Appendix 2

Tables for X-ray Crystal Structures

Structures for Chapter 1

Compound 21

Table 1. Crystal data and structure refinement for 21 (CCDC 258068).

Empirical formula	$C_{54}H_{54}Cl_6N_2O_2P_4Cr_2 \cdot 4(CH_2Cl_2)$
Formula weight	1543.28
Crystallization Solvent	Dichloromethane/petroleum ether
Crystal Habit	Block
Crystal size	0.41 x 0.16 x 0.15 mm^3
Crystal color	Sapphire blue

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 19148 reflections used in lattice determination	2.19 to 33.48°
Unit cell dimensions	a = 11.3376(5) Å b = 18.5701(7) Å β= 108.7220(10)° c = 16.7264(7) Å
Volume	3335.2(2) $Å^3$
Z	2
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.537 Mg/m^3
F(000)	1572
θ range for data collection	1.69 to 33.74°
Completeness to θ = 33.74°	90.1 %
Index ranges	$-16 \le h \le 16$, $-28 < k < 28$, $-25 < l < 25$
Data collection scan type	ω scans at 3 ϕ settings of 2θ=-28º and 2 at 2θ=-40º
Reflections collected	54219
Independent reflections	12015 [R_{int}= 0.0669]
Absorption coefficient	1.026 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8614 and 0.6785

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12015 / 0 / 491
Treatment of hydrogen atoms	Unrestrained, disordered riding
Goodness-of-fit on F^2	1.596
Final R indices [$I>2\sigma(I)$, 7974 reflections]	R1 = 0.0458, *w*R2 = 0.0749
R indices (all data)	R1 = 0.0776, *w*R2 = 0.0783
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.183 and -0.759 e.Å^{-3}

Special Refinement Details

There is disorder in the methyl-ethyl keytone ligand attached to nitrogen. The disorder was modeled with alternate positions for the ethyl carbon atom alpha to oxygen (C26A & B) with the corresponding changes in the methyl carbon (C27A & B). The oxygen atom (O1) was refined at a single position. The molecule sits on a center of symmetry, therefore, only the unique atoms are labeled in the figures. Disorder is also observed in the dichloromethane solvents (not shown in the figures).

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 21 (CCDC 258068). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Cr(1)	10258(1)	5437(1)	9145(1)	16(1)	1
Cl(1)	9270(1)	6364(1)	8313(1)	21(1)	1
Cl(2)	11971(1)	6091(1)	9890(1)	23(1)	1
Cl(3)	11000(1)	4392(1)	9962(1)	18(1)	1
P(1)	11095(1)	5139(1)	8022(1)	19(1)	1
P(2)	8871(1)	4635(1)	8053(1)	18(1)	1
O(1)	8632(1)	4810(1)	5551(1)	42(1)	1
N(1)	9828(1)	4661(1)	7445(1)	20(1)	1
C(1)	12508(2)	4597(1)	8274(1)	20(1)	1
C(2)	12868(2)	4222(1)	7671(2)	30(1)	1
C(3)	13952(2)	3818(1)	7916(2)	34(1)	1
C(4)	14698(2)	3807(1)	8740(2)	32(1)	1
C(5)	14381(2)	4191(1)	9333(2)	28(1)	1
C(6)	13280(2)	4581(1)	9109(1)	26(1)	1
C(7)	11338(2)	5868(1)	7377(1)	22(1)	1
C(8)	10389(2)	6115(1)	6669(1)	29(1)	1
C(9)	10589(2)	6705(1)	6231(2)	37(1)	1
C(10)	11706(2)	7060(1)	6487(2)	37(1)	1
C(11)	12635(2)	6838(1)	7192(2)	34(1)	1
C(12)	12458(2)	6242(1)	7641(2)	29(1)	1
C(13)	8569(2)	3684(1)	8144(1)	21(1)	1
C(14)	7365(2)	3413(1)	7947(1)	27(1)	1
C(15)	7165(2)	2691(1)	8037(2)	33(1)	1
C(16)	8149(2)	2226(1)	8309(2)	36(1)	1
C(17)	9354(2)	2485(1)	8501(1)	30(1)	1
C(18)	9564(2)	3203(1)	8424(1)	24(1)	1
C(19)	7343(2)	5008(1)	7514(1)	21(1)	1
C(20)	6889(2)	5165(1)	6672(2)	33(1)	1
C(21)	5683(2)	5441(1)	6328(2)	39(1)	1
C(22)	4971(2)	5564(1)	6842(2)	34(1)	1
C(23)	5430(2)	5418(1)	7683(2)	33(1)	1
C(24)	6614(2)	5135(1)	8024(2)	28(1)	1
C(25)	9770(2)	4142(1)	6756(1)	32(1)	1
C(26A)	9747(3)	4423(2)	5930(2)	29(1)	0.606(4)
C(27A)	7688(4)	4691(2)	4830(2)	46(1)	0.606(4)
C(26B)	8771(5)	4127(3)	6040(3)	28(1)	0.394(4)
C(27B)	8508(6)	5082(3)	4772(4)	38(2)	0.394(4)
C(31)	3736(2)	2840(1)	5658(2)	41(1)	1
Cl(11)	4592(1)	3648(1)	5838(1)	53(1)	1
Cl(12)	2282(4)	2929(2)	5855(3)	43(1)	0.54(2)
Cl(13)	2215(5)	3022(5)	5595(12)	90(2)	0.46(2)
C(32)	3105(2)	2924(2)	1044(2)	52(1)	1
Cl(21)	4595(1)	2819(1)	976(1)	49(1)	1
Cl(22)	1989(2)	2464(3)	290(4)	55(1)	0.551(12)
Cl(23)	2129(3)	2175(4)	548(2)	64(1)	0.449(12)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 21 (CCDC 258068). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	146(1)	168(1)	161(2)	-8(1)	54(1)	10(1)
Cl(1)	200(2)	197(2)	221(2)	23(2)	67(2)	44(2)
Cl(2)	179(2)	222(2)	269(3)	-15(2)	35(2)	-19(2)
Cl(3)	179(2)	194(2)	176(2)	5(2)	73(2)	32(2)
P(1)	183(2)	193(2)	201(3)	20(2)	91(2)	34(2)
P(2)	171(2)	201(2)	177(3)	-24(2)	55(2)	4(2)
O(1)	413(9)	553(10)	206(9)	-80(7)	-12(7)	202(8)
N(1)	196(8)	237(8)	180(8)	-47(7)	69(6)	7(6)
C(1)	186(9)	169(9)	288(11)	59(8)	131(8)	31(7)
C(2)	300(12)	319(12)	324(14)	21(10)	163(10)	62(9)
C(3)	315(12)	296(12)	492(16)	-33(11)	241(12)	66(9)
C(4)	197(11)	229(11)	556(16)	75(10)	170(11)	48(9)
C(5)	192(10)	311(11)	347(14)	91(10)	84(10)	0(9)
C(6)	225(10)	266(10)	328(13)	25(9)	141(9)	8(8)
C(7)	250(10)	219(9)	233(11)	13(8)	147(8)	64(8)
C(8)	358(13)	282(11)	235(12)	19(9)	97(10)	45(10)
C(9)	537(16)	308(12)	251(13)	74(10)	126(12)	139(11)
C(10)	590(16)	247(11)	409(15)	115(10)	336(13)	109(11)
C(11)	364(13)	264(11)	495(16)	81(10)	263(12)	29(10)
C(12)	252(11)	279(11)	370(13)	86(10)	159(10)	67(9)
C(13)	250(10)	200(9)	173(10)	-59(8)	54(8)	-25(8)
C(14)	247(11)	278(11)	270(12)	-48(9)	73(9)	-7(9)
C(15)	317(12)	299(12)	387(14)	-113(10)	112(10)	-124(10)
C(16)	480(15)	240(11)	329(13)	-57(10)	93(11)	-88(10)
C(17)	323(12)	238(11)	294(13)	-31(9)	36(10)	21(9)
C(18)	241(11)	235(10)	212(11)	-38(8)	33(8)	-21(8)
C(19)	159(9)	181(9)	272(11)	-40(8)	51(8)	4(7)
C(20)	268(12)	442(13)	304(13)	27(10)	112(10)	113(10)
C(21)	327(13)	473(14)	342(15)	113(12)	54(11)	105(11)
C(22)	178(11)	277(11)	544(16)	-10(10)	107(10)	36(9)
C(23)	216(11)	377(12)	433(15)	-89(11)	149(10)	-7(9)
C(24)	215(10)	363(12)	280(13)	-68(10)	90(9)	-26(9)
C(25)	435(13)	322(11)	240(12)	-49(9)	145(10)	91(10)
C(26A)	330(20)	340(20)	185(18)	-30(14)	65(15)	131(16)
C(27A)	420(20)	670(30)	280(20)	-130(20)	117(19)	-120(20)
C(26B)	300(30)	270(30)	280(30)	-70(20)	100(20)	-30(20)
C(27B)	400(40)	480(40)	280(30)	60(30)	120(30)	90(30)
C(31)	435(14)	302(12)	447(15)	-52(11)	94(12)	53(10)
Cl(11)	696(4)	395(3)	501(4)	-26(3)	207(3)	-103(3)
Cl(12)	305(12)	390(15)	557(17)	-125(9)	86(10)	-39(10)
Cl(13)	435(14)	990(30)	1050(60)	-380(30)	-90(20)	275(17)
C(32)	420(15)	601(17)	495(17)	-85(14)	90(12)	141(13)
Cl(21)	384(3)	423(3)	689(5)	85(3)	228(3)	46(3)
Cl(22)	310(8)	610(20)	690(20)	-305(15)	121(9)	2(9)
Cl(23)	412(10)	666(19)	692(14)	210(17)	-12(9)	66(11)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 21 (CCDC 258068).

	x	y	z	U_{iso}
H(2A)	12402(19)	4242(11)	7132(15)	34(6)
H(3A)	14110(20)	3590(13)	7527(16)	48(8)
H(4A)	15380(20)	3571(11)	8898(14)	37(7)
H(5A)	14786(17)	4189(10)	9851(12)	14(5)
H(6A)	13060(17)	4830(10)	9505(12)	20(5)
H(8A)	9677(19)	5851(11)	6475(13)	32(6)
H(9A)	10003(19)	6848(11)	5795(14)	31(6)
H(10A)	11830(20)	7455(12)	6182(15)	43(7)
H(11A)	13348(19)	7070(11)	7394(13)	29(6)
H(12A)	13040(20)	6109(11)	8143(14)	32(6)
H(14A)	6731(19)	3716(11)	7755(14)	31(6)
H(15A)	6361(19)	2530(11)	7890(13)	30(6)
H(16A)	8029(19)	1713(12)	8366(13)	36(6)
H(17A)	9992(19)	2202(11)	8672(14)	33(6)
H(18A)	10311(17)	3362(10)	8564(12)	16(5)
H(20A)	7298(19)	5108(11)	6307(14)	31(6)
H(21A)	5432(19)	5533(11)	5755(15)	38(6)
H(22A)	4209(19)	5747(11)	6637(13)	30(6)
H(23A)	5000(20)	5506(12)	8013(15)	41(7)
H(24A)	6897(19)	5009(12)	8583(15)	38(7)
H(25A)	10497	3817	6960	39
H(25B)	9016	3842	6666	39
H(25C)	10516	4226	6583	39
H(25D)	9856	3653	7005	39
H(26A)	10471	4743	6003	35
H(26B)	9806	4018	5560	35
H(27A)	7441	5146	4526	69
H(27B)	6977	4487	4965	69
H(27C)	7960	4352	4475	69
H(26C)	8007	4042	6191	34
H(26D)	8865	3721	5681	34
H(27D)	7756	5380	4581	57
H(27E)	8439	4685	4374	57
H(27F)	9238	5376	4800	57
H(31A)	4236	2459	6029	49
H(31B)	3577	2688	5066	49
H(31C)	3795	2596	5146	49
H(31D)	4058	2511	6145	49
H(32A)	3106	2758	1606	62
H(32B)	2890	3442	996	62
H(32C)	2739	3379	766	62
H(32D)	3153	2951	1644	62

Compound 24

Table 1. Crystal data and structure refinement for 24 (CCDC 690602).

Empirical formula	$C_{64}H_{58}N_2O_2P_4Cl_6Cr_2$, $4(CH_2Cl_2)$
Formula weight	1667.41
Crystallization Solvent	Dichloromethane
Crystal Habit	Plate
Crystal size	0.25 x 0.16 x 0.04 mm^3
Crystal color	Purple

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 2632 reflections used in lattice determination	2.44 to 25.55°
Unit cell dimensions	a = 13.378(4) Å b = 21.561(7) Å β= 113.178(5)° c = 14.246(5) Å
Volume	3778(2) $Å^3$
Z	2
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.466 Mg/m^3
F(000)	1700
Data collection program	Bruker SMART v5.630
θ range for data collection	1.77 to 20.10°
Completeness to θ = 20.10°	99.2 %
Index ranges	$-12 \le h \le 12$, $-20 \le k \le 20$, $-13 \le l \le 13$
Data collection scan type	ω scans at 3 settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	14486
Independent reflections	3554 [R_{int}= 0.1408]
Absorption coefficient	0.912 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9644 and 0.8041

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	3554 / 18 / 416
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.774
Final R indices [$I>2\sigma(I)$, 2190 reflections]	R1 = 0.0788, *w*R2 = 0.1305
R indices (all data)	R1 = 0.1392, *w*R2 = 0.1399
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.272 and -1.235 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

This is a weakly diffracting crystal and data extends to only $2\theta=40^o$. Three atoms C5, C9 and C19 had restraints on the anisotropic displacement parameter in order to similar isotropic behavior.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 24 (CCDC 690602). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cr(1)	9731(2)	10158(1)	8698(2)	24(1)
Cl(1)	8811(2)	10240(1)	9822(3)	26(1)
Cl(2)	10718(2)	9959(1)	7735(2)	27(1)
Cl(3)	10137(3)	11194(1)	8864(3)	34(1)
P(1)	8607(3)	9192(1)	7936(3)	24(1)
P(2)	8161(3)	10360(1)	7132(3)	24(1)
O(1)	6287(7)	8215(3)	6423(7)	39(3)
N(1)	7660(7)	9626(4)	6989(8)	22(3)
C(1)	9236(11)	8615(5)	7393(11)	27(4)
C(2)	10322(11)	8462(5)	7994(11)	32(4)
C(3)	10887(11)	8026(6)	7662(13)	35(4)
C(4)	10369(13)	7769(6)	6728(15)	53(5)
C(5)	9287(13)	7916(5)	6096(12)	43(4)
C(6)	8705(11)	8359(5)	6441(12)	36(4)
C(7)	7912(9)	8731(5)	8582(9)	17(3)
C(8)	8155(10)	8115(5)	8801(10)	28(4)
C(9)	7669(11)	7789(5)	9373(10)	37(4)
C(10)	6936(10)	8073(6)	9696(11)	44(4)
C(11)	6663(10)	8700(6)	9450(10)	30(4)
C(12)	7157(10)	9029(5)	8889(10)	24(4)
C(13)	8445(9)	10548(5)	6018(10)	20(3)
C(14)	8444(9)	10096(5)	5311(11)	27(4)
C(15)	8737(10)	10254(6)	4517(11)	37(4)
C(16)	9029(9)	10857(6)	4396(11)	34(4)
C(17)	9033(10)	11299(6)	5087(11)	32(4)
C(18)	8758(10)	11157(6)	5898(12)	37(4)
C(19)	7043(10)	10897(5)	6985(11)	19(3)
C(20)	6335(10)	11113(5)	6056(10)	27(4)
C(21)	5479(11)	11493(5)	5996(11)	29(4)
C(22)	5313(11)	11631(6)	6841(14)	45(4)
C(23)	5987(12)	11429(7)	7778(13)	64(5)
C(24)	6885(11)	11048(6)	7861(12)	47(4)
C(25)	6619(10)	9447(5)	6152(10)	26(4)
C(26)	5719(10)	9242(6)	6462(10)	28(4)
C(27)	4988(11)	9650(6)	6577(10)	38(4)
C(28)	4136(11)	9470(8)	6836(12)	52(5)
C(29)	3981(12)	8865(8)	6918(12)	58(5)
C(30)	4686(13)	8402(7)	6802(11)	50(4)
C(31)	5550(11)	8615(6)	6555(10)	32(4)
C(32)	6123(11)	7551(5)	6487(12)	67(5)
C(41)	6472(13)	577(7)	651(13)	93(6)
Cl(4)	5680(5)	304(2)	-596(5)	153(3)
Cl(5)	6463(5)	1388(2)	644(5)	123(2)
C(42)	1733(11)	1376(5)	7457(13)	54(5)
Cl(6)	3001(4)	1141(2)	7501(5)	108(2)
Cl(7)	1484(3)	2176(1)	7092(3)	58(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 24 (CCDC 690602). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	233(13)	156(11)	346(15)	0(11)	146(12)	-14(10)
Cl(1)	250(20)	206(17)	370(20)	-1(17)	171(18)	59(16)
Cl(2)	290(20)	156(18)	430(20)	9(17)	200(20)	-5(15)
Cl(3)	340(20)	181(17)	490(30)	-21(18)	180(20)	-24(16)
P(1)	260(20)	154(18)	370(30)	37(18)	180(20)	19(17)
P(2)	250(20)	104(17)	390(30)	28(17)	160(20)	24(16)
O(1)	400(70)	110(50)	540(70)	-20(50)	70(60)	-130(50)
N(1)	180(70)	90(50)	330(80)	30(50)	50(60)	30(50)
C(1)	430(110)	110(70)	340(110)	-90(70)	230(90)	-10(70)
C(2)	360(100)	100(70)	490(110)	30(70)	150(90)	-60(70)
C(3)	290(100)	160(80)	660(130)	60(80)	240(100)	30(80)
C(4)	540(130)	310(90)	890(160)	90(100)	450(120)	20(90)
C(5)	600(80)	220(60)	500(80)	30(60)	250(70)	-130(60)
C(6)	460(100)	170(70)	600(130)	-10(80)	360(100)	90(70)
C(7)	220(80)	100(70)	210(90)	-60(60)	100(70)	-20(60)
C(8)	330(90)	170(80)	390(100)	-10(70)	210(80)	50(70)
C(9)	440(80)	140(60)	420(80)	70(60)	40(70)	-80(60)
C(10)	450(110)	440(100)	670(130)	-120(90)	490(100)	-180(80)
C(11)	190(90)	360(90)	310(100)	-190(80)	60(80)	0(70)
C(12)	260(90)	150(70)	270(100)	50(70)	70(80)	-10(70)
C(13)	120(80)	140(70)	380(100)	80(70)	130(70)	-30(60)
C(14)	100(80)	140(80)	510(110)	-80(80)	50(80)	-30(60)
C(15)	430(100)	170(80)	610(120)	10(80)	320(90)	-30(70)
C(16)	320(100)	270(80)	580(120)	0(80)	350(90)	50(70)
C(17)	380(100)	290(90)	380(110)	110(90)	250(90)	-50(70)
C(18)	340(100)	240(90)	470(120)	-40(80)	110(90)	60(70)
C(19)	220(70)	100(60)	250(80)	-100(60)	120(60)	-40(50)
C(20)	230(90)	300(80)	200(100)	30(70)	-10(80)	0(70)
C(21)	430(110)	140(80)	260(110)	-30(70)	90(90)	-40(70)
C(22)	390(110)	260(90)	480(130)	-100(90)	-70(110)	110(70)
C(23)	550(120)	890(130)	380(130)	-210(110)	50(110)	330(100)
C(24)	420(110)	370(90)	520(130)	-10(90)	80(90)	210(80)
C(25)	390(100)	180(70)	240(90)	20(70)	160(80)	30(70)
C(26)	220(90)	250(90)	400(100)	50(70)	150(80)	-60(70)
C(27)	220(90)	390(90)	470(110)	60(80)	60(80)	60(80)
C(28)	310(110)	790(130)	590(130)	20(100)	300(90)	10(90)
C(29)	360(110)	770(120)	670(140)	70(110)	280(100)	-280(110)
C(30)	400(110)	510(100)	460(120)	-30(90)	30(100)	-190(100)
C(31)	310(110)	320(100)	370(110)	-40(80)	180(90)	-40(80)
C(32)	650(130)	370(90)	850(140)	30(90)	150(110)	-150(80)
C(41)	740(140)	1200(160)	580(150)	-270(130)	-40(120)	-140(120)
Cl(4)	1340(50)	1130(40)	1690(70)	-410(50)	120(50)	150(40)
Cl(5)	1530(60)	1090(40)	1140(50)	-150(40)	590(50)	-300(40)
C(42)	640(120)	310(80)	1030(150)	50(90)	710(110)	-10(80)
Cl(6)	670(40)	600(30)	2320(70)	-220(40)	970(40)	-40(30)
Cl(7)	710(30)	280(20)	910(40)	-10(20)	510(30)	-70(20)

Structures for Chapter 2

Compound 17

Table 1. Crystal data and structure refinement for 17.

Empirical formula	C41 H33 B Cl2 F3 O4 P2 Re	
Formula weight	976.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.165(2) Å	α= 95.935(2)°
	b = 12.498(2) Å	β= 97.794(2)°
	c = 14.550(3) Å	γ = 113.704(2)°
Volume	1976.2(6) $Å^3$	
Z	2	
Density (calculated)	1.641 g/cm^3	
Absorption coefficient	3.346 mm^{-1}	
F(000)	964	
Crystal size	0.30 x 0.20 x 0.06 mm^3	
Theta range for data collection	1.81 to 28.23°	
Index ranges	-15<=h<=15, -16<=k<=16, -18<=l<=18	
Reflections collected	16967	
Independent reflections	8763 [R(int) = 0.0197]	
Completeness to theta = 25.00°	99.0 %	
Absorption correction	multi-scan (Sadabs)	
Max. and min. transmission	0.8245 and 0.4335	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8763 / 0 / 487	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0259, wR2 = 0.0647	
R indices (all data)	R1 = 0.0275, wR2 = 0.0654	
Largest diff. peak and hole	2.021 and -1.306 e $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 17. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	5771(1)	6215(1)	7555(1)	13(1)
P(1)	7837(1)	6450(1)	8128(1)	14(1)
P(2)	3648(1)	5915(1)	7085(1)	14(1)
Cl(1)	3672(2)	1045(2)	7605(3)	172(2)
Cl(2)	5352(2)	257(1)	8589(1)	75(1)
F(1)	6399(2)	10146(2)	6468(2)	36(1)
F(2)	8351(2)	10529(2)	7068(2)	37(1)
F(3)	7396(3)	9281(2)	5683(2)	50(1)
O(1)	4810(2)	4177(2)	8722(2)	27(1)
O(2)	5802(2)	4735(2)	5706(2)	29(1)
O(3)	6165(2)	8223(2)	9201(2)	32(1)
O(4)	6823(2)	8702(2)	7123(2)	21(1)
C(1)	5151(3)	4906(3)	8276(2)	17(1)
C(2)	5742(3)	5226(3)	6392(2)	19(1)
C(3)	5994(3)	7464(3)	8614(2)	20(1)
C(4)	6428(3)	7604(3)	6796(2)	18(1)
B(1)	7261(3)	9703(3)	6537(3)	23(1)
C(6)	4450(6)	1081(6)	8679(4)	86(2)
C(11)	8487(3)	7235(3)	9341(2)	16(1)
C(12)	9644(3)	8175(3)	9628(2)	20(1)
C(13)	10074(3)	8711(3)	10565(2)	22(1)
C(14)	9369(3)	8314(3)	11232(2)	24(1)
C(15)	8222(3)	7376(3)	10962(2)	25(1)
C(16)	7784(3)	6842(3)	10026(2)	22(1)
C(21)	8042(3)	5083(3)	8183(2)	17(1)
C(22)	7153(3)	3977(3)	7730(2)	19(1)
C(23)	7365(3)	2964(3)	7757(2)	22(1)
C(24)	8470(3)	3056(3)	8235(2)	25(1)
C(25)	9366(3)	4146(3)	8691(2)	25(1)
C(26)	9158(3)	5164(3)	8670(2)	22(1)

C(31)	8954(2)	7223(3)	7428(2)	16(1)
C(32)	9356(3)	6588(3)	6817(2)	21(1)
C(33)	10158(3)	7166(3)	6248(2)	26(1)
C(34)	10575(3)	8374(3)	6291(2)	27(1)
C(35)	10175(3)	9012(3)	6885(2)	25(1)
C(36)	9352(3)	8440(3)	7446(2)	21(1)
C(41)	3105(2)	6510(3)	8042(2)	16(1)
C(42)	3162(3)	6108(3)	8901(2)	22(1)
C(43)	2780(3)	6545(3)	9645(2)	25(1)
C(44)	2350(3)	7413(3)	9553(2)	24(1)
C(45)	2282(3)	7805(3)	8705(2)	26(1)
C(46)	2652(3)	7358(3)	7952(2)	22(1)
C(51)	2513(3)	4373(3)	6766(2)	17(1)
C(52)	2767(3)	3518(3)	6266(3)	27(1)
C(53)	1874(3)	2374(3)	5947(3)	32(1)
C(54)	709(3)	2060(3)	6136(2)	24(1)
C(55)	448(3)	2899(3)	6641(2)	21(1)
C(56)	1338(3)	4050(3)	6952(2)	20(1)
C(61)	3262(3)	6582(3)	6102(2)	16(1)
C(62)	3914(3)	7797(3)	6140(2)	19(1)
C(63)	3617(3)	8356(3)	5427(2)	24(1)
C(64)	2663(3)	7694(3)	4675(2)	23(1)
C(65)	2022(3)	6488(3)	4633(2)	22(1)
C(66)	2314(3)	5921(3)	5336(2)	18(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 17. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	11(1)	14(1)	14(1)	4(1)	3(1)	6(1)
P(1)	12(1)	14(1)	15(1)	3(1)	2(1)	6(1)
P(2)	12(1)	15(1)	15(1)	5(1)	4(1)	6(1)
Cl(1)	105(2)	129(2)	234(3)	-70(2)	-86(2)	62(2)

Cl(2)	79(1)	42(1)	82(1)	4(1)	4(1)	8(1)
F(1)	25(1)	24(1)	61(2)	19(1)	6(1)	10(1)
F(2)	21(1)	23(1)	53(1)	13(1)	-1(1)	-2(1)
F(3)	89(2)	30(1)	39(1)	15(1)	35(1)	25(1)
O(1)	27(1)	25(1)	33(1)	15(1)	10(1)	11(1)
O(2)	30(1)	39(1)	21(1)	-1(1)	4(1)	20(1)
O(3)	36(1)	30(1)	29(1)	-6(1)	3(1)	15(1)
O(4)	21(1)	16(1)	23(1)	5(1)	4(1)	6(1)
C(1)	14(1)	17(1)	19(1)	1(1)	3(1)	7(1)
C(2)	16(1)	20(2)	21(2)	5(1)	3(1)	9(1)
C(3)	16(1)	23(2)	23(2)	5(1)	4(1)	8(1)
C(4)	15(1)	19(2)	20(1)	5(1)	4(1)	6(1)
B(1)	22(2)	14(2)	31(2)	8(1)	6(1)	5(1)
C(6)	77(4)	74(4)	75(4)	-31(3)	24(3)	7(3)
C(11)	16(1)	19(1)	16(1)	5(1)	3(1)	10(1)
C(12)	19(1)	22(2)	22(2)	4(1)	4(1)	9(1)
C(13)	19(2)	20(2)	24(2)	-1(1)	0(1)	6(1)
C(14)	29(2)	26(2)	17(2)	1(1)	-1(1)	16(1)
C(15)	27(2)	32(2)	17(2)	8(1)	5(1)	11(1)
C(16)	18(1)	23(2)	21(2)	7(1)	3(1)	4(1)
C(21)	19(1)	18(1)	17(1)	5(1)	5(1)	10(1)
C(22)	22(2)	21(2)	17(1)	5(1)	5(1)	10(1)
C(23)	31(2)	18(2)	19(1)	4(1)	12(1)	12(1)
C(24)	38(2)	26(2)	24(2)	13(1)	16(1)	23(2)
C(25)	28(2)	34(2)	25(2)	12(1)	10(1)	22(2)
C(26)	20(2)	24(2)	25(2)	8(1)	5(1)	12(1)
C(31)	11(1)	19(1)	16(1)	5(1)	2(1)	6(1)
C(32)	23(2)	22(2)	20(2)	2(1)	5(1)	10(1)
C(33)	28(2)	35(2)	20(2)	4(1)	10(1)	15(2)
C(34)	22(2)	37(2)	23(2)	12(1)	10(1)	11(1)
C(35)	25(2)	24(2)	28(2)	12(1)	9(1)	10(1)
C(36)	20(2)	22(2)	22(2)	6(1)	6(1)	10(1)
C(41)	11(1)	17(1)	16(1)	2(1)	3(1)	3(1)
C(42)	23(2)	26(2)	21(2)	7(1)	6(1)	14(1)
C(43)	24(2)	34(2)	18(2)	7(1)	7(1)	12(1)
C(44)	23(2)	28(2)	23(2)	0(1)	10(1)	10(1)

C(45)	28(2)	28(2)	32(2)	8(1)	14(1)	18(2)
C(46)	21(2)	26(2)	23(2)	9(1)	8(1)	12(1)
C(51)	15(1)	16(1)	17(1)	4(1)	2(1)	5(1)
C(52)	20(2)	22(2)	37(2)	0(1)	10(1)	6(1)
C(53)	29(2)	19(2)	43(2)	-3(1)	9(2)	8(1)
C(54)	25(2)	16(2)	23(2)	5(1)	-1(1)	1(1)
C(55)	16(1)	24(2)	21(2)	8(1)	3(1)	4(1)
C(56)	18(1)	21(2)	21(2)	7(1)	6(1)	8(1)
C(61)	15(1)	22(2)	14(1)	6(1)	6(1)	10(1)
C(62)	16(1)	21(2)	22(2)	8(1)	3(1)	7(1)
C(63)	21(2)	22(2)	30(2)	12(1)	7(1)	9(1)
C(64)	30(2)	26(2)	19(2)	11(1)	8(1)	16(1)
C(65)	28(2)	26(2)	14(1)	2(1)	1(1)	14(1)
C(66)	23(2)	18(1)	16(1)	3(1)	5(1)	10(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 17.

	x	y	z	U(eq)
H(4A)	6430	7393	6150	22
H(6A)	3862	744	9093	103
H(6B)	4991	1915	8969	103
H(12A)	10142	8449	9177	24
H(13A)	10860	9356	10751	27
H(14A)	9671	8684	11874	28
H(15A)	7735	7099	11420	30
H(16A)	6996	6200	9845	26
H(22A)	6393	3910	7399	23
H(23A)	6751	2211	7448	26
H(24A)	8614	2365	8250	30
H(25A)	10123	4204	9019	30
H(26A)	9773	5913	8986	26
H(32A)	9080	5756	6790	25
H(33A)	10419	6725	5827	31
H(34A)	11138	8768	5912	33
H(35A)	10461	9845	6913	30
H(36A)	9062	8880	7841	25
H(42A)	3468	5526	8973	26
H(43A)	2811	6253	10221	29
H(44A)	2106	7731	10068	29
H(45A)	1977	8389	8636	32
H(46A)	2596	7635	7371	26
H(52A)	3566	3722	6140	33
H(53A)	2060	1804	5599	38
H(54A)	94	1275	5920	29
H(55A)	-347	2685	6777	26
H(56A)	1145	4621	7292	24
H(62A)	4566	8249	6656	23
H(63A)	4065	9185	5456	28
H(64A)	2451	8070	4189	27

H(65A)	1372	6039	4115	27
H(66A)	1871	5090	5296	22

Compound 18

Table 1. Crystal data and structure refinement for 18 (CCDC 685990).

Empirical formula	$C_{58}H_{31}BF_{15}O_4P_2Re \bullet 0.51(CH_2Cl_2), 0.49(C_5H_{12})$
Formula weight	1414.34
Crystallization Solvent	Dichloromethane/petroleum ether
Crystal Habit	Plate
Crystal size	0.18 x 0.13 x 0.05 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9891 reflections used in lattice determination	2.34 to 24.00°
Unit cell dimensions	a = 12.6862(8) Å b = 29.8277(19) Å β= 102.822(4)° c = 15.0080(9) Å
Volume	5537.4(6) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.697 Mg/m^3
F(000)	2792
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.55 to 33.13°
Completeness to θ = 33.13°	99.7 %
Index ranges	$-19 \le h \le 19, -45 \le k \le 45, -23 \le l \le 23$
Data collection scan type	ω scans; 24 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	177247
Independent reflections	21028 [R_{int}= 0.1340]
Absorption coefficient	2.401 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8894 and 0.6718

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	21028 / 16 / 778
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.739
Final R indices [$I>2\sigma(I)$, 12708 reflections]	R1 = 0.0639, *w*R2 = 0.0939
R indices (all data)	R1 = 0.1212, *w*R2 = 0.0975
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	7.047 and -4.595 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a loop using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The solvent area is disordered and contains CH_2Cl_2 and some ill defined solvent mixture modeled as pentane. Distances and angles of the solvent were restrained, CH_2Cl_2 refined anistropically and C_5H_{12} refined with isotropic temperature parameters.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 18 (CCDC 685990). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Re(1)	2775(1)	7010(1)	2366(1)	14(1)
P(1)	4729(1)	6963(1)	2837(1)	15(1)
P(2)	840(1)	7110(1)	1824(1)	16(1)
O(1)	2751(3)	7709(1)	3903(2)	29(1)
O(2)	3187(3)	7659(1)	853(2)	26(1)
O(3)	2681(3)	6215(1)	998(2)	34(1)
O(4)	1959(2)	6142(1)	3083(2)	17(1)
F(42)	3848(2)	5762(1)	2913(2)	24(1)
F(43)	4567(2)	5212(1)	1785(2)	32(1)
F(44)	3525(2)	4416(1)	1276(2)	35(1)
F(45)	1762(2)	4202(1)	1934(2)	39(1)
F(46)	976(2)	4760(1)	2986(2)	32(1)
F(48)	3438(2)	4963(1)	4510(2)	26(1)
F(49)	4609(2)	4972(1)	6188(2)	28(1)
F(50)	4559(2)	5689(1)	7304(2)	37(1)
F(51)	3250(2)	6395(1)	6681(2)	37(1)
F(52)	2028(2)	6394(1)	4986(2)	27(1)
F(54)	230(2)	5644(1)	1992(2)	27(1)
F(55)	-1878(2)	5536(1)	1854(2)	36(1)
F(56)	-2672(2)	5405(1)	3383(2)	39(1)
F(57)	-1291(2)	5418(1)	5056(2)	34(1)
F(58)	795(2)	5559(1)	5224(2)	27(1)
B(1)	1927(4)	5686(2)	3607(3)	19(1)
C(1)	2758(4)	7454(2)	3343(3)	17(1)
C(2)	3021(4)	7436(2)	1423(3)	14(1)
C(3)	2723(4)	6516(2)	1474(3)	18(1)
C(4)	2619(4)	6472(2)	3256(3)	15(1)
C(5)	5340(3)	6729(2)	1930(3)	15(1)
C(6)	5756(3)	7018(2)	1373(3)	20(1)
C(7)	6159(4)	6847(2)	651(3)	25(1)
C(8)	6164(4)	6394(2)	498(3)	27(1)
C(9)	5728(4)	6102(2)	1037(3)	24(1)
C(10)	5301(4)	6277(2)	1752(3)	20(1)
C(11)	5274(3)	6658(2)	3905(3)	14(1)
C(12)	5911(3)	6280(2)	3997(3)	18(1)
C(13)	6282(4)	6083(2)	4858(3)	23(1)
C(14)	6006(4)	6269(2)	5622(3)	24(1)
C(15)	5371(4)	6644(2)	5535(3)	23(1)
C(16)	4996(4)	6844(2)	4694(3)	20(1)
C(17)	5488(4)	7485(2)	3100(3)	16(1)
C(18)	6607(4)	7455(2)	3424(3)	22(1)
C(19)	7243(4)	7832(2)	3569(3)	26(1)
C(20)	6788(4)	8251(2)	3392(3)	27(1)
C(21)	5670(4)	8291(2)	3092(3)	21(1)
C(22)	5038(4)	7910(2)	2933(3)	22(1)
C(23)	376(3)	6867(2)	687(3)	15(1)
C(24)	433(4)	7130(2)	-71(3)	21(1)

C(25)	217(4)	6939(2)	-940(3)	27(1)
C(26)	-64(4)	6496(2)	-1056(3)	35(1)
C(27)	-125(5)	6236(2)	-301(3)	40(2)
C(28)	112(4)	6426(2)	567(3)	32(1)
C(29)	311(4)	7683(2)	1654(3)	20(1)
C(30)	977(4)	8057(2)	1774(3)	24(1)
C(31)	550(5)	8489(2)	1631(3)	32(1)
C(32)	-561(5)	8549(2)	1363(3)	34(1)
C(33)	-1225(5)	8182(2)	1242(4)	38(2)
C(34)	-798(4)	7752(2)	1378(3)	29(1)
C(35)	-21(4)	6876(2)	2527(3)	17(1)
C(36)	345(4)	6891(2)	3478(3)	16(1)
C(37)	-319(4)	6753(2)	4050(3)	18(1)
C(38)	-1345(4)	6592(2)	3674(3)	21(1)
C(39)	-1719(4)	6569(2)	2742(3)	23(1)
C(40)	-1070(4)	6715(2)	2169(3)	24(1)
C(41)	2327(4)	5313(2)	2953(3)	19(1)
C(42)	3247(4)	5390(2)	2629(3)	18(1)
C(43)	3658(4)	5104(2)	2070(3)	23(1)
C(44)	3146(4)	4704(2)	1813(3)	24(1)
C(45)	2248(4)	4601(2)	2148(3)	28(1)
C(46)	1856(4)	4901(2)	2682(3)	21(1)
C(47)	2705(4)	5694(2)	4636(3)	18(1)
C(48)	3372(4)	5335(2)	4996(3)	16(1)
C(49)	3988(4)	5329(2)	5878(3)	20(1)
C(50)	3963(4)	5685(2)	6447(3)	24(1)
C(51)	3288(4)	6046(2)	6137(3)	23(1)
C(52)	2699(4)	6035(2)	5240(3)	21(1)
C(53)	646(4)	5622(2)	3616(3)	19(1)
C(54)	-112(4)	5600(2)	2780(3)	22(1)
C(55)	-1198(4)	5530(2)	2689(3)	26(1)
C(56)	-1596(4)	5464(2)	3456(4)	28(1)
C(57)	-899(4)	5479(2)	4297(3)	26(1)
C(58)	168(4)	5552(2)	4361(3)	24(1)
Cl(1)	1931(2)	5569(1)	7968(2)	50(1)
Cl(2)	3509(5)	5297(2)	9523(3)	142(3)
C(101)	3057(12)	5747(3)	8790(10)	144(10)
C(204)	724(7)	4996(3)	10004(6)	22(2)
C(205)	1512(8)	5308(3)	10234(6)	25(2)
C(206)	1860(20)	5433(10)	9319(13)	223(15)
C(207)	2670(20)	5763(6)	8990(20)	168(14)
C(208)	3258(8)	6220(3)	8948(6)	22(2)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 18 (CCDC 685990). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	106(1)	199(1)	108(1)	17(1)	24(1)	5(1)
P(1)	120(6)	204(8)	133(5)	-4(5)	46(4)	2(6)
P(2)	127(6)	217(8)	136(5)	39(5)	30(4)	13(5)
O(1)	230(20)	410(20)	236(18)	-62(17)	68(15)	14(17)
O(2)	320(20)	280(20)	181(16)	55(15)	93(15)	-46(17)
O(3)	330(20)	350(30)	320(20)	-99(18)	46(17)	-11(18)
O(4)	182(17)	170(19)	182(15)	6(13)	62(13)	38(14)
F(42)	220(15)	216(17)	285(14)	-42(12)	79(12)	-53(12)
F(43)	340(18)	360(20)	327(16)	0(14)	223(14)	3(14)
F(44)	386(19)	360(20)	296(16)	-140(14)	31(14)	99(15)
F(45)	326(18)	249(19)	570(20)	-157(16)	27(16)	-41(14)
F(46)	225(17)	276(19)	469(18)	-9(14)	96(14)	-69(13)
F(48)	279(16)	251(18)	232(14)	26(12)	50(12)	78(13)
F(49)	212(16)	280(18)	303(15)	68(13)	-12(12)	60(13)
F(50)	348(18)	380(20)	259(15)	-14(14)	-171(13)	36(15)
F(51)	450(20)	310(20)	270(16)	-76(14)	-92(14)	90(15)
F(52)	321(17)	266(17)	207(13)	-10(12)	30(12)	125(13)
F(54)	261(16)	390(20)	166(13)	76(13)	26(12)	23(14)
F(55)	214(17)	480(20)	328(17)	-4(15)	-34(13)	19(15)
F(56)	167(16)	460(20)	560(20)	-13(16)	129(15)	-48(14)
F(57)	318(18)	390(20)	376(17)	-4(14)	211(14)	-19(14)
F(58)	256(16)	348(19)	219(14)	28(13)	60(12)	-3(13)
B(1)	210(30)	180(30)	180(20)	30(20)	50(20)	40(20)
C(1)	100(20)	220(30)	180(20)	90(20)	-10(19)	50(20)
C(2)	110(20)	160(30)	150(20)	-38(19)	24(18)	-10(20)
C(3)	160(30)	190(30)	180(20)	50(20)	18(19)	20(20)
C(4)	110(20)	260(30)	94(19)	-41(19)	25(17)	-10(20)
C(5)	100(20)	230(30)	122(19)	-10(18)	36(17)	30(20)
C(6)	190(20)	240(30)	178(19)	0(20)	47(17)	0(20)
C(7)	230(30)	350(40)	180(20)	30(20)	80(20)	20(20)
C(8)	240(30)	390(40)	190(20)	-20(20)	70(20)	30(20)
C(9)	220(30)	290(30)	210(20)	-70(20)	50(20)	-30(20)
C(10)	160(20)	290(30)	130(20)	-10(20)	34(18)	-30(20)
C(11)	120(20)	170(30)	140(20)	-12(18)	30(17)	-10(20)
C(12)	120(20)	230(30)	180(20)	10(20)	60(18)	-20(20)
C(13)	160(30)	230(30)	290(30)	60(20)	40(20)	-20(20)
C(14)	190(30)	310(30)	180(20)	60(20)	0(20)	-50(20)
C(15)	180(30)	360(30)	170(20)	-10(20)	50(20)	-20(20)
C(16)	170(30)	250(30)	170(20)	-21(19)	20(19)	40(20)
C(17)	160(20)	160(30)	160(20)	-15(19)	87(19)	-10(20)
C(18)	230(30)	180(30)	270(20)	-30(20)	90(20)	-20(20)
C(19)	170(30)	330(30)	270(30)	-30(20)	70(20)	-50(20)
C(20)	400(40)	230(30)	200(20)	0(20)	140(20)	-100(30)
C(21)	330(30)	150(30)	140(20)	20(19)	20(20)	20(20)
C(22)	210(30)	310(40)	160(20)	20(20)	50(19)	0(20)
C(23)	60(20)	220(30)	150(20)	23(18)	-22(17)	-4(18)
C(24)	190(30)	210(30)	220(20)	46(19)	50(20)	10(20)

C(25)	220(30)	430(40)	150(20)	60(20)	39(18)	-80(30)
C(26)	380(40)	510(40)	130(20)	-20(20)	40(20)	-140(30)
C(27)	570(40)	390(40)	230(30)	-20(20)	50(30)	-210(30)
C(28)	490(40)	290(40)	170(20)	40(20)	30(20)	-130(30)
C(29)	300(30)	190(30)	130(20)	65(19)	90(20)	90(20)
C(30)	290(30)	280(30)	180(20)	30(20)	120(20)	70(20)
C(31)	550(40)	230(30)	220(20)	50(20)	190(30)	70(30)
C(32)	480(40)	370(40)	220(20)	80(20)	190(30)	180(30)
C(33)	320(30)	480(40)	340(30)	140(30)	120(30)	220(30)
C(34)	240(30)	350(40)	290(30)	90(20)	80(20)	70(30)
C(35)	110(20)	150(30)	230(20)	51(19)	-17(19)	52(19)
C(36)	150(20)	180(30)	149(19)	34(17)	17(18)	14(19)
C(37)	150(30)	200(30)	200(20)	0(20)	62(19)	10(20)
C(38)	200(30)	210(30)	260(20)	60(20)	130(20)	30(20)
C(39)	100(20)	300(30)	270(20)	30(20)	20(20)	-10(20)
C(40)	180(30)	310(30)	200(20)	30(20)	-30(20)	10(20)
C(41)	190(30)	170(30)	210(20)	50(20)	50(20)	20(20)
C(42)	190(30)	140(30)	210(20)	33(19)	53(19)	10(20)
C(43)	260(30)	220(30)	200(20)	40(20)	40(20)	30(20)
C(44)	210(30)	240(30)	240(20)	-70(20)	0(20)	110(20)
C(45)	240(30)	200(30)	310(30)	-50(20)	-100(20)	-60(20)
C(46)	110(20)	250(30)	240(20)	40(20)	10(20)	0(20)
C(47)	190(30)	140(30)	220(20)	14(19)	100(20)	20(20)
C(48)	180(20)	170(30)	180(20)	1(19)	99(19)	0(20)
C(49)	130(20)	170(30)	290(20)	80(20)	10(20)	20(20)
C(50)	220(30)	250(30)	220(20)	30(20)	-50(20)	-30(20)
C(51)	270(30)	150(30)	220(20)	-30(20)	-30(20)	-10(20)
C(52)	190(30)	200(30)	220(20)	40(20)	10(20)	20(20)
C(53)	170(30)	190(30)	210(20)	50(20)	47(19)	20(20)
C(54)	220(30)	210(30)	240(20)	50(20)	80(20)	20(20)
C(55)	180(30)	290(30)	280(30)	-20(20)	-10(20)	10(20)
C(56)	150(30)	210(30)	480(30)	10(20)	90(20)	20(20)
C(57)	290(30)	220(30)	310(30)	20(20)	150(20)	0(20)
C(58)	230(30)	240(30)	240(20)	10(20)	60(20)	30(20)
Cl(1)	790(30)	310(19)	323(15)	36(13)	-27(15)	61(16)
Cl(2)	1720(60)	1540(60)	740(30)	-320(30)	-290(40)	140(40)
C(101)	1680(130)	1740(140)	1160(120)	140(90)	890(100)	140(90)

Compound 20

Table 1. Crystal data and structure refinement for 20 (CCDC 686292).

Empirical formula	$C_{58}H_{31}BF_{15}O_4P_2Mn \cdot 1.37(CH_2Cl_2)$
Formula weight	1320.44
Crystallization Solvent	Dichloromethane/petroleum ether
Crystal Habit	Block
Crystal size	0.31 x 0.24 x 0.14 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9253 reflections used in lattice determination	2.37 to 29.67°
Unit cell dimensions	a = 12.5140(10) Å b = 29.9230(10) Å β= 101.670(4)° c = 14.9910(10) Å
Volume	5497.4(6) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.595 Mg/m^3
F(000)	2653
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.66 to 29.68°
Completeness to θ = 29.68°	97.4 %
Index ranges	$-17 \le h \le 16$, $-41 \le k \le 41$, $-19 \le l \le 20$
Data collection scan type	ω scans; 20 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	103862
Independent reflections	15189 [R_{int}= 0.0536]
Absorption coefficient	0.531 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9293 and 0.8526

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	15189 / 8 / 795
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.805
Final R indices [$I>2\sigma(I)$, 11251 reflections]	R1 = 0.0525, *w*R2 = 0.0843
R indices (all data)	R1 = 0.0766, *w*R2 = 0.0855
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.962 and -1.484 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 20 (CCDC 686292). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn(1)	2836(1)	6958(1)	2313(1)	12(1)
P(1)	4712(1)	6936(1)	2754(1)	13(1)
P(2)	985(1)	7071(1)	1804(1)	13(1)
O(1)	2753(1)	7597(1)	3821(1)	23(1)
O(2)	3259(1)	7575(1)	860(1)	22(1)
O(3)	2788(1)	6184(1)	1052(1)	24(1)
O(4)	2000(1)	6136(1)	3013(1)	14(1)
F(42)	3939(1)	5743(1)	2883(1)	19(1)
F(43)	4687(1)	5181(1)	1776(1)	27(1)
F(44)	3610(1)	4396(1)	1266(1)	32(1)
F(45)	1781(1)	4202(1)	1906(1)	35(1)
F(46)	983(1)	4767(1)	2945(1)	27(1)
F(48)	3412(1)	4956(1)	4487(1)	19(1)
F(49)	4587(1)	4973(1)	6150(1)	21(1)
F(50)	4603(1)	5708(1)	7226(1)	26(1)
F(51)	3363(1)	6430(1)	6575(1)	26(1)
F(52)	2132(1)	6419(1)	4903(1)	21(1)
F(54)	255(1)	5637(1)	1982(1)	22(1)
F(55)	-1862(1)	5509(1)	1884(1)	29(1)
F(56)	-2654(1)	5380(1)	3432(1)	33(1)
F(57)	-1264(1)	5421(1)	5081(1)	30(1)
F(58)	834(1)	5572(1)	5204(1)	23(1)
B(1)	1962(2)	5683(1)	3565(2)	14(1)
C(1)	2793(2)	7356(1)	3238(2)	14(1)
C(2)	3084(2)	7352(1)	1437(2)	16(1)
C(3)	2804(2)	6490(1)	1512(2)	15(1)
C(4)	2684(2)	6456(1)	3155(2)	13(1)
C(5)	5371(2)	6710(1)	1865(2)	14(1)
C(6)	5788(2)	7001(1)	1298(2)	19(1)
C(7)	6230(2)	6838(1)	584(2)	25(1)
C(8)	6269(2)	6386(1)	431(2)	23(1)
C(9)	5838(2)	6092(1)	978(2)	21(1)
C(10)	5377(2)	6254(1)	1682(2)	17(1)
C(11)	5275(2)	6652(1)	3835(2)	13(1)
C(12)	5896(2)	6264(1)	3934(2)	16(1)
C(13)	6282(2)	6087(1)	4800(2)	20(1)
C(14)	6059(2)	6292(1)	5562(2)	21(1)
C(15)	5436(2)	6682(1)	5467(2)	20(1)
C(16)	5053(2)	6858(1)	4612(2)	17(1)
C(17)	5448(2)	7468(1)	2990(2)	14(1)
C(18)	6581(2)	7443(1)	3279(2)	20(1)
C(19)	7212(2)	7823(1)	3410(2)	23(1)
C(20)	6727(2)	8239(1)	3278(2)	22(1)
C(21)	5606(2)	8272(1)	3016(2)	20(1)
C(22)	4971(2)	7887(1)	2867(2)	17(1)
C(23)	511(2)	6854(1)	658(2)	14(1)
C(24)	508(2)	7124(1)	-94(2)	18(1)

C(25)	243(2)	6951(1)	-965(2)	23(1)
C(26)	-30(2)	6508(1)	-1096(2)	27(1)
C(27)	-28(2)	6234(1)	-354(2)	34(1)
C(28)	261(2)	6403(1)	518(2)	25(1)
C(29)	480(2)	7650(1)	1663(2)	15(1)
C(30)	1162(2)	8023(1)	1786(2)	20(1)
C(31)	736(2)	8453(1)	1646(2)	24(1)
C(32)	-376(2)	8518(1)	1391(2)	26(1)
C(33)	-1062(2)	8152(1)	1276(2)	26(1)
C(34)	-643(2)	7725(1)	1408(2)	22(1)
C(35)	70(2)	6846(1)	2498(2)	13(1)
C(36)	388(2)	6875(1)	3438(2)	15(1)
C(37)	-297(2)	6746(1)	4010(2)	18(1)
C(38)	-1328(2)	6584(1)	3637(2)	18(1)
C(39)	-1658(2)	6553(1)	2702(2)	20(1)
C(40)	-975(2)	6679(1)	2132(2)	18(1)
C(41)	2376(2)	5308(1)	2918(2)	13(1)
C(42)	3329(2)	5373(1)	2601(2)	14(1)
C(43)	3752(2)	5084(1)	2053(2)	18(1)
C(44)	3221(2)	4688(1)	1807(2)	20(1)
C(45)	2296(2)	4596(1)	2127(2)	22(1)
C(46)	1894(2)	4898(1)	2656(2)	18(1)
C(47)	2747(2)	5700(1)	4575(2)	13(1)
C(48)	3386(2)	5340(1)	4953(2)	14(1)
C(49)	3999(2)	5336(1)	5829(2)	16(1)
C(50)	4003(2)	5701(1)	6374(2)	19(1)
C(51)	3374(2)	6069(1)	6037(2)	17(1)
C(52)	2771(2)	6056(1)	5169(2)	15(1)
C(53)	671(2)	5623(1)	3593(2)	14(1)
C(54)	-87(2)	5596(1)	2780(2)	18(1)
C(55)	-1188(2)	5516(1)	2700(2)	20(1)
C(56)	-1577(2)	5451(1)	3478(2)	23(1)
C(57)	-877(2)	5476(1)	4314(2)	21(1)
C(58)	219(2)	5559(1)	4352(2)	18(1)
C(70)	3108(3)	9221(1)	3962(2)	149(2)
Cl(1)	2139(1)	9419(1)	3013(1)	113(1)
Cl(2)	3142(1)	8631(1)	3898(1)	64(1)
Cl(3)	3467(3)	9721(1)	4584(2)	103(2)
C(72)	452(3)	5024(3)	9469(3)	43(2)
Cl(5)	1504(2)	5281(1)	10272(1)	45(1)
Cl(6)	-753(2)	4995(1)	9913(2)	45(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 20 (CCDC 686292). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	111(2)	134(2)	120(2)	7(2)	18(1)	-1(1)
P(1)	117(3)	133(3)	135(3)	-2(3)	24(2)	1(2)
P(2)	120(3)	147(3)	126(4)	20(3)	14(3)	5(2)
O(1)	231(9)	240(10)	212(11)	-75(8)	54(8)	2(7)
O(2)	246(9)	221(9)	186(11)	54(8)	60(8)	-29(7)
O(3)	226(9)	245(10)	241(11)	-72(8)	17(8)	11(7)
O(4)	132(8)	123(8)	161(10)	12(7)	44(7)	-7(6)
F(42)	171(7)	151(7)	269(9)	-31(6)	84(6)	-30(5)
F(43)	287(8)	258(8)	325(10)	-10(7)	190(7)	28(6)
F(44)	348(8)	293(8)	296(10)	-143(7)	47(7)	83(6)
F(45)	249(8)	196(8)	577(12)	-163(7)	-12(7)	-33(6)
F(46)	188(7)	175(7)	467(11)	-20(7)	103(7)	-56(6)
F(48)	232(7)	146(7)	189(8)	13(6)	33(6)	42(5)
F(49)	177(7)	180(7)	243(9)	49(6)	-11(6)	48(5)
F(50)	283(8)	268(8)	180(9)	-6(6)	-98(6)	42(6)
F(51)	313(8)	208(8)	217(9)	-60(6)	-33(6)	47(6)
F(52)	231(7)	174(7)	209(9)	-1(6)	14(6)	79(5)
F(54)	168(7)	279(8)	194(9)	60(6)	26(6)	-17(6)
F(55)	160(7)	358(9)	320(10)	15(7)	-39(7)	-25(6)
F(56)	151(7)	318(9)	542(11)	19(8)	106(7)	-42(6)
F(57)	261(8)	319(9)	362(10)	41(7)	202(7)	-6(6)
F(58)	220(7)	296(8)	185(9)	21(6)	65(6)	-12(6)
B(1)	149(14)	111(13)	167(16)	35(11)	31(12)	-2(10)
C(1)	86(11)	150(12)	194(15)	39(11)	13(10)	1(9)
C(2)	108(12)	161(12)	199(15)	-29(11)	3(10)	1(9)
C(3)	107(12)	192(13)	164(15)	36(11)	27(10)	-9(9)
C(4)	104(11)	145(12)	162(14)	-26(10)	45(10)	28(9)
C(5)	75(11)	188(12)	135(14)	-9(10)	2(10)	9(9)
C(6)	202(13)	186(13)	175(15)	-12(11)	37(11)	12(10)
C(7)	287(15)	276(15)	198(16)	52(12)	105(12)	4(11)
C(8)	247(14)	302(15)	175(15)	-46(12)	91(11)	39(11)
C(9)	211(13)	208(13)	217(16)	-68(11)	43(11)	8(10)
C(10)	126(12)	202(13)	166(14)	-5(10)	12(10)	-11(9)
C(11)	84(11)	170(12)	135(14)	0(10)	19(10)	-41(9)
C(12)	134(12)	170(12)	171(14)	-4(10)	52(10)	-8(9)
C(13)	160(12)	182(13)	251(16)	53(11)	29(11)	10(9)
C(14)	173(13)	255(14)	170(15)	63(11)	-4(11)	-54(10)
C(15)	177(13)	283(14)	148(15)	-31(11)	35(11)	-24(10)
C(16)	136(12)	204(13)	166(15)	-13(10)	12(10)	28(9)
C(17)	153(12)	157(12)	119(14)	-6(10)	56(10)	-24(9)
C(18)	173(13)	185(13)	246(16)	-20(11)	55(11)	-12(10)
C(19)	170(13)	259(14)	282(17)	-44(12)	74(11)	-71(10)
C(20)	274(14)	214(13)	182(15)	-17(11)	65(11)	-123(11)
C(21)	297(14)	127(12)	164(15)	3(10)	48(11)	-16(10)
C(22)	189(13)	206(13)	115(14)	-4(10)	53(10)	-5(10)
C(23)	65(11)	209(13)	148(14)	28(10)	8(9)	0(9)
C(24)	149(12)	198(12)	195(15)	41(11)	39(10)	-4(9)

C(25)	199(13)	358(15)	142(15)	76(12)	46(11)	-34(11)
C(26)	272(14)	406(17)	131(15)	-35(13)	13(11)	-120(12)
C(27)	448(17)	323(16)	240(18)	-46(13)	19(14)	-194(13)
C(28)	343(15)	265(14)	134(15)	35(11)	12(12)	-73(11)
C(29)	191(12)	167(12)	94(13)	30(10)	53(10)	41(9)
C(30)	222(13)	198(13)	188(15)	7(11)	79(11)	32(10)
C(31)	361(16)	164(13)	236(16)	11(11)	121(12)	8(11)
C(32)	396(16)	207(14)	200(16)	34(11)	135(12)	132(11)
C(33)	205(14)	326(16)	277(17)	63(12)	81(12)	125(11)
C(34)	197(13)	231(14)	227(16)	45(11)	54(11)	33(10)
C(35)	103(11)	140(12)	163(14)	34(10)	42(10)	22(8)
C(36)	120(11)	146(12)	170(14)	10(10)	22(10)	9(9)
C(37)	218(13)	163(12)	158(14)	19(10)	68(11)	48(10)
C(38)	161(13)	167(12)	250(16)	39(11)	108(11)	20(9)
C(39)	117(12)	195(13)	275(17)	43(11)	18(11)	-6(9)
C(40)	143(12)	222(13)	178(15)	44(11)	5(11)	23(10)
C(41)	107(11)	129(11)	140(14)	33(10)	-1(10)	13(8)
C(42)	157(12)	91(11)	166(14)	1(10)	-8(10)	-14(9)
C(43)	165(13)	210(13)	174(15)	14(11)	54(11)	31(10)
C(44)	253(14)	163(12)	178(15)	-67(11)	8(11)	86(10)
C(45)	163(13)	129(12)	321(17)	-61(11)	-64(11)	-16(9)
C(46)	107(12)	169(12)	247(15)	18(11)	13(11)	5(9)
C(47)	101(11)	145(12)	162(14)	27(10)	50(10)	-2(9)
C(48)	150(12)	115(11)	191(14)	-3(10)	85(10)	-11(9)
C(49)	98(12)	148(12)	229(15)	63(10)	51(10)	16(9)
C(50)	148(12)	207(13)	188(15)	30(11)	-18(11)	-12(10)
C(51)	187(13)	143(12)	189(15)	-31(10)	29(11)	1(9)
C(52)	132(12)	124(12)	200(15)	56(10)	30(10)	48(9)
C(53)	143(12)	99(11)	193(15)	24(10)	57(10)	15(9)
C(54)	183(13)	151(12)	230(16)	53(11)	102(11)	14(9)
C(55)	142(13)	171(12)	264(17)	34(11)	0(12)	-2(9)
C(56)	105(13)	171(13)	428(19)	-6(12)	95(12)	-21(9)
C(57)	219(14)	156(12)	283(17)	49(11)	148(12)	11(10)
C(58)	173(13)	131(12)	224(16)	13(10)	39(11)	10(9)
C(70)	2880(70)	1200(40)	380(30)	100(30)	300(40)	-680(50)
Cl(1)	2066(13)	558(7)	816(9)	15(6)	381(9)	141(8)
Cl(2)	804(10)	622(9)	544(10)	-132(7)	233(7)	110(7)
Cl(3)	1190(30)	1100(30)	760(30)	200(20)	120(20)	-250(20)
C(72)	430(60)	410(50)	380(60)	-120(50)	-100(50)	-40(40)
Cl(5)	421(12)	547(14)	327(14)	-13(10)	-51(10)	19(10)
Cl(6)	468(14)	342(12)	497(17)	103(12)	-8(12)	-62(10)

Compound 24

Table 1. Crystal data and structure refinement for 24 (CCDC 644905).

Empirical formula	$[C_{41}H_{34}O_4P_2Re]^+ [BC_{24}H_{20}]^- \bullet \frac{1}{2}(CH_2Cl_2)$
Formula weight	1242.96
Crystallization Solvent	Dichloromethane
Crystal Habit	Tabular
Crystal size	0.30 x 0.30 x 0.08 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 35109 reflections used in lattice determination	2.30 to 39.58°
Unit cell dimensions	a = 20.2321(5) Å b = 8.8558(2) Å c = 15.6377(4) Å
Volume	2801.83(12) $Å^3$
Z	2
Crystal system	Orthorhombic
Space group	$Pmn2_1$
Density (calculated)	1.473 Mg/m^3
F(000)	1256
Data collection program	Bruker SMART v5.630
θ range for data collection	1.65 to 40.56°
Completeness to θ = 40.56°	96.1 %
Index ranges	$-36 \le h \le 36$, $-15 \le k \le 15$, $-28 \le l \le 26$
Data collection scan type	ω scans at 6 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	74440
Independent reflections	16931 [R_{int}= 0.0676]
Absorption coefficient	2.370 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7445 and 0.3248

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	16931 / 1 / 371
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.016
Final R indices [I>2σ(I), 14911 reflections]	R1 = 0.0316, *w*R2 = 0.0606
R indices (all data)	R1 = 0.0404, *w*R2 = 0.0637
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.004
Average shift/error	0.000
Absolute structure determination	Anomalous differences
Absolute structure parameter	-0.001(3)
Largest diff. peak and hole	2.141 and -1.452 e.Å^{-3}

Special Refinement Details

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 24 (CCDC 644905). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Re	10000	9550(1)	7500(1)	11(1)
P(1)	8798(1)	9351(1)	7519(1)	13(1)
O(1)	10000	13007(3)	7898(2)	37(1)
O(2)	10000	10376(2)	5540(1)	22(1)
O(3)	10000	6029(2)	7434(3)	29(1)
O(4)	10000	7907(3)	9164(1)	20(1)
C(1)	10000	11745(3)	7742(2)	20(1)
C(2)	10000	10045(3)	6250(2)	14(1)
C(3)	10000	7303(3)	7426(3)	18(1)
C(4)	10000	9220(3)	8806(2)	15(1)
C(5)	10000	7772(5)	10094(2)	31(1)
C(6)	8421(1)	8249(3)	6649(2)	18(1)
C(7)	8793(1)	7620(2)	5989(1)	18(1)
C(8)	8488(1)	6855(2)	5315(2)	23(1)
C(9)	7808(1)	6684(3)	5311(2)	30(1)
C(10)	7431(1)	7269(3)	5980(2)	36(1)
C(11)	7731(1)	8054(3)	6643(2)	27(1)
C(12)	8311(1)	11090(2)	7486(2)	16(1)
C(13)	8525(1)	12251(2)	6941(1)	21(1)
C(14)	8155(1)	13564(2)	6855(2)	26(1)
C(15)	7570(1)	13732(2)	7311(2)	26(1)
C(16)	7347(1)	12590(3)	7841(2)	24(1)
C(17)	7712(1)	11258(2)	7926(1)	20(1)
C(18)	8526(1)	8354(3)	8479(2)	18(1)
C(19)	8482(1)	6784(2)	8458(2)	24(1)
C(20)	8367(1)	5983(3)	9219(2)	32(1)
C(21)	8295(1)	6733(4)	9976(2)	36(1)
C(22)	8342(1)	8292(3)	10010(2)	32(1)
C(23)	8466(1)	9104(3)	9261(2)	25(1)
B	10000	584(2)	2506(5)	14(1)
C(24)	9357(1)	1119(2)	3082(1)	14(1)
C(25)	9064(1)	2551(2)	2996(1)	18(1)
C(26)	8557(1)	3056(3)	3535(2)	23(1)
C(27)	8327(1)	2135(3)	4192(2)	24(1)
C(28)	8604(1)	712(2)	4298(1)	22(1)
C(29)	9108(1)	223(2)	3753(1)	18(1)
C(30)	10000	1386(3)	1558(2)	16(1)
C(31)	9415(1)	1729(2)	1113(1)	21(1)
C(32)	9410(1)	2490(3)	335(2)	27(1)
C(33)	10000	2926(4)	-46(2)	29(1)
C(34)	10000	-1235(3)	2324(1)	15(1)
C(35)	9412(1)	-2049(2)	2194(1)	17(1)
C(36)	9409(1)	-3577(2)	1963(1)	19(1)
C(37)	10000	-4346(3)	1842(2)	20(1)
C(41)	0	3772(4)	4709(2)	23(1)
Cl(1)	0	5479(1)	4116(1)	29(1)
Cl(2)	0	4151(1)	5824(1)	26(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 24 (CCDC 644905). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re	160(1)	82(1)	88(1)	3(1)	0	0
P(1)	163(2)	113(2)	115(2)	14(3)	2(3)	-13(1)
O(1)	810(20)	94(9)	216(11)	8(8)	0	0
O(2)	286(10)	234(10)	124(9)	44(7)	0	0
O(3)	529(12)	121(7)	234(13)	18(10)	0	0
O(4)	228(9)	240(10)	126(9)	64(7)	0	0
C(1)	366(15)	150(11)	74(9)	18(7)	0	0
C(2)	158(11)	147(11)	124(11)	26(8)	0	0
C(3)	270(10)	111(9)	147(15)	-51(10)	0	0
C(4)	180(11)	147(11)	121(11)	2(8)	0	0
C(5)	246(14)	540(20)	127(13)	137(13)	0	0
C(6)	222(10)	136(9)	165(10)	2(7)	-41(8)	-8(7)
C(7)	238(9)	162(8)	153(8)	15(6)	-21(6)	-33(6)
C(8)	305(11)	194(9)	193(10)	-15(7)	-40(8)	-38(7)
C(9)	334(12)	253(11)	303(12)	-70(9)	-127(9)	-19(8)
C(10)	238(11)	362(13)	480(17)	-168(11)	-117(10)	3(9)
C(11)	202(9)	267(10)	345(12)	-90(9)	-63(8)	25(7)
C(12)	179(6)	135(6)	179(6)	-9(11)	17(12)	1(4)
C(13)	206(8)	182(9)	231(10)	63(7)	57(7)	22(6)
C(14)	240(10)	167(9)	374(13)	57(8)	38(8)	14(7)
C(15)	232(9)	157(8)	403(17)	-13(7)	14(7)	51(6)
C(16)	188(9)	247(10)	284(10)	-74(8)	29(7)	13(7)
C(17)	197(8)	176(8)	213(9)	-15(7)	36(6)	-14(6)
C(18)	170(9)	212(10)	164(10)	57(7)	17(7)	-45(7)
C(19)	222(9)	212(9)	273(11)	100(7)	4(7)	-33(7)
C(20)	233(10)	334(12)	398(14)	239(11)	-20(9)	-51(8)
C(21)	216(10)	563(17)	286(13)	254(12)	-21(9)	-97(10)
C(22)	243(10)	558(16)	165(10)	99(10)	-28(7)	-96(10)
C(23)	234(10)	341(11)	174(9)	38(8)	-15(7)	-88(8)
B	155(8)	123(9)	132(9)	-6(17)	0	0
C(24)	147(7)	148(8)	131(7)	-4(5)	-14(5)	-13(5)
C(25)	204(8)	162(8)	171(8)	-1(6)	2(6)	24(6)
C(26)	216(9)	226(9)	257(10)	-18(7)	0(7)	86(7)
C(27)	179(9)	292(10)	233(10)	-38(8)	35(7)	33(7)
C(28)	200(9)	270(10)	181(9)	23(7)	46(7)	-9(7)
C(29)	188(8)	187(9)	154(8)	21(6)	10(6)	6(6)
C(30)	229(11)	98(10)	136(11)	-2(8)	0	0
C(31)	264(9)	200(9)	163(9)	5(6)	-34(7)	16(7)
C(32)	421(13)	235(10)	150(9)	-11(7)	-75(8)	58(8)
C(33)	600(20)	169(13)	94(12)	-3(9)	0	0
C(34)	205(10)	124(10)	118(13)	22(6)	0	0
C(35)	209(8)	151(8)	158(8)	21(6)	-21(6)	-5(6)
C(36)	260(9)	144(8)	150(8)	11(6)	-32(6)	-30(6)
C(37)	335(15)	113(11)	146(12)	21(8)	0	0
C(41)	360(16)	217(13)	126(12)	-26(9)	0	0
Cl(1)	402(4)	293(4)	188(3)	68(3)	0	0
Cl(2)	401(4)	241(3)	123(3)	-10(2)	0	0

Compound 26

Table 1. Crystal data and structure refinement for 26 (CCDC 685551).

Empirical formula	$C_{41}H_{35}O_4P_2Mn$
Formula weight	708.57
Crystallization Solvent	THF/petroleum ether
Crystal Habit	Needle
Crystal size	0.41 x 0.08 x 0.03 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9881 reflections used in lattice determination	2.22 to 27.18°
Unit cell dimensions	a = b = 43.9520(16) Å c = 11.9031(5) Å
Volume	19913.5(13) $Å^3$
Z	18
Crystal system	Rhombohedral
Space group	R-3
Density (calculated)	1.064 Mg/m^3
F(000)	6624
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.79 to 27.20°
Completeness to θ = 27.20°	99.8 %
Index ranges	$-49 \leq h \leq 56$, $-56 \leq k \leq 32$, $-15 \leq l \leq 15$
Data collection scan type	ω scans; 6 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	46126
Independent reflections	9850 [R_{int}= 0.0768]
Absorption coefficient	0.403 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9880 and 0.8520

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	9850 / 0 / 434
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.519
Final R indices [$I>2\sigma(I)$, 6210 reflections]	R1 = 0.0419, *w*R2 = 0.0766
R indices (all data)	R1 = 0.0713, *w*R2 = 0.0783
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	0.457 and -0.285 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The solvent region (25.5% of the unit cell volume) contains two severely disordered THF molecules and other ill-defined density. The program SQUEEZE was used to flatten the solvent area. The three solvent voids are located at 0.000 0.000 -0.010, 0.333 0.667 0.829 and 0.667 0.333 0.496 each with a volume of 1692 Å and electron density equaling 310 electrons. The THF would contribute 288 electrons to each void (two THF times three) which is in reasonable agreement with the 310 electrons accounted for by solvent flattening.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 26 (CCDC 685551). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn(1)	7299(1)	1358(1)	5897(1)	21(1)
P(1)	7496(1)	1520(1)	4097(1)	22(1)
P(2)	7174(1)	1224(1)	7762(1)	20(1)
O(1)	6743(1)	662(1)	5072(2)	41(1)
O(2)	7913(1)	1263(1)	6272(1)	27(1)
O(3)	7632(1)	2120(1)	6487(1)	31(1)
O(4)	6880(1)	1737(1)	5845(2)	40(1)
C(1)	6973(1)	928(1)	5414(2)	30(1)
C(2)	7671(1)	1301(1)	6122(2)	22(1)
C(3)	7508(1)	1828(1)	6267(2)	24(1)
C(4)	6831(1)	1390(1)	5621(2)	33(1)
C(5)	6562(1)	1745(1)	5653(3)	54(1)
C(6)	7640(1)	1250(1)	3344(2)	22(1)
C(7)	7558(1)	917(1)	3718(2)	26(1)
C(8)	7656(1)	712(1)	3103(2)	30(1)
C(9)	7839(1)	836(1)	2101(2)	29(1)
C(10)	7925(1)	1169(1)	1724(2)	28(1)
C(11)	7829(1)	1375(1)	2338(2)	26(1)
C(12)	7893(1)	1956(1)	3966(2)	21(1)
C(13)	8183(1)	2026(1)	4624(2)	26(1)
C(14)	8490(1)	2349(1)	4573(2)	28(1)
C(15)	8509(1)	2607(1)	3885(2)	29(1)
C(16)	8225(1)	2545(1)	3222(2)	31(1)
C(17)	7918(1)	2218(1)	3258(2)	27(1)
C(18)	7184(1)	1528(1)	3087(2)	24(1)
C(19)	7075(1)	1775(1)	3213(2)	33(1)
C(20)	6824(1)	1775(1)	2504(2)	39(1)
C(21)	6673(1)	1520(1)	1676(2)	42(1)
C(22)	6772(1)	1271(1)	1558(2)	39(1)
C(23)	7028(1)	1273(1)	2252(2)	30(1)
C(24)	7206(1)	848(1)	8302(2)	20(1)
C(25)	7148(1)	570(1)	7608(2)	30(1)
C(26)	7134(1)	271(1)	8039(2)	37(1)
C(27)	7176(1)	243(1)	9182(2)	32(1)
C(28)	7241(1)	521(1)	9880(2)	26(1)
C(29)	7258(1)	821(1)	9443(2)	22(1)
C(30)	7479(1)	1575(1)	8712(2)	20(1)
C(31)	7838(1)	1694(1)	8623(2)	29(1)
C(32)	8079(1)	1961(1)	9310(2)	29(1)
C(33)	7967(1)	2116(1)	10088(2)	29(1)
C(34)	7614(1)	1998(1)	10190(2)	34(1)
C(35)	7370(1)	1728(1)	9515(2)	28(1)
C(36)	6741(1)	1116(1)	8301(2)	22(1)
C(37)	6631(1)	1364(1)	8209(2)	32(1)
C(38)	6307(1)	1294(1)	8613(2)	44(1)
C(39)	6082(1)	969(1)	9096(2)	45(1)
C(40)	6181(1)	719(1)	9168(2)	38(1)

C(41)	6509(1)	791(1)	8765(2)	27(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 26 (CCDC 685551). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	199(2)	246(2)	123(2)	-20(2)	-2(2)	55(2)
P(1)	205(4)	238(4)	138(3)	-13(3)	-6(3)	43(3)
P(2)	183(4)	220(4)	133(3)	-25(3)	5(3)	62(3)
O(1)	309(11)	366(12)	307(12)	-67(9)	-19(9)	-8(10)
O(2)	298(11)	287(10)	211(10)	-10(8)	7(8)	144(9)
O(3)	343(11)	269(11)	260(11)	-29(9)	-24(8)	109(9)
O(4)	372(12)	526(13)	370(12)	-55(10)	-87(9)	269(11)
C(1)	272(16)	399(18)	150(14)	-5(13)	44(12)	102(15)
C(2)	294(16)	190(14)	95(13)	-19(10)	45(11)	65(12)
C(3)	163(14)	376(17)	131(13)	34(12)	18(11)	103(13)
C(4)	289(16)	399(18)	217(16)	-1(13)	1(12)	114(14)
C(5)	500(20)	820(30)	440(20)	-59(18)	-130(16)	444(19)
C(6)	196(14)	247(14)	132(13)	-45(11)	-6(11)	40(12)
C(7)	289(15)	278(15)	130(14)	-13(11)	26(11)	70(13)
C(8)	353(16)	260(15)	193(15)	-37(12)	-9(12)	91(13)
C(9)	272(15)	346(17)	189(15)	-117(12)	-33(12)	97(13)
C(10)	231(15)	342(17)	136(13)	-33(12)	29(11)	46(13)
C(11)	244(15)	259(15)	160(14)	-12(11)	-18(11)	38(12)
C(12)	181(13)	215(14)	155(13)	-29(11)	27(11)	46(11)
C(13)	233(15)	305(16)	186(14)	24(12)	11(11)	85(13)
C(14)	211(15)	376(17)	197(15)	-53(13)	-17(11)	106(13)
C(15)	215(15)	205(15)	344(17)	-110(12)	42(12)	30(12)
C(16)	294(16)	243(15)	368(17)	44(13)	73(13)	109(13)
C(17)	247(15)	289(16)	235(15)	1(12)	-14(12)	100(13)
C(18)	162(14)	293(16)	148(14)	41(12)	0(11)	16(12)
C(19)	250(15)	365(17)	254(16)	8(13)	-43(12)	68(14)
C(20)	268(16)	480(19)	387(19)	101(15)	-23(14)	155(15)
C(21)	186(15)	640(20)	247(17)	102(16)	-42(13)	71(16)
C(22)	247(16)	500(20)	188(16)	-14(14)	-14(12)	7(15)
C(23)	223(15)	327(16)	184(15)	23(12)	31(12)	21(13)
C(24)	141(13)	228(14)	172(14)	-24(11)	24(10)	40(11)
C(25)	393(17)	309(16)	180(14)	-24(12)	21(12)	155(14)
C(26)	530(19)	270(16)	292(17)	-75(13)	19(14)	180(15)
C(27)	375(17)	258(16)	332(17)	46(13)	46(13)	159(14)
C(28)	247(15)	300(16)	208(14)	2(12)	-10(11)	115(13)
C(29)	188(14)	231(14)	192(14)	-39(11)	1(11)	77(12)
C(30)	212(14)	194(13)	122(13)	4(10)	-14(11)	52(11)
C(31)	264(16)	359(17)	199(15)	-100(12)	-25(12)	117(13)
C(32)	201(14)	314(16)	249(15)	-41(12)	-28(12)	53(13)
C(33)	317(17)	223(15)	229(15)	-59(12)	-90(12)	61(13)
C(34)	414(18)	365(17)	243(16)	-120(13)	-41(13)	205(15)
C(35)	239(15)	333(16)	210(15)	-55(12)	-27(12)	100(13)
C(36)	211(14)	310(15)	122(13)	-70(11)	-51(11)	106(13)
C(37)	338(17)	425(18)	199(15)	-54(13)	-34(13)	204(15)

C(38)	450(20)	730(20)	325(18)	-178(17)	-111(15)	434(19)
C(39)	233(17)	770(30)	343(18)	-211(17)	-43(14)	237(18)
C(40)	212(16)	484(19)	282(17)	-124(14)	2(12)	49(15)
C(41)	197(14)	352(16)	188(14)	-86(12)	-11(11)	78(13)

Structures for Appendix 1

Compound 10

Table 1. Crystal data and structure refinement for 10 (CCDC 237454).

Empirical formula	$C_{48}H_{47}Cl_2O_4P_2Cr$
Formula weight	872.70
Crystallization Solvent	Dichloromethane/petroleum ether
Crystal Habit	Fragment
Crystal size	0.38 x 0.26 x 0.19 mm^3
Crystal color	Pink/purple

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 19252 reflections used in lattice determination	2.29 to 28.06°
Unit cell dimensions	a = 32.667(2) Å b = 15.4563(9) Å β= 132.245(2)° c = 22.6716(16) Å
Volume	8474.1(10) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/c
Density (calculated)	1.368 Mg/m^3
F(000)	3640
θ range for data collection	1.56 to 28.44°
Completeness to θ = 28.44°	93.6 %
Index ranges	$-43 \le h \le 42$, $-20 \le k \le 20$, $-28 \le l \le 30$
Data collection scan type	ω scans at 5 ϕ settings
Reflections collected	61900
Independent reflections	10011 [R_{int}= 0.0726]
Absorption coefficient	0.516 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9083 and 0.8280

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10011 / 51 / 592
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.861
Final R indices [$I>2\sigma(I)$, 7089 reflections]	R1 = 0.0487, *w*R2 = 0.0809
R indices (all data)	R1 = 0.0745, *w*R2 = 0.0827
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.004
Average shift/error	0.000
Largest diff. peak and hole	0.652 and -0.484 e.Å^{-3}

Special Refinement Details

The molecule contains two very different chromium to phosphorus interactions. One of these, Cr-P1, appears to be an average chromium-phosphorus bond. The other, Cr-P2, is 0.4Å longer (see Table 2). For this reason no bond was drawn from Cr to P2 in the figures. Additionally, one methoxyphenyl ligand on P2 is disordered. The disorder appears to be more complex than a simple rotation around the P-C bond that would result in the methoxy group on one side or the other of the phenyl ring. There is an accompanying displacement in the ring carbons. The SAME command was applied to both disordered groups to restrain them to imitate the unbonded methoxyphenyl ligand on P1.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 10 (CCDC 237454). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Cr(1)	2494(1)	8840(1)	1357(1)	20(1)	1
P(1)	2693(1)	10420(1)	1531(1)	18(1)	1
P(2)	1647(1)	9990(1)	970(1)	18(1)	1
O(1)	2243(1)	9233(1)	215(1)	22(1)	1
C(1)	2328(1)	10736(1)	510(1)	18(1)	1
C(2)	2207(1)	11586(2)	250(1)	22(1)	1
C(3)	1930(1)	11801(2)	-530(1)	28(1)	1
C(4)	1787(1)	11149(2)	-1056(1)	31(1)	1
C(5)	1907(1)	10294(2)	-814(1)	27(1)	1
C(6)	2161(1)	10087(2)	-40(1)	20(1)	1
C(7)	2133(1)	8561(2)	-325(1)	32(1)	1
O(2)	3498(1)	10835(1)	1384(1)	26(1)	1
C(8)	3287(1)	11130(1)	2166(1)	19(1)	1
C(9)	3422(1)	11508(1)	2835(1)	25(1)	1
C(10)	3890(1)	12018(2)	3345(1)	33(1)	1
C(11)	4223(1)	12157(2)	3186(1)	33(1)	1
C(12)	4105(1)	11779(2)	2533(1)	27(1)	1
C(13)	3644(1)	11256(1)	2031(1)	21(1)	1
C(14)	3885(1)	10830(2)	1280(2)	34(1)	1
O(3)	1000(1)	9559(2)	-717(2)	25(1)	0.663(3)
C(15)	1181(7)	10712(6)	108(4)	19(2)	0.663(3)
C(16)	1083(2)	11559(3)	180(3)	18(1)	0.663(3)
C(17)	741(2)	12112(3)	-471(3)	26(1)	0.663(3)
C(18)	492(3)	11793(4)	-1220(3)	27(1)	0.663(3)
C(19)	571(3)	10941(3)	-1319(3)	23(1)	0.663(3)
C(20)	905(3)	10405(3)	-664(4)	21(1)	0.663(3)
C(21)	664(2)	9180(2)	-1492(2)	34(1)	0.663(3)
O(3B)	1094(2)	11725(3)	539(3)	23(1)	0.337(3)
C(15B)	1149(13)	10509(11)	-19(7)	13(3)	0.337(3)
C(16B)	975(5)	10062(7)	-682(5)	14(3)	0.337(3)
C(17B)	639(3)	10446(5)	-1428(4)	30(2)	0.337(3)
C(18B)	471(5)	11284(6)	-1497(5)	29(3)	0.337(3)
C(19B)	606(5)	11748(6)	-864(5)	20(3)	0.337(3)
C(20B)	937(4)	11340(6)	-126(4)	19(3)	0.337(3)
C(21B)	842(3)	12544(4)	432(4)	28(2)	0.337(3)
O(4)	669(1)	9035(1)	236(1)	32(1)	1
C(22)	1271(1)	9966(1)	1302(1)	18(1)	1
C(23)	1419(1)	10432(1)	1944(1)	21(1)	1
C(24)	1107(1)	10397(2)	2151(1)	24(1)	1
C(25)	646(1)	9878(2)	1726(2)	29(1)	1
C(26)	481(1)	9411(2)	1078(2)	28(1)	1
C(27)	795(1)	9454(1)	869(1)	22(1)	1
C(28)	195(1)	8490(2)	-235(2)	37(1)	1
C(29)	2220(1)	10751(1)	1656(1)	20(1)	1
C(30)	3247(1)	8411(1)	1780(1)	22(1)	1
C(31)	3470(1)	8691(2)	1454(1)	28(1)	1
C(32)	3987(1)	8435(2)	1750(2)	36(1)	1

C(33)	4306(1)	7882(2)	2395(2)	39(1)	1
C(34)	4102(1)	7586(2)	2729(2)	35(1)	1
C(35)	3587(1)	7849(1)	2426(1)	26(1)	1
C(36)	2081(1)	7672(1)	939(1)	21(1)	1
C(37)	2326(1)	6861(2)	1256(1)	25(1)	1
C(38)	2024(1)	6095(2)	978(1)	27(1)	1
C(39)	1457(1)	6112(2)	362(2)	31(1)	1
C(40)	1198(1)	6904(2)	34(2)	31(1)	1
C(41)	1503(1)	7658(2)	316(1)	28(1)	1
C(42)	2688(1)	8764(1)	2423(1)	22(1)	1
C(43)	3189(1)	9053(2)	3147(1)	32(1)	1
C(44)	3316(1)	8983(2)	3861(2)	45(1)	1
C(45)	2941(1)	8624(2)	3885(2)	46(1)	1
C(46)	2440(1)	8340(2)	3190(2)	35(1)	1
C(47)	2318(1)	8407(1)	2473(1)	26(1)	1
C(48)	419(1)	5328(2)	6331(2)	36(1)	1
Cl(1)	135(1)	6005(1)	5508(1)	48(1)	1
Cl(2)	-93(1)	4988(1)	6338(1)	61(1)	1

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 10 (CCDC 237454). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	211(2)	216(2)	184(2)	0(2)	141(2)	-1(2)
P(1)	173(3)	219(3)	167(3)	2(3)	123(3)	2(3)
P(2)	164(3)	235(3)	147(3)	-5(3)	102(3)	0(3)
O(1)	304(10)	215(9)	184(9)	-11(7)	183(8)	33(7)
C(1)	145(12)	248(13)	165(12)	1(10)	116(11)	-2(10)
C(2)	201(13)	236(14)	254(14)	-2(11)	162(12)	-12(10)
C(3)	236(14)	293(15)	258(15)	85(12)	143(13)	-5(11)
C(4)	271(14)	423(17)	182(14)	65(13)	131(12)	-12(13)
C(5)	292(15)	349(16)	187(13)	-32(11)	165(13)	-34(12)
C(6)	185(13)	242(14)	205(13)	27(11)	142(11)	20(10)
C(7)	491(18)	258(14)	335(16)	-27(12)	325(15)	59(12)
O(2)	231(9)	388(10)	247(10)	-41(8)	193(8)	-23(7)
C(8)	147(12)	233(13)	171(12)	28(10)	98(11)	34(10)
C(9)	200(13)	331(15)	226(14)	-16(11)	149(12)	2(11)
C(10)	214(14)	459(17)	245(15)	-121(12)	129(13)	-44(12)
C(11)	196(14)	398(16)	336(16)	-133(13)	152(13)	-85(12)
C(12)	205(14)	322(15)	322(15)	-23(12)	194(13)	-27(11)
C(13)	197(13)	223(13)	211(13)	24(11)	136(12)	28(11)
C(14)	312(15)	480(17)	386(16)	-34(13)	296(14)	-4(13)
O(3)	272(16)	269(19)	166(15)	-44(16)	132(13)	31(17)
C(15)	160(40)	270(50)	170(30)	-20(30)	130(40)	-10(40)
C(16)	140(30)	240(30)	110(30)	0(20)	70(30)	0(20)
C(17)	250(20)	210(30)	360(30)	0(20)	220(20)	4(19)
C(18)	200(30)	340(30)	230(40)	60(30)	140(40)	10(20)
C(19)	230(30)	310(40)	150(30)	40(30)	130(30)	20(30)

C(20)	190(30)	170(30)	330(30)	-20(30)	200(30)	10(20)
C(21)	310(20)	400(30)	210(20)	-118(18)	140(20)	-13(19)
O(3B)	290(30)	170(30)	200(30)	-10(20)	150(30)	40(20)
C(15B)	120(60)	190(70)	60(60)	-70(50)	50(60)	-40(70)
C(16B)	70(50)	320(90)	20(40)	-20(60)	20(30)	60(70)
C(17B)	300(50)	460(60)	150(40)	-90(40)	150(40)	-80(50)
C(18B)	170(60)	430(90)	50(50)	120(50)	-10(50)	-30(60)
C(19B)	180(70)	180(50)	260(80)	80(50)	150(70)	40(40)
C(20B)	130(50)	390(70)	30(50)	-70(40)	50(50)	-100(50)
C(21B)	280(40)	160(40)	320(50)	-50(30)	160(40)	-10(30)
O(4)	229(9)	379(11)	290(10)	-143(8)	152(9)	-76(8)
C(22)	170(12)	205(12)	149(12)	37(10)	104(11)	28(10)
C(23)	187(13)	240(13)	153(12)	30(10)	99(11)	9(10)
C(24)	258(14)	306(14)	184(13)	54(11)	162(12)	73(11)
C(25)	311(15)	351(16)	345(16)	103(13)	277(14)	82(12)
C(26)	188(13)	263(15)	385(16)	47(12)	190(13)	6(11)
C(27)	195(13)	238(14)	179(13)	27(10)	102(11)	33(11)
C(28)	226(15)	330(15)	330(16)	-81(13)	93(13)	-33(12)
C(29)	220(13)	233(13)	168(13)	13(10)	138(11)	23(10)
C(30)	234(13)	201(13)	207(13)	-28(10)	135(12)	-11(11)
C(31)	295(15)	287(15)	292(15)	53(11)	212(13)	69(11)
C(32)	347(17)	426(17)	443(18)	12(14)	318(15)	59(13)
C(33)	246(15)	359(17)	459(18)	-32(14)	196(15)	95(13)
C(34)	276(15)	260(15)	332(16)	16(12)	137(14)	54(12)
C(35)	241(14)	236(14)	259(14)	-39(11)	145(12)	-42(11)
C(36)	270(14)	257(14)	187(13)	-26(11)	189(12)	5(11)
C(37)	227(13)	333(15)	197(13)	-29(11)	151(12)	-42(11)
C(38)	334(15)	239(14)	286(14)	11(12)	230(13)	16(12)
C(39)	367(16)	269(15)	356(16)	-97(13)	266(14)	-79(13)
C(40)	251(15)	348(16)	289(15)	-51(12)	163(13)	-15(12)
C(41)	344(16)	245(14)	292(15)	-9(12)	227(14)	27(12)
C(42)	291(14)	169(12)	235(13)	9(11)	191(12)	16(11)
C(43)	412(17)	248(15)	297(15)	-11(12)	242(14)	-77(12)
C(44)	640(20)	373(17)	248(16)	-99(13)	268(16)	-199(15)
C(45)	820(20)	363(18)	330(17)	-65(13)	442(19)	-116(16)
C(46)	557(19)	273(15)	403(17)	25(13)	404(17)	-5(13)
C(47)	327(15)	225(14)	292(15)	35(11)	231(13)	44(11)
C(48)	268(15)	369(16)	417(17)	64(13)	220(14)	58(12)
Cl(1)	565(5)	399(4)	442(5)	47(3)	327(4)	52(4)
Cl(2)	336(4)	754(6)	744(6)	276(5)	362(5)	112(4)

Compound 12

Table 1. Crystal data and structure refinement for 12 (CCDC 237455).

Empirical formula	$C_{33}H_{30}O_8P_2Cr$, CH_2Cl_2	
Formula weight	753.44	
Crystallization Solvent	Dichloromethane/petroleum ether	
Crystal Habit	Fragment	
Crystal size	0.28 x 0.26 x 0.12 mm^3	
Crystal color	Yellow	
Data Collection		
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9204 reflections used in lattice determination	2.15 to 25.13°	
Unit cell dimensions	a = 11.7302(12) Å b = 17.6390(18) Å c = 17.7569(18) Å	α= 80.294(2)° β= 86.804(2)° γ = 74.673(2)°
Volume	3492.4(6) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.433 Mg/m^3	
F(000)	1552	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.54 to 25.11°	
Completeness to θ = 25.11°	99.6 %	
Index ranges	$-13 \le h \le 13$, $-21 \le k \le 21$, $-21 \le l \le 21$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.45	
Reflections collected	56515	
Independent reflections	12378 [R_{int}= 0.1033]	
Absorption coefficient	0.622 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9291 and 0.8452	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12378 / 0 / 855
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.371
Final R indices [$I>2\sigma(I)$, 6803 reflections]	R1 = 0.0559, *w*R2 = 0.0952
R indices (all data)	R1 = 0.1158, *w*R2 = 0.1024
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	1.777 and -0.795 e.Å^{-3}

Special Refinement Details

The largest peak in the final difference Fourier is near a methoxy oxygen and can not be explained by any chemically reasonable hypothesis. It is therefore assumed to be an artifact. All other difference peaks represent less than one electron.

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

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 12 (CCDC 237455). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cr(1)	8797(1)	1186(1)	2267(1)	14(1)
P(1A)	9622(1)	2247(1)	1741(1)	13(1)
P(2A)	8279(1)	2168(1)	3061(1)	13(1)
O(1A)	9689(3)	186(2)	1030(2)	36(1)
O(2A)	7652(3)	-20(2)	3171(2)	32(1)
O(3A)	10993(3)	474(2)	3215(2)	22(1)
O(4A)	6514(3)	1961(2)	1402(2)	42(1)
O(5A)	9527(3)	1908(2)	234(2)	19(1)
O(6A)	10989(3)	3460(2)	1572(2)	23(1)
O(7A)	8654(3)	3232(2)	4095(2)	20(1)
O(8A)	6159(3)	1739(2)	3563(2)	24(1)
C(1A)	9369(4)	566(3)	1502(3)	23(1)
C(2A)	8082(4)	450(3)	2822(3)	21(1)
C(3A)	10167(4)	738(2)	2850(3)	14(1)
C(4A)	7389(5)	1665(3)	1729(3)	22(1)
C(5A)	8966(4)	2976(2)	918(2)	14(1)
C(6A)	8423(4)	3766(3)	958(3)	23(1)
C(7A)	7900(4)	4282(3)	319(3)	29(1)
C(8A)	7919(4)	3996(3)	-362(3)	26(1)
C(9A)	8450(4)	3206(3)	-421(3)	20(1)
C(10A)	8960(4)	2701(3)	221(3)	17(1)
C(11A)	9452(4)	1572(3)	-433(2)	24(1)
C(12A)	11219(4)	2093(3)	1591(2)	14(1)
C(13A)	11934(4)	1330(3)	1565(2)	20(1)
C(14A)	13149(4)	1188(3)	1518(3)	30(1)
C(15A)	13653(5)	1817(3)	1498(3)	34(1)
C(16A)	12964(4)	2589(3)	1510(3)	28(1)
C(17A)	11751(4)	2718(3)	1555(2)	20(1)
C(18A)	11497(5)	4135(3)	1453(3)	34(1)
C(19A)	8655(4)	1919(3)	4064(2)	13(1)
C(20A)	8815(4)	1142(3)	4441(3)	18(1)
C(21A)	9158(4)	925(3)	5195(3)	20(1)
C(22A)	9352(4)	1478(3)	5590(3)	23(1)
C(23A)	9172(4)	2264(3)	5244(3)	20(1)
C(24A)	8840(4)	2477(3)	4485(3)	16(1)
C(25A)	8884(4)	3824(3)	4490(3)	27(1)
C(26A)	6837(4)	2862(3)	3068(2)	14(1)
C(27A)	6623(4)	3682(2)	2852(3)	18(1)
C(28A)	5498(4)	4173(3)	2909(3)	31(1)
C(29A)	4575(4)	3857(3)	3176(3)	34(1)
C(30A)	4743(4)	3052(3)	3393(3)	28(1)
C(31A)	5872(4)	2551(3)	3340(3)	18(1)
C(32A)	5238(4)	1388(3)	3854(3)	31(1)
C(33A)	9303(4)	2727(2)	2592(2)	12(1)
Cr(2)	7767(1)	6191(1)	3275(1)	16(1)
P(1B)	8728(1)	7158(1)	2676(1)	14(1)
P(2B)	7315(1)	7263(1)	3971(1)	13(1)

O(1B)	8621(3)	4970(2)	2235(2)	31(1)
O(2B)	6369(3)	5199(2)	4278(2)	33(1)
O(3B)	9995(3)	5491(2)	4208(2)	23(1)
O(4B)	5573(3)	6876(2)	2317(2)	46(1)
O(5B)	8635(3)	6711(2)	1210(2)	23(1)
O(6B)	10414(3)	8195(2)	2547(2)	18(1)
O(7B)	7591(3)	8469(2)	4872(2)	18(1)
O(8B)	5156(3)	6942(2)	4542(2)	22(1)
C(1B)	8291(4)	5439(3)	2628(3)	23(1)
C(2B)	6917(4)	5581(3)	3899(3)	24(1)
C(3B)	9133(4)	5749(3)	3862(3)	17(1)
C(4B)	6414(5)	6639(3)	2678(3)	25(1)
C(5B)	8184(4)	7846(3)	1814(2)	14(1)
C(6B)	7762(4)	8663(3)	1777(3)	21(1)
C(7B)	7356(4)	9148(3)	1098(3)	31(1)
C(8B)	7354(4)	8830(3)	452(3)	29(1)
C(9B)	7754(4)	8016(3)	464(3)	25(1)
C(10B)	8169(4)	7528(3)	1141(3)	18(1)
C(11B)	8620(4)	6351(3)	565(2)	26(1)
C(12B)	10327(4)	6885(2)	2536(2)	14(1)
C(13B)	10923(4)	6091(3)	2478(2)	20(1)
C(14B)	12114(4)	5841(3)	2398(3)	21(1)
C(15B)	12793(4)	6381(3)	2382(3)	22(1)
C(16B)	12238(4)	7186(3)	2434(3)	20(1)
C(17B)	11028(4)	7422(3)	2501(2)	14(1)
C(18B)	11082(4)	8780(2)	2413(3)	23(1)
C(19B)	7686(4)	7114(3)	4980(2)	13(1)
C(20B)	7883(4)	6357(3)	5407(3)	17(1)
C(21B)	8225(4)	6224(3)	6160(3)	20(1)
C(22B)	8339(4)	6842(3)	6501(3)	21(1)
C(23B)	8119(4)	7612(3)	6084(3)	18(1)
C(24B)	7810(4)	7736(3)	5335(3)	15(1)
C(25B)	7654(4)	9143(3)	5209(3)	25(1)
C(26B)	5876(4)	7991(2)	3917(2)	13(1)
C(27B)	5700(4)	8783(2)	3577(3)	18(1)
C(28B)	4579(4)	9304(3)	3538(3)	22(1)
C(29B)	3638(4)	9015(3)	3841(3)	23(1)
C(30B)	3771(4)	8236(3)	4175(3)	23(1)
C(31B)	4899(4)	7723(3)	4210(3)	16(1)
C(32B)	4186(4)	6614(3)	4818(3)	30(1)
C(33B)	8424(4)	7741(2)	3461(2)	13(1)
C(41)	4574(5)	8353(3)	1046(3)	50(2)
Cl(1)	3871(2)	8800(1)	204(1)	95(1)
Cl(2)	4103(2)	8861(1)	1804(1)	63(1)
C(42)	4733(6)	6558(3)	9746(3)	62(2)
Cl(3)	5276(1)	5873(1)	9105(1)	64(1)
Cl(4)	5275(2)	6254(1)	10648(1)	68(1)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 12 (CCDC 237455). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	178(5)	107(4)	152(4)	-38(3)	21(4)	-42(4)
P(1A)	131(7)	120(7)	140(7)	-26(5)	19(6)	-41(6)
P(2A)	117(7)	122(7)	142(7)	-21(5)	9(6)	-25(5)
O(1A)	640(30)	157(19)	260(20)	-125(17)	80(20)	-24(19)
O(2A)	420(20)	230(20)	370(20)	-14(17)	132(19)	-209(19)
O(3A)	220(20)	184(19)	180(20)	18(15)	0(17)	31(17)
O(4A)	320(20)	460(30)	460(30)	30(20)	-160(20)	-120(20)
O(5A)	250(20)	142(18)	135(18)	-63(14)	-4(15)	41(15)
O(6A)	250(20)	201(19)	280(20)	-53(15)	65(16)	-142(16)
O(7A)	219(19)	171(19)	240(20)	-100(15)	10(16)	-62(15)
O(8A)	157(19)	132(18)	390(20)	-7(16)	97(17)	-29(15)
C(1A)	320(30)	200(30)	160(30)	10(20)	0(20)	-90(20)
C(2A)	240(30)	210(30)	180(30)	-120(20)	20(20)	-20(20)
C(3A)	190(30)	60(20)	140(30)	-20(20)	90(20)	-30(20)
C(4A)	200(30)	200(30)	300(30)	-30(20)	60(30)	-130(30)
C(5A)	130(30)	130(30)	120(30)	30(20)	-40(20)	-30(20)
C(6A)	320(30)	180(30)	170(30)	-60(20)	0(20)	-30(20)
C(7A)	410(40)	100(30)	300(30)	-10(20)	-70(30)	40(20)
C(8A)	340(30)	220(30)	170(30)	30(20)	-40(20)	-10(30)
C(9A)	260(30)	180(30)	150(30)	-20(20)	-20(20)	-40(20)
C(10A)	210(30)	120(30)	180(30)	-10(20)	30(20)	-80(20)
C(11A)	340(30)	240(30)	150(30)	-120(20)	10(20)	-30(20)
C(12A)	110(30)	220(30)	80(20)	10(20)	30(20)	-40(20)
C(13A)	210(30)	250(30)	120(30)	0(20)	50(20)	-50(20)
C(14A)	220(30)	370(30)	220(30)	-40(30)	60(30)	40(30)
C(15A)	160(30)	560(40)	330(30)	-30(30)	20(30)	-180(30)
C(16A)	180(30)	350(30)	310(30)	-30(30)	70(30)	-120(30)
C(17A)	210(30)	300(30)	100(30)	-20(20)	30(20)	-110(20)
C(18A)	480(40)	280(30)	330(30)	-70(30)	80(30)	-250(30)
C(19A)	80(30)	180(30)	150(30)	-80(20)	50(20)	-40(20)
C(20A)	130(30)	200(30)	180(30)	-20(20)	50(20)	-20(20)
C(21A)	150(30)	240(30)	150(30)	20(20)	30(20)	20(20)
C(22A)	130(30)	340(30)	140(30)	20(20)	40(20)	10(20)
C(23A)	140(30)	320(30)	160(30)	-150(20)	70(20)	-60(20)
C(24A)	120(30)	140(30)	200(30)	-30(20)	10(20)	10(20)
C(25A)	310(30)	260(30)	320(30)	-190(30)	50(30)	-140(30)
C(26A)	110(30)	150(30)	170(30)	-40(20)	-10(20)	-10(20)
C(27A)	130(30)	110(30)	270(30)	20(20)	0(20)	-10(20)
C(28A)	220(30)	180(30)	470(40)	10(30)	20(30)	40(20)
C(29A)	130(30)	220(30)	570(40)	0(30)	0(30)	70(20)
C(30A)	160(30)	300(30)	370(30)	-40(30)	50(30)	-60(30)
C(31A)	150(30)	220(30)	170(30)	-50(20)	10(20)	-60(20)
C(32A)	180(30)	230(30)	510(40)	-40(30)	70(30)	-80(20)
C(33A)	120(30)	120(20)	130(30)	-40(20)	-30(20)	-20(20)
Cr(2)	175(5)	135(4)	179(5)	-45(3)	29(4)	-42(4)
P(1B)	157(7)	139(7)	131(7)	-47(5)	29(6)	-39(6)
P(2B)	134(7)	125(7)	140(7)	-29(5)	18(6)	-33(6)

O(1B)	430(20)	230(20)	330(20)	-204(18)	170(19)	-123(18)
O(2B)	320(20)	230(20)	450(20)	-40(18)	137(19)	-127(18)
O(3B)	250(20)	220(20)	200(20)	-35(16)	7(17)	-3(17)
O(4B)	400(30)	460(30)	530(30)	10(20)	-260(20)	-120(20)
O(5B)	350(20)	190(19)	167(19)	-70(15)	29(16)	-73(16)
O(6B)	185(19)	135(18)	244(19)	-48(14)	71(15)	-72(15)
O(7B)	210(19)	129(17)	205(19)	-65(14)	13(15)	-49(15)
O(8B)	126(19)	139(18)	360(20)	-3(16)	53(16)	-25(15)
C(1B)	230(30)	290(30)	210(30)	-10(20)	40(20)	-150(30)
C(2B)	190(30)	160(30)	370(30)	-140(20)	10(30)	-20(20)
C(3B)	240(30)	120(30)	170(30)	-70(20)	60(20)	-40(20)
C(4B)	360(40)	220(30)	190(30)	-80(20)	-50(30)	-80(30)
C(5B)	140(30)	150(30)	130(30)	-10(20)	20(20)	-30(20)
C(6B)	260(30)	180(30)	170(30)	-20(20)	0(20)	-40(20)
C(7B)	360(40)	190(30)	310(30)	10(30)	-40(30)	30(30)
C(8B)	350(30)	300(30)	170(30)	60(20)	-60(30)	-30(30)
C(9B)	290(30)	330(30)	150(30)	-80(20)	20(20)	-80(30)
C(10B)	170(30)	210(30)	150(30)	0(20)	-10(20)	-30(20)
C(11B)	400(30)	290(30)	100(30)	-40(20)	10(20)	-90(30)
C(12B)	150(30)	120(30)	130(30)	-10(20)	20(20)	-20(20)
C(13B)	260(30)	170(30)	170(30)	20(20)	50(20)	-110(20)
C(14B)	160(30)	180(30)	190(30)	-10(20)	20(20)	100(20)
C(15B)	170(30)	240(30)	210(30)	20(20)	10(20)	-30(20)
C(16B)	230(30)	200(30)	220(30)	-30(20)	-10(20)	-120(20)
C(17B)	180(30)	130(30)	90(30)	0(20)	50(20)	-20(20)
C(18B)	280(30)	120(30)	320(30)	-50(20)	60(30)	-110(20)
C(19B)	60(30)	180(30)	140(30)	-60(20)	30(20)	-20(20)
C(20B)	80(30)	190(30)	220(30)	-70(20)	60(20)	10(20)
C(21B)	180(30)	230(30)	170(30)	0(20)	70(20)	-40(20)
C(22B)	130(30)	380(30)	130(30)	-10(20)	40(20)	-100(20)
C(23B)	180(30)	200(30)	180(30)	-70(20)	40(20)	-60(20)
C(24B)	60(30)	170(30)	230(30)	-60(20)	50(20)	-30(20)
C(25B)	260(30)	180(30)	370(30)	-150(20)	30(30)	-120(20)
C(26B)	80(30)	110(30)	180(30)	-40(20)	-40(20)	20(20)
C(27B)	180(30)	110(30)	260(30)	-50(20)	30(20)	-60(20)
C(28B)	210(30)	80(30)	350(30)	-70(20)	0(30)	20(20)
C(29B)	150(30)	170(30)	330(30)	-60(20)	-20(20)	50(20)
C(30B)	120(30)	200(30)	340(30)	-70(20)	10(20)	0(20)
C(31B)	170(30)	150(30)	150(30)	-50(20)	20(20)	-20(20)
C(32B)	230(30)	200(30)	440(40)	-20(30)	150(30)	-60(20)
C(33B)	70(30)	110(20)	200(30)	-50(20)	10(20)	-20(20)
C(41)	520(40)	600(40)	330(40)	-130(30)	-90(30)	10(30)
Cl(1)	1230(19)	993(16)	527(13)	104(11)	-288(12)	-202(14)
Cl(2)	736(13)	666(12)	651(12)	-351(10)	259(10)	-345(10)
C(42)	620(50)	440(40)	620(50)	10(30)	260(40)	50(30)
Cl(3)	576(11)	641(11)	811(13)	-219(10)	143(10)	-330(10)
Cl(4)	669(13)	616(12)	738(13)	-157(10)	-128(10)	-67(10)