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Figure 1: Expansion of the ^{1}H NMR spectrum of **13b** showing the signal of the BH_3-moiety a) without decoupling, and under b) continuous-wave ^{11}B decoupling; c) ^{11}B and selective ^{31}P decoupling at $\delta^{31}P = 217$, the remaining splitting was assigned to $^{2}J_{P\text{-}B\text{-}H} = 5.1$ Hz; d) ^{11}B and ^{31}P decoupling. Evaluation of the ^{183}W satellites in b) – d) gave $^{1}J_{WH} = 14$ Hz.

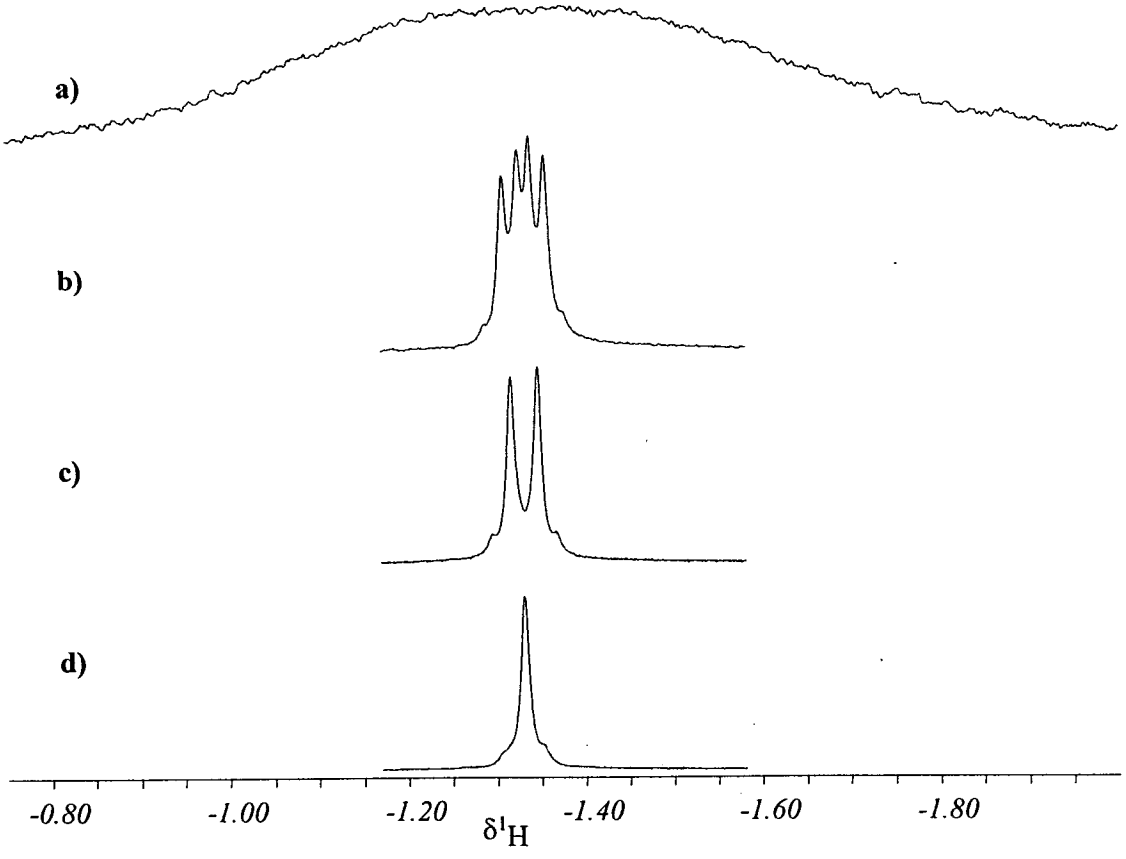


Table 1-6. Crystal data and structure refinement for **6**.

	6
Formula	$C_{43}H_{29}CrO_5P_3$ - CH_2Cl_2
Formula weight	855.50
Crystal size	0.35 x 0.15 x 0.02 mm
Crystal System, space group	Triclinic, P-1 (No.2)
Unit cell dimensions	a = 9.5017(2) Å
	b = 12.4747(2) Å
	c = 18.3005(4) Å
	α = 76.515(1)°
	β = 80.180(1)°
	γ = 74.624(1)°
Volume	2020.15(7) $Å^3$
Z, ρ_{calc}	2, 1.42 Mg/m^3
μ	0.58 mm^{-1}
$F(000)$	876
Theta range for data collection	2.95 to 25.32°
Completeness of data	96.8 %
Max. and min. transmission	
Limiting indices	$-11 \le h \le 11$,
	$-14 \le k \le 15$,
	$-21 \le l \le 22$
Reflections collected / unique	27049 / 7152 [R_{int} = 0.0372]
Absorption Correction	None
Data / restraints / parameters	7152 / 0 / 496
Goodness-of-fit on F^2	1.065
R1 [$I > 2\sigma(I)$]	0.037
wR2 R (all data)	0.010
Largest diff. peak and hole	0.352 and -0.391 e $Å^{-3}$

Table 2-6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr(1)	3558(1)	1183(1)	2680(1)	22(1)
C(1A)	3766(3)	107(2)	2107(2)	33(1)
O(1A)	3940(3)	-555(2)	1734(1)	52(1)
C(1B)	5013(3)	162(2)	3262(1)	27(1)
O(1B)	5877(2)	-487(2)	3600(1)	42(1)
C(1C)	1993(3)	2128(2)	2132(2)	29(1)
O(1C)	1019(3)	2597(2)	1802(1)	47(1)
C(1D)	5007(3)	1734(2)	1956(2)	28(1)
O(1D)	5916(2)	1978(2)	1496(1)	40(1)
C(1E)	2114(3)	524(2)	3340(2)	29(1)
O(1E)	1252(2)	64(2)	3701(1)	42(1)
P(1)	2998(1)	4484(1)	1995(1)	20(1)
C(2)	3290(3)	4028(2)	2939(1)	19(1)
C(3)	3454(3)	4931(2)	3267(1)	18(1)
C(4)	3702(3)	4894(2)	4015(1)	22(1)
C(5)	3853(3)	5853(2)	4211(1)	24(1)
C(6)	3757(3)	6877(2)	3684(1)	25(1)
C(7)	3498(3)	6945(2)	2956(1)	23(1)
C(8)	3339(3)	5972(2)	2734(1)	20(1)
C(9)	3089(3)	5863(2)	2002(1)	19(1)
P(2)	3519(1)	2578(1)	3409(1)	18(1)
C(10)	2161(3)	2550(2)	4250(1)	19(1)
C(11)	2209(3)	1540(2)	4790(1)	24(1)
C(12)	1173(3)	1497(2)	5419(1)	27(1)
C(13)	67(3)	2438(2)	5520(1)	29(1)
C(14)	-17(3)	3435(2)	4979(1)	28(1)
C(15)	1028(3)	3489(2)	4347(1)	22(1)
C(16)	5317(3)	2298(2)	3762(1)	20(1)
C(17)	5588(3)	1870(2)	4513(1)	25(1)
C(18)	7006(3)	1638(2)	4702(2)	33(1)
C(19)	8156(3)	1825(2)	4165(2)	37(1)
C(20)	7901(3)	2259(3)	3419(2)	37(1)
C(21)	6486(3)	2496(2)	3225(2)	31(1)
P(3)	2856(1)	6967(1)	1225(1)	21(1)
C(22)	4520(3)	7461(2)	883(1)	23(1)
C(23)	5694(3)	7076(2)	1320(1)	27(1)
C(24)	6935(3)	7491(2)	1095(2)	39(1)
C(25)	7047(4)	8271(3)	427(2)	43(1)
C(26)	5939(4)	8616(2)	-22(2)	39(1)
C(27)	4663(3)	8218(2)	202(1)	31(1)
C(28)	1380(3)	8131(2)	1465(1)	26(1)
C(29)	376(3)	7915(3)	2095(2)	37(1)
C(30)	-786(4)	8780(3)	2302(2)	50(1)
C(31)	-918(4)	9864(3)	1893(2)	62(1)
C(32)	57(5)	10095(3)	1251(2)	68(1)
C(33)	1199(4)	9228(2)	1040(2)	49(1)
C(34)	2363(3)	6526(2)	453(1)	23(1)
C(35)	889(3)	6617(2)	403(2)	34(1)
C(36)	489(4)	6282(3)	-187(2)	44(1)
C(37)	1568(4)	5848(3)	-723(2)	41(1)
C(38)	3014(4)	5757(2)	-682(2)	34(1)
C(39)	3423(3)	6099(2)	-90(1)	30(1)
C(1)	7464(4)	5230(3)	3366(2)	44(1)

Cl(1)	7751(1)	6234(1)	3824(1)	59(1)
Cl(2)	8781(1)	5048(1)	2576(1)	57(1)

Table 3-6. Bond lengths [A] and angles [deg] for **6**.

Cr(1)-C(1A)	1.840(3)
Cr(1)-C(1D)	1.892(3)
Cr(1)-C(1E)	1.893(3)
Cr(1)-C(1B)	1.899(3)
Cr(1)-C(1C)	1.906(3)
Cr(1)-P(2)	2.4170(7)
C(1A)-O(1A)	1.151(3)
C(1B)-O(1B)	1.140(3)
C(1C)-O(1C)	1.142(3)
C(1D)-O(1D)	1.148(3)
C(1E)-O(1E)	1.151(3)
P(1)-C(2)	1.734(2)
P(1)-C(9)	1.748(2)
C(2)-C(3)	1.446(3)
C(2)-P(2)	1.786(2)
C(3)-C(4)	1.417(3)
C(3)-C(8)	1.421(3)
C(4)-C(5)	1.375(3)
C(5)-C(6)	1.401(3)
C(6)-C(7)	1.374(3)
C(7)-C(8)	1.418(3)
C(8)-C(9)	1.443(3)
C(9)-P(3)	1.732(2)
P(2)-C(10)	1.832(2)
P(2)-C(16)	1.847(3)
C(10)-C(15)	1.388(4)
C(10)-C(11)	1.404(3)
C(11)-C(12)	1.383(4)
C(12)-C(13)	1.376(4)
C(13)-C(14)	1.390(4)
C(14)-C(15)	1.391(4)
C(16)-C(21)	1.387(4)
C(16)-C(17)	1.394(3)
C(17)-C(18)	1.387(4)
C(18)-C(19)	1.370(4)
C(19)-C(20)	1.384(4)
C(20)-C(21)	1.387(4)
P(3)-C(34)	1.801(2)
P(3)-C(22)	1.809(3)
P(3)-C(28)	1.810(3)
C(22)-C(27)	1.388(3)
C(22)-C(23)	1.398(4)
C(23)-C(24)	1.374(4)
C(24)-C(25)	1.380(4)
C(25)-C(26)	1.364(4)
C(26)-C(27)	1.392(4)
C(28)-C(29)	1.389(4)
C(28)-C(33)	1.390(4)
C(29)-C(30)	1.394(4)
C(30)-C(31)	1.370(5)
C(31)-C(32)	1.390(5)
C(32)-C(33)	1.388(5)
C(34)-C(39)	1.380(4)
C(34)-C(35)	1.392(4)
C(35)-C(36)	1.384(4)
C(36)-C(37)	1.384(4)
C(37)-C(38)	1.362(4)
C(38)-C(39)	1.398(4)
C(1)-Cl(1)	1.758(3)
C(1)-Cl(2)	1.759(3)
C(1A)-Cr(1)-C(1D)	86.03(11)
C(1A)-Cr(1)-C(1E)	88.01(11)
C(1D)-Cr(1)-C(1E)	174.02(11)
C(1A)-Cr(1)-C(1B)	88.80(12)
C(1D)-Cr(1)-C(1B)	91.51(12)
C(1E)-Cr(1)-C(1B)	88.90(11)
C(1A)-Cr(1)-C(1C)	89.60(12)
C(1D)-Cr(1)-C(1C)	92.73(11)
C(1E)-Cr(1)-C(1C)	86.68(11)
C(1B)-Cr(1)-C(1C)	175.35(11)
C(1A)-Cr(1)-P(2)	174.89(10)
C(1D)-Cr(1)-P(2)	89.95(8)
C(1E)-Cr(1)-P(2)	96.03(8)
C(1B)-Cr(1)-P(2)	88.16(8)
C(1C)-Cr(1)-P(2)	93.74(8)
O(1A)-C(1A)-Cr(1)	177.6(3)
O(1B)-C(1B)-Cr(1)	177.1(2)
O(1C)-C(1C)-Cr(1)	173.2(2)
O(1D)-C(1D)-Cr(1)	173.9(2)
O(1E)-C(1E)-Cr(1)	174.5(2)
C(2)-P(1)-C(9)	91.93(11)
C(3)-C(2)-P(1)	112.19(16)
C(3)-C(2)-P(2)	124.95(17)
P(1)-C(2)-P(2)	122.63(13)
C(4)-C(3)-C(8)	119.0(2)
C(4)-C(3)-C(2)	129.0(2)
C(8)-C(3)-C(2)	112.0(2)
C(5)-C(4)-C(3)	119.9(2)
C(4)-C(5)-C(6)	121.2(2)
C(7)-C(6)-C(5)	120.5(2)
C(6)-C(7)-C(8)	119.9(2)
C(7)-C(8)-C(3)	119.6(2)
C(7)-C(8)-C(9)	128.4(2)
C(3)-C(8)-C(9)	112.00(19)
C(8)-C(9)-P(3)	124.54(17)
C(8)-C(9)-P(1)	111.87(17)
P(3)-C(9)-P(1)	123.57(13)
C(2)-P(2)-C(10)	106.58(11)
C(2)-P(2)-C(16)	101.40(11)
C(10)-P(2)-C(16)	105.74(11)
C(2)-P(2)-Cr(1)	118.54(8)
C(10)-P(2)-Cr(1)	113.37(7)
C(16)-P(2)-Cr(1)	109.89(8)
C(15)-C(10)-C(11)	118.8(2)

C(15)-C(10)-P(2)	121.51(18)
C(11)-C(10)-P(2)	119.6(2)
C(12)-C(11)-C(10)	120.4(3)
C(13)-C(12)-C(11)	120.5(2)
C(12)-C(13)-C(14)	119.7(2)
C(13)-C(14)-C(15)	120.2(3)
C(10)-C(15)-C(14)	120.4(2)
C(21)-C(16)-C(17)	118.3(2)
C(21)-C(16)-P(2)	116.40(18)
C(17)-C(16)-P(2)	125.2(2)
C(18)-C(17)-C(16)	119.9(3)
C(19)-C(18)-C(17)	121.3(3)
C(18)-C(19)-C(20)	119.5(3)
C(19)-C(20)-C(21)	119.6(3)
C(20)-C(21)-C(16)	121.4(3)
C(9)-P(3)-C(34)	110.93(11)
C(9)-P(3)-C(22)	111.82(12)
C(34)-P(3)-C(22)	107.09(12)
C(9)-P(3)-C(28)	109.95(12)
C(34)-P(3)-C(28)	107.31(12)
C(22)-P(3)-C(28)	109.59(11)
C(27)-C(22)-C(23)	119.0(2)
C(27)-C(22)-P(3)	121.9(2)
C(23)-C(22)-P(3)	119.11(18)

C(24)-C(23)-C(22)	120.2(2)
C(23)-C(24)-C(25)	120.3(3)
C(26)-C(25)-C(24)	120.2(3)
C(25)-C(26)-C(27)	120.3(3)
C(22)-C(27)-C(26)	119.9(3)
C(29)-C(28)-C(33)	118.6(3)
C(29)-C(28)-P(3)	118.6(2)
C(33)-C(28)-P(3)	122.8(2)
C(28)-C(29)-C(30)	120.9(3)
C(31)-C(30)-C(29)	119.7(3)
C(30)-C(31)-C(32)	120.4(3)
C(33)-C(32)-C(31)	119.7(3)
C(32)-C(33)-C(28)	120.7(3)
C(39)-C(34)-C(35)	119.5(2)
C(39)-C(34)-P(3)	121.0(2)
C(35)-C(34)-P(3)	119.5(2)
C(36)-C(35)-C(34)	120.3(3)
C(37)-C(36)-C(35)	119.4(3)
C(38)-C(37)-C(36)	120.9(3)
C(37)-C(38)-C(39)	119.9(3)
C(34)-C(39)-C(38)	120.0(3)
Cl(1)-C(1)-Cl(2)	111.04(17)

Table 4-6. Anisotropic displacement parameters (A^2 x 10^3) for **6**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr(1)	28(1)	19(1)	20(1)	-2(1)	-5(1)	-6(1)
C(1A)	51(2)	24(2)	25(1)	-1(1)	-2(1)	-13(2)
O(1A)	93(2)	28(1)	38(1)	-9(1)	-8(1)	-18(1)
C(1B)	33(2)	24(1)	25(1)	-5(1)	0(1)	-8(1)
O(1B)	43(1)	33(1)	43(1)	1(1)	-16(1)	4(1)
C(1C)	36(2)	25(2)	29(2)	-4(1)	-7(1)	-14(1)
O(1C)	48(2)	39(1)	55(1)	3(1)	-30(1)	-11(1)
C(1D)	37(2)	22(1)	24(1)	-3(1)	-8(1)	-3(1)
O(1D)	44(1)	43(1)	29(1)	-2(1)	7(1)	-13(1)
C(1E)	33(2)	24(1)	30(2)	-3(1)	-11(1)	-3(1)
O(1E)	38(1)	40(1)	48(1)	3(1)	-2(1)	-20(1)
P(1)	26(1)	17(1)	17(1)	-1(1)	-4(1)	-6(1)
C(2)	21(2)	17(1)	18(1)	-1(1)	-2(1)	-4(1)
C(3)	16(2)	19(1)	20(1)	-3(1)	0(1)	-4(1)
C(4)	22(2)	23(1)	18(1)	-2(1)	-1(1)	-4(1)
C(5)	25(2)	31(2)	18(1)	-7(1)	-4(1)	-6(1)
C(6)	27(2)	22(1)	30(2)	-13(1)	-3(1)	-6(1)
C(7)	25(2)	18(1)	26(1)	-3(1)	-1(1)	-6(1)
C(8)	18(2)	19(1)	21(1)	-4(1)	0(1)	-3(1)
C(9)	21(2)	18(1)	17(1)	-2(1)	0(1)	-6(1)
P(2)	20(1)	17(1)	16(1)	0(1)	-3(1)	-5(1)
C(10)	22(2)	21(1)	17(1)	-3(1)	-3(1)	-9(1)
C(11)	26(2)	24(1)	22(1)	-2(1)	-6(1)	-8(1)
C(12)	30(2)	33(2)	20(1)	4(1)	-5(1)	-16(1)
C(13)	26(2)	48(2)	21(1)	-9(1)	3(1)	-21(2)
C(14)	19(2)	32(2)	34(2)	-14(1)	-1(1)	-5(1)
C(15)	22(2)	25(1)	20(1)	-4(1)	-4(1)	-8(1)
C(16)	22(2)	16(1)	24(1)	-4(1)	-6(1)	-4(1)

C(17)	29(2)	22(1)	26(1)	-6(1)	-6(1)	-5(1)
C(18)	38(2)	30(2)	32(2)	-11(1)	-19(2)	1(1)
C(19)	26(2)	36(2)	55(2)	-21(2)	-17(2)	0(1)
C(20)	24(2)	46(2)	45(2)	-14(2)	-2(1)	-11(2)
C(21)	29(2)	34(2)	30(2)	-4(1)	-6(1)	-9(1)
P(3)	25(1)	17(1)	18(1)	-1(1)	-3(1)	-5(1)
C(22)	29(2)	19(1)	22(1)	-5(1)	1(1)	-9(1)
C(23)	28(2)	26(1)	25(1)	-2(1)	0(1)	-7(1)
C(24)	32(2)	42(2)	42(2)	-2(1)	-5(2)	-12(2)
C(25)	34(2)	42(2)	50(2)	0(2)	4(2)	-17(2)
C(26)	49(2)	34(2)	31(2)	5(1)	5(2)	-19(2)
C(27)	41(2)	25(1)	26(2)	-2(1)	-3(1)	-8(1)
C(28)	26(2)	23(1)	28(2)	-5(1)	-6(1)	-2(1)
C(29)	35(2)	37(2)	32(2)	-5(1)	-5(1)	4(2)
C(30)	38(2)	61(2)	39(2)	-14(2)	4(2)	8(2)
C(31)	48(3)	48(2)	79(3)	-27(2)	0(2)	16(2)
C(32)	57(3)	24(2)	101(3)	1(2)	2(2)	7(2)
C(33)	44(2)	27(2)	61(2)	2(2)	9(2)	1(2)
C(34)	30(2)	17(1)	19(1)	2(1)	-5(1)	-5(1)
C(35)	31(2)	44(2)	32(2)	-14(1)	-4(1)	-9(2)
C(36)	34(2)	55(2)	47(2)	-15(2)	-14(2)	-9(2)
C(37)	56(2)	39(2)	33(2)	-10(1)	-19(2)	-9(2)
C(38)	42(2)	32(2)	29(2)	-13(1)	-1(1)	-6(2)
C(39)	33(2)	27(2)	29(2)	-5(1)	-4(1)	-6(1)
C(1)	39(2)	53(2)	46(2)	-19(2)	-3(2)	-12(2)
Cl(1)	70(1)	67(1)	53(1)	-23(1)	-9(1)	-29(1)
Cl(2)	60(1)	61(1)	43(1)	-11(1)	8(1)	-9(1)

Table 5-6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6**.

	x	y	z	U(eq)
H(4)	3764	4209	4381	26
H(5)	4026	5822	4713	29
H(6)	3871	7528	3830	30
H(7)	3426	7643	2602	28
H(11)	2958	882	4722	29
H(12)	1224	813	5786	33
H(13)	-636	2405	5956	35
H(14)	-790	4081	5042	33
H(15)	965	4173	3980	26
H(17)	4804	1738	4893	31
H(18)	7182	1344	5215	39
H(19)	9121	1659	4304	44
H(20)	8690	2392	3042	44
H(21)	6315	2802	2713	37
H(23)	5633	6526	1774	33
H(24)	7720	7241	1400	47
H(25)	7899	8568	280	52
H(26)	6038	9130	-490	47
H(27)	3891	8465	-111	37
H(29)	483	7168	2389	45
H(30)	-1483	8618	2725	60
H(31)	-1680	10461	2048	74
H(32)	-59	10843	958	81
H(33)	1864	9386	601	59
H(35)	154	6910	775	41

H(36)	-518	6350	-223	52
H(37)	1295	5611	-1125	49
H(38)	3743	5461	-1055	41
H(39)	4431	6037	-61	36
H(1A)	6468	5486	3201	53
H(1B)	7521	4495	3725	53

Table 6-6. Hydrogen bonds for **6** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(7)-H(7)...O(1A)#1	0.95	2.54	3.467(3)	164.4
C(26)-H(26)...O(1A)#2	0.95	2.54	3.489(3)	175.0
Symmetry transformations use	d to generat	e equivalent	atoms:	
#1 x,y+1,z #2 -x+1,-y+1,-	z			

Table 1-10a. Crystal data and structure refinement for **10a**.

	10a
Formula	$C_{46}H_{37}CrO_5P_3S$
Formula weight	846.73
Crystal size	0.18 x 0.05 x 0.02 mm
Crystal System, space group	Monoclinic, P21/c
Unit cell dimensions	a = 10.9086(2) Å
	b = 22.0459(5) Å
	c = 17.3373(3) Å
	β = 101.930(2)°
Volume	4079.39(14) Å^3
Z, ρ_{calc}	4, 1.38 Mg/m^3
μ	0.50 mm^{-1}
F(000)	1752
Theta range for data collection	3.67 to 25.03°
Completeness of data	
Max. and min. transmission	1.035 and 0.973
Limiting indices	$-12 \le h \le 12$,
	$-26 \le k \le 26$,
	$-20 \le l \le 19$
Reflections collected / unique	41298 / 7154 [R_{int} = 0.0770]
Absorption Correction	Multi-scan
Data / restraints / parameters	7148 / 0 / 592
Goodness-of-fit on F^2	1.080
R1 [I > 2σ(I)]	0.048
wR2 R (all data)	0.117
Largest diff. peak and hole	0.574 and -0.418 e Å^{-3}

Table 2-10a. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr	8973(1)	3176(1)	7772(1)	32(1)
P(1)	7328(1)	3832(1)	7277(1)	27(1)
C(1)	5916(3)	3734(1)	7547(2)	26(1)
C(2)	5175(3)	4285(1)	7423(2)	26(1)
C(3)	5799(3)	4760(1)	7091(2)	23(1)
C(4)	7006(3)	4567(1)	6950(2)	25(1)
C(5)	3985(3)	4396(2)	7586(2)	34(1)
C(6)	3422(4)	4949(2)	7428(2)	40(1)
C(7)	4019(4)	5410(2)	7097(2)	41(1)
C(8)	5182(3)	5321(2)	6927(2)	33(1)
P(2)	5671(1)	3013(1)	7921(1)	28(1)
C(9)	5375(3)	3052(1)	8912(2)	31(1)
C(10)	6351(4)	2959(2)	9563(3)	47(1)
C(11)	6114(5)	2997(2)	10324(3)	60(1)
C(12)	4934(5)	3132(2)	10434(3)	58(1)
C(13)	3974(5)	3226(2)	9797(3)	54(1)
C(14)	4182(4)	3184(2)	9035(2)	39(1)
C(15)	4298(3)	2646(1)	7353(2)	29(1)
C(16)	4091(4)	2038(2)	7481(2)	40(1)
C(17)	3063(4)	1738(2)	7043(3)	48(1)
C(18)	2226(4)	2044(2)	6476(3)	48(1)
C(19)	2417(4)	2650(2)	6344(3)	55(1)
C(20)	3444(4)	2949(2)	6777(3)	44(1)
S	7186(1)	2494(1)	7893(1)	40(1)
P(3)	8060(1)	4975(1)	6512(1)	26(1)
C(21)	8794(3)	4458(2)	5934(2)	35(1)
C(22)	10079(4)	4468(2)	5965(3)	49(1)
C(23)	10599(5)	4077(2)	5493(3)	65(2)
C(24)	9854(6)	3692(3)	4990(3)	71(2)
C(25)	8579(6)	3672(2)	4945(3)	61(1)
C(26)	8051(4)	4057(2)	5424(2)	46(1)
C(27)	9221(3)	5370(2)	7224(2)	32(1)
C(28)	10102(4)	5749(2)	6985(3)	48(1)
C(29)	10898(4)	6096(2)	7541(4)	64(2)
C(30)	10803(5)	6071(2)	8316(4)	69(2)
C(31)	9946(5)	5706(2)	8561(3)	61(1)
C(32)	9150(4)	5352(2)	8006(2)	41(1)
C(33)	7250(3)	5554(1)	5855(2)	27(1)
C(34)	6447(4)	5397(2)	5155(2)	40(1)
C(35)	5734(4)	5838(2)	4699(2)	48(1)
C(36)	5823(4)	6432(2)	4934(2)	45(1)
C(37)	6630(4)	6597(2)	5615(2)	40(1)
C(38)	7341(3)	6162(2)	6079(2)	32(1)
C(39)	9040(4)	2811(2)	6789(3)	42(1)
O(1)	9143(3)	2577(1)	6214(2)	64(1)
C(40)	10275(3)	3669(2)	7679(2)	42(1)
O(2)	11155(3)	3971(2)	7672(2)	64(1)
C(41)	10131(4)	2622(2)	8277(3)	50(1)
O(3)	10899(3)	2298(2)	8600(2)	83(1)
C(42)	9045(4)	3530(2)	8768(3)	48(1)
O(4)	9173(4)	3744(2)	9387(2)	84(1)
O(5)	2481(4)	4405(2)	10506(3)	88(1)

C(43)	3641(6)	4674(3)	10868(3)	90(2)
C(44)	3650(7)	5272(3)	10563(5)	114(2)
C(45)	2948(7)	5245(4)	9783(5)	128(3)
C(46)	2133(8)	4673(3)	9752(4)	137(4)

Table 3-10a. Selected bond lengths [A] and angles [deg] for **10a**.

Cr-C(40)	1.821(4)
Cr-C(41)	1.844(4)
Cr-C(42)	1.882(5)
Cr-C(39)	1.899(5)
Cr-P(1)	2.3262(10)
Cr-S	2.5056(10)
P(1)-C(1)	1.714(3)
P(1)-C(4)	1.729(3)
C(1)-C(2)	1.450(4)
C(1)-P(2)	1.758(3)
C(2)-C(5)	1.406(5)
C(2)-C(3)	1.432(4)
C(3)-C(8)	1.410(4)
C(3)-C(4)	1.451(4)
C(4)-P(3)	1.751(3)
C(5)-C(6)	1.367(5)
C(6)-C(7)	1.393(5)
C(7)-C(8)	1.374(5)
P(2)-C(15)	1.805(3)
P(2)-C(9)	1.815(4)
P(2)-S	2.0184(12)
C(9)-C(14)	1.391(5)
C(9)-C(10)	1.397(5)
C(10)-C(11)	1.399(6)
C(11)-C(12)	1.373(7)
C(12)-C(13)	1.371(7)
C(13)-C(14)	1.390(6)
C(15)-C(16)	1.384(5)
C(15)-C(20)	1.388(5)
C(16)-C(17)	1.385(6)
C(17)-C(18)	1.372(6)
C(18)-C(19)	1.378(6)
C(19)-C(20)	1.381(6)
P(3)-C(27)	1.800(3)
P(3)-C(21)	1.810(3)
P(3)-C(33)	1.815(3)
C(21)-C(26)	1.387(6)
C(21)-C(22)	1.392(5)
C(22)-C(23)	1.387(6)
C(23)-C(24)	1.360(8)
C(24)-C(25)	1.377(8)
C(25)-C(26)	1.392(6)
C(27)-C(32)	1.376(5)
C(27)-C(28)	1.399(5)
C(28)-C(29)	1.387(7)
C(29)-C(30)	1.370(8)
C(30)-C(31)	1.366(8)
C(31)-C(32)	1.393(6)
C(33)-C(34)	1.385(5)
C(33)-C(38)	1.395(5)

C(34)-C(35)	1.386(5)
C(35)-C(36)	1.368(6)
C(36)-C(37)	1.370(5)
C(37)-C(38)	1.382(5)
C(39)-O(1)	1.149(5)
C(40)-O(2)	1.171(4)
C(41)-O(3)	1.153(5)
C(42)-O(4)	1.155(5)
O(5)-C(46)	1.412(8)
O(5)-C(43)	1.421(7)
C(43)-C(44)	1.422(8)
C(44)-C(45)	1.410(9)
C(45)-C(46)	1.537(10)
C(40)-Cr-C(41)	88.1(2)
C(40)-Cr-C(42)	87.0(2)
C(41)-Cr-C(42)	86.8(2)
C(40)-Cr-C(39)	89.9(2)
C(41)-Cr-C(39)	89.7(2)
C(42)-Cr-C(39)	175.5(2)
C(40)-Cr-P(1)	98.83(12)
C(41)-Cr-P(1)	171.04(14)
C(42)-Cr-P(1)	87.89(13)
C(39)-Cr-P(1)	95.91(12)
C(40)-Cr-S	179.65(12)
C(41)-Cr-S	91.75(13)
C(42)-Cr-S	93.27(13)
C(39)-Cr-S	89.77(12)
P(1)-Cr-S	81.36(3)
C(1)-P(1)-C(4)	94.3(2)
C(1)-P(1)-Cr	119.32(11)
C(4)-P(1)-Cr	142.40(11)
C(2)-C(1)-P(1)	111.0(2)
C(2)-C(1)-P(2)	133.6(2)
P(1)-C(1)-P(2)	115.3(2)
C(5)-C(2)-C(3)	119.3(3)
C(5)-C(2)-C(1)	128.6(3)
C(3)-C(2)-C(1)	112.0(3)
C(8)-C(3)-C(2)	118.4(3)
C(8)-C(3)-C(4)	129.4(3)
C(2)-C(3)-C(4)	112.2(3)
C(3)-C(4)-P(1)	110.4(2)
C(3)-C(4)-P(3)	128.6(2)
P(1)-C(4)-P(3)	121.1(2)
C(6)-C(5)-C(2)	120.6(3)
C(5)-C(6)-C(7)	120.3(3)
C(8)-C(7)-C(6)	121.0(3)
C(7)-C(8)-C(3)	120.4(3)
C(1)-P(2)-C(15)	112.1(2)
C(1)-P(2)-C(9)	112.1(2)

C(15)-P(2)-C(9)	104.3(2)
C(1)-P(2)-S	108.47(11)
C(15)-P(2)-S	108.92(11)
C(9)-P(2)-S	110.91(12)
C(14)-C(9)-C(10)	119.2(4)
C(14)-C(9)-P(2)	120.6(3)
C(10)-C(9)-P(2)	120.1(3)
C(9)-C(10)-C(11)	119.6(4)
C(12)-C(11)-C(10)	120.4(5)
C(13)-C(12)-C(11)	120.2(4)
C(12)-C(13)-C(14)	120.6(4)
C(13)-C(14)-C(9)	120.0(4)
C(16)-C(15)-C(20)	118.3(3)
C(16)-C(15)-P(2)	119.4(3)
C(20)-C(15)-P(2)	122.3(3)
C(15)-C(16)-C(17)	121.0(4)
C(18)-C(17)-C(16)	120.1(4)
C(17)-C(18)-C(19)	119.6(4)
C(18)-C(19)-C(20)	120.4(4)
C(19)-C(20)-C(15)	120.6(4)
P(2)-S-Cr	108.45(4)
C(4)-P(3)-C(27)	112.6(2)
C(4)-P(3)-C(21)	108.8(2)
C(27)-P(3)-C(21)	110.8(2)
C(4)-P(3)-C(33)	110.8(2)
C(27)-P(3)-C(33)	105.8(2)
C(21)-P(3)-C(33)	108.0(2)
C(26)-C(21)-C(22)	119.1(4)
C(26)-C(21)-P(3)	119.2(3)
C(22)-C(21)-P(3)	121.7(3)
C(23)-C(22)-C(21)	119.9(5)
C(24)-C(23)-C(22)	120.2(5)
C(23)-C(24)-C(25)	121.2(5)
C(24)-C(25)-C(26)	119.0(5)
C(21)-C(26)-C(25)	120.6(5)
C(32)-C(27)-C(28)	119.4(4)
C(32)-C(27)-P(3)	119.1(3)
C(28)-C(27)-P(3)	121.1(3)
C(29)-C(28)-C(27)	119.6(5)
C(30)-C(29)-C(28)	119.7(5)
C(31)-C(30)-C(29)	121.6(4)
C(30)-C(31)-C(32)	119.0(5)
C(27)-C(32)-C(31)	120.6(4)
C(34)-C(33)-C(38)	118.6(3)
C(34)-C(33)-P(3)	120.8(3)
C(38)-C(33)-P(3)	120.3(3)
C(33)-C(34)-C(35)	120.3(4)
C(36)-C(35)-C(34)	120.3(4)
C(35)-C(36)-C(37)	120.3(4)
C(36)-C(37)-C(38)	120.0(4)
C(37)-C(38)-C(33)	120.4(3)
O(1)-C(39)-Cr	176.3(4)
O(2)-C(40)-Cr	175.3(3)
O(3)-C(41)-Cr	176.5(4)
O(4)-C(42)-Cr	175.5(4)
C(46)-O(5)-C(43)	106.2(5)
O(5)-C(43)-C(44)	107.2(5)
C(45)-C(44)-C(43)	105.8(6)
C(44)-C(45)-C(46)	105.3(6)
O(5)-C(46)-C(45)	105.5(5)

Table 4-10a. Anisotropic displacement parameters (A^2 x 10^3) for **10a**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr	24(1)	27(1)	46(1)	8(1)	11(1)	4(1)
P(1)	23(1)	22(1)	39(1)	4(1)	11(1)	1(1)
C(1)	24(2)	21(2)	36(2)	1(1)	12(1)	-2(1)
C(2)	24(2)	21(2)	33(2)	-1(1)	6(1)	0(1)
C(3)	20(2)	20(2)	29(2)	-3(1)	7(1)	-1(1)
C(4)	25(2)	19(2)	32(2)	-1(1)	9(1)	-3(1)
C(5)	29(2)	30(2)	47(2)	4(2)	15(2)	-1(2)
C(6)	27(2)	33(2)	66(3)	6(2)	21(2)	5(2)
C(7)	34(2)	27(2)	63(3)	9(2)	16(2)	11(2)
C(8)	31(2)	22(2)	47(2)	4(2)	15(2)	1(1)
P(2)	26(1)	21(1)	39(1)	3(1)	12(1)	0(1)
C(9)	36(2)	19(2)	40(2)	2(1)	12(2)	-5(1)
C(10)	45(2)	45(2)	51(3)	8(2)	10(2)	-7(2)
C(11)	74(4)	62(3)	40(3)	6(2)	2(2)	-17(3)
C(12)	93(4)	46(3)	42(3)	-2(2)	27(3)	-8(2)
C(13)	73(3)	36(2)	63(3)	2(2)	40(3)	5(2)
C(14)	46(2)	30(2)	45(2)	4(2)	21(2)	2(2)
C(15)	32(2)	25(2)	34(2)	0(1)	16(2)	-4(1)
C(16)	50(3)	30(2)	40(2)	5(2)	9(2)	-8(2)
C(17)	60(3)	33(2)	53(3)	2(2)	16(2)	-19(2)
C(18)	41(2)	48(2)	56(3)	-6(2)	8(2)	-15(2)
C(19)	45(3)	42(2)	69(3)	5(2)	-7(2)	-3(2)
C(20)	40(2)	29(2)	59(3)	2(2)	3(2)	-5(2)
S	33(1)	24(1)	69(1)	9(1)	22(1)	5(1)
P(3)	24(1)	23(1)	32(1)	2(1)	9(1)	-2(1)
C(21)	40(2)	31(2)	39(2)	10(2)	21(2)	6(2)
C(22)	47(3)	50(2)	57(3)	21(2)	31(2)	12(2)
C(23)	68(3)	64(3)	77(4)	25(3)	49(3)	28(3)
C(24)	106(5)	62(3)	62(3)	19(3)	58(3)	40(3)
C(25)	100(4)	39(2)	48(3)	-1(2)	29(3)	13(3)
C(26)	58(3)	37(2)	48(3)	-3(2)	20(2)	7(2)
C(27)	24(2)	24(2)	46(2)	6(2)	0(2)	-3(1)
C(28)	32(2)	38(2)	69(3)	15(2)	1(2)	-5(2)
C(29)	35(3)	33(2)	113(5)	13(3)	-10(3)	-11(2)
C(30)	56(3)	33(2)	98(5)	-10(2)	-32(3)	-6(2)
C(31)	69(3)	45(3)	56(3)	-12(2)	-14(2)	4(2)
C(32)	41(2)	33(2)	44(2)	-1(2)	-2(2)	-2(2)
C(33)	28(2)	25(2)	30(2)	2(1)	9(1)	-3(1)
C(34)	45(2)	32(2)	38(2)	0(2)	0(2)	-7(2)
C(35)	49(3)	48(2)	40(2)	3(2)	-10(2)	-7(2)
C(36)	44(2)	37(2)	49(3)	15(2)	-3(2)	0(2)
C(37)	40(2)	25(2)	52(3)	2(2)	4(2)	1(2)
C(38)	32(2)	29(2)	35(2)	1(2)	4(2)	-2(2)
C(39)	35(2)	35(2)	58(3)	9(2)	16(2)	6(2)
O(1)	81(2)	54(2)	65(2)	-5(2)	30(2)	7(2)
C(40)	29(2)	44(2)	52(3)	11(2)	9(2)	6(2)
O(2)	34(2)	72(2)	86(2)	16(2)	11(2)	-18(2)
C(41)	39(2)	43(2)	66(3)	10(2)	11(2)	3(2)
O(3)	59(2)	60(2)	120(3)	33(2)	-7(2)	26(2)
C(42)	36(2)	48(2)	58(3)	4(2)	9(2)	-2(2)
O(4)	83(3)	105(3)	63(2)	-24(2)	12(2)	-19(2)
O(5)	85(3)	78(3)	100(3)	8(2)	15(2)	-10(2)

C(43)	112(5)	89(4)	65(4)	-4(3)	9(3)	-14(4)
C(44)	102(5)	70(4)	155(7)	-2(4)	-9(5)	16(4)
C(45)	98(6)	158(8)	121(6)	72(6)	9(5)	-4(5)
C(46)	164(8)	91(5)	110(6)	-13(4)	-77(5)	25(5)

Table 5-10a. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **10a**.

	x	y	z	U(eq)
H(5)	3588(35)	4079(17)	7800(22)	41
H(6)	2585(38)	5035(17)	7528(22)	48
H(7)	3652(38)	5760(19)	7015(23)	49
H(8)	5565(34)	5622(17)	6660(21)	39
H(10)	7098(42)	2842(19)	9456(25)	56
H(11)	6838(46)	2927(21)	10770(29)	72
H(12)	4695(43)	3155(20)	10981(29)	70
H(13)	3201(45)	3300(20)	9879(27)	64
H(14)	3531(38)	3239(17)	8573(24)	46
H(16)	4612(39)	1865(18)	7835(25)	48
H(17)	2960(39)	1311(21)	7123(24)	58
H(18)	1478(42)	1863(19)	6197(25)	58
H(19)	1853(44)	2835(21)	5954(27)	66
H(20)	3551(39)	3318(19)	6642(24)	52
H(22)	10649(40)	4778(20)	6336(25)	58
H(23)	11542(50)	4099(22)	5556(28)	78
H(24)	10175(50)	3448(24)	4675(31)	85
H(25)	8012(45)	3402(23)	4619(29)	73
H(26)	7220(42)	4027(19)	5386(25)	55
H(28)	10036(41)	5792(20)	6470(26)	57
H(29)	11443(48)	6303(24)	7397(30)	77
H(30)	11285(50)	6263(24)	8659(31)	83
H(31)	9887(45)	5676(22)	9097(30)	73
H(32)	8597(40)	5133(19)	8137(24)	49
H(34)	6378(37)	4997(19)	5012(23)	47
H(35)	5181(40)	5717(18)	4182(26)	58
H(36)	5306(39)	6738(19)	4610(24)	54
H(37)	6699(36)	7031(18)	5770(22)	48
H(38)	7835(35)	6276(17)	6551(22)	39
H(43A)	4333(6)	4441(3)	10749(3)	108
H(43B)	3723(6)	4686(3)	11436(3)	108
H(44A)	3272(7)	5554(3)	10874(5)	137
H(44B)	4501(7)	5403(3)	10568(5)	137
H(45A)	3498(7)	5214(4)	9411(5)	153
H(45B)	2430(7)	5603(4)	9660(5)	153
H(46A)	1251(8)	4779(3)	9640(4)	164
H(46B)	2290(8)	4397(3)	9348(4)	164

Table 1-10b. Crystal data and structure refinement for **10b**.

	10b
Formula	$C_{42}H_{29}O_4P_3SW$
Formula weight	906.47
Crystal size	0.30 x 0.10 x 0.05 mm
Crystal System, space group	Monoclinic, Cc (No.9)
Unit cell dimensions	a = 17.8938(5) Å
	b = 13.2188(3) Å
	c = 16.4646(4) Å
	β = 106.520(1)°
Volume	3733.69(16) Å^3
Z, ρ_{calc}	4, 1.61 Mg/m^3
μ	3.32 mm^{-1}
F(000)	1792
Theta range for data collection	2.58 to 25.00°
Completeness of data	
Max. and min. transmission	0.5444 and 0.4481
Limiting indices	$-21 \le h \le 21$,
	$-15 \le k \le 15$,
	$-19 \le l \le 19$
Reflections collected / unique	38503 / 6561 [R_{int} = 0.0878]
Absorption Correction	Empirical from multiple refl.
Data / restraints / parameters	6561 / 2 / 461
Goodness-of-fit on F^2	0.997
R1 [I > 2σ(I)]	0.034
wR2 R (all data)	0.073
Largest diff. peak and hole	0.662 and -1.424 e Å^{-3}

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Table 2-10b. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **10b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
W(1)	6297(1)	2584(1)	3507(1)	18(1)
C(1A)	6605(7)	2602(6)	2394(8)	27(3)
O(1A)	6823(8)	2622(5)	1821(7)	41(3)
C(1B)	5989(8)	2551(5)	4589(8)	29(4)
O(1B)	5776(8)	2498(4)	5206(8)	45(3)
C(1C)	7412(6)	2494(5)	4157(5)	26(2)
O(1C)	8054(3)	2412(4)	4505(4)	33(2)
C(1D)	6301(5)	1082(4)	3469(6)	25(1)
O(1D)	6320(5)	218(3)	3450(5)	38(1)
S(1)	4801(1)	2693(1)	2798(1)	22(1)
P(1)	6142(1)	4427(1)	3322(1)	19(1)
P(2)	7526(1)	5711(1)	4219(1)	19(1)
P(3)	4651(1)	3945(1)	2072(1)	18(1)
C(2)	6606(3)	5591(4)	3480(4)	16(1)
C(3)	6130(4)	6344(4)	2931(4)	18(1)
C(4)	6260(4)	7385(4)	2844(4)	24(2)
C(5)	5719(4)	7990(5)	2285(4)	24(2)
C(6)	5013(8)	7568(5)	1786(8)	21(3)
C(7)	4852(4)	6566(5)	1869(4)	21(2)
C(8)	5402(3)	5933(4)	2420(4)	18(1)
C(9)	5332(4)	4875(4)	2570(4)	18(1)
C(10)	7518(3)	5010(4)	5164(4)	19(1)
C(11)	6849(4)	5047(5)	5451(4)	25(2)
C(12)	6828(4)	4508(5)	6161(4)	30(2)
C(13)	7454(4)	3922(5)	6583(4)	29(2)
C(14)	8125(4)	3897(6)	6314(5)	30(2)
C(15)	8150(4)	4443(5)	5607(4)	25(2)
C(16)	7761(4)	7018(5)	4491(4)	20(1)
C(17)	8193(4)	7583(4)	4070(4)	28(2)
C(18)	8304(4)	8603(5)	4233(5)	32(2)
C(19)	7980(4)	9074(5)	4797(5)	38(2)
C(20)	7540(5)	8521(5)	5213(5)	37(2)
C(21)	7447(9)	7498(5)	5064(8)	30(3)
C(22)	8322(4)	5215(5)	3872(4)	21(2)
C(23)	8178(4)	4529(4)	3206(4)	23(2)
C(24)	8792(4)	4114(5)	2964(4)	30(2)
C(25)	9551(4)	4402(5)	3369(5)	35(2)
C(26)	9697(4)	5089(5)	4024(5)	33(2)
C(27)	9083(4)	5502(5)	4288(4)	24(2)
C(28)	3668(3)	4389(5)	1939(4)	20(1)
C(29)	3045(4)	3913(5)	1375(4)	25(2)
C(30)	2292(4)	4156(5)	1353(5)	33(2)
C(31)	2164(4)	4904(5)	1891(5)	31(2)
C(32)	2776(4)	5392(5)	2440(5)	28(2)
C(33)	3524(4)	5134(5)	2472(4)	23(2)
C(34)	4759(4)	3666(5)	1023(4)	20(2)
C(35)	4899(4)	2684(5)	821(5)	30(2)
C(36)	5010(5)	2488(6)	36(5)	39(2)
C(37)	4978(4)	3257(6)	-544(5)	37(2)
C(38)	4846(4)	4224(6)	-327(4)	33(2)
C(39)	4741(4)	4443(5)	457(4)	27(2)

Table 3-10b. Bond lengths [A] and angles [deg] for **10b**.

W(1)-C(1C)	1.982(10)
W(1)-C(1D)	1.986(5)
W(1)-C(1B)	2.010(15)
W(1)-C(1A)	2.059(11)
W(1)-P(1)	2.4605(15)
W(1)-S(1)	2.602(3)
C(1A)-O(1A)	1.119(16)
C(1B)-O(1B)	1.183(18)
C(1C)-O(1C)	1.133(10)
C(1D)-O(1D)	1.144(6)
S(1)-P(3)	2.015(2)
P(1)-C(9)	1.722(6)
P(1)-C(2)	1.733(6)
P(2)-C(2)	1.753(6)
P(2)-C(22)	1.803(6)
P(2)-C(16)	1.804(6)
P(2)-C(10)	1.813(6)
P(3)-C(9)	1.760(6)
P(3)-C(28)	1.807(6)
P(3)-C(34)	1.828(7)
C(2)-C(3)	1.448(8)
C(3)-C(4)	1.409(8)
C(3)-C(8)	1.442(8)
C(4)-C(5)	1.384(9)
C(5)-C(6)	1.412(13)
C(6)-C(7)	1.370(9)
C(7)-C(8)	1.408(8)
C(8)-C(9)	1.432(8)
C(10)-C(15)	1.380(8)
C(10)-C(11)	1.407(8)
C(11)-C(12)	1.379(9)
C(12)-C(13)	1.377(10)
C(13)-C(14)	1.393(10)
C(14)-C(15)	1.381(9)
C(16)-C(21)	1.383(15)
C(16)-C(17)	1.392(9)
C(17)-C(18)	1.379(8)
C(18)-C(19)	1.377(10)
C(19)-C(20)	1.389(10)
C(20)-C(21)	1.375(9)
C(22)-C(23)	1.391(9)
C(22)-C(27)	1.391(9)
C(23)-C(24)	1.384(9)
C(24)-C(25)	1.385(10)
C(25)-C(26)	1.377(10)
C(26)-C(27)	1.402(9)
C(28)-C(29)	1.384(9)
C(28)-C(33)	1.391(9)
C(29)-C(30)	1.376(9)
C(30)-C(31)	1.389(10)
C(31)-C(32)	1.366(9)
C(32)-C(33)	1.368(9)
C(34)-C(39)	1.381(9)
C(34)-C(35)	1.381(9)
C(35)-C(36)	1.387(10)
C(36)-C(37)	1.385(10)
C(37)-C(38)	1.365(10)
C(38)-C(39)	1.388(9)

C(1C)-W(1)-C(1D)	86.8(3)
C(1C)-W(1)-C(1B)	90.5(4)
C(1D)-W(1)-C(1B)	90.6(3)
C(1C)-W(1)-C(1A)	89.9(4)
C(1D)-W(1)-C(1A)	88.8(3)
C(1B)-W(1)-C(1A)	179.3(4)
C(1C)-W(1)-P(1)	100.76(19)
C(1D)-W(1)-P(1)	170.7(3)
C(1B)-W(1)-P(1)	94.7(2)
C(1A)-W(1)-P(1)	85.8(2)
C(1C)-W(1)-S(1)	174.3(2)
C(1D)-W(1)-S(1)	93.1(3)
C(1B)-W(1)-S(1)	83.8(3)
C(1A)-W(1)-S(1)	95.9(4)
P(1)-W(1)-S(1)	79.88(6)
O(1A)-C(1A)-W(1)	175.4(12)
O(1B)-C(1B)-W(1)	176.6(10)
O(1C)-C(1C)-W(1)	177.1(7)
O(1D)-C(1D)-W(1)	178.6(9)
P(3)-S(1)-W(1)	104.97(10)
C(9)-P(1)-C(2)	94.1(3)
C(9)-P(1)-W(1)	118.1(2)
C(2)-P(1)-W(1)	145.9(2)
C(2)-P(2)-C(22)	114.7(3)
C(2)-P(2)-C(16)	111.5(3)
C(22)-P(2)-C(16)	106.0(3)
C(2)-P(2)-C(10)	108.3(3)
C(22)-P(2)-C(10)	106.6(3)
C(16)-P(2)-C(10)	109.5(3)
C(9)-P(3)-C(28)	110.5(3)
C(9)-P(3)-C(34)	109.6(3)
C(28)-P(3)-C(34)	108.1(3)
C(9)-P(3)-S(1)	109.8(2)
C(28)-P(3)-S(1)	107.4(2)
C(34)-P(3)-S(1)	111.2(2)
C(3)-C(2)-P(1)	110.2(4)
C(3)-C(2)-P(2)	129.8(4)
P(1)-C(2)-P(2)	120.0(3)
C(4)-C(3)-C(8)	117.2(5)
C(4)-C(3)-C(2)	130.6(6)
C(8)-C(3)-C(2)	112.2(5)
C(5)-C(4)-C(3)	121.8(6)
C(4)-C(5)-C(6)	120.0(6)
C(7)-C(6)-C(5)	120.1(9)
C(6)-C(7)-C(8)	120.7(8)
C(7)-C(8)-C(9)	127.7(6)
C(7)-C(8)-C(3)	120.1(5)
C(9)-C(8)-C(3)	112.1(5)
C(8)-C(9)-P(1)	111.3(4)
C(8)-C(9)-P(3)	133.2(5)
P(1)-C(9)-P(3)	115.1(3)
C(15)-C(10)-C(11)	119.2(6)
C(15)-C(10)-P(2)	121.8(5)
C(11)-C(10)-P(2)	119.0(5)

C(12)-C(11)-C(10)	119.9(6)
C(13)-C(12)-C(11)	120.3(7)
C(12)-C(13)-C(14)	120.2(7)
C(15)-C(14)-C(13)	119.6(7)
C(10)-C(15)-C(14)	120.8(6)
C(21)-C(16)-C(17)	119.0(7)
C(21)-C(16)-P(2)	119.8(6)
C(17)-C(16)-P(2)	120.9(5)
C(18)-C(17)-C(16)	119.9(6)
C(19)-C(18)-C(17)	120.5(7)
C(18)-C(19)-C(20)	120.1(7)
C(21)-C(20)-C(19)	119.1(9)
C(20)-C(21)-C(16)	121.3(11)
C(23)-C(22)-C(27)	120.1(6)
C(23)-C(22)-P(2)	120.1(5)
C(27)-C(22)-P(2)	119.8(5)
C(24)-C(23)-C(22)	120.1(6)
C(23)-C(24)-C(25)	120.1(6)
C(26)-C(25)-C(24)	120.0(7)

C(25)-C(26)-C(27)	120.5(7)
C(22)-C(27)-C(26)	119.1(7)
C(29)-C(28)-C(33)	119.1(6)
C(29)-C(28)-P(3)	120.3(5)
C(33)-C(28)-P(3)	120.1(5)
C(30)-C(29)-C(28)	120.5(7)
C(29)-C(30)-C(31)	119.2(7)
C(32)-C(31)-C(30)	120.8(7)
C(31)-C(32)-C(33)	120.0(7)
C(32)-C(33)-C(28)	120.5(6)
C(39)-C(34)-C(35)	120.4(7)
C(39)-C(34)-P(3)	119.9(5)
C(35)-C(34)-P(3)	119.5(5)
C(34)-C(35)-C(36)	119.0(7)
C(37)-C(36)-C(35)	121.1(7)
C(38)-C(37)-C(36)	118.9(7)
C(37)-C(38)-C(39)	121.2(7)
C(34)-C(39)-C(38)	119.4(7)

Table 4-10b. Anisotropic displacement parameters (A^2 x 10^3) for **10b**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W(1)	18(1)	20(1)	18(1)	1(1)	8(1)	0(1)
C(1A)	36(7)	25(6)	36(8)	2(4)	35(6)	2(4)
O(1A)	52(7)	53(5)	28(6)	5(3)	26(5)	6(3)
C(1B)	31(7)	20(6)	21(7)	4(3)	-18(5)	1(3)
O(1B)	57(7)	57(6)	26(6)	4(3)	21(5)	2(3)
C(1C)	34(5)	27(4)	22(4)	5(3)	18(4)	6(4)
O(1C)	20(3)	39(4)	38(4)	3(2)	3(3)	4(2)
C(1D)	20(3)	24(3)	33(4)	20(5)	13(3)	21(5)
O(1D)	39(3)	21(2)	65(4)	6(4)	32(2)	9(4)
S(1)	22(1)	22(1)	23(1)	1(1)	8(1)	-3(1)
P(1)	21(1)	18(1)	19(1)	0(1)	9(1)	-1(1)
P(2)	18(1)	21(1)	18(1)	-1(1)	9(1)	-3(1)
P(3)	18(1)	21(1)	16(1)	-1(1)	7(1)	0(1)
C(2)	21(3)	19(3)	13(3)	-3(3)	11(3)	-1(3)
C(3)	25(4)	12(3)	18(3)	-2(3)	12(3)	2(3)
C(4)	26(4)	25(4)	23(3)	-5(3)	11(3)	-5(3)
C(5)	33(4)	16(3)	27(4)	6(3)	16(3)	6(3)
C(6)	25(5)	26(5)	16(5)	10(3)	9(4)	9(3)
C(7)	16(3)	27(4)	22(4)	-1(3)	9(3)	-2(3)
C(8)	23(3)	20(3)	13(3)	1(3)	11(3)	6(3)
C(9)	23(3)	21(3)	13(3)	-3(3)	10(3)	-4(3)
C(10)	20(3)	20(3)	19(4)	1(3)	9(3)	-1(3)
C(11)	21(4)	33(4)	20(4)	3(3)	4(3)	4(3)
C(12)	27(4)	42(4)	23(4)	0(3)	11(3)	-8(3)
C(13)	44(5)	27(4)	16(4)	1(3)	8(3)	2(4)
C(14)	29(5)	32(4)	25(4)	3(4)	3(4)	2(4)
C(15)	20(4)	31(4)	25(4)	-4(3)	8(3)	-4(3)
C(16)	18(3)	25(3)	16(4)	-2(3)	3(3)	-5(3)
C(17)	30(4)	30(4)	23(4)	-5(3)	8(3)	-8(3)
C(18)	30(4)	29(4)	36(4)	3(3)	6(3)	-6(3)
C(19)	52(5)	23(4)	33(5)	-6(3)	2(4)	-6(4)
C(20)	54(5)	33(4)	30(4)	-12(3)	21(4)	-4(4)
C(21)	39(7)	31(6)	22(6)	-4(3)	10(5)	-6(4)

C(22)	22(4)	24(3)	21(4)	4(3)	12(3)	3(3)
C(23)	22(4)	26(4)	22(4)	6(3)	8(3)	-2(3)
C(24)	44(5)	27(4)	27(4)	-2(3)	24(4)	6(3)
C(25)	35(5)	37(4)	42(5)	5(4)	25(4)	3(3)
C(26)	26(4)	39(4)	39(5)	4(4)	16(4)	-1(3)
C(27)	26(4)	22(4)	27(4)	1(3)	10(3)	2(3)
C(28)	21(4)	23(3)	19(4)	8(3)	11(3)	1(3)
C(29)	28(4)	23(3)	29(4)	0(3)	14(3)	-1(3)
C(30)	22(4)	26(4)	50(5)	3(3)	8(4)	-6(3)
C(31)	25(4)	34(4)	37(4)	15(3)	14(3)	-2(3)
C(32)	25(4)	31(4)	29(4)	5(3)	11(3)	9(3)
C(33)	27(4)	24(4)	17(4)	-2(3)	5(3)	-2(3)
C(34)	18(4)	25(4)	18(4)	-5(3)	7(3)	-3(3)
C(35)	30(4)	36(4)	26(4)	-5(3)	10(3)	5(3)
C(36)	42(5)	45(5)	32(4)	-12(4)	12(4)	7(4)
C(37)	23(4)	69(6)	20(4)	-12(4)	6(3)	-6(4)
C(38)	27(4)	53(5)	20(4)	2(3)	9(3)	-3(3)
C(39)	24(4)	32(4)	23(4)	-4(3)	7(3)	0(3)

Table 5-10b. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **10b**.

	x	y	z	U(eq)
H(4)	6731	7680	3178	28
H(5)	5823	8688	2238	29
H(6)	4648	7979	1391	26
H(7)	4365	6295	1551	25
H(11)	6413	5443	5156	30
H(12)	6379	4540	6359	36
H(13)	7429	3533	7060	35
H(14)	8562	3508	6615	36
H(15)	8608	4427	5423	30
H(17)	8410	7265	3672	33
H(18)	8607	8984	3953	39
H(19)	8057	9779	4902	45
H(20)	7307	8844	5595	45
H(21)	7160	7114	5361	36
H(23)	7657	4344	2917	27
H(24)	8693	3630	2519	36
H(25)	9970	4127	3194	42
H(26)	10219	5285	4300	40
H(27)	9185	5971	4743	29
H(29)	3138	3414	999	30
H(30)	1865	3816	976	40
H(31)	1646	5079	1877	37
H(32)	2681	5909	2798	33
H(33)	3948	5466	2861	28
H(35)	4918	2150	1213	36
H(36)	5110	1815	-106	47
H(37)	5047	3115	-1084	44
H(38)	4826	4756	-721	39
H(39)	4658	5120	603	32

Table 1-13b. Crystal data and structure refinement **13b**.

	13b
Formula	$C_{44.50}H_{32}BO_4P_3W$
Formula weight	918.27
Crystal size	0.34 x 0.16 x 0.1 mm
Crystal System, space group	Monoclinic, P21/c
Unit cell dimensions	a = 11.06270(10) Å
	b = 21.8693(2) Å
	c = 17.3806(2) Å
	β = 102.36°
Volume	4107.41(7) Å^3
Z, ρ_{calc}	4, 1.49 Mg/m^3
μ	2.86 mm^{-1}
F(000)	1820
Theta range for data collection	3.04 to 27.43°
Completeness of data	
Max. and min. transmission	1.073 and 0.948
Limiting indices	$-14 \le h \le 14$,
	$-28 \le k \le 28$,
	$-22 \le l \le 22$
Reflections collected / unique	74507 / 9350 [R_{int} = 0.0541]
Absorption Correction	Multi-scan
Data / restraints / parameters	9350 / 0 / 504
Goodness-of-fit on F^2	1.081
R1 [I > 2σ(I)]	0.027
wR2 R (all data)	0.069
Largest diff. peak and hole	0.833 and -1.153 e Å^{-3}

Table 2-13b. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **13b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
W	1103(1)	1826(1)	2198(1)	29(1)
P(1)	2871(1)	1163(1)	2773(1)	26(1)
P(2)	4626(1)	1989(1)	2209(1)	29(1)
P(3)	2035(1)	-5(1)	3454(1)	23(1)
B	3256(4)	2544(2)	2214(2)	40(1)
C(1)	3125(2)	407(1)	3074(2)	24(1)
C(2)	4347(2)	217(1)	2989(2)	24(1)
C(3)	5022(2)	707(1)	2723(2)	26(1)
C(4)	4325(2)	1265(1)	2586(2)	27(1)
C(5)	6238(2)	599(1)	2629(2)	34(1)
C(6)	6775(3)	36(1)	2783(2)	40(1)
C(7)	6115(3)	-444(1)	3036(2)	39(1)
C(8)	4926(3)	-357(1)	3141(2)	32(1)
C(9)	6003(3)	2342(1)	2802(2)	33(1)
C(10)	6801(3)	2049(2)	3411(2)	53(1)
C(11)	7801(4)	2357(2)	3852(3)	66(1)
C(12)	8018(4)	2955(2)	3699(2)	57(1)
C(13)	7217(4)	3258(2)	3109(2)	60(1)
C(14)	6214(4)	2956(2)	2662(2)	49(1)
C(15)	4940(3)	1888(1)	1235(2)	39(1)
C(16)	3960(4)	1939(2)	587(2)	63(1)
C(17)	4164(6)	1852(3)	-168(3)	88(2)
C(18)	5332(6)	1715(2)	-278(3)	81(2)
C(19)	6309(5)	1665(2)	358(3)	67(1)
C(20)	6120(4)	1753(1)	1120(2)	48(1)
C(21)	2798(2)	-603(1)	4094(2)	26(1)
C(22)	2709(3)	-1212(1)	3857(2)	33(1)
C(23)	3431(3)	-1656(1)	4314(2)	43(1)
C(24)	4243(3)	-1496(2)	4997(2)	47(1)
C(25)	4323(3)	-890(2)	5244(2)	45(1)
C(26)	3598(3)	-449(1)	4802(2)	35(1)
C(27)	1287(3)	494(1)	4043(2)	31(1)
C(28)	1986(3)	912(1)	4551(2)	43(1)
C(29)	1435(4)	1276(2)	5037(2)	59(1)
C(30)	181(4)	1216(2)	5009(2)	63(1)
C(31)	-515(4)	808(2)	4511(2)	59(1)
C(32)	25(3)	440(2)	4025(2)	42(1)
C(33)	889(2)	-362(1)	2689(2)	29(1)
C(34)	26(3)	-779(1)	2859(2)	38(1)
C(35)	-813(3)	-1056(2)	2254(2)	50(1)
C(36)	-798(3)	-913(2)	1476(2)	57(1)
C(37)	43(4)	-505(2)	1304(2)	54(1)
C(38)	884(3)	-227(1)	1907(2)	37(1)
C(39)	1095(3)	2258(2)	3243(2)	44(1)
O(1)	1064(3)	2499(1)	3823(2)	70(1)
C(40)	-260(3)	1299(2)	2346(2)	42(1)
O(2)	-1088(2)	991(1)	2384(2)	68(1)
C(41)	-139(3)	2402(2)	1620(2)	51(1)
O(3)	-864(3)	2727(2)	1264(2)	87(1)
C(42)	982(3)	1383(2)	1166(2)	48(1)
O(4)	836(4)	1119(2)	581(2)	88(1)
C(43)	5463(24)	42(9)	636(12)	38(5)

C(44)	6626(16)	27(7)	599(9)	44(5)
C(45)	7073(24)	105(11)	-253(16)	64(6)
C(46)	4351(20)	-61(8)	821(11)	57(6)
O(5)	4391(13)	10(7)	163(9)	112(4)
C(47)	3430(23)	-42(10)	520(14)	79(6)
C(48)	5159(17)	-65(8)	758(10)	50(5)
C(49)	5850(21)	-30(9)	632(11)	58(6)
C(50)	6770(19)	-24(8)	-41(12)	63(5)

Table 3-13b. Bond lengths [A] and angles [deg] for **13b**.

W-C(40)	1.958(3)
W-C(41)	1.972(3)
W-C(42)	2.019(4)
W-HB1	2.02(3)
W-C(39)	2.049(4)
W-P(1)	2.4684(7)
P(1)-C(4)	1.722(3)
P(1)-C(1)	1.738(3)
P(2)-C(4)	1.772(3)
P(2)-C(15)	1.814(3)
P(2)-C(9)	1.818(3)
P(2)-B	1.943(4)
P(3)-C(1)	1.744(2)
P(3)-C(21)	1.805(3)
P(3)-C(33)	1.806(3)
P(3)-C(27)	1.813(3)
B-HB1	1.15(3)
B-HB2	1.15(5)
B-HB3	0.90(3)
C(1)-C(2)	1.452(3)
C(2)-C(8)	1.410(4)
C(2)-C(3)	1.437(3)
C(3)-C(5)	1.409(4)
C(3)-C(4)	1.435(3)
C(5)-C(6)	1.369(4)
C(5)-H(5)	0.93
C(6)-C(7)	1.403(4)
C(6)-H(6)	0.93
C(7)-C(8)	1.379(4)
C(7)-H(7)	0.93
C(8)-H(8)	0.93
C(9)-C(10)	1.381(5)
C(9)-C(14)	1.395(4)
C(10)-C(11)	1.379(5)
C(10)-H(10)	0.93
C(11)-C(12)	1.368(6)
C(11)-H(11)	0.93
C(12)-C(13)	1.373(6)
C(12)-H(12)	0.93
C(13)-C(14)	1.379(5)
C(13)-H(13)	0.93
C(14)-H(14)	0.93
C(15)-C(16)	1.391(5)
C(15)-C(20)	1.394(5)
C(16)-C(17)	1.391(6)
C(16)-H(16)	0.93

C(17)-C(18)	1.379(8)
C(17)-H(17)	0.93
C(18)-C(19)	1.375(7)
C(18)-H(18)	0.93
C(19)-C(20)	1.396(5)
C(19)-H(19)	0.93
C(20)-H(20)	0.93
C(21)-C(22)	1.391(4)
C(21)-C(26)	1.395(4)
C(22)-C(23)	1.392(4)
C(22)-H(22)	0.93
C(23)-C(24)	1.373(5)
C(23)-H(23)	0.93
C(24)-C(25)	1.392(5)
C(24)-H(24)	0.93
C(25)-C(26)	1.378(4)
C(25)-H(25)	0.93
C(26)-H(26)	0.93
C(27)-C(28)	1.385(4)
C(27)-C(32)	1.395(4)
C(28)-C(29)	1.393(5)
C(28)-H(28)	0.93
C(29)-C(30)	1.383(6)
C(29)-H(29)	0.93
C(30)-C(31)	1.361(6)
C(30)-H(30)	0.93
C(31)-C(32)	1.390(5)
C(31)-H(31)	0.93
C(32)-H(32)	0.93
C(33)-C(38)	1.389(4)
C(33)-C(34)	1.398(4)
C(34)-C(35)	1.384(5)
C(34)-H(34)	0.93
C(35)-C(36)	1.392(6)
C(35)-H(35)	0.93
C(36)-C(37)	1.368(5)
C(36)-H(36)	0.93
C(37)-C(38)	1.384(4)
C(37)-H(37)	0.93
C(38)-H(38)	0.93
C(39)-O(1)	1.144(4)
C(40)-O(2)	1.151(4)
C(41)-O(3)	1.149(4)
C(42)-O(4)	1.149(5)
C(43)-O(5)	1.29(2)
C(43)-C(44)	1.30(3)

C(43)-C(46)	1.36(3)
C(43)-O(5)#1	1.44(2)
C(44)-C(49)	0.88(2)
C(44)-C(50)	1.16(2)
C(44)-O(5)#1	1.55(2)
C(44)-C(45)	1.67(3)
C(44)-C(48)	1.71(2)
C(44)-C(47)#1	1.93(3)
C(45)-C(50)	0.62(3)
C(45)-C(47)#1	0.66(3)
C(45)-C(46)#1	1.67(3)
C(45)-O(5)#1	1.68(3)
C(46)-C(48)	0.92(2)
C(46)-C(47)	1.04(3)
C(46)-O(5)	1.16(2)
C(46)-C(50)#1	1.64(3)
C(46)-C(45)#1	1.67(3)
C(46)-C(49)	1.76(3)
O(5)-C(48)	1.20(2)
O(5)-C(50)#1	1.26(2)
O(5)-C(47)	1.35(3)
O(5)-C(49)#1	1.35(2)
O(5)-C(43)#1	1.44(2)
O(5)-C(44)#1	1.55(2)
O(5)-O(5)#1	1.57(3)
O(5)-C(49)	1.65(2)
O(5)-C(45)#1	1.68(3)
O(5)-C(48)#1	1.78(2)
C(47)-C(45)#1	0.66(3)
C(47)-C(50)#1	0.83(3)
C(47)-C(48)	1.87(3)
C(47)-C(44)#1	1.93(3)
C(48)-C(49)	0.84(3)
C(48)-O(5)#1	1.78(2)
C(49)-O(5)#1	1.35(2)
C(49)-C(50)	1.71(3)
C(50)-C(47)#1	0.83(3)
C(50)-O(5)#1	1.26(2)
C(50)-C(46)#1	1.64(3)
W-HB1-B	125,74(0)
C(40)-W-C(41)	88.32(13)
C(40)-W-C(42)	85.84(15)
C(41)-W-C(42)	86.9(2)
C(40)-W-HB1	168.8(10)
C(41)-W-HB1	87.1(10)
C(42)-W-HB1	83.8(10)
C(40)-W-C(39)	90.35(14)
C(41)-W-C(39)	91.3(2)
C(42)-W-C(39)	175.85(14)
HB1-W-C(39)	99.9(10)
C(40)-W-P(1)	99.59(9)
C(41)-W-P(1)	170.53(11)
C(42)-W-P(1)	88.48(10)
C(39)-W-P(1)	93.78(9)
C(4)-P(1)-C(1)	94.74(12)
C(4)-P(1)-W	122.64(9)

C(1)-P(1)-W	138.03(9)
C(4)-P(2)-C(15)	108.95(13)
C(4)-P(2)-C(9)	111.76(13)
C(15)-P(2)-C(9)	106.00(14)
C(4)-P(2)-B	110.37(14)
C(15)-P(2)-B	112.7(2)
C(9)-P(2)-B	107.0(2)
C(1)-P(3)-C(21)	109.76(12)
C(1)-P(3)-C(33)	112.18(13)
C(21)-P(3)-C(33)	107.58(12)
C(1)-P(3)-C(27)	109.82(12)
C(21)-P(3)-C(27)	107.34(12)
C(33)-P(3)-C(27)	110.02(13)
P(2)-B-HB1	107.2(18)
P(2)-B-HB2	103.1(22)
HB1-B-HB2	97.5(27)
P(2)-B-HB3	104.7(20)
HB1-B-HB3	125.2(26)
HB2-B-HB3	117.0(30)
C(2)-C(1)-P(1)	109.6(2)
C(2)-C(1)-P(3)	128.7(2)
P(1)-C(1)-P(3)	121.67(14)
C(8)-C(2)-C(3)	118.6(2)
C(8)-C(2)-C(1)	129.2(2)
C(3)-C(2)-C(1)	112.3(2)
C(5)-C(3)-C(4)	127.9(2)
C(5)-C(3)-C(2)	119.2(2)
C(4)-C(3)-C(2)	112.9(2)
C(3)-C(4)-P(1)	110.4(2)
C(3)-C(4)-P(2)	133.2(2)
P(1)-C(4)-P(2)	116.21(14)
C(6)-C(5)-C(3)	120.9(3)
C(6)-C(5)-H(5)	119.6(2)
C(3)-C(5)-H(5)	119.6(2)
C(5)-C(6)-C(7)	120.1(3)
C(5)-C(6)-H(6)	119.9(2)
C(7)-C(6)-H(6)	119.9(2)
C(8)-C(7)-C(6)	120.9(3)
C(8)-C(7)-H(7)	119.6(2)
C(6)-C(7)-H(7)	119.6(2)
C(7)-C(8)-C(2)	120.4(2)
C(7)-C(8)-H(8)	119.8(2)
C(2)-C(8)-H(8)	119.79(15)
C(10)-C(9)-C(14)	118.4(3)
C(10)-C(9)-P(2)	124.0(2)
C(14)-C(9)-P(2)	117.5(3)
C(11)-C(10)-C(9)	120.4(3)
C(11)-C(10)-H(10)	119.8(2)
C(9)-C(10)-H(10)	119.8(2)
C(12)-C(11)-C(10)	120.8(4)
C(12)-C(11)-H(11)	119.6(2)
C(10)-C(11)-H(11)	119.6(2)
C(11)-C(12)-C(13)	119.7(3)
C(11)-C(12)-H(12)	120.2(2)
C(13)-C(12)-H(12)	120.2(2)
C(12)-C(13)-C(14)	120.2(3)
C(12)-C(13)-H(13)	119.9(2)

C(14)-C(13)-H(13)	119.9(2)
C(13)-C(14)-C(9)	120.5(4)
C(13)-C(14)-H(14)	119.8(2)
C(9)-C(14)-H(14)	119.8(2)
C(16)-C(15)-C(20)	119.5(3)
C(16)-C(15)-P(2)	118.4(3)
C(20)-C(15)-P(2)	122.2(3)
C(15)-C(16)-C(17)	119.8(4)
C(15)-C(16)-H(16)	120.1(2)
C(17)-C(16)-H(16)	120.1(3)
C(18)-C(17)-C(16)	120.5(5)
C(18)-C(17)-H(17)	119.8(3)
C(16)-C(17)-H(17)	119.8(3)
C(19)-C(18)-C(17)	120.2(4)
C(19)-C(18)-H(18)	119.9(3)
C(17)-C(18)-H(18)	119.9(3)
C(18)-C(19)-C(20)	120.0(4)
C(18)-C(19)-H(19)	120.0(3)
C(20)-C(19)-H(19)	120.0(3)
C(15)-C(20)-C(19)	120.0(4)
C(15)-C(20)-H(20)	120.0(2)
C(19)-C(20)-H(20)	120.0(3)
C(22)-C(21)-C(26)	119.0(3)
C(22)-C(21)-P(3)	121.2(2)
C(26)-C(21)-P(3)	119.5(2)
C(21)-C(22)-C(23)	120.2(3)
C(21)-C(22)-H(22)	119.9(2)
C(23)-C(22)-H(22)	119.9(2)
C(24)-C(23)-C(22)	120.4(3)
C(24)-C(23)-H(23)	119.8(2)
C(22)-C(23)-H(23)	119.8(2)
C(23)-C(24)-C(25)	119.7(3)
C(23)-C(24)-H(24)	120.2(2)
C(25)-C(24)-H(24)	120.2(2)
C(26)-C(25)-C(24)	120.3(3)
C(26)-C(25)-H(25)	119.8(2)
C(24)-C(25)-H(25)	119.8(2)
C(25)-C(26)-C(21)	120.4(3)
C(25)-C(26)-H(26)	119.8(2)
C(21)-C(26)-H(26)	119.8(2)
C(28)-C(27)-C(32)	119.3(3)
C(28)-C(27)-P(3)	119.8(2)
C(32)-C(27)-P(3)	120.8(2)
C(27)-C(28)-C(29)	120.4(3)
C(27)-C(28)-H(28)	119.8(2)
C(29)-C(28)-H(28)	119.8(2)
C(30)-C(29)-C(28)	119.3(4)
C(30)-C(29)-H(29)	120.4(2)
C(28)-C(29)-H(29)	120.4(2)
C(31)-C(30)-C(29)	120.8(3)
C(31)-C(30)-H(30)	119.6(2)
C(29)-C(30)-H(30)	119.6(2)
C(30)-C(31)-C(32)	120.4(4)
C(30)-C(31)-H(31)	119.8(2)
C(32)-C(31)-H(31)	119.8(2)
C(31)-C(32)-C(27)	119.7(4)
C(31)-C(32)-H(32)	120.1(2)
C(27)-C(32)-H(32)	120.1(2)
C(38)-C(33)-C(34)	119.0(3)
C(38)-C(33)-P(3)	118.9(2)
C(34)-C(33)-P(3)	122.0(2)
C(35)-C(34)-C(33)	120.1(3)
C(35)-C(34)-H(34)	119.9(2)
C(33)-C(34)-H(34)	119.9(2)
C(34)-C(35)-C(36)	119.6(3)
C(34)-C(35)-H(35)	120.2(2)
C(36)-C(35)-H(35)	120.2(2)
C(37)-C(36)-C(35)	120.6(3)
C(37)-C(36)-H(36)	119.7(2)
C(35)-C(36)-H(36)	119.7(2)
C(36)-C(37)-C(38)	120.0(3)
C(36)-C(37)-H(37)	120.0(2)
C(38)-C(37)-H(37)	120.0(2)
C(37)-C(38)-C(33)	120.6(3)
C(37)-C(38)-H(38)	119.7(2)
C(33)-C(38)-H(38)	119.7(2)
O(1)-C(39)-W	178.5(3)
O(2)-C(40)-W	175.8(3)
O(3)-C(41)-W	178.2(4)
O(4)-C(42)-W	175.5(4)
O(5)-C(43)-C(44)	138.5(21)
O(5)-C(43)-C(46)	52.1(13)
C(44)-C(43)-C(46)	164.6(21)
O(5)-C(43)-O(5)#1	70.0(14)
C(44)-C(43)-O(5)#1	68.5(15)
C(46)-C(43)-O(5)#1	120.8(18)
C(49)-C(44)-C(50)	112.7(23)
C(49)-C(44)-C(43)	9.6(20)
C(50)-C(44)-C(43)	112.9(18)
C(49)-C(44)-O(5)#1	60.6(17)
C(50)-C(44)-O(5)#1	53.1(12)
C(43)-C(44)-O(5)#1	59.9(12)
C(49)-C(44)-C(45)	123.5(21)
C(50)-C(44)-C(45)	14.6(14)
C(43)-C(44)-C(45)	121.7(16)
O(5)#1-C(44)-C(45)	62.9(12)
C(49)-C(44)-C(48)	5.6(14)
C(50)-C(44)-C(48)	118.2(16)
C(43)-C(44)-C(48)	10.3(12)
O(5)#1-C(44)-C(48)	65.9(10)
C(45)-C(44)-C(48)	128.8(14)
C(49)-C(44)-C(47)#1	104.3(20)
C(50)-C(44)-C(47)#1	11.5(12)
C(43)-C(44)-C(47)#1	103.3(15)
O(5)#1-C(44)-C(47)#1	43.8(9)
C(45)-C(44)-C(47)#1	19.3(10)
C(48)-C(44)-C(47)#1	109.7(13)
C(50)-C(45)-C(47)#1	80.8(41)
C(50)-C(45)-C(44)	28.3(30)
C(47)#1-C(45)-C(44)	103.7(39)
C(50)-C(45)-C(46)#1	76.3(35)
C(47)#1-C(45)-C(46)#1	12.9(27)
C(44)-C(45)-C(46)#1	95.6(15)
C(50)-C(45)-O(5)#1	38.6(29)

C(47)#1-C(45)-O(5)#1	49.3(31)
C(44)-C(45)-O(5)#1	55.0(11)
C(46)#1-C(45)-O(5)#1	40.7(10)
C(48)-C(46)-C(47)	143.9(28)
C(48)-C(46)-O(5)	69.1(18)
C(47)-C(46)-O(5)	74.9(19)
C(48)-C(46)-C(43)	12.2(17)
C(47)-C(46)-C(43)	135.5(23)
O(5)-C(46)-C(43)	61.1(14)
C(48)-C(46)-C(50)#1	118.9(21)
C(47)-C(46)-C(50)#1	25.2(16)
O(5)-C(46)-C(50)#1	49.8(12)
C(43)-C(46)-C(50)#1	110.4(16)
C(48)-C(46)-C(45)#1	137.9(22)
C(47)-C(46)-C(45)#1	8.1(17)
O(5)-C(46)-C(45)#1	69.9(15)
C(43)-C(46)-C(45)#1	131.0(17)
C(50)#1-C(46)-C(45)#1	21.4(9)
C(48)-C(46)-C(49)	4.7(15)
C(47)-C(46)-C(49)	139.8(22)
O(5)-C(46)-C(49)	64.9(14)
C(43)-C(46)-C(49)	8.0(13)
C(50)#1-C(46)-C(49)	114.7(15)
C(45)#1-C(46)-C(49)	134.3(16)
C(46)-O(5)-C(48)	45.9(12)
C(46)-O(5)-C(50)#1	85.2(16)
C(48)-O(5)-C(50)#1	131.1(19)
C(46)-O(5)-C(43)	66.8(17)
C(48)-O(5)-C(43)	22.4(11)
C(50)#1-O(5)-C(43)	150.7(20)
C(46)-O(5)-C(47)	48.4(13)
C(48)-O(5)-C(47)	94.3(17)
C(50)#1-O(5)-C(47)	36.8(12)
C(43)-O(5)-C(47)	114.8(20)
C(46)-O(5)-C(49)#1	165.6(20)
C(48)-O(5)-C(49)#1	146.5(18)
C(50)#1-O(5)-C(49)#1	81.7(17)
C(43)-O(5)-C(49)#1	127.0(18)
C(47)-O(5)-C(49)#1	118.2(19)
C(46)-O(5)-C(43)#1	167.2(18)
C(48)-O(5)-C(43)#1	128.1(18)
C(50)#1-O(5)-C(43)#1	99.3(18)
C(43)-O(5)-C(43)#1	110.0(14)
C(47)-O(5)-C(43)#1	134.6(20)
C(49)#1-O(5)-C(43)#1	18.6(11)
C(46)-O(5)-C(44)#1	131.4(17)
C(48)-O(5)-C(44)#1	169.2(16)
C(50)#1-O(5)-C(44)#1	47.7(12)
C(43)-O(5)-C(44)#1	161.6(17)
C(47)-O(5)-C(44)#1	83.6(15)
C(49)#1-O(5)-C(44)#1	34.6(10)
C(43)#1-O(5)-C(44)#1	51.6(13)
C(46)-O(5)-O(5)#1	124.6(20)
C(48)-O(5)-O(5)#1	78.7(15)
C(50)#1-O(5)-O(5)#1	149.9(20)
C(43)-O(5)-O(5)#1	59.3(13)
C(47)-O(5)-O(5)#1	171.1(21)

C(49)#1-O(5)-O(5)#1	68.2(13)
C(43)#1-O(5)-O(5)#1	50.6(12)
C(44)#1-O(5)-O(5)#1	102.3(15)
C(46)-O(5)-C(49)	75.3(16)
C(48)-O(5)-C(49)	29.4(12)
C(50)#1-O(5)-C(49)	160.5(17)
C(43)-O(5)-C(49)	11.3(13)
C(47)-O(5)-C(49)	123.7(17)
C(49)#1-O(5)-C(49)	117.8(13)
C(43)#1-O(5)-C(49)	100.0(13)
C(44)#1-O(5)-C(49)	151.4(13)
O(5)#1-O(5)-C(49)	49.6(10)
C(46)-O(5)-C(45)#1	69.4(15)
C(48)-O(5)-C(45)#1	114.7(17)
C(50)#1-O(5)-C(45)#1	17.8(12)
C(43)-O(5)-C(45)#1	136.1(19)
C(47)-O(5)-C(45)#1	21.8(12)
C(49)#1-O(5)-C(45)#1	96.7(17)
C(43)#1-O(5)-C(45)#1	112.9(18)
C(44)#1-O(5)-C(45)#1	62.1(13)
O(5)#1-O(5)-C(45)#1	161.6(19)
C(49)-O(5)-C(45)#1	143.9(16)
C(46)-O(5)-C(48)#1	165.8(16)
C(48)-O(5)-C(48)#1	120.1(13)
C(50)#1-O(5)-C(48)#1	108.6(15)
C(43)-O(5)-C(48)#1	100.0(14)
C(47)-O(5)-C(48)#1	145.2(17)
C(49)#1-O(5)-C(48)#1	27.0(11)
C(43)#1-O(5)-C(48)#1	12.7(11)
C(44)#1-O(5)-C(48)#1	61.6(10)
O(5)#1-O(5)-C(48)#1	41.4(9)
C(49)-O(5)-C(48)#1	90.9(11)
C(45)#1-O(5)-C(48)#1	123.7(15)
C(45)#1-C(47)-C(50)#1	47.4(28)
C(45)#1-C(47)-C(46)	159.1(44)
C(50)#1-C(47)-C(46)	122.4(35)
C(45)#1-C(47)-O(5)	109.0(39)
C(50)#1-C(47)-O(5)	65.8(24)
C(46)-C(47)-O(5)	56.7(17)
C(45)#1-C(47)-C(48)	145.2(39)
C(50)#1-C(47)-C(48)	105.6(28)
C(46)-C(47)-C(48)	16.9(14)
O(5)-C(47)-C(48)	39.8(11)
C(45)#1-C(47)-C(44)#1	56.9(34)
C(50)#1-C(47)-C(44)#1	16.3(18)
C(46)-C(47)-C(44)#1	108.9(21)
O(5)-C(47)-C(44)#1	52.6(12)
C(48)-C(47)-C(44)#1	92.0(12)
C(49)-C(48)-C(46)	170.2(31)
C(49)-C(48)-O(5)	106.1(22)
C(46)-C(48)-O(5)	65.0(17)
C(49)-C(48)-C(44)	5.8(14)
C(46)-C(48)-C(44)	172.4(22)
O(5)-C(48)-C(44)	111.3(16)
C(49)-C(48)-O(5)#1	46.8(16)
C(46)-C(48)-O(5)#1	124.8(20)
O(5)-C(48)-O(5)#1	59.9(13)

C(44)-C(48)-O(5)#1	52.4(9)
C(49)-C(48)-C(47)	151.9(22)
C(46)-C(48)-C(47)	19.2(15)
O(5)-C(48)-C(47)	45.9(11)
C(44)-C(48)-C(47)	156.9(14)
O(5)#1-C(48)-C(47)	105.6(12)
C(48)-C(49)-C(44)	168.6(28)
C(48)-C(49)-O(5)#1	106.1(22)
C(44)-C(49)-O(5)#1	84.8(20)
C(48)-C(49)-O(5)	44.5(16)
C(44)-C(49)-O(5)	145.5(23)
O(5)#1-C(49)-O(5)	62.2(13)
C(48)-C(49)-C(50)	152.4(22)
C(44)-C(49)-C(50)	38.9(15)
O(5)#1-C(49)-C(50)	46.8(11)
O(5)-C(49)-C(50)	109.0(14)
C(48)-C(49)-C(46)	5.1(16)
C(44)-C(49)-C(46)	171.0(22)

O(5)#1-C(49)-C(46)	101.8(16)
O(5)-C(49)-C(46)	39.8(9)
C(50)-C(49)-C(46)	148.5(15)
C(45)-C(50)-C(47)#1	51.8(29)
C(45)-C(50)-C(44)	137.1(42)
C(47)#1-C(50)-C(44)	152.2(29)
C(45)-C(50)-O(5)#1	123.7(39)
C(47)#1-C(50)-O(5)#1	77.4(26)
C(44)-C(50)-O(5)#1	79.3(17)
C(45)-C(50)-C(46)#1	82.3(36)
C(47)#1-C(50)-C(46)#1	32.4(22)
C(44)-C(50)-C(46)#1	123.0(18)
O(5)#1-C(50)-C(46)#1	45.0(11)
C(45)-C(50)-C(49)	153.3(36)
C(47)#1-C(50)-C(49)	128.3(29)
C(44)-C(50)-C(49)	28.4(10)
O(5)#1-C(50)-C(49)	51.5(12)
C(46)#1-C(50)-C(49)	96.4(14)

Table 4-13b. Anisotropic displacement parameters (A^2 x 10^3) for **13b**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
W	22(1)	24(1)	43(1)	8(1)	9(1)	5(1)
P(1)	20(1)	19(1)	39(1)	5(1)	9(1)	1(1)
P(2)	27(1)	21(1)	41(1)	5(1)	12(1)	-3(1)
P(3)	21(1)	20(1)	29(1)	1(1)	7(1)	-2(1)
C(1)	23(1)	19(1)	30(1)	0(1)	7(1)	-1(1)
C(2)	22(1)	19(1)	31(1)	-1(1)	6(1)	-2(1)
C(3)	22(1)	21(1)	36(2)	0(1)	6(1)	-1(1)
C(4)	21(1)	21(1)	39(2)	5(1)	9(1)	-1(1)
C(5)	24(1)	28(1)	52(2)	3(1)	12(1)	-2(1)
C(6)	22(1)	36(2)	64(2)	3(1)	15(1)	4(1)
C(7)	31(2)	25(1)	63(2)	3(1)	16(1)	6(1)
C(8)	30(1)	20(1)	48(2)	3(1)	12(1)	-1(1)
C(9)	33(2)	28(1)	42(2)	-2(1)	16(1)	-8(1)
C(10)	42(2)	39(2)	71(3)	4(2)	-3(2)	-4(2)
C(11)	49(2)	50(2)	86(3)	-3(2)	-12(2)	-4(2)
C(12)	46(2)	57(2)	67(3)	-16(2)	12(2)	-26(2)
C(13)	76(3)	48(2)	56(2)	0(2)	15(2)	-36(2)
C(14)	63(2)	36(2)	47(2)	6(2)	8(2)	-19(2)
C(15)	47(2)	29(2)	44(2)	4(1)	18(1)	-12(1)
C(16)	56(2)	86(3)	47(2)	8(2)	10(2)	-23(2)
C(17)	97(4)	120(5)	46(3)	0(2)	12(2)	-44(3)
C(18)	123(5)	76(3)	54(3)	-11(2)	41(3)	-33(3)
C(19)	95(3)	45(2)	76(3)	-1(2)	54(3)	0(2)
C(20)	61(2)	35(2)	54(2)	6(1)	29(2)	2(2)
C(21)	25(1)	22(1)	30(1)	3(1)	7(1)	-3(1)
C(22)	32(1)	24(1)	39(2)	0(1)	2(1)	-4(1)
C(23)	43(2)	21(1)	60(2)	5(1)	4(2)	0(1)
C(24)	46(2)	38(2)	52(2)	13(2)	-2(2)	6(1)
C(25)	46(2)	44(2)	38(2)	5(1)	-5(1)	-3(2)
C(26)	40(2)	28(1)	34(2)	-2(1)	3(1)	-4(1)
C(27)	33(1)	28(1)	36(2)	6(1)	14(1)	6(1)
C(28)	52(2)	34(2)	43(2)	-5(1)	13(2)	5(1)
C(29)	95(3)	44(2)	41(2)	-6(2)	18(2)	17(2)
C(30)	91(3)	63(3)	45(2)	12(2)	38(2)	38(2)

C(31)	58(2)	66(3)	66(3)	20(2)	39(2)	26(2)
C(32)	37(2)	43(2)	52(2)	10(2)	21(1)	8(1)
C(33)	24(1)	24(1)	38(2)	-2(1)	4(1)	-2(1)
C(34)	31(2)	35(2)	49(2)	4(1)	7(1)	-6(1)
C(35)	32(2)	36(2)	76(3)	-3(2)	-1(2)	-10(1)
C(36)	49(2)	44(2)	65(3)	-11(2)	-15(2)	-7(2)
C(37)	67(2)	48(2)	38(2)	-6(2)	-7(2)	-4(2)
C(38)	42(2)	30(2)	37(2)	0(1)	2(1)	-3(1)
C(39)	45(2)	33(2)	59(2)	6(2)	20(2)	10(1)
O(1)	93(2)	59(2)	66(2)	-10(2)	33(2)	11(2)
C(40)	27(2)	40(2)	58(2)	14(2)	11(1)	6(1)
O(2)	31(1)	72(2)	99(2)	31(2)	13(1)	-11(1)
C(41)	35(2)	42(2)	74(3)	17(2)	11(2)	8(2)
O(3)	61(2)	64(2)	126(3)	38(2)	1(2)	31(2)
C(42)	48(2)	44(2)	51(2)	7(2)	8(2)	4(2)
O(4)	113(3)	93(3)	56(2)	-24(2)	11(2)	-6(2)

Table 5-13b. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **13b**.

	x	y	z	U(eq)
HB1	2393(32)	2332(16)	1822(20)	48(10)
HB2	3411(40)	2925(21)	1790(25)	77(13)
HB3	3331(28)	2646(14)	2723(19)	31(8)
H(5)	6681(2)	915(1)	2460(2)	41
H(6)	7579(3)	-28(1)	2720(2)	48
H(7)	6485(3)	-827(1)	3135(2)	47
H(8)	4503(3)	-680(1)	3312(2)	38
H(10)	6663(3)	1643(2)	3524(2)	64
H(11)	8335(4)	2154(2)	4259(3)	79
H(12)	8704(4)	3157(2)	3993(2)	68
H(13)	7352(4)	3667(2)	3010(2)	72
H(14)	5673(4)	3165(2)	2265(2)	59
H(16)	3171(4)	2032(2)	657(2)	76
H(17)	3509(6)	1886(3)	-601(3)	105
H(18)	5459(6)	1655(2)	-785(3)	97
H(19)	7095(5)	1573(2)	282(3)	80
H(20)	6782(4)	1722(1)	1550(2)	57
H(22)	2167(3)	-1323(1)	3392(2)	39
H(23)	3362(3)	-2063(1)	4154(2)	51
H(24)	4738(3)	-1793(2)	5294(2)	56
H(25)	4868(3)	-781(2)	5709(2)	54
H(26)	3642(3)	-46(1)	4977(2)	42
H(28)	2828(3)	950(1)	4568(2)	51
H(29)	1905(4)	1557(2)	5378(2)	71
H(30)	-190(4)	1457(2)	5334(2)	75
H(31)	-1358(4)	775(2)	4495(2)	71
H(32)	-453(3)	160(2)	3690(2)	51
H(34)	16(3)	-871(1)	3380(2)	46
H(35)	-1383(3)	-1336(2)	2367(2)	60
H(36)	-1366(3)	-1096(2)	1069(2)	68
H(37)	51(4)	-414(2)	782(2)	64
H(38)	1450(3)	53(1)	1788(2)	45