

P-Chirogenic Phosphines Supported by Calix[4]arene : New Insight on Pd-Catalyzed Asymmetric Allylic Substitution

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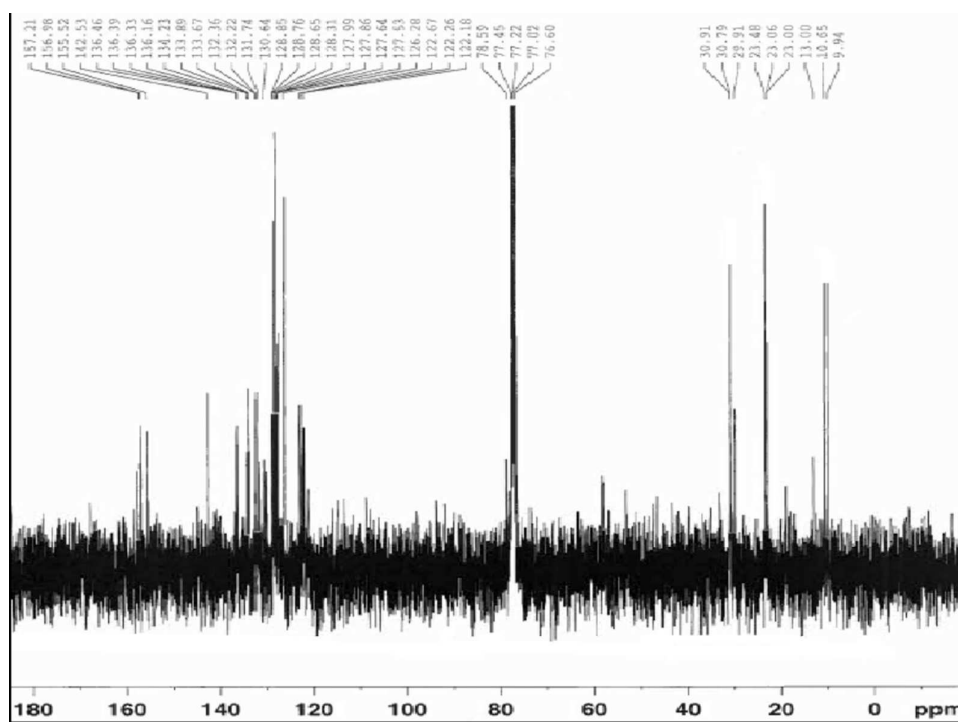
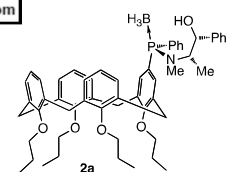
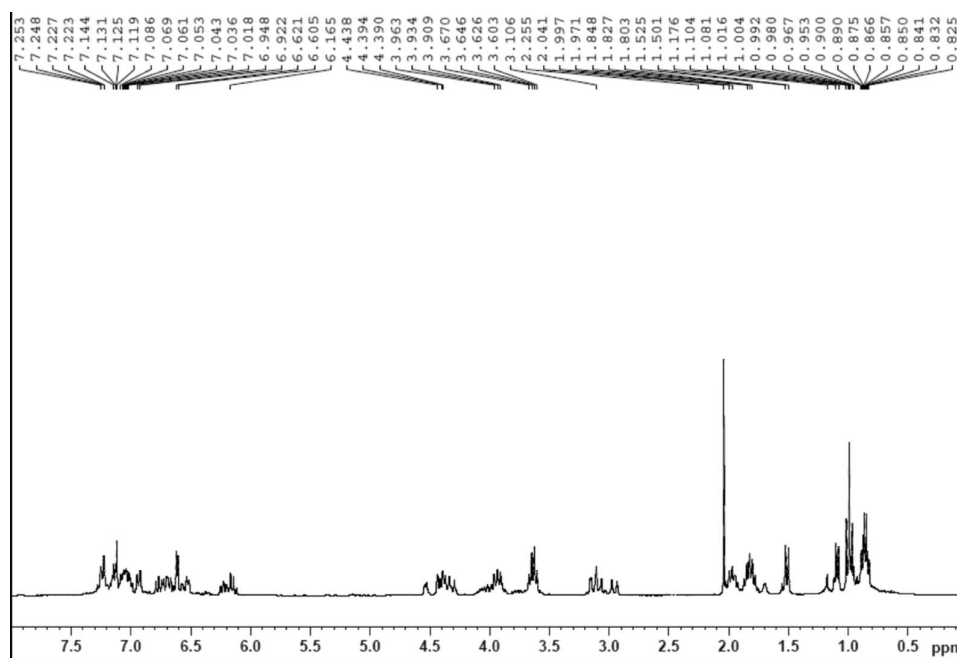
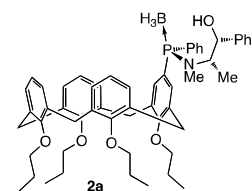
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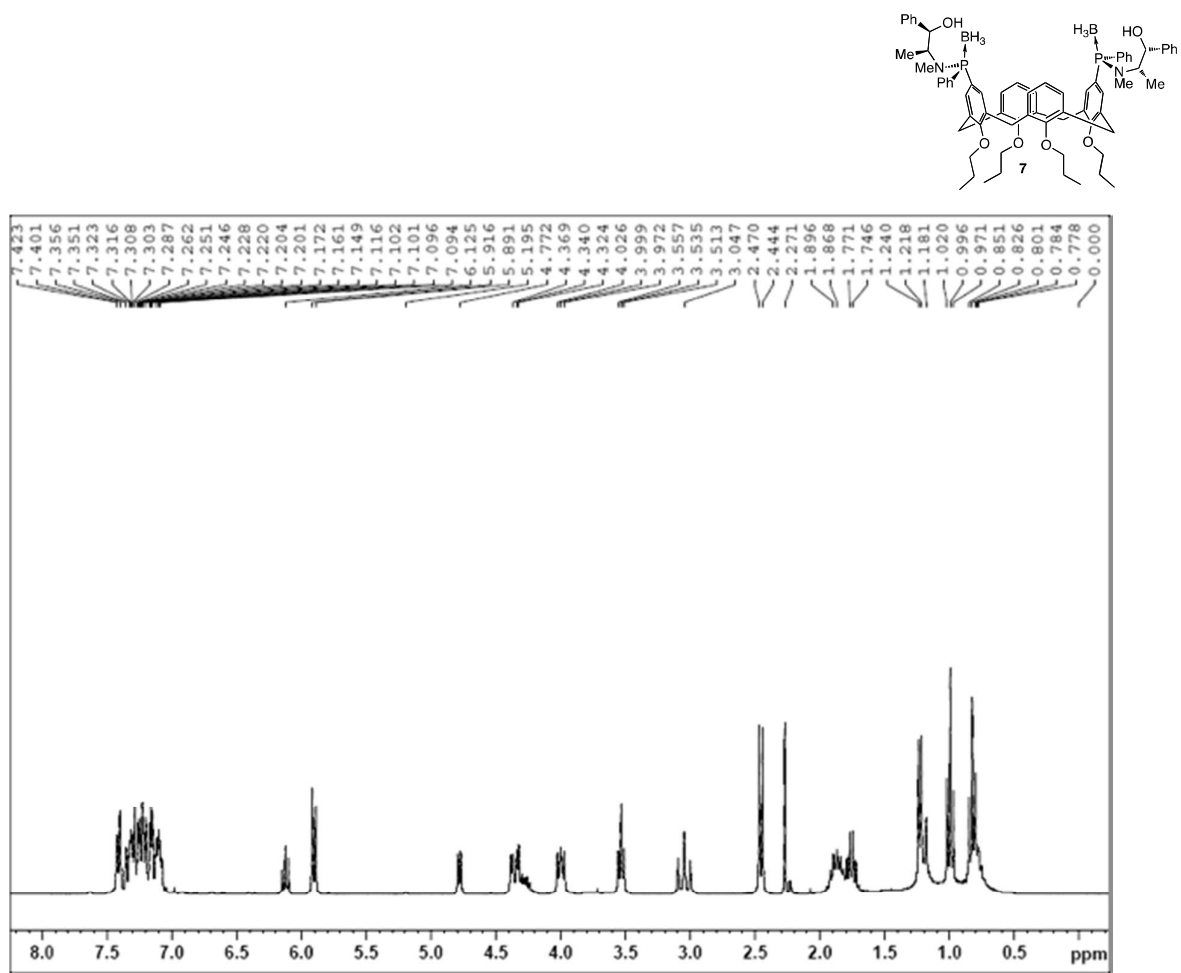
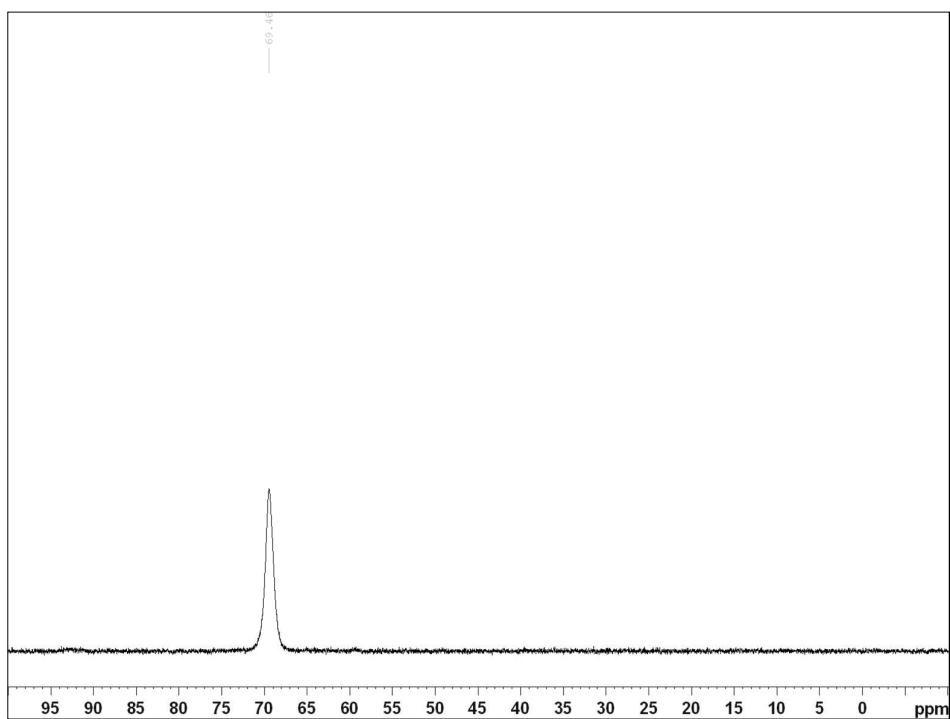
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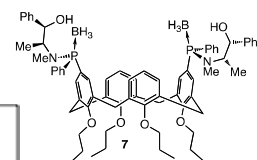
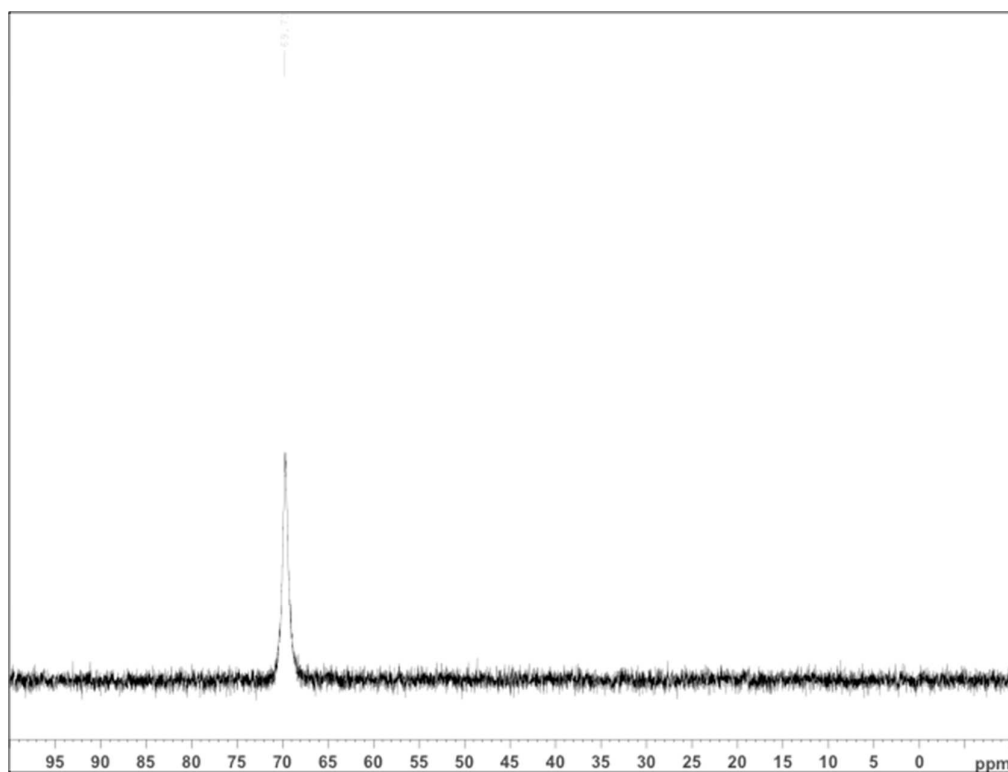
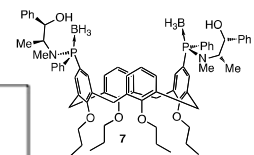
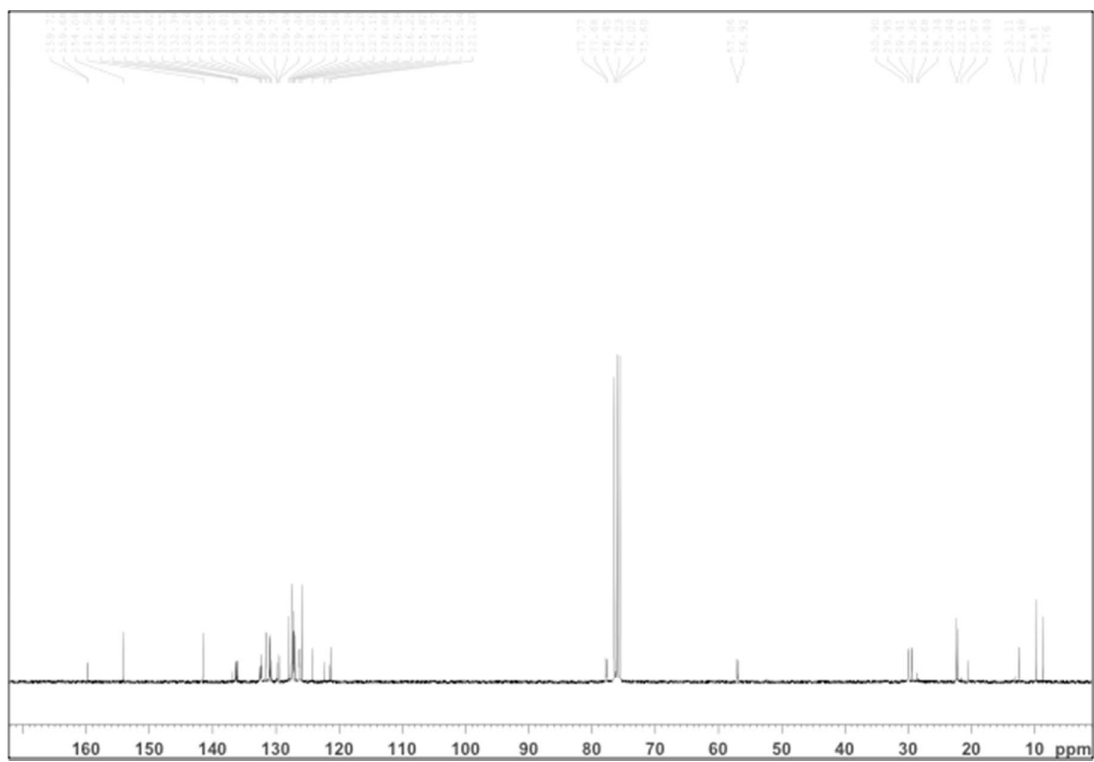
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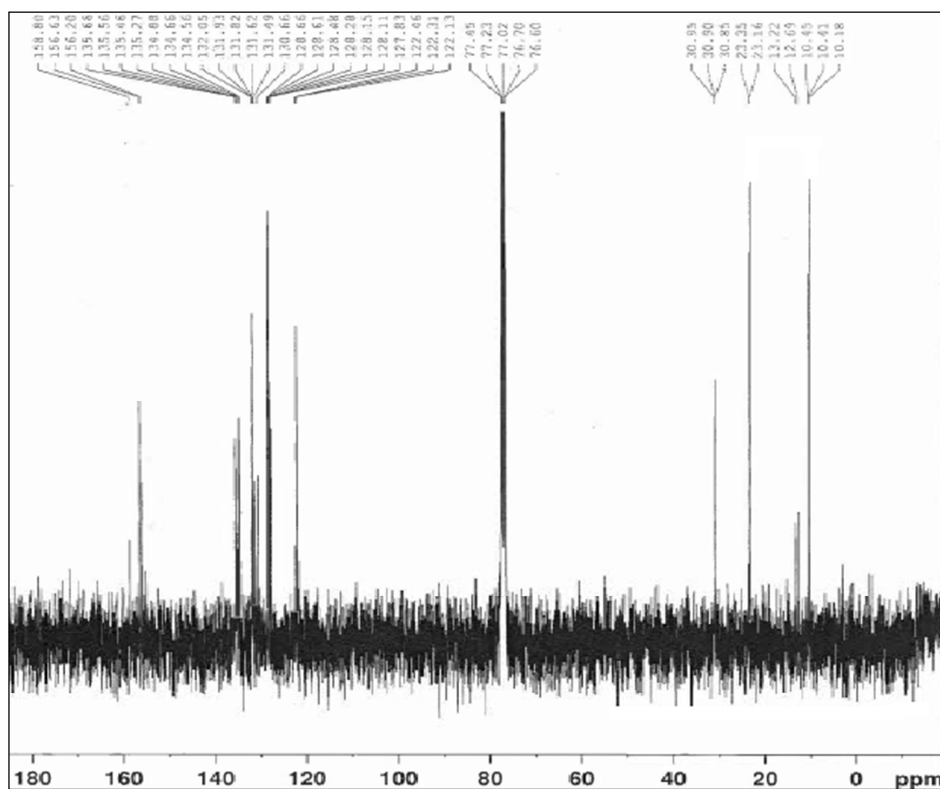
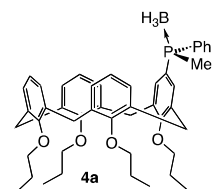
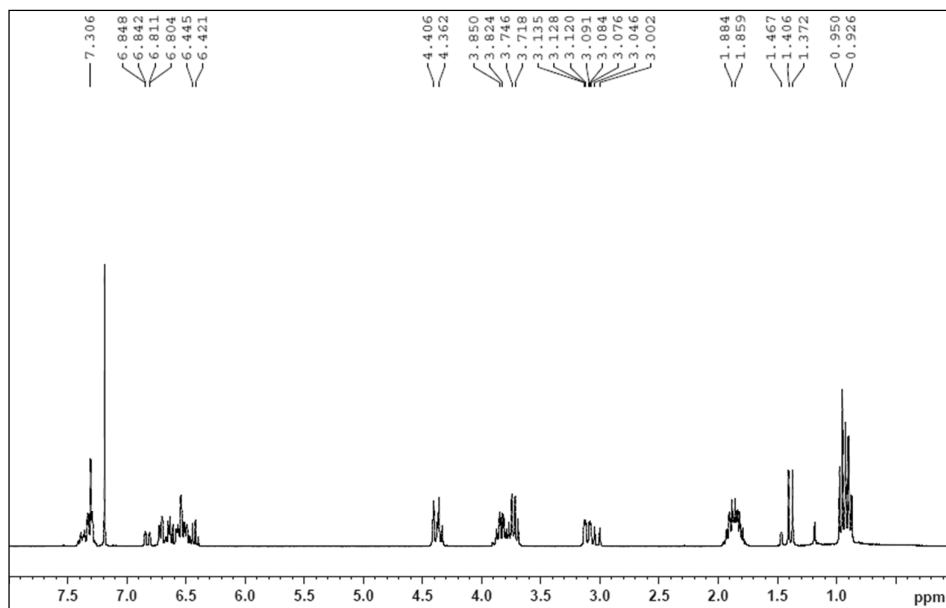
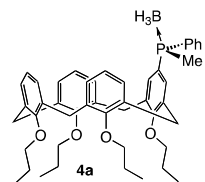
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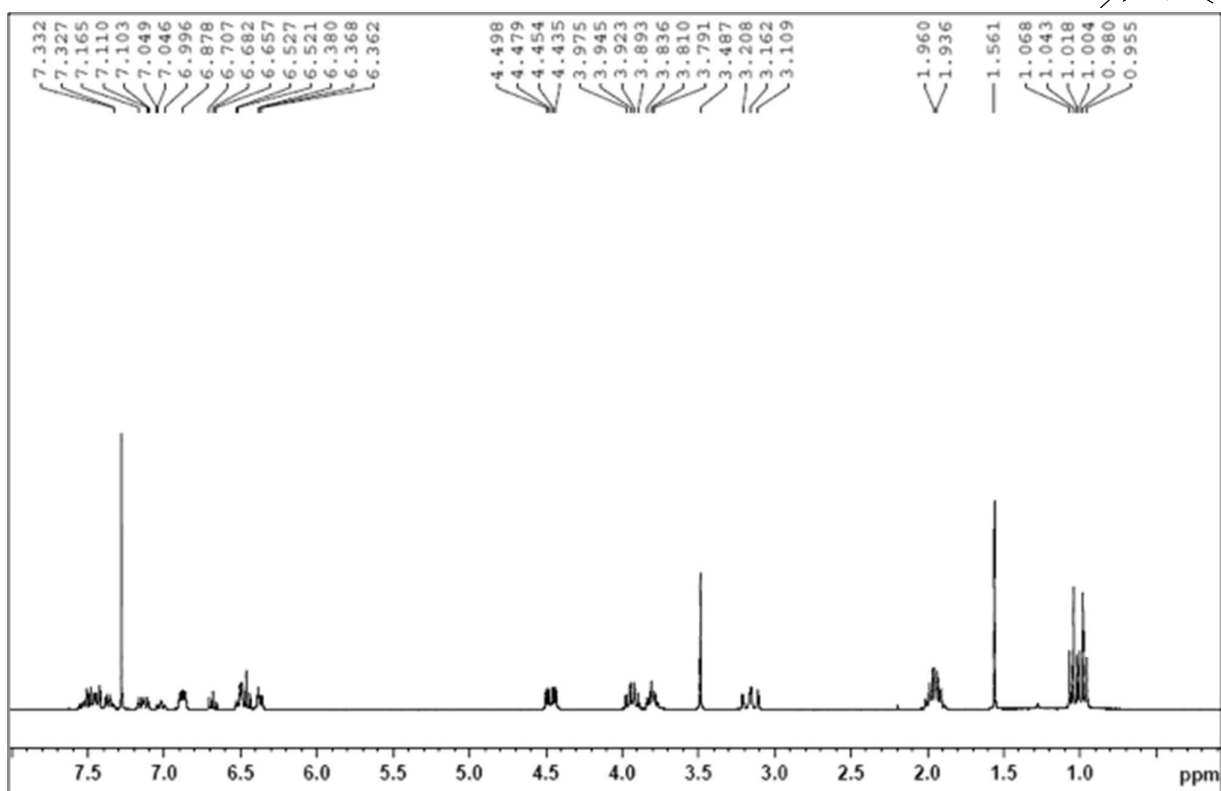
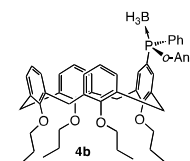
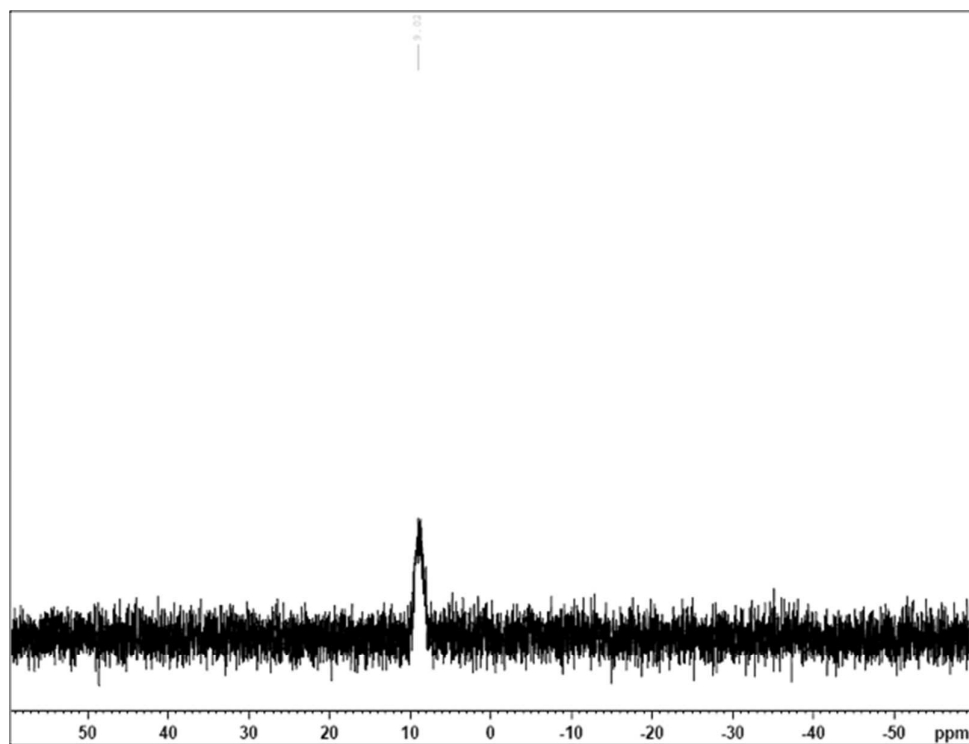
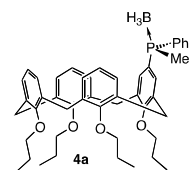
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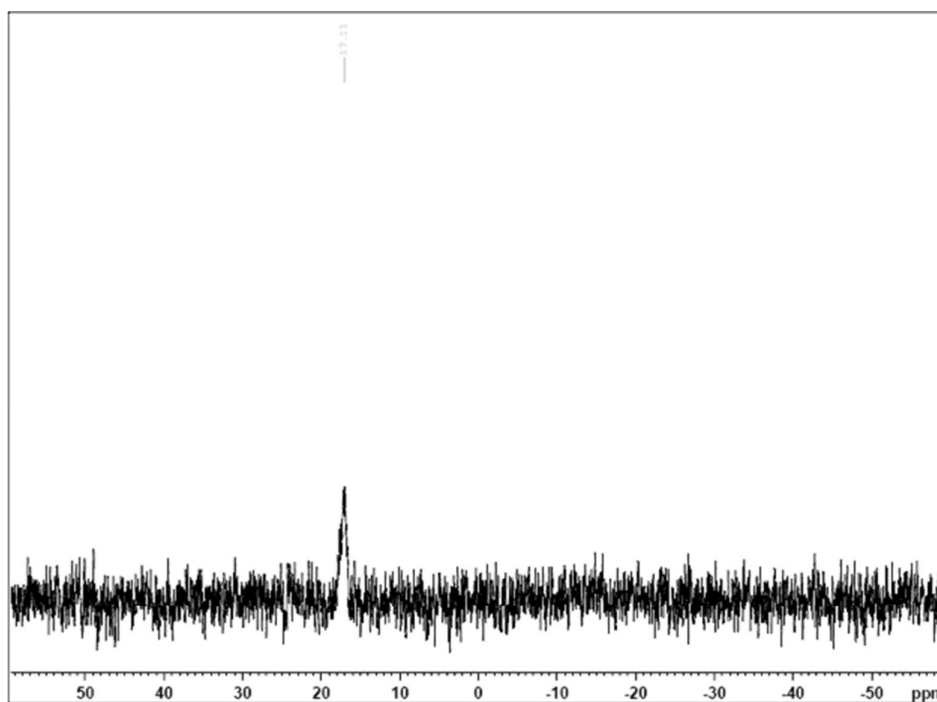
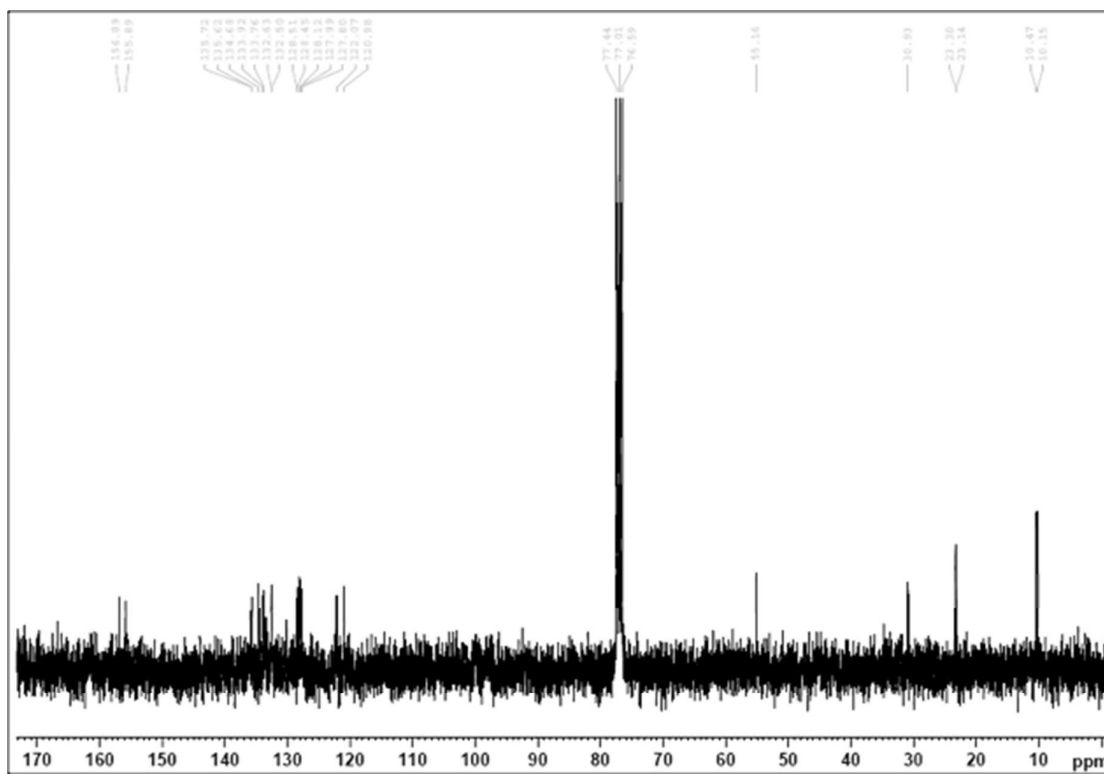


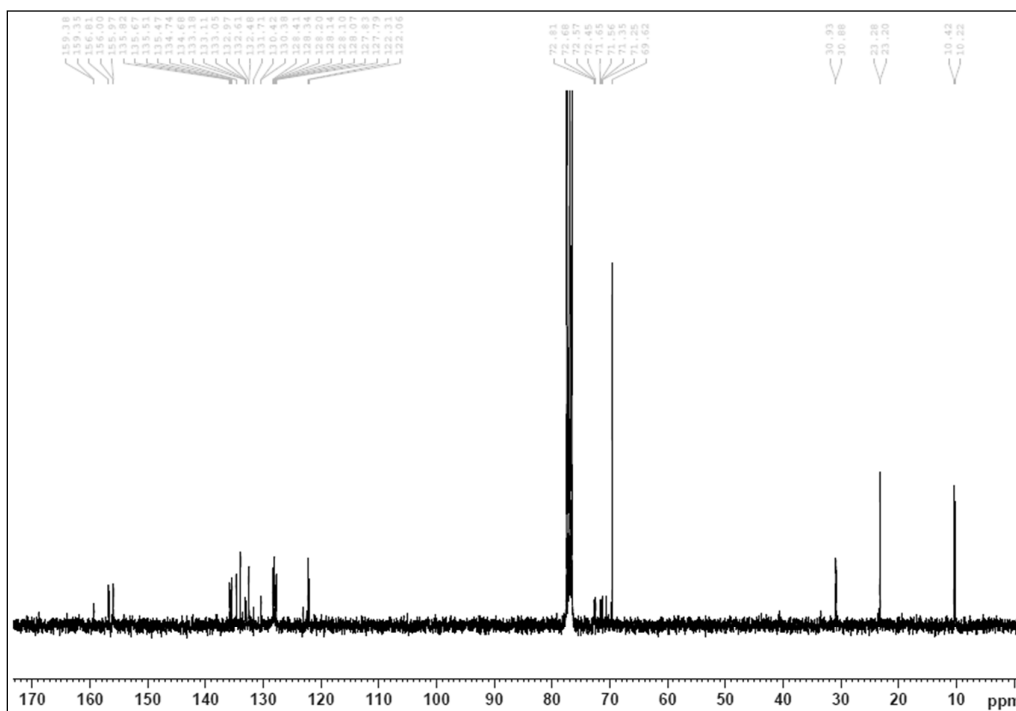
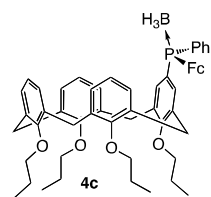
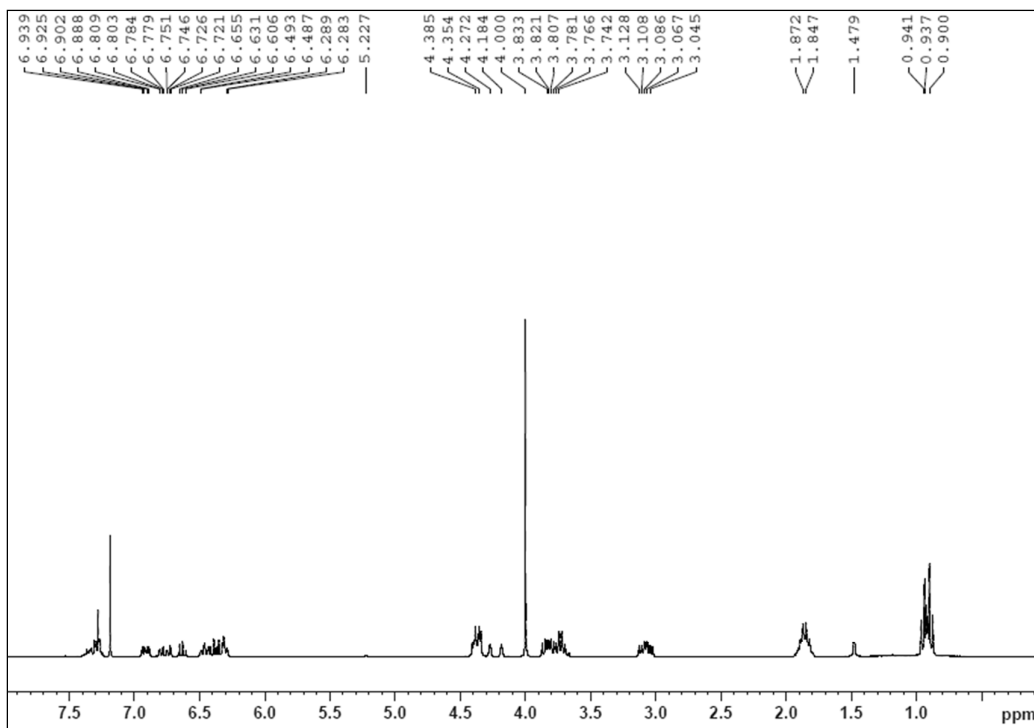
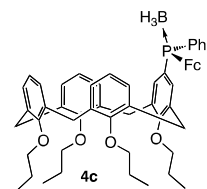


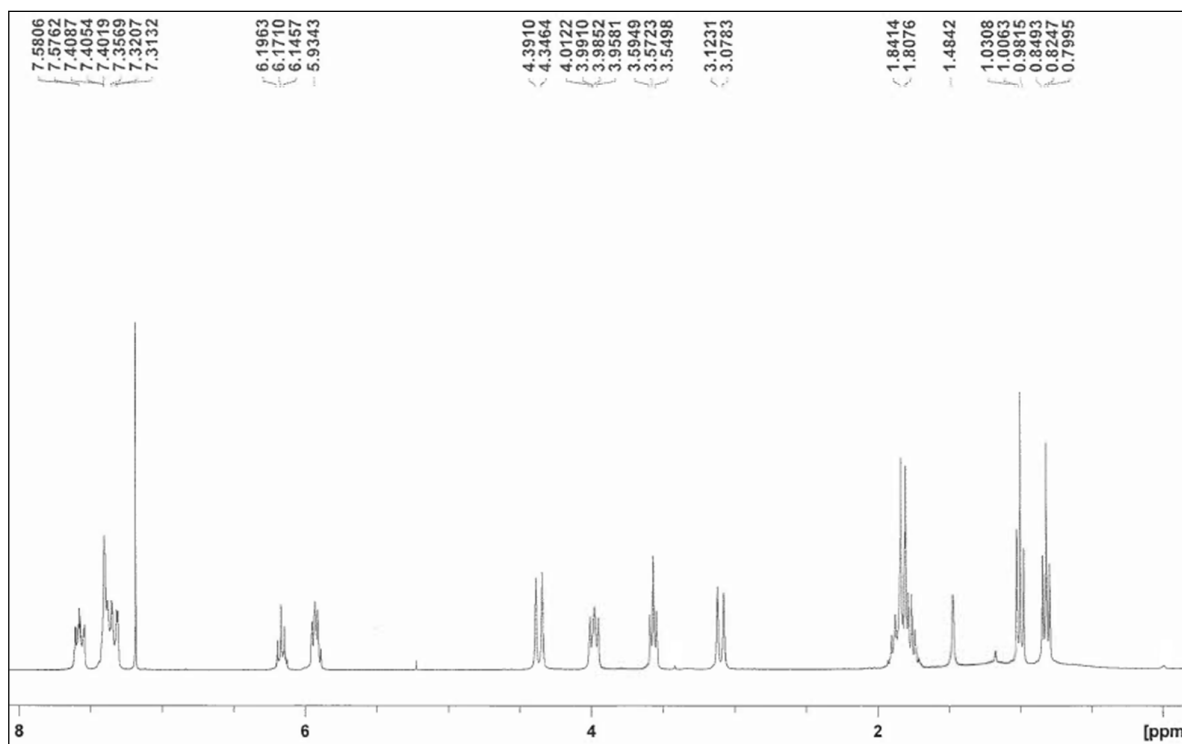
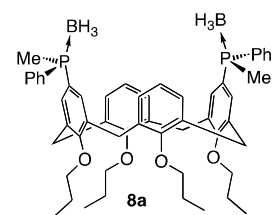
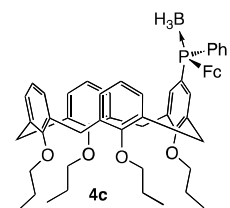
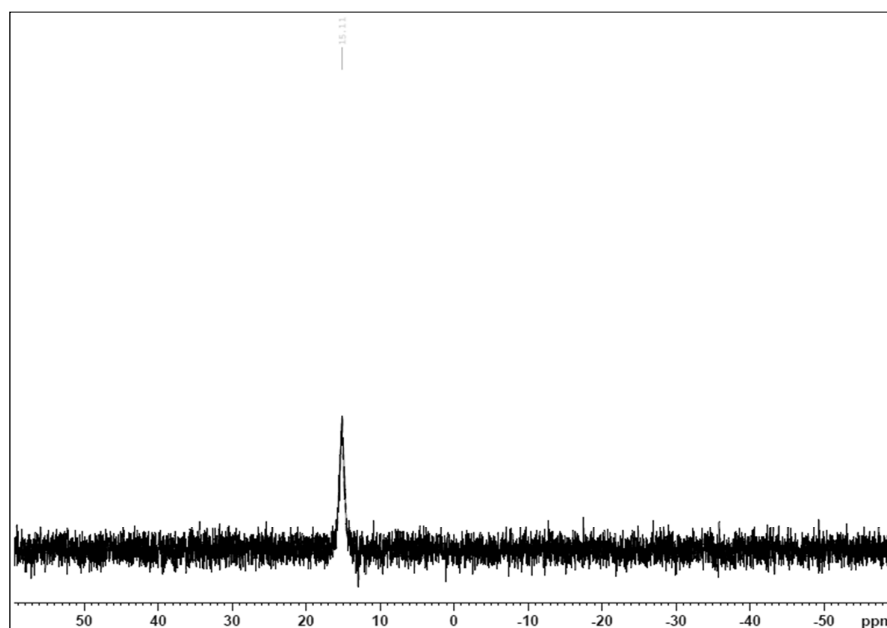


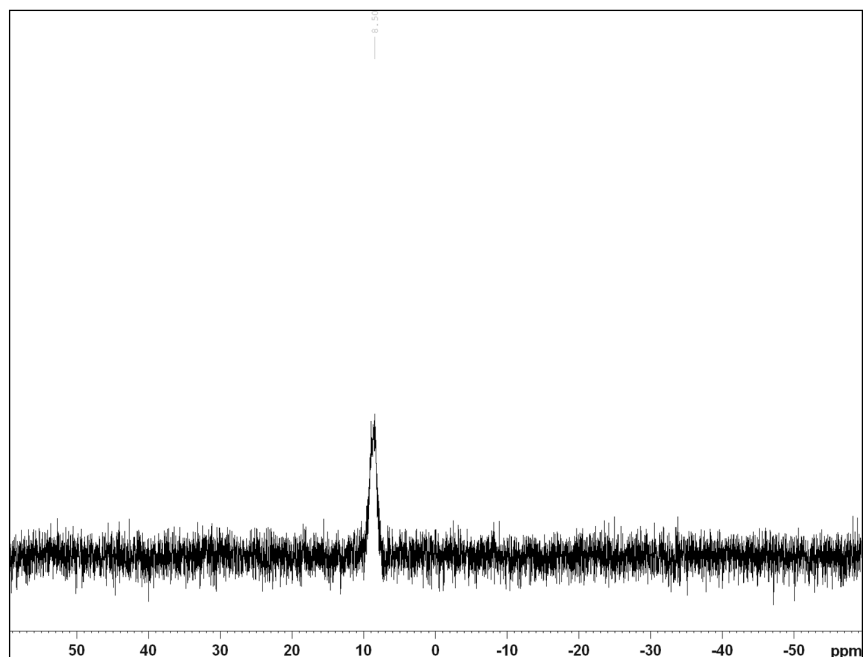
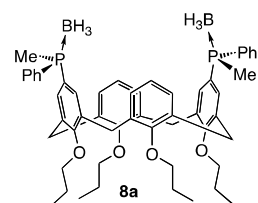
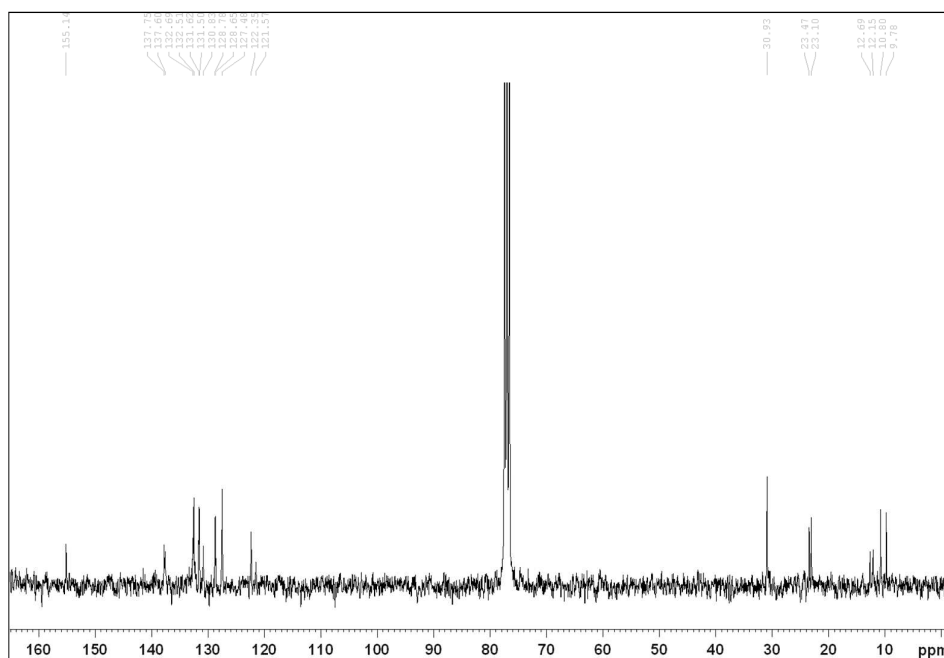
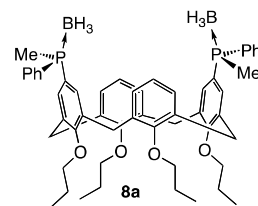


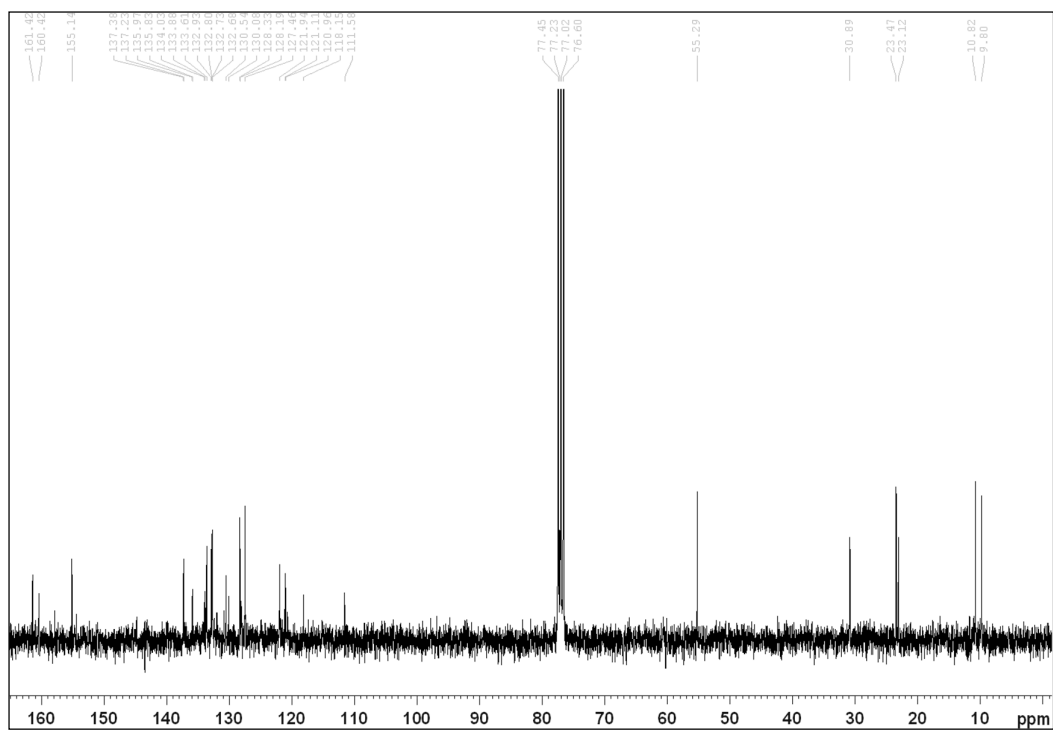
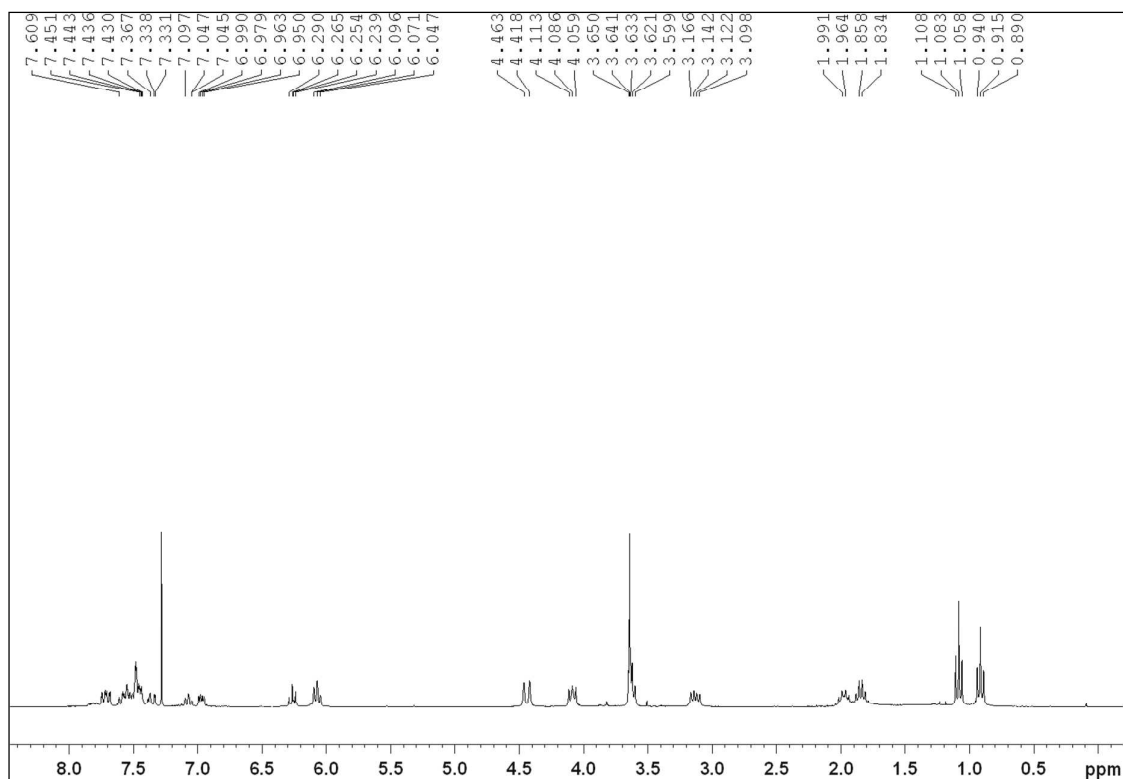
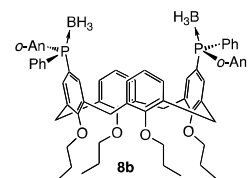


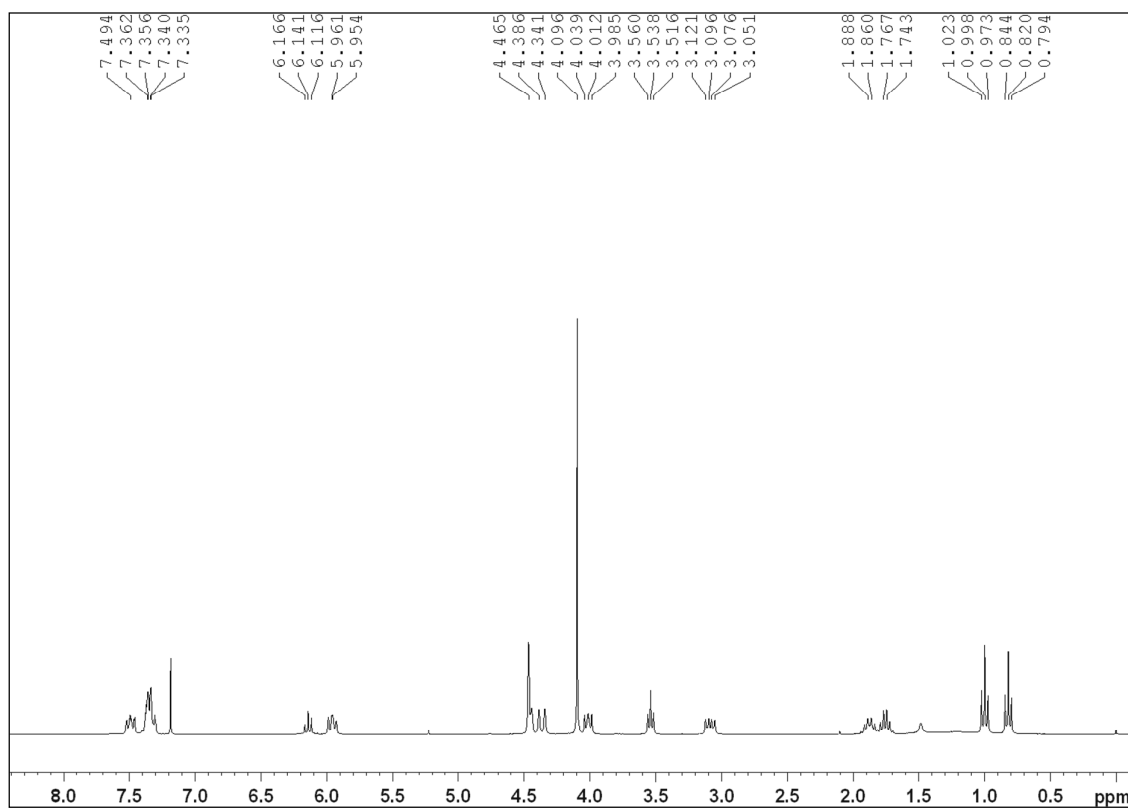
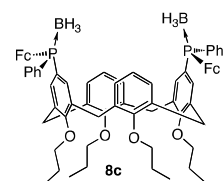
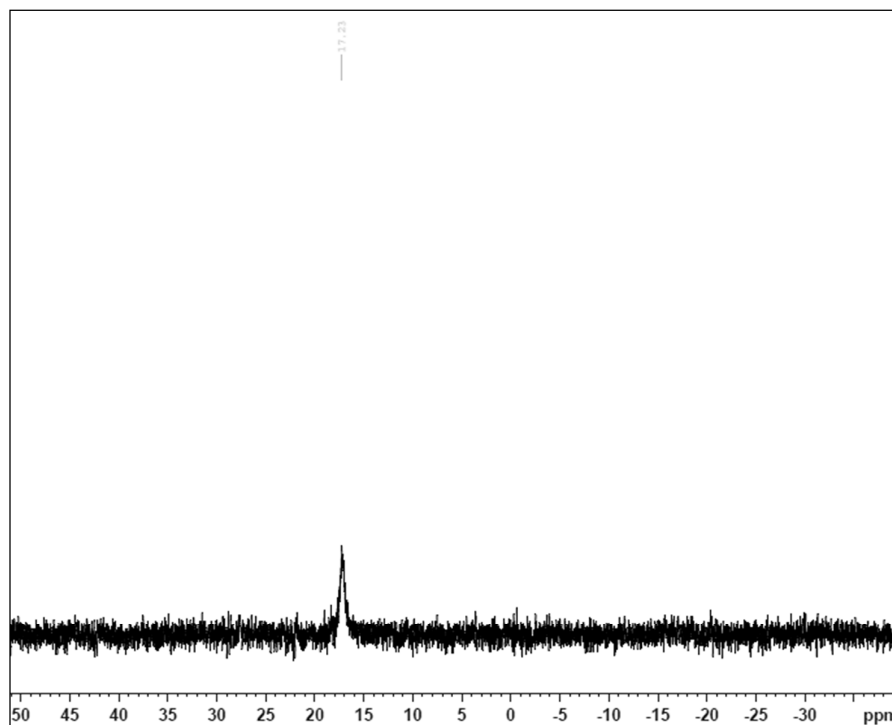
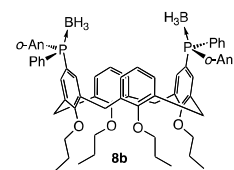


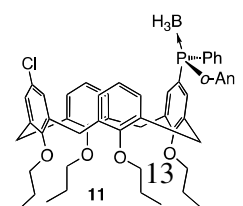
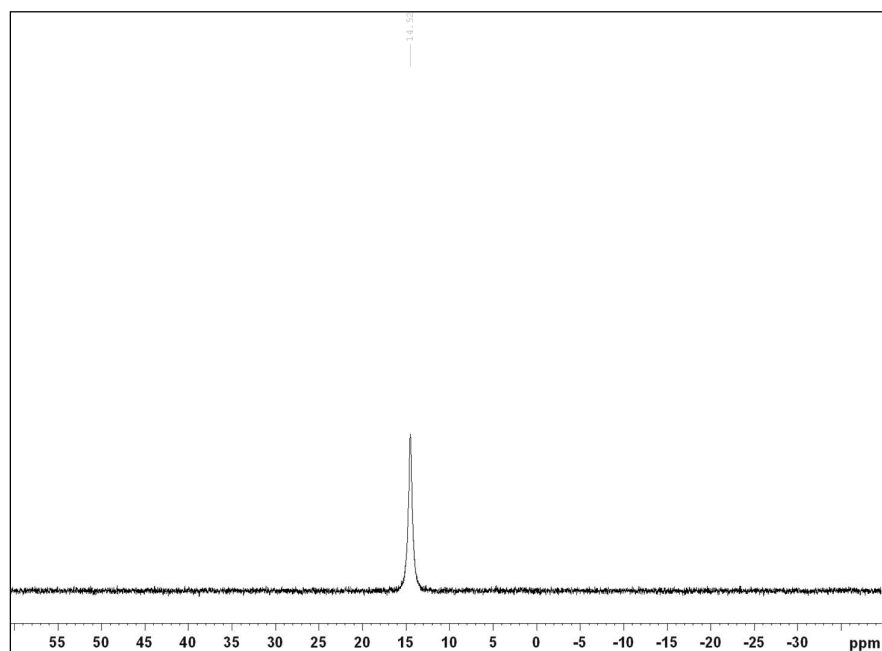
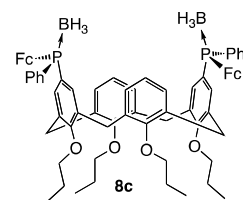
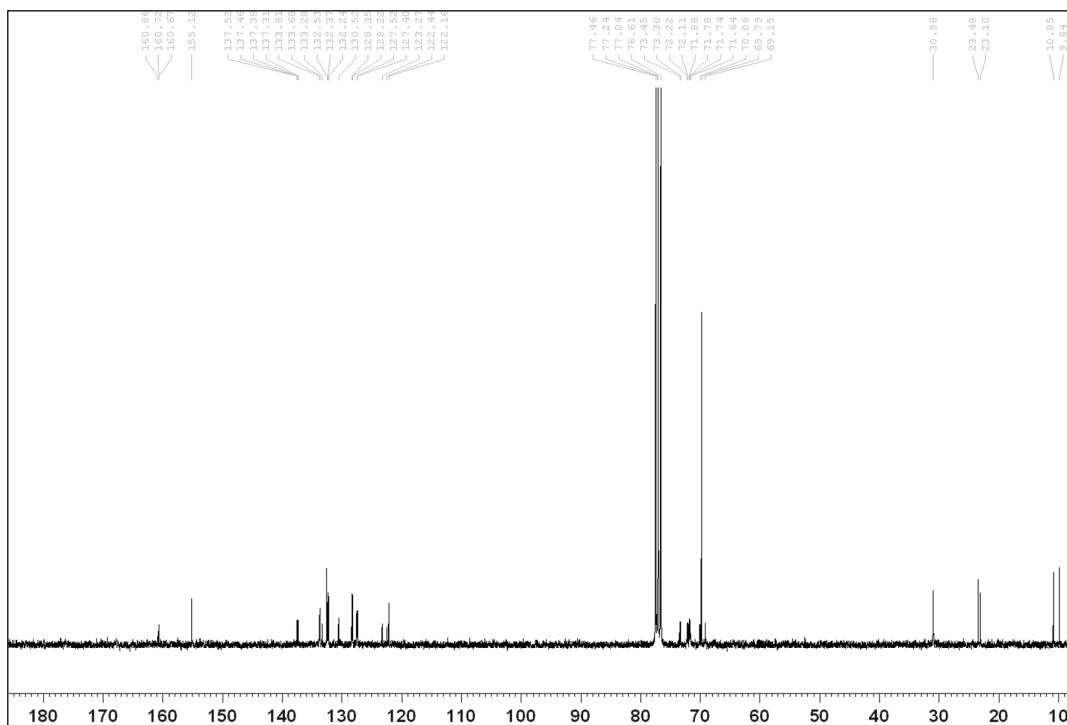
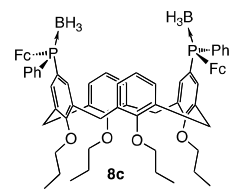


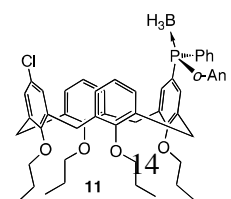
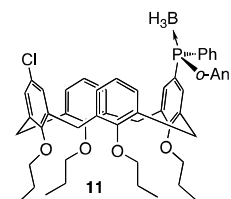
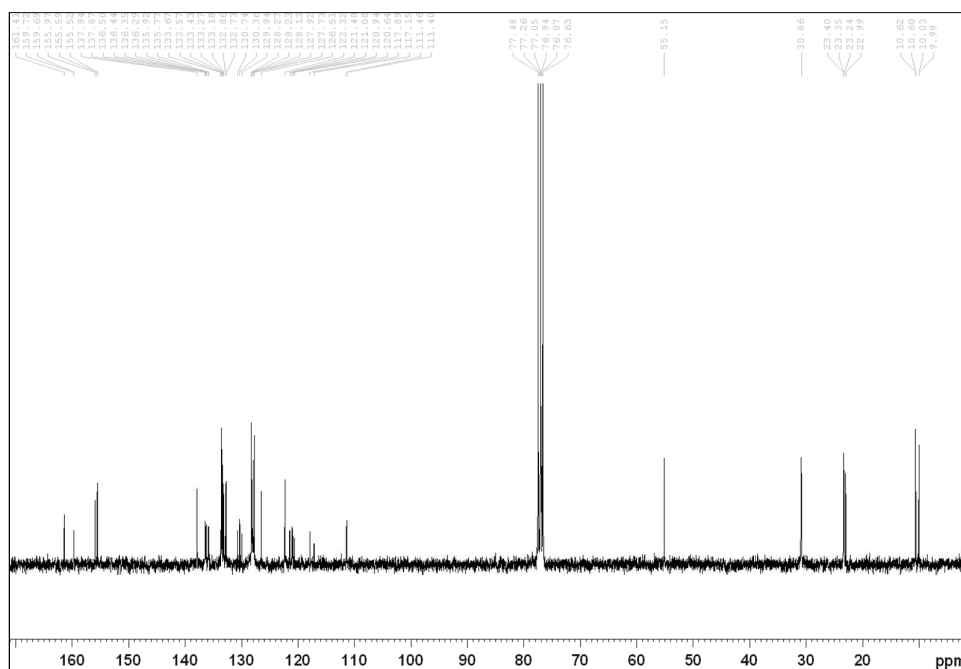
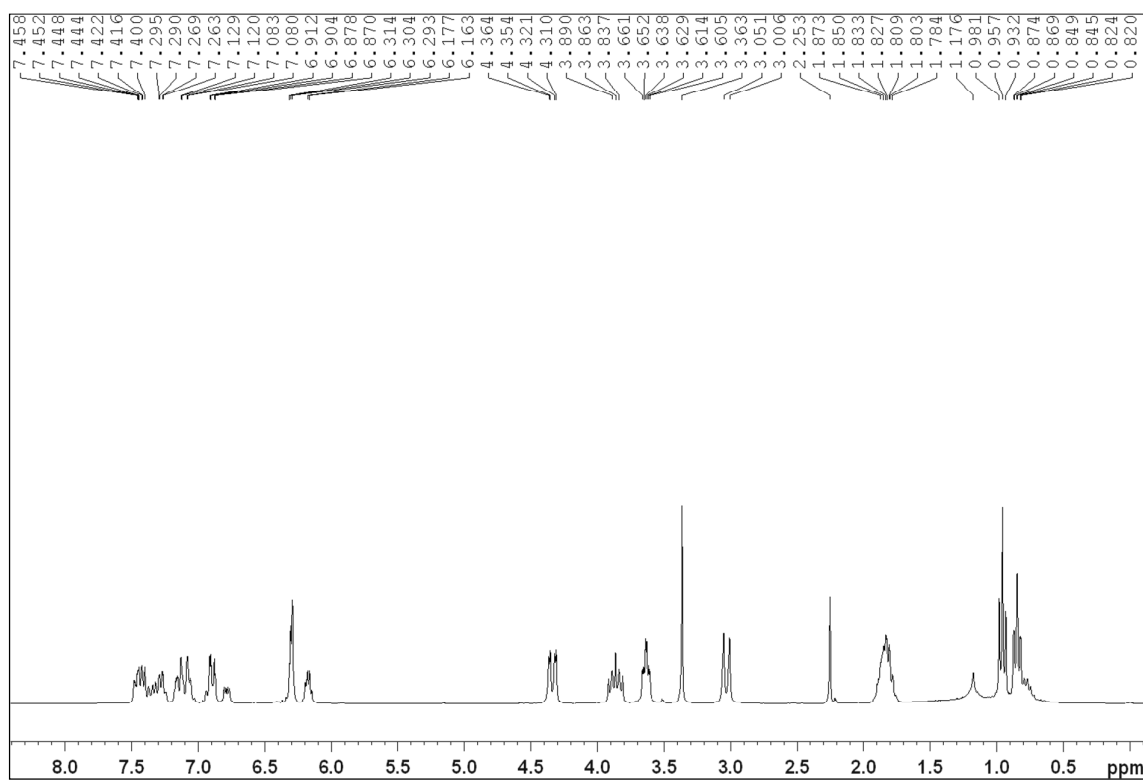


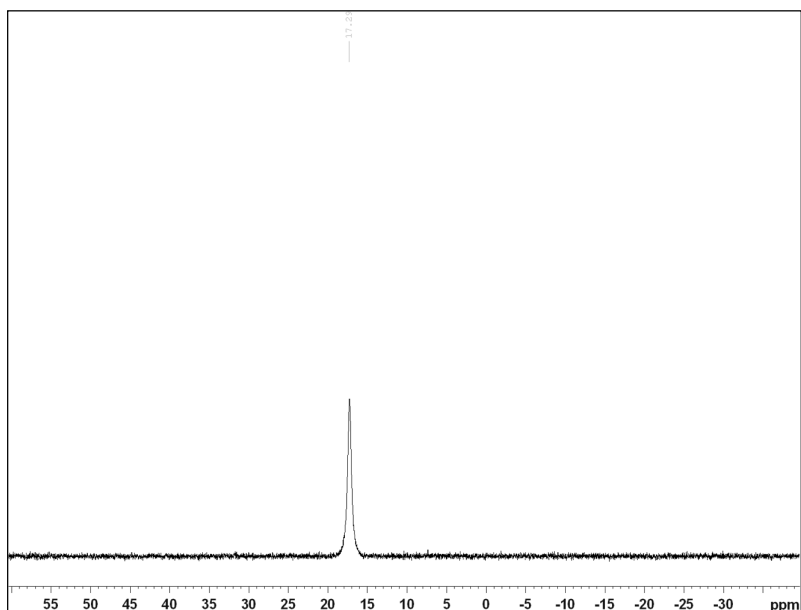












Crystal Structure Refinement

For compound **4c**, anisotropic thermal parameters were used for non-hydrogen atoms. Two propyl groups from the calix[4]arene and phenyl group attached to the phosphine borane adduct exhibit disorder with the ratios 0.50(1) / 0.50(1). The geometric parameters of disordered components in each group were restrained by using SADI¹ restraints and using EADP¹ constraints. Similar U^{ij} constraints were applied within the disordered parts to maintain a reasonable model.

For compound (*R*)-**4b**, all non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms attached to carbon atoms were included in their calculated positions and refined with a riding model while the H-B distances were refined. The methoxy group included in the anisole group was found disordered over two positions and refined with an occupation factor of 0.54/0.46. In these groups, the oxygen-carbon distance was restrained to 1.42 Å. One propoxy group from the calix[4]arene was found disordered with an occupation factor of 0.55/0.45. All bonds and angles of the four propoxy group linked to the calix[4]arene were restrained to be identical (SAME¹ instruction).

For compound **8c**, anisotropic thermal parameters were used for non-hydrogen atoms. One dichloromethane molecule, two cyclopentadienyl groups linked to Fe(1) and the ending propyl carbon C33 from the calix[4]arene exhibit disorder with the ratios 0.60(1) / 0.40(1), 0.65(1) / 0.35(1) and 0.73(1) / 0.27(1) respectively. The geometric parameters of disordered components in each group were restrained by using EADP¹ constraints. SADI¹ restraints were used only for the ending propyl group containing C32 and C33. Similar U^{ij} constraints were applied within the disordered parts to maintain a reasonable model. H atoms on boron atom B2 seemed to be disordered over two positions in the Fourier difference map and for this reason idealized methyl group were placed over two positions.

For compound **11**, all non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms attached to carbon atoms were included in their calculated positions and refined with a riding model while the B-H distances were refined. The methoxy group included in the anisyl group was found disordered over two positions and refined with an occupation factor of 0.59/0.41. In these groups, the oxygen-carbon distance was restrained to 1.42Å. Two propoxy group from the calix[4]arene were found disordered with an occupation factor equal respectively to 0.66/0.34 and 0.72/0.28. All bonds and angles of the four propoxy group linked to the calix[4]arene were restrained to be identical (SAME¹ instruction).

(1) (a) Sheldrick, G., A short history of SHELX. *Acta Cryst. Sect. A* **2008**, *64* (1), 112-122. (b) Sheldrick, G. M. *SHELX-97, Program for the Refinement of Crystal Structures*, 1997, University of Göttingen, Göttingen, Germany.

Identification code	4b (jug1)	4c (09kn250)	8c (09kn1)	11 (etjug1)
Empirical formula	C ₅₃ H ₆₂ BO ₅ P	C ₅₆ H ₆₄ BFeO ₄ P	C ₇₃ H ₈₂ B ₂ Cl ₂ Fe ₂ O ₄ P ₇	C ₅₃ H ₆₁ BClO ₅ P
Formula weight (g.mol ⁻¹)	820.81	898.70	1289.55	855.25
Temperature (K)	115(2)	115(2)	115(2)	115(2) K
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Orthorhombic
Space group	<i>P</i> 21 21 21	<i>P</i> 21	<i>C</i> 2	<i>P</i> 21 21 21
a (Å)	15.5827(4)	9.5379(4)	34.5194(10)	15.7555(4)
b (Å)	15.7535(4)	14.2348(5)	9.5372(2)	15.9369(4)
c (Å)	18.4561(5)	18.0710(8)	24.9507(8)	18.3866(5)
β (°)		98.527(2)	125.8800(10)	
Volume (Å ³)	4530.6(2)	2426.38(17)	6655.5(3)	4616.8(2)
Z	4	2	4	4
Dc (Mg.m ³)	1.203	1.230	1.287	1.230
μ (mm ⁻¹)	0.108	0.389	0.612	0.165
F(000)	1760	956	2712	1824
Crystal size (mm ³)	0.33 x 0.12 x 0.12	0.15 x 0.15 x 0.12	0.20 x 0.10 x 0.10	0.40 x 0.25 x 0.22
θ range for data collection (°)	2.90 to 27.54	1.83 to 27.48	1.66 to 27.46	2.79 to 27.49
Index ranges	-20<=h<=12	-12<=h<=12	-44<=h<=44	-20<=h<=20
	-19<=k<=20	-18<=k<=16	-12<=k<=8	-20<=k<=20
	-20<=l<=23	-23<=l<=23	-32<=l<=32	-23<=l<=23
Reflections collected	22793	10485	12953	10441
Independent reflections	10049	10485	12953	10441
[(Rint)]	0.078	0.0000	0.0000	0.041
Completeness to θ = 27.5°	98.9 %	98.9 %	98.4 %	99.4 %
Data / restraints / parameters	10049 / 52 / 583	10485 / 14 / 545	12953 / 2 / 769	10441 / 77 / 618
Goodness-of-fit on F ²	1.009	1.110	1.088	1.018
Final R1, wR2 indices [I>2σ(I)]	0.0586, 0.1187	0.0827, 0.1705	0.0601, 0.1203	0.0470, 0.0919
R1, wR2 indices (all data)	0.1162, 0.1389	0.1054, 0.1899	0.0678, 0.1270	0.0692, 0.1021
Absolute structure parameter	0.00(12)	0.06(3)	0.070(18)	0.00(5)
Largest diff. peak and hole (e. Å ⁻³)	0.632 and -0.430	0.553 and -0.565	0.771 and -0.872	0.253 and -0.268

Table S1. Crystal data and structure refinement for compound **4b** (**jug1**).

Compound	jug1
Formula	C₅₃H₆₂BO₅P
M	820.81
T; K	115(2)
Crystal system	orthorombic
Space group	P2₁2₁2₁
a; Å	15.5827(4)
b; Å	15.7535(4)
c; Å	18.4561(5)
V; Å ³	4530.6(2)
Z	4
F(000)	1760
D _{calc} ; g/cm ³	1.203
diffractometer	Enraf-Nonius KappaCCD
scan type	mixture of ϕ rotations and ω scans
λ ; Å	0.71073
μ ; mm ⁻¹	0.108
Crystal size; mm ³	0.325 x 0.12 x 0.12
$\sin(\theta)/\lambda$ max; Å ⁻¹	0.65
Index ranges	h: -20; 12
	k: -19; 20
	l: -20; 23
RC = Refl. Collected	22793
IRC = independent RC	10049 [R(int) = 0.0693]
IRCGT = RC and [I>2 σ (I)]	6177
Refinement method	Full-matrix least-squares on F²
Data / restraints / parameters	10049 / 14 / 563
R for IRCGT	R1^a = 0.0603 , wR2^b = 0.1250
R for IRC	R1^a = 0.1179 , wR2^b = 0.1457
Goodness-of-fit ^c	1.025
Abs. structure parameter	-0.13(12)
Largest diff. peak and hole; e.Å ⁻³	0.635 and -0.416

^a $R1 = \sum(|F_o| - |F_c|) / \sum|F_o|$.

^b $wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ where $w = 1 / [\sigma^2(F_o^2) + (0.0662P)^2]$ where $P = (\text{Max}(F_o^2, 0) + 2 * F_c^2) / 3$

^c Goodness of fit = $[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **4b** (**jug1**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3139(2)	1418(2)	10369(2)	37(1)
C(2)	2799(3)	962(2)	10954(2)	47(1)
C(3)	3283(3)	847(2)	11579(2)	57(1)
C(4)	4090(3)	1177(2)	11634(2)	56(1)
C(5)	4445(3)	1619(2)	11063(2)	48(1)
C(6)	3971(2)	1727(2)	10429(2)	38(1)
C(7)	3070(2)	1157(2)	8787(2)	33(1)
C(8)	2939(2)	311(2)	8603(2)	38(1)
C(9)	3370(2)	-48(2)	8023(2)	39(1)
C(10)	3927(2)	446(2)	7619(2)	40(1)
C(11)	4053(2)	1288(2)	7791(2)	40(1)
C(12)	3629(2)	1643(2)	8374(2)	37(1)
C(13)	5168(3)	2214(6)	9776(3)	159(4)
C(14)	2379(2)	2701(2)	9417(2)	32(1)
C(15)	2624(2)	3306(2)	9931(2)	32(1)
C(16)	2449(2)	4161(2)	9839(2)	29(1)
C(17)	2005(2)	4411(2)	9220(2)	32(1)
C(18)	1816(2)	3840(2)	8658(2)	34(1)
C(19)	1996(2)	2988(2)	8778(2)	35(1)
C(20)	1506(2)	4158(2)	7929(2)	36(1)
C(21)	2171(2)	4719(2)	7567(2)	32(1)
C(22)	2018(2)	5576(2)	7404(2)	33(1)
C(23)	2661(2)	6104(2)	7135(1)	32(1)
C(24)	3453(2)	5748(2)	6982(2)	35(1)
C(25)	3614(2)	4903(2)	7106(2)	36(1)
C(26)	2978(2)	4396(2)	7416(2)	34(1)
C(27)	2537(2)	7057(2)	7052(2)	37(1)
C(28)	3255(2)	7523(2)	7434(2)	32(1)
C(29)	3337(2)	7454(2)	8191(2)	30(1)
C(30)	4082(2)	7713(2)	8554(2)	31(1)
C(31)	4717(2)	8111(2)	8145(2)	36(1)
C(32)	4625(2)	8239(2)	7408(2)	39(1)
C(33)	3903(2)	7937(2)	7060(2)	40(1)
C(34)	4202(2)	7506(2)	9348(2)	30(1)
C(35)	4213(2)	6560(2)	9483(1)	28(1)
C(36)	3583(2)	6161(2)	9902(1)	25(1)
C(37)	3563(2)	5274(2)	9980(1)	28(1)
C(38)	4228(2)	4808(2)	9676(2)	33(1)
C(39)	4877(2)	5202(2)	9279(2)	35(1)
C(40)	4858(2)	6065(2)	9181(2)	33(1)
C(41)	2818(2)	4832(2)	10349(1)	29(1)
C(42)	890(2)	5424(2)	9253(2)	49(1)
C(43)	627(2)	5444(2)	10033(2)	48(1)
C(44)	-344(2)	5465(3)	10101(3)	71(1)
C(45)	636(3)	5896(4)	6942(2)	89(2)
C(46A)	-320(6)	5823(5)	7312(4)	48(2)
C(47A)	-482(5)	6719(6)	7593(4)	56(2)
C(46B)	-101(5)	6559(5)	7096(4)	38(2)
C(47B)	-715(7)	6025(9)	7547(6)	55(3)

C (48)	2066 (3)	7585 (4)	8901 (2)	86 (2)
C (49)	1500 (4)	8066 (3)	8529 (3)	97 (2)
C (50)	801 (2)	8521 (3)	8926 (2)	53 (1)
C (51)	3144 (2)	6861 (2)	10970 (2)	36 (1)
C (52)	2454 (3)	7434 (2)	11261 (2)	42 (1)
C (53)	2442 (3)	8316 (2)	10937 (2)	51 (1)
O (1)	4287 (2)	2142 (2)	9838 (1)	46 (1)
O (2)	1796 (1)	5258 (1)	9139 (1)	37 (1)
O (3)	1210 (1)	5905 (1)	7559 (1)	39 (1)
O (4)	2698 (1)	7056 (1)	8580 (1)	38 (1)
O (5)	2947 (1)	6651 (1)	10224 (1)	29 (1)
P (1)	2491 (1)	1569 (1)	9567 (1)	37 (1)
B (1)	1424 (3)	1011 (3)	9686 (3)	61 (1)

Table S3. Bond lengths [Å] and angles [deg] for compound **4b(jug1)**.

C(1)–C(6)	1.390(5)
C(1)–C(2)	1.402(4)
C(1)–P(1)	1.808(4)
C(2)–C(3)	1.389(5)
C(2)–H(2)	0.9300
C(3)–C(4)	1.364(6)
C(3)–H(3)	0.9300
C(4)–C(5)	1.379(5)
C(4)–H(4)	0.9300
C(5)–C(6)	1.395(5)
C(5)–H(5)	0.9300
C(6)–O(1)	1.362(4)
C(7)–C(12)	1.387(4)
C(7)–C(8)	1.390(4)
C(7)–P(1)	1.820(3)
C(8)–C(9)	1.385(4)
C(8)–H(8)	0.9300
C(9)–C(10)	1.384(5)
C(9)–H(9)	0.9300
C(10)–C(11)	1.377(4)
C(10)–H(10)	0.9300
C(11)–C(12)	1.382(4)
C(11)–H(11)	0.9300
C(12)–H(12)	0.9300
C(13)–O(1)	1.382(5)
C(13)–H(13A)	0.9600
C(13)–H(13B)	0.9600
C(13)–H(13C)	0.9600
C(14)–C(15)	1.398(4)
C(14)–C(19)	1.399(4)
C(14)–P(1)	1.812(3)
C(15)–C(16)	1.384(4)
C(15)–H(15)	0.9300
C(16)–C(17)	1.392(4)
C(16)–C(41)	1.528(4)
C(17)–O(2)	1.383(4)
C(17)–C(18)	1.404(4)
C(18)–C(19)	1.388(4)
C(18)–C(20)	1.514(4)
C(19)–H(19)	0.9300
C(20)–C(21)	1.516(4)
C(20)–H(20A)	0.9700
C(20)–H(20B)	0.9700
C(21)–C(26)	1.385(4)
C(21)–C(22)	1.404(4)
C(22)–O(3)	1.391(4)
C(22)–C(23)	1.394(5)
C(23)–C(24)	1.385(4)
C(23)–C(27)	1.520(4)
C(24)–C(25)	1.375(4)
C(24)–H(24)	0.9300
C(25)–C(26)	1.395(5)
C(25)–H(25)	0.9300
C(26)–H(26)	0.9300
C(27)–C(28)	1.513(5)

C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-C(33)	1.386(5)
C(28)-C(29)	1.407(4)
C(29)-O(4)	1.379(4)
C(29)-C(30)	1.401(4)
C(30)-C(31)	1.393(4)
C(30)-C(34)	1.512(4)
C(31)-C(32)	1.384(4)
C(31)-H(31)	0.9300
C(32)-C(33)	1.379(5)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-C(35)	1.510(4)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(35)-C(40)	1.389(4)
C(35)-C(36)	1.398(4)
C(36)-O(5)	1.389(3)
C(36)-C(37)	1.406(4)
C(37)-C(38)	1.388(4)
C(37)-C(41)	1.516(4)
C(38)-C(39)	1.394(4)
C(38)-H(38)	0.9300
C(39)-C(40)	1.371(5)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(42)-O(2)	1.450(4)
C(42)-C(43)	1.498(5)
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700
C(43)-C(44)	1.519(5)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(44)-H(44A)	0.9600
C(44)-H(44B)	0.9600
C(44)-H(44C)	0.9600
C(45)-O(3)	1.447(4)
C(45)-C(46B)	1.578(8)
C(45)-C(46A)	1.643(10)
C(45)-H(45A)	0.9700
C(45)-H(45B)	0.9700
C(46A)-C(47A)	1.524(10)
C(46A)-H(46A)	0.9700
C(46A)-H(46B)	0.9700
C(47A)-H(47A)	0.9600
C(47A)-H(47B)	0.9600
C(47A)-H(47C)	0.9600
C(46B)-C(47B)	1.521(11)
C(46B)-H(46C)	0.9700
C(46B)-H(46D)	0.9700
C(47B)-H(47D)	0.9600
C(47B)-H(47E)	0.9600
C(47B)-H(47F)	0.9600
C(48)-C(49)	1.350(6)
C(48)-O(4)	1.420(4)

C(48)–H(48A)	0.9700
C(48)–H(48B)	0.9700
C(49)–C(50)	1.495(5)
C(49)–H(49A)	0.9700
C(49)–H(49B)	0.9700
C(50)–H(50A)	0.9600
C(50)–H(50B)	0.9600
C(50)–H(50C)	0.9600
C(51)–O(5)	1.449(3)
C(51)–C(52)	1.503(5)
C(51)–H(51A)	0.9700
C(51)–H(51B)	0.9700
C(52)–C(53)	1.513(5)
C(52)–H(52A)	0.9700
C(52)–H(52B)	0.9700
C(53)–H(53A)	0.9600
C(53)–H(53B)	0.9600
C(53)–H(53C)	0.9600
P(1)–B(1)	1.893(4)
B(1)–H(1A)	1.1208
B(1)–H(1B)	1.1208
B(1)–H(1C)	1.1208
C(6)–C(1)–C(2)	118.1(3)
C(6)–C(1)–P(1)	122.7(2)
C(2)–C(1)–P(1)	119.2(3)
C(3)–C(2)–C(1)	120.1(4)
C(3)–C(2)–H(2)	119.9
C(1)–C(2)–H(2)	119.9
C(4)–C(3)–C(2)	120.8(4)
C(4)–C(3)–H(3)	119.6
C(2)–C(3)–H(3)	119.6
C(3)–C(4)–C(5)	120.4(4)
C(3)–C(4)–H(4)	119.8
C(5)–C(4)–H(4)	119.8
C(4)–C(5)–C(6)	119.4(4)
C(4)–C(5)–H(5)	120.3
C(6)–C(5)–H(5)	120.3
O(1)–C(6)–C(1)	116.2(3)
O(1)–C(6)–C(5)	122.6(3)
C(1)–C(6)–C(5)	121.2(3)
C(12)–C(7)–C(8)	119.2(3)
C(12)–C(7)–P(1)	123.3(2)
C(8)–C(7)–P(1)	117.5(2)
C(9)–C(8)–C(7)	120.6(3)
C(9)–C(8)–H(8)	119.7
C(7)–C(8)–H(8)	119.7
C(10)–C(9)–C(8)	119.4(3)
C(10)–C(9)–H(9)	120.3
C(8)–C(9)–H(9)	120.3
C(11)–C(10)–C(9)	120.5(3)
C(11)–C(10)–H(10)	119.8
C(9)–C(10)–H(10)	119.8
C(10)–C(11)–C(12)	120.0(3)
C(10)–C(11)–H(11)	120.0
C(12)–C(11)–H(11)	120.0
C(11)–C(12)–C(7)	120.3(3)
C(11)–C(12)–H(12)	119.8

C(7)-C(12)-H(12)	119.8
O(1)-C(13)-H(13A)	109.5
O(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	117.9(3)
C(15)-C(14)-P(1)	122.8(2)
C(19)-C(14)-P(1)	119.2(2)
C(16)-C(15)-C(14)	121.8(3)
C(16)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1
C(15)-C(16)-C(17)	118.3(3)
C(15)-C(16)-C(41)	121.5(3)
C(17)-C(16)-C(41)	119.9(3)
O(2)-C(17)-C(16)	118.6(3)
O(2)-C(17)-C(18)	119.3(3)
C(16)-C(17)-C(18)	122.0(3)
C(19)-C(18)-C(17)	117.3(3)
C(19)-C(18)-C(20)	121.7(3)
C(17)-C(18)-C(20)	120.7(3)
C(18)-C(19)-C(14)	122.2(3)
C(18)-C(19)-H(19)	118.9
C(14)-C(19)-H(19)	118.9
C(18)-C(20)-C(21)	111.5(3)
C(18)-C(20)-H(20A)	109.3
C(21)-C(20)-H(20A)	109.3
C(18)-C(20)-H(20B)	109.3
C(21)-C(20)-H(20B)	109.3
H(20A)-C(20)-H(20B)	108.0
C(26)-C(21)-C(22)	117.6(3)
C(26)-C(21)-C(20)	119.7(3)
C(22)-C(21)-C(20)	122.6(3)
O(3)-C(22)-C(23)	120.0(3)
O(3)-C(22)-C(21)	117.9(3)
C(23)-C(22)-C(21)	121.9(3)
C(24)-C(23)-C(22)	118.1(3)
C(24)-C(23)-C(27)	119.5(3)
C(22)-C(23)-C(27)	122.3(3)
C(25)-C(24)-C(23)	121.4(3)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3
C(24)-C(25)-C(26)	119.5(3)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(21)-C(26)-C(25)	121.2(3)
C(21)-C(26)-H(26)	119.4
C(25)-C(26)-H(26)	119.4
C(28)-C(27)-C(23)	109.8(3)
C(28)-C(27)-H(27A)	109.7
C(23)-C(27)-H(27A)	109.7
C(28)-C(27)-H(27B)	109.7
C(23)-C(27)-H(27B)	109.7
H(27A)-C(27)-H(27B)	108.2
C(33)-C(28)-C(29)	117.7(3)
C(33)-C(28)-C(27)	122.4(3)
C(29)-C(28)-C(27)	119.5(3)

O(4)–C(29)–C(30)	118.8(3)
O(4)–C(29)–C(28)	119.1(3)
C(30)–C(29)–C(28)	121.8(3)
C(31)–C(30)–C(29)	117.4(3)
C(31)–C(30)–C(34)	122.3(3)
C(29)–C(30)–C(34)	120.2(3)
C(32)–C(31)–C(30)	121.6(3)
C(32)–C(31)–H(31)	119.2
C(30)–C(31)–H(31)	119.2
C(33)–C(32)–C(31)	119.5(3)
C(33)–C(32)–H(32)	120.3
C(31)–C(32)–H(32)	120.3
C(32)–C(33)–C(28)	121.6(3)
C(32)–C(33)–H(33)	119.2
C(28)–C(33)–H(33)	119.2
C(35)–C(34)–C(30)	112.1(2)
C(35)–C(34)–H(34A)	109.2
C(30)–C(34)–H(34A)	109.2
C(35)–C(34)–H(34B)	109.2
C(30)–C(34)–H(34B)	109.2
H(34A)–C(34)–H(34B)	107.9
C(40)–C(35)–C(36)	118.5(3)
C(40)–C(35)–C(34)	119.7(3)
C(36)–C(35)–C(34)	121.8(3)
O(5)–C(36)–C(35)	119.2(3)
O(5)–C(36)–C(37)	119.5(3)
C(35)–C(36)–C(37)	121.3(3)
C(38)–C(37)–C(36)	117.8(3)
C(38)–C(37)–C(41)	120.8(3)
C(36)–C(37)–C(41)	121.3(3)
C(37)–C(38)–C(39)	121.3(3)
C(37)–C(38)–H(38)	119.4
C(39)–C(38)–H(38)	119.4
C(40)–C(39)–C(38)	119.6(3)
C(40)–C(39)–H(39)	120.2
C(38)–C(39)–H(39)	120.2
C(39)–C(40)–C(35)	121.3(3)
C(39)–C(40)–H(40)	119.3
C(35)–C(40)–H(40)	119.3
C(37)–C(41)–C(16)	109.2(2)
C(37)–C(41)–H(41A)	109.8
C(16)–C(41)–H(41A)	109.8
C(37)–C(41)–H(41B)	109.8
C(16)–C(41)–H(41B)	109.8
H(41A)–C(41)–H(41B)	108.3
O(2)–C(42)–C(43)	114.1(3)
O(2)–C(42)–H(42A)	108.7
C(43)–C(42)–H(42A)	108.7
O(2)–C(42)–H(42B)	108.7
C(43)–C(42)–H(42B)	108.7
H(42A)–C(42)–H(42B)	107.6
C(42)–C(43)–C(44)	110.7(3)
C(42)–C(43)–H(43A)	109.5
C(44)–C(43)–H(43A)	109.5
C(42)–C(43)–H(43B)	109.5
C(44)–C(43)–H(43B)	109.5
H(43A)–C(43)–H(43B)	108.1
C(43)–C(44)–H(44A)	109.5

C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
O(3)-C(45)-C(46B)	107.6(4)
O(3)-C(45)-C(46A)	103.6(4)
C(46B)-C(45)-C(46A)	46.5(4)
O(3)-C(45)-H(45A)	111.0
C(46B)-C(45)-H(45A)	139.4
C(46A)-C(45)-H(45A)	111.0
O(3)-C(45)-H(45B)	111.0
C(46B)-C(45)-H(45B)	66.6
C(46A)-C(45)-H(45B)	111.0
H(45A)-C(45)-H(45B)	109.0
C(47A)-C(46A)-C(45)	103.1(6)
C(47A)-C(46A)-H(46A)	111.1
C(45)-C(46A)-H(46A)	111.1
C(47A)-C(46A)-H(46B)	111.1
C(45)-C(46A)-H(46B)	111.1
H(46A)-C(46A)-H(46B)	109.1
C(46A)-C(47A)-H(47A)	109.5
C(46A)-C(47A)-H(47B)	109.5
H(47A)-C(47A)-H(47B)	109.5
C(46A)-C(47A)-H(47C)	109.5
H(47A)-C(47A)-H(47C)	109.5
H(47B)-C(47A)-H(47C)	109.5
C(47B)-C(46B)-C(45)	100.9(7)
C(47B)-C(46B)-H(46C)	111.6
C(45)-C(46B)-H(46C)	111.6
C(47B)-C(46B)-H(46D)	111.6
C(45)-C(46B)-H(46D)	111.6
H(46C)-C(46B)-H(46D)	109.4
C(46B)-C(47B)-H(47D)	109.5
C(46B)-C(47B)-H(47E)	109.5
H(47D)-C(47B)-H(47E)	109.5
C(46B)-C(47B)-H(47F)	109.5
H(47D)-C(47B)-H(47F)	109.5
H(47E)-C(47B)-H(47F)	109.5
C(49)-C(48)-O(4)	124.8(4)
C(49)-C(48)-H(48A)	106.1
O(4)-C(48)-H(48A)	106.1
C(49)-C(48)-H(48B)	106.1
O(4)-C(48)-H(48B)	106.1
H(48A)-C(48)-H(48B)	106.3
C(48)-C(49)-C(50)	119.7(4)
C(48)-C(49)-H(49A)	107.4
C(50)-C(49)-H(49A)	107.4
C(48)-C(49)-H(49B)	107.4
C(50)-C(49)-H(49B)	107.4
H(49A)-C(49)-H(49B)	106.9
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
O(5)-C(51)-C(52)	109.0(3)

O(5)-C(51)-H(51A)	109.9
C(52)-C(51)-H(51A)	109.9
O(5)-C(51)-H(51B)	109.9
C(52)-C(51)-H(51B)	109.9
H(51A)-C(51)-H(51B)	108.3
C(51)-C(52)-C(53)	114.8(3)
C(51)-C(52)-H(52A)	108.6
C(53)-C(52)-H(52A)	108.6
C(51)-C(52)-H(52B)	108.6
C(53)-C(52)-H(52B)	108.6
H(52A)-C(52)-H(52B)	107.6
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(6)-O(1)-C(13)	117.6(3)
C(17)-O(2)-C(42)	112.8(3)
C(22)-O(3)-C(45)	113.3(2)
C(29)-O(4)-C(48)	116.9(3)
C(36)-O(5)-C(51)	112.4(2)
C(1)-P(1)-C(14)	107.95(14)
C(1)-P(1)-C(7)	108.84(15)
C(14)-P(1)-C(7)	106.12(14)
C(1)-P(1)-B(1)	109.5(2)
C(14)-P(1)-B(1)	113.0(2)
C(7)-P(1)-B(1)	111.23(17)
P(1)-B(1)-H(1A)	109.5
P(1)-B(1)-H(1B)	109.5
H(1A)-B(1)-H(1B)	109.5
P(1)-B(1)-H(1C)	109.5
H(1A)-B(1)-H(1C)	109.5
H(1B)-B(1)-H(1C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **4b** (**jug1**).

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	51(2)	25(2)	33(2)	-3(1)	14(2)	4(2)
C(2)	71(3)	28(2)	40(2)	-6(2)	20(2)	5(2)
C(3)	90(4)	43(2)	39(2)	14(2)	24(2)	25(2)
C(4)	82(3)	47(2)	38(2)	2(2)	10(2)	29(2)
C(5)	70(3)	36(2)	40(2)	-8(2)	-1(2)	15(2)
C(6)	56(2)	29(2)	28(2)	-4(2)	7(2)	3(2)
C(7)	41(2)	33(2)	26(2)	-2(1)	4(2)	-3(2)
C(8)	46(2)	34(2)	32(2)	-1(2)	4(2)	-4(2)
C(9)	51(2)	30(2)	36(2)	-8(2)	-1(2)	-1(2)
C(10)	58(2)	36(2)	24(2)	-4(2)	2(2)	3(2)
C(11)	49(2)	36(2)	34(2)	2(2)	10(2)	-4(2)
C(12)	46(2)	31(2)	35(2)	-7(2)	4(2)	-5(2)
C(13)	51(4)	309(10)	116(5)	125(6)	-12(3)	-75(5)
C(14)	33(2)	36(2)	27(2)	-9(1)	7(2)	-4(2)
C(15)	42(2)	34(2)	21(1)	0(1)	4(1)	-6(2)
C(16)	31(2)	34(2)	23(1)	-4(1)	9(1)	-4(2)
C(17)	32(2)	38(2)	27(2)	-5(2)	1(2)	-1(2)
C(18)	33(2)	43(2)	25(2)	-9(2)	3(1)	-1(2)
C(19)	29(2)	41(2)	34(2)	-16(2)	2(2)	-8(2)
C(20)	34(2)	46(2)	28(2)	-17(2)	-4(2)	2(2)
C(21)	35(2)	42(2)	17(1)	-11(1)	-7(1)	6(2)
C(22)	29(2)	49(2)	20(2)	-15(2)	-4(1)	12(2)
C(23)	38(2)	40(2)	18(1)	-5(1)	-9(1)	10(2)
C(24)	34(2)	41(2)	30(2)	-9(2)	-2(2)	2(2)
C(25)	35(2)	42(2)	31(2)	-10(2)	0(2)	11(2)
C(26)	41(2)	31(2)	30(2)	-11(1)	-7(2)	6(2)
C(27)	49(2)	42(2)	21(2)	-7(1)	-10(2)	14(2)
C(28)	42(2)	29(2)	24(2)	-3(1)	-4(2)	14(2)
C(29)	36(2)	29(2)	26(2)	2(1)	4(1)	6(2)
C(30)	38(2)	32(2)	24(2)	-1(1)	-3(2)	0(2)
C(31)	38(2)	33(2)	36(2)	5(2)	0(2)	1(2)
C(32)	50(2)	36(2)	29(2)	7(2)	8(2)	5(2)
C(33)	64(3)	33(2)	22(2)	5(2)	10(2)	12(2)
C(34)	30(2)	33(2)	26(2)	4(1)	-4(1)	-2(1)
C(35)	32(2)	32(2)	18(1)	3(1)	-8(1)	-1(2)
C(36)	27(2)	33(2)	14(1)	-3(1)	-5(1)	3(1)
C(37)	34(2)	33(2)	17(1)	1(1)	-3(1)	0(1)
C(38)	44(2)	29(2)	24(2)	3(1)	-1(2)	6(2)
C(39)	30(2)	44(2)	31(2)	5(2)	2(2)	10(2)
C(40)	31(2)	40(2)	28(2)	5(2)	-2(2)	-4(2)
C(41)	45(2)	28(2)	15(1)	-2(1)	-2(1)	-2(1)
C(42)	42(2)	62(2)	42(2)	-19(2)	-12(2)	16(2)
C(43)	47(2)	51(2)	46(2)	-20(2)	5(2)	0(2)
C(44)	47(3)	61(3)	105(4)	-43(3)	14(3)	-6(2)
C(45)	51(3)	173(5)	42(2)	-43(3)	-21(2)	57(3)
C(46A)	61(6)	40(5)	42(5)	7(4)	-15(4)	2(5)
C(47A)	39(5)	78(6)	53(5)	-2(5)	-4(4)	24(4)
C(46B)	27(4)	48(5)	40(4)	19(4)	-8(4)	5(4)
C(47B)	42(7)	74(9)	49(6)	8(6)	12(5)	5(6)

C(48)	71(3)	133(5)	52(3)	36(3)	27(2)	47(3)
C(49)	129(5)	71(3)	91(4)	38(3)	61(4)	48(3)
C(50)	53(3)	61(2)	46(2)	-12(2)	5(2)	6(2)
C(51)	45(2)	39(2)	22(2)	-3(1)	-3(2)	2(2)
C(52)	49(2)	45(2)	33(2)	-7(2)	7(2)	-4(2)
C(53)	56(2)	47(2)	51(2)	-4(2)	13(2)	10(2)
O(1)	47(2)	49(1)	41(1)	3(1)	6(1)	-7(1)
O(2)	39(2)	39(1)	32(1)	-3(1)	-3(1)	6(1)
O(3)	32(1)	58(2)	26(1)	-14(1)	-8(1)	16(1)
O(4)	35(1)	46(1)	32(1)	-8(1)	6(1)	-5(1)
O(5)	34(1)	32(1)	21(1)	-3(1)	-1(1)	1(1)
P(1)	49(1)	33(1)	30(1)	-7(1)	12(1)	-11(1)
B(1)	58(3)	73(3)	51(3)	-25(2)	21(2)	-30(3)

Table S5. Crystal data and structure refinement for compound **4c** (09kn250).

Identification code	09kn250	
Empirical formula	C ₅₆ H ₆₄ B Fe O ₄ P	
Formula weight	898.70	
Temperature	115(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 9.5379(4) Å	a = 90°.
	b = 14.2348(5) Å	b = 98.527(2)°.
	c = 18.0710(8) Å	g = 90°.
Volume	2426.38(17) Å ³	
Z	2	
Density (calculated)	1.230 Mg/m ³	
Absorption coefficient	0.389 mm ⁻¹	
F(000)	956	
Crystal size	0.15 x 0.15 x 0.12 mm ³	
Theta range for data collection	1.83 to 27.48°.	
Index ranges	-12<=h<=12, -18<=k<=16, -23<=l<=23	
Reflections collected	10485	
Independent reflections	10485 [R(int) = 0.0000]	
Completeness to theta = 27.48°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10485 / 14 / 545	
Goodness-of-fit on F ²	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0827, wR2 = 0.1705	
R indices (all data)	R1 = 0.1054, wR2 = 0.1899	
Absolute structure parameter	0.06(3)	
Largest diff. peak and hole	0.553 and -0.565 e.Å ⁻³	

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **4c** (09kn250). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-439(5)	1162(5)	555(2)	34(1)
C(2)	19(6)	331(4)	929(3)	34(1)
C(3)	938(6)	345(4)	1599(3)	30(1)
C(4)	1412(5)	1234(4)	1888(2)	28(1)
C(5)	889(6)	2062(4)	1563(3)	31(1)
C(6)	-33(6)	2026(4)	887(3)	32(1)
C(7)	1285(7)	2987(4)	1963(3)	31(1)
C(8)	747(6)	3035(4)	2714(3)	31(1)
C(9)	-667(7)	2866(4)	2763(3)	36(1)
C(10)	-1154(7)	2842(4)	3446(3)	37(1)
C(11)	-187(6)	2956(4)	4100(3)	33(1)
C(12)	1241(6)	3125(3)	4078(3)	29(1)
C(13)	1682(6)	3185(3)	3384(3)	27(1)
C(14)	2272(6)	3169(4)	4806(3)	31(1)
C(15)	2147(6)	2275(4)	5247(3)	28(1)
C(16)	1413(6)	2268(4)	5865(3)	36(1)
C(17)	1124(6)	1426(4)	6197(3)	38(1)
C(18)	1465(6)	583(4)	5901(3)	34(1)
C(19)	2196(6)	561(4)	5280(3)	30(1)
C(20)	2581(5)	1416(4)	4994(3)	30(1)
C(21)	2400(6)	-349(4)	4875(3)	30(1)
C(22)	1351(6)	-392(3)	4157(3)	29(1)
C(23)	-61(6)	-202(4)	4173(3)	33(1)
C(24)	-1036(6)	-187(4)	3524(3)	34(1)
C(25)	-588(6)	-324(4)	2837(3)	34(1)
C(26)	836(6)	-500(3)	2796(3)	28(1)
C(27)	1781(6)	-549(3)	3460(3)	26(1)
C(28)	1327(7)	-553(4)	2037(3)	33(1)
C(29A)	3752(12)	967(10)	2481(9)	53(2)
C(30A)	4553(13)	1751(10)	2212(8)	53(2)
C(31A)	6043(13)	1603(12)	1984(8)	53(2)
C(33A)	4846(14)	4607(10)	3233(10)	55(1)
C(34A)	4836(17)	5691(9)	3077(8)	55(1)

C(42A)	-3390(15)	-28(11)	310(8)	50(1)
C(43A)	-4474(15)	-711(11)	331(9)	50(1)
C(44A)	-4920(17)	-1181(12)	-326(8)	50(1)
C(45A)	-4395(16)	-1033(11)	-979(8)	50(1)
C(46A)	-3307(19)	-361(14)	-970(9)	50(1)
C(29B)	3812(12)	1328(13)	2559(8)	53(2)
C(30B)	4454(12)	1459(11)	1883(7)	53(2)
C(31B)	6143(12)	1353(13)	2233(7)	53(2)
C(33B)	4844(14)	4387(10)	3079(10)	55(1)
C(34B)	5257(17)	5396(10)	2851(8)	55(1)
C(42B)	-3644(14)	396(11)	278(8)	50(1)
C(43B)	-4734(15)	-237(11)	386(8)	50(1)
C(44B)	-5010(18)	-973(11)	-86(9)	50(1)
C(45B)	-4234(16)	-1071(11)	-660(8)	50(1)
C(46B)	-3175(19)	-457(14)	-761(9)	50(1)
C(32)	3338(8)	4364(5)	3244(4)	55(1)
C(35)	4770(7)	1687(5)	4558(3)	49(2)
C(36)	5699(7)	878(5)	4817(4)	52(2)
C(37)	7266(6)	1220(7)	5009(4)	65(2)
C(38)	3550(8)	-1702(5)	3418(4)	57(2)
C(39)	5104(8)	-1771(6)	3369(5)	71(2)
C(40)	5493(8)	-1404(7)	2648(5)	81(3)
C(41)	-2827(7)	219(5)	-289(4)	50(1)
C(47)	-303(6)	564(4)	-949(3)	35(1)
C(48)	869(6)	-58(4)	-731(3)	36(1)
C(49)	1485(7)	-274(4)	-1381(3)	42(1)
C(50)	691(7)	185(4)	-2000(3)	45(2)
C(51)	-410(7)	705(4)	-1748(3)	40(1)
C(52)	2926(9)	1809(6)	-418(5)	72(2)
C(53)	1801(9)	2427(5)	-715(5)	62(2)
C(54)	1805(9)	2503(5)	-1484(5)	67(2)
C(55)	2903(8)	1931(6)	-1688(6)	70(2)
C(56)	3583(8)	1503(6)	-1034(6)	75(2)
B(1)	-2308(8)	2259(6)	-732(4)	47(2)
Fe(1)	1512(1)	1143(1)	-1206(1)	39(1)
O(1)	3209(4)	-721(3)	3430(2)	33(1)
O(2)	2361(3)	1258(3)	2542(2)	36(1)
O(3)	3098(4)	3379(3)	3345(2)	33(1)

O(4)	3305(4)	1407(2)	4378(2)	32(1)
P(1)	-1464(1)	1101(1)	-366(1)	35(1)

Table S7. Bond lengths [Å] and angles [°] for compound **4c** (09kn250).

C(1)-C(6)	1.398(8)
C(1)-C(2)	1.401(8)
C(1)-P(1)	1.803(5)
C(2)-C(3)	1.386(8)
C(2)-H(2)	0.9500
C(3)-C(4)	1.417(8)
C(3)-C(28)	1.521(8)
C(4)-C(5)	1.377(8)
C(4)-O(2)	1.378(5)
C(5)-C(6)	1.397(8)
C(5)-C(7)	1.523(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.521(7)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.386(8)
C(8)-C(13)	1.411(8)
C(9)-C(10)	1.382(8)
C(9)-H(9)	0.9500
C(10)-C(11)	1.396(8)
C(10)-H(10)	0.9500
C(11)-C(12)	1.390(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.383(7)
C(12)-C(14)	1.522(7)
C(13)-O(3)	1.390(7)
C(14)-C(15)	1.515(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.391(7)
C(15)-C(16)	1.404(8)
C(16)-C(17)	1.386(8)
C(16)-H(16)	0.9500
C(17)-C(18)	1.372(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.407(7)

C(18)-H(18)	0.9500
C(19)-C(20)	1.393(7)
C(19)-C(21)	1.514(7)
C(20)-O(4)	1.394(5)
C(21)-C(22)	1.518(7)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.378(8)
C(22)-C(27)	1.398(7)
C(23)-C(24)	1.384(8)
C(23)-H(23)	0.9500
C(24)-C(25)	1.385(8)
C(24)-H(24)	0.9500
C(25)-C(26)	1.394(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.391(7)
C(26)-C(28)	1.515(8)
C(27)-O(1)	1.393(7)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29A)-O(2)	1.410(11)
C(29A)-C(30A)	1.475(13)
C(29A)-H(29A)	0.9900
C(29A)-H(29B)	0.9900
C(30A)-C(31A)	1.552(13)
C(30A)-H(30A)	0.9900
C(30A)-H(30B)	0.9900
C(31A)-H(31A)	0.9800
C(31A)-H(31B)	0.9800
C(31A)-H(31C)	0.9800
C(33A)-C(32)	1.482(13)
C(33A)-C(34A)	1.568(13)
C(33A)-H(33A)	0.9900
C(33A)-H(33B)	0.9900
C(34A)-H(34A)	0.9800
C(34A)-H(34B)	0.9800
C(34A)-H(34C)	0.9800
C(42A)-C(41)	1.326(15)

C(42A)-C(43A)	1.423(19)
C(42A)-H(42A)	0.9500
C(43A)-C(44A)	1.38(2)
C(43A)-H(43A)	0.9500
C(44A)-C(45A)	1.364(19)
C(44A)-H(44A)	0.9500
C(45A)-C(46A)	1.41(2)
C(45A)-H(45A)	0.9500
C(46A)-C(41)	1.50(2)
C(46A)-H(46A)	0.9500
C(29B)-O(2)	1.383(11)
C(29B)-C(30B)	1.457(13)
C(29B)-H(29C)	0.9900
C(29B)-H(29D)	0.9900
C(30B)-C(31B)	1.647(13)
C(30B)-H(30C)	0.9900
C(30B)-H(30D)	0.9900
C(31B)-H(31D)	0.9800
C(31B)-H(31E)	0.9800
C(31B)-H(31F)	0.9800
C(33B)-C(32)	1.510(13)
C(33B)-C(34B)	1.560(13)
C(33B)-H(33C)	0.9900
C(33B)-H(33D)	0.9900
C(34B)-H(34D)	0.9800
C(34B)-H(34E)	0.9800
C(34B)-H(34F)	0.9800
C(42B)-C(41)	1.399(15)
C(42B)-C(43B)	1.411(19)
C(42B)-H(42B)	0.9500
C(43B)-C(44B)	1.35(2)
C(43B)-H(43B)	0.9500
C(44B)-C(45B)	1.37(2)
C(44B)-H(44B)	0.9500
C(45B)-C(46B)	1.37(2)
C(45B)-H(45B)	0.9500
C(46B)-C(41)	1.30(2)
C(46B)-H(46B)	0.9500

C(32)-O(3)	1.436(8)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(35)-O(4)	1.444(7)
C(35)-C(36)	1.486(9)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(37)	1.561(9)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-O(1)	1.435(7)
C(38)-C(39)	1.501(10)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.502(13)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-P(1)	1.827(6)
C(47)-C(48)	1.435(8)
C(47)-C(51)	1.446(7)
C(47)-P(1)	1.806(6)
C(47)-Fe(1)	2.032(5)
C(48)-C(49)	1.423(8)
C(48)-Fe(1)	2.048(6)
C(48)-H(48)	0.9500
C(49)-C(50)	1.415(9)
C(49)-Fe(1)	2.043(6)
C(49)-H(49)	0.9500
C(50)-C(51)	1.414(9)
C(50)-Fe(1)	2.050(6)
C(50)-H(50)	0.9500
C(51)-Fe(1)	2.044(6)

C(51)-H(51)	0.9500
C(52)-C(56)	1.423(11)
C(52)-C(53)	1.430(12)
C(52)-Fe(1)	2.043(7)
C(52)-H(52)	0.9500
C(53)-C(54)	1.394(11)
C(53)-Fe(1)	2.031(7)
C(53)-H(53)	0.9500
C(54)-C(55)	1.418(11)
C(54)-Fe(1)	2.029(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.400(12)
C(55)-Fe(1)	2.030(7)
C(55)-H(55)	0.9500
C(56)-Fe(1)	2.020(7)
C(56)-H(56)	0.9500
B(1)-P(1)	1.909(7)
B(1)-H(1A)	0.9800
B(1)-H(1B)	0.9800
B(1)-H(1C)	0.9800

C(6)-C(1)-C(2)	119.3(4)
C(6)-C(1)-P(1)	121.2(4)
C(2)-C(1)-P(1)	119.5(5)
C(3)-C(2)-C(1)	121.4(5)
C(3)-C(2)-H(2)	119.3
C(1)-C(2)-H(2)	119.3
C(2)-C(3)-C(4)	117.5(5)
C(2)-C(3)-C(28)	121.1(5)
C(4)-C(3)-C(28)	121.2(5)
C(5)-C(4)-O(2)	119.6(5)
C(5)-C(4)-C(3)	122.1(4)
O(2)-C(4)-C(3)	118.2(5)
C(4)-C(5)-C(6)	118.8(5)
C(4)-C(5)-C(7)	119.3(5)
C(6)-C(5)-C(7)	121.8(5)
C(5)-C(6)-C(1)	120.5(5)
C(5)-C(6)-H(6)	119.8

C(1)-C(6)-H(6)	119.8
C(8)-C(7)-C(5)	111.6(5)
C(8)-C(7)-H(7A)	109.3
C(5)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7B)	109.3
C(5)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	108.0
C(9)-C(8)-C(13)	118.0(5)
C(9)-C(8)-C(7)	120.6(5)
C(13)-C(8)-C(7)	121.2(5)
C(10)-C(9)-C(8)	121.3(6)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.3
C(9)-C(10)-C(11)	119.1(6)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	121.6(5)
C(12)-C(11)-H(11)	119.2
C(10)-C(11)-H(11)	119.2
C(13)-C(12)-C(11)	117.9(5)
C(13)-C(12)-C(14)	122.4(5)
C(11)-C(12)-C(14)	119.6(5)
C(12)-C(13)-O(3)	119.2(5)
C(12)-C(13)-C(8)	122.1(5)
O(3)-C(13)-C(8)	118.8(5)
C(15)-C(14)-C(12)	109.2(4)
C(15)-C(14)-H(14A)	109.8
C(12)-C(14)-H(14A)	109.8
C(15)-C(14)-H(14B)	109.8
C(12)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.3
C(20)-C(15)-C(16)	117.6(5)
C(20)-C(15)-C(14)	121.0(4)
C(16)-C(15)-C(14)	120.8(5)
C(17)-C(16)-C(15)	120.3(5)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	121.0(5)

C(18)-C(17)-H(17)	119.5
C(16)-C(17)-H(17)	119.5
C(17)-C(18)-C(19)	120.2(5)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(20)-C(19)-C(18)	117.8(5)
C(20)-C(19)-C(21)	120.6(4)
C(18)-C(19)-C(21)	121.2(5)
C(15)-C(20)-C(19)	122.6(4)
C(15)-C(20)-O(4)	118.5(4)
C(19)-C(20)-O(4)	118.5(4)
C(19)-C(21)-C(22)	109.4(4)
C(19)-C(21)-H(21A)	109.8
C(22)-C(21)-H(21A)	109.8
C(19)-C(21)-H(21B)	109.8
C(22)-C(21)-H(21B)	109.8
H(21A)-C(21)-H(21B)	108.2
C(23)-C(22)-C(27)	118.0(5)
C(23)-C(22)-C(21)	119.7(5)
C(27)-C(22)-C(21)	122.1(5)
C(22)-C(23)-C(24)	121.4(5)
C(22)-C(23)-H(23)	119.3
C(24)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	120.0(5)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.3(5)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(27)-C(26)-C(25)	118.4(5)
C(27)-C(26)-C(28)	122.0(5)
C(25)-C(26)-C(28)	119.4(5)
C(26)-C(27)-O(1)	119.2(4)
C(26)-C(27)-C(22)	121.9(5)
O(1)-C(27)-C(22)	118.8(5)
C(26)-C(28)-C(3)	110.2(4)
C(26)-C(28)-H(28A)	109.6
C(3)-C(28)-H(28A)	109.6

C(26)-C(28)-H(28B)	109.6
C(3)-C(28)-H(28B)	109.6
H(28A)-C(28)-H(28B)	108.1
O(2)-C(29A)-C(30A)	110.0(11)
O(2)-C(29A)-H(29A)	109.7
C(30A)-C(29A)-H(29A)	109.7
O(2)-C(29A)-H(29B)	109.7
C(30A)-C(29A)-H(29B)	109.7
H(29A)-C(29A)-H(29B)	108.2
C(29A)-C(30A)-C(31A)	121.6(12)
C(29A)-C(30A)-H(30A)	106.9
C(31A)-C(30A)-H(30A)	106.9
C(29A)-C(30A)-H(30B)	106.9
C(31A)-C(30A)-H(30B)	106.9
H(30A)-C(30A)-H(30B)	106.7
C(30A)-C(31A)-H(31A)	109.5
C(30A)-C(31A)-H(31B)	109.5
H(31A)-C(31A)-H(31B)	109.5
C(30A)-C(31A)-H(31C)	109.5
H(31A)-C(31A)-H(31C)	109.5
H(31B)-C(31A)-H(31C)	109.5
C(32)-C(33A)-C(34A)	104.6(11)
C(32)-C(33A)-H(33A)	110.8
C(34A)-C(33A)-H(33A)	110.8
C(32)-C(33A)-H(33B)	110.8
C(34A)-C(33A)-H(33B)	110.8
H(33A)-C(33A)-H(33B)	108.9
C(33A)-C(34A)-H(34A)	109.5
C(33A)-C(34A)-H(34B)	109.5
H(34A)-C(34A)-H(34B)	109.5
C(33A)-C(34A)-H(34C)	109.5
H(34A)-C(34A)-H(34C)	109.5
H(34B)-C(34A)-H(34C)	109.5
C(41)-C(42A)-C(43A)	125.9(14)
C(41)-C(42A)-H(42A)	117.0
C(43A)-C(42A)-H(42A)	117.0
C(44A)-C(43A)-C(42A)	116.3(13)
C(44A)-C(43A)-H(43A)	121.9

C(42A)-C(43A)-H(43A)	121.9
C(45A)-C(44A)-C(43A)	124.4(15)
C(45A)-C(44A)-H(44A)	117.8
C(43A)-C(44A)-H(44A)	117.8
C(44A)-C(45A)-C(46A)	117.3(15)
C(44A)-C(45A)-H(45A)	121.3
C(46A)-C(45A)-H(45A)	121.3
C(45A)-C(46A)-C(41)	121.2(13)
C(45A)-C(46A)-H(46A)	119.4
C(41)-C(46A)-H(46A)	119.4
O(2)-C(29B)-C(30B)	122.3(12)
O(2)-C(29B)-H(29C)	106.8
C(30B)-C(29B)-H(29C)	106.8
O(2)-C(29B)-H(29D)	106.8
C(30B)-C(29B)-H(29D)	106.8
H(29C)-C(29B)-H(29D)	106.6
C(29B)-C(30B)-C(31B)	100.1(10)
C(29B)-C(30B)-H(30C)	111.7
C(31B)-C(30B)-H(30C)	111.7
C(29B)-C(30B)-H(30D)	111.7
C(31B)-C(30B)-H(30D)	111.7
H(30C)-C(30B)-H(30D)	109.5
C(30B)-C(31B)-H(31D)	109.5
C(30B)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31E)	109.5
C(30B)-C(31B)-H(31F)	109.5
H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
C(32)-C(33B)-C(34B)	111.0(12)
C(32)-C(33B)-H(33C)	109.4
C(34B)-C(33B)-H(33C)	109.4
C(32)-C(33B)-H(33D)	109.4
C(34B)-C(33B)-H(33D)	109.4
H(33C)-C(33B)-H(33D)	108.0
C(33B)-C(34B)-H(34D)	109.5
C(33B)-C(34B)-H(34E)	109.5
H(34D)-C(34B)-H(34E)	109.5
C(33B)-C(34B)-H(34F)	109.5

H(34D)-C(34B)-H(34F)	109.5
H(34E)-C(34B)-H(34F)	109.5
C(41)-C(42B)-C(43B)	119.2(13)
C(41)-C(42B)-H(42B)	120.4
C(43B)-C(42B)-H(42B)	120.4
C(44B)-C(43B)-C(42B)	119.1(14)
C(44B)-C(43B)-H(43B)	120.4
C(42B)-C(43B)-H(43B)	120.4
C(43B)-C(44B)-C(45B)	118.7(14)
C(43B)-C(44B)-H(44B)	120.7
C(45B)-C(44B)-H(44B)	120.7
C(46B)-C(45B)-C(44B)	122.0(16)
C(46B)-C(45B)-H(45B)	119.0
C(44B)-C(45B)-H(45B)	119.0
C(41)-C(46B)-C(45B)	120.6(15)
C(41)-C(46B)-H(46B)	119.7
C(45B)-C(46B)-H(46B)	119.7
O(3)-C(32)-C(33A)	113.8(8)
O(3)-C(32)-C(33B)	102.8(8)
O(3)-C(32)-H(32A)	108.8
C(33A)-C(32)-H(32A)	108.8
C(33B)-C(32)-H(32A)	124.6
O(3)-C(32)-H(32B)	108.8
C(33A)-C(32)-H(32B)	108.8
C(33B)-C(32)-H(32B)	103.4
H(32A)-C(32)-H(32B)	107.7
O(4)-C(35)-C(36)	111.6(5)
O(4)-C(35)-H(35A)	109.3
C(36)-C(35)-H(35A)	109.3
O(4)-C(35)-H(35B)	109.3
C(36)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-C(37)	109.5(6)
C(35)-C(36)-H(36A)	109.8
C(37)-C(36)-H(36A)	109.8
C(35)-C(36)-H(36B)	109.8
C(37)-C(36)-H(36B)	109.8
H(36A)-C(36)-H(36B)	108.2

C(36)-C(37)-H(37A)	109.5
C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
O(1)-C(38)-C(39)	107.0(6)
O(1)-C(38)-H(38A)	110.3
C(39)-C(38)-H(38A)	110.3
O(1)-C(38)-H(38B)	110.3
C(39)-C(38)-H(38B)	110.3
H(38A)-C(38)-H(38B)	108.6
C(38)-C(39)-C(40)	113.7(6)
C(38)-C(39)-H(39A)	108.8
C(40)-C(39)-H(39A)	108.8
C(38)-C(39)-H(39B)	108.8
C(40)-C(39)-H(39B)	108.8
H(39A)-C(39)-H(39B)	107.7
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(46B)-C(41)-C(42A)	104.2(11)
C(46B)-C(41)-C(42B)	119.9(11)
C(42A)-C(41)-C(46A)	114.5(10)
C(42B)-C(41)-C(46A)	124.5(10)
C(46B)-C(41)-P(1)	125.1(9)
C(42A)-C(41)-P(1)	128.6(8)
C(42B)-C(41)-P(1)	114.4(8)
C(46A)-C(41)-P(1)	116.8(7)
C(48)-C(47)-C(51)	107.2(5)
C(48)-C(47)-P(1)	128.3(4)
C(51)-C(47)-P(1)	124.4(4)
C(48)-C(47)-Fe(1)	70.0(3)
C(51)-C(47)-Fe(1)	69.6(3)
P(1)-C(47)-Fe(1)	125.3(3)

C(49)-C(48)-C(47)	107.9(5)
C(49)-C(48)-Fe(1)	69.4(3)
C(47)-C(48)-Fe(1)	68.8(3)
C(49)-C(48)-H(48)	126.1
C(47)-C(48)-H(48)	126.1
Fe(1)-C(48)-H(48)	127.2
C(50)-C(49)-C(48)	108.3(5)
C(50)-C(49)-Fe(1)	70.1(4)
C(48)-C(49)-Fe(1)	69.8(3)
C(50)-C(49)-H(49)	125.8
C(48)-C(49)-H(49)	125.8
Fe(1)-C(49)-H(49)	125.8
C(51)-C(50)-C(49)	108.9(5)
C(51)-C(50)-Fe(1)	69.6(3)
C(49)-C(50)-Fe(1)	69.5(4)
C(51)-C(50)-H(50)	125.6
C(49)-C(50)-H(50)	125.6
Fe(1)-C(50)-H(50)	126.9
C(50)-C(51)-C(47)	107.7(5)
C(50)-C(51)-Fe(1)	70.0(4)
C(47)-C(51)-Fe(1)	68.8(3)
C(50)-C(51)-H(51)	126.2
C(47)-C(51)-H(51)	126.2
Fe(1)-C(51)-H(51)	126.6
C(56)-C(52)-C(53)	106.7(8)
C(56)-C(52)-Fe(1)	68.6(4)
C(53)-C(52)-Fe(1)	69.0(4)
C(56)-C(52)-H(52)	126.7
C(53)-C(52)-H(52)	126.7
Fe(1)-C(52)-H(52)	127.2
C(54)-C(53)-C(52)	108.0(7)
C(54)-C(53)-Fe(1)	69.8(4)
C(52)-C(53)-Fe(1)	69.9(4)
C(54)-C(53)-H(53)	126.0
C(52)-C(53)-H(53)	126.0
Fe(1)-C(53)-H(53)	125.9
C(53)-C(54)-C(55)	109.0(8)
C(53)-C(54)-Fe(1)	70.0(4)

C(55)-C(54)-Fe(1)	69.6(4)
C(53)-C(54)-H(54)	125.5
C(55)-C(54)-H(54)	125.5
Fe(1)-C(54)-H(54)	126.5
C(56)-C(55)-C(54)	107.3(8)
C(56)-C(55)-Fe(1)	69.4(4)
C(54)-C(55)-Fe(1)	69.5(4)
C(56)-C(55)-H(55)	126.4
C(54)-C(55)-H(55)	126.4
Fe(1)-C(55)-H(55)	126.3
C(55)-C(56)-C(52)	109.0(8)
C(55)-C(56)-Fe(1)	70.2(4)
C(52)-C(56)-Fe(1)	70.4(4)
C(55)-C(56)-H(56)	125.5
C(52)-C(56)-H(56)	125.5
Fe(1)-C(56)-H(56)	125.5
P(1)-B(1)-H(1A)	109.5
P(1)-B(1)-H(1B)	109.5
H(1A)-B(1)-H(1B)	109.5
P(1)-B(1)-H(1C)	109.5
H(1A)-B(1)-H(1C)	109.5
H(1B)-B(1)-H(1C)	109.5
C(56)-Fe(1)-C(54)	68.2(4)
C(56)-Fe(1)-C(55)	40.5(3)
C(54)-Fe(1)-C(55)	40.9(3)
C(56)-Fe(1)-C(53)	68.8(3)
C(54)-Fe(1)-C(53)	40.1(3)
C(55)-Fe(1)-C(53)	68.6(3)
C(56)-Fe(1)-C(47)	156.2(3)
C(54)-Fe(1)-C(47)	126.6(3)
C(55)-Fe(1)-C(47)	162.8(3)
C(53)-Fe(1)-C(47)	109.3(3)
C(56)-Fe(1)-C(49)	105.3(3)
C(54)-Fe(1)-C(49)	154.5(3)
C(55)-Fe(1)-C(49)	118.2(3)
C(53)-Fe(1)-C(49)	162.6(3)
C(47)-Fe(1)-C(49)	69.1(2)
C(56)-Fe(1)-C(52)	41.0(3)

C(54)-Fe(1)-C(52)	68.3(4)
C(55)-Fe(1)-C(52)	68.7(4)
C(53)-Fe(1)-C(52)	41.1(3)
C(47)-Fe(1)-C(52)	121.8(3)
C(49)-Fe(1)-C(52)	123.9(3)
C(56)-Fe(1)-C(51)	159.8(3)
C(54)-Fe(1)-C(51)	108.6(3)
C(55)-Fe(1)-C(51)	124.0(3)
C(53)-Fe(1)-C(51)	122.6(3)
C(47)-Fe(1)-C(51)	41.6(2)
C(49)-Fe(1)-C(51)	68.5(3)
C(52)-Fe(1)-C(51)	158.2(3)
C(56)-Fe(1)-C(48)	119.6(3)
C(54)-Fe(1)-C(48)	164.0(3)
C(55)-Fe(1)-C(48)	153.7(3)
C(53)-Fe(1)-C(48)	126.8(3)
C(47)-Fe(1)-C(48)	41.2(2)
C(49)-Fe(1)-C(48)	40.7(2)
C(52)-Fe(1)-C(48)	107.7(3)
C(51)-Fe(1)-C(48)	69.1(2)
C(56)-Fe(1)-C(50)	122.7(3)
C(54)-Fe(1)-C(50)	120.9(3)
C(55)-Fe(1)-C(50)	105.8(3)
C(53)-Fe(1)-C(50)	156.5(3)
C(47)-Fe(1)-C(50)	68.9(2)
C(49)-Fe(1)-C(50)	40.5(2)
C(52)-Fe(1)-C(50)	160.2(3)
C(51)-Fe(1)-C(50)	40.4(2)
C(48)-Fe(1)-C(50)	68.3(2)
C(27)-O(1)-C(38)	113.3(5)
C(4)-O(2)-C(29B)	123.3(7)
C(4)-O(2)-C(29A)	115.5(7)
C(13)-O(3)-C(32)	112.0(5)
C(20)-O(4)-C(35)	113.3(4)
C(1)-P(1)-C(47)	105.3(2)
C(1)-P(1)-C(41)	104.9(3)
C(47)-P(1)-C(41)	105.0(3)
C(1)-P(1)-B(1)	114.9(3)

C(47)-P(1)-B(1)	115.2(3)
C(41)-P(1)-B(1)	110.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **4c** (09kn250). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(2)	41(3)	25(2)	2(3)	5(2)	1(3)
C(2)	43(4)	38(3)	22(3)	-3(2)	4(2)	-1(2)
C(3)	36(3)	35(3)	20(2)	-5(2)	8(2)	1(2)
C(4)	30(2)	32(3)	23(2)	-5(2)	6(2)	-2(2)
C(5)	36(3)	30(3)	28(3)	0(2)	10(2)	-1(2)
C(6)	35(3)	37(3)	26(3)	2(2)	8(2)	5(2)
C(7)	41(3)	27(3)	24(2)	0(2)	8(2)	3(2)
C(8)	41(3)	22(2)	29(3)	2(2)	5(2)	5(2)
C(9)	45(4)	35(3)	28(3)	0(2)	5(2)	-4(2)
C(10)	32(3)	39(3)	42(3)	6(2)	7(2)	5(2)
C(11)	43(3)	25(3)	33(3)	2(2)	14(2)	7(2)
C(12)	40(3)	19(2)	27(2)	1(2)	4(2)	4(2)
C(13)	32(3)	19(2)	33(3)	3(2)	12(2)	2(2)
C(14)	41(3)	31(3)	23(2)	-7(2)	7(2)	-7(2)
C(15)	30(3)	31(3)	23(2)	-2(2)	0(2)	-4(2)
C(16)	45(3)	35(3)	27(3)	-4(2)	1(2)	4(2)
C(17)	45(3)	43(3)	27(2)	1(2)	14(2)	3(2)
C(18)	40(3)	37(3)	26(2)	9(2)	7(2)	1(2)
C(19)	35(3)	31(3)	22(2)	-3(2)	2(2)	1(2)
C(20)	30(2)	35(3)	24(2)	1(2)	1(2)	-1(2)
C(21)	36(3)	27(3)	26(2)	5(2)	4(2)	5(2)
C(22)	38(3)	23(2)	26(2)	-1(2)	5(2)	-2(2)
C(23)	40(3)	32(3)	28(2)	6(2)	12(2)	-3(2)
C(24)	32(3)	38(3)	35(3)	-1(2)	11(2)	-3(2)
C(25)	34(3)	30(3)	34(3)	0(2)	-2(2)	-4(2)
C(26)	41(3)	19(2)	27(2)	-2(2)	11(2)	-2(2)
C(27)	33(3)	18(2)	28(2)	3(2)	7(2)	-3(2)
C(28)	39(3)	29(3)	30(3)	-4(2)	6(2)	5(2)
C(29A)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(30A)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(31A)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(33A)	62(3)	52(3)	52(3)	2(2)	4(2)	-21(2)
C(34A)	62(3)	52(3)	52(3)	2(2)	4(2)	-21(2)
C(42A)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(43A)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)

C(44A)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(45A)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(46A)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(29B)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(30B)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(31B)	47(2)	67(5)	47(3)	0(3)	9(2)	-2(3)
C(33B)	62(3)	52(3)	52(3)	2(2)	4(2)	-21(2)
C(34B)	62(3)	52(3)	52(3)	2(2)	4(2)	-21(2)
C(42B)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(43B)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(44B)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(45B)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(46B)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(32)	62(3)	52(3)	52(3)	2(2)	4(2)	-21(2)
C(35)	42(3)	75(5)	34(3)	3(3)	15(3)	-2(3)
C(36)	56(4)	60(4)	43(3)	1(3)	19(3)	4(3)
C(37)	37(3)	90(5)	70(4)	-13(5)	18(3)	12(4)
C(38)	60(5)	47(4)	69(5)	21(3)	22(4)	22(3)
C(39)	50(4)	72(5)	84(6)	-20(4)	-15(4)	38(4)
C(40)	50(5)	105(7)	92(6)	-46(5)	30(4)	-6(4)
C(41)	42(2)	55(2)	55(2)	8(2)	11(2)	-5(2)
C(47)	35(3)	42(3)	28(2)	2(2)	5(2)	-9(2)
C(48)	39(3)	37(3)	31(3)	1(2)	2(2)	-3(2)
C(49)	51(4)	37(3)	39(3)	-1(2)	9(3)	4(3)
C(50)	57(4)	50(4)	28(3)	0(2)	10(3)	-11(3)
C(51)	52(4)	43(3)	27(2)	7(2)	9(2)	0(3)
C(52)	60(5)	72(5)	79(6)	-19(4)	-8(4)	-29(4)
C(53)	69(5)	43(4)	82(5)	-20(4)	33(4)	-19(4)
C(54)	69(5)	39(4)	100(7)	19(4)	35(5)	-3(4)
C(55)	59(5)	56(5)	104(7)	9(4)	42(5)	-12(4)
C(56)	33(3)	73(6)	119(7)	-16(5)	16(4)	-13(3)
B(1)	47(4)	55(4)	39(4)	12(3)	4(3)	10(3)
Fe(1)	36(1)	40(1)	42(1)	-2(1)	12(1)	-4(1)
O(1)	36(2)	33(2)	30(2)	-3(2)	5(2)	9(2)
O(2)	36(2)	38(2)	31(2)	-2(2)	-2(1)	2(2)
O(3)	36(2)	30(2)	34(2)	1(2)	8(2)	-1(2)
O(4)	36(2)	38(2)	23(2)	-1(1)	9(1)	-2(2)
P(1)	33(1)	46(1)	25(1)	2(1)	2(1)	-1(1)

Table S9. Crystal data and structure refinement for compound **8c** (09kn1).

Identification code	09kn1	
Empirical formula	C73 H82 B2 Cl2 Fe2 O4 P2	
Formula weight	1289.55	
Temperature	115(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 34.5194(10) Å	a = 90°.
	b = 9.5372(2) Å	b = 125.8800(10)°.
	c = 24.9507(8) Å	g = 90°.
Volume	6655.5(3) Å ³	
Z	4	
Density (calculated)	1.287 Mg/m ³	
Absorption coefficient	0.612 mm ⁻¹	
F(000)	2712	
Crystal size	0.20 x 0.10 x 0.10 mm ³	
Theta range for data collection	1.66 to 27.46°.	
Index ranges	-44<=h<=44, -12<=k<=8, -32<=l<=32	
Reflections collected	12953	
Independent reflections	12953 [R(int) = 0.0000]	
Completeness to theta = 27.46°	98.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	12953 / 2 / 769	
Goodness-of-fit on F ²	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1203	
R indices (all data)	R1 = 0.0678, wR2 = 0.1270	
Absolute structure parameter	0.070(18)	
Largest diff. peak and hole	0.771 and -0.872 e.Å ⁻³	

Table S10. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **8c** (09kn1). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(80A)	5616(4)	4396(15)	3159(5)	64(3)
Cl(1A)	5061(1)	3478(4)	2581(2)	70(1)
Cl(2A)	5641(1)	5929(4)	2803(2)	70(1)
C(80B)	5790(6)	5460(20)	3186(9)	64(3)
Cl(1B)	5321(2)	4059(6)	2655(2)	70(1)
Cl(2B)	5531(2)	7006(6)	2687(2)	70(1)
C(1)	6969(2)	5928(5)	8850(2)	28(1)
C(2A)	6661(3)	7175(9)	8743(3)	23(1)
C(3A)	6916(2)	7957(9)	9340(3)	23(1)
C(4A)	7349(3)	7288(8)	9801(4)	23(1)
C(5A)	7377(3)	6070(9)	9493(4)	23(1)
C(4B)	7488(5)	6935(16)	9877(7)	23(1)
C(5B)	7493(5)	5808(18)	9503(8)	23(1)
C(3B)	7040(6)	7565(16)	9524(6)	23(1)
C(2B)	6742(6)	6873(18)	8905(7)	23(1)
C(6)	7454(2)	7889(6)	8292(3)	37(1)
C(7A)	7195(4)	9119(13)	8242(7)	34(1)
C(8A)	7463(4)	9810(13)	8843(6)	34(1)
C(9A)	7887(4)	9010(12)	9266(6)	34(1)
C(10A)	7867(5)	7814(14)	8891(7)	34(1)
C(7B)	7103(5)	8851(15)	8165(7)	34(1)
C(8B)	7295(4)	9729(15)	8729(6)	34(1)
C(9B)	7772(5)	9368(13)	9209(7)	34(1)
C(10B)	7886(6)	8161(14)	8969(8)	34(1)
C(11)	6491(2)	3254(5)	8327(2)	24(1)
C(12)	6382(2)	3350(5)	8781(2)	32(1)
C(13)	6122(2)	2307(6)	8819(3)	40(1)
C(14)	5965(2)	1172(6)	8409(3)	45(1)
C(15)	6080(2)	1047(6)	7966(3)	54(2)
C(16)	6349(2)	2082(6)	7936(3)	46(1)
C(17)	6377(2)	5431(5)	7451(2)	21(1)
C(18)	5933(2)	5782(5)	7302(2)	23(1)
C(19)	5604(2)	6561(5)	6740(2)	23(1)

C(20)	5739(2)	6984(5)	6330(2)	22(1)
C(21)	6164(2)	6544(5)	6438(2)	23(1)
C(22)	6486(2)	5776(5)	7010(2)	20(1)
C(23)	5099(2)	6775(5)	6534(2)	25(1)
C(24)	6257(1)	6801(5)	5926(2)	22(1)
C(25)	5901(1)	6023(5)	5286(2)	19(1)
C(26)	5839(2)	4593(5)	5305(2)	27(1)
C(27)	5502(2)	3860(6)	4736(2)	28(1)
C(28)	5205(2)	4582(5)	4145(2)	26(1)
C(29)	4740(1)	6007(5)	5887(2)	21(1)
C(30)	5615(1)	6712(5)	4680(2)	18(1)
C(31)	6048(2)	8428(5)	4552(3)	30(1)
C(32)	6094(2)	10008(6)	4530(3)	44(1)
C(33B)	5732(16)	10880(70)	3960(30)	62(4)
C(33A)	5660(5)	10580(20)	3913(11)	62(4)
C(34)	5378(2)	9227(6)	5912(3)	42(1)
C(35)	5768(2)	10130(7)	6036(3)	47(2)
C(36)	5683(2)	11667(7)	6140(3)	50(2)
C(37)	8286(2)	2694(7)	6724(3)	48(1)
C(38)	8316(2)	3625(6)	6305(2)	36(1)
C(39)	7952(2)	3246(6)	5638(3)	37(1)
C(40)	7696(2)	2094(6)	5642(3)	46(1)
C(41)	7899(2)	1745(6)	6306(4)	53(2)
C(42)	7583(2)	5674(5)	6402(2)	24(1)
C(43)	7467(2)	4588(5)	6688(2)	28(1)
C(44)	7081(2)	3794(6)	6163(2)	31(1)
C(45)	6954(2)	4379(5)	5557(2)	33(1)
C(46)	7263(2)	5534(5)	5700(2)	28(1)
C(47)	7797(2)	8358(5)	7027(2)	28(1)
C(48)	7321(2)	8750(5)	6565(3)	34(1)
C(49)	7126(2)	9875(6)	6677(3)	43(1)
C(50)	7406(2)	10645(6)	7249(3)	48(2)
C(51)	7877(2)	10279(6)	7715(3)	51(2)
C(52)	8072(2)	9134(6)	7602(3)	45(1)
C(53)	8528(2)	6178(5)	7586(2)	24(1)
C(54)	8467(2)	5788(5)	8068(2)	26(1)
C(55)	8817(2)	5043(5)	8629(2)	24(1)
C(56)	9230(2)	4674(6)	8682(2)	26(1)

C(57)	9328(2)	5170(5)	8248(2)	23(1)
C(58)	8967(2)	5915(5)	7691(2)	25(1)
C(59)	9819(2)	4998(5)	8387(2)	26(1)
C(60)	10204(1)	5688(5)	9043(2)	22(1)
C(61)	10180(2)	7127(5)	9113(2)	28(1)
C(62)	10505(2)	7776(6)	9714(2)	30(1)
C(63)	10846(2)	6997(5)	10255(2)	28(1)
C(64)	10881(2)	5552(5)	10206(2)	25(1)
C(65)	10566(2)	4920(5)	9590(2)	21(1)
C(66)	8770(2)	4694(5)	9179(2)	25(1)
C(67)	10996(2)	3108(5)	9510(3)	32(1)
C(68)	11008(2)	1516(6)	9482(3)	40(1)
C(69)	10594(2)	930(7)	8847(4)	54(2)
C(70)	9612(2)	2457(6)	9074(3)	37(1)
C(71)	9259(2)	1490(7)	9021(3)	44(1)
C(72)	9354(2)	-2(7)	8903(3)	50(2)
O(1)	5429(1)	7788(4)	5778(1)	25(1)
O(2)	5679(1)	8145(3)	4645(1)	21(1)
O(3)	9568(1)	3894(4)	9228(2)	28(1)
O(4)	10598(1)	3490(3)	9525(2)	24(1)
P(1)	6824(1)	4616(1)	8240(1)	21(1)
P(2)	8049(1)	6969(1)	6817(1)	24(1)
Fe(1)	7310(1)	7757(1)	8976(1)	26(1)
Fe(2)	7656(1)	3761(1)	6119(1)	26(1)
B(1)	7362(2)	3834(7)	8308(3)	33(1)
B(2)	8232(2)	7767(7)	6294(3)	35(1)

Table S11. Bond lengths [Å] and angles [°] for compound **8c** (09kn1).

C(80A)-Cl(2A)	1.739(14)
C(80A)-Cl(1A)	1.810(12)
C(80A)-H(80A)	0.9900
C(80A)-H(80B)	0.9900
C(80B)-Cl(2B)	1.80(2)
C(80B)-Cl(1B)	1.91(2)
C(80B)-H(80C)	0.9900
C(80B)-H(80D)	0.9900
C(1)-C(2B)	1.255(19)
C(1)-C(5A)	1.388(9)
C(1)-C(2A)	1.511(10)
C(1)-C(5B)	1.576(17)
C(1)-P(1)	1.799(5)
C(1)-Fe(1)	2.023(5)
C(2A)-C(3A)	1.420(10)
C(2A)-Fe(1)	2.034(9)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.396(9)
C(3A)-Fe(1)	2.039(7)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.427(10)
C(4A)-Fe(1)	2.031(7)
C(4A)-H(4A)	0.9500
C(5A)-Fe(1)	1.989(9)
C(5A)-H(5A)	0.9500
C(4B)-C(3B)	1.389(18)
C(4B)-C(5B)	1.430(19)
C(4B)-Fe(1)	2.104(14)
C(4B)-H(4B)	0.9500
C(5B)-Fe(1)	2.147(18)
C(5B)-H(5B)	0.9500
C(3B)-C(2B)	1.421(18)
C(3B)-Fe(1)	2.065(14)
C(3B)-H(3B)	0.9500
C(2B)-Fe(1)	2.044(17)
C(2B)-H(2B)	0.9500

C(6)-C(10A)	1.330(16)
C(6)-C(7B)	1.400(18)
C(6)-C(7A)	1.435(16)
C(6)-C(10B)	1.480(16)
C(6)-Fe(1)	2.042(4)
C(6)-H(6)	0.9500
C(7A)-C(8A)	1.382(15)
C(7A)-Fe(1)	2.086(14)
C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.425(16)
C(8A)-Fe(1)	2.105(12)
C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.451(15)
C(9A)-Fe(1)	2.058(12)
C(9A)-H(9A)	0.9500
C(10A)-Fe(1)	2.054(15)
C(10A)-H(10A)	0.9500
C(7B)-C(8B)	1.423(17)
C(7B)-Fe(1)	2.000(15)
C(7B)-H(7B)	0.9500
C(8B)-C(9B)	1.397(17)
C(8B)-Fe(1)	1.971(14)
C(8B)-H(8B)	0.9500
C(9B)-C(10B)	1.455(17)
C(9B)-Fe(1)	2.039(13)
C(9B)-H(9B)	0.9500
C(10B)-Fe(1)	2.037(16)
C(10B)-H(10B)	0.9500
C(11)-C(16)	1.372(7)
C(11)-C(12)	1.387(6)
C(11)-P(1)	1.831(4)
C(12)-C(13)	1.380(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.364(8)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.386(8)

C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.388(6)
C(17)-C(22)	1.394(5)
C(17)-P(1)	1.818(4)
C(18)-C(19)	1.394(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.408(6)
C(19)-C(23)	1.514(6)
C(20)-O(1)	1.379(5)
C(20)-C(21)	1.392(6)
C(21)-C(22)	1.395(6)
C(21)-C(24)	1.510(5)
C(22)-H(22)	0.9500
C(23)-C(29)	1.527(6)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.521(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.386(7)
C(25)-C(30)	1.394(6)
C(26)-C(27)	1.385(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.389(7)
C(27)-H(27)	0.9500
C(28)-C(29)#1	1.381(7)
C(28)-H(28)	0.9500
C(29)-C(28)#1	1.381(7)
C(29)-C(30)#1	1.387(6)
C(30)-C(29)#1	1.387(6)
C(30)-O(2)	1.396(5)
C(31)-O(2)	1.448(5)
C(31)-C(32)	1.520(8)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33B)	1.485(18)
C(32)-C(33A)	1.487(11)

C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33B)-H(33D)	0.9800
C(33B)-H(33E)	0.9800
C(33B)-H(33F)	0.9800
C(33A)-H(33A)	0.9800
C(33A)-H(33B)	0.9800
C(33A)-H(33C)	0.9800
C(34)-O(1)	1.448(7)
C(34)-C(35)	1.470(8)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.546(9)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.421(8)
C(37)-C(41)	1.434(9)
C(37)-Fe(2)	2.049(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.424(7)
C(38)-Fe(2)	2.047(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.413(7)
C(39)-Fe(2)	2.039(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.408(9)
C(40)-Fe(2)	2.038(5)
C(40)-H(40)	0.9500
C(41)-Fe(2)	2.039(6)
C(41)-H(41)	0.9500
C(42)-C(46)	1.427(6)
C(42)-C(43)	1.442(6)
C(42)-P(2)	1.797(5)
C(42)-Fe(2)	2.025(5)
C(43)-C(44)	1.420(7)

C(43)-Fe(2)	2.038(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.418(7)
C(44)-Fe(2)	2.050(4)
C(44)-H(44)	0.9500
C(45)-C(46)	1.425(7)
C(45)-Fe(2)	2.050(5)
C(45)-H(45)	0.9500
C(46)-Fe(2)	2.032(5)
C(46)-H(46)	0.9500
C(47)-C(52)	1.381(7)
C(47)-C(48)	1.398(6)
C(47)-P(2)	1.821(5)
C(48)-C(49)	1.379(7)
C(48)-H(48)	0.9500
C(49)-C(50)	1.375(8)
C(49)-H(49)	0.9500
C(50)-C(51)	1.379(9)
C(50)-H(50)	0.9500
C(51)-C(52)	1.398(8)
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500
C(53)-C(54)	1.389(6)
C(53)-C(58)	1.401(6)
C(53)-P(2)	1.808(4)
C(54)-C(55)	1.393(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.398(6)
C(55)-C(66)	1.511(6)
C(56)-O(3)	1.380(5)
C(56)-C(57)	1.393(6)
C(57)-C(58)	1.399(6)
C(57)-C(59)	1.527(6)
C(58)-H(58)	0.9500
C(59)-C(60)	1.526(6)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.391(7)

C(60)-C(65)	1.400(6)
C(61)-C(62)	1.386(7)
C(61)-H(61)	0.9500
C(62)-C(63)	1.378(7)
C(62)-H(62)	0.9500
C(63)-C(64)	1.395(7)
C(63)-H(63)	0.9500
C(64)-C(65)	1.395(6)
C(64)-C(66)#2	1.520(6)
C(65)-O(4)	1.386(6)
C(66)-C(64)#2	1.520(6)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-O(4)	1.442(5)
C(67)-C(68)	1.521(8)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(68)-C(69)	1.488(9)
C(68)-H(68A)	0.9900
C(68)-H(68B)	0.9900
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-O(3)	1.454(7)
C(70)-C(71)	1.471(8)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
C(71)-C(72)	1.527(9)
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900
C(72)-H(72E)	0.9800
C(72)-H(72F)	0.9800
C(72)-H(72G)	0.9800
P(1)-B(1)	1.914(5)
P(2)-B(2)	1.910(5)
B(1)-H(1A)	0.9800
B(1)-H(1B)	0.9800
B(1)-H(1C)	0.9800

B(2)-H(2C)	0.9800
B(2)-H(2D)	0.9800
B(2)-H(2E)	0.9800
B(2)-H(2F)	0.9800
B(2)-H(2G)	0.9800
B(2)-H(2H)	0.9800
Cl(2A)-C(80A)-Cl(1A)	110.2(6)
Cl(2A)-C(80A)-H(80A)	109.6
Cl(1A)-C(80A)-H(80A)	109.6
Cl(2A)-C(80A)-H(80B)	109.6
Cl(1A)-C(80A)-H(80B)	109.6
H(80A)-C(80A)-H(80B)	108.1
Cl(2B)-C(80B)-Cl(1B)	102.6(9)
Cl(2B)-C(80B)-H(80C)	111.2
Cl(1B)-C(80B)-H(80C)	111.2
Cl(2B)-C(80B)-H(80D)	111.2
Cl(1B)-C(80B)-H(80D)	111.2
H(80C)-C(80B)-H(80D)	109.2
C(2B)-C(1)-C(5A)	94.5(8)
C(5A)-C(1)-C(2A)	105.0(6)
C(2B)-C(1)-C(5B)	110.5(10)
C(2A)-C(1)-C(5B)	120.1(7)
C(2B)-C(1)-P(1)	135.3(8)
C(5A)-C(1)-P(1)	129.5(5)
C(2A)-C(1)-P(1)	125.4(4)
C(5B)-C(1)-P(1)	114.0(6)
C(2B)-C(1)-Fe(1)	73.0(8)
C(5A)-C(1)-Fe(1)	68.4(4)
C(2A)-C(1)-Fe(1)	68.5(4)
C(5B)-C(1)-Fe(1)	72.0(7)
P(1)-C(1)-Fe(1)	125.5(2)
C(3A)-C(2A)-C(1)	106.8(6)
C(3A)-C(2A)-Fe(1)	69.8(4)
C(1)-C(2A)-Fe(1)	67.8(4)
C(3A)-C(2A)-H(2A)	126.6
C(1)-C(2A)-H(2A)	126.6
Fe(1)-C(2A)-H(2A)	127.4

C(4A)-C(3A)-C(2A)	109.2(7)
C(4A)-C(3A)-Fe(1)	69.6(4)
C(2A)-C(3A)-Fe(1)	69.4(4)
C(4A)-C(3A)-H(3A)	125.4
C(2A)-C(3A)-H(3A)	125.4
Fe(1)-C(3A)-H(3A)	127.2
C(3A)-C(4A)-C(5A)	107.9(6)
C(3A)-C(4A)-Fe(1)	70.3(4)
C(5A)-C(4A)-Fe(1)	67.6(4)
C(3A)-C(4A)-H(4A)	126.1
C(5A)-C(4A)-H(4A)	126.1
Fe(1)-C(4A)-H(4A)	127.6
C(1)-C(5A)-C(4A)	111.0(6)
C(1)-C(5A)-Fe(1)	71.1(4)
C(4A)-C(5A)-Fe(1)	70.8(4)
C(1)-C(5A)-H(5A)	124.5
C(4A)-C(5A)-H(5A)	124.5
Fe(1)-C(5A)-H(5A)	125.2
C(3B)-C(4B)-C(5B)	110.2(11)
C(3B)-C(4B)-Fe(1)	69.0(8)
C(5B)-C(4B)-Fe(1)	71.9(8)
C(3B)-C(4B)-H(4B)	124.9
C(5B)-C(4B)-H(4B)	124.9
Fe(1)-C(4B)-H(4B)	125.8
C(4B)-C(5B)-C(1)	100.1(10)
C(4B)-C(5B)-Fe(1)	68.7(8)
C(1)-C(5B)-Fe(1)	63.7(6)
C(4B)-C(5B)-H(5B)	130.0
C(1)-C(5B)-H(5B)	130.0
Fe(1)-C(5B)-H(5B)	128.9
C(4B)-C(3B)-C(2B)	108.4(12)
C(4B)-C(3B)-Fe(1)	72.1(9)
C(2B)-C(3B)-Fe(1)	69.0(8)
C(4B)-C(3B)-H(3B)	125.8
C(2B)-C(3B)-H(3B)	125.8
Fe(1)-C(3B)-H(3B)	124.7
C(1)-C(2B)-C(3B)	110.6(11)
C(1)-C(2B)-Fe(1)	71.1(8)

C(3B)-C(2B)-Fe(1)	70.5(8)
C(1)-C(2B)-H(2B)	124.7
C(3B)-C(2B)-H(2B)	124.7
Fe(1)-C(2B)-H(2B)	125.2
C(10A)-C(6)-C(7B)	120.3(9)
C(10A)-C(6)-C(7A)	110.1(9)
C(7B)-C(6)-C(10B)	107.6(9)
C(7A)-C(6)-C(10B)	96.7(8)
C(10A)-C(6)-Fe(1)	71.6(6)
C(7B)-C(6)-Fe(1)	68.1(6)
C(7A)-C(6)-Fe(1)	71.3(6)
C(10B)-C(6)-Fe(1)	68.5(6)
C(10A)-C(6)-H(6)	124.9
C(7B)-C(6)-H(6)	113.9
C(7A)-C(6)-H(6)	124.9
C(10B)-C(6)-H(6)	138.3
Fe(1)-C(6)-H(6)	123.8
C(8A)-C(7A)-C(6)	108.0(11)
C(8A)-C(7A)-Fe(1)	71.5(7)
C(6)-C(7A)-Fe(1)	68.0(6)
C(8A)-C(7A)-H(7A)	126.0
C(6)-C(7A)-H(7A)	126.0
Fe(1)-C(7A)-H(7A)	126.0
C(7A)-C(8A)-C(9A)	106.9(11)
C(7A)-C(8A)-Fe(1)	70.0(7)
C(9A)-C(8A)-Fe(1)	68.2(7)
C(7A)-C(8A)-H(8A)	126.5
C(9A)-C(8A)-H(8A)	126.5
Fe(1)-C(8A)-H(8A)	126.8
C(8A)-C(9A)-C(10A)	107.6(12)
C(8A)-C(9A)-Fe(1)	71.8(6)
C(10A)-C(9A)-Fe(1)	69.2(7)
C(8A)-C(9A)-H(9A)	126.2
C(10A)-C(9A)-H(9A)	126.2
Fe(1)-C(9A)-H(9A)	124.4
C(6)-C(10A)-C(9A)	107.3(12)
C(6)-C(10A)-Fe(1)	70.6(7)
C(9A)-C(10A)-Fe(1)	69.5(7)

C(6)-C(10A)-H(10A)	126.4
C(9A)-C(10A)-H(10A)	126.4
Fe(1)-C(10A)-H(10A)	125.2
C(6)-C(7B)-C(8B)	108.8(11)
C(6)-C(7B)-Fe(1)	71.4(7)
C(8B)-C(7B)-Fe(1)	67.9(8)
C(6)-C(7B)-H(7B)	125.6
C(8B)-C(7B)-H(7B)	125.6
Fe(1)-C(7B)-H(7B)	126.7
C(9B)-C(8B)-C(7B)	109.5(12)
C(9B)-C(8B)-Fe(1)	72.2(8)
C(7B)-C(8B)-Fe(1)	70.1(8)
C(9B)-C(8B)-H(8B)	125.2
C(7B)-C(8B)-H(8B)	125.2
Fe(1)-C(8B)-H(8B)	124.0
C(8B)-C(9B)-C(10B)	108.0(13)
C(8B)-C(9B)-Fe(1)	67.0(8)
C(10B)-C(9B)-Fe(1)	69.0(8)
C(8B)-C(9B)-H(9B)	126.0
C(10B)-C(9B)-H(9B)	126.0
Fe(1)-C(9B)-H(9B)	129.6
C(9B)-C(10B)-C(6)	105.9(13)
C(9B)-C(10B)-Fe(1)	69.1(8)
C(6)-C(10B)-Fe(1)	68.9(6)
C(9B)-C(10B)-H(10B)	127.1
C(6)-C(10B)-H(10B)	127.1
Fe(1)-C(10B)-H(10B)	126.4
C(16)-C(11)-C(12)	118.7(4)
C(16)-C(11)-P(1)	118.7(3)
C(12)-C(11)-P(1)	122.6(4)
C(13)-C(12)-C(11)	120.4(5)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	120.6(5)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(13)-C(14)-C(15)	119.6(5)
C(13)-C(14)-H(14)	120.2

C(15)-C(14)-H(14)	120.2
C(14)-C(15)-C(16)	119.8(6)
C(14)-C(15)-H(15)	120.1
C(16)-C(15)-H(15)	120.1
C(11)-C(16)-C(15)	120.8(5)
C(11)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6
C(18)-C(17)-C(22)	119.8(4)
C(18)-C(17)-P(1)	119.7(3)
C(22)-C(17)-P(1)	120.4(3)
C(17)-C(18)-C(19)	121.3(4)
C(17)-C(18)-H(18)	119.4
C(19)-C(18)-H(18)	119.4
C(18)-C(19)-C(20)	117.5(4)
C(18)-C(19)-C(23)	120.7(4)
C(20)-C(19)-C(23)	121.3(4)
O(1)-C(20)-C(21)	118.2(4)
O(1)-C(20)-C(19)	119.5(4)
C(21)-C(20)-C(19)	122.1(4)
C(20)-C(21)-C(22)	118.4(4)
C(20)-C(21)-C(24)	120.7(4)
C(22)-C(21)-C(24)	120.8(4)
C(17)-C(22)-C(21)	120.5(4)
C(17)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(19)-C(23)-C(29)	110.8(3)
C(19)-C(23)-H(23A)	109.5
C(29)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
C(29)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	108.1
C(21)-C(24)-C(25)	111.6(3)
C(21)-C(24)-H(24A)	109.3
C(25)-C(24)-H(24A)	109.3
C(21)-C(24)-H(24B)	109.3
C(25)-C(24)-H(24B)	109.3
H(24A)-C(24)-H(24B)	108.0
C(26)-C(25)-C(30)	118.4(4)

C(26)-C(25)-C(24)	119.4(4)
C(30)-C(25)-C(24)	122.1(4)
C(27)-C(26)-C(25)	121.1(4)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	119.4(5)
C(26)-C(27)-H(27)	120.3
C(28)-C(27)-H(27)	120.3
C(29)#1-C(28)-C(27)	120.6(4)
C(29)#1-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)#1-C(29)-C(30)#1	119.1(4)
C(28)#1-C(29)-C(23)	118.6(4)
C(30)#1-C(29)-C(23)	122.1(4)
C(29)#1-C(30)-C(25)	121.3(4)
C(29)#1-C(30)-O(2)	119.2(4)
C(25)-C(30)-O(2)	119.5(4)
O(2)-C(31)-C(32)	108.1(4)
O(2)-C(31)-H(31A)	110.1
C(32)-C(31)-H(31A)	110.1
O(2)-C(31)-H(31B)	110.1
C(32)-C(31)-H(31B)	110.1
H(31A)-C(31)-H(31B)	108.4
C(33B)-C(32)-C(31)	123(3)
C(33A)-C(32)-C(31)	109.8(9)
C(33B)-C(32)-H(32A)	106.6
C(33A)-C(32)-H(32A)	110.3
C(31)-C(32)-H(32A)	106.6
C(33B)-C(32)-H(32B)	106.6
C(33A)-C(32)-H(32B)	116.6
C(31)-C(32)-H(32B)	106.6
H(32A)-C(32)-H(32B)	106.5
C(32)-C(33B)-H(33D)	109.5
C(32)-C(33B)-H(33E)	109.5
C(32)-C(33B)-H(33F)	109.5
C(32)-C(33A)-H(33A)	109.5
C(32)-C(33A)-H(33B)	109.5
H(33A)-C(33A)-H(33B)	109.5

C(32)-C(33A)-H(33C)	109.5
H(33A)-C(33A)-H(33C)	109.5
H(33B)-C(33A)-H(33C)	109.5
O(1)-C(34)-C(35)	112.4(4)
O(1)-C(34)-H(34A)	109.1
C(35)-C(34)-H(34A)	109.1
O(1)-C(34)-H(34B)	109.1
C(35)-C(34)-H(34B)	109.1
H(34A)-C(34)-H(34B)	107.9
C(34)-C(35)-C(36)	110.5(5)
C(34)-C(35)-H(35A)	109.5
C(36)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	108.1
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(41)	107.3(5)
C(38)-C(37)-Fe(2)	69.6(3)
C(41)-C(37)-Fe(2)	69.1(3)
C(38)-C(37)-H(37)	126.3
C(41)-C(37)-H(37)	126.3
Fe(2)-C(37)-H(37)	126.5
C(37)-C(38)-C(39)	107.8(5)
C(37)-C(38)-Fe(2)	69.8(3)
C(39)-C(38)-Fe(2)	69.3(3)
C(37)-C(38)-H(38)	126.1
C(39)-C(38)-H(38)	126.1
Fe(2)-C(38)-H(38)	126.4
C(40)-C(39)-C(38)	108.5(5)
C(40)-C(39)-Fe(2)	69.7(3)
C(38)-C(39)-Fe(2)	69.9(3)
C(40)-C(39)-H(39)	125.8
C(38)-C(39)-H(39)	125.8

Fe(2)-C(39)-H(39)	126.3
C(41)-C(40)-C(39)	108.0(6)
C(41)-C(40)-Fe(2)	69.9(3)
C(39)-C(40)-Fe(2)	69.8(3)
C(41)-C(40)-H(40)	126.0
C(39)-C(40)-H(40)	126.0
Fe(2)-C(40)-H(40)	126.0
C(40)-C(41)-C(37)	108.4(5)
C(40)-C(41)-Fe(2)	69.7(3)
C(37)-C(41)-Fe(2)	69.8(3)
C(40)-C(41)-H(41)	125.8
C(37)-C(41)-H(41)	125.8
Fe(2)-C(41)-H(41)	126.2
C(46)-C(42)-C(43)	107.5(4)
C(46)-C(42)-P(2)	124.0(3)
C(43)-C(42)-P(2)	128.5(3)
C(46)-C(42)-Fe(2)	69.7(3)
C(43)-C(42)-Fe(2)	69.7(3)
P(2)-C(42)-Fe(2)	124.6(2)
C(44)-C(43)-C(42)	107.9(4)
C(44)-C(43)-Fe(2)	70.1(3)
C(42)-C(43)-Fe(2)	68.8(2)
C(44)-C(43)-H(43)	126.0
C(42)-C(43)-H(43)	126.0
Fe(2)-C(43)-H(43)	126.6
C(45)-C(44)-C(43)	108.2(4)
C(45)-C(44)-Fe(2)	69.8(3)
C(43)-C(44)-Fe(2)	69.2(2)
C(45)-C(44)-H(44)	125.9
C(43)-C(44)-H(44)	125.9
Fe(2)-C(44)-H(44)	126.7
C(44)-C(45)-C(46)	108.5(4)
C(44)-C(45)-Fe(2)	69.8(3)
C(46)-C(45)-Fe(2)	68.9(3)
C(44)-C(45)-H(45)	125.7
C(46)-C(45)-H(45)	125.7
Fe(2)-C(45)-H(45)	127.2
C(45)-C(46)-C(42)	107.9(4)

C(45)-C(46)-Fe(2)	70.2(3)
C(42)-C(46)-Fe(2)	69.2(3)
C(45)-C(46)-H(46)	126.0
C(42)-C(46)-H(46)	126.0
Fe(2)-C(46)-H(46)	126.1
C(52)-C(47)-C(48)	118.3(5)
C(52)-C(47)-P(2)	122.4(4)
C(48)-C(47)-P(2)	119.1(4)
C(49)-C(48)-C(47)	121.2(5)
C(49)-C(48)-H(48)	119.4
C(47)-C(48)-H(48)	119.4
C(50)-C(49)-C(48)	119.8(5)
C(50)-C(49)-H(49)	120.1
C(48)-C(49)-H(49)	120.1
C(49)-C(50)-C(51)	120.2(6)
C(49)-C(50)-H(50)	119.9
C(51)-C(50)-H(50)	119.9
C(50)-C(51)-C(52)	119.8(5)
C(50)-C(51)-H(51)	120.1
C(52)-C(51)-H(51)	120.1
C(47)-C(52)-C(51)	120.7(5)
C(47)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7
C(54)-C(53)-C(58)	119.2(4)
C(54)-C(53)-P(2)	121.4(3)
C(58)-C(53)-P(2)	119.4(3)
C(53)-C(54)-C(55)	121.5(4)
C(53)-C(54)-H(54)	119.2
C(55)-C(54)-H(54)	119.2
C(54)-C(55)-C(56)	117.5(4)
C(54)-C(55)-C(66)	122.2(4)
C(56)-C(55)-C(66)	120.3(4)
O(3)-C(56)-C(57)	120.1(4)
O(3)-C(56)-C(55)	117.1(4)
C(57)-C(56)-C(55)	122.5(4)
C(56)-C(57)-C(58)	117.8(4)
C(56)-C(57)-C(59)	121.9(4)
C(58)-C(57)-C(59)	120.2(4)

C(57)-C(58)-C(53)	120.7(4)
C(57)-C(58)-H(58)	119.6
C(53)-C(58)-H(58)	119.6
C(60)-C(59)-C(57)	110.6(3)
C(60)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59A)	109.5
C(60)-C(59)-H(59B)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	108.1
C(61)-C(60)-C(65)	118.6(4)
C(61)-C(60)-C(59)	118.8(4)
C(65)-C(60)-C(59)	122.6(4)
C(62)-C(61)-C(60)	120.5(5)
C(62)-C(61)-H(61)	119.8
C(60)-C(61)-H(61)	119.8
C(63)-C(62)-C(61)	120.3(5)
C(63)-C(62)-H(62)	119.9
C(61)-C(62)-H(62)	119.9
C(62)-C(63)-C(64)	121.0(5)
C(62)-C(63)-H(63)	119.5
C(64)-C(63)-H(63)	119.5
C(65)-C(64)-C(63)	118.2(4)
C(65)-C(64)-C(66)#2	121.6(4)
C(63)-C(64)-C(66)#2	120.0(4)
O(4)-C(65)-C(64)	119.3(4)
O(4)-C(65)-C(60)	119.2(4)
C(64)-C(65)-C(60)	121.4(4)
C(55)-C(66)-C(64)#2	110.8(4)
C(55)-C(66)-H(66A)	109.5
C(64)#2-C(66)-H(66A)	109.5
C(55)-C(66)-H(66B)	109.5
C(64)#2-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	108.1
O(4)-C(67)-C(68)	107.8(4)
O(4)-C(67)-H(67A)	110.1
C(68)-C(67)-H(67A)	110.1
O(4)-C(67)-H(67B)	110.1
C(68)-C(67)-H(67B)	110.1

H(67A)-C(67)-H(67B)	108.5
C(69)-C(68)-C(67)	112.9(5)
C(69)-C(68)-H(68A)	109.0
C(67)-C(68)-H(68A)	109.0
C(69)-C(68)-H(68B)	109.0
C(67)-C(68)-H(68B)	109.0
H(68A)-C(68)-H(68B)	107.8
C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(68)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
O(3)-C(70)-C(71)	114.0(4)
O(3)-C(70)-H(70A)	108.8
C(71)-C(70)-H(70A)	108.8
O(3)-C(70)-H(70B)	108.8
C(71)-C(70)-H(70B)	108.8
H(70A)-C(70)-H(70B)	107.7
C(70)-C(71)-C(72)	109.9(5)
C(70)-C(71)-H(71A)	109.7
C(72)-C(71)-H(71A)	109.7
C(70)-C(71)-H(71B)	109.7
C(72)-C(71)-H(71B)	109.7
H(71A)-C(71)-H(71B)	108.2
C(71)-C(72)-H(72E)	109.5
C(71)-C(72)-H(72F)	109.5
H(72E)-C(72)-H(72F)	109.5
C(71)-C(72)-H(72G)	109.5
H(72E)-C(72)-H(72G)	109.5
H(72F)-C(72)-H(72G)	109.5
C(20)-O(1)-C(34)	115.1(4)
C(30)-O(2)-C(31)	112.3(3)
C(56)-O(3)-C(70)	114.0(4)
C(65)-O(4)-C(67)	113.3(3)
C(1)-P(1)-C(17)	104.9(2)
C(1)-P(1)-C(11)	106.0(2)
C(17)-P(1)-C(11)	103.8(2)

C(1)-P(1)-B(1)	114.9(2)
C(17)-P(1)-B(1)	115.2(2)
C(11)-P(1)-B(1)	111.0(2)
C(42)-P(2)-C(53)	106.2(2)
C(42)-P(2)-C(47)	104.4(2)
C(53)-P(2)-C(47)	107.0(2)
C(42)-P(2)-B(2)	115.1(2)
C(53)-P(2)-B(2)	115.3(2)
C(47)-P(2)-B(2)	108.1(2)
C(8B)-Fe(1)-C(5A)	161.3(4)
C(8B)-Fe(1)-C(7B)	42.0(5)
C(5A)-Fe(1)-C(7B)	156.2(4)
C(8B)-Fe(1)-C(1)	150.2(3)
C(5A)-Fe(1)-C(1)	40.5(3)
C(7B)-Fe(1)-C(1)	117.5(3)
C(8B)-Fe(1)-C(4A)	120.1(4)
C(5A)-Fe(1)-C(4A)	41.6(3)
C(7B)-Fe(1)-C(4A)	155.8(5)
C(1)-Fe(1)-C(4A)	69.8(3)
C(8B)-Fe(1)-C(2A)	110.4(4)
C(5A)-Fe(1)-C(2A)	69.8(3)
C(7B)-Fe(1)-C(2A)	99.9(4)
C(1)-Fe(1)-C(2A)	43.7(3)
C(4A)-Fe(1)-C(2A)	68.8(3)
C(8B)-Fe(1)-C(10B)	70.3(6)
C(5A)-Fe(1)-C(10B)	114.6(5)
C(7B)-Fe(1)-C(10B)	70.3(7)
C(1)-Fe(1)-C(10B)	130.0(4)
C(4A)-Fe(1)-C(10B)	124.5(5)
C(2A)-Fe(1)-C(10B)	165.1(4)
C(8B)-Fe(1)-C(9B)	40.8(4)
C(5A)-Fe(1)-C(9B)	130.6(5)
C(7B)-Fe(1)-C(9B)	69.6(5)
C(1)-Fe(1)-C(9B)	168.8(4)
C(4A)-Fe(1)-C(9B)	107.5(5)
C(2A)-Fe(1)-C(9B)	146.5(4)
C(10B)-Fe(1)-C(9B)	41.8(4)
C(8B)-Fe(1)-C(3A)	98.5(4)

C(5A)-Fe(1)-C(3A)	69.0(3)
C(7B)-Fe(1)-C(3A)	117.8(5)
C(1)-Fe(1)-C(3A)	70.8(3)
C(4A)-Fe(1)-C(3A)	40.1(3)
C(2A)-Fe(1)-C(3A)	40.8(3)
C(10B)-Fe(1)-C(3A)	153.7(4)
C(9B)-Fe(1)-C(3A)	114.7(4)
C(8B)-Fe(1)-C(6)	69.8(4)
C(5A)-Fe(1)-C(6)	126.8(3)
C(7B)-Fe(1)-C(6)	40.5(5)
C(1)-Fe(1)-C(6)	109.1(2)
C(4A)-Fe(1)-C(6)	162.9(2)
C(2A)-Fe(1)-C(6)	123.0(3)
C(10B)-Fe(1)-C(6)	42.5(4)
C(9B)-Fe(1)-C(6)	70.0(4)
C(3A)-Fe(1)-C(6)	156.8(2)
C(8B)-Fe(1)-C(2B)	121.2(6)
C(5A)-Fe(1)-C(2B)	57.6(5)
C(7B)-Fe(1)-C(2B)	111.8(5)
C(1)-Fe(1)-C(2B)	35.9(5)
C(4A)-Fe(1)-C(2B)	59.2(5)
C(2A)-Fe(1)-C(2B)	12.3(4)
C(10B)-Fe(1)-C(2B)	165.8(6)
C(9B)-Fe(1)-C(2B)	152.4(6)
C(3A)-Fe(1)-C(2B)	38.8(6)
C(6)-Fe(1)-C(2B)	130.1(5)
C(8B)-Fe(1)-C(10A)	78.3(5)
C(5A)-Fe(1)-C(10A)	109.2(5)
C(7B)-Fe(1)-C(10A)	71.5(6)
C(1)-Fe(1)-C(10A)	120.0(4)
C(4A)-Fe(1)-C(10A)	126.9(5)
C(2A)-Fe(1)-C(10A)	156.5(4)
C(10B)-Fe(1)-C(10A)	10.4(5)
C(9B)-Fe(1)-C(10A)	52.2(5)
C(3A)-Fe(1)-C(10A)	162.3(4)
C(6)-Fe(1)-C(10A)	37.9(4)
C(2B)-Fe(1)-C(10A)	155.4(6)
C(42)-Fe(2)-C(46)	41.18(17)

C(42)-Fe(2)-C(43)	41.57(18)
C(46)-Fe(2)-C(43)	69.27(19)
C(42)-Fe(2)-C(40)	166.2(2)
C(46)-Fe(2)-C(40)	127.0(2)
C(43)-Fe(2)-C(40)	150.2(2)
C(42)-Fe(2)-C(39)	129.0(2)
C(46)-Fe(2)-C(39)	108.1(2)
C(43)-Fe(2)-C(39)	168.1(2)
C(40)-Fe(2)-C(39)	40.6(2)
C(42)-Fe(2)-C(41)	152.7(2)
C(46)-Fe(2)-C(41)	164.4(3)
C(43)-Fe(2)-C(41)	117.6(2)
C(40)-Fe(2)-C(41)	40.4(3)
C(39)-Fe(2)-C(41)	68.1(2)
C(42)-Fe(2)-C(38)	109.1(2)
C(46)-Fe(2)-C(38)	119.2(2)
C(43)-Fe(2)-C(38)	129.5(2)
C(40)-Fe(2)-C(38)	68.6(2)
C(39)-Fe(2)-C(38)	40.8(2)
C(41)-Fe(2)-C(38)	68.5(2)
C(42)-Fe(2)-C(37)	119.1(2)
C(46)-Fe(2)-C(37)	153.2(2)
C(43)-Fe(2)-C(37)	108.4(2)
C(40)-Fe(2)-C(37)	68.7(3)
C(39)-Fe(2)-C(37)	68.4(2)
C(41)-Fe(2)-C(37)	41.1(3)
C(38)-Fe(2)-C(37)	40.6(2)
C(42)-Fe(2)-C(44)	69.2(2)
C(46)-Fe(2)-C(44)	68.8(2)
C(43)-Fe(2)-C(44)	40.66(19)
C(40)-Fe(2)-C(44)	116.2(2)
C(39)-Fe(2)-C(44)	150.3(2)
C(41)-Fe(2)-C(44)	106.5(2)
C(38)-Fe(2)-C(44)	166.7(2)
C(37)-Fe(2)-C(44)	127.7(2)
C(42)-Fe(2)-C(45)	68.92(19)
C(46)-Fe(2)-C(45)	40.86(19)
C(43)-Fe(2)-C(45)	68.42(19)

C(40)-Fe(2)-C(45)	106.4(2)
C(39)-Fe(2)-C(45)	117.7(2)
C(41)-Fe(2)-C(45)	126.2(2)
C(38)-Fe(2)-C(45)	152.4(2)
C(37)-Fe(2)-C(45)	165.0(2)
C(44)-Fe(2)-C(45)	40.46(19)
P(1)-B(1)-H(1A)	109.5
P(1)-B(1)-H(1B)	109.5
H(1A)-B(1)-H(1B)	109.5
P(1)-B(1)-H(1C)	109.5
H(1A)-B(1)-H(1C)	109.5
H(1B)-B(1)-H(1C)	109.5
P(2)-B(2)-H(2C)	109.5
P(2)-B(2)-H(2D)	109.5
H(2C)-B(2)-H(2D)	109.5
P(2)-B(2)-H(2E)	109.5
H(2C)-B(2)-H(2E)	109.5
H(2D)-B(2)-H(2E)	109.5
P(2)-B(2)-H(2F)	109.5
H(2C)-B(2)-H(2F)	141.1
H(2D)-B(2)-H(2F)	56.3
H(2E)-B(2)-H(2F)	56.3
P(2)-B(2)-H(2G)	109.5
H(2C)-B(2)-H(2G)	56.3
H(2D)-B(2)-H(2G)	141.1
H(2E)-B(2)-H(2G)	56.3
H(2F)-B(2)-H(2G)	109.5
P(2)-B(2)-H(2H)	109.5
H(2C)-B(2)-H(2H)	56.3
H(2D)-B(2)-H(2H)	56.3
H(2E)-B(2)-H(2H)	141.1
H(2F)-B(2)-H(2H)	109.5
H(2G)-B(2)-H(2H)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1 #2 -x+2,y,-z+2

Table S12. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **8c** (09kn1). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(80A)	37(5)	106(10)	43(5)	-10(6)	21(4)	1(5)
Cl(1A)	63(1)	83(2)	73(1)	-3(1)	45(1)	0(1)
Cl(2A)	63(1)	83(2)	73(1)	-3(1)	45(1)	0(1)
C(80B)	37(5)	106(10)	43(5)	-10(6)	21(4)	1(5)
Cl(1B)	63(1)	83(2)	73(1)	-3(1)	45(1)	0(1)
Cl(2B)	63(1)	83(2)	73(1)	-3(1)	45(1)	0(1)
C(1)	23(2)	36(3)	18(2)	0(2)	9(2)	-9(2)
C(2A)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(3A)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(4A)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(5A)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(4B)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(5B)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(3B)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(2B)	17(2)	30(3)	16(2)	2(2)	6(2)	4(2)
C(6)	44(3)	41(3)	40(3)	0(2)	31(2)	-8(3)
C(7A)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(8A)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(9A)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(10A)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(7B)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(8B)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(9B)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(10B)	31(2)	27(3)	38(2)	-7(2)	18(2)	-15(2)
C(11)	18(2)	24(2)	26(2)	10(2)	11(2)	5(2)
C(12)	30(2)	34(3)	34(2)	3(2)	21(2)	-2(2)
C(13)	38(3)	45(3)	43(3)	7(2)	28(2)	-4(2)
C(14)	42(3)	34(3)	63(4)	18(3)	32(3)	1(3)
C(15)	70(4)	34(3)	61(4)	-14(3)	41(4)	-21(3)
C(16)	61(4)	40(3)	52(3)	-9(3)	42(3)	-16(3)
C(17)	20(2)	24(2)	14(2)	-2(2)	8(2)	-3(2)
C(18)	23(2)	26(2)	19(2)	0(2)	11(2)	-2(2)
C(19)	20(2)	26(2)	18(2)	-4(2)	9(2)	-2(2)

C(20)	20(2)	23(2)	14(2)	0(2)	5(2)	-4(2)
C(21)	22(2)	25(2)	20(2)	-1(2)	12(2)	-2(2)
C(22)	17(2)	22(2)	17(2)	-3(2)	8(2)	0(2)
C(23)	20(2)	33(3)	18(2)	2(2)	9(2)	7(2)
C(24)	16(2)	27(3)	22(2)	1(2)	10(2)	-2(2)
C(25)	15(2)	26(2)	18(2)	0(2)	11(2)	1(2)
C(26)	22(2)	31(3)	25(2)	7(2)	12(2)	3(2)
C(27)	31(2)	21(2)	35(2)	-1(2)	21(2)	-5(2)
C(28)	22(2)	29(3)	25(2)	-8(2)	13(2)	-9(2)
C(29)	16(2)	27(2)	23(2)	-1(2)	13(2)	0(2)
C(30)	17(2)	22(2)	19(2)	0(2)	13(2)	1(2)
C(31)	26(2)	32(3)	37(3)	8(2)	22(2)	-1(2)
C(32)	47(3)	40(3)	66(4)	0(3)	44(3)	-7(3)
C(33B)	67(7)	38(10)	97(6)	34(7)	57(6)	9(6)
C(33A)	67(7)	38(10)	97(6)	34(7)	57(6)	9(6)
C(34)	37(3)	47(4)	46(3)	13(3)	26(3)	12(3)
C(35)	38(3)	56(4)	41(3)	11(3)	20(3)	3(3)
C(36)	65(4)	36(4)	59(4)	7(3)	41(4)	-1(3)
C(37)	51(3)	54(4)	50(3)	19(3)	35(3)	31(3)
C(38)	27(2)	44(3)	41(3)	-2(2)	23(2)	6(2)
C(39)	45(3)	35(3)	45(3)	-8(2)	35(3)	-5(2)
C(40)	55(3)	32(3)	74(4)	-21(3)	50(3)	-10(3)
C(41)	75(4)	31(3)	91(5)	20(3)	70(4)	20(3)
C(42)	22(2)	26(2)	22(2)	4(2)	12(2)	4(2)
C(43)	27(2)	32(3)	33(2)	3(2)	22(2)	3(2)
C(44)	26(2)	29(3)	41(3)	3(2)	22(2)	1(2)
C(45)	25(2)	34(3)	30(2)	2(2)	11(2)	1(2)
C(46)	22(2)	28(3)	25(2)	3(2)	9(2)	2(2)
C(47)	30(2)	25(2)	29(2)	0(2)	17(2)	-3(2)
C(48)	27(2)	24(2)	49(3)	-5(2)	20(2)	-4(2)
C(49)	39(3)	27(3)	70(4)	-4(3)	36(3)	-2(2)
C(50)	68(4)	37(3)	66(4)	6(3)	55(4)	5(3)
C(51)	72(4)	43(4)	40(3)	-11(3)	35(3)	-6(3)
C(52)	45(3)	44(3)	35(3)	-2(2)	17(2)	1(3)
C(53)	18(2)	25(3)	19(2)	-1(2)	5(2)	-2(2)
C(54)	21(2)	28(3)	28(2)	1(2)	13(2)	2(2)
C(55)	19(2)	28(3)	19(2)	-1(2)	8(2)	-2(2)
C(56)	21(2)	30(3)	19(2)	0(2)	8(2)	2(2)

C(57)	21(2)	27(2)	24(2)	-2(2)	14(2)	-2(2)
C(58)	22(2)	31(3)	18(2)	2(2)	9(2)	-1(2)
C(59)	22(2)	33(3)	19(2)	0(2)	10(2)	4(2)
C(60)	14(2)	31(3)	23(2)	3(2)	12(2)	1(2)
C(61)	31(2)	25(3)	34(2)	4(2)	22(2)	3(2)
C(62)	28(2)	28(3)	37(2)	-5(2)	21(2)	-1(2)
C(63)	23(2)	30(3)	32(2)	-6(2)	17(2)	-2(2)
C(64)	16(2)	31(3)	26(2)	-2(2)	12(2)	-1(2)
C(65)	20(2)	25(2)	25(2)	-3(2)	18(2)	-2(2)
C(66)	18(2)	32(3)	20(2)	-1(2)	8(2)	-6(2)
C(67)	31(2)	37(3)	40(3)	0(2)	27(2)	3(2)
C(68)	49(3)	35(3)	54(3)	9(3)	41(3)	13(3)
C(69)	63(4)	36(4)	79(5)	-4(3)	50(4)	4(3)
C(70)	29(3)	41(3)	37(3)	9(2)	17(2)	4(2)
C(71)	27(3)	54(4)	44(3)	13(3)	17(3)	7(3)
C(72)	48(4)	35(3)	60(4)	2(3)	28(3)	-4(3)
O(1)	19(1)	31(2)	20(1)	7(2)	9(1)	4(2)
O(2)	17(1)	25(2)	23(1)	2(1)	12(1)	-1(1)
O(3)	22(2)	33(2)	24(2)	6(2)	11(1)	7(2)
O(4)	20(1)	27(2)	26(2)	-1(1)	14(1)	2(1)
P(1)	18(1)	24(1)	18(1)	3(1)	9(1)	0(1)
P(2)	21(1)	26(1)	20(1)	3(1)	10(1)	2(1)
Fe(1)	25(1)	28(1)	24(1)	-3(1)	14(1)	-5(1)
Fe(2)	29(1)	24(1)	28(1)	1(1)	19(1)	3(1)
B(1)	30(3)	34(3)	38(3)	13(3)	22(2)	8(3)
B(2)	35(3)	34(3)	40(3)	8(3)	25(3)	0(3)

Table S13. Crystal data and structure refinement for compound **11** (**etjugl**).

Compound	etjugl
Formula	C₅₃H₆₁O₅PBCL
M	855.25
T; K	115 (2)
Crystal system	orthorhombic
Space group	P 2₁2₁2₁
a; Å	15.7555 (4)
b; Å	15.9369 (4)
c; Å	18.3866 (5)
V; Å ³	4616.8 (2)
Z	4
F(000)	1824
D _{calc} ; g/cm ³	1.23
diffractometer	Enraf-Nonius KappaCCD
scan type	mixture of ϕ rotations and ω scans
λ ; Å	0.71073
μ ; mm ⁻¹	0.165
Crystal size; mm ³	0.4 x 0.25 x 0.225
$\sin(\theta)/\lambda$ max; Å ⁻¹	0.70
Index ranges	h: -20; 20
	k: -20; 20
	l: -23; 23
RC = Refl. Collected	10441
IRC = independent RC	10441 [R(int) = 0.000]
IRCGT = RC and [I>2 σ (I)]	8402
Refinement method	Full-matrix least-squares on F²
Data / restraints / parameters	10441 / 0 / 557
R for IRCGT	R1^a = 0.0572 , wR2^b = 0.1179
R for IRC	R1^a = 0.0799 , wR2^b = 0.1304
Goodness-of-fit ^c	1.020
Abs. structure parameter	0.00 (7)
Largest diff. peak and hole; e.Å ⁻³	0.789 and -0.519

^a $R1 = \Sigma (||F_o| - |F_c||) / \Sigma |F_o|$.

^b $wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma [w(F_o^2)^2]]^{1/2}$ where $w = 1 / [\sigma^2(F_o^2) + 4.866P + (0.0347P)^2]$ where $P = (\text{Max}(F_o^2, 0) + 2 * F_c^2) / 3$

^c Goodness of fit = $[\Sigma w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$.

Table S14. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **11** (**etjugl**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3081(2)	1183(2)	6212(2)	30(1)
C(2)	3643(2)	1661(2)	6621(2)	36(1)
C(3)	4064(2)	1315(2)	7205(2)	42(1)
C(4)	3926(2)	484(2)	7394(2)	42(1)
C(5)	3355(2)	4(2)	7003(2)	40(1)
C(6)	2935(2)	352(2)	6415(2)	36(1)
C(7)	3169(2)	1432(2)	4623(2)	32(1)
C(8)	2827(2)	972(2)	4040(2)	42(1)
C(9)	3290(3)	842(2)	3405(2)	51(1)
C(10)	4091(3)	1169(2)	3353(2)	49(1)
C(11)	4454(2)	1618(2)	3920(2)	41(1)
C(12)	3995(2)	1739(2)	4557(2)	34(1)
C(13)	5184(3)	2249(5)	5190(4)	129(3)
C(14)	2408(2)	2712(2)	5566(2)	29(1)
C(15)	2665(2)	3312(2)	5058(2)	28(1)
C(16)	2479(2)	4162(2)	5148(2)	26(1)
C(17)	2009(2)	4397(2)	5752(2)	28(1)
C(18)	1813(2)	3826(2)	6315(2)	30(1)
C(19)	2002(2)	2985(2)	6200(2)	30(1)
C(20)	2832(2)	4819(2)	4636(2)	28(1)
C(21)	3547(2)	5311(2)	4997(2)	26(1)
C(22)	3513(2)	6180(2)	5082(1)	24(1)
C(23)	4122(2)	6610(2)	5484(2)	25(1)
C(24)	4806(2)	6166(2)	5762(2)	31(1)
C(25)	4881(2)	5313(2)	5646(2)	33(1)
C(26)	4247(2)	4889(2)	5275(2)	29(1)
C(27)	4056(2)	7548(2)	5636(2)	30(1)
C(28)	3922(2)	7714(2)	6440(2)	29(1)
C(29)	3168(2)	7450(2)	6778(2)	30(1)
C(30)	3064(2)	7497(2)	7532(2)	29(1)
C(31)	3690(2)	7884(2)	7942(2)	31(1)
C(32)	4424(2)	8174(2)	7611(2)	29(1)
C(33)	4553(2)	8077(2)	6862(2)	29(1)
C(34)	2343(2)	7040(2)	7906(2)	31(1)
C(35)	2506(2)	6100(2)	7837(2)	29(1)
C(36)	1898(2)	5553(2)	7558(2)	29(1)
C(37)	2084(2)	4708(2)	7410(2)	30(1)
C(38)	2891(2)	4418(2)	7588(2)	33(1)
C(39)	3489(2)	4936(2)	7905(2)	33(1)
C(40)	3297(2)	5778(2)	8019(2)	32(1)
C(41)	1459(2)	4135(2)	7033(2)	34(1)
C(42)	878(2)	5361(2)	5687(2)	42(1)
C(43)	650(2)	5390(2)	4890(2)	47(1)
C(44)	-312(3)	5382(3)	4797(3)	69(1)
C(45)	3044(2)	6868(2)	4028(2)	32(1)
C(46)	2354(2)	7433(2)	3742(2)	37(1)
C(47)	2333(3)	8293(2)	4095(2)	48(1)
C(48)	1808(3)	7454(3)	6177(3)	80(2)
C(49)	1616(4)	8261(3)	6320(3)	103(2)
C(50)	753(3)	8611(3)	6105(2)	53(1)
C(51)	512(2)	5801(4)	7989(2)	68(1)

C (52)	-427 (3)	5896 (3)	7632 (3)	83 (2)
C (53)	-508 (4)	6731 (3)	7416 (4)	100 (2)
O (1)	4304 (2)	2147 (2)	5150 (1)	40 (1)
O (2)	1773 (1)	5227 (1)	5824 (1)	33 (1)
O (3)	2852 (1)	6635 (1)	4765 (1)	27 (1)
O (4)	2576 (2)	7061 (1)	6347 (1)	37 (1)
O (5)	1089 (1)	5851 (1)	7388 (1)	33 (1)
P	2518 (1)	1589 (1)	5424 (1)	31 (1)
B	1479 (3)	1062 (3)	5315 (3)	51 (1)
C1	5200 (1)	8655 (1)	8148 (1)	30 (1)

Table S15. Bond lengths [Å] and angles [deg] for compound **11(etjug1)**.

C(1)–C(2)	1.389(4)
C(1)–C(6)	1.395(4)
C(1)–P	1.819(3)
C(2)–C(3)	1.379(5)
C(2)–H(2)	0.9300
C(3)–C(4)	1.386(5)
C(3)–H(3)	0.9300
C(4)–C(5)	1.383(5)
C(4)–H(4)	0.9300
C(5)–C(6)	1.383(5)
C(5)–H(5)	0.9300
C(6)–H(6)	0.9300
C(7)–C(12)	1.395(5)
C(7)–C(8)	1.406(4)
C(7)–P	1.812(3)
C(8)–C(9)	1.393(5)
C(8)–H(8)	0.9300
C(9)–C(10)	1.368(6)
C(9)–H(9)	0.9300
C(10)–C(11)	1.389(5)
C(10)–H(10)	0.9300
C(11)–C(12)	1.390(5)
C(11)–H(11)	0.9300
C(12)–O(1)	1.360(4)
C(13)–O(1)	1.398(5)
C(13)–H(13A)	0.9600
C(13)–H(13B)	0.9600
C(13)–H(13C)	0.9600
C(14)–C(15)	1.397(4)
C(14)–C(19)	1.399(4)
C(14)–P	1.818(3)
C(15)–C(16)	1.395(4)
C(15)–H(15)	0.9300
C(16)–C(17)	1.387(4)
C(16)–C(20)	1.513(4)
C(17)–O(2)	1.381(3)
C(17)–C(18)	1.412(4)
C(18)–C(19)	1.388(4)
C(18)–C(41)	1.515(4)
C(19)–H(19)	0.9300
C(20)–C(21)	1.523(4)
C(20)–H(20A)	0.9700
C(20)–H(20B)	0.9700
C(21)–C(26)	1.389(4)
C(21)–C(22)	1.396(4)
C(22)–C(23)	1.392(4)
C(22)–O(3)	1.396(3)
C(23)–C(24)	1.387(4)
C(23)–C(27)	1.523(4)
C(24)–C(25)	1.381(4)
C(24)–H(24)	0.9300
C(25)–C(26)	1.385(4)
C(25)–H(25)	0.9300
C(26)–H(26)	0.9300
C(27)–C(28)	1.517(4)
C(27)–H(27A)	0.9700
C(27)–H(27B)	0.9700

C(28)–C(33)	1.388(4)
C(28)–C(29)	1.405(4)
C(29)–O(4)	1.372(4)
C(29)–C(30)	1.399(4)
C(30)–C(31)	1.386(4)
C(30)–C(34)	1.514(4)
C(31)–C(32)	1.387(4)
C(31)–H(31)	0.9300
C(32)–C(33)	1.401(4)
C(32)–Cl	1.749(3)
C(33)–H(33)	0.9300
C(34)–C(35)	1.526(4)
C(34)–H(34A)	0.9700
C(34)–H(34B)	0.9700
C(35)–C(40)	1.389(4)
C(35)–C(36)	1.393(4)
C(36)–O(5)	1.396(4)
C(36)–C(37)	1.405(4)
C(37)–C(38)	1.391(4)
C(37)–C(41)	1.511(5)
C(38)–C(39)	1.382(5)
C(38)–H(38)	0.9300
C(39)–C(40)	1.391(4)
C(39)–H(39)	0.9300
C(40)–H(40)	0.9300
C(41)–H(41A)	0.9700
C(41)–H(41B)	0.9700
C(42)–O(2)	1.448(4)
C(42)–C(43)	1.508(5)
C(42)–H(42A)	0.9700
C(42)–H(42B)	0.9700
C(43)–C(44)	1.525(5)
C(43)–H(43A)	0.9700
C(43)–H(43B)	0.9700
C(44)–H(44A)	0.9600
C(44)–H(44B)	0.9600
C(44)–H(44C)	0.9600
C(45)–O(3)	1.437(3)
C(45)–C(46)	1.507(4)
C(45)–H(45A)	0.9700
C(45)–H(45B)	0.9700
C(46)–C(47)	1.517(5)
C(46)–H(46A)	0.9700
C(46)–H(46B)	0.9700
C(47)–H(47A)	0.9600
C(47)–H(47B)	0.9600
C(47)–H(47C)	0.9600
C(48)–C(49)	1.348(6)
C(48)–O(4)	1.398(5)
C(48)–H(48A)	0.9700
C(48)–H(48B)	0.9700
C(49)–C(50)	1.521(6)
C(49)–H(49A)	0.9700
C(49)–H(49B)	0.9700
C(50)–H(50A)	0.9600
C(50)–H(50B)	0.9600
C(50)–H(50C)	0.9600
C(51)–O(5)	1.433(4)
C(51)–C(52)	1.626(7)
C(51)–H(51A)	0.9700
C(51)–H(51B)	0.9700

C(52)-C(53)	1.394(7)
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600
C(53)-H(53C)	0.9600
P-B	1.851(4)
B-H(0A)	0.9600
B-H(0B)	0.9600
B-H(0C)	0.9600
C(2)-C(1)-C(6)	118.8(3)
C(2)-C(1)-P	123.1(2)
C(6)-C(1)-P	118.1(2)
C(3)-C(2)-C(1)	120.6(3)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(2)-C(3)-C(4)	120.2(3)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	120.0(3)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	119.8(3)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(5)-C(6)-C(1)	120.7(3)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
C(12)-C(7)-C(8)	118.3(3)
C(12)-C(7)-P	123.4(2)
C(8)-C(7)-P	118.3(3)
C(9)-C(8)-C(7)	121.1(4)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	119.0(3)
C(10)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5
C(9)-C(10)-C(11)	121.6(4)
C(9)-C(10)-H(10)	119.2
C(11)-C(10)-H(10)	119.2
C(10)-C(11)-C(12)	119.3(4)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
O(1)-C(12)-C(11)	123.7(3)
O(1)-C(12)-C(7)	115.6(3)
C(11)-C(12)-C(7)	120.7(3)
O(1)-C(13)-H(13A)	109.5
O(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	118.5(3)
C(15)-C(14)-P	123.3(2)
C(19)-C(14)-P	118.1(2)
C(16)-C(15)-C(14)	121.6(3)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(17)-C(16)-C(15)	117.9(3)
C(17)-C(16)-C(20)	120.5(3)

C(15)-C(16)-C(20)	121.4(3)
O(2)-C(17)-C(16)	118.6(3)
O(2)-C(17)-C(18)	119.3(3)
C(16)-C(17)-C(18)	122.0(3)
C(19)-C(18)-C(17)	117.6(3)
C(19)-C(18)-C(41)	121.6(3)
C(17)-C(18)-C(41)	120.7(3)
C(18)-C(19)-C(14)	121.6(3)
C(18)-C(19)-H(19)	119.2
C(14)-C(19)-H(19)	119.2
C(16)-C(20)-C(21)	110.9(2)
C(16)-C(20)-H(20A)	109.5
C(21)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
C(21)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.0
C(26)-C(21)-C(22)	118.0(3)
C(26)-C(21)-C(20)	119.9(3)
C(22)-C(21)-C(20)	122.1(3)
C(23)-C(22)-C(21)	121.5(3)
C(23)-C(22)-O(3)	118.7(2)
C(21)-C(22)-O(3)	119.8(3)
C(24)-C(23)-C(22)	118.7(3)
C(24)-C(23)-C(27)	119.1(3)
C(22)-C(23)-C(27)	122.2(3)
C(25)-C(24)-C(23)	120.7(3)
C(25)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(24)-C(25)-C(26)	119.7(3)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(25)-C(26)-C(21)	121.2(3)
C(25)-C(26)-H(26)	119.4
C(21)-C(26)-H(26)	119.4
C(28)-C(27)-C(23)	111.1(2)
C(28)-C(27)-H(27A)	109.4
C(23)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27B)	109.4
C(23)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	108.0
C(33)-C(28)-C(29)	118.9(3)
C(33)-C(28)-C(27)	121.2(3)
C(29)-C(28)-C(27)	119.8(3)
O(4)-C(29)-C(30)	121.1(3)
O(4)-C(29)-C(28)	117.0(3)
C(30)-C(29)-C(28)	121.5(3)
C(31)-C(30)-C(29)	118.6(3)
C(31)-C(30)-C(34)	120.0(3)
C(29)-C(30)-C(34)	120.9(3)
C(30)-C(31)-C(32)	120.2(3)
C(30)-C(31)-H(31)	119.9
C(32)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	121.1(3)
C(31)-C(32)-Cl	118.8(2)
C(33)-C(32)-Cl	120.1(2)
C(28)-C(33)-C(32)	119.4(3)
C(28)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
C(30)-C(34)-C(35)	108.0(2)
C(30)-C(34)-H(34A)	110.1
C(35)-C(34)-H(34A)	110.1

C(30)–C(34)–H(34B)	110.1
C(35)–C(34)–H(34B)	110.1
H(34A)–C(34)–H(34B)	108.4
C(40)–C(35)–C(36)	118.3(3)
C(40)–C(35)–C(34)	119.6(3)
C(36)–C(35)–C(34)	122.0(3)
C(35)–C(36)–O(5)	119.8(3)
C(35)–C(36)–C(37)	121.9(3)
O(5)–C(36)–C(37)	118.2(3)
C(38)–C(37)–C(36)	117.6(3)
C(38)–C(37)–C(41)	120.2(3)
C(36)–C(37)–C(41)	122.2(3)
C(39)–C(38)–C(37)	121.6(3)
C(39)–C(38)–H(38)	119.2
C(37)–C(38)–H(38)	119.2
C(38)–C(39)–C(40)	119.4(3)
C(38)–C(39)–H(39)	120.3
C(40)–C(39)–H(39)	120.3
C(35)–C(40)–C(39)	121.0(3)
C(35)–C(40)–H(40)	119.5
C(39)–C(40)–H(40)	119.5
C(37)–C(41)–C(18)	110.9(3)
C(37)–C(41)–H(41A)	109.5
C(18)–C(41)–H(41A)	109.5
C(37)–C(41)–H(41B)	109.5
C(18)–C(41)–H(41B)	109.5
H(41A)–C(41)–H(41B)	108.1
O(2)–C(42)–C(43)	113.9(3)
O(2)–C(42)–H(42A)	108.8
C(43)–C(42)–H(42A)	108.8
O(2)–C(42)–H(42B)	108.8
C(43)–C(42)–H(42B)	108.8
H(42A)–C(42)–H(42B)	107.7
C(42)–C(43)–C(44)	110.2(4)
C(42)–C(43)–H(43A)	109.6
C(44)–C(43)–H(43A)	109.6
C(42)–C(43)–H(43B)	109.6
C(44)–C(43)–H(43B)	109.6
H(43A)–C(43)–H(43B)	108.1
C(43)–C(44)–H(44A)	109.5
C(43)–C(44)–H(44B)	109.5
H(44A)–C(44)–H(44B)	109.5
C(43)–C(44)–H(44C)	109.5
H(44A)–C(44)–H(44C)	109.5
H(44B)–C(44)–H(44C)	109.5
O(3)–C(45)–C(46)	109.4(3)
O(3)–C(45)–H(45A)	109.8
C(46)–C(45)–H(45A)	109.8
O(3)–C(45)–H(45B)	109.8
C(46)–C(45)–H(45B)	109.8
H(45A)–C(45)–H(45B)	108.2
C(45)–C(46)–C(47)	114.0(3)
C(45)–C(46)–H(46A)	108.8
C(47)–C(46)–H(46A)	108.8
C(45)–C(46)–H(46B)	108.8
C(47)–C(46)–H(46B)	108.8
H(46A)–C(46)–H(46B)	107.6
C(46)–C(47)–H(47A)	109.5
C(46)–C(47)–H(47B)	109.5
H(47A)–C(47)–H(47B)	109.5
C(46)–C(47)–H(47C)	109.5

H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(49)-C(48)-O(4)	125.3(4)
C(49)-C(48)-H(48A)	106.0
O(4)-C(48)-H(48A)	106.0
C(49)-C(48)-H(48B)	106.0
O(4)-C(48)-H(48B)	106.0
H(48A)-C(48)-H(48B)	106.3
C(48)-C(49)-C(50)	119.9(5)
C(48)-C(49)-H(49A)	107.3
C(50)-C(49)-H(49A)	107.3
C(48)-C(49)-H(49B)	107.3
C(50)-C(49)-H(49B)	107.3
H(49A)-C(49)-H(49B)	106.9
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
O(5)-C(51)-C(52)	105.1(3)
O(5)-C(51)-H(51A)	110.7
C(52)-C(51)-H(51A)	110.7
O(5)-C(51)-H(51B)	110.7
C(52)-C(51)-H(51B)	110.7
H(51A)-C(51)-H(51B)	108.8
C(53)-C(52)-C(51)	106.6(5)
C(53)-C(52)-H(52A)	110.4
C(51)-C(52)-H(52A)	110.4
C(53)-C(52)-H(52B)	110.4
C(51)-C(52)-H(52B)	110.4
H(52A)-C(52)-H(52B)	108.6
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(12)-O(1)-C(13)	116.9(3)
C(17)-O(2)-C(42)	112.7(3)
C(22)-O(3)-C(45)	111.8(2)
C(29)-O(4)-C(48)	121.0(3)
C(36)-O(5)-C(51)	112.8(2)
C(7)-P-C(14)	107.91(14)
C(7)-P-C(1)	108.81(15)
C(14)-P-C(1)	106.37(14)
C(7)-P-B	110.55(19)
C(14)-P-B	112.23(19)
C(1)-P-B	110.81(17)
P-B-H(0A)	109.5
P-B-H(0B)	109.5
H(0A)-B-H(0B)	109.5
P-B-H(0C)	109.5
H(0A)-B-H(0C)	109.5
H(0B)-B-H(0C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for compound **11** (**etjug1**).

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(4)	55(2)	45(2)	26(2)	8(2)	-3(2)	11(2)
C(5)	55(2)	26(2)	39(2)	9(1)	2(2)	7(2)
C(6)	47(2)	27(2)	34(2)	5(1)	-2(2)	-3(1)
C(7)	48(2)	20(1)	29(2)	2(1)	-8(1)	1(1)
C(8)	55(2)	26(2)	43(2)	1(2)	-12(2)	7(2)
C(9)	72(3)	45(2)	35(2)	-15(2)	-17(2)	24(2)
C(10)	70(3)	50(2)	28(2)	-5(2)	0(2)	32(2)
C(11)	56(2)	32(2)	35(2)	5(2)	1(2)	14(2)
C(12)	49(2)	26(2)	27(2)	2(1)	-4(2)	5(1)
C(13)	47(3)	222(8)	119(5)	-117(6)	20(3)	-56(4)
C(14)	30(2)	30(1)	26(2)	7(1)	-7(1)	-4(1)
C(15)	33(2)	28(1)	22(1)	3(1)	-1(1)	-4(1)
C(16)	34(2)	24(1)	22(1)	4(1)	-4(1)	-4(1)
C(17)	32(2)	25(1)	26(2)	6(1)	-2(1)	1(1)
C(18)	29(2)	33(2)	27(2)	5(1)	1(1)	-2(1)
C(19)	32(2)	31(2)	28(2)	9(1)	-1(1)	-6(1)
C(20)	41(2)	25(1)	18(1)	2(1)	-2(1)	-4(1)
C(21)	36(2)	26(1)	17(1)	3(1)	4(1)	-2(1)
C(22)	28(2)	29(2)	15(1)	3(1)	3(1)	2(1)
C(23)	32(2)	25(1)	17(1)	1(1)	3(1)	-1(1)
C(24)	31(2)	36(2)	25(2)	0(1)	0(1)	-4(1)
C(25)	34(2)	37(2)	27(2)	2(1)	0(1)	6(1)
C(26)	37(2)	24(1)	26(2)	0(1)	3(1)	4(1)
C(27)	41(2)	28(1)	21(2)	1(1)	5(1)	-4(1)
C(28)	39(2)	25(1)	23(2)	0(1)	2(1)	1(1)
C(29)	39(2)	26(1)	24(2)	0(1)	0(1)	1(1)
C(30)	35(2)	27(1)	24(2)	1(1)	2(1)	9(1)
C(31)	46(2)	26(1)	20(2)	1(1)	1(1)	9(1)
C(32)	38(2)	23(1)	26(2)	-4(1)	-5(1)	7(1)
C(33)	35(2)	25(1)	26(2)	0(1)	3(1)	3(1)
C(34)	38(2)	33(2)	22(2)	1(1)	5(1)	6(1)
C(35)	33(2)	34(2)	19(1)	6(1)	7(1)	5(1)
C(36)	29(2)	37(2)	21(1)	9(1)	7(1)	6(1)
C(37)	35(2)	34(2)	22(2)	10(1)	5(1)	0(1)
C(38)	35(2)	31(2)	31(2)	7(1)	4(1)	6(1)
C(39)	33(2)	37(2)	30(2)	8(1)	2(1)	7(1)
C(40)	33(2)	37(2)	26(2)	3(1)	2(1)	2(1)
C(41)	38(2)	36(2)	30(2)	9(1)	4(1)	0(1)
C(42)	41(2)	41(2)	44(2)	14(2)	5(2)	8(2)
C(43)	46(2)	45(2)	50(2)	19(2)	-9(2)	-5(2)
C(44)	47(2)	56(2)	103(4)	46(3)	-20(3)	-11(2)
C(45)	47(2)	31(2)	17(1)	4(1)	0(1)	2(1)
C(46)	44(2)	34(2)	32(2)	7(1)	-7(2)	1(2)
C(47)	56(2)	43(2)	46(2)	4(2)	-6(2)	11(2)
C(48)	59(3)	118(4)	61(3)	-48(3)	-29(2)	42(3)
C(49)	144(5)	77(3)	88(4)	-46(3)	-77(4)	61(4)
C(50)	59(2)	53(2)	46(2)	10(2)	-7(2)	7(2)
C(51)	36(2)	118(4)	50(2)	34(3)	20(2)	27(2)
C(52)	90(4)	55(3)	103(4)	-22(3)	56(3)	-20(3)
C(53)	80(4)	76(4)	146(6)	-23(4)	56(4)	13(3)
O(1)	40(1)	45(1)	33(1)	-6(1)	1(1)	-7(1)

O(2)	41(1)	28(1)	30(1)	6(1)	3(1)	4(1)
O(3)	32(1)	29(1)	19(1)	6(1)	-1(1)	4(1)
O(4)	37(1)	40(1)	34(1)	1(1)	-6(1)	-5(1)
O(5)	31(1)	40(1)	30(1)	10(1)	7(1)	9(1)
P	40(1)	25(1)	30(1)	6(1)	-8(1)	-7(1)
B	45(2)	58(3)	50(3)	25(2)	-1(2)	-8(2)
Cl	33(1)	28(1)	28(1)	-1(1)	-6(1)	-1(1)
