Ground State Singlet L_3Fe-(μ-N)-FeL_3 and $L_3Fe(NR)$ Complexes Featuring Pseudotetrahedral Fe(II) Centers

Steven D. Brown and Jonas C. Peters

Division of Chemistry and Chemical Engineering, Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, California 91125

Supporting Information

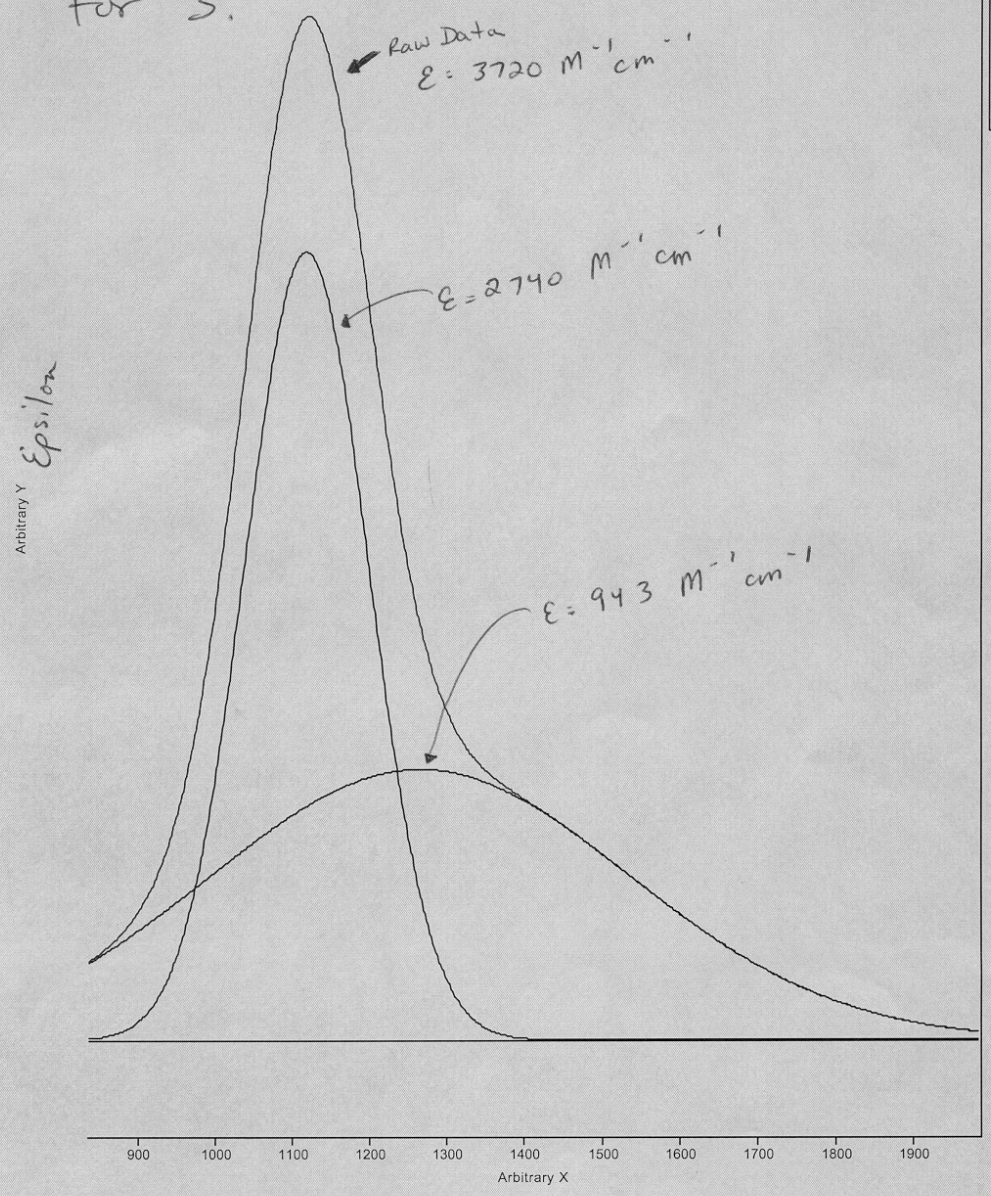
The synthesis and characterization of $\{[PhBP_3]Fe(MeCN)_3\}\{PF_6\}$ was originally executed by Duimstra, J. and Peters, J. C. but never reported. Briefly, $[^nBu_4N][PhBP_3]$[1] (0.584 g, 0.63 mmol) was stirred with $FeCl_2{\cdot}xH_2O$ (0.213 g, 1.07 mmol if x = 4) in 5 mL of acetonitrile. After stirring for 45 minutes at room temperature the reaction was cooled to -30 °C for 30 minutes and the resulting red solids were isolated on a sintered glass frit and washed with fresh acetonitrile (2 x 10 mL). Drying under reduced pressure yielded 0.510 g (84%) of $\{[PhBP_3]Fe(CH_3CN)_3\}\{[FeCl_4]_{0.5}\}$ as a red powder. ^{1}H NMR (CD_3CN, 300 MHz): δ 7.5- 7.0 (m, 35H); 1.95 (s, 9H); 1.27 (br s, 6H). $^{31}P\{^1H\}$ NMR (CD_3CN, 121.4 MHz): δ 43.8 (s).

A partially dissolved solution of $[K][PF_6]$ (0.824 g, 4.48 mmol) in acetonitrile (35 mL) was added to a benzene solution (15 mL) of $\{[PhBP_3]Fe(CH_3CN)_3\}\{[FeCl_4]_{0.5}\}$ (2.38 g, 2.24 mmol). The resulting red/violet solution was allowed to stir overnight. After this time the crude reaction was filtered over Celite and the solvent was removed under reduced pressure. The resulting solids were redissolved in CH_2Cl_2 (25 mL) and filtered to remove excess $[K][PF_6]$. Crystalline material was obtained from vapor diffusion of Et_2O into a CH_2Cl_2 solution. Two crops of crystals yielded 1.52 g (67%) of $\{[PhBP_3]Fe(MeCN)_3\}\{PF_6\}$. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.1- 7.6 (m, 35H); 2.17 (s, 9H); 1.40 (br s, 6H). $^{31}P\{^1H\}$ NMR ($CDCl_3$, 121.4 MHz): δ 45.0 (s); -142.9 (septet, J = 709 Hz). $^{19}F\{^1H\}$ NMR ($CDCl_3$, 282.1 MHz): δ 73.2 (d, J = 709 Hz). Anal. Calcd. for $C_{51}H_{50}BF_6FeN_3P_4$: C, 60.98; H, 4.99; N, 4.16. Found: C, 60.37; H, 5.06; N, 4.00.

---

[1] Thomas, J. C.; Peters, J. C. *Inorg. Synth.* **2004,** *34,* 8.

Grams Curve Fitting Data For The NIR data from 850 to 2000 nm for 3.



sdb.spc

Curve Fit

Peaks

Fit Peak Report

Raw Data File: C:\My Documents\sdb.spc

Thermo Galactic GRAMS v. 3.2

Peak #1: Gaussian
Area: 546998.8

	Center	Height	Width
Value	1119.739	2738.12	187.7092
Fixed	NO	NO	NO
Lo Limit	None	0	1.111
Hi Limit	None	None	None
Std. Error	.1132226	4.045055	.3346712

Peak #2: Gaussian
Area: 602326.4

	Center	Height	Width
Value	1265.941	942.8226	639.0497
Fixed	NO	NO	NO
Lo Limit	None	0	1.111
Hi Limit	None	None	None
Std. Error	.9268096	3.717261	3.071308

Baseline: Offset

	Offset
Value	108.138
Fixed	NO
Lo Limit	None
Hi Limit	None
Std. Error	3.297936

Fit Statistics Summary

Solution has CONVERGED.
Total data points: 1035 Fit region: 836.7829 to 1985.557
Fitted equations: 3
Total parameters: 7 # Fitted: 7 # Fixed: 0
Reduced Chi²: 1.381188 RMS Noise: 24.64199
Correlation (R^2): .9992013
Standard Error: 28.86214

Figure 1. Core labeled drawing of $\{[PhBP_3]FeN_3\}_2$, (**2**). Hydrogen atoms and a benzene solvent molecule have been removed for clarity.

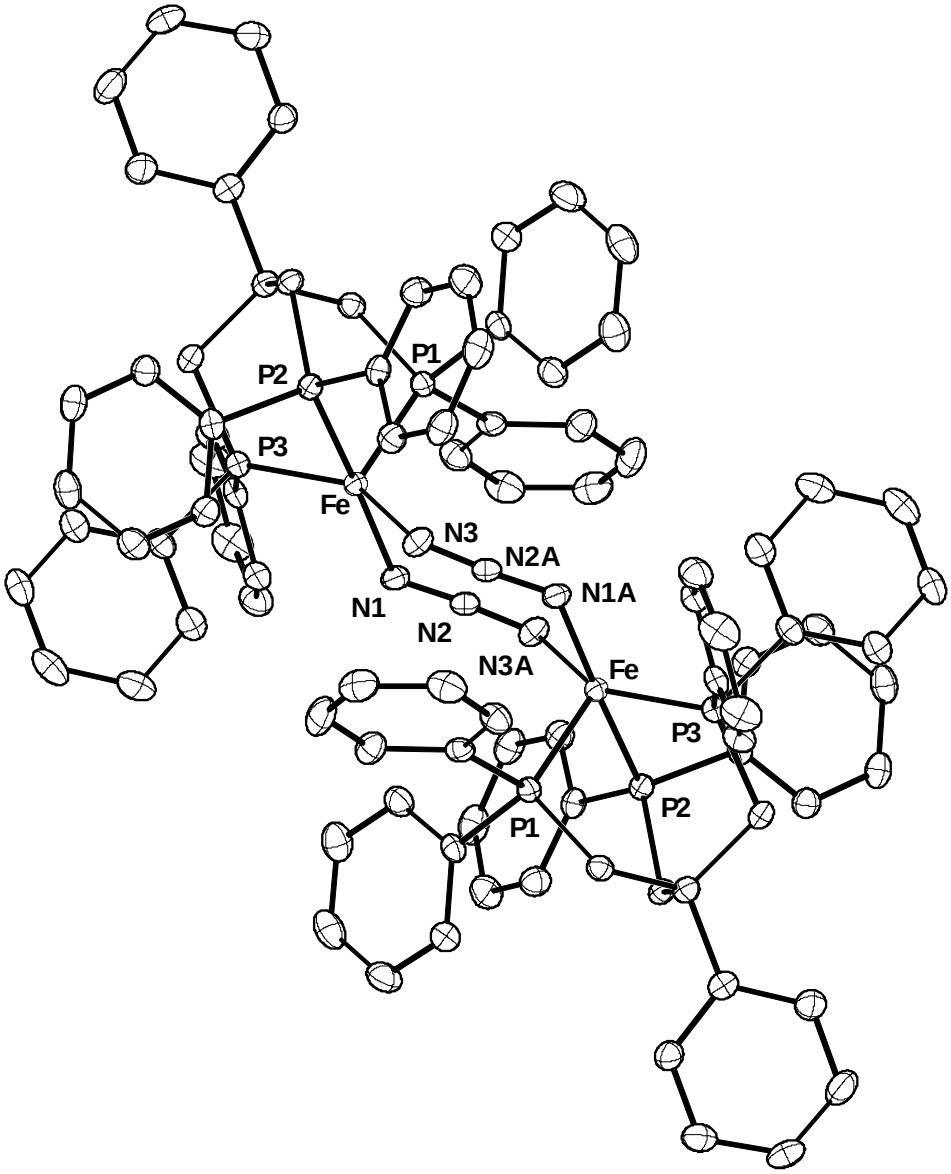


Figure 2. Core labeled drawing of $[([PhBP_3]Fe)_2N][Na(THF_5)]$, (**3**) showing the more populated position of the nitride ligand. Hydrogen atoms and a molecule of THF solvent have been removed for clarity.

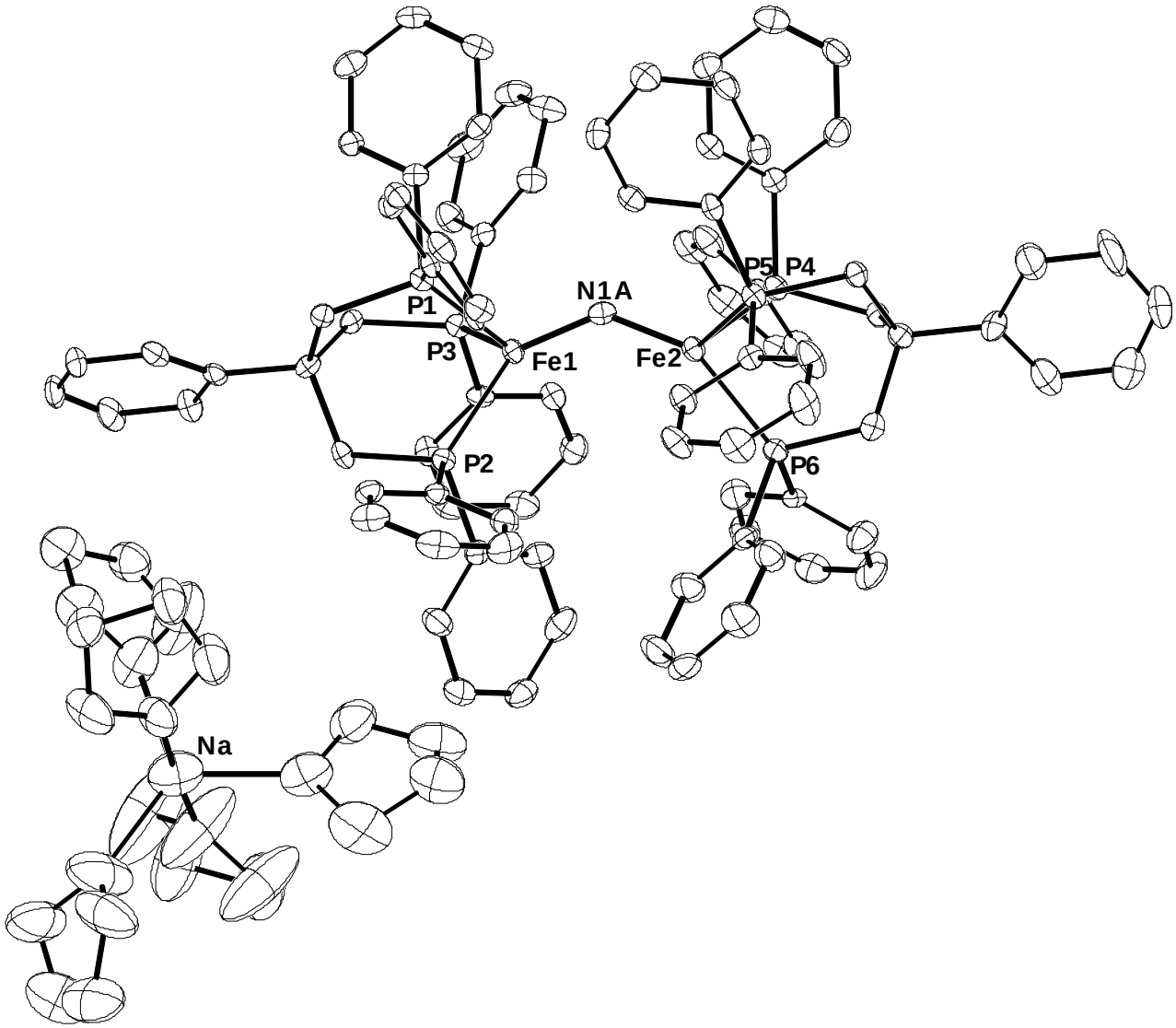


Figure 3. Core labeled drawing of {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}, (**4**). Hydrogen atoms and a molecule of THF solvent have been removed for clarity.

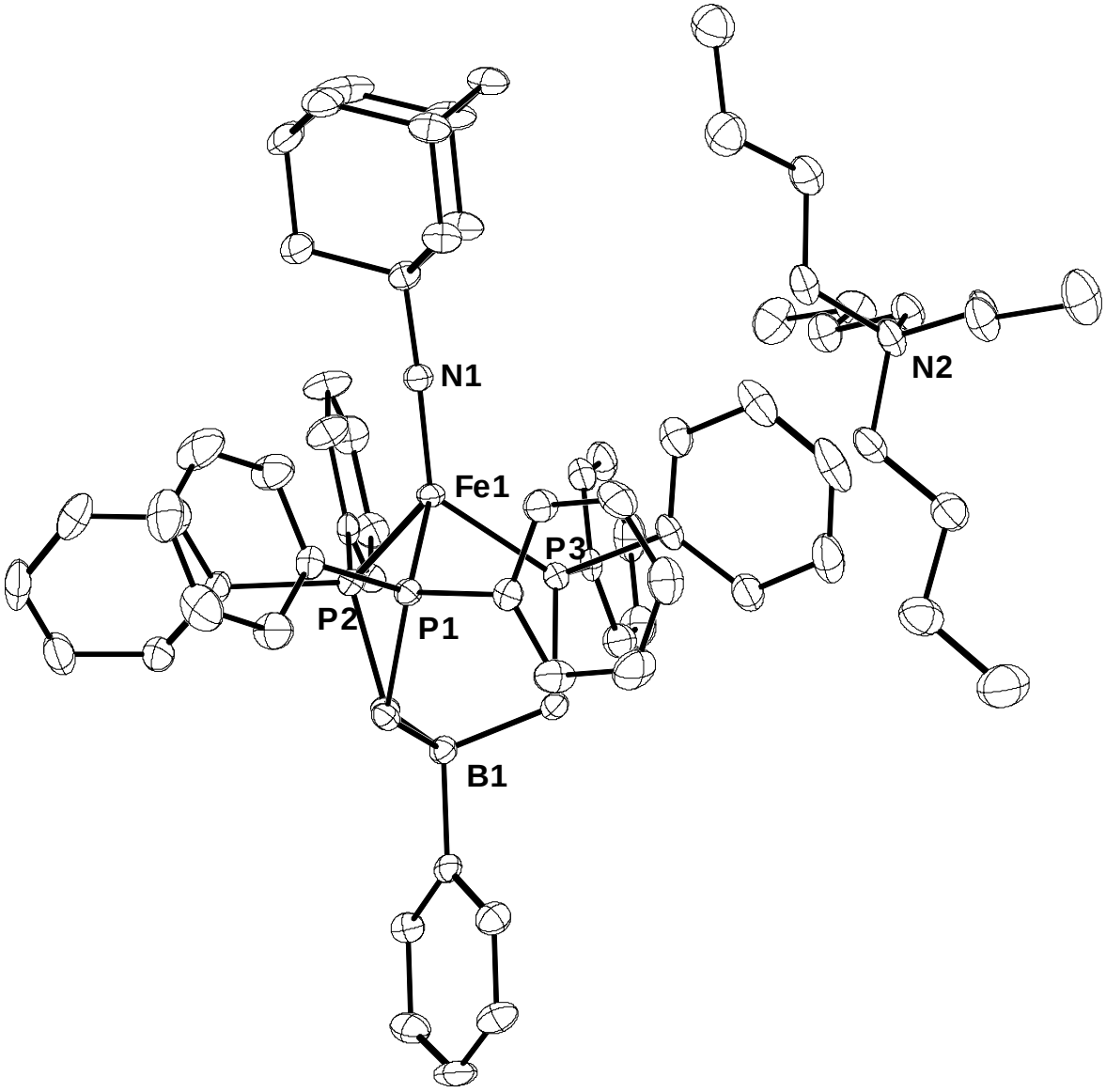


Figure 4. Core labeled drawing of $[PhBP_3]Fe{\equiv}N(1\text{-}Ad)$, (**5**). Hydrogen atoms have been removed for clarity.

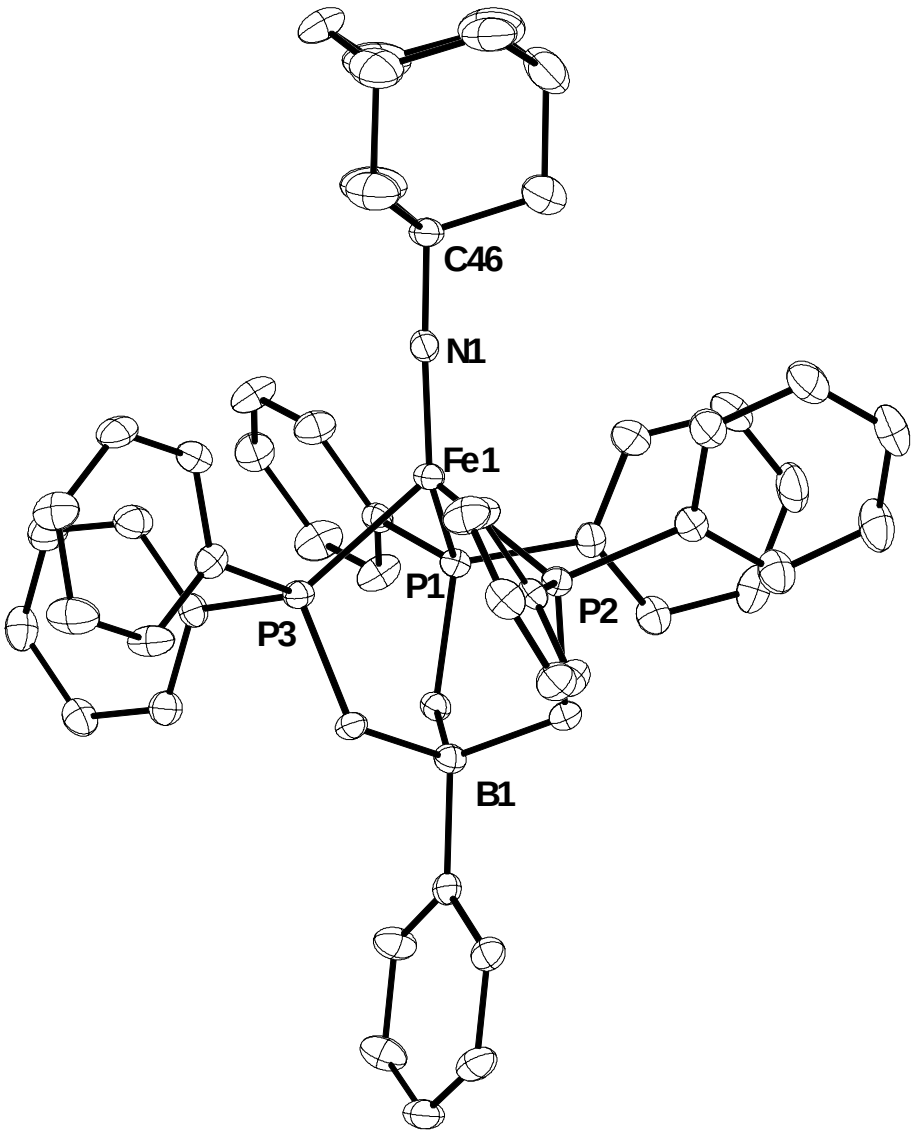


Table 1. Crystal data and structure refinement for $\{[PhBP_3]FeN_3\}_2 \cdot C_6D_6$, (**2**).

Identification code	sdb31	
Empirical formula	$C_{51}\ H_{47}\ B\ Fe\ N_3\ P_3$	
Formula weight	861.49 (monomer + one benzene)	
Temperature	96(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.0738(10) Å	α= 118.2270(10)°.
	b = 14.2209(11) Å	β= 95.2290(10)°.
	c = 14.6878(12) Å	γ = 111.0900(10)°.
Volume	2128.4(3) $Å^3$	
Z	2	
Density (calculated)	1.344 Mg/m^3	
Absorption coefficient	0.508 mm^{-1}	
F(000)	900	
Crystal size	0.23 x 0.27 x 0.33 mm^3	
Theta range for data collection	1.66 to 28.59°.	
Index ranges	-17<=h<=17, -18<=k<=18, -19<=l<=19	
Reflections collected	44993	
Independent reflections	9998 [R(int) = 0.0528]	
Completeness to theta = 28.59°	91.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9998 / 0 / 532	
Goodness-of-fit on F^2	1.809	
Final R indices [I>2sigma(I)]	R1 = 0.0396, wR2 = 0.0858	
R indices (all data)	R1 = 0.0562, wR2 = 0.0893	
Largest diff. peak and hole	0.605 and -0.482 $e.Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\{[PhBP_3]FeN_3\}_2 \cdot C_6D_6$, (**2**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe	3682(1)	5131(1)	3773(1)	15(1)
P(1)	2050(1)	3859(1)	3639(1)	15(1)
P(2)	3164(1)	4145(1)	1962(1)	15(1)
P(3)	2959(1)	6328(1)	3806(1)	16(1)
N(1)	4275(1)	6062(1)	5410(1)	19(1)
N(2)	4656(1)	5650(1)	5801(1)	16(1)
N(3)	4963(1)	4732(1)	3780(1)	21(1)
B(1)	974(2)	4207(2)	2072(2)	17(1)
C(1)	-297(2)	3697(2)	1252(2)	18(1)
C(2)	-1226(2)	2594(2)	914(2)	23(1)
C(3)	-2287(2)	2118(2)	173(2)	26(1)
C(4)	-2463(2)	2718(2)	-285(2)	27(1)
C(5)	-1575(2)	3797(2)	13(2)	33(1)
C(6)	-516(2)	4276(2)	771(2)	28(1)
C(7)	826(2)	3930(2)	3052(2)	17(1)
C(8)	1629(2)	3498(2)	1300(1)	17(1)
C(9)	1769(2)	5672(2)	2616(2)	18(1)
C(10)	1942(2)	4020(2)	4940(2)	18(1)
C(11)	1822(2)	5000(2)	5709(2)	24(1)
C(12)	1757(2)	5168(2)	6707(2)	29(1)
C(13)	1809(2)	4364(2)	6959(2)	31(1)
C(14)	1929(2)	3393(2)	6215(2)	32(1)
C(15)	2000(2)	3221(2)	5213(2)	24(1)
C(16)	1797(2)	2297(2)	2819(2)	17(1)
C(17)	2693(2)	2034(2)	3002(2)	23(1)
C(18)	2536(2)	863(2)	2445(2)	29(1)
C(19)	1491(2)	-59(2)	1682(2)	30(1)
C(20)	599(2)	187(2)	1470(2)	30(1)
C(21)	748(2)	1356(2)	2040(2)	23(1)
C(22)	3597(2)	2948(2)	1270(2)	17(1)
C(23)	4768(2)	3231(2)	1476(2)	21(1)

C(24)	5114(2)	2354(2)	966(2)	25(1)
C(25)	4302(2)	1175(2)	224(2)	29(1)
C(26)	3146(2)	878(2)	15(2)	29(1)
C(27)	2794(2)	1754(2)	533(2)	23(1)
C(28)	3962(2)	5146(2)	1544(2)	17(1)
C(29)	5109(2)	5981(2)	2176(2)	20(1)
C(30)	5770(2)	6748(2)	1893(2)	24(1)
C(31)	5293(2)	6690(2)	977(2)	25(1)
C(32)	4163(2)	5865(2)	339(2)	24(1)
C(33)	3497(2)	5096(2)	624(2)	21(1)
C(34)	4176(2)	7600(2)	3940(2)	19(1)
C(35)	5265(2)	8034(2)	4616(2)	25(1)
C(36)	6210(2)	8994(2)	4743(2)	32(1)
C(37)	6070(2)	9516(2)	4185(2)	32(1)
C(38)	4993(2)	9092(2)	3510(2)	29(1)
C(39)	4045(2)	8136(2)	3384(2)	24(1)
C(40)	2541(2)	7153(2)	4992(2)	19(1)
C(41)	3360(2)	7891(2)	6030(2)	22(1)
C(42)	3083(2)	8530(2)	6942(2)	28(1)
C(43)	1986(2)	8447(2)	6827(2)	33(1)
C(44)	1174(2)	7727(2)	5814(2)	32(1)
C(45)	1446(2)	7078(2)	4900(2)	24(1)
C(46)	-389(3)	1857(4)	7200(4)	89(1)
C(47)	525(2)	2464(3)	8141(2)	53(1)
C(48)	1278(2)	2007(2)	8160(2)	43(1)
C(49)	1149(3)	957(2)	7289(3)	67(1)
C(50)	245(4)	364(4)	6374(3)	106(2)
C(51)	-519(3)	793(5)	6306(3)	116(2)

Table 3. Bond lengths [Å] and angles [°] for $\{[PhBP_3]FeN_3\}_2 \cdot C_6D_6$, (**2**).

Fe-N(3)	1.9516(16)	C(8)-H(8A)	0.9900
Fe-N(1)	2.0107(15)	C(8)-H(8B)	0.9900
Fe-P(1)	2.1610(5)	C(9)-H(9A)	0.9900
Fe-P(3)	2.2101(6)	C(9)-H(9B)	0.9900
Fe-P(2)	2.2279(6)	C(10)-C(11)	1.393(3)
P(1)-C(7)	1.8044(18)	C(10)-C(15)	1.395(3)
P(1)-C(16)	1.8338(18)	C(11)-C(12)	1.385(3)
P(1)-C(10)	1.8399(19)	C(11)-H(11)	0.9500
P(2)-C(8)	1.8136(18)	C(12)-C(13)	1.378(3)
P(2)-C(28)	1.8351(18)	C(12)-H(12)	0.9500
P(2)-C(22)	1.8474(18)	C(13)-C(14)	1.374(3)
P(3)-C(9)	1.8063(18)	C(13)-H(13)	0.9500
P(3)-C(34)	1.8371(19)	C(14)-C(15)	1.390(3)
P(3)-C(40)	1.8468(19)	C(14)-H(14)	0.9500
N(1)-N(2)	1.181(2)	C(15)-H(15)	0.9500
N(2)-N(3)#1	1.175(2)	C(16)-C(21)	1.388(3)
N(3)-N(2)#1	1.175(2)	C(16)-C(17)	1.393(3)
B(1)-C(1)	1.636(3)	C(17)-C(18)	1.385(3)
B(1)-C(8)	1.660(3)	C(17)-H(17)	0.9500
B(1)-C(9)	1.665(3)	C(18)-C(19)	1.372(3)
B(1)-C(7)	1.673(3)	C(18)-H(18)	0.9500
C(1)-C(6)	1.394(3)	C(19)-C(20)	1.381(3)
C(1)-C(2)	1.402(3)	C(19)-H(19)	0.9500
C(2)-C(3)	1.386(3)	C(20)-C(21)	1.387(3)
C(2)-H(2)	0.9500	C(20)-H(20)	0.9500
C(3)-C(4)	1.373(3)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(27)	1.388(3)
C(4)-C(5)	1.372(3)	C(22)-C(23)	1.397(3)
C(4)-H(4)	0.9500	C(23)-C(24)	1.381(3)
C(5)-C(6)	1.394(3)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(24)-C(25)	1.380(3)
C(6)-H(6)	0.9500	C(24)-H(24)	0.9500
C(7)-H(7A)	0.9900	C(25)-C(26)	1.375(3)
C(7)-H(7B)	0.9900	C(25)-H(25)	0.9500

C(26)-C(27)	1.386(3)	C(46)-C(47)	1.383(4)
C(26)-H(26)	0.9500	C(46)-C(51)	1.392(6)
C(27)-H(27)	0.9500	C(46)-H(46)	0.9500
C(28)-C(33)	1.389(3)	C(47)-C(48)	1.366(4)
C(28)-C(29)	1.394(3)	C(47)-H(47)	0.9500
C(29)-C(30)	1.388(3)	C(48)-C(49)	1.366(3)
C(29)-H(29)	0.9500	C(48)-H(48)	0.9500
C(30)-C(31)	1.382(3)	C(49)-C(50)	1.355(5)
C(30)-H(30)	0.9500	C(49)-H(49)	0.9500
C(31)-C(32)	1.377(3)	C(50)-C(51)	1.363(6)
C(31)-H(31)	0.9500	C(50)-H(50)	0.9500
C(32)-C(33)	1.394(3)	C(51)-H(51)	0.9500
C(32)-H(32)	0.9500		
C(33)-H(33)	0.9500	N(3)-Fe-N(1)	87.06(6)
C(34)-C(35)	1.387(3)	N(3)-Fe-P(1)	116.91(5)
C(34)-C(39)	1.392(3)	N(1)-Fe-P(1)	94.52(5)
C(35)-C(36)	1.390(3)	N(3)-Fe-P(3)	150.84(5)
C(35)-H(35)	0.9500	N(1)-Fe-P(3)	91.92(5)
C(36)-C(37)	1.379(3)	P(1)-Fe-P(3)	92.23(2)
C(36)-H(36)	0.9500	N(3)-Fe-P(2)	89.44(5)
C(37)-C(38)	1.377(3)	N(1)-Fe-P(2)	175.64(5)
C(37)-H(37)	0.9500	P(1)-Fe-P(2)	89.37(2)
C(38)-C(39)	1.387(3)	P(3)-Fe-P(2)	89.88(2)
C(38)-H(38)	0.9500	C(7)-P(1)-C(16)	107.09(9)
C(39)-H(39)	0.9500	C(7)-P(1)-C(10)	107.35(8)
C(40)-C(45)	1.386(3)	C(16)-P(1)-C(10)	101.39(8)
C(40)-C(41)	1.398(3)	C(7)-P(1)-Fe	112.88(6)
C(41)-C(42)	1.387(3)	C(16)-P(1)-Fe	113.22(6)
C(41)-H(41)	0.9500	C(10)-P(1)-Fe	114.04(6)
C(42)-C(43)	1.385(3)	C(8)-P(2)-C(28)	108.67(9)
C(42)-H(42)	0.9500	C(8)-P(2)-C(22)	107.11(8)
C(43)-C(44)	1.371(3)	C(28)-P(2)-C(22)	99.23(8)
C(43)-H(43)	0.9500	C(8)-P(2)-Fe	114.07(6)
C(44)-C(45)	1.389(3)	C(28)-P(2)-Fe	110.07(6)
C(44)-H(44)	0.9500	C(22)-P(2)-Fe	116.50(6)
C(45)-H(45)	0.9500	C(9)-P(3)-C(34)	109.32(9)

C(9)-P(3)-C(40)	105.96(9)	P(1)-C(7)-H(7B)	108.8
C(34)-P(3)-C(40)	99.54(8)	H(7A)-C(7)-H(7B)	107.7
C(9)-P(3)-Fe	115.49(6)	B(1)-C(8)-P(2)	114.00(12)
C(34)-P(3)-Fe	104.76(6)	B(1)-C(8)-H(8A)	108.8
C(40)-P(3)-Fe	120.24(6)	P(2)-C(8)-H(8A)	108.8
N(2)-N(1)-Fe	116.86(12)	B(1)-C(8)-H(8B)	108.8
N(3)#1-N(2)-N(1)	177.95(18)	P(2)-C(8)-H(8B)	108.8
N(2)#1-N(3)-Fe	136.05(13)	H(8A)-C(8)-H(8B)	107.6
C(1)-B(1)-C(8)	105.94(14)	B(1)-C(9)-P(3)	111.23(12)
C(1)-B(1)-C(9)	111.29(15)	B(1)-C(9)-H(9A)	109.4
C(8)-B(1)-C(9)	107.61(15)	P(3)-C(9)-H(9A)	109.4
C(1)-B(1)-C(7)	110.25(15)	B(1)-C(9)-H(9B)	109.4
C(8)-B(1)-C(7)	111.21(15)	P(3)-C(9)-H(9B)	109.4
C(9)-B(1)-C(7)	110.44(15)	H(9A)-C(9)-H(9B)	108.0
C(6)-C(1)-C(2)	114.70(17)	C(11)-C(10)-C(15)	117.69(17)
C(6)-C(1)-B(1)	122.80(17)	C(11)-C(10)-P(1)	119.02(14)
C(2)-C(1)-B(1)	122.32(17)	C(15)-C(10)-P(1)	123.27(15)
C(3)-C(2)-C(1)	122.96(19)	C(12)-C(11)-C(10)	121.05(19)
C(3)-C(2)-H(2)	118.5	C(12)-C(11)-H(11)	119.5
C(1)-C(2)-H(2)	118.5	C(10)-C(11)-H(11)	119.5
C(4)-C(3)-C(2)	120.32(19)	C(13)-C(12)-C(11)	120.4(2)
C(4)-C(3)-H(3)	119.8	C(13)-C(12)-H(12)	119.8
C(2)-C(3)-H(3)	119.8	C(11)-C(12)-H(12)	119.8
C(5)-C(4)-C(3)	118.89(19)	C(14)-C(13)-C(12)	119.65(19)
C(5)-C(4)-H(4)	120.6	C(14)-C(13)-H(13)	120.2
C(3)-C(4)-H(4)	120.6	C(12)-C(13)-H(13)	120.2
C(4)-C(5)-C(6)	120.4(2)	C(13)-C(14)-C(15)	120.3(2)
C(4)-C(5)-H(5)	119.8	C(13)-C(14)-H(14)	119.9
C(6)-C(5)-H(5)	119.8	C(15)-C(14)-H(14)	119.9
C(5)-C(6)-C(1)	122.73(19)	C(14)-C(15)-C(10)	120.96(19)
C(5)-C(6)-H(6)	118.6	C(14)-C(15)-H(15)	119.5
C(1)-C(6)-H(6)	118.6	C(10)-C(15)-H(15)	119.5
B(1)-C(7)-P(1)	113.96(12)	C(21)-C(16)-C(17)	118.13(17)
B(1)-C(7)-H(7A)	108.8	C(21)-C(16)-P(1)	123.37(15)
P(1)-C(7)-H(7A)	108.8	C(17)-C(16)-P(1)	118.49(14)
B(1)-C(7)-H(7B)	108.8	C(18)-C(17)-C(16)	121.07(19)

C(18)-C(17)-H(17)	119.5	C(30)-C(29)-H(29)	119.7
C(16)-C(17)-H(17)	119.5	C(28)-C(29)-H(29)	119.7
C(19)-C(18)-C(17)	120.1(2)	C(31)-C(30)-C(29)	120.09(19)
C(19)-C(18)-H(18)	120.0	C(31)-C(30)-H(30)	120.0
C(17)-C(18)-H(18)	120.0	C(29)-C(30)-H(30)	120.0
C(18)-C(19)-C(20)	119.72(19)	C(32)-C(31)-C(30)	120.06(18)
C(18)-C(19)-H(19)	120.1	C(32)-C(31)-H(31)	120.0
C(20)-C(19)-H(19)	120.1	C(30)-C(31)-H(31)	120.0
C(19)-C(20)-C(21)	120.35(19)	C(31)-C(32)-C(33)	119.95(18)
C(19)-C(20)-H(20)	119.8	C(31)-C(32)-H(32)	120.0
C(21)-C(20)-H(20)	119.8	C(33)-C(32)-H(32)	120.0
C(20)-C(21)-C(16)	120.62(19)	C(28)-C(33)-C(32)	120.71(18)
C(20)-C(21)-H(21)	119.7	C(28)-C(33)-H(33)	119.6
C(16)-C(21)-H(21)	119.7	C(32)-C(33)-H(33)	119.6
C(27)-C(22)-C(23)	117.76(17)	C(35)-C(34)-C(39)	118.98(17)
C(27)-C(22)-P(2)	122.25(14)	C(35)-C(34)-P(3)	118.64(14)
C(23)-C(22)-P(2)	119.99(14)	C(39)-C(34)-P(3)	122.39(15)
C(24)-C(23)-C(22)	121.10(18)	C(34)-C(35)-C(36)	120.61(19)
C(24)-C(23)-H(23)	119.4	C(34)-C(35)-H(35)	119.7
C(22)-C(23)-H(23)	119.4	C(36)-C(35)-H(35)	119.7
C(25)-C(24)-C(23)	120.25(19)	C(37)-C(36)-C(35)	119.8(2)
C(25)-C(24)-H(24)	119.9	C(37)-C(36)-H(36)	120.1
C(23)-C(24)-H(24)	119.9	C(35)-C(36)-H(36)	120.1
C(26)-C(25)-C(24)	119.43(19)	C(38)-C(37)-C(36)	120.11(19)
C(26)-C(25)-H(25)	120.3	C(38)-C(37)-H(37)	119.9
C(24)-C(25)-H(25)	120.3	C(36)-C(37)-H(37)	119.9
C(25)-C(26)-C(27)	120.55(19)	C(37)-C(38)-C(39)	120.3(2)
C(25)-C(26)-H(26)	119.7	C(37)-C(38)-H(38)	119.9
C(27)-C(26)-H(26)	119.7	C(39)-C(38)-H(38)	119.9
C(26)-C(27)-C(22)	120.90(18)	C(38)-C(39)-C(34)	120.17(19)
C(26)-C(27)-H(27)	119.5	C(38)-C(39)-H(39)	119.9
C(22)-C(27)-H(27)	119.5	C(34)-C(39)-H(39)	119.9
C(33)-C(28)-C(29)	118.62(17)	C(45)-C(40)-C(41)	118.10(18)
C(33)-C(28)-P(2)	123.76(15)	C(45)-C(40)-P(3)	122.89(15)
C(29)-C(28)-P(2)	117.60(14)	C(41)-C(40)-P(3)	119.02(15)
C(30)-C(29)-C(28)	120.57(18)	C(42)-C(41)-C(40)	120.87(19)

C(42)-C(41)-H(41)	119.6	C(51)-C(46)-H(46)	120.5
C(40)-C(41)-H(41)	119.6	C(48)-C(47)-C(46)	118.9(3)
C(43)-C(42)-C(41)	119.9(2)	C(48)-C(47)-H(47)	120.5
C(43)-C(42)-H(42)	120.1	C(46)-C(47)-H(47)	120.5
C(41)-C(42)-H(42)	120.1	C(47)-C(48)-C(49)	122.5(3)
C(44)-C(43)-C(42)	119.8(2)	C(47)-C(48)-H(48)	118.8
C(44)-C(43)-H(43)	120.1	C(49)-C(48)-H(48)	118.8
C(42)-C(43)-H(43)	120.1	C(50)-C(49)-C(48)	118.1(4)
C(43)-C(44)-C(45)	120.4(2)	C(50)-C(49)-H(49)	120.9
C(43)-C(44)-H(44)	119.8	C(48)-C(49)-H(49)	120.9
C(45)-C(44)-H(44)	119.8	C(49)-C(50)-C(51)	121.7(4)
C(40)-C(45)-C(44)	120.91(19)	C(49)-C(50)-H(50)	119.1
C(40)-C(45)-H(45)	119.5	C(51)-C(50)-H(50)	119.1
C(44)-C(45)-H(45)	119.5	C(50)-C(51)-C(46)	119.8(4)
C(47)-C(46)-C(51)	118.9(4)	C(50)-C(51)-H(51)	120.1
C(47)-C(46)-H(46)	120.5	C(46)-C(51)-H(51)	120.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for $\{[PhBP_3]FeN_3\}_2 \cdot C_6D_6$, (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe	14(1)	16(1)	16(1)	9(1)	4(1)	6(1)
P(1)	16(1)	15(1)	15(1)	9(1)	5(1)	6(1)
P(2)	14(1)	17(1)	16(1)	10(1)	6(1)	8(1)
P(3)	16(1)	15(1)	17(1)	10(1)	5(1)	7(1)
N(1)	17(1)	19(1)	17(1)	8(1)	3(1)	8(1)
N(2)	13(1)	18(1)	13(1)	6(1)	4(1)	6(1)
N(3)	20(1)	27(1)	18(1)	13(1)	7(1)	12(1)
B(1)	16(1)	19(1)	17(1)	10(1)	5(1)	8(1)
C(1)	18(1)	22(1)	16(1)	9(1)	8(1)	12(1)
C(2)	25(1)	20(1)	22(1)	10(1)	4(1)	12(1)
C(3)	20(1)	22(1)	26(1)	9(1)	4(1)	9(1)
C(4)	17(1)	37(1)	25(1)	14(1)	3(1)	14(1)
C(5)	25(1)	46(1)	38(1)	31(1)	7(1)	17(1)
C(6)	19(1)	32(1)	34(1)	22(1)	5(1)	8(1)
C(7)	15(1)	16(1)	19(1)	8(1)	5(1)	7(1)
C(8)	14(1)	21(1)	17(1)	11(1)	4(1)	8(1)
C(9)	19(1)	22(1)	18(1)	13(1)	5(1)	11(1)
C(10)	13(1)	21(1)	17(1)	11(1)	5(1)	4(1)
C(11)	25(1)	21(1)	24(1)	12(1)	10(1)	8(1)
C(12)	28(1)	27(1)	22(1)	9(1)	10(1)	8(1)
C(13)	26(1)	43(1)	21(1)	19(1)	9(1)	10(1)
C(14)	33(1)	45(1)	35(1)	31(1)	14(1)	20(1)
C(15)	24(1)	31(1)	24(1)	18(1)	10(1)	14(1)
C(16)	21(1)	15(1)	17(1)	10(1)	8(1)	7(1)
C(17)	20(1)	21(1)	28(1)	14(1)	8(1)	7(1)
C(18)	31(1)	29(1)	39(1)	22(1)	19(1)	19(1)
C(19)	41(1)	18(1)	31(1)	12(1)	17(1)	15(1)
C(20)	31(1)	19(1)	25(1)	7(1)	3(1)	5(1)
C(21)	22(1)	22(1)	24(1)	13(1)	6(1)	9(1)
C(22)	21(1)	21(1)	16(1)	13(1)	10(1)	12(1)
C(23)	22(1)	24(1)	20(1)	14(1)	9(1)	11(1)

C(24)	25(1)	35(1)	29(1)	22(1)	14(1)	20(1)
C(25)	39(1)	31(1)	29(1)	17(1)	16(1)	26(1)
C(26)	34(1)	20(1)	26(1)	9(1)	8(1)	13(1)
C(27)	21(1)	24(1)	24(1)	13(1)	6(1)	11(1)
C(28)	21(1)	18(1)	19(1)	11(1)	11(1)	12(1)
C(29)	20(1)	24(1)	21(1)	14(1)	8(1)	11(1)
C(30)	20(1)	23(1)	29(1)	14(1)	11(1)	9(1)
C(31)	29(1)	27(1)	33(1)	22(1)	20(1)	17(1)
C(32)	31(1)	28(1)	24(1)	19(1)	14(1)	18(1)
C(33)	21(1)	22(1)	22(1)	13(1)	8(1)	11(1)
C(34)	22(1)	15(1)	20(1)	9(1)	9(1)	8(1)
C(35)	25(1)	23(1)	29(1)	15(1)	10(1)	10(1)
C(36)	21(1)	25(1)	36(1)	13(1)	6(1)	3(1)
C(37)	31(1)	21(1)	39(1)	16(1)	16(1)	5(1)
C(38)	36(1)	23(1)	33(1)	19(1)	16(1)	12(1)
C(39)	26(1)	20(1)	28(1)	13(1)	10(1)	11(1)
C(40)	22(1)	14(1)	21(1)	11(1)	9(1)	8(1)
C(41)	23(1)	19(1)	25(1)	13(1)	6(1)	8(1)
C(42)	32(1)	22(1)	22(1)	10(1)	8(1)	9(1)
C(43)	35(1)	31(1)	29(1)	13(1)	19(1)	14(1)
C(44)	23(1)	33(1)	37(1)	16(1)	16(1)	12(1)
C(45)	20(1)	22(1)	26(1)	12(1)	7(1)	6(1)
C(46)	53(2)	132(4)	108(3)	100(3)	20(2)	21(2)
C(47)	48(2)	58(2)	64(2)	44(2)	18(2)	20(2)
C(48)	44(2)	34(1)	38(2)	17(1)	14(1)	9(1)
C(49)	78(2)	38(2)	65(2)	24(2)	42(2)	9(2)
C(50)	103(3)	66(2)	44(2)	11(2)	15(2)	-33(2)
C(51)	44(2)	158(5)	62(3)	65(3)	-15(2)	-34(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for $\{[PhBP_3]FeN_3\}_2 \cdot C_6D_6$, (**2**).

	x	y	z	U(eq)
H(2)	-1124	2152	1207	27
H(3)	-2895	1374	-21	31
H(4)	-3187	2391	-798	33
H(5)	-1684	4220	-300	39
H(6)	81	5028	967	33
H(7A)	128	3156	2746	20
H(7B)	703	4567	3638	20
H(8A)	1521	3506	629	20
H(8B)	1253	2649	1082	20
H(9A)	1277	6080	2821	22
H(9B)	2075	5795	2068	22
H(11)	1786	5561	5547	29
H(12)	1675	5841	7221	35
H(13)	1762	4482	7643	37
H(14)	1964	2836	6385	38
H(15)	2090	2549	4707	29
H(17)	3425	2668	3517	27
H(18)	3151	697	2592	35
H(19)	1381	-863	1301	36
H(20)	-120	-448	931	36
H(21)	125	1514	1895	28
H(23)	5335	4042	1975	25
H(24)	5913	2562	1126	30
H(25)	4540	574	-138	34
H(26)	2584	67	-489	34
H(27)	1992	1535	381	27
H(29)	5442	6024	2806	24
H(30)	6551	7314	2329	29
H(31)	5745	7219	786	29
H(32)	3838	5821	-294	28

H(33)	2717	4531	183	25
H(35)	5365	7671	4996	30
H(36)	6952	9291	5213	38
H(37)	6716	10169	4267	39
H(38)	4899	9455	3128	34
H(39)	3305	7847	2917	29
H(41)	4116	7956	6113	27
H(42)	3646	9023	7644	33
H(43)	1796	8889	7449	39
H(44)	421	7670	5735	38
H(45)	874	6577	4203	29
H(46)	-920	2161	7164	107
H(47)	628	3188	8764	63
H(48)	1914	2435	8802	52
H(49)	1678	651	7325	80
H(50)	141	-370	5763	127
H(51)	-1138	367	5651	139

Table 6. Crystal data and structure refinement for $\{([PhBP_3]Fe)_2N\}\{Na(THF)_5\}\cdot THF$, (**3**).

Identification code	sdb47	
Empirical formula	$C_{114}\ H_{130}\ B_2\ Fe_2\ N\ Na\ O_6\ P_6$	
Formula weight	1952.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 16.7910(8) Å	α= 90°.
	b = 13.7352(6) Å	β= 93.6530(10)°.
	c = 43.299(2) Å	γ = 90°.
Volume	9965.8(8) $Å^3$	
Z	4	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	0.449 mm^{-1}	
F(000)	4128	
Crystal size	0.18 x 0.26 x 0.41 mm^3	
Theta range for data collection	1.22 to 30.53°.	
Index ranges	-21<=h<=17, -19<=k<=18, -54<=l<=60	
Reflections collected	81503	
Independent reflections	22334 [R(int) = 0.0899]	
Completeness to theta = 30.53°	73.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	22334 / 0 / 1209	
Goodness-of-fit on F^2	1.508	
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.0940	
R indices (all data)	R1 = 0.1239, wR2 = 0.1004	
Largest diff. peak and hole	1.076 and -0.764 $e.Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. The bridging nitride ligand was located in two positions and the population of each position was determined as a free variable during the refinement process.

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\{([PhBP_3]Fe)_2N\}\{Na(THF)_5\}\cdot THF$, (**3**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5938(1)	8119(1)	6495(1)	16(1)
Fe(2)	7602(1)	8100(1)	6206(1)	16(1)
N(1A)	6917(3)	8317(3)	6472(1)	17(2)
N(1B)	6774(5)	7631(7)	6335(2)	30(3)
P(1)	5630(1)	7664(1)	6967(1)	16(1)
P(2)	4879(1)	7348(1)	6273(1)	16(1)
P(3)	5222(1)	9455(1)	6547(1)	16(1)
P(4)	8344(1)	9436(1)	6167(1)	17(1)
P(5)	8666(1)	7291(1)	6391(1)	17(1)
P(6)	7890(1)	7625(1)	5728(1)	18(1)
B(1)	3975(2)	8150(3)	6777(1)	17(1)
B(2)	9537(2)	8189(3)	5905(1)	19(1)
Na	1678(1)	3500(1)	5916(1)	71(1)
O(1)	9825(2)	3144(2)	6908(1)	75(1)
O(2)	687(2)	2462(4)	5765(1)	125(2)
O(3)	1256(3)	4692(3)	5552(1)	151(2)
O(4)	2838(2)	3588(2)	5688(1)	62(1)
O(5)	1642(2)	4669(2)	6288(1)	67(1)
O(6)	2145(2)	2346(2)	6278(1)	52(1)
C(1)	8936(3)	4320(3)	7081(1)	66(2)
C(2)	8447(3)	3431(3)	6989(1)	48(1)
C(3)	9054(3)	2704(3)	6904(1)	62(2)
C(4)	9760(3)	3959(3)	7129(1)	68(2)
C(5)	780(4)	1489(4)	5699(1)	103(2)
C(6)	235(4)	1246(4)	5420(1)	98(2)
C(7)	-300(4)	2130(6)	5397(2)	122(3)
C(8A)	-157(7)	2450(12)	5690(3)	106(7)
C(8B)	168(9)	3088(11)	5478(4)	67(6)
C(9)	1493(4)	4710(5)	5235(1)	150(3)
C(10)	1227(4)	5701(4)	5120(2)	108(2)

C(11)	528(4)	5919(4)	5323(2)	108(2)
C(12)	675(5)	5455(6)	5607(2)	197(5)
C(13)	3193(3)	2962(3)	5458(1)	88(2)
C(14)	4068(3)	3321(3)	5478(1)	73(2)
C(15)	3996(3)	4389(3)	5509(1)	72(2)
C(16)	3334(3)	4442(4)	5723(1)	66(2)
C(17)	2947(3)	2397(4)	6405(1)	67(2)
C(18)	2983(3)	2062(3)	6729(1)	55(1)
C(19)	2133(3)	1824(3)	6793(1)	46(1)
C(20)	1727(3)	1719(3)	6476(1)	73(2)
C(21)	2026(4)	5605(4)	6287(2)	141(3)
C(22)	1757(3)	6172(3)	6523(1)	51(1)
C(23)	1404(3)	5495(3)	6754(1)	55(1)
C(24)	1483(3)	4504(3)	6604(1)	60(1)
C(25)	3073(2)	8187(2)	6894(1)	18(1)
C(26)	2498(2)	8822(2)	6752(1)	27(1)
C(27)	1717(2)	8874(2)	6844(1)	29(1)
C(28)	1485(2)	8307(3)	7081(1)	29(1)
C(29)	2016(2)	7660(2)	7223(1)	25(1)
C(30)	2797(2)	7611(2)	7130(1)	22(1)
C(31)	4571(2)	7478(2)	7013(1)	16(1)
C(32)	3921(2)	7629(2)	6430(1)	17(1)
C(33)	4324(2)	9276(2)	6758(1)	16(1)
C(34)	6090(2)	6529(2)	7124(1)	14(1)
C(35)	6128(2)	6328(2)	7438(1)	20(1)
C(36)	6475(2)	5467(2)	7550(1)	21(1)
C(37)	6758(2)	4795(2)	7351(1)	24(1)
C(38)	6706(2)	4975(2)	7037(1)	24(1)
C(39)	6377(2)	5848(2)	6923(1)	18(1)
C(40)	5946(2)	8507(2)	7288(1)	15(1)
C(41)	5413(2)	8996(2)	7465(1)	18(1)
C(42)	5685(2)	9634(2)	7701(1)	26(1)
C(43)	6492(2)	9759(2)	7765(1)	27(1)
C(44)	7032(2)	9268(2)	7595(1)	25(1)
C(45)	6761(2)	8655(2)	7353(1)	20(1)
C(46)	4980(2)	6003(2)	6291(1)	17(1)

C(47)	4538(2)	5403(2)	6471(1)	23(1)
C(48)	4670(2)	4400(2)	6476(1)	31(1)
C(49)	5233(2)	3996(3)	6301(1)	33(1)
C(50)	5674(2)	4591(3)	6119(1)	33(1)
C(51)	5554(2)	5587(2)	6118(1)	25(1)
C(52)	4625(2)	7472(2)	5852(1)	18(1)
C(53)	4015(2)	6919(3)	5710(1)	31(1)
C(54)	3793(2)	7020(3)	5398(1)	34(1)
C(55)	4177(2)	7674(3)	5221(1)	31(1)
C(56)	4780(2)	8243(3)	5359(1)	32(1)
C(57)	4999(2)	8135(2)	5671(1)	24(1)
C(58)	5688(2)	10522(2)	6743(1)	17(1)
C(59)	6458(2)	10477(2)	6875(1)	23(1)
C(60)	6797(2)	11263(2)	7038(1)	29(1)
C(61)	6354(2)	12100(2)	7068(1)	31(1)
C(62)	5590(2)	12162(2)	6939(1)	30(1)
C(63)	5260(2)	11375(2)	6778(1)	26(1)
C(64)	4870(2)	10038(2)	6182(1)	17(1)
C(65)	5412(2)	10520(2)	6011(1)	22(1)
C(66)	5182(2)	10951(2)	5728(1)	26(1)
C(67)	4405(2)	10876(2)	5609(1)	30(1)
C(68)	3850(2)	10405(2)	5776(1)	28(1)
C(69)	4079(2)	9991(2)	6062(1)	22(1)
C(70)	10418(2)	8283(2)	5778(1)	22(1)
C(71)	10542(3)	8514(3)	5475(1)	56(1)
C(72)	11304(3)	8634(4)	5358(1)	70(2)
C(73)	11980(3)	8500(3)	5555(1)	47(1)
C(74)	11883(3)	8376(3)	5851(1)	64(2)
C(75)	11129(3)	8254(3)	5965(1)	51(1)
C(76)	9607(2)	7730(2)	6260(1)	17(1)
C(77)	8953(2)	7465(2)	5678(1)	19(1)
C(78)	9152(2)	9299(2)	5910(1)	18(1)
C(79)	7877(2)	10619(2)	6054(1)	17(1)
C(80)	7530(2)	11177(2)	6277(1)	28(1)
C(81)	7113(2)	12032(2)	6196(1)	31(1)
C(82)	7054(2)	12336(2)	5894(1)	34(1)

C(83)	7411(2)	11801(3)	5672(1)	32(1)
C(84)	7815(2)	10945(2)	5749(1)	26(1)
C(85)	8850(2)	9778(2)	6543(1)	17(1)
C(86)	8546(2)	9455(2)	6813(1)	20(1)
C(87)	8936(2)	9634(2)	7103(1)	24(1)
C(88)	9646(2)	10142(2)	7121(1)	28(1)
C(89)	9952(2)	10491(2)	6855(1)	29(1)
C(90)	9557(2)	10309(2)	6568(1)	26(1)
C(91)	8833(2)	7151(2)	6812(1)	17(1)
C(92)	9599(2)	7105(2)	6958(1)	20(1)
C(93)	9700(2)	6964(2)	7273(1)	25(1)
C(94)	9048(2)	6860(2)	7448(1)	25(1)
C(95)	8285(2)	6890(2)	7309(1)	22(1)
C(96)	8183(2)	7039(2)	6991(1)	21(1)
C(97)	8642(2)	5974(2)	6298(1)	18(1)
C(98)	9321(2)	5434(2)	6247(1)	32(1)
C(99)	9270(2)	4444(3)	6191(1)	38(1)
C(100)	8544(2)	3975(3)	6187(1)	34(1)
C(101)	7873(2)	4494(2)	6245(1)	30(1)
C(102)	7919(2)	5487(2)	6301(1)	23(1)
C(103)	7400(2)	6524(2)	5559(1)	20(1)
C(104)	6594(2)	6578(3)	5459(1)	33(1)
C(105)	6176(2)	5751(3)	5350(1)	40(1)
C(106)	6563(3)	4869(3)	5338(1)	34(1)
C(107)	7354(3)	4806(3)	5431(1)	39(1)
C(108)	7764(2)	5635(3)	5541(1)	31(1)
C(109)	7551(2)	8513(2)	5425(1)	18(1)
C(110)	6890(2)	9077(2)	5479(1)	28(1)
C(111)	6588(2)	9735(2)	5256(1)	29(1)
C(112)	6959(2)	9871(2)	4989(1)	30(1)
C(113)	7622(3)	9333(3)	4937(1)	39(1)
C(114)	7914(2)	8637(3)	5152(1)	31(1)

Table 8. Bond lengths [Å] and angles [°] for $\{([PhBP_3]Fe)_2N\}\{Na(THF)_5\}\cdot THF$, (**3**).

Fe(1)-N(1A)	1.675(5)	B(2)-C(76)	1.657(5)
Fe(1)-N(1B)	1.739(9)	B(2)-C(78)	1.657(5)
Fe(1)-P(3)	2.2127(10)	B(2)-C(77)	1.671(5)
Fe(1)-P(1)	2.2295(10)	Na-O(4)	2.244(4)
Fe(1)-P(2)	2.2338(10)	Na-O(2)	2.256(5)
Fe(2)-N(1B)	1.661(9)	Na-O(5)	2.276(3)
Fe(2)-N(1A)	1.705(5)	Na-O(6)	2.328(3)
Fe(2)-P(5)	2.2106(10)	Na-O(3)	2.351(4)
Fe(2)-P(4)	2.2299(10)	O(1)-C(3)	1.428(5)
Fe(2)-P(6)	2.2534(10)	O(1)-C(4)	1.482(5)
N(1A)-N(1B)	1.132(8)	O(2)-C(5)	1.378(6)
P(1)-C(31)	1.818(3)	O(2)-C(8A)	1.434(11)
P(1)-C(34)	1.849(3)	O(2)-C(8B)	1.704(14)
P(1)-C(40)	1.859(3)	O(3)-C(9)	1.454(6)
P(2)-C(32)	1.828(3)	O(3)-C(12)	1.461(6)
P(2)-C(46)	1.857(3)	O(4)-C(16)	1.441(5)
P(2)-C(52)	1.855(3)	O(4)-C(13)	1.471(5)
P(3)-C(33)	1.827(3)	O(5)-C(24)	1.432(5)
P(3)-C(64)	1.835(3)	O(5)-C(21)	1.437(5)
P(3)-C(58)	1.842(3)	O(6)-C(17)	1.424(5)
P(4)-C(78)	1.820(3)	O(6)-C(20)	1.430(4)
P(4)-C(85)	1.848(3)	C(1)-C(4)	1.473(6)
P(4)-C(79)	1.856(3)	C(1)-C(2)	1.510(5)
P(5)-C(76)	1.815(3)	C(1)-H(1A)	0.9900
P(5)-C(91)	1.838(3)	C(1)-H(1B)	0.9900
P(5)-C(97)	1.853(3)	C(2)-C(3)	1.490(5)
P(6)-C(77)	1.825(3)	C(2)-H(2A)	0.9900
P(6)-C(103)	1.850(3)	C(2)-H(2B)	0.9900
P(6)-C(109)	1.852(3)	C(3)-H(3A)	0.9900
B(1)-C(25)	1.628(5)	C(3)-H(3B)	0.9900
B(1)-C(32)	1.659(4)	C(4)-H(4A)	0.9900
B(1)-C(31)	1.663(4)	C(4)-H(4B)	0.9900
B(1)-C(33)	1.658(5)	C(5)-C(6)	1.504(6)
B(2)-C(70)	1.616(5)	C(5)-H(5A)	0.9900

C(5)-H(5B)	0.9900	C(17)-H(17B)	0.9900
C(6)-C(7)	1.511(7)	C(18)-C(19)	1.507(5)
C(6)-H(6A)	0.9900	C(18)-H(18A)	0.9900
C(6)-H(6B)	0.9900	C(18)-H(18B)	0.9900
C(7)-C(8A)	1.351(10)	C(19)-C(20)	1.502(5)
C(7)-C(8B)	1.560(15)	C(19)-H(19A)	0.9900
C(7)-H(7A)	0.9900	C(19)-H(19B)	0.9900
C(7)-H(7B)	0.9900	C(20)-H(20A)	0.9900
C(8A)-H(8A)	0.9900	C(20)-H(20B)	0.9900
C(8A)-H(8B)	0.9900	C(21)-C(22)	1.385(6)
C(8B)-H(8C)	0.9900	C(21)-H(21A)	0.9900
C(8B)-H(8D)	0.9900	C(21)-H(21B)	0.9900
C(9)-C(10)	1.507(7)	C(22)-C(23)	1.513(5)
C(9)-H(9A)	0.9900	C(22)-H(22A)	0.9900
C(9)-H(9B)	0.9900	C(22)-H(22B)	0.9900
C(10)-C(11)	1.541(7)	C(23)-C(24)	1.516(5)
C(10)-H(10A)	0.9900	C(23)-H(23A)	0.9900
C(10)-H(10B)	0.9900	C(23)-H(23B)	0.9900
C(11)-C(12)	1.394(7)	C(24)-H(24A)	0.9900
C(11)-H(11A)	0.9900	C(24)-H(24B)	0.9900
C(11)-H(11B)	0.9900	C(25)-C(30)	1.394(4)
C(12)-H(12A)	0.9900	C(25)-C(26)	1.413(4)
C(12)-H(12B)	0.9900	C(26)-C(27)	1.396(5)
C(13)-C(14)	1.546(6)	C(26)-H(26)	0.9500
C(13)-H(13A)	0.9900	C(27)-C(28)	1.366(5)
C(13)-H(13B)	0.9900	C(27)-H(27)	0.9500
C(14)-C(15)	1.478(6)	C(28)-C(29)	1.376(5)
C(14)-H(14A)	0.9900	C(28)-H(28)	0.9500
C(14)-H(14B)	0.9900	C(29)-C(30)	1.398(5)
C(15)-C(16)	1.494(6)	C(29)-H(29)	0.9500
C(15)-H(15A)	0.9900	C(30)-H(30)	0.9500
C(15)-H(15B)	0.9900	C(31)-H(31A)	0.9900
C(16)-H(16A)	0.9900	C(31)-H(31B)	0.9900
C(16)-H(16B)	0.9900	C(32)-H(32A)	0.9900
C(17)-C(18)	1.476(5)	C(32)-H(32B)	0.9900
C(17)-H(17A)	0.9900	C(33)-H(33A)	0.9900

C(33)-H(33B)	0.9900	C(53)-C(54)	1.383(4)
C(34)-C(35)	1.385(4)	C(53)-H(53)	0.9500
C(34)-C(39)	1.385(4)	C(54)-C(55)	1.370(5)
C(35)-C(36)	1.393(4)	C(54)-H(54)	0.9500
C(35)-H(35)	0.9500	C(55)-C(56)	1.385(5)
C(36)-C(37)	1.371(4)	C(55)-H(55)	0.9500
C(36)-H(36)	0.9500	C(56)-C(57)	1.386(4)
C(37)-C(38)	1.378(4)	C(56)-H(56)	0.9500
C(37)-H(37)	0.9500	C(57)-H(57)	0.9500
C(38)-C(39)	1.397(4)	C(58)-C(59)	1.381(4)
C(38)-H(38)	0.9500	C(58)-C(63)	1.388(4)
C(39)-H(39)	0.9500	C(59)-C(60)	1.393(4)
C(40)-C(41)	1.391(4)	C(59)-H(59)	0.9500
C(40)-C(45)	1.393(4)	C(60)-C(61)	1.380(5)
C(41)-C(42)	1.398(4)	C(60)-H(60)	0.9500
C(41)-H(41)	0.9500	C(61)-C(62)	1.369(5)
C(42)-C(43)	1.375(5)	C(61)-H(61)	0.9500
C(42)-H(42)	0.9500	C(62)-C(63)	1.384(4)
C(43)-C(44)	1.379(5)	C(62)-H(62)	0.9500
C(43)-H(43)	0.9500	C(63)-H(63)	0.9500
C(44)-C(45)	1.398(4)	C(64)-C(65)	1.380(5)
C(44)-H(44)	0.9500	C(64)-C(69)	1.398(4)
C(45)-H(45)	0.9500	C(65)-C(66)	1.392(4)
C(46)-C(51)	1.382(5)	C(65)-H(65)	0.9500
C(46)-C(47)	1.383(5)	C(66)-C(67)	1.376(5)
C(47)-C(48)	1.395(4)	C(66)-H(66)	0.9500
C(47)-H(47)	0.9500	C(67)-C(68)	1.379(5)
C(48)-C(49)	1.367(5)	C(67)-H(67)	0.9500
C(48)-H(48)	0.9500	C(68)-C(69)	1.392(4)
C(49)-C(50)	1.383(5)	C(68)-H(68)	0.9500
C(49)-H(49)	0.9500	C(69)-H(69)	0.9500
C(50)-C(51)	1.383(4)	C(70)-C(71)	1.380(5)
C(50)-H(50)	0.9500	C(70)-C(75)	1.399(5)
C(51)-H(51)	0.9500	C(71)-C(72)	1.415(6)
C(52)-C(57)	1.378(4)	C(71)-H(71)	0.9500
C(52)-C(53)	1.387(4)	C(72)-C(73)	1.387(6)

C(72)-H(72)	0.9500	C(92)-C(93)	1.374(4)
C(73)-C(74)	1.316(5)	C(92)-H(92)	0.9500
C(73)-H(73)	0.9500	C(93)-C(94)	1.378(5)
C(74)-C(75)	1.397(6)	C(93)-H(93)	0.9500
C(74)-H(74)	0.9500	C(94)-C(95)	1.381(4)
C(75)-H(75)	0.9500	C(94)-H(94)	0.9500
C(76)-H(76A)	0.9900	C(95)-C(96)	1.391(4)
C(76)-H(76B)	0.9900	C(95)-H(95)	0.9500
C(77)-H(77A)	0.9900	C(96)-H(96)	0.9500
C(77)-H(77B)	0.9900	C(97)-C(98)	1.390(5)
C(78)-H(78A)	0.9900	C(97)-C(102)	1.386(4)
C(78)-H(78B)	0.9900	C(98)-C(99)	1.383(4)
C(79)-C(80)	1.389(5)	C(98)-H(98)	0.9500
C(79)-C(84)	1.391(4)	C(99)-C(100)	1.377(5)
C(80)-C(81)	1.400(4)	C(99)-H(99)	0.9500
C(80)-H(80)	0.9500	C(100)-C(101)	1.371(5)
C(81)-C(82)	1.372(5)	C(100)-H(100)	0.9500
C(81)-H(81)	0.9500	C(101)-C(102)	1.386(4)
C(82)-C(83)	1.374(5)	C(101)-H(101)	0.9500
C(82)-H(82)	0.9500	C(102)-H(102)	0.9500
C(83)-C(84)	1.388(4)	C(103)-C(108)	1.369(4)
C(83)-H(83)	0.9500	C(103)-C(104)	1.396(5)
C(84)-H(84)	0.9500	C(104)-C(105)	1.400(4)
C(85)-C(86)	1.378(4)	C(104)-H(104)	0.9500
C(85)-C(90)	1.393(4)	C(105)-C(106)	1.378(5)
C(86)-C(87)	1.399(4)	C(105)-H(105)	0.9500
C(86)-H(86)	0.9500	C(106)-C(107)	1.366(5)
C(87)-C(88)	1.380(5)	C(106)-H(106)	0.9500
C(87)-H(87)	0.9500	C(107)-C(108)	1.399(5)
C(88)-C(89)	1.378(5)	C(107)-H(107)	0.9500
C(88)-H(88)	0.9500	C(108)-H(108)	0.9500
C(89)-C(90)	1.393(4)	C(109)-C(114)	1.377(5)
C(89)-H(89)	0.9500	C(109)-C(110)	1.385(5)
C(90)-H(90)	0.9500	C(110)-C(111)	1.394(4)
C(91)-C(96)	1.387(5)	C(110)-H(110)	0.9500
C(91)-C(92)	1.398(4)	C(111)-C(112)	1.360(5)

C(111)-H(111)	0.9500	C(31)-P(1)-Fe(1)	115.11(10)
C(112)-C(113)	1.367(5)	C(34)-P(1)-Fe(1)	117.16(12)
C(112)-H(112)	0.9500	C(40)-P(1)-Fe(1)	115.93(11)
C(113)-C(114)	1.400(4)	C(32)-P(2)-C(46)	105.91(16)
C(113)-H(113)	0.9500	C(32)-P(2)-C(52)	101.24(15)
C(114)-H(114)	0.9500	C(46)-P(2)-C(52)	98.47(14)
		C(32)-P(2)-Fe(1)	115.77(10)
N(1A)-Fe(1)-N(1B)	38.7(3)	C(46)-P(2)-Fe(1)	112.69(11)
N(1A)-Fe(1)-P(3)	114.45(15)	C(52)-P(2)-Fe(1)	120.46(12)
N(1B)-Fe(1)-P(3)	144.9(3)	C(33)-P(3)-C(64)	104.97(16)
N(1A)-Fe(1)-P(1)	112.69(14)	C(33)-P(3)-C(58)	102.54(15)
N(1B)-Fe(1)-P(1)	119.9(3)	C(64)-P(3)-C(58)	98.76(14)
P(3)-Fe(1)-P(1)	88.83(4)	C(33)-P(3)-Fe(1)	114.26(10)
N(1A)-Fe(1)-P(2)	143.93(16)	C(64)-P(3)-Fe(1)	114.90(11)
N(1B)-Fe(1)-P(2)	106.6(3)	C(58)-P(3)-Fe(1)	119.23(12)
P(3)-Fe(1)-P(2)	90.79(4)	C(78)-P(4)-C(85)	104.25(16)
P(1)-Fe(1)-P(2)	92.10(4)	C(78)-P(4)-C(79)	104.34(15)
N(1B)-Fe(2)-N(1A)	39.3(3)	C(85)-P(4)-C(79)	99.94(14)
N(1B)-Fe(2)-P(5)	111.0(3)	C(78)-P(4)-Fe(2)	113.80(10)
N(1A)-Fe(2)-P(5)	114.02(13)	C(85)-P(4)-Fe(2)	111.74(11)
N(1B)-Fe(2)-P(4)	145.9(3)	C(79)-P(4)-Fe(2)	120.77(11)
N(1A)-Fe(2)-P(4)	108.14(16)	C(76)-P(5)-C(91)	105.34(15)
P(5)-Fe(2)-P(4)	89.90(4)	C(76)-P(5)-C(97)	105.30(16)
N(1B)-Fe(2)-P(6)	115.4(3)	C(91)-P(5)-C(97)	96.43(13)
N(1A)-Fe(2)-P(6)	149.92(15)	C(76)-P(5)-Fe(2)	114.77(10)
P(5)-Fe(2)-P(6)	88.36(4)	C(91)-P(5)-Fe(2)	118.74(12)
P(4)-Fe(2)-P(6)	90.88(4)	C(97)-P(5)-Fe(2)	114.00(11)
N(1B)-N(1A)-Fe(1)	73.7(5)	C(77)-P(6)-C(103)	105.56(16)
N(1B)-N(1A)-Fe(2)	68.2(5)	C(77)-P(6)-C(109)	104.71(16)
Fe(1)-N(1A)-Fe(2)	135.9(3)	C(103)-P(6)-C(109)	98.62(14)
N(1A)-N(1B)-Fe(2)	72.5(5)	C(77)-P(6)-Fe(2)	114.37(10)
N(1A)-N(1B)-Fe(1)	67.6(5)	C(103)-P(6)-Fe(2)	118.98(12)
Fe(2)-N(1B)-Fe(1)	134.3(6)	C(109)-P(6)-Fe(2)	112.62(12)
C(31)-P(1)-C(34)	103.36(14)	C(25)-B(1)-C(32)	107.3(3)
C(31)-P(1)-C(40)	103.96(15)	C(25)-B(1)-C(31)	111.2(3)
C(34)-P(1)-C(40)	99.11(13)	C(32)-B(1)-C(31)	108.2(3)

C(25)-B(1)-C(33)	109.0(3)	C(17)-O(6)-Na	119.7(3)
C(32)-B(1)-C(33)	110.9(3)	C(20)-O(6)-Na	131.0(3)
C(31)-B(1)-C(33)	110.3(3)	C(4)-C(1)-C(2)	104.8(4)
C(70)-B(2)-C(76)	109.4(3)	C(4)-C(1)-H(1A)	110.8
C(70)-B(2)-C(78)	107.3(3)	C(2)-C(1)-H(1A)	110.8
C(76)-B(2)-C(78)	110.0(3)	C(4)-C(1)-H(1B)	110.8
C(70)-B(2)-C(77)	111.3(3)	C(2)-C(1)-H(1B)	110.8
C(76)-B(2)-C(77)	108.9(3)	H(1A)-C(1)-H(1B)	108.9
C(78)-B(2)-C(77)	109.9(3)	C(3)-C(2)-C(1)	103.8(4)
O(4)-Na-O(2)	123.35(15)	C(3)-C(2)-H(2A)	111.0
O(4)-Na-O(5)	109.66(14)	C(1)-C(2)-H(2A)	111.0
O(2)-Na-O(5)	126.85(16)	C(3)-C(2)-H(2B)	111.0
O(4)-Na-O(6)	93.93(12)	C(1)-C(2)-H(2B)	111.0
O(2)-Na-O(6)	88.61(16)	H(2A)-C(2)-H(2B)	109.0
O(5)-Na-O(6)	91.65(12)	O(1)-C(3)-C(2)	110.3(4)
O(4)-Na-O(3)	84.21(15)	O(1)-C(3)-H(3A)	109.6
O(2)-Na-O(3)	93.4(2)	C(2)-C(3)-H(3A)	109.6
O(5)-Na-O(3)	87.85(15)	O(1)-C(3)-H(3B)	109.6
O(6)-Na-O(3)	177.79(19)	C(2)-C(3)-H(3B)	109.6
C(3)-O(1)-C(4)	103.0(4)	H(3A)-C(3)-H(3B)	108.1
C(5)-O(2)-C(8A)	93.8(7)	C(1)-C(4)-O(1)	105.6(4)
C(5)-O(2)-C(8B)	113.5(6)	C(1)-C(4)-H(4A)	110.6
C(8A)-O(2)-C(8B)	52.3(6)	O(1)-C(4)-H(4A)	110.6
C(5)-O(2)-Na	125.6(4)	C(1)-C(4)-H(4B)	110.6
C(8A)-O(2)-Na	140.6(6)	O(1)-C(4)-H(4B)	110.6
C(8B)-O(2)-Na	103.1(6)	H(4A)-C(4)-H(4B)	108.8
C(9)-O(3)-C(12)	111.6(4)	O(2)-C(5)-C(6)	108.0(5)
C(9)-O(3)-Na	123.9(3)	O(2)-C(5)-H(5A)	110.1
C(12)-O(3)-Na	124.4(4)	C(6)-C(5)-H(5A)	110.1
C(16)-O(4)-C(13)	106.9(4)	O(2)-C(5)-H(5B)	110.1
C(16)-O(4)-Na	120.6(3)	C(6)-C(5)-H(5B)	110.1
C(13)-O(4)-Na	132.0(3)	H(5A)-C(5)-H(5B)	108.4
C(24)-O(5)-C(21)	104.8(4)	C(7)-C(6)-C(5)	101.8(5)
C(24)-O(5)-Na	125.4(2)	C(7)-C(6)-H(6A)	111.4
C(21)-O(5)-Na	126.7(3)	C(5)-C(6)-H(6A)	111.4
C(17)-O(6)-C(20)	106.6(3)	C(7)-C(6)-H(6B)	111.4

C(5)-C(6)-H(6B)	111.4	C(12)-C(11)-C(10)	108.5(6)
H(6A)-C(6)-H(6B)	109.3	C(12)-C(11)-H(11A)	110.0
C(8A)-C(7)-C(6)	97.4(7)	C(10)-C(11)-H(11A)	110.0
C(8A)-C(7)-C(8B)	57.2(7)	C(12)-C(11)-H(11B)	110.0
C(6)-C(7)-C(8B)	111.9(7)	C(10)-C(11)-H(11B)	110.0
C(8A)-C(7)-H(7A)	112.3	H(11A)-C(11)-H(11B)	108.4
C(6)-C(7)-H(7A)	112.3	C(11)-C(12)-O(3)	105.4(5)
C(8B)-C(7)-H(7A)	55.4	C(11)-C(12)-H(12A)	110.7
C(8A)-C(7)-H(7B)	112.3	O(3)-C(12)-H(12A)	110.7
C(6)-C(7)-H(7B)	112.3	C(11)-C(12)-H(12B)	110.7
C(8B)-C(7)-H(7B)	135.6	O(3)-C(12)-H(12B)	110.7
H(7A)-C(7)-H(7B)	109.9	H(12A)-C(12)-H(12B)	108.8
C(7)-C(8A)-O(2)	109.2(9)	O(4)-C(13)-C(14)	101.5(4)
C(7)-C(8A)-H(8A)	109.8	O(4)-C(13)-H(13A)	111.5
O(2)-C(8A)-H(8A)	109.8	C(14)-C(13)-H(13A)	111.5
C(7)-C(8A)-H(8B)	109.8	O(4)-C(13)-H(13B)	111.5
O(2)-C(8A)-H(8B)	109.8	C(14)-C(13)-H(13B)	111.5
H(8A)-C(8A)-H(8B)	108.3	H(13A)-C(13)-H(13B)	109.3
C(7)-C(8B)-O(2)	88.0(8)	C(15)-C(14)-C(13)	103.9(4)
C(7)-C(8B)-H(8C)	114.0	C(15)-C(14)-H(14A)	111.0
O(2)-C(8B)-H(8C)	114.0	C(13)-C(14)-H(14A)	111.0
C(7)-C(8B)-H(8D)	114.0	C(15)-C(14)-H(14B)	111.0
O(2)-C(8B)-H(8D)	114.0	C(13)-C(14)-H(14B)	111.0
H(8C)-C(8B)-H(8D)	111.2	H(14A)-C(14)-H(14B)	109.0
O(3)-C(9)-C(10)	103.6(5)	C(14)-C(15)-C(16)	100.0(4)
O(3)-C(9)-H(9A)	111.0	C(14)-C(15)-H(15A)	111.8
C(10)-C(9)-H(9A)	111.0	C(16)-C(15)-H(15A)	111.8
O(3)-C(9)-H(9B)	111.0	C(14)-C(15)-H(15B)	111.8
C(10)-C(9)-H(9B)	111.0	C(16)-C(15)-H(15B)	111.8
H(9A)-C(9)-H(9B)	109.0	H(15A)-C(15)-H(15B)	109.5
C(9)-C(10)-C(11)	101.9(5)	O(4)-C(16)-C(15)	110.0(4)
C(9)-C(10)-H(10A)	111.4	O(4)-C(16)-H(16A)	109.7
C(11)-C(10)-H(10A)	111.4	C(15)-C(16)-H(16A)	109.7
C(9)-C(10)-H(10B)	111.4	O(4)-C(16)-H(16B)	109.7
C(11)-C(10)-H(10B)	111.4	C(15)-C(16)-H(16B)	109.7
H(10A)-C(10)-H(10B)	109.3	H(16A)-C(16)-H(16B)	108.2

O(6)-C(17)-C(18)	109.5(4)	C(22)-C(23)-C(24)	102.7(4)
O(6)-C(17)-H(17A)	109.8	C(22)-C(23)-H(23A)	111.2
C(18)-C(17)-H(17A)	109.8	C(24)-C(23)-H(23A)	111.2
O(6)-C(17)-H(17B)	109.8	C(22)-C(23)-H(23B)	111.2
C(18)-C(17)-H(17B)	109.8	C(24)-C(23)-H(23B)	111.2
H(17A)-C(17)-H(17B)	108.2	H(23A)-C(23)-H(23B)	109.1
C(17)-C(18)-C(19)	105.1(3)	O(5)-C(24)-C(23)	107.1(4)
C(17)-C(18)-H(18A)	110.7	O(5)-C(24)-H(24A)	110.3
C(19)-C(18)-H(18A)	110.7	C(23)-C(24)-H(24A)	110.3
C(17)-C(18)-H(18B)	110.7	O(5)-C(24)-H(24B)	110.3
C(19)-C(18)-H(18B)	110.7	C(23)-C(24)-H(24B)	110.3
H(18A)-C(18)-H(18B)	108.8	H(24A)-C(24)-H(24B)	108.5
C(18)-C(19)-C(20)	103.5(4)	C(30)-C(25)-C(26)	114.7(3)
C(18)-C(19)-H(19A)	111.1	C(30)-C(25)-B(1)	124.8(3)
C(20)-C(19)-H(19A)	111.1	C(26)-C(25)-B(1)	120.5(3)
C(18)-C(19)-H(19B)	111.1	C(27)-C(26)-C(25)	122.4(4)
C(20)-C(19)-H(19B)	111.1	C(27)-C(26)-H(26)	118.8
H(19A)-C(19)-H(19B)	109.0	C(25)-C(26)-H(26)	118.8
O(6)-C(20)-C(19)	106.2(3)	C(28)-C(27)-C(26)	120.3(3)
O(6)-C(20)-H(20A)	110.5	C(28)-C(27)-H(27)	119.9
C(19)-C(20)-H(20A)	110.5	C(26)-C(27)-H(27)	119.9
O(6)-C(20)-H(20B)	110.5	C(27)-C(28)-C(29)	119.7(4)
C(19)-C(20)-H(20B)	110.5	C(27)-C(28)-H(28)	120.1
H(20A)-C(20)-H(20B)	108.7	C(29)-C(28)-H(28)	120.1
C(22)-C(21)-O(5)	109.5(4)	C(28)-C(29)-C(30)	119.7(4)
C(22)-C(21)-H(21A)	109.8	C(28)-C(29)-H(29)	120.2
O(5)-C(21)-H(21A)	109.8	C(30)-C(29)-H(29)	120.2
C(22)-C(21)-H(21B)	109.8	C(25)-C(30)-C(29)	123.2(3)
O(5)-C(21)-H(21B)	109.8	C(25)-C(30)-H(30)	118.4
H(21A)-C(21)-H(21B)	108.2	C(29)-C(30)-H(30)	118.4
C(21)-C(22)-C(23)	107.6(4)	B(1)-C(31)-P(1)	114.2(2)
C(21)-C(22)-H(22A)	110.2	B(1)-C(31)-H(31A)	108.7
C(23)-C(22)-H(22A)	110.2	P(1)-C(31)-H(31A)	108.7
C(21)-C(22)-H(22B)	110.2	B(1)-C(31)-H(31B)	108.7
C(23)-C(22)-H(22B)	110.2	P(1)-C(31)-H(31B)	108.7
H(22A)-C(22)-H(22B)	108.5	H(31A)-C(31)-H(31B)	107.6

B(1)-C(32)-P(2)	115.4(2)	C(43)-C(42)-C(41)	119.9(3)
B(1)-C(32)-H(32A)	108.4	C(43)-C(42)-H(42)	120.1
P(2)-C(32)-H(32A)	108.4	C(41)-C(42)-H(42)	120.1
B(1)-C(32)-H(32B)	108.4	C(42)-C(43)-C(44)	120.2(3)
P(2)-C(32)-H(32B)	108.4	C(42)-C(43)-H(43)	119.9
H(32A)-C(32)-H(32B)	107.5	C(44)-C(43)-H(43)	119.9
B(1)-C(33)-P(3)	117.1(2)	C(43)-C(44)-C(45)	120.0(3)
B(1)-C(33)-H(33A)	108.0	C(43)-C(44)-H(44)	120.0
P(3)-C(33)-H(33A)	108.0	C(45)-C(44)-H(44)	120.0
B(1)-C(33)-H(33B)	108.0	C(44)-C(45)-C(40)	120.5(3)
P(3)-C(33)-H(33B)	108.0	C(44)-C(45)-H(45)	119.7
H(33A)-C(33)-H(33B)	107.3	C(40)-C(45)-H(45)	119.7
C(35)-C(34)-C(39)	119.1(3)	C(51)-C(46)-C(47)	118.5(3)
C(35)-C(34)-P(1)	121.3(3)	C(51)-C(46)-P(2)	117.0(3)
C(39)-C(34)-P(1)	119.5(2)	C(47)-C(46)-P(2)	124.5(3)
C(36)-C(35)-C(34)	120.3(3)	C(46)-C(47)-C(48)	120.4(4)
C(36)-C(35)-H(35)	119.8	C(46)-C(47)-H(47)	119.8
C(34)-C(35)-H(35)	119.8	C(48)-C(47)-H(47)	119.8
C(37)-C(36)-C(35)	120.4(3)	C(49)-C(48)-C(47)	120.5(4)
C(37)-C(36)-H(36)	119.8	C(49)-C(48)-H(48)	119.8
C(35)-C(36)-H(36)	119.8	C(47)-C(48)-H(48)	119.8
C(36)-C(37)-C(38)	119.9(3)	C(48)-C(49)-C(50)	119.3(3)
C(36)-C(37)-H(37)	120.1	C(48)-C(49)-H(49)	120.3
C(38)-C(37)-H(37)	120.1	C(50)-C(49)-H(49)	120.3
C(37)-C(38)-C(39)	120.2(3)	C(51)-C(50)-C(49)	120.3(4)
C(37)-C(38)-H(38)	119.9	C(51)-C(50)-H(50)	119.8
C(39)-C(38)-H(38)	119.9	C(49)-C(50)-H(50)	119.8
C(34)-C(39)-C(38)	120.1(3)	C(46)-C(51)-C(50)	120.8(4)
C(34)-C(39)-H(39)	119.9	C(46)-C(51)-H(51)	119.6
C(38)-C(39)-H(39)	119.9	C(50)-C(51)-H(51)	119.6
C(41)-C(40)-C(45)	118.4(3)	C(57)-C(52)-C(53)	117.5(3)
C(41)-C(40)-P(1)	123.4(3)	C(57)-C(52)-P(2)	122.3(2)
C(45)-C(40)-P(1)	118.2(3)	C(53)-C(52)-P(2)	120.2(3)
C(40)-C(41)-C(42)	120.9(3)	C(54)-C(53)-C(52)	121.5(4)
C(40)-C(41)-H(41)	119.6	C(54)-C(53)-H(53)	119.2
C(42)-C(41)-H(41)	119.6	C(52)-C(53)-H(53)	119.2

C(55)-C(54)-C(53)	120.3(3)	C(67)-C(66)-C(65)	120.1(3)
C(55)-C(54)-H(54)	119.8	C(67)-C(66)-H(66)	119.9
C(53)-C(54)-H(54)	119.8	C(65)-C(66)-H(66)	119.9
C(54)-C(55)-C(56)	119.0(3)	C(66)-C(67)-C(68)	119.7(3)
C(54)-C(55)-H(55)	120.5	C(66)-C(67)-H(67)	120.2
C(56)-C(55)-H(55)	120.5	C(68)-C(67)-H(67)	120.2
C(55)-C(56)-C(57)	120.2(3)	C(67)-C(68)-C(69)	120.0(3)
C(55)-C(56)-H(56)	119.9	C(67)-C(68)-H(68)	120.0
C(57)-C(56)-H(56)	119.9	C(69)-C(68)-H(68)	120.0
C(52)-C(57)-C(56)	121.4(3)	C(68)-C(69)-C(64)	121.0(3)
C(52)-C(57)-H(57)	119.3	C(68)-C(69)-H(69)	119.5
C(56)-C(57)-H(57)	119.3	C(64)-C(69)-H(69)	119.5
C(59)-C(58)-C(63)	118.0(3)	C(71)-C(70)-C(75)	112.5(4)
C(59)-C(58)-P(3)	120.9(3)	C(71)-C(70)-B(2)	122.5(3)
C(63)-C(58)-P(3)	120.9(3)	C(75)-C(70)-B(2)	124.6(3)
C(58)-C(59)-C(60)	121.2(3)	C(70)-C(71)-C(72)	124.1(4)
C(58)-C(59)-H(59)	119.4	C(70)-C(71)-H(71)	117.9
C(60)-C(59)-H(59)	119.4	C(72)-C(71)-H(71)	117.9
C(61)-C(60)-C(59)	119.2(3)	C(73)-C(72)-C(71)	119.2(5)
C(61)-C(60)-H(60)	120.4	C(73)-C(72)-H(72)	120.4
C(59)-C(60)-H(60)	120.4	C(71)-C(72)-H(72)	120.4
C(62)-C(61)-C(60)	120.7(3)	C(74)-C(73)-C(72)	118.0(4)
C(62)-C(61)-H(61)	119.6	C(74)-C(73)-H(73)	121.0
C(60)-C(61)-H(61)	119.6	C(72)-C(73)-H(73)	121.0
C(61)-C(62)-C(63)	119.4(3)	C(73)-C(74)-C(75)	122.1(4)
C(61)-C(62)-H(62)	120.3	C(73)-C(74)-H(74)	119.0
C(63)-C(62)-H(62)	120.3	C(75)-C(74)-H(74)	119.0
C(62)-C(63)-C(58)	121.4(3)	C(70)-C(75)-C(74)	123.4(4)
C(62)-C(63)-H(63)	119.3	C(70)-C(75)-H(75)	118.3
C(58)-C(63)-H(63)	119.3	C(74)-C(75)-H(75)	118.3
C(65)-C(64)-C(69)	117.7(3)	B(2)-C(76)-P(5)	113.9(2)
C(65)-C(64)-P(3)	119.0(3)	B(2)-C(76)-H(76A)	108.8
C(69)-C(64)-P(3)	123.2(3)	P(5)-C(76)-H(76A)	108.8
C(64)-C(65)-C(66)	121.4(3)	B(2)-C(76)-H(76B)	108.8
C(64)-C(65)-H(65)	119.3	P(5)-C(76)-H(76B)	108.8
C(66)-C(65)-H(65)	119.3	H(76A)-C(76)-H(76B)	107.7

B(2)-C(77)-P(6)	113.6(2)	C(88)-C(87)-C(86)	119.6(3)
B(2)-C(77)-H(77A)	108.8	C(88)-C(87)-H(87)	120.2
P(6)-C(77)-H(77A)	108.8	C(86)-C(87)-H(87)	120.2
B(2)-C(77)-H(77B)	108.8	C(89)-C(88)-C(87)	119.6(3)
P(6)-C(77)-H(77B)	108.8	C(89)-C(88)-H(88)	120.2
H(77A)-C(77)-H(77B)	107.7	C(87)-C(88)-H(88)	120.2
B(2)-C(78)-P(4)	114.2(2)	C(88)-C(89)-C(90)	120.2(4)
B(2)-C(78)-H(78A)	108.7	C(88)-C(89)-H(89)	119.9
P(4)-C(78)-H(78A)	108.7	C(90)-C(89)-H(89)	119.9
B(2)-C(78)-H(78B)	108.7	C(89)-C(90)-C(85)	121.1(3)
P(4)-C(78)-H(78B)	108.7	C(89)-C(90)-H(90)	119.5
H(78A)-C(78)-H(78B)	107.6	C(85)-C(90)-H(90)	119.5
C(80)-C(79)-C(84)	118.1(3)	C(96)-C(91)-C(92)	118.5(3)
C(80)-C(79)-P(4)	119.3(3)	C(96)-C(91)-P(5)	119.3(3)
C(84)-C(79)-P(4)	122.5(3)	C(92)-C(91)-P(5)	122.1(3)
C(79)-C(80)-C(81)	120.9(3)	C(93)-C(92)-C(91)	120.3(3)
C(79)-C(80)-H(80)	119.5	C(93)-C(92)-H(92)	119.8
C(81)-C(80)-H(80)	119.5	C(91)-C(92)-H(92)	119.8
C(82)-C(81)-C(80)	120.0(4)	C(94)-C(93)-C(92)	120.5(3)
C(82)-C(81)-H(81)	120.0	C(94)-C(93)-H(93)	119.7
C(80)-C(81)-H(81)	120.0	C(92)-C(93)-H(93)	119.7
C(81)-C(82)-C(83)	119.6(3)	C(93)-C(94)-C(95)	120.3(3)
C(81)-C(82)-H(82)	120.2	C(93)-C(94)-H(94)	119.9
C(83)-C(82)-H(82)	120.2	C(95)-C(94)-H(94)	119.9
C(82)-C(83)-C(84)	120.9(4)	C(94)-C(95)-C(96)	119.3(3)
C(82)-C(83)-H(83)	119.5	C(94)-C(95)-H(95)	120.4
C(84)-C(83)-H(83)	119.5	C(96)-C(95)-H(95)	120.4
C(83)-C(84)-C(79)	120.4(3)	C(91)-C(96)-C(95)	121.1(3)
C(83)-C(84)-H(84)	119.8	C(91)-C(96)-H(96)	119.5
C(79)-C(84)-H(84)	119.8	C(95)-C(96)-H(96)	119.5
C(86)-C(85)-C(90)	117.7(3)	C(98)-C(97)-C(102)	118.1(3)
C(86)-C(85)-P(4)	119.4(3)	C(98)-C(97)-P(5)	123.3(3)
C(90)-C(85)-P(4)	122.9(3)	C(102)-C(97)-P(5)	118.5(3)
C(85)-C(86)-C(87)	121.8(3)	C(99)-C(98)-C(97)	120.6(4)
C(85)-C(86)-H(86)	119.1	C(99)-C(98)-H(98)	119.7
C(87)-C(86)-H(86)	119.1	C(97)-C(98)-H(98)	119.7

C(100)-C(99)-C(98)	120.5(4)	C(106)-C(107)-C(108)	119.8(4)
C(100)-C(99)-H(99)	119.7	C(106)-C(107)-H(107)	120.1
C(98)-C(99)-H(99)	119.7	C(108)-C(107)-H(107)	120.1
C(101)-C(100)-C(99)	119.4(3)	C(103)-C(108)-C(107)	122.2(4)
C(101)-C(100)-H(100)	120.3	C(103)-C(108)-H(108)	118.9
C(99)-C(100)-H(100)	120.3	C(107)-C(108)-H(108)	118.9
C(100)-C(101)-C(102)	120.4(4)	C(114)-C(109)-C(110)	118.5(3)
C(100)-C(101)-H(101)	119.8	C(114)-C(109)-P(6)	123.8(3)
C(102)-C(101)-H(101)	119.8	C(110)-C(109)-P(6)	117.7(3)
C(101)-C(102)-C(97)	120.9(3)	C(109)-C(110)-C(111)	120.5(4)
C(101)-C(102)-H(102)	119.6	C(109)-C(110)-H(110)	119.8
C(97)-C(102)-H(102)	119.6	C(111)-C(110)-H(110)	119.8
C(108)-C(103)-C(104)	117.3(3)	C(112)-C(111)-C(110)	120.8(4)
C(108)-C(103)-P(6)	124.2(3)	C(112)-C(111)-H(111)	119.6
C(104)-C(103)-P(6)	118.4(3)	C(110)-C(111)-H(111)	119.6
C(103)-C(104)-C(105)	121.1(4)	C(111)-C(112)-C(113)	119.1(3)
C(103)-C(104)-H(104)	119.5	C(111)-C(112)-H(112)	120.5
C(105)-C(104)-H(104)	119.5	C(113)-C(112)-H(112)	120.5
C(106)-C(105)-C(104)	119.9(4)	C(112)-C(113)-C(114)	120.9(4)
C(106)-C(105)-H(105)	120.1	C(112)-C(113)-H(113)	119.5
C(104)-C(105)-H(105)	120.1	C(114)-C(113)-H(113)	119.5
C(107)-C(106)-C(105)	119.8(3)	C(109)-C(114)-C(113)	120.1(4)
C(107)-C(106)-H(106)	120.1	C(109)-C(114)-H(114)	120.0
C(105)-C(106)-H(106)	120.1	C(113)-C(114)-H(114)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2$x 10^3) for $\{([PhBP_3]Fe)_2N\}\{Na(THF)_5\}\cdot THF$, (**3**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	14(1)	15(1)	18(1)	2(1)	0(1)	0(1)
Fe(2)	14(1)	16(1)	19(1)	2(1)	0(1)	0(1)
N(1A)	22(3)	11(3)	18(3)	-2(2)	-1(2)	3(2)
N(1B)	22(6)	37(6)	31(5)	-3(5)	0(4)	-3(5)
P(1)	15(1)	14(1)	18(1)	0(1)	-1(1)	0(1)
P(2)	16(1)	16(1)	17(1)	0(1)	0(1)	1(1)
P(3)	16(1)	14(1)	18(1)	0(1)	-1(1)	1(1)
P(4)	16(1)	16(1)	20(1)	1(1)	0(1)	-1(1)
P(5)	16(1)	16(1)	20(1)	2(1)	0(1)	0(1)
P(6)	18(1)	17(1)	19(1)	0(1)	0(1)	-1(1)
B(1)	22(3)	16(2)	13(2)	0(2)	3(2)	1(2)
B(2)	17(3)	18(2)	21(2)	1(2)	-1(2)	1(2)
Na	90(2)	54(1)	67(1)	-7(1)	-4(1)	13(1)
O(1)	68(3)	79(3)	76(2)	-12(2)	-1(2)	13(2)
O(2)	61(3)	163(4)	144(4)	-92(3)	-34(3)	40(3)
O(3)	225(6)	163(4)	71(3)	39(3)	53(3)	143(4)
O(4)	90(3)	33(2)	62(2)	-5(2)	4(2)	2(2)
O(5)	95(3)	36(2)	74(3)	-7(2)	31(2)	-13(2)
O(6)	50(2)	56(2)	49(2)	15(2)	-2(2)	-21(2)
C(1)	89(5)	39(3)	69(4)	9(2)	-9(3)	11(3)
C(2)	66(4)	45(3)	32(3)	6(2)	-6(2)	14(3)
C(3)	78(4)	44(3)	60(3)	-2(2)	-20(3)	14(3)
C(4)	88(5)	47(3)	69(4)	-10(3)	-7(3)	-7(3)
C(5)	112(6)	107(5)	84(5)	34(4)	-32(4)	-70(5)
C(6)	145(7)	97(5)	50(4)	24(3)	-11(4)	-49(5)
C(7)	93(6)	153(7)	114(6)	-11(5)	-31(5)	-13(5)
C(8A)	81(10)	140(13)	95(11)	-73(10)	-10(8)	26(8)
C(8B)	62(11)	70(10)	67(11)	16(9)	-16(8)	-8(8)
C(9)	228(9)	170(7)	55(4)	27(4)	32(5)	144(6)
C(10)	87(5)	111(5)	131(6)	-8(5)	39(4)	10(4)
C(11)	123(6)	83(5)	125(6)	9(4)	63(5)	37(4)

C(12)	253(11)	214(9)	134(7)	83(6)	89(7)	194(8)
C(13)	89(5)	34(3)	138(5)	-41(3)	-10(4)	23(3)
C(14)	87(5)	48(3)	83(4)	4(3)	-7(3)	-11(3)
C(15)	79(5)	62(4)	71(4)	-7(3)	-24(3)	8(3)
C(16)	83(5)	72(4)	45(3)	2(3)	10(3)	-4(3)
C(17)	41(4)	89(4)	72(4)	16(3)	8(3)	-1(3)
C(18)	34(3)	76(4)	55(3)	20(3)	4(2)	1(3)
C(19)	49(3)	51(3)	39(3)	13(2)	4(2)	0(2)
C(20)	72(4)	86(4)	61(3)	39(3)	-15(3)	-49(3)
C(21)	196(8)	77(4)	164(7)	-64(5)	121(6)	-64(5)
C(22)	54(4)	43(3)	56(3)	-1(3)	1(3)	-10(2)
C(23)	56(4)	40(3)	70(3)	-10(3)	2(3)	12(2)
C(24)	63(4)	45(3)	73(4)	-4(3)	2(3)	7(3)
C(25)	16(2)	14(2)	22(2)	-8(2)	1(2)	-3(2)
C(26)	18(3)	30(2)	33(2)	1(2)	4(2)	0(2)
C(27)	14(3)	30(2)	43(3)	-5(2)	0(2)	9(2)
C(28)	15(2)	35(2)	38(3)	-11(2)	12(2)	-3(2)
C(29)	19(3)	30(2)	27(2)	-1(2)	8(2)	-8(2)
C(30)	18(2)	20(2)	27(2)	-4(2)	-3(2)	-1(2)
C(31)	18(2)	13(2)	18(2)	-1(1)	3(2)	0(2)
C(32)	12(2)	14(2)	27(2)	2(2)	1(2)	0(2)
C(33)	14(2)	17(2)	17(2)	-1(1)	1(2)	6(2)
C(34)	11(2)	13(2)	20(2)	3(2)	2(2)	-1(2)
C(35)	18(2)	21(2)	22(2)	-1(2)	2(2)	1(2)
C(36)	20(2)	25(2)	19(2)	7(2)	-2(2)	-4(2)
C(37)	20(2)	15(2)	36(2)	6(2)	-1(2)	-3(2)
C(38)	21(2)	19(2)	31(2)	-4(2)	-2(2)	5(2)
C(39)	10(2)	21(2)	23(2)	2(2)	1(2)	-3(2)
C(40)	21(2)	11(2)	14(2)	4(1)	-2(2)	1(2)
C(41)	16(2)	19(2)	19(2)	-1(2)	0(2)	5(2)
C(42)	36(3)	21(2)	22(2)	-3(2)	2(2)	7(2)
C(43)	33(3)	27(2)	21(2)	-8(2)	-5(2)	-3(2)
C(44)	23(3)	24(2)	27(2)	-3(2)	-5(2)	-3(2)
C(45)	23(2)	17(2)	19(2)	0(2)	3(2)	3(2)
C(46)	16(2)	17(2)	18(2)	-4(2)	-1(2)	2(2)
C(47)	25(2)	21(2)	21(2)	-6(2)	1(2)	1(2)

C(48)	46(3)	21(2)	25(2)	2(2)	-5(2)	-3(2)
C(49)	43(3)	18(2)	37(3)	-3(2)	-15(2)	9(2)
C(50)	38(3)	28(2)	34(3)	-8(2)	0(2)	16(2)
C(51)	23(2)	26(2)	24(2)	-3(2)	-1(2)	1(2)
C(52)	16(2)	18(2)	19(2)	-2(2)	1(2)	6(2)
C(53)	26(3)	39(2)	27(2)	4(2)	-3(2)	-12(2)
C(54)	25(3)	49(3)	26(2)	0(2)	-6(2)	-5(2)
C(55)	31(3)	42(2)	18(2)	0(2)	-2(2)	10(2)
C(56)	45(3)	28(2)	24(2)	4(2)	12(2)	0(2)
C(57)	31(3)	17(2)	23(2)	-5(2)	1(2)	2(2)
C(58)	22(2)	14(2)	16(2)	3(2)	2(2)	-3(2)
C(59)	25(2)	20(2)	22(2)	2(2)	-4(2)	3(2)
C(60)	35(3)	24(2)	28(2)	2(2)	-10(2)	-5(2)
C(61)	51(3)	20(2)	22(2)	-1(2)	-3(2)	-9(2)
C(62)	43(3)	19(2)	29(2)	-3(2)	3(2)	5(2)
C(63)	21(2)	24(2)	33(2)	0(2)	1(2)	1(2)
C(64)	22(2)	12(2)	18(2)	-2(2)	-2(2)	0(2)
C(65)	17(2)	23(2)	25(2)	1(2)	1(2)	-1(2)
C(66)	29(3)	26(2)	25(2)	6(2)	5(2)	-4(2)
C(67)	37(3)	28(2)	24(2)	7(2)	-7(2)	-2(2)
C(68)	24(3)	32(2)	28(2)	3(2)	-9(2)	0(2)
C(69)	18(2)	23(2)	26(2)	3(2)	3(2)	-1(2)
C(70)	26(3)	24(2)	17(2)	9(2)	4(2)	4(2)
C(71)	27(3)	96(4)	45(3)	-3(3)	0(2)	-17(3)
C(72)	57(4)	112(4)	44(3)	-8(3)	21(3)	-32(3)
C(73)	20(3)	66(3)	55(3)	-4(3)	14(2)	-3(2)
C(74)	17(3)	114(4)	59(4)	24(3)	-3(2)	-17(3)
C(75)	30(3)	88(4)	34(3)	7(2)	1(2)	-11(3)
C(76)	14(2)	17(2)	20(2)	1(2)	0(2)	2(2)
C(77)	20(2)	16(2)	21(2)	4(2)	4(2)	5(2)
C(78)	14(2)	18(2)	20(2)	2(2)	1(2)	-2(2)
C(79)	9(2)	14(2)	27(2)	-2(2)	1(2)	-1(2)
C(80)	22(2)	21(2)	41(3)	-2(2)	-1(2)	-6(2)
C(81)	26(3)	16(2)	49(3)	-10(2)	0(2)	-1(2)
C(82)	30(3)	15(2)	55(3)	-1(2)	-10(2)	2(2)
C(83)	32(3)	24(2)	39(2)	7(2)	-11(2)	-3(2)

C(84)	23(3)	20(2)	37(2)	0(2)	-1(2)	3(2)
C(85)	19(2)	11(2)	21(2)	-2(2)	2(2)	2(2)
C(86)	17(2)	13(2)	28(2)	-1(2)	-1(2)	1(2)
C(87)	28(3)	22(2)	20(2)	2(2)	1(2)	0(2)
C(88)	32(3)	21(2)	30(2)	-3(2)	-6(2)	2(2)
C(89)	19(2)	29(2)	38(3)	-11(2)	0(2)	-7(2)
C(90)	28(3)	26(2)	25(2)	-3(2)	8(2)	-1(2)
C(91)	14(2)	11(2)	25(2)	2(2)	2(2)	-1(2)
C(92)	19(2)	18(2)	24(2)	4(2)	4(2)	-1(2)
C(93)	15(2)	30(2)	28(2)	5(2)	-4(2)	-1(2)
C(94)	27(3)	25(2)	23(2)	7(2)	-3(2)	1(2)
C(95)	22(2)	22(2)	23(2)	9(2)	5(2)	3(2)
C(96)	19(2)	20(2)	25(2)	2(2)	-4(2)	0(2)
C(97)	21(2)	15(2)	17(2)	3(2)	0(2)	2(2)
C(98)	21(3)	19(2)	55(3)	0(2)	3(2)	-3(2)
C(99)	23(3)	25(2)	68(3)	-4(2)	10(2)	11(2)
C(100)	35(3)	19(2)	48(3)	-1(2)	2(2)	2(2)
C(101)	22(3)	23(2)	43(3)	2(2)	-2(2)	-6(2)
C(102)	18(2)	21(2)	30(2)	2(2)	0(2)	1(2)
C(103)	25(3)	20(2)	15(2)	-3(2)	5(2)	-4(2)
C(104)	32(3)	29(2)	37(2)	-10(2)	1(2)	-4(2)
C(105)	27(3)	41(3)	51(3)	-12(2)	-3(2)	-10(2)
C(106)	50(3)	28(2)	23(2)	-9(2)	9(2)	-20(2)
C(107)	43(3)	24(2)	50(3)	-10(2)	3(2)	0(2)
C(108)	28(3)	27(2)	36(2)	-4(2)	2(2)	-3(2)
C(109)	19(2)	22(2)	13(2)	-4(2)	0(2)	-4(2)
C(110)	28(3)	31(2)	24(2)	7(2)	0(2)	1(2)
C(111)	22(3)	32(2)	32(2)	3(2)	-1(2)	6(2)
C(112)	34(3)	27(2)	28(2)	6(2)	-6(2)	-1(2)
C(113)	46(3)	52(3)	20(2)	13(2)	10(2)	1(2)
C(114)	32(3)	38(2)	25(2)	3(2)	3(2)	8(2)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for $\{([PhBP_3]Fe)_2N\}\{Na(THF)_5\}\cdot THF$, (**3**).

	x	y	z	U(eq)
H(1A)	8895	4816	6915	79
H(1B)	8753	4611	7273	79
H(2A)	8148	3194	7164	58
H(2B)	8065	3573	6811	58
H(3A)	9065	2154	7052	74
H(3B)	8908	2444	6695	74
H(4A)	9866	3730	7344	82
H(4B)	10147	4480	7087	82
H(5A)	642	1088	5878	124
H(5B)	1341	1353	5656	124
H(6A)	537	1168	5233	118
H(6B)	-73	645	5454	118
H(7A)	-130	2606	5242	146
H(7B)	-867	1956	5351	146
H(8A)	-420	2015	5835	127
H(8B)	-378	3114	5711	127
H(8C)	-168	3619	5553	81
H(8D)	499	3319	5312	81
H(9A)	1223	4187	5110	180
H(9B)	2077	4633	5227	180
H(10A)	1047	5683	4897	130
H(10B)	1659	6188	5152	130
H(11A)	480	6630	5354	129
H(11B)	22	5679	5221	129
H(12A)	178	5170	5679	237
H(12B)	895	5919	5765	237
H(13A)	2936	3062	5248	105
H(13B)	3158	2265	5514	105
H(14A)	4371	3038	5660	88
H(14B)	4337	3148	5289	88

H(15A)	3850	4704	5308	86
H(15B)	4494	4683	5602	86
H(16A)	3558	4489	5940	79
H(16B)	3009	5032	5677	79
H(17A)	3142	3076	6395	80
H(17B)	3293	1982	6283	80
H(18A)	3197	2580	6870	66
H(18B)	3327	1479	6756	66
H(19A)	1890	2355	6910	55
H(19B)	2104	1211	6912	55
H(20A)	1753	1036	6404	88
H(20B)	1160	1914	6477	88
H(21A)	2611	5522	6316	169
H(21B)	1903	5931	6085	169
H(22A)	1347	6637	6440	61
H(22B)	2205	6546	6624	61
H(23A)	838	5655	6782	66
H(23B)	1708	5523	6957	66
H(24A)	1925	4133	6711	72
H(24B)	983	4128	6617	72
H(26)	2647	9228	6588	32
H(27)	1346	9306	6741	35
H(28)	958	8359	7148	35
H(29)	1854	7250	7384	30
H(30)	3156	7163	7231	26
H(31A)	4444	6783	6976	20
H(31B)	4458	7630	7229	20
H(32A)	3618	8065	6284	21
H(32B)	3613	7017	6443	21
H(33A)	4437	9514	6972	19
H(33B)	3897	9692	6661	19
H(35)	5916	6780	7577	24
H(36)	6515	5345	7767	26
H(37)	6990	4206	7428	28
H(38)	6894	4505	6898	28
H(39)	6349	5975	6706	22

H(41)	4856	8895	7427	22
H(42)	5315	9980	7816	32
H(43)	6677	10186	7926	33
H(44)	7588	9346	7643	30
H(45)	7135	8337	7231	23
H(47)	4141	5675	6592	27
H(48)	4367	3995	6603	37
H(49)	5321	3312	6305	40
H(50)	6060	4315	5994	40
H(51)	5871	5991	5996	29
H(53)	3743	6461	5829	37
H(54)	3372	6633	5307	40
H(55)	4031	7736	5006	37
H(56)	5045	8708	5239	38
H(57)	5417	8528	5763	29
H(59)	6761	9900	6853	27
H(60)	7328	11224	7127	35
H(61)	6581	12638	7180	37
H(62)	5289	12741	6960	36
H(63)	4729	11419	6689	31
H(65)	5954	10560	6088	26
H(66)	5562	11297	5617	32
H(67)	4253	11148	5412	36
H(68)	3310	10363	5697	34
H(69)	3691	9672	6176	27
H(71)	10086	8597	5335	67
H(72)	11352	8804	5147	84
H(73)	12497	8498	5478	56
H(74)	12339	8370	5992	76
H(75)	11098	8146	6181	61
H(76A)	9820	8237	6405	21
H(76B)	9993	7185	6266	21
H(77A)	9098	6779	5722	23
H(77B)	9055	7597	5459	23
H(78A)	8951	9474	5697	21
H(78B)	9582	9765	5974	21

H(80)	7577	10976	6487	34
H(81)	6871	12400	6350	37
H(82)	6768	12913	5837	41
H(83)	7380	12021	5464	39
H(84)	8051	10580	5593	32
H(86)	8059	9101	6802	24
H(87)	8712	9408	7285	28
H(88)	9923	10251	7316	34
H(89)	10433	10856	6867	35
H(90)	9775	10553	6386	31
H(92)	10053	7170	6839	24
H(93)	10223	6937	7370	30
H(94)	9124	6769	7665	30
H(95)	7835	6809	7429	26
H(96)	7659	7064	6895	25
H(98)	9826	5748	6250	38
H(99)	9738	4084	6155	46
H(100)	8509	3297	6144	41
H(101)	7373	4171	6248	36
H(102)	7450	5838	6340	28
H(104)	6325	7185	5465	40
H(105)	5626	5799	5285	48
H(106)	6281	4307	5264	40
H(107)	7625	4200	5421	47
H(108)	8314	5580	5606	37
H(110)	6641	9016	5668	33
H(111)	6118	10093	5291	34
H(112)	6759	10334	4840	36
H(113)	7889	9432	4752	47
H(114)	8363	8251	5109	37

Table 11. Crystal data and structure refinement for {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}·THF, (**4**).

Identification code	sdb42	
Empirical formula	C_{75} H_{100} B Fe N_2 O P_3	
Formula weight	1205.14	
Temperature	96(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.173(3) Å	α= 71.610(4)°.
	b = 14.051(4) Å	β= 79.790(4)°.
	c = 22.131(6) Å	γ = 68.373(4)°.
Volume	3331.1(14) $Å^3$	
Z	2	
Density (calculated)	1.202 Mg/m^3	
Absorption coefficient	0.344 mm^{-1}	
F(000)	1296	
Crystal size	0.15 x 0.37 x 0.37 mm^3	
Theta range for data collection	1.62 to 28.59°.	
Index ranges	-16<=h<=15, -18<=k<=18, -29<=l<=29	
Reflections collected	70679	
Independent reflections	15685 [R(int) = 0.0634]	
Completeness to theta = 28.59°	92.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15685 / 0 / 752	
Goodness-of-fit on F^2	1.826	
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.0972	
R indices (all data)	R1 = 0.0755, wR2 = 0.1030	
Largest diff. peak and hole	0.983 and -0.534 e.$Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}·THF, (**4**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3757(1)	8835(1)	2881(1)	15(1)
P(1)	3533(1)	10344(1)	2198(1)	15(1)
P(2)	5036(1)	8998(1)	3358(1)	15(1)
P(3)	5200(1)	8126(1)	2270(1)	15(1)
N(1)	2649(1)	8421(1)	3256(1)	16(1)
N(2)	5645(2)	3657(1)	2258(1)	22(1)
B(1)	6080(2)	9849(2)	2122(1)	16(1)
O(1)	463(2)	6755(2)	1787(1)	63(1)
C(1)	7091(2)	10383(2)	1743(1)	17(1)
C(2)	7042(2)	10919(2)	1090(1)	23(1)
C(3)	7851(2)	11406(2)	750(1)	27(1)
C(4)	8770(2)	11380(2)	1052(1)	29(1)
C(5)	8860(2)	10860(2)	1692(1)	26(1)
C(6)	8044(2)	10368(2)	2027(1)	20(1)
C(7)	4776(2)	10826(2)	2049(1)	16(1)
C(8)	6090(2)	8939(2)	1785(1)	16(1)
C(9)	6332(2)	9275(2)	2886(1)	16(1)
C(10)	2239(2)	11483(2)	2339(1)	18(1)
C(11)	1305(2)	11315(2)	2756(1)	32(1)
C(12)	321(2)	12167(2)	2854(1)	41(1)
C(13)	258(2)	13187(2)	2537(1)	37(1)
C(14)	1180(2)	13374(2)	2119(1)	37(1)
C(15)	2163(2)	12528(2)	2022(1)	28(1)
C(16)	3159(2)	10410(2)	1407(1)	17(1)
C(17)	2258(2)	10033(2)	1401(1)	24(1)

C(18)	1951(2)	9996(2)	843(1)	30(1)
C(19)	2558(2)	10311(2)	271(1)	31(1)
C(20)	3464(2)	10679(2)	269(1)	35(1)
C(21)	3751(2)	10747(2)	829(1)	27(1)
C(22)	4467(2)	10001(2)	3818(1)	19(1)
C(23)	5198(2)	10348(2)	4047(1)	26(1)
C(24)	4744(2)	11070(2)	4406(1)	33(1)
C(25)	3546(2)	11445(2)	4551(1)	36(1)
C(26)	2806(2)	11098(2)	4340(1)	38(1)
C(27)	3260(2)	10378(2)	3971(1)	28(1)
C(28)	5592(2)	7812(2)	4036(1)	16(1)
C(29)	4756(2)	7429(2)	4446(1)	26(1)
C(30)	5084(2)	6528(2)	4953(1)	31(1)
C(31)	6269(2)	5980(2)	5055(1)	26(1)
C(32)	7108(2)	6345(2)	4650(1)	23(1)
C(33)	6779(2)	7255(2)	4147(1)	19(1)
C(34)	6288(2)	6858(2)	2693(1)	16(1)
C(35)	5843(2)	6163(2)	3179(1)	21(1)
C(36)	6590(2)	5224(2)	3538(1)	28(1)
C(37)	7811(2)	4968(2)	3430(1)	30(1)
C(38)	8262(2)	5660(2)	2954(1)	29(1)
C(39)	7513(2)	6587(2)	2588(1)	23(1)
C(40)	4758(2)	7631(2)	1702(1)	19(1)
C(41)	3727(2)	7363(2)	1844(1)	25(1)
C(42)	3333(2)	7049(2)	1414(1)	34(1)
C(43)	3946(2)	7029(2)	828(1)	37(1)
C(44)	4963(2)	7280(2)	682(1)	38(1)
C(45)	5385(2)	7563(2)	1121(1)	29(1)
C(46)	1684(2)	8075(2)	3594(1)	18(1)
C(47)	1168(2)	8542(2)	4165(1)	27(1)

C(48)	688(2)	8410(2)	3151(1)	22(1)
C(49)	2132(2)	6857(2)	3842(1)	25(1)
C(50)	160(2)	8132(2)	4525(1)	36(1)
C(51)	-819(2)	8476(2)	4079(1)	32(1)
C(52)	-325(2)	8009(2)	3510(1)	24(1)
C(53)	147(2)	6797(2)	3743(1)	26(1)
C(54)	1118(2)	6450(2)	4197(1)	30(1)
C(55)	623(2)	6915(2)	4760(1)	41(1)
C(56)	6367(2)	4398(2)	1968(1)	25(1)
C(57)	7477(2)	3975(2)	1565(1)	32(1)
C(58)	8101(2)	4798(2)	1287(1)	37(1)
C(59)	9172(2)	4424(2)	837(1)	52(1)
C(60)	6358(2)	2618(2)	2703(1)	24(1)
C(61)	6817(2)	2707(2)	3271(1)	26(1)
C(62)	7563(2)	1611(2)	3639(1)	28(1)
C(63)	7991(2)	1617(2)	4242(1)	36(1)
C(64)	4567(2)	4262(2)	2614(1)	24(1)
C(65)	3700(2)	3685(2)	2960(1)	28(1)
C(66)	2567(2)	4471(2)	3168(1)	37(1)
C(67)	1690(2)	3969(2)	3586(1)	38(1)
C(68)	5286(2)	3341(2)	1747(1)	24(1)
C(69)	4472(2)	4235(2)	1271(1)	30(1)
C(70)	4325(2)	3851(2)	732(1)	29(1)
C(71)	3376(2)	4670(2)	299(1)	43(1)
C(72)	16(2)	7888(2)	1659(1)	46(1)
C(73)	-240(3)	8322(2)	985(1)	54(1)
C(74)	-532(3)	7480(2)	840(1)	61(1)
C(75)	280(3)	6495(2)	1257(2)	74(1)

Table 13. Bond lengths [Å] and angles [°] for {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}·THF, (**4**).

Fe(1)-N(1)	1.6507(16)	C(4)-C(5)	1.377(3)
Fe(1)-P(1)	2.1330(7)	C(5)-C(6)	1.390(3)
Fe(1)-P(2)	2.1432(7)	C(10)-C(11)	1.375(3)
Fe(1)-P(3)	2.1504(7)	C(10)-C(15)	1.390(3)
P(1)-C(7)	1.8158(19)	C(11)-C(12)	1.388(3)
P(1)-C(10)	1.849(2)	C(12)-C(13)	1.362(3)
P(1)-C(16)	1.851(2)	C(13)-C(14)	1.372(3)
P(2)-C(9)	1.8280(19)	C(14)-C(15)	1.383(3)
P(2)-C(22)	1.853(2)	C(16)-C(21)	1.387(3)
P(2)-C(28)	1.854(2)	C(16)-C(17)	1.387(3)
P(3)-C(8)	1.8323(19)	C(17)-C(18)	1.372(3)
P(3)-C(40)	1.850(2)	C(18)-C(19)	1.379(3)
P(3)-C(34)	1.858(2)	C(19)-C(20)	1.379(3)
N(1)-C(46)	1.434(2)	C(20)-C(21)	1.386(3)
N(2)-C(64)	1.516(3)	C(22)-C(27)	1.384(3)
N(2)-C(68)	1.518(2)	C(22)-C(23)	1.387(3)
N(2)-C(60)	1.522(2)	C(23)-C(24)	1.380(3)
N(2)-C(56)	1.524(3)	C(24)-C(25)	1.371(3)
B(1)-C(1)	1.643(3)	C(25)-C(26)	1.372(3)
B(1)-C(9)	1.657(3)	C(26)-C(27)	1.394(3)
B(1)-C(7)	1.666(3)	C(28)-C(29)	1.385(3)
B(1)-C(8)	1.668(3)	C(28)-C(33)	1.389(3)
O(1)-C(75)	1.408(4)	C(29)-C(30)	1.383(3)
O(1)-C(72)	1.429(3)	C(30)-C(31)	1.382(3)
C(1)-C(2)	1.402(3)	C(31)-C(32)	1.373(3)
C(1)-C(6)	1.404(3)	C(32)-C(33)	1.384(3)
C(2)-C(3)	1.382(3)	C(34)-C(35)	1.386(3)
C(3)-C(4)	1.385(3)	C(34)-C(39)	1.393(3)

C(35)-C(36)	1.383(3)	C(66)-C(67)	1.512(3)
C(36)-C(37)	1.389(3)	C(68)-C(69)	1.511(3)
C(37)-C(38)	1.377(3)	C(69)-C(70)	1.517(3)
C(38)-C(39)	1.380(3)	C(70)-C(71)	1.515(3)
C(40)-C(45)	1.385(3)	C(72)-C(73)	1.466(4)
C(40)-C(41)	1.396(3)	C(73)-C(74)	1.490(4)
C(41)-C(42)	1.384(3)	C(74)-C(75)	1.501(4)
C(42)-C(43)	1.378(3)		
C(43)-C(44)	1.368(3)	N(1)-Fe(1)-P(1)	123.87(6)
C(44)-C(45)	1.392(3)	N(1)-Fe(1)-P(2)	123.64(6)
C(46)-C(49)	1.534(3)	P(1)-Fe(1)-P(2)	92.68(3)
C(46)-C(47)	1.536(3)	N(1)-Fe(1)-P(3)	128.81(6)
C(46)-C(48)	1.538(3)	P(1)-Fe(1)-P(3)	88.91(3)
C(47)-C(50)	1.536(3)	P(2)-Fe(1)-P(3)	87.77(3)
C(48)-C(52)	1.534(3)	C(7)-P(1)-C(10)	104.27(9)
C(49)-C(54)	1.537(3)	C(7)-P(1)-C(16)	106.14(9)
C(50)-C(51)	1.523(3)	C(10)-P(1)-C(16)	96.97(9)
C(50)-C(55)	1.531(3)	C(7)-P(1)-Fe(1)	116.08(7)
C(51)-C(52)	1.529(3)	C(10)-P(1)-Fe(1)	117.34(7)
C(52)-C(53)	1.525(3)	C(16)-P(1)-Fe(1)	113.78(7)
C(53)-C(54)	1.528(3)	C(9)-P(2)-C(22)	103.93(9)
C(54)-C(55)	1.517(3)	C(9)-P(2)-C(28)	107.00(9)
C(56)-C(57)	1.513(3)	C(22)-P(2)-C(28)	97.44(9)
C(57)-C(58)	1.525(3)	C(9)-P(2)-Fe(1)	118.30(7)
C(58)-C(59)	1.529(3)	C(22)-P(2)-Fe(1)	116.36(7)
C(60)-C(61)	1.518(3)	C(28)-P(2)-Fe(1)	111.43(7)
C(61)-C(62)	1.517(3)	C(8)-P(3)-C(40)	105.17(9)
C(62)-C(63)	1.519(3)	C(8)-P(3)-C(34)	105.18(9)
C(64)-C(65)	1.519(3)	C(40)-P(3)-C(34)	98.73(9)
C(65)-C(66)	1.519(3)	C(8)-P(3)-Fe(1)	117.41(6)

C(40)-P(3)-Fe(1)	114.12(7)	C(10)-C(11)-C(12)	120.7(2)
C(34)-P(3)-Fe(1)	114.15(6)	C(13)-C(12)-C(11)	120.8(2)
C(46)-N(1)-Fe(1)	178.57(14)	C(12)-C(13)-C(14)	119.5(2)
C(64)-N(2)-C(68)	111.01(16)	C(13)-C(14)-C(15)	119.9(2)
C(64)-N(2)-C(60)	111.21(15)	C(14)-C(15)-C(10)	121.3(2)
C(68)-N(2)-C(60)	105.60(15)	C(21)-C(16)-C(17)	117.74(19)
C(64)-N(2)-C(56)	106.18(15)	C(21)-C(16)-P(1)	125.30(16)
C(68)-N(2)-C(56)	111.28(15)	C(17)-C(16)-P(1)	116.85(15)
C(60)-N(2)-C(56)	111.66(16)	C(18)-C(17)-C(16)	121.6(2)
C(1)-B(1)-C(9)	111.36(16)	C(17)-C(18)-C(19)	120.4(2)
C(1)-B(1)-C(7)	107.11(15)	C(18)-C(19)-C(20)	118.8(2)
C(9)-B(1)-C(7)	110.16(15)	C(19)-C(20)-C(21)	120.8(2)
C(1)-B(1)-C(8)	109.14(15)	C(20)-C(21)-C(16)	120.6(2)
C(9)-B(1)-C(8)	109.10(16)	C(27)-C(22)-C(23)	118.22(19)
C(7)-B(1)-C(8)	109.94(15)	C(27)-C(22)-P(2)	118.55(16)
C(75)-O(1)-C(72)	108.0(2)	C(23)-C(22)-P(2)	123.13(16)
C(2)-C(1)-C(6)	114.41(18)	C(24)-C(23)-C(22)	121.5(2)
C(2)-C(1)-B(1)	120.84(17)	C(25)-C(24)-C(23)	119.9(2)
C(6)-C(1)-B(1)	124.74(18)	C(24)-C(25)-C(26)	119.8(2)
C(3)-C(2)-C(1)	123.37(19)	C(25)-C(26)-C(27)	120.6(2)
C(2)-C(3)-C(4)	120.2(2)	C(22)-C(27)-C(26)	120.1(2)
C(5)-C(4)-C(3)	118.7(2)	C(29)-C(28)-C(33)	117.81(18)
C(4)-C(5)-C(6)	120.5(2)	C(29)-C(28)-P(2)	116.99(15)
C(5)-C(6)-C(1)	122.87(19)	C(33)-C(28)-P(2)	125.14(15)
B(1)-C(7)-P(1)	112.92(13)	C(30)-C(29)-C(28)	121.37(19)
B(1)-C(8)-P(3)	111.76(13)	C(31)-C(30)-C(29)	120.1(2)
B(1)-C(9)-P(2)	111.97(13)	C(32)-C(31)-C(30)	119.2(2)
C(11)-C(10)-C(15)	117.82(19)	C(31)-C(32)-C(33)	120.72(19)
C(11)-C(10)-P(1)	120.48(16)	C(32)-C(33)-C(28)	120.83(19)
C(15)-C(10)-P(1)	121.69(15)	C(35)-C(34)-C(39)	117.71(19)

C(35)-C(34)-P(3)	117.22(15)	C(55)-C(50)-C(47)	109.96(19)
C(39)-C(34)-P(3)	124.94(15)	C(50)-C(51)-C(52)	109.50(17)
C(36)-C(35)-C(34)	121.2(2)	C(53)-C(52)-C(51)	109.97(18)
C(35)-C(36)-C(37)	120.4(2)	C(53)-C(52)-C(48)	109.13(16)
C(38)-C(37)-C(36)	118.9(2)	C(51)-C(52)-C(48)	109.41(17)
C(37)-C(38)-C(39)	120.5(2)	C(52)-C(53)-C(54)	109.35(17)
C(38)-C(39)-C(34)	121.3(2)	C(55)-C(54)-C(53)	109.81(18)
C(45)-C(40)-C(41)	118.30(19)	C(55)-C(54)-C(49)	109.02(18)
C(45)-C(40)-P(3)	122.24(16)	C(53)-C(54)-C(49)	109.25(18)
C(41)-C(40)-P(3)	119.38(15)	C(54)-C(55)-C(50)	109.87(18)
C(42)-C(41)-C(40)	120.9(2)	C(57)-C(56)-N(2)	115.70(17)
C(43)-C(42)-C(41)	119.7(2)	C(56)-C(57)-C(58)	110.74(19)
C(44)-C(43)-C(42)	120.2(2)	C(57)-C(58)-C(59)	111.8(2)
C(43)-C(44)-C(45)	120.3(2)	C(61)-C(60)-N(2)	116.46(16)
C(40)-C(45)-C(44)	120.5(2)	C(62)-C(61)-C(60)	109.44(17)
N(1)-C(46)-C(49)	109.00(15)	C(61)-C(62)-C(63)	112.91(18)
N(1)-C(46)-C(47)	111.47(16)	N(2)-C(64)-C(65)	116.85(16)
C(49)-C(46)-C(47)	108.64(17)	C(66)-C(65)-C(64)	109.56(18)
N(1)-C(46)-C(48)	110.70(16)	C(67)-C(66)-C(65)	114.42(19)
C(49)-C(46)-C(48)	108.52(16)	C(69)-C(68)-N(2)	116.02(16)
C(47)-C(46)-C(48)	108.46(16)	C(68)-C(69)-C(70)	110.90(18)
C(50)-C(47)-C(46)	110.03(17)	C(71)-C(70)-C(69)	112.71(19)
C(52)-C(48)-C(46)	110.39(16)	O(1)-C(72)-C(73)	107.0(2)
C(46)-C(49)-C(54)	110.68(16)	C(72)-C(73)-C(74)	104.1(2)
C(51)-C(50)-C(55)	109.00(19)	C(73)-C(74)-C(75)	100.9(2)
C(51)-C(50)-C(47)	109.43(19)	O(1)-C(75)-C(74)	108.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2$x 10^3) for {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}·THF, (**4**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	13(1)	15(1)	17(1)	-5(1)	1(1)	-6(1)
P(1)	12(1)	15(1)	18(1)	-5(1)	0(1)	-4(1)
P(2)	14(1)	15(1)	14(1)	-5(1)	1(1)	-5(1)
P(3)	16(1)	14(1)	16(1)	-5(1)	-1(1)	-5(1)
N(1)	16(1)	17(1)	17(1)	-5(1)	0(1)	-6(1)
N(2)	33(1)	15(1)	21(1)	-5(1)	-6(1)	-9(1)
B(1)	14(1)	17(1)	16(1)	-5(1)	0(1)	-5(1)
O(1)	63(1)	54(1)	66(1)	4(1)	-26(1)	-21(1)
C(1)	15(1)	13(1)	19(1)	-6(1)	2(1)	-2(1)
C(2)	18(1)	26(1)	23(1)	-6(1)	-2(1)	-7(1)
C(3)	27(1)	28(1)	21(1)	0(1)	3(1)	-11(1)
C(4)	24(1)	28(1)	35(1)	-4(1)	8(1)	-16(1)
C(5)	19(1)	29(1)	33(1)	-7(1)	-2(1)	-11(1)
C(6)	19(1)	20(1)	21(1)	-4(1)	-1(1)	-7(1)
C(7)	18(1)	14(1)	19(1)	-5(1)	-1(1)	-7(1)
C(8)	15(1)	15(1)	15(1)	-4(1)	1(1)	-4(1)
C(9)	12(1)	19(1)	18(1)	-6(1)	0(1)	-7(1)
C(10)	15(1)	20(1)	19(1)	-7(1)	-4(1)	-2(1)
C(11)	23(1)	26(1)	40(1)	-7(1)	4(1)	-5(1)
C(12)	20(1)	44(2)	49(2)	-15(1)	10(1)	-2(1)
C(13)	26(1)	34(1)	45(2)	-21(1)	-8(1)	8(1)
C(14)	31(1)	20(1)	56(2)	-12(1)	-9(1)	1(1)
C(15)	24(1)	22(1)	35(1)	-6(1)	-1(1)	-5(1)
C(16)	16(1)	14(1)	19(1)	-4(1)	-3(1)	-1(1)
C(17)	23(1)	27(1)	23(1)	-6(1)	-1(1)	-10(1)

C(18)	26(1)	32(1)	37(1)	-11(1)	-10(1)	-11(1)
C(19)	35(1)	34(1)	26(1)	-10(1)	-14(1)	-6(1)
C(20)	42(1)	46(2)	16(1)	-3(1)	0(1)	-19(1)
C(21)	26(1)	33(1)	23(1)	-2(1)	-5(1)	-15(1)
C(22)	26(1)	16(1)	14(1)	-5(1)	3(1)	-7(1)
C(23)	33(1)	26(1)	21(1)	-9(1)	3(1)	-14(1)
C(24)	51(2)	31(1)	27(1)	-13(1)	-2(1)	-20(1)
C(25)	58(2)	24(1)	24(1)	-14(1)	3(1)	-8(1)
C(26)	32(1)	41(2)	35(1)	-20(1)	10(1)	-3(1)
C(27)	28(1)	30(1)	28(1)	-15(1)	3(1)	-9(1)
C(28)	23(1)	14(1)	12(1)	-5(1)	-2(1)	-5(1)
C(29)	18(1)	31(1)	23(1)	-2(1)	0(1)	-5(1)
C(30)	27(1)	35(1)	25(1)	4(1)	4(1)	-15(1)
C(31)	31(1)	21(1)	20(1)	1(1)	-6(1)	-7(1)
C(32)	19(1)	23(1)	27(1)	-7(1)	-6(1)	-5(1)
C(33)	20(1)	19(1)	21(1)	-6(1)	-1(1)	-9(1)
C(34)	21(1)	14(1)	16(1)	-8(1)	-1(1)	-4(1)
C(35)	26(1)	20(1)	22(1)	-10(1)	-1(1)	-9(1)
C(36)	47(2)	18(1)	20(1)	-5(1)	1(1)	-14(1)
C(37)	39(1)	17(1)	26(1)	-7(1)	-11(1)	3(1)
C(38)	22(1)	24(1)	34(1)	-10(1)	-4(1)	1(1)
C(39)	23(1)	19(1)	26(1)	-7(1)	0(1)	-6(1)
C(40)	25(1)	12(1)	21(1)	-5(1)	-7(1)	-4(1)
C(41)	22(1)	22(1)	33(1)	-12(1)	-7(1)	-2(1)
C(42)	31(1)	22(1)	53(2)	-15(1)	-18(1)	-4(1)
C(43)	58(2)	20(1)	38(2)	-8(1)	-28(1)	-8(1)
C(44)	70(2)	26(1)	21(1)	-8(1)	-4(1)	-19(1)
C(45)	44(1)	25(1)	23(1)	-9(1)	0(1)	-18(1)
C(46)	13(1)	19(1)	19(1)	-4(1)	-1(1)	-4(1)
C(47)	23(1)	40(1)	27(1)	-17(1)	6(1)	-17(1)

C(48)	19(1)	22(1)	24(1)	0(1)	-5(1)	-8(1)
C(49)	18(1)	20(1)	34(1)	1(1)	-4(1)	-8(1)
C(50)	28(1)	61(2)	30(1)	-24(1)	14(1)	-25(1)
C(51)	17(1)	31(1)	48(2)	-15(1)	9(1)	-11(1)
C(52)	14(1)	26(1)	31(1)	-2(1)	-6(1)	-8(1)
C(53)	18(1)	25(1)	34(1)	-4(1)	0(1)	-11(1)
C(54)	22(1)	23(1)	37(1)	8(1)	-5(1)	-11(1)
C(55)	33(1)	66(2)	24(1)	10(1)	-5(1)	-33(1)
C(56)	37(1)	19(1)	25(1)	-5(1)	-6(1)	-15(1)
C(57)	38(1)	33(1)	30(1)	-10(1)	-2(1)	-17(1)
C(58)	44(2)	44(2)	29(1)	-6(1)	-6(1)	-25(1)
C(59)	49(2)	78(2)	40(2)	-18(2)	3(1)	-36(2)
C(60)	31(1)	16(1)	24(1)	-4(1)	-6(1)	-7(1)
C(61)	30(1)	24(1)	25(1)	-8(1)	-6(1)	-8(1)
C(62)	30(1)	26(1)	30(1)	-3(1)	-8(1)	-12(1)
C(63)	34(1)	43(2)	27(1)	-8(1)	-7(1)	-7(1)
C(64)	34(1)	18(1)	22(1)	-7(1)	-7(1)	-7(1)
C(65)	34(1)	21(1)	29(1)	-8(1)	-5(1)	-9(1)
C(66)	40(1)	29(1)	38(2)	-9(1)	-1(1)	-9(1)
C(67)	35(1)	35(1)	44(2)	-13(1)	-3(1)	-10(1)
C(68)	36(1)	19(1)	23(1)	-9(1)	-6(1)	-12(1)
C(69)	45(1)	22(1)	24(1)	-5(1)	-11(1)	-12(1)
C(70)	39(1)	29(1)	22(1)	-8(1)	-5(1)	-15(1)
C(71)	63(2)	40(2)	32(1)	-11(1)	-19(1)	-14(1)
C(72)	39(2)	51(2)	53(2)	-21(2)	-5(1)	-14(1)
C(73)	64(2)	43(2)	59(2)	-12(2)	-19(2)	-15(2)
C(74)	79(2)	62(2)	48(2)	-17(2)	-14(2)	-25(2)
C(75)	91(3)	35(2)	106(3)	-28(2)	-32(2)	-12(2)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for {[$PhBP_3$]Fe≡N(1-Ad)}{$^nBu_4$}·THF, (**4**).

	x	y	z	U(eq)
H(2)	6422	10949	871	27
H(3)	7776	11759	309	32
H(4)	9328	11715	822	35
H(5)	9483	10837	1907	32
H(6)	8136	10006	2466	24
H(7A)	4757	11311	1612	20
H(7B)	4691	11241	2352	20
H(8A)	6916	8471	1726	19
H(8B)	5774	9300	1358	19
H(9A)	6553	9747	3057	19
H(9B)	7006	8600	2927	19
H(11)	1332	10608	2980	38
H(12)	-315	12036	3146	50
H(13)	-421	13764	2605	45
H(14)	1143	14083	1896	44
H(15)	2799	12665	1732	34
H(17)	1843	9795	1791	29
H(18)	1316	9752	852	35
H(19)	2355	10275	-115	37
H(20)	3897	10888	-122	42
H(21)	4358	11027	816	33
H(23)	6030	10084	3955	31
H(24)	5259	11306	4553	40
H(25)	3230	11944	4797	43

H(26)	1978	11350	4446	45
H(27)	2741	10147	3825	34
H(29)	3939	7793	4377	32
H(30)	4495	6285	5232	37
H(31)	6499	5358	5402	31
H(32)	7924	5970	4715	28
H(33)	7371	7501	3873	23
H(35)	5010	6335	3265	26
H(36)	6267	4750	3862	33
H(37)	8326	4327	3679	36
H(38)	9095	5497	2878	34
H(39)	7840	7049	2257	28
H(41)	3290	7396	2242	30
H(42)	2643	6849	1521	40
H(43)	3661	6839	526	44
H(44)	5383	7262	278	45
H(45)	6107	7711	1022	34
H(47A)	1798	8334	4456	33
H(47B)	863	9329	4012	33
H(48A)	384	9196	2989	27
H(48B)	1005	8114	2780	27
H(49A)	2767	6628	4134	30
H(49B)	2471	6544	3479	30
H(50)	-165	8434	4898	43
H(51A)	-1131	9263	3926	38
H(51B)	-1477	8225	4310	38
H(52)	-967	8237	3217	29
H(53A)	472	6496	3374	31
H(53B)	-504	6527	3966	31
H(54)	1425	5655	4354	36

H(55A)	1251	6683	5057	49
H(55B)	-28	6655	4994	49
H(56A)	5852	5072	1701	30
H(56B)	6596	4568	2319	30
H(57A)	7266	3793	1214	38
H(57B)	8020	3317	1831	38
H(58A)	8363	4938	1640	44
H(58B)	7535	5474	1052	44
H(59A)	9736	3757	1069	78
H(59B)	9555	4968	672	78
H(59C)	8911	4307	480	78
H(60A)	5857	2161	2866	28
H(60B)	7044	2250	2450	28
H(61A)	7300	3181	3121	31
H(61B)	6142	3019	3553	31
H(62A)	8258	1325	3360	33
H(62B)	7090	1129	3756	33
H(63A)	8443	2106	4131	54
H(63B)	8498	898	4449	54
H(63C)	7308	1851	4534	54
H(64A)	4130	4924	2304	29
H(64B)	4844	4472	2930	29
H(65A)	3520	3352	2674	33
H(65B)	4057	3116	3339	33
H(66A)	2774	4869	3403	44
H(66B)	2179	4991	2782	44
H(67A)	1559	3495	3384	56
H(67B)	938	4527	3642	56
H(67C)	2005	3558	4004	56
H(68A)	6014	2992	1509	29

H(68B)	4891	2807	1960	29
H(69A)	4803	4822	1094	36
H(69B)	3688	4515	1490	36
H(70A)	5089	3672	476	34
H(70B)	4120	3193	916	34
H(71A)	2610	4825	546	65
H(71B)	3330	4390	-46	65
H(71C)	3574	5324	116	65
H(72A)	611	8147	1746	55
H(72B)	-714	8112	1934	55
H(73A)	458	8453	714	65
H(73B)	-918	8997	916	65
H(74A)	-351	7498	383	73
H(74B)	-1374	7543	960	73
H(75A)	-80	5926	1400	89
H(75B)	1045	6235	1016	89

Table 16. Crystal data and structure refinement for $[PhBP_3]Fe{\equiv}N(1\text{-}Ad)$, (**5**).

Identification code	sdb22	
Empirical formula	$C_{55}H_{56}BFeNP_3$	
Formula weight	890.58	
Temperature	98(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.4143(15) Å	α= 90°.
	b = 14.1225(13) Å	β= 109.186(2)°.
	c = 20.7686(19) Å	γ = 90°.
Volume	4547.0(7) $Å^3$	
Z	4	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	0.476 mm^{-1}	
F(000)	1876	
Crystal size	0.20 x 0.31 x 0.33 mm^3	
Theta range for data collection	1.38 to 28.49°.	
Index ranges	-21<=h<=21, -18<=k<=18, -27<=l<=27	
Reflections collected	66856	
Independent reflections	10793 [R(int) = 0.0652]	
Completeness to theta = 28.49°	93.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10793 / 0 / 550	
Goodness-of-fit on F^2	1.887	
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.0982	
R indices (all data)	R1 = 0.0798, wR2 = 0.1031	
Largest diff. peak and hole	1.098 and -0.510 $e.Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]Fe{\equiv}N(1\text{-}Ad)$, (**5**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4598(1)	4916(1)	2192(1)	16(1)
N(1)	3722(1)	5113(1)	1541(1)	17(1)
P(1)	5253(1)	6058(1)	2909(1)	15(1)
P(2)	4691(1)	4015(1)	3126(1)	16(1)
P(3)	5922(1)	4479(1)	2188(1)	15(1)
B(1)	6464(2)	4614(2)	3668(1)	16(1)
C(1)	7372(1)	4433(2)	4288(1)	16(1)
C(2)	7550(2)	3590(2)	4666(1)	19(1)
C(3)	8349(2)	3400(2)	5147(1)	24(1)
C(4)	9011(2)	4056(2)	5276(1)	25(1)
C(5)	8859(2)	4891(2)	4921(1)	27(1)
C(6)	8061(2)	5074(2)	4439(1)	24(1)
C(7)	6309(1)	5766(2)	3508(1)	16(1)
C(8)	5630(1)	4216(2)	3870(1)	17(1)
C(9)	6569(1)	4017(2)	3006(1)	16(1)
C(10)	4578(2)	6459(2)	3407(1)	17(1)
C(11)	3694(2)	6510(2)	3063(1)	28(1)
C(12)	3135(2)	6826(2)	3393(2)	34(1)
C(13)	3449(2)	7086(2)	4064(2)	32(1)
C(14)	4325(2)	7033(2)	4414(1)	28(1)
C(15)	4886(2)	6719(2)	4088(1)	22(1)
C(16)	5404(1)	7179(2)	2515(1)	16(1)
C(17)	5044(2)	7316(2)	1816(1)	23(1)
C(18)	5179(2)	8156(2)	1518(1)	27(1)
C(19)	5671(2)	8868(2)	1916(1)	24(1)
C(20)	6018(2)	8742(2)	2613(1)	28(1)
C(21)	5887(2)	7906(2)	2905(1)	25(1)
C(22)	3729(2)	4050(2)	3396(1)	18(1)
C(23)	2945(2)	3759(2)	2937(1)	28(1)
C(24)	2205(2)	3767(2)	3117(2)	35(1)
C(25)	2237(2)	4084(2)	3754(2)	32(1)

C(26)	3011(2)	4372(2)	4213(2)	34(1)
C(27)	3756(2)	4350(2)	4034(1)	27(1)
C(28)	4711(1)	2755(2)	2909(1)	16(1)
C(29)	4329(2)	2474(2)	2236(1)	23(1)
C(30)	4271(2)	1523(2)	2058(1)	28(1)
C(31)	4612(2)	842(2)	2545(1)	24(1)
C(32)	5018(2)	1113(2)	3211(1)	25(1)
C(33)	5056(2)	2060(2)	3394(1)	23(1)
C(34)	5935(2)	3615(2)	1535(1)	17(1)
C(35)	5259(2)	3548(2)	923(1)	22(1)
C(36)	5328(2)	2985(2)	398(1)	24(1)
C(37)	6076(2)	2481(2)	476(1)	26(1)
C(38)	6752(2)	2537(2)	1084(1)	32(1)
C(39)	6681(2)	3093(2)	1614(1)	25(1)
C(40)	6589(1)	5375(2)	1962(1)	16(1)
C(41)	6270(2)	5808(2)	1327(1)	23(1)
C(42)	6770(2)	6440(2)	1114(1)	27(1)
C(43)	7599(2)	6647(2)	1528(1)	23(1)
C(44)	7927(2)	6225(2)	2158(1)	21(1)
C(45)	7424(2)	5591(2)	2375(1)	19(1)
C(46)	2938(2)	5313(2)	1004(1)	19(1)
C(47)	2177(2)	5276(2)	1295(2)	43(1)
C(48)	2956(2)	6261(2)	683(2)	46(1)
C(49)	2767(2)	4531(2)	460(1)	37(1)
C(50)	1913(2)	4726(2)	-120(2)	39(1)
C(51)	1963(2)	5661(3)	-430(2)	51(1)
C(52)	2094(2)	6473(2)	97(2)	50(1)
C(53)	1382(2)	6431(2)	409(2)	54(1)
C(54)	1318(2)	5480(2)	705(2)	45(1)
C(55)	1199(2)	4710(2)	176(1)	39(1)

Table 18. Bond lengths [Å] and angles [°] for [PhBP$_3$]Fe≡N(1-Ad), (**5**).

Fe(1)-N(1)	1.6410(19)	C(9)-H(9B)	0.9900
Fe(1)-P(1)	2.2174(7)	C(10)-C(15)	1.386(3)
Fe(1)-P(3)	2.2626(7)	C(10)-C(11)	1.393(3)
Fe(1)-P(2)	2.2829(7)	C(11)-C(12)	1.387(4)
N(1)-C(46)	1.428(3)	C(11)-H(11)	0.9500
P(1)-C(7)	1.818(2)	C(12)-C(13)	1.368(4)
P(1)-C(16)	1.836(2)	C(12)-H(12)	0.9500
P(1)-C(10)	1.837(2)	C(13)-C(14)	1.383(4)
P(2)-C(8)	1.811(2)	C(13)-H(13)	0.9500
P(2)-C(28)	1.839(2)	C(14)-C(15)	1.384(3)
P(2)-C(22)	1.841(2)	C(14)-H(14)	0.9500
P(3)-C(9)	1.804(2)	C(15)-H(15)	0.9500
P(3)-C(34)	1.829(2)	C(16)-C(21)	1.385(3)
P(3)-C(40)	1.833(2)	C(16)-C(17)	1.389(3)
B(1)-C(1)	1.638(3)	C(17)-C(18)	1.389(3)
B(1)-C(8)	1.657(3)	C(17)-H(17)	0.9500
B(1)-C(7)	1.663(3)	C(18)-C(19)	1.380(3)
B(1)-C(9)	1.669(3)	C(18)-H(18)	0.9500
C(1)-C(6)	1.400(3)	C(19)-C(20)	1.382(3)
C(1)-C(2)	1.404(3)	C(19)-H(19)	0.9500
C(2)-C(3)	1.389(3)	C(20)-C(21)	1.376(3)
C(2)-H(2)	0.9500	C(20)-H(20)	0.9500
C(3)-C(4)	1.384(3)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(27)	1.378(3)
C(4)-C(5)	1.371(3)	C(22)-C(23)	1.388(3)
C(4)-H(4)	0.9500	C(23)-C(24)	1.383(3)
C(5)-C(6)	1.386(3)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(24)-C(25)	1.381(4)
C(6)-H(6)	0.9500	C(24)-H(24)	0.9500
C(7)-H(7A)	0.9900	C(25)-C(26)	1.376(4)
C(7)-H(7B)	0.9900	C(25)-H(25)	0.9500
C(8)-H(8A)	0.9900	C(26)-C(27)	1.391(3)
C(8)-H(8B)	0.9900	C(26)-H(26)	0.9500
C(9)-H(9A)	0.9900	C(27)-H(27)	0.9500

C(28)-C(33)	1.387(3)	C(47)-C(54)	1.562(4)
C(28)-C(29)	1.389(3)	C(47)-H(47A)	0.9900
C(29)-C(30)	1.387(3)	C(47)-H(47B)	0.9900
C(29)-H(29)	0.9500	C(48)-C(52)	1.562(4)
C(30)-C(31)	1.375(4)	C(48)-H(48A)	0.9900
C(30)-H(30)	0.9500	C(48)-H(48B)	0.9900
C(31)-C(32)	1.377(3)	C(49)-C(50)	1.544(4)
C(31)-H(31)	0.9500	C(49)-H(49A)	0.9900
C(32)-C(33)	1.387(3)	C(49)-H(49B)	0.9900
C(32)-H(32)	0.9500	C(50)-C(51)	1.483(4)
C(33)-H(33)	0.9500	C(50)-C(55)	1.493(4)
C(34)-C(35)	1.388(3)	C(50)-H(50)	1.0000
C(34)-C(39)	1.391(3)	C(51)-C(52)	1.551(5)
C(35)-C(36)	1.385(3)	C(51)-H(51A)	0.9900
C(35)-H(35)	0.9500	C(51)-H(51B)	0.9900
C(36)-C(37)	1.382(3)	C(52)-C(53)	1.512(5)
C(36)-H(36)	0.9500	C(52)-H(52)	1.0000
C(37)-C(38)	1.382(3)	C(53)-C(54)	1.495(5)
C(37)-H(37)	0.9500	C(53)-H(53A)	0.9900
C(38)-C(39)	1.389(4)	C(53)-H(53B)	0.9900
C(38)-H(38)	0.9500	C(54)-C(55)	1.512(4)
C(39)-H(39)	0.9500	C(54)-H(54)	1.0000
C(40)-C(45)	1.389(3)	C(55)-H(55A)	0.9900
C(40)-C(41)	1.391(3)	C(55)-H(55B)	0.9900
C(41)-C(42)	1.380(3)		
C(41)-H(41)	0.9500	N(1)-Fe(1)-P(1)	122.02(7)
C(42)-C(43)	1.382(3)	N(1)-Fe(1)-P(3)	128.68(7)
C(42)-H(42)	0.9500	P(1)-Fe(1)-P(3)	86.92(3)
C(43)-C(44)	1.376(3)	N(1)-Fe(1)-P(2)	126.22(7)
C(43)-H(43)	0.9500	P(1)-Fe(1)-P(2)	87.30(3)
C(44)-C(45)	1.389(3)	P(3)-Fe(1)-P(2)	93.14(2)
C(44)-H(44)	0.9500	C(46)-N(1)-Fe(1)	176.33(17)
C(45)-H(45)	0.9500	C(7)-P(1)-C(16)	105.20(10)
C(46)-C(48)	1.500(4)	C(7)-P(1)-C(10)	107.45(11)
C(46)-C(49)	1.538(4)	C(16)-P(1)-C(10)	100.34(10)
C(46)-C(47)	1.556(4)	C(7)-P(1)-Fe(1)	115.99(8)

C(16)-P(1)-Fe(1)	115.77(8)	C(5)-C(6)-H(6)	118.5
C(10)-P(1)-Fe(1)	110.67(8)	C(1)-C(6)-H(6)	118.5
C(8)-P(2)-C(28)	106.41(11)	B(1)-C(7)-P(1)	114.01(15)
C(8)-P(2)-C(22)	108.12(11)	B(1)-C(7)-H(7A)	108.7
C(28)-P(2)-C(22)	100.77(10)	P(1)-C(7)-H(7A)	108.7
C(8)-P(2)-Fe(1)	115.98(8)	B(1)-C(7)-H(7B)	108.7
C(28)-P(2)-Fe(1)	109.44(8)	P(1)-C(7)-H(7B)	108.7
C(22)-P(2)-Fe(1)	114.74(8)	H(7A)-C(7)-H(7B)	107.6
C(9)-P(3)-C(34)	108.06(11)	B(1)-C(8)-P(2)	112.29(16)
C(9)-P(3)-C(40)	105.92(11)	B(1)-C(8)-H(8A)	109.1
C(34)-P(3)-C(40)	96.75(10)	P(2)-C(8)-H(8A)	109.1
C(9)-P(3)-Fe(1)	111.33(8)	B(1)-C(8)-H(8B)	109.1
C(34)-P(3)-Fe(1)	115.50(8)	P(2)-C(8)-H(8B)	109.1
C(40)-P(3)-Fe(1)	117.91(8)	H(8A)-C(8)-H(8B)	107.9
C(1)-B(1)-C(8)	111.19(19)	B(1)-C(9)-P(3)	113.89(16)
C(1)-B(1)-C(7)	110.45(18)	B(1)-C(9)-H(9A)	108.8
C(8)-B(1)-C(7)	107.28(18)	P(3)-C(9)-H(9A)	108.8
C(1)-B(1)-C(9)	104.83(18)	B(1)-C(9)-H(9B)	108.8
C(8)-B(1)-C(9)	110.76(19)	P(3)-C(9)-H(9B)	108.8
C(7)-B(1)-C(9)	112.39(19)	H(9A)-C(9)-H(9B)	107.7
C(6)-C(1)-C(2)	114.8(2)	C(15)-C(10)-C(11)	118.6(2)
C(6)-C(1)-B(1)	122.3(2)	C(15)-C(10)-P(1)	124.87(18)
C(2)-C(1)-B(1)	122.7(2)	C(11)-C(10)-P(1)	116.55(18)
C(3)-C(2)-C(1)	122.7(2)	C(12)-C(11)-C(10)	120.7(3)
C(3)-C(2)-H(2)	118.7	C(12)-C(11)-H(11)	119.6
C(1)-C(2)-H(2)	118.7	C(10)-C(11)-H(11)	119.6
C(4)-C(3)-C(2)	120.4(2)	C(13)-C(12)-C(11)	120.0(3)
C(4)-C(3)-H(3)	119.8	C(13)-C(12)-H(12)	120.0
C(2)-C(3)-H(3)	119.8	C(11)-C(12)-H(12)	120.0
C(5)-C(4)-C(3)	118.6(2)	C(12)-C(13)-C(14)	120.0(3)
C(5)-C(4)-H(4)	120.7	C(12)-C(13)-H(13)	120.0
C(3)-C(4)-H(4)	120.7	C(14)-C(13)-H(13)	120.0
C(4)-C(5)-C(6)	120.7(2)	C(13)-C(14)-C(15)	120.2(3)
C(4)-C(5)-H(5)	119.7	C(13)-C(14)-H(14)	119.9
C(6)-C(5)-H(5)	119.7	C(15)-C(14)-H(14)	119.9
C(5)-C(6)-C(1)	122.9(2)	C(14)-C(15)-C(10)	120.5(2)

C(14)-C(15)-H(15)	119.8	C(22)-C(27)-H(27)	119.6
C(10)-C(15)-H(15)	119.8	C(26)-C(27)-H(27)	119.6
C(21)-C(16)-C(17)	118.2(2)	C(33)-C(28)-C(29)	118.1(2)
C(21)-C(16)-P(1)	120.94(18)	C(33)-C(28)-P(2)	122.85(18)
C(17)-C(16)-P(1)	120.83(18)	C(29)-C(28)-P(2)	119.01(18)
C(16)-C(17)-C(18)	120.6(2)	C(30)-C(29)-C(28)	120.9(2)
C(16)-C(17)-H(17)	119.7	C(30)-C(29)-H(29)	119.6
C(18)-C(17)-H(17)	119.7	C(28)-C(29)-H(29)	119.6
C(19)-C(18)-C(17)	120.3(2)	C(31)-C(30)-C(29)	120.3(2)
C(19)-C(18)-H(18)	119.9	C(31)-C(30)-H(30)	119.8
C(17)-C(18)-H(18)	119.9	C(29)-C(30)-H(30)	119.8
C(18)-C(19)-C(20)	119.4(2)	C(30)-C(31)-C(32)	119.4(2)
C(18)-C(19)-H(19)	120.3	C(30)-C(31)-H(31)	120.3
C(20)-C(19)-H(19)	120.3	C(32)-C(31)-H(31)	120.3
C(21)-C(20)-C(19)	120.2(2)	C(31)-C(32)-C(33)	120.4(2)
C(21)-C(20)-H(20)	119.9	C(31)-C(32)-H(32)	119.8
C(19)-C(20)-H(20)	119.9	C(33)-C(32)-H(32)	119.8
C(20)-C(21)-C(16)	121.4(2)	C(32)-C(33)-C(28)	120.8(2)
C(20)-C(21)-H(21)	119.3	C(32)-C(33)-H(33)	119.6
C(16)-C(21)-H(21)	119.3	C(28)-C(33)-H(33)	119.6
C(27)-C(22)-C(23)	118.7(2)	C(35)-C(34)-C(39)	118.6(2)
C(27)-C(22)-P(2)	122.74(19)	C(35)-C(34)-P(3)	121.54(18)
C(23)-C(22)-P(2)	118.57(19)	C(39)-C(34)-P(3)	119.36(18)
C(24)-C(23)-C(22)	120.7(2)	C(36)-C(35)-C(34)	120.8(2)
C(24)-C(23)-H(23)	119.6	C(36)-C(35)-H(35)	119.6
C(22)-C(23)-H(23)	119.6	C(34)-C(35)-H(35)	119.6
C(25)-C(24)-C(23)	120.1(3)	C(37)-C(36)-C(35)	120.2(2)
C(25)-C(24)-H(24)	120.0	C(37)-C(36)-H(36)	119.9
C(23)-C(24)-H(24)	120.0	C(35)-C(36)-H(36)	119.9
C(26)-C(25)-C(24)	119.7(2)	C(36)-C(37)-C(38)	119.5(2)
C(26)-C(25)-H(25)	120.1	C(36)-C(37)-H(37)	120.2
C(24)-C(25)-H(25)	120.1	C(38)-C(37)-H(37)	120.2
C(25)-C(26)-C(27)	120.0(3)	C(37)-C(38)-C(39)	120.3(2)
C(25)-C(26)-H(26)	120.0	C(37)-C(38)-H(38)	119.8
C(27)-C(26)-H(26)	120.0	C(39)-C(38)-H(38)	119.8
C(22)-C(27)-C(26)	120.8(2)	C(38)-C(39)-C(34)	120.4(2)

C(38)-C(39)-H(39)	119.8	C(52)-C(48)-H(48B)	109.3
C(34)-C(39)-H(39)	119.8	H(48A)-C(48)-H(48B)	107.9
C(45)-C(40)-C(41)	118.5(2)	C(46)-C(49)-C(50)	110.2(2)
C(45)-C(40)-P(3)	123.00(18)	C(46)-C(49)-H(49A)	109.6
C(41)-C(40)-P(3)	118.36(18)	C(50)-C(49)-H(49A)	109.6
C(42)-C(41)-C(40)	120.6(2)	C(46)-C(49)-H(49B)	109.6
C(42)-C(41)-H(41)	119.7	C(50)-C(49)-H(49B)	109.6
C(40)-C(41)-H(41)	119.7	H(49A)-C(49)-H(49B)	108.1
C(41)-C(42)-C(43)	120.3(2)	C(51)-C(50)-C(55)	110.9(3)
C(41)-C(42)-H(42)	119.8	C(51)-C(50)-C(49)	109.3(2)
C(43)-C(42)-H(42)	119.8	C(55)-C(50)-C(49)	108.1(2)
C(44)-C(43)-C(42)	119.9(2)	C(51)-C(50)-H(50)	109.5
C(44)-C(43)-H(43)	120.1	C(55)-C(50)-H(50)	109.5
C(42)-C(43)-H(43)	120.1	C(49)-C(50)-H(50)	109.5
C(43)-C(44)-C(45)	119.9(2)	C(50)-C(51)-C(52)	111.5(2)
C(43)-C(44)-H(44)	120.0	C(50)-C(51)-H(51A)	109.3
C(45)-C(44)-H(44)	120.0	C(52)-C(51)-H(51A)	109.3
C(44)-C(45)-C(40)	120.8(2)	C(50)-C(51)-H(51B)	109.3
C(44)-C(45)-H(45)	119.6	C(52)-C(51)-H(51B)	109.3
C(40)-C(45)-H(45)	119.6	H(51A)-C(51)-H(51B)	108.0
N(1)-C(46)-C(48)	112.3(2)	C(53)-C(52)-C(51)	109.0(3)
N(1)-C(46)-C(49)	109.35(19)	C(53)-C(52)-C(48)	106.8(3)
C(48)-C(46)-C(49)	109.9(2)	C(51)-C(52)-C(48)	106.8(3)
N(1)-C(46)-C(47)	108.81(19)	C(53)-C(52)-H(52)	111.3
C(48)-C(46)-C(47)	109.8(2)	C(51)-C(52)-H(52)	111.3
C(49)-C(46)-C(47)	106.6(2)	C(48)-C(52)-H(52)	111.3
C(46)-C(47)-C(54)	108.8(2)	C(54)-C(53)-C(52)	112.4(3)
C(46)-C(47)-H(47A)	109.9	C(54)-C(53)-H(53A)	109.1
C(54)-C(47)-H(47A)	109.9	C(52)-C(53)-H(53A)	109.1
C(46)-C(47)-H(47B)	109.9	C(54)-C(53)-H(53B)	109.1
C(54)-C(47)-H(47B)	109.9	C(52)-C(53)-H(53B)	109.1
H(47A)-C(47)-H(47B)	108.3	H(53A)-C(53)-H(53B)	107.9
C(46)-C(48)-C(52)	111.8(2)	C(53)-C(54)-C(55)	110.9(3)
C(46)-C(48)-H(48A)	109.3	C(53)-C(54)-C(47)	108.7(3)
C(52)-C(48)-H(48A)	109.3	C(55)-C(54)-C(47)	107.8(2)
C(46)-C(48)-H(48B)	109.3	C(53)-C(54)-H(54)	109.8

C(55)-C(54)-H(54)	109.8	C(50)-C(55)-H(55B)	109.5
C(47)-C(54)-H(54)	109.8	C(54)-C(55)-H(55B)	109.5
C(50)-C(55)-C(54)	110.9(2)	H(55A)-C(55)-H(55B)	108.0
C(50)-C(55)-H(55A)	109.5		
C(54)-C(55)-H(55A)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 19. Anisotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]Fe{\equiv}N(1\text{-}Ad)$, (**5**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2\, a^{*2}U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	12(1)	18(1)	15(1)	1(1)	2(1)	0(1)
N(1)	15(1)	19(1)	17(1)	-2(1)	6(1)	-1(1)
P(1)	14(1)	16(1)	15(1)	1(1)	4(1)	1(1)
P(2)	14(1)	17(1)	15(1)	-1(1)	4(1)	-1(1)
P(3)	14(1)	16(1)	14(1)	1(1)	3(1)	-1(1)
B(1)	14(1)	17(1)	16(1)	-1(1)	4(1)	-1(1)
C(1)	17(1)	17(1)	14(1)	-2(1)	7(1)	2(1)
C(2)	21(1)	20(1)	16(1)	-2(1)	5(1)	-1(1)
C(3)	29(1)	23(1)	17(1)	3(1)	4(1)	6(1)
C(4)	17(1)	31(2)	21(1)	-3(1)	0(1)	5(1)
C(5)	18(1)	25(1)	33(2)	-5(1)	2(1)	-1(1)
C(6)	19(1)	20(1)	28(1)	4(1)	3(1)	3(1)
C(7)	13(1)	18(1)	16(1)	-2(1)	4(1)	0(1)
C(8)	17(1)	21(1)	13(1)	0(1)	3(1)	0(1)
C(9)	15(1)	18(1)	13(1)	3(1)	3(1)	1(1)
C(10)	20(1)	14(1)	20(1)	2(1)	10(1)	2(1)
C(11)	21(1)	35(2)	26(2)	2(1)	7(1)	8(1)
C(12)	20(1)	46(2)	37(2)	2(1)	10(1)	10(1)
C(13)	33(2)	33(2)	38(2)	4(1)	25(1)	10(1)
C(14)	38(2)	28(2)	24(2)	-2(1)	17(1)	-2(1)
C(15)	21(1)	22(1)	24(1)	-2(1)	10(1)	-1(1)
C(16)	14(1)	16(1)	19(1)	2(1)	6(1)	4(1)
C(17)	24(1)	21(1)	20(1)	0(1)	2(1)	-2(1)
C(18)	35(2)	25(2)	16(1)	4(1)	2(1)	-1(1)
C(19)	27(1)	18(1)	28(2)	5(1)	10(1)	3(1)
C(20)	34(2)	20(1)	25(2)	-3(1)	4(1)	-6(1)
C(21)	32(2)	21(1)	17(1)	1(1)	3(1)	-1(1)
C(22)	19(1)	14(1)	22(1)	2(1)	8(1)	0(1)
C(23)	21(1)	40(2)	24(2)	-3(1)	8(1)	-3(1)
C(24)	19(1)	49(2)	38(2)	-3(2)	9(1)	-6(1)
C(25)	27(2)	32(2)	47(2)	0(1)	24(1)	-1(1)

C(26)	35(2)	36(2)	38(2)	-13(1)	23(1)	-6(1)
C(27)	24(1)	29(2)	29(2)	-8(1)	12(1)	-6(1)
C(28)	12(1)	17(1)	19(1)	-1(1)	6(1)	-1(1)
C(29)	24(1)	21(1)	19(1)	1(1)	2(1)	2(1)
C(30)	33(2)	26(2)	21(1)	-8(1)	2(1)	-2(1)
C(31)	23(1)	20(1)	30(2)	-4(1)	9(1)	-1(1)
C(32)	27(1)	21(1)	26(2)	5(1)	8(1)	2(1)
C(33)	26(1)	25(1)	18(1)	0(1)	6(1)	-3(1)
C(34)	20(1)	13(1)	17(1)	1(1)	6(1)	-5(1)
C(35)	15(1)	27(1)	22(1)	0(1)	4(1)	2(1)
C(36)	22(1)	28(2)	16(1)	-3(1)	-1(1)	-4(1)
C(37)	31(2)	21(1)	23(1)	-8(1)	4(1)	1(1)
C(38)	30(2)	27(2)	33(2)	-8(1)	1(1)	12(1)
C(39)	24(1)	22(1)	21(1)	-3(1)	-2(1)	4(1)
C(40)	16(1)	15(1)	18(1)	-2(1)	8(1)	0(1)
C(41)	19(1)	24(1)	24(1)	2(1)	4(1)	-3(1)
C(42)	31(2)	25(2)	25(2)	6(1)	9(1)	-2(1)
C(43)	27(1)	19(1)	26(2)	-5(1)	15(1)	-7(1)
C(44)	18(1)	23(1)	23(1)	-9(1)	7(1)	-5(1)
C(45)	19(1)	20(1)	19(1)	-1(1)	6(1)	1(1)
C(46)	15(1)	22(1)	17(1)	-1(1)	2(1)	2(1)
C(47)	23(2)	71(2)	32(2)	-3(2)	6(1)	3(2)
C(48)	33(2)	37(2)	51(2)	11(2)	-9(2)	-7(1)
C(49)	29(2)	40(2)	34(2)	-7(1)	-1(1)	4(1)
C(50)	28(2)	47(2)	33(2)	-13(2)	-1(1)	-3(1)
C(51)	40(2)	89(3)	22(2)	22(2)	6(1)	20(2)
C(52)	35(2)	47(2)	51(2)	7(2)	-11(2)	-6(2)
C(53)	54(2)	51(2)	45(2)	-1(2)	2(2)	34(2)
C(54)	22(2)	70(2)	44(2)	-15(2)	12(1)	1(2)
C(55)	29(2)	47(2)	30(2)	1(1)	-5(1)	5(1)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for $[PhBP_3]Fe{\equiv}N(1\text{-}Ad)$, (**5**).

	x	y	z	U(eq)
H(2)	7106	3130	4590	23
H(3)	8442	2818	5389	28
H(4)	9558	3929	5605	29
H(5)	9305	5350	5005	32
H(6)	7977	5659	4200	28
H(7A)	6757	6002	3325	19
H(7B)	6385	6102	3943	19
H(8A)	5484	4682	4171	21
H(8B)	5793	3616	4127	21
H(9A)	6406	3348	3039	19
H(9B)	7182	4028	3034	19
H(11)	3472	6327	2597	33
H(12)	2533	6862	3152	41
H(13)	3066	7303	4289	38
H(14)	4541	7213	4880	34
H(15)	5486	6681	4332	26
H(17)	4703	6831	1539	27
H(18)	4933	8241	1040	32
H(19)	5769	9440	1712	29
H(20)	6347	9233	2891	33
H(21)	6132	7826	3384	30
H(23)	2916	3552	2495	34
H(24)	1674	3554	2802	43
H(25)	1727	4102	3875	39
H(26)	3037	4588	4653	40
H(27)	4290	4543	4355	32
H(29)	4104	2938	1892	28
H(30)	3994	1342	1597	34
H(31)	4568	191	2424	29
H(32)	5274	647	3547	30

H(33)	5321	2235	3858	28
H(35)	4743	3893	864	26
H(36)	4860	2945	-17	29
H(37)	6126	2099	114	32
H(38)	7268	2192	1139	39
H(39)	7144	3118	2033	29
H(41)	5702	5667	1036	28
H(42)	6543	6733	680	33
H(43)	7942	7080	1379	27
H(44)	8496	6366	2444	26
H(45)	7653	5301	2810	23
H(47A)	2265	5756	1660	51
H(47B)	2151	4644	1493	51
H(48A)	3440	6278	498	55
H(48B)	3058	6760	1036	55
H(49A)	2736	3910	670	45
H(49B)	3249	4510	272	45
H(50)	1814	4221	-475	47
H(51A)	1424	5774	-815	62
H(51B)	2449	5659	-614	62
H(52)	2112	7104	-116	60
H(53A)	1490	6916	771	65
H(53B)	825	6582	54	65
H(54)	823	5474	886	54
H(55A)	1186	4085	389	47
H(55B)	640	4800	-191	47