14(1)
C(29)	3285(1)	-1702(1)	4195(1)	15(1)

C(11)	5595(1)	3382(1)	4250(1)	15(1)
C(23)	5651(1)	-1582(1)	2387(1)	24(1)
C(20)	6349(1)	19(1)	3199(1)	19(1)
C(18)	7296(1)	1606(1)	1650(1)	19(1)
C(39)	-777(1)	2335(1)	2951(1)	26(1)
C(36)	1852(1)	-1876(1)	1857(1)	17(1)
C(10)	4625(1)	3359(1)	4832(1)	15(1)
C(24)	5238(1)	-589(1)	2240(1)	17(1)
C(4)	-110(1)	3185(1)	5443(1)	28(1)
C(33)	-415(1)	-1817(1)	1809(1)	26(1)
C(35)	1433(1)	-2669(1)	1498(1)	23(1)
C(45)	2198(1)	2338(1)	80(1)	20(1)
C(32)	-1(1)	-1020(1)	2178(1)	19(1)
C(14)	5926(1)	2873(1)	1246(1)	20(1)
C(16)	7870(1)	2934(1)	684(1)	25(1)
C(34)	299(1)	-2631(1)	1465(1)	28(1)
C(47)	3709(1)	-792(1)	339(1)	18(1)
C(17)	8132(1)	2070(1)	1134(1)	22(1)
C(46)	3082(1)	1412(1)	74(1)	16(1)
C(44)	3808(1)	3935(1)	-111(1)	30(1)
C(22)	6410(1)	-1775(1)	2940(1)	25(1)
C(21)	6756(1)	-975(1)	3344(1)	24(1)
C(15)	6767(1)	3331(1)	734(1)	27(1)
O(1)	3108(1)	5420(1)	2096(1)	43(1)
C(49)	2383(1)	5497(1)	2881(1)	38(1)
C(52)	4238(1)	5440(2)	2233(1)	52(1)
C(50)	3100(1)	5320(1)	3558(1)	43(1)
C(51)	4216(1)	5684(2)	3146(1)	32(1)
C(51A)	4145(8)	5178(15)	3068(5)	51(4)
O(2)	2942(1)	4429(1)	6652(1)	35(1)
C(54)	1629(1)	4667(1)	7877(1)	43(1)
C(55)	1005(1)	4611(1)	7127(1)	36(1)
C(53)	2802(1)	4809(1)	7483(1)	39(1)
C(56)	1914(1)	4722(2)	6373(1)	28(1)
C(56A)	1850(8)	4300(20)	6420(10)	56(5)
B(1)	2784(1)	1639(1)	3756(1)	11(1)

C(43)	1393(1)	4489(1)	676(1)	32(1)

Table S27. Bond lengths [Å] and angles [°] for **8**.

Fe(1)-N(1)	1.8996(7)
Fe(1)-N(2)	2.0194(6)
Fe(1)-P(1)	2.4248(2)
Fe(1)-B(1)	2.8335(8)
Fe(1)-H(101)	1.813(12)
P(2)-N(2)	1.6064(6)
P(2)-C(37)	1.7964(7)
P(2)-C(31)	1.8139(7)
P(2)-C(25)	1.8177(7)
P(1)-C(19)	1.8221(7)
P(1)-C(7)	1.8240(7)
P(1)-C(13)	1.8277(7)
Si(2)-N(2)	1.7529(6)
Si(2)-C(48)	1.8682(7)
Si(2)-C(47)	1.8715(8)
Si(2)-C(46)	1.8734(8)
Si(1)-N(1)	1.6974(7)
Si(1)-C(45)	1.8710(8)
Si(1)-C(43)	1.8769(10)
Si(1)-C(44)	1.8783(10)
C(7)-C(12)	1.4005(9)
C(7)-C(8)	1.4208(9)
C(8)-C(9)	1.4095(9)
C(8)-B(1)	1.6461(9)
C(6)-C(1)	1.3991(10)
C(6)-C(5)	1.4011(11)
C(6)-H(6)	0.9500
C(37)-C(38)	1.3918(11)
C(37)-C(42)	1.4014(11)
N(2)-N(1)	3.4974(9)
N(1)-H(102)	0.68(2)
C(1)-C(2)	1.4052(10)
C(1)-B(1)	1.6262(10)
C(9)-C(10)	1.3940(10)

C(9)-H(9)	0.9500
C(28)-C(29)	1.3879(10)
C(28)-C(27)	1.3922(10)
C(28)-H(28)	0.9500
C(30)-C(29)	1.3911(10)
C(30)-C(25)	1.4045(9)
C(30)-H(30)	0.9500
C(42)-C(41)	1.3869(11)
C(42)-H(42)	0.9500
C(25)-C(26)	1.4240(9)
C(3)-C(4)	1.3871(15)
C(3)-C(2)	1.3929(11)
C(3)-H(3)	0.9500
C(27)-C(26)	1.4093(9)
C(27)-H(27)	0.9500
C(40)-C(39)	1.3866(15)
C(40)-C(41)	1.3883(15)
C(40)-H(40)	0.9500
C(19)-C(24)	1.3969(10)
C(19)-C(20)	1.4011(10)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(13)-C(14)	1.3973(11)
C(13)-C(18)	1.3985(10)
C(26)-B(1)	1.6304(10)
C(41)-H(41)	0.9500
C(38)-C(39)	1.3969(11)
C(38)-H(38)	0.9500
C(31)-C(32)	1.4004(10)
C(31)-C(36)	1.4012(11)
C(5)-C(4)	1.3867(15)
C(5)-H(5)	0.9500
C(2)-H(2)	0.9500
C(12)-C(11)	1.3930(10)
C(12)-H(12)	0.9500

C(29)-H(29)	0.9500
C(11)-C(10)	1.3922(10)
C(11)-H(11)	0.9500
C(23)-C(22)	1.3895(14)
C(23)-C(24)	1.3932(11)
C(23)-H(23)	0.9500
C(20)-C(21)	1.3926(12)
C(20)-H(20)	0.9500
C(18)-C(17)	1.3965(11)
C(18)-H(18)	0.9500
C(39)-H(39)	0.9500
C(36)-C(35)	1.3892(11)
C(36)-H(36)	0.9500
C(10)-H(10)	0.9500
C(24)-H(24)	0.9500
C(4)-H(4)	0.9500
C(33)-C(34)	1.3848(15)
C(33)-C(32)	1.3962(11)
C(33)-H(33)	0.9500
C(35)-C(34)	1.3910(15)
C(35)-H(35)	0.9500
C(45)-C(46)	1.5542(11)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(32)-H(32)	0.9500
C(14)-C(15)	1.3936(12)
C(14)-H(14)	0.9500
C(16)-C(17)	1.3842(14)
C(16)-C(15)	1.3880(14)
C(16)-H(16)	0.9500
C(34)-H(34)	0.9500
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(17)-H(17)	0.9500
C(46)-H(46A)	0.9900

C(46)-H(46B)	0.9900
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(22)-C(21)	1.3893(14)
C(22)-H(22)	0.9500
C(21)-H(21)	0.9500
C(15)-H(15)	0.9500
O(1)-C(49)	1.4245(16)
O(1)-C(52)	1.4343(16)
C(49)-C(50)	1.5079(19)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(52)-C(51)	1.510(2)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(50)-C(51)	1.5364(19)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
O(2)-C(56)	1.4174(19)
O(2)-C(53)	1.4198(15)
C(54)-C(53)	1.4995(16)
C(54)-C(55)	1.5363(17)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.527(2)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
B(1)-H(101)	1.183(12)
C(43)-H(43A)	0.9800

C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800

N(1)-Fe(1)-N(2)	126.33(3)
N(1)-Fe(1)-P(1)	112.75(2)
N(2)-Fe(1)-P(1)	116.926(17)
N(1)-Fe(1)-B(1)	114.56(3)
N(2)-Fe(1)-B(1)	96.97(2)
P(1)-Fe(1)-B(1)	75.004(15)
N(1)-Fe(1)-H(101)	104.2(4)
N(2)-Fe(1)-H(101)	95.8(4)
P(1)-Fe(1)-H(101)	89.1(4)
B(1)-Fe(1)-H(101)	15.2(4)
N(2)-P(2)-C(37)	113.77(3)
N(2)-P(2)-C(31)	109.07(3)
C(37)-P(2)-C(31)	104.29(3)
N(2)-P(2)-C(25)	113.88(3)
C(37)-P(2)-C(25)	106.10(3)
C(31)-P(2)-C(25)	109.23(3)
C(19)-P(1)-C(7)	106.44(3)
C(19)-P(1)-C(13)	104.18(3)
C(7)-P(1)-C(13)	104.21(3)
C(19)-P(1)-Fe(1)	119.78(2)
C(7)-P(1)-Fe(1)	103.56(2)
C(13)-P(1)-Fe(1)	117.18(2)
N(2)-Si(2)-C(48)	113.27(3)
N(2)-Si(2)-C(47)	112.32(3)
C(48)-Si(2)-C(47)	109.88(4)
N(2)-Si(2)-C(46)	108.07(3)
C(48)-Si(2)-C(46)	106.92(4)
C(47)-Si(2)-C(46)	105.96(4)
N(1)-Si(1)-C(45)	107.72(4)
N(1)-Si(1)-C(43)	113.04(5)
C(45)-Si(1)-C(43)	108.78(4)
N(1)-Si(1)-C(44)	112.01(4)
C(45)-Si(1)-C(44)	106.73(5)

C(43)-Si(1)-C(44)	108.33(5)
C(12)-C(7)-C(8)	121.61(6)
C(12)-C(7)-P(1)	120.61(5)
C(8)-C(7)-P(1)	117.70(5)
C(9)-C(8)-C(7)	115.35(6)
C(9)-C(8)-B(1)	119.91(6)
C(7)-C(8)-B(1)	124.72(5)
C(1)-C(6)-C(5)	121.70(8)
C(1)-C(6)-H(6)	119.1
C(5)-C(6)-H(6)	119.1
C(38)-C(37)-C(42)	120.36(7)
C(38)-C(37)-P(2)	121.44(6)
C(42)-C(37)-P(2)	118.13(6)
P(2)-N(2)-Si(2)	130.62(4)
P(2)-N(2)-Fe(1)	115.76(3)
Si(2)-N(2)-Fe(1)	113.00(3)
P(2)-N(2)-N(1)	124.28(3)
Si(2)-N(2)-N(1)	97.25(3)
Fe(1)-N(2)-N(1)	25.950(15)
Si(1)-N(1)-Fe(1)	130.10(4)
Si(1)-N(1)-N(2)	106.15(3)
Fe(1)-N(1)-N(2)	27.722(15)
Si(1)-N(1)-H(102)	112.5(18)
Fe(1)-N(1)-H(102)	117.4(18)
N(2)-N(1)-H(102)	138.6(18)
C(6)-C(1)-C(2)	116.52(6)
C(6)-C(1)-B(1)	124.20(6)
C(2)-C(1)-B(1)	119.02(6)
C(10)-C(9)-C(8)	123.27(6)
C(10)-C(9)-H(9)	118.4
C(8)-C(9)-H(9)	118.4
C(29)-C(28)-C(27)	119.47(6)
C(29)-C(28)-H(28)	120.3
C(27)-C(28)-H(28)	120.3
C(29)-C(30)-C(25)	121.08(6)
C(29)-C(30)-H(30)	119.5

C(25)-C(30)-H(30)	119.5
C(41)-C(42)-C(37)	120.05(8)
C(41)-C(42)-H(42)	120.0
C(37)-C(42)-H(42)	120.0
C(30)-C(25)-C(26)	120.82(6)
C(30)-C(25)-P(2)	117.91(5)
C(26)-C(25)-P(2)	121.25(5)
C(4)-C(3)-C(2)	119.88(8)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(28)-C(27)-C(26)	123.51(6)
C(28)-C(27)-H(27)	118.2
C(26)-C(27)-H(27)	118.2
C(39)-C(40)-C(41)	120.54(8)
C(39)-C(40)-H(40)	119.7
C(41)-C(40)-H(40)	119.7
C(24)-C(19)-C(20)	119.14(7)
C(24)-C(19)-P(1)	117.98(5)
C(20)-C(19)-P(1)	122.88(6)
Si(2)-C(48)-H(48A)	109.5
Si(2)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
Si(2)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(14)-C(13)-C(18)	119.09(7)
C(14)-C(13)-P(1)	117.06(5)
C(18)-C(13)-P(1)	123.85(6)
C(27)-C(26)-C(25)	115.65(6)
C(27)-C(26)-B(1)	116.72(5)
C(25)-C(26)-B(1)	127.49(6)
C(42)-C(41)-C(40)	119.60(8)
C(42)-C(41)-H(41)	120.2
C(40)-C(41)-H(41)	120.2
C(37)-C(38)-C(39)	119.02(8)
C(37)-C(38)-H(38)	120.5

C(39)-C(38)-H(38)	120.5
C(32)-C(31)-C(36)	118.87(7)
C(32)-C(31)-P(2)	121.11(6)
C(36)-C(31)-P(2)	119.53(5)
C(4)-C(5)-C(6)	120.16(8)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(3)-C(2)-C(1)	122.22(8)
C(3)-C(2)-H(2)	118.9
C(1)-C(2)-H(2)	118.9
C(11)-C(12)-C(7)	120.88(6)
C(11)-C(12)-H(12)	119.6
C(7)-C(12)-H(12)	119.6
C(28)-C(29)-C(30)	119.37(6)
C(28)-C(29)-H(29)	120.3
C(30)-C(29)-H(29)	120.3
C(10)-C(11)-C(12)	118.94(6)
C(10)-C(11)-H(11)	120.5
C(12)-C(11)-H(11)	120.5
C(22)-C(23)-C(24)	120.02(8)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(21)-C(20)-C(19)	119.96(8)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(17)-C(18)-C(13)	120.05(8)
C(17)-C(18)-H(18)	120.0
C(13)-C(18)-H(18)	120.0
C(40)-C(39)-C(38)	120.43(9)
C(40)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(35)-C(36)-C(31)	120.83(8)
C(35)-C(36)-H(36)	119.6
C(31)-C(36)-H(36)	119.6
C(11)-C(10)-C(9)	119.85(6)
C(11)-C(10)-H(10)	120.1

C(9)-C(10)-H(10)	120.1
C(23)-C(24)-C(19)	120.55(7)
C(23)-C(24)-H(24)	119.7
C(19)-C(24)-H(24)	119.7
C(5)-C(4)-C(3)	119.50(7)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(34)-C(33)-C(32)	120.45(8)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(36)-C(35)-C(34)	119.77(8)
C(36)-C(35)-H(35)	120.1
C(34)-C(35)-H(35)	120.1
C(46)-C(45)-Si(1)	112.61(5)
C(46)-C(45)-H(45A)	109.1
Si(1)-C(45)-H(45A)	109.1
C(46)-C(45)-H(45B)	109.1
Si(1)-C(45)-H(45B)	109.1
H(45A)-C(45)-H(45B)	107.8
C(33)-C(32)-C(31)	119.98(8)
C(33)-C(32)-H(32)	120.0
C(31)-C(32)-H(32)	120.0
C(15)-C(14)-C(13)	120.37(8)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(17)-C(16)-C(15)	119.83(8)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(33)-C(34)-C(35)	120.07(8)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
Si(2)-C(47)-H(47A)	109.5
Si(2)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
Si(2)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5

H(47B)-C(47)-H(47C)	109.5
C(16)-C(17)-C(18)	120.44(8)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(45)-C(46)-Si(2)	116.24(6)
C(45)-C(46)-H(46A)	108.2
Si(2)-C(46)-H(46A)	108.2
C(45)-C(46)-H(46B)	108.2
Si(2)-C(46)-H(46B)	108.2
H(46A)-C(46)-H(46B)	107.4
Si(1)-C(44)-H(44A)	109.5
Si(1)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
Si(1)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(21)-C(22)-C(23)	119.78(8)
C(21)-C(22)-H(22)	120.1
C(23)-C(22)-H(22)	120.1
C(22)-C(21)-C(20)	120.55(8)
C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(16)-C(15)-C(14)	120.19(9)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(49)-O(1)-C(52)	109.39(10)
O(1)-C(49)-C(50)	107.17(10)
O(1)-C(49)-H(49A)	110.3
C(50)-C(49)-H(49A)	110.3
O(1)-C(49)-H(49B)	110.3
C(50)-C(49)-H(49B)	110.3
H(49A)-C(49)-H(49B)	108.5
O(1)-C(52)-C(51)	107.93(10)
O(1)-C(52)-H(52A)	110.1
C(51)-C(52)-H(52A)	110.1
O(1)-C(52)-H(52B)	110.1

C(51)-C(52)-H(52B)	110.1
H(52A)-C(52)-H(52B)	108.4
C(49)-C(50)-C(51)	102.94(10)
C(49)-C(50)-H(50A)	111.2
C(51)-C(50)-H(50A)	111.2
C(49)-C(50)-H(50B)	111.2
C(51)-C(50)-H(50B)	111.2
H(50A)-C(50)-H(50B)	109.1
C(52)-C(51)-C(50)	102.10(12)
C(52)-C(51)-H(51A)	111.4
C(50)-C(51)-H(51A)	111.4
C(52)-C(51)-H(51B)	111.3
C(50)-C(51)-H(51B)	111.3
H(51A)-C(51)-H(51B)	109.2
C(56)-O(2)-C(53)	104.79(12)
C(53)-C(54)-C(55)	104.15(10)
C(53)-C(54)-H(54A)	110.9
C(55)-C(54)-H(54A)	110.9
C(53)-C(54)-H(54B)	110.9
C(55)-C(54)-H(54B)	110.9
H(54A)-C(54)-H(54B)	108.9
C(56)-C(55)-C(54)	103.04(11)
C(56)-C(55)-H(55A)	111.2
C(54)-C(55)-H(55A)	111.2
C(56)-C(55)-H(55B)	111.2
C(54)-C(55)-H(55B)	111.2
H(55A)-C(55)-H(55B)	109.1
O(2)-C(53)-C(54)	106.73(9)
O(2)-C(53)-H(53A)	110.4
C(54)-C(53)-H(53A)	110.4
O(2)-C(53)-H(53B)	110.4
C(54)-C(53)-H(53B)	110.4
H(53A)-C(53)-H(53B)	108.6
O(2)-C(56)-C(55)	106.30(12)
O(2)-C(56)-H(56A)	110.5
C(55)-C(56)-H(56A)	110.5

O(2)-C(56)-H(56B)	110.5
C(55)-C(56)-H(56B)	110.5
H(56A)-C(56)-H(56B)	108.7
C(1)-B(1)-C(26)	113.53(5)
C(1)-B(1)-C(8)	108.64(5)
C(26)-B(1)-C(8)	113.76(5)
C(1)-B(1)-Fe(1)	125.67(4)
C(26)-B(1)-Fe(1)	97.49(4)
C(8)-B(1)-Fe(1)	96.70(4)
C(1)-B(1)-H(101)	102.0(6)
C(26)-B(1)-H(101)	109.9(6)
C(8)-B(1)-H(101)	108.2(6)
Fe(1)-B(1)-H(101)	23.7(6)
Si(1)-C(43)-H(43A)	109.5
Si(1)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
Si(1)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5

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