

ORGANOMETALLICS

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Table 1. Crystal data and structure refinement for **14**·2CHCl₃.

Empirical formula	C ₆₁ H ₅₂ Cl ₈ NO ₉ P ₃ Pd
Formula weight	1425.95
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P $\bar{1}$
Unit cell dimensions	$a = 9.6940(10)$ Å $\alpha = 79.150(10)^\circ$ $b = 13.299(2)$ Å $\beta = 86.530(10)^\circ$ $c = 25.154(3)$ Å $\gamma = 73.900(10)^\circ$
Volume	3059.9(7) Å ³
Z	2
Density (calculated)	1.548 Mg/m ³
Absorption coefficient	0.788 mm ⁻¹
F(000)	1448
Crystal size	0.26 × 0.12 × 0.09 mm
θ range for data collection	2.09 - 22.50 °
Index ranges	$0 \leq h \leq 10, -13 \leq k \leq 14, -27 \leq l \leq 27$
Reflections collected	8619
Independent reflections	8008 ($R_{\text{int}} = 0.0574$)
Absorption correction	Ψ -scan
Max. and min. transmission	0.932 and 0.821
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8008 / 0 / 748
Goodness-of-fit on F ²	1.025
R indices [$I > 2\sigma(I)$]	$R1 = 0.0617, wR2 = 0.1279$
Final R indices (all data)	$R1 = 0.1245, wR2 = 0.1472$
Largest diff. peak and hole	0.990 and -1.819 eÅ ⁻³

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

$$wR2 = [\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$$

$$\text{Goodness-of-fit} = [\sum w (F_o^2 - F_c^2)^2 / (N_{\text{obs}} - N_{\text{param}})]^{1/2}$$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $14\cdot 2\text{CHCl}_3$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	9718(1)	7244(1)	7144(1)	19(1)
P(1)	9254(2)	7303(2)	6245(1)	23(1)
C(1)	10528(8)	7610(6)	5714(3)	22(2)
C(2)	11558(9)	6805(7)	5511(3)	31(2)
C(3)	12563(10)	7039(8)	5131(4)	38(2)
C(4)	12588(10)	8066(8)	4944(4)	41(2)
C(5)	11600(9)	8885(7)	5147(4)	36(2)
C(6)	10575(9)	8646(7)	5528(3)	29(2)
C(7)	8945(8)	6060(6)	6138(3)	26(2)
C(8)	8730(8)	5321(6)	6579(3)	25(2)
C(9)	8451(9)	4393(7)	6507(4)	34(2)
C(10)	8413(9)	4190(7)	5995(4)	35(2)
C(11)	8606(9)	4934(7)	5549(3)	32(2)
C(12)	8877(9)	5853(7)	5624(3)	31(2)
C(13)	7578(9)	8321(6)	6055(3)	27(2)
C(14)	6545(9)	8131(7)	5756(3)	34(2)
C(15)	5267(10)	8908(8)	5636(4)	47(3)
C(16)	5009(10)	9854(7)	5806(4)	42(2)
C(17)	6029(9)	10057(7)	6102(4)	35(2)
C(18)	7296(8)	9295(6)	6217(3)	26(2)
P(2)	9892(2)	9281(2)	8815(1)	22(1)
C(19)	11047(9)	10137(6)	8726(3)	29(2)
C(20)	10789(10)	10947(6)	9026(4)	36(2)
C(21)	11673(12)	11617(7)	8971(4)	48(3)
C(22)	12806(12)	11485(7)	8613(5)	52(3)
C(23)	13100(11)	10686(9)	8310(5)	62(3)
C(24)	12212(11)	10010(8)	8376(5)	58(3)
C(25)	8220(9)	10027(6)	9063(3)	23(2)
C(26)	7451(9)	10934(7)	8730(4)	36(2)
C(27)	6234(10)	11576(7)	8930(4)	42(2)
C(28)	5775(9)	11321(7)	9462(4)	35(2)
C(29)	6524(9)	10413(7)	9791(3)	29(2)
C(30)	7749(9)	9767(6)	9594(3)	29(2)
C(31)	10551(9)	8123(6)	9301(3)	23(2)
C(32)	11707(9)	8026(7)	9620(4)	33(2)
C(33)	12140(10)	7152(7)	10018(4)	41(2)
C(34)	11446(10)	6350(7)	10098(4)	41(2)
C(35)	10317(10)	6436(7)	9780(4)	36(2)
C(36)	9872(9)	7319(6)	9386(3)	28(2)
P(3)	11249(2)	5732(2)	8060(1)	20(1)
C(37)	12452(9)	5831(6)	7491(3)	25(2)
C(38)	11836(8)	6644(6)	7061(3)	20(2)
C(39)	12799(9)	6907(6)	6663(3)	27(2)
C(40)	14253(9)	6352(7)	6668(3)	36(2)
C(41)	14778(10)	5514(7)	7070(4)	43(3)
C(42)	13891(9)	5250(6)	7492(3)	30(2)
C(43)	12276(8)	5196(6)	8660(3)	17(2)
C(44)	12000(9)	4339(6)	9024(3)	26(2)
C(45)	12849(9)	3896(6)	9478(3)	29(2)
C(46)	13981(9)	4285(6)	9560(3)	28(2)
C(47)	14251(9)	5133(6)	9205(3)	31(2)

C(48)	13405(9)	5588(6)	8754(3)	27(2)
C(49)	10128(9)	4864(6)	8026(3)	22(2)
C(50)	10695(9)	3953(6)	7809(3)	31(2)
C(51)	9873(11)	3259(7)	7802(4)	40(2)
C(52)	8489(10)	3473(7)	8006(4)	38(2)
C(53)	7933(10)	4376(7)	8226(4)	41(2)
C(54)	8732(9)	5070(7)	8243(3)	34(2)
N(1)	7518(8)	7734(5)	7310(3)	28(2)
C(55)	6325(10)	8030(7)	7382(3)	29(2)
C(56)	4779(9)	8433(9)	7450(4)	53(3)
C(57)	10103(8)	7035(6)	8000(3)	22(2)
C(58)	10701(9)	7887(6)	8078(3)	24(2)
C(59)	9605(8)	8908(6)	8186(3)	21(2)
O(9)	11971(6)	7834(4)	8069(2)	27(1)
Cl(1)	6041(2)	7571(2)	8986(1)	34(1)
O(1)	4748(9)	7534(7)	8791(4)	101(3)
O(2)	6738(7)	8182(6)	8598(3)	57(2)
O(3)	5752(10)	8046(6)	9450(3)	92(3)
O(4)	6977(7)	6517(5)	9136(3)	54(2)
Cl(2)	6760(3)	11672(2)	7207(1)	49(1)
O(5)	6349(13)	10733(8)	7336(3)	116(4)
O(6)	6872(9)	11994(7)	6634(3)	80(3)
O(7)	8203(8)	11454(7)	7403(3)	73(2)
O(8)	5878(9)	12471(7)	7468(4)	103(3)
C(100)	9290(11)	9051(8)	3419(4)	49(3)
Cl(3)	9016(3)	10439(2)	3225(1)	50(1)
Cl(4)	9292(3)	8704(2)	4129(1)	60(1)
Cl(5)	7841(4)	8701(2)	3170(1)	70(1)
C(101)	13936(11)	3504(8)	6097(4)	46(3)
Cl(6)	12319(3)	4077(2)	6426(1)	66(1)
Cl(7)	13565(3)	2875(2)	5586(1)	64(1)
Cl(8)	14746(3)	4498(2)	5787(1)	68(1)

Table 3. Selected bond lengths (Å) and angles (°) for **14**·2CHCl₃.

Pd-C(38)	1.999(8)	Pd-N(1)	2.091(7)
Pd-C(57)	2.161(8)	Pd-P(1)	2.315(2)
P(2)-C(31)	1.766(8)	P(2)-C(19)	1.784(8)
P(2)-C(25)	1.795(8)	P(2)-C(59)	1.801(7)
P(3)-C(57)	1.764(7)	P(3)-C(43)	1.778(7)
P(3)-C(37)	1.801(8)	P(3)-C(49)	1.808(8)
C(37)-C(38)	1.405(11)	C(38)-C(39)	1.390(10)
N(1)-C(55)	1.129(10)	C(55)-C(56)	1.456(12)
C(57)-C(58)	1.456(11)	C(58)-O(9)	1.212(9)
C(58)-C(59)	1.533(10)		
C(38)-Pd-N(1)	173.3(3)	C(38)-Pd-C(57)	86.7(3)
N(1)-Pd-C(57)	88.4(3)	C(38)-Pd-P(1)	93.8(2)
N(1)-Pd-P(1)	90.59(19)	C(57)-Pd-P(1)	174.2(2)
N(1)-C(55)-C(56)	177.5(9)	C(58)-C(57)-P(3)	118.7(6)
C(58)-C(57)-Pd	107.2(5)	O(9)-C(58)-C(57)	124.9(7)
O(9)-C(58)-C(59)	119.5(7)	C(57)-C(58)-C(59)	115.6(7)
C(58)-C(59)-P(2)	113.4(5)		

Table 4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $14\cdot 2\text{CHCl}_3$.

Pd-C(38)	1.999(8)	Pd-N(1)	2.091(7)
Pd-C(57)	2.161(8)	Pd-P(1)	2.315(2)
Pd-P(3)	2.928(2)	P(1)-C(13)	1.825(8)
P(1)-C(7)	1.829(8)	P(1)-C(1)	1.830(8)
C(1)-C(6)	1.381(11)	C(1)-C(2)	1.397(11)
C(2)-C(3)	1.378(11)	C(3)-C(4)	1.365(12)
C(4)-C(5)	1.392(12)	C(5)-C(6)	1.396(11)
C(7)-C(12)	1.380(11)	C(7)-C(8)	1.384(11)
C(8)-C(9)	1.380(11)	C(9)-C(10)	1.367(11)
C(10)-C(11)	1.390(12)	C(11)-C(12)	1.369(11)
C(13)-C(18)	1.381(11)	C(13)-C(14)	1.390(11)
C(14)-C(15)	1.382(12)	C(15)-C(16)	1.358(12)
C(16)-C(17)	1.384(12)	C(17)-C(18)	1.364(11)
P(2)-C(31)	1.766(8)	P(2)-C(19)	1.784(8)
P(2)-C(25)	1.795(8)	P(2)-C(59)	1.801(7)
C(19)-C(24)	1.382(12)	C(19)-C(20)	1.387(11)
C(20)-C(21)	1.381(12)	C(21)-C(22)	1.372(14)
C(22)-C(23)	1.379(14)	C(23)-C(24)	1.390(13)
C(25)-C(26)	1.381(11)	C(25)-C(30)	1.397(11)
C(26)-C(27)	1.380(12)	C(27)-C(28)	1.394(12)
C(28)-C(29)	1.370(12)	C(29)-C(30)	1.384(11)
C(31)-C(32)	1.381(11)	C(31)-C(36)	1.381(11)
C(32)-C(33)	1.367(12)	C(33)-C(34)	1.391(13)
C(34)-C(35)	1.361(13)	C(35)-C(36)	1.371(11)
P(3)-C(57)	1.764(7)	P(3)-C(43)	1.778(7)
P(3)-C(37)	1.801(8)	P(3)-C(49)	1.808(8)
C(37)-C(42)	1.395(11)	C(37)-C(38)	1.405(11)
C(38)-C(39)	1.390(10)	C(39)-C(40)	1.398(11)
C(40)-C(41)	1.359(12)	C(41)-C(42)	1.381(11)
C(43)-C(48)	1.385(11)	C(43)-C(44)	1.398(10)
C(44)-C(45)	1.386(11)	C(45)-C(46)	1.377(11)
C(46)-C(47)	1.376(11)	C(47)-C(48)	1.381(11)
C(49)-C(50)	1.383(10)	C(49)-C(54)	1.402(11)
C(50)-C(51)	1.378(12)	C(51)-C(52)	1.380(12)
C(52)-C(53)	1.377(12)	C(53)-C(54)	1.367(11)
N(1)-C(55)	1.129(10)	C(55)-C(56)	1.456(12)
C(57)-C(58)	1.456(11)	C(58)-O(9)	1.212(9)
C(58)-C(59)	1.533(10)	Cl(1)-O(1)	1.390(7)
Cl(1)-O(3)	1.408(7)	Cl(1)-O(2)	1.413(6)
Cl(1)-O(4)	1.437(7)	Cl(2)-O(5)	1.390(8)
Cl(2)-O(8)	1.407(8)	Cl(2)-O(6)	1.431(7)
Cl(2)-O(7)	1.445(8)	C(100)-Cl(4)	1.759(10)
C(100)-Cl(3)	1.766(10)	C(100)-Cl(5)	1.777(10)
C(101)-Cl(8)	1.757(10)	C(101)-Cl(7)	1.763(10)
C(101)-Cl(6)	1.773(9)		
C(38)-Pd-N(1)	173.3(3)	C(38)-Pd-C(57)	86.7(3)
N(1)-Pd-C(57)	88.4(3)	C(38)-Pd-P(1)	93.8(2)
N(1)-Pd-P(1)	90.59(19)	C(57)-Pd-P(1)	174.2(2)
C(38)-Pd-P(3)	62.5(2)	N(1)-Pd-P(3)	110.96(19)
C(57)-Pd-P(3)	36.81(19)	P(1)-Pd-P(3)	139.19(7)
C(13)-P(1)-C(1)	105.2(4)	C(13)-P(1)-C(1)	104.2(4)
C(7)-P(1)-C(1)	105.4(3)	C(13)-P(1)-Pd	108.8(3)
C(7)-P(1)-Pd	111.6(3)	C(1)-P(1)-Pd	120.4(3)
C(6)-C(1)-C(2)	117.5(7)	C(6)-C(1)-P(1)	120.9(6)

C(2)-C(1)-P(1)	121.5(6)
C(4)-C(3)-C(2)	120.9(8)
C(4)-C(5)-C(6)	119.6(8)
C(12)-C(7)-C(8)	118.8(7)
C(8)-C(7)-P(1)	119.7(6)
C(10)-C(9)-C(8)	119.8(8)
C(12)-C(11)-C(10)	119.6(8)
C(18)-C(13)-C(14)	118.5(8)
C(14)-C(13)-P(1)	121.2(6)
C(16)-C(15)-C(14)	120.8(9)
C(18)-C(17)-C(16)	119.0(8)
C(31)-P(2)-C(19)	112.1(4)
C(19)-P(2)-C(25)	105.8(4)
C(19)-P(2)-C(59)	111.7(4)
C(24)-C(19)-C(20)	118.5(8)
C(20)-C(19)-P(2)	119.2(7)
C(22)-C(21)-C(20)	119.6(9)
C(22)-C(23)-C(24)	118.2(10)
C(26)-C(25)-C(30)	119.7(8)
C(30)-C(25)-P(2)	121.8(6)
C(26)-C(27)-C(28)	120.8(9)
C(28)-C(29)-C(30)	119.5(8)
C(32)-C(31)-C(36)	118.9(8)
C(36)-C(31)-P(2)	120.3(7)
C(32)-C(33)-C(34)	120.7(9)
C(34)-C(35)-C(36)	119.4(9)
C(57)-P(3)-C(43)	117.9(4)
C(43)-P(3)-C(37)	109.0(4)
C(43)-P(3)-C(49)	106.5(4)
C(57)-P(3)-Pd	47.2(3)
C(37)-P(3)-Pd	70.0(3)
C(42)-C(37)-C(38)	122.8(7)
C(38)-C(37)-P(3)	112.8(6)
C(39)-C(38)-Pd	131.4(6)
C(38)-C(39)-C(40)	122.5(8)
C(40)-C(41)-C(42)	119.8(8)
C(48)-C(43)-C(44)	119.7(7)
C(44)-C(43)-P(3)	120.2(6)
C(46)-C(45)-C(44)	119.7(8)
C(46)-C(47)-C(48)	120.1(8)
C(50)-C(49)-C(54)	119.9(7)
C(54)-C(49)-P(3)	121.0(6)
C(50)-C(51)-C(52)	120.5(8)
C(54)-C(53)-C(52)	120.9(9)
C(55)-N(1)-Pd	177.2(7)
C(58)-C(57)-P(3)	118.7(6)
P(3)-C(57)-Pd	96.0(3)
O(9)-C(58)-C(59)	119.5(7)
C(58)-C(59)-P(2)	113.4(5)
O(1)-Cl(1)-O(2)	111.2(5)
O(1)-Cl(1)-O(4)	110.8(5)
O(2)-Cl(1)-O(4)	109.4(4)
O(5)-Cl(2)-O(6)	111.5(5)
O(5)-Cl(2)-O(7)	107.5(6)
O(6)-Cl(2)-O(7)	104.8(5)
Cl(4)-C(100)-Cl(5)	108.2(5)
Cl(8)-C(101)-Cl(7)	107.7(5)
Cl(7)-C(101)-Cl(6)	109.9(6)

C(3)-C(2)-C(1)	121.2(8)
C(3)-C(4)-C(5)	119.3(8)
C(1)-C(6)-C(5)	121.5(8)
C(12)-C(7)-P(1)	121.4(6)
C(9)-C(8)-C(7)	120.7(8)
C(9)-C(10)-C(11)	120.1(8)
C(11)-C(12)-C(7)	120.9(8)
C(18)-C(13)-P(1)	120.3(7)
C(15)-C(14)-C(13)	119.6(8)
C(15)-C(16)-C(17)	120.3(9)
C(17)-C(18)-C(13)	121.8(8)
C(31)-P(2)-C(25)	108.0(4)
C(31)-P(2)-C(59)	109.4(4)
C(25)-P(2)-C(59)	109.7(4)
C(24)-C(19)-P(2)	122.3(6)
C(21)-C(20)-C(19)	120.6(9)
C(21)-C(22)-C(23)	121.4(9)
C(19)-C(24)-C(23)	121.6(9)
C(26)-C(25)-P(2)	118.3(6)
C(27)-C(26)-C(25)	119.4(9)
C(29)-C(28)-C(27)	120.0(8)
C(29)-C(30)-C(25)	120.6(8)
C(32)-C(31)-P(2)	120.7(6)
C(33)-C(32)-C(31)	119.7(8)
C(35)-C(34)-C(33)	119.8(8)
C(35)-C(36)-C(31)	121.5(8)
C(57)-P(3)-C(37)	103.0(4)
C(57)-P(3)-C(49)	106.9(4)
C(37)-P(3)-C(49)	113.8(4)
C(43)-P(3)-Pd	161.5(3)
C(49)-P(3)-Pd	90.2(3)
C(42)-C(37)-P(3)	124.1(6)
C(39)-C(38)-C(37)	115.0(7)
C(37)-C(38)-Pd	113.6(5)
C(41)-C(40)-C(39)	120.3(8)
C(41)-C(42)-C(37)	119.2(8)
C(48)-C(43)-P(3)	120.0(6)
C(45)-C(44)-C(43)	119.7(8)
C(47)-C(46)-C(45)	120.7(8)
C(47)-C(48)-C(43)	120.0(7)
C(50)-C(49)-P(3)	119.0(6)
C(51)-C(50)-C(49)	119.6(8)
C(53)-C(52)-C(51)	119.7(8)
C(53)-C(54)-C(49)	119.4(8)
N(1)-C(55)-C(56)	177.5(9)
C(58)-C(57)-Pd	107.2(5)
O(9)-C(58)-C(57)	124.9(7)
C(57)-C(58)-C(59)	115.6(7)
O(1)-Cl(1)-O(3)	108.5(6)
O(3)-Cl(1)-O(2)	108.6(5)
O(3)-Cl(1)-O(4)	108.3(4)
O(5)-Cl(2)-O(8)	111.5(6)
O(8)-Cl(2)-O(6)	113.7(6)
O(8)-Cl(2)-O(7)	107.4(5)
Cl(4)-C(100)-Cl(3)	109.8(5)
Cl(3)-C(100)-Cl(5)	108.4(6)
Cl(8)-C(101)-Cl(6)	110.1(5)

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14-2CHCl₃**. The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}].$$

	U11	U22	U33	U23	U13	U12
Pd	15(1)	21(1)	22(1)	-7(1)	5(1)	-6(1)
P(1)	20(1)	25(1)	24(1)	-9(1)	6(1)	-6(1)
C(1)	17(5)	28(5)	23(4)	-7(4)	0(4)	-11(4)
C(2)	24(5)	37(5)	39(5)	-9(4)	4(4)	-18(4)
C(3)	31(6)	52(6)	37(6)	-23(5)	10(5)	-14(5)
C(4)	38(6)	64(7)	29(5)	-9(5)	13(4)	-29(5)
C(5)	33(6)	33(5)	43(6)	5(4)	-5(5)	-15(5)
C(6)	25(5)	33(5)	31(5)	-3(4)	-2(4)	-10(4)
C(7)	17(5)	32(5)	32(5)	-13(4)	13(4)	-11(4)
C(8)	15(5)	39(5)	26(5)	-15(4)	9(4)	-10(4)
C(9)	25(5)	34(5)	43(6)	-6(4)	11(4)	-11(4)
C(10)	28(5)	37(5)	49(6)	-26(5)	14(5)	-15(4)
C(11)	35(6)	42(6)	28(5)	-23(4)	8(4)	-14(5)
C(12)	32(5)	33(5)	34(5)	-15(4)	7(4)	-12(4)
C(13)	23(5)	25(5)	35(5)	-8(4)	11(4)	-9(4)
C(14)	27(5)	43(6)	38(5)	-17(4)	-3(4)	-15(5)
C(15)	27(6)	52(7)	62(7)	-16(5)	-16(5)	-4(5)
C(16)	27(6)	39(6)	48(6)	0(5)	0(5)	4(5)
C(17)	31(6)	31(5)	43(6)	-11(4)	6(5)	-8(5)
C(18)	17(5)	29(5)	26(5)	-3(4)	0(4)	1(4)
P(2)	22(1)	21(1)	27(1)	-9(1)	4(1)	-9(1)
C(19)	28(5)	24(5)	37(5)	-6(4)	1(4)	-9(4)
C(20)	41(6)	32(5)	36(5)	-1(4)	-9(5)	-15(5)
C(21)	65(8)	36(6)	50(7)	-5(5)	-12(6)	-26(6)
C(22)	55(7)	33(6)	78(8)	6(6)	-27(6)	-31(5)
C(23)	37(7)	69(8)	100(9)	-30(7)	24(6)	-41(6)
C(24)	51(7)	52(7)	92(9)	-37(6)	21(6)	-38(6)
C(25)	30(5)	16(4)	26(5)	-12(4)	9(4)	-8(4)
C(26)	30(6)	32(5)	50(6)	-6(5)	0(5)	-13(5)
C(27)	30(6)	36(5)	54(7)	-17(5)	-1(5)	4(5)
C(28)	16(5)	38(6)	54(6)	-17(5)	9(5)	-8(4)
C(29)	22(5)	40(5)	30(5)	-14(4)	8(4)	-14(4)
C(30)	28(5)	29(5)	36(5)	-9(4)	3(4)	-18(4)
C(31)	22(5)	24(4)	25(5)	-12(4)	12(4)	-8(4)
C(32)	25(5)	25(5)	46(6)	-3(4)	1(5)	-6(4)
C(33)	33(6)	46(6)	40(6)	-8(5)	-3(5)	-1(5)
C(34)	33(6)	31(5)	44(6)	-2(5)	0(5)	13(5)
C(35)	35(6)	23(5)	45(6)	-7(4)	18(5)	-4(4)
C(36)	32(5)	31(5)	27(5)	-10(4)	7(4)	-14(4)
P(3)	19(1)	20(1)	22(1)	-6(1)	2(1)	-6(1)
C(37)	23(5)	24(5)	33(5)	-12(4)	10(4)	-11(4)
C(38)	22(5)	17(4)	24(5)	-8(4)	3(4)	-9(4)
C(39)	32(5)	27(5)	22(5)	-5(4)	14(4)	-10(4)
C(40)	19(5)	58(6)	31(5)	-6(5)	17(4)	-13(5)
C(41)	23(5)	50(6)	51(6)	-6(5)	15(5)	-8(5)
C(42)	24(5)	28(5)	29(5)	0(4)	-2(4)	3(4)
C(43)	17(4)	19(4)	15(4)	-1(3)	-10(3)	-2(4)
C(44)	25(5)	25(5)	31(5)	-10(4)	7(4)	-9(4)
C(45)	32(5)	27(5)	27(5)	-3(4)	2(4)	-10(4)
C(46)	20(5)	32(5)	26(5)	1(4)	-11(4)	2(4)
C(47)	28(5)	34(5)	30(5)	-5(4)	4(4)	-9(4)

C(48)	28(5)	35(5)	17(4)	3(4)	2(4)	-15(4)
C(49)	28(5)	16(4)	24(4)	-8(3)	-3(4)	-7(4)
C(50)	31(5)	28(5)	35(5)	-7(4)	-4(4)	-8(4)
C(51)	57(7)	26(5)	40(6)	-8(4)	-6(5)	-14(5)
C(52)	49(7)	37(6)	40(6)	-8(5)	1(5)	-31(5)
C(53)	36(6)	49(6)	52(6)	-14(5)	0(5)	-33(5)
C(54)	35(6)	30(5)	41(6)	-12(4)	5(4)	-14(4)
N(1)	17(4)	31(4)	31(4)	-6(3)	1(3)	0(3)
C(55)	32(6)	38(5)	17(5)	-5(4)	-6(4)	-8(5)
C(56)	17(6)	89(8)	46(6)	-8(6)	6(5)	-9(5)
C(57)	16(5)	21(4)	29(5)	-10(4)	3(4)	-6(4)
C(58)	29(6)	24(5)	17(4)	-5(4)	8(4)	-8(4)
C(59)	20(5)	27(4)	22(4)	-5(4)	2(4)	-13(4)
O(9)	15(3)	33(3)	37(3)	-10(3)	4(3)	-10(3)
Cl(1)	25(1)	48(1)	33(1)	-8(1)	8(1)	-17(1)
O(1)	64(6)	87(6)	158(9)	38(6)	-51(6)	-60(5)
O(2)	44(4)	81(5)	49(4)	10(4)	4(3)	-36(4)
O(3)	139(8)	64(5)	41(5)	-16(4)	27(5)	21(5)
O(4)	45(4)	46(4)	73(5)	-26(4)	-7(4)	-3(4)
Cl(2)	56(2)	48(2)	49(2)	-11(1)	-4(1)	-22(1)
O(5)	205(12)	115(8)	73(6)	-27(6)	24(7)	-115(8)
O(6)	90(6)	104(7)	49(5)	16(4)	-12(4)	-47(5)
O(7)	49(5)	101(6)	59(5)	-20(4)	3(4)	1(5)
O(8)	69(6)	79(6)	145(9)	-45(6)	3(6)	19(5)
C(100)	61(7)	45(6)	47(6)	-11(5)	1(5)	-21(6)
Cl(3)	62(2)	36(1)	51(2)	-9(1)	3(1)	-16(1)
Cl(4)	68(2)	48(2)	59(2)	0(1)	-16(2)	-11(1)
Cl(5)	100(3)	67(2)	61(2)	-20(2)	-1(2)	-47(2)
C(101)	48(7)	47(6)	44(6)	-20(5)	10(5)	-8(5)
Cl(6)	56(2)	53(2)	78(2)	-14(2)	36(2)	-1(1)
Cl(7)	66(2)	65(2)	67(2)	-25(2)	5(2)	-23(2)
Cl(8)	54(2)	70(2)	95(2)	-42(2)	30(2)	-28(2)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14**·2CHCl₃.

	x	y	z	U(eq)
H(2)	11566	6099	5635	37
H(3)	13233	6489	5001	45
H(4)	13258	8217	4683	49
H(5)	11622	9586	5031	44
H(6)	9909	9196	5659	35
H(8)	8774	5451	6927	30
H(9)	8289	3907	6805	41
H(10)	8259	3554	5946	42
H(11)	8550	4807	5200	39
H(12)	9019	6345	5325	38
H(14)	6713	7486	5638	40
H(15)	4575	8780	5437	56
H(16)	4144	10369	5722	50
H(17)	5852	10702	6221	42
H(18)	7990	9435	6409	31
H(20)	10014	11041	9265	43
H(21)	11501	12153	9176	58
H(22)	13389	11945	8573	63
H(23)	13871	10601	8069	75
H(24)	12407	9459	8180	69
H(26)	7752	11111	8375	44
H(27)	5713	12187	8707	50
H(28)	4962	11766	9593	42
H(29)	6210	10232	10143	34
H(30)	8264	9155	9817	34
H(32)	12189	8553	9565	39
H(33)	12907	7094	10237	50
H(34)	11752	5756	10367	50
H(35)	9853	5900	9829	43
H(36)	9095	7379	9172	34
H(39)	12462	7474	6382	33
H(40)	14864	6558	6396	44
H(41)	15732	5119	7061	51
H(42)	14249	4691	7774	36
H(44)	11251	4067	8961	32
H(45)	12654	3338	9727	34
H(46)	14570	3970	9858	34
H(47)	15004	5400	9270	37
H(48)	13593	6158	8513	32
H(50)	11624	3809	7668	37
H(51)	10255	2642	7660	48
H(52)	7934	3008	7994	46
H(53)	7002	4515	8365	49
H(54)	8353	5673	8397	41
H(56A)	4329	8636	7102	79
H(56B)	4577	9040	7626	79
H(56C)	4412	7887	7668	79
H(57)	9218	7047	8212	26
H(59A)	8649	8810	8191	26
H(59B)	9650	9485	7891	26