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Summary of Crystal Data and Intensity Collection of Complex **4**.

Empirical Formula	$C_{46}\ H_{44}\ Br_2\ O_4\ P_2\ Pd\cdot(\ CH_2Cl_2)\cdot(H_2O)$
Color; Habit	Colerless; Bladed
Crystal Size (mm)	0.22 x 0.12 x 0.04
Space Group	$P\bar{1}$; Triclinic
Unit Cell Dimensions	$\underline{a}$ = 9.610(2) Å; α = 69.32(2)°
	$\underline{b}$ = 15.542(4) Å; β = 84.82(2)°
	$\underline{c}$ = 17.559(5) Å; γ = 75.36(2)°
No. Reflns. for Indexing	13 (9.11° ≤ 2θ ≤ 18.64°)
Volume	2373.8(11) Å^3
Z	2
Formula Weight	1089.9
Density(calc.)	1.525 Mg/m^3
Absorption Coefficient	2.297 mm^{-1}
F(000)	1096
Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	295
2θ Range	2.5 to 45.0°
Scan Type	$\theta/2\theta$
Scan Speed	Variable; 2.49 to 14.65°/min. in ω
Scan Range (ω)	1.00° plus Kα-separation
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 50 reflections
Index Ranges	$-10 \le h \le 10, -17 \le k \le 17, 0 \le \ell \le 20$
Reflections Collected	7488 (3559 ≥ 3.0σ(I))
Independent Reflections	6977 (3177 ≥ 3.0σ(I))(R_{int} =4.66%)
Min./Max. Transmission	0.7913 / 0.9442
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0002F^2$
Number of Parameters Refined	542
Final R Indices (obs. data)	R = 0.0457, Rw = 0.0389
Goodness-of-Fit	1.21
Largest and Mean Δ/σ	0.003, 0.000
Data-to-Parameter Ratio	5.9:1
Largest Difference Peak/Hole	0.48/-0.52 eÅ^{-3}

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Pd(1)	-1233(1)	11221(1)	2634(1)	27(1)
Br(1)	-2073(1)	11208(1)	4023(1)	43(1)
Br(2)	-3772(2)	13860(1)	-1739(1)	68(1)
Cl(1)	1331(5)	5164(3)	4113(3)	112(3)
Cl(2)	2322(5)	3653(3)	3481(3)	112(3)
P(1)	-1371(3)	8914(2)	3381(2)	28(1)
P(2)	-1861(3)	13525(2)	2207(2)	29(1)
O(1)	-3252(9)	11168(6)	1044(4)	59(4)
O(2)	-1021(8)	11094(5)	543(4)	47(4)
O(3)	2316(8)	11323(6)	2329(5)	58(4)
O(4)	1835(9)	11307(6)	1125(5)	69(5)
O(5)	5208(9)	7806(6)	463(5)	88(5)
C(1)	-2130(12)	8829(7)	4369(6)	31(5)
C(2)	-1341(12)	8794(7)	5005(6)	37(5)
C(3)	-2028(15)	8781(8)	5723(7)	49(6)
C(4)	-3474(16)	8804(9)	5825(8)	63(7)
C(5)	-4230(13)	8829(9)	5197(8)	67(7)
C(6)	-3562(13)	8857(8)	4462(7)	50(6)
C(7)	-2002(10)	8073(7)	3095(6)	27(5)
C(8)	-1970(12)	7178(8)	3648(7)	50(6)
C(9)	-2488(14)	6545(8)	3437(9)	65(7)
C(10)	-3049(14)	6767(9)	2692(9)	62(7)
C(11)	-3092(13)	7669(10)	2144(8)	62(7)
C(12)	-2602(11)	8331(9)	2339(7)	50(6)
C(13)	553(11)	8629(7)	3399(6)	29(5)
C(14)	1332(12)	7871(8)	3144(6)	40(5)
C(15)	2811(14)	7656(9)	3148(7)	62(7)
C(16)	3532(13)	8164(10)	3414(7)	64(7)
C(17)	2748(13)	8916(9)	3665(7)	53(7)
C(18)	1284(12)	9146(8)	3649(6)	41(6)
C(19)	-2021(10)	10062(6)	2651(5)	28(5)
C(20)	-1207(10)	10364(7)	1933(5)	26(4)
C(21)	-2013(13)	10929(8)	1146(7)	37(6)
C(22)	-1558(13)	11659(8)	-281(6)	57(6)
C(23)	-310(14)	11625(9)	-839(7)	76(8)
C(24)	-3374(11)	13446(7)	1722(6)	34(5)
C(25)	-4360(12)	12972(7)	2172(7)	41(5)
C(26)	-5501(12)	12877(9)	1788(8)	54(7)
C(27)	-5604(13)	13251(9)	952(8)	55(7)
C(28)	-4634(14)	13713(8)	509(7)	57(7)
C(29)	-3483(12)	13815(7)	874(6)	45(6)
C(30)	-2423(11)	13715(7)	3150(6)	27(5)
C(31)	-1451(13)	13390(8)	3792(6)	49(6)
C(32)	-1876(16)	13561(8)	4505(7)	57(7)
C(33)	-3274(18)	14038(10)	4594(8)	68(8)
C(34)	-4198(13)	14362(9)	3967(9)	64(7)
C(35)	-3805(12)	14195(8)	3239(6)	48(6)
C(36)	-1160(12)	14513(8)	1554(6)	33(5)
C(37)	316(13)	14394(8)	1450(6)	46(6)
C(38)	894(14)	15157(10)	1015(7)	63(7)
C(39)	18(17)	16021(9)	686(7)	61(7)
C(40)	-1476(15)	16158(8)	794(7)	60(7)
C(41)	-2057(12)	15394(8)	1248(6)	44(6)
C(42)	-477(10)	12464(6)	2379(6)	27(4)

C(43)	-28(11)	12088(7)	1757(6)	32(5)
C(44)	1485(12)	11528(8)	1780(7)	34(5)
C(45)	3236(15)	10739(12)	1087(10)	96(11)
C(46)	3364(38)	10297(23)	454(16)	135(25)
C(46A)	3173(30)	9765(13)	1202(21)	95(18)
C(47)	1488(14)	4850(9)	3259(8)	80(8)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Pd(1)-Br(1)	2.494 (2)	Pd(1)-C(19)	2.112 (11)
Pd(1)-C(20)	2.103 (11)	Pd(1)-C(42)	2.122 (10)
Pd(1)-C(43)	2.129 (10)	Cl(1)-C(47)	1.717 (16)
Cl(2)-C(47)	1.746 (13)	P(1)-C(1)	1.794 (11)
P(1)-C(7)	1.802 (13)	P(1)-C(13)	1.790 (10)
P(1)-C(19)	1.784 (8)	P(2)-C(24)	1.801 (13)
P(2)-C(30)	1.795 (11)	P(2)-C(36)	1.807 (11)
P(2)-C(42)	1.786 (9)	O(1)-C(21)	1.164 (15)
O(2)-C(21)	1.358 (14)	O(2)-C(22)	1.463 (11)
O(3)-C(44)	1.209 (15)	O(4)-C(44)	1.304 (16)
O(4)-C(45)	1.422 (16)	C(1)-C(2)	1.384 (17)
C(1)-C(6)	1.362 (17)	C(2)-C(3)	1.365 (16)
C(3)-C(4)	1.379 (21)	C(4)-C(5)	1.358 (22)
C(5)-C(6)	1.378 (18)	C(7)-C(8)	1.382 (14)
C(7)-C(12)	1.378 (16)	C(8)-C(9)	1.376 (22)
C(9)-C(10)	1.354 (21)	C(10)-C(11)	1.386 (18)
C(11)-C(12)	1.386 (23)	C(13)-C(14)	1.420 (16)
C(13)-C(18)	1.387 (19)	C(14)-C(15)	1.375 (17)
C(15)-C(16)	1.385 (23)	C(16)-C(17)	1.409 (20)
C(17)-C(18)	1.362 (16)	C(19)-C(20)	1.418 (12)
C(20)-C(21)	1.507 (14)	C(22)-C(23)	1.481 (17)
C(24)-C(25)	1.368 (15)	C(24)-C(29)	1.397 (15)
C(25)-C(26)	1.403 (19)	C(26)-C(27)	1.377 (18)
C(27)-C(28)	1.343 (19)	C(28)-C(29)	1.395 (20)
C(30)-C(31)	1.397 (15)	C(30)-C(35)	1.375 (15)
C(31)-C(32)	1.376 (18)	C(32)-C(33)	1.385 (20)
C(33)-C(34)	1.346 (20)	C(34)-C(35)	1.394 (20)
C(36)-C(37)	1.387 (16)	C(36)-C(41)	1.369 (14)
C(37)-C(38)	1.385 (18)	C(38)-C(39)	1.347 (17)
C(39)-C(40)	1.403 (21)	C(40)-C(41)	1.394 (17)
C(42)-C(43)	1.398 (16)	C(43)-C(44)	1.490 (14)
C(45)-C(46)	1.482 (42)	C(45)-C(46A)	1.472 (30)

Table 3. Bond angles (°)

Br(1)-Pd(1)-C(19)	96.9(3)	Br(1)-Pd(1)-C(20)	135.9(2)
C(19)-Pd(1)-C(20)	39.3(4)	Br(1)-Pd(1)-C(42)	92.8(3)
C(19)-Pd(1)-C(42)	169.3(4)	C(20)-Pd(1)-C(42)	131.3(4)
Br(1)-Pd(1)-C(43)	130.7(3)	C(19)-Pd(1)-C(43)	132.4(4)
C(20)-Pd(1)-C(43)	93.1(4)	C(42)-Pd(1)-C(43)	38.4(4)
C(1)-P(1)-C(7)	105.0(5)	C(1)-P(1)-C(13)	112.0(5)
C(7)-P(1)-C(13)	110.3(5)	C(1)-P(1)-C(19)	111.5(5)
C(7)-P(1)-C(19)	108.2(5)	C(13)-P(1)-C(19)	109.7(5)
C(24)-P(2)-C(30)	109.7(5)	C(24)-P(2)-C(36)	109.6(5)
C(30)-P(2)-C(36)	108.6(6)	C(24)-P(2)-C(42)	109.7(5)
C(30)-P(2)-C(42)	110.6(4)	C(36)-P(2)-C(42)	108.7(5)
C(21)-O(2)-C(22)	117.2(8)	C(44)-O(4)-C(45)	117.8(11)
P(1)-C(1)-C(2)	122.5(9)	P(1)-C(1)-C(6)	117.1(9)
C(2)-C(1)-C(6)	120.2(10)	C(1)-C(2)-C(3)	118.5(11)
C(2)-C(3)-C(4)	121.7(13)	C(3)-C(4)-C(5)	119.0(12)
C(4)-C(5)-C(6)	120.2(12)	C(1)-C(6)-C(5)	120.4(12)
P(1)-C(7)-C(8)	120.3(9)	P(1)-C(7)-C(12)	120.5(8)
C(8)-C(7)-C(12)	119.0(12)	C(7)-C(8)-C(9)	120.3(11)
C(8)-C(9)-C(10)	122.1(11)	C(9)-C(10)-C(11)	117.2(15)
C(10)-C(11)-C(12)	122.3(13)	C(7)-C(12)-C(11)	119.0(10)
P(1)-C(13)-C(14)	119.3(9)	P(1)-C(13)-C(18)	120.7(8)
C(14)-C(13)-C(18)	120.0(10)	C(13)-C(14)-C(15)	119.5(13)
C(14)-C(15)-C(16)	120.1(12)	C(15)-C(16)-C(17)	119.9(12)
C(16)-C(17)-C(18)	120.4(14)	C(13)-C(18)-C(17)	120.0(11)
Pd(1)-C(19)-P(1)	120.5(6)	Pd(1)-C(19)-C(20)	70.0(6)
P(1)-C(19)-C(20)	118.8(7)	Pd(1)-C(20)-C(19)	70.7(6)
Pd(1)-C(20)-C(21)	110.9(7)	C(19)-C(20)-C(21)	117.9(9)
O(1)-C(21)-O(2)	124.5(10)	O(1)-C(21)-C(20)	128.1(10)
O(2)-C(21)-C(20)	107.4(9)	O(2)-C(22)-C(23)	107.1(9)
P(2)-C(24)-C(25)	120.5(8)	P(2)-C(24)-C(29)	119.5(9)
C(25)-C(24)-C(29)	119.9(12)	C(24)-C(25)-C(26)	120.3(10)
C(25)-C(26)-C(27)	119.3(11)	C(26)-C(27)-C(28)	120.5(14)
C(27)-C(28)-C(29)	121.6(11)	C(24)-C(29)-C(28)	118.5(10)
P(2)-C(30)-C(31)	120.2(8)	P(2)-C(30)-C(35)	120.3(8)
C(31)-C(30)-C(35)	119.6(10)	C(30)-C(31)-C(32)	119.9(11)
C(31)-C(32)-C(33)	120.2(12)	C(32)-C(33)-C(34)	119.5(13)
C(33)-C(34)-C(35)	121.7(12)	C(30)-C(35)-C(34)	119.1(11)
P(2)-C(36)-C(37)	119.0(7)	P(2)-C(36)-C(41)	120.3(9)
C(37)-C(36)-C(41)	120.2(11)	C(36)-C(37)-C(38)	120.4(10)
C(37)-C(38)-C(39)	119.8(12)	C(38)-C(39)-C(40)	120.5(13)
C(39)-C(40)-C(41)	119.7(10)	C(36)-C(41)-C(40)	119.2(11)
Pd(1)-C(42)-P(2)	114.5(5)	Pd(1)-C(42)-C(43)	71.1(6)
P(2)-C(42)-C(43)	121.0(7)	Pd(1)-C(43)-C(42)	70.5(6)
Pd(1)-C(43)-C(44)	108.1(6)	C(42)-C(43)-C(44)	117.7(10)
O(3)-C(44)-O(4)	123.4(10)	O(3)-C(44)-C(43)	124.2(12)
O(4)-C(44)-C(43)	112.4(10)	O(4)-C(45)-C(46)	112.7(18)
O(4)-C(45)-C(46A)	110.7(16)	Cl(1)-C(47)-Cl(2)	111.3(7)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd(1)	27(1)	28(1)	27(1)	-9(1)	3(1)	-9(1)
Br(1)	52(1)	44(1)	36(1)	-18(1)	14(1)	-16(1)
Br(2)	75(1)	63(1)	53(1)	-14(1)	-4(1)	-4(1)
Cl(1)	117(4)	113(4)	113(3)	-2(3)	-4(3)	-65(3)
Cl(2)	92(3)	80(3)	170(4)	-15(3)	18(3)	-58(3)
P(1)	22(2)	32(2)	31(2)	-8(1)	-1(1)	-9(1)
P(2)	31(2)	28(2)	27(2)	-9(2)	2(1)	-8(1)
O(1)	38(6)	80(7)	45(5)	-7(5)	-17(5)	-8(5)
O(2)	46(5)	57(6)	32(5)	-14(5)	-3(4)	-6(4)
O(3)	40(6)	77(7)	54(6)	-12(5)	-2(5)	-21(5)
O(4)	42(6)	103(8)	71(6)	-3(5)	18(5)	-53(6)
O(5)	76(7)	89(7)	96(7)	-23(6)	-21(6)	-20(6)
C(1)	29(8)	32(7)	32(7)	-8(6)	7(6)	-14(5)
C(2)	39(8)	29(7)	33(7)	-3(6)	8(6)	-2(6)
C(3)	68(10)	38(8)	35(8)	-3(7)	-3(7)	-10(6)
C(4)	66(12)	64(10)	44(9)	-3(9)	14(8)	-11(7)
C(5)	39(9)	92(11)	61(10)	-15(8)	22(8)	-21(9)
C(6)	40(9)	76(10)	43(8)	-20(7)	3(7)	-28(7)
C(7)	23(7)	26(7)	36(7)	-6(5)	-5(5)	-14(5)
C(8)	64(9)	33(8)	54(8)	-8(7)	-31(7)	-10(6)
C(9)	82(11)	32(8)	90(11)	-35(8)	-10(9)	-12(8)
C(10)	92(11)	37(9)	79(10)	-22(8)	-6(9)	-39(8)
C(11)	59(9)	86(12)	59(9)	-16(9)	-6(7)	-48(9)
C(12)	47(8)	63(9)	55(8)	-24(7)	0(7)	-31(7)
C(13)	26(7)	29(7)	25(6)	-3(6)	-6(5)	-3(5)
C(14)	26(8)	42(8)	51(8)	2(6)	-5(6)	-18(6)
C(15)	48(10)	65(10)	76(10)	-2(8)	2(7)	-35(8)
C(16)	26(8)	79(11)	77(10)	3(8)	-2(7)	-26(9)
C(17)	29(9)	62(10)	80(10)	-14(7)	-7(7)	-34(8)
C(18)	25(8)	44(8)	55(8)	0(6)	-9(6)	-21(7)
C(19)	32(7)	18(6)	28(6)	1(5)	-8(5)	-3(5)
C(20)	33(7)	25(6)	15(6)	-5(5)	1(5)	-4(5)
C(21)	35(8)	38(8)	53(8)	-23(7)	7(7)	-27(7)
C(22)	81(11)	53(9)	27(7)	-12(8)	-18(7)	0(6)
C(23)	101(13)	75(11)	41(8)	-13(9)	12(8)	-16(8)
C(24)	28(7)	42(7)	36(7)	-12(6)	-5(5)	-12(6)
C(25)	34(8)	39(8)	41(7)	-3(6)	2(6)	-6(6)
C(26)	41(9)	71(10)	63(9)	-27(7)	6(7)	-31(8)
C(27)	51(9)	60(10)	61(10)	-15(8)	-11(8)	-26(8)
C(28)	66(10)	55(9)	50(9)	-12(8)	-31(8)	-13(7)
C(29)	50(9)	48(8)	33(7)	0(7)	0(6)	-18(6)
C(30)	28(7)	30(7)	23(6)	-10(6)	9(6)	-8(5)
C(31)	53(9)	67(9)	36(7)	-15(7)	-5(7)	-26(7)
C(32)	89(12)	46(9)	35(8)	-2(8)	-18(7)	-18(7)
C(33)	108(14)	79(12)	33(8)	-31(10)	22(9)	-36(8)
C(34)	31(9)	86(11)	85(11)	-4(8)	15(8)	-50(9)
C(35)	40(9)	67(9)	38(8)	3(7)	-1(6)	-29(7)
C(36)	27(7)	32(7)	49(7)	-10(6)	12(6)	-24(6)
C(37)	52(9)	35(8)	39(7)	-20(7)	5(6)	6(6)
C(38)	55(9)	54(10)	72(10)	-13(8)	12(8)	-15(8)
C(39)	90(12)	43(9)	60(9)	-43(9)	20(8)	-16(7)
C(40)	70(11)	35(8)	78(10)	-18(8)	-4(8)	-18(7)
C(41)	51(8)	29(7)	60(8)	-18(7)	23(7)	-25(6)
C(42)	27(7)	17(6)	34(6)	-9(5)	0(5)	-6(5)
C(43)	31(7)	24(6)	40(7)	-10(6)	6(5)	-9(5)

C(44)	28(8)	37(8)	43(8)	-21(6)	18(6)	-15(6)
C(45)	64(12)	141(17)	116(14)	-31(12)	43(10)	-89(14)
C(46)	161(37)	54(24)	201(42)	-52(26)	43(34)	-50(28)
C(46A)	57(22)	57(24)	131(30)	4(18)	3(20)	4(21)
C(47)	75(11)	79(11)	91(11)	-33(9)	6(9)	-27(9)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(2A)	-333	8777	4939	80
H(3A)	-1499	8763	6169	80
H(4A)	-3935	8784	6337	80
H(5A)	-5237	8844	5259	80
H(6A)	-4096	8902	4008	80
H(8A)	-1579	6999	4181	80
H(9A)	-2446	5922	3825	80
H(10A)	-3425	6323	2555	80
H(11A)	-3475	7841	1610	80
H(12A)	-2668	8960	1959	80
H(14A)	814	7522	2967	80
H(15A)	3344	7146	2974	80
H(16A)	4564	8000	3429	80
H(17A)	3253	9267	3848	80
H(18A)	742	9669	3805	80
H(19A)	-3034	10214	2547	80
H(20A)	-306	9936	1901	80
H(22A)	-2002	12301	-324	80
H(22B)	-2252	11393	-425	80
H(23A)	-598	11981	-1394	80
H(23B)	373	11891	-685	80
H(23C)	123	10979	-787	80
H(25A)	-4252	12700	2753	80
H(26A)	-6206	12554	2102	80
H(27A)	-6377	13190	679	80
H(28A)	-4727	13967	-73	80
H(29A)	-2783	14138	556	80
H(31A)	-488	13054	3726	80
H(32A)	-1206	13350	4945	80
H(33A)	-3595	14133	5098	80
H(34A)	-5153	14719	4021	80
H(35A)	-4480	14410	2801	80
H(37A)	931	13773	1676	80
H(38A)	1918	15076	958	80
H(39A)	414	16546	366	80
H(40A)	-2091	16777	557	80
H(41A)	-3075	15480	1338	80
H(42A)	295	12398	2721	80
H(43A)	-458	12456	1233	80
H(45A)	3651	10503	1621	80
H(45B)	3817	11125	718	80
H(46A)	3516	10754	-62	80
H(46B)	4162	9754	573	80
H(46C)	2495	10107	434	80
H(46D)	3017	9414	1761	80
H(46E)	2392	9804	877	80
H(46F)	4059	9450	1016	80
H(47A)	2040	5226	2855	80
H(47B)	548	4974	3042	80