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Table 4. Crystal Data and Structure Refinement of 3a

Identification code	2518	
Empirical formula	$C_{22}H_{38}P_2Pd$	
Formula weight	470.86 g · mol^{-1}	
Temperature	293 K	
Wavelength	0.71069 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$ (no. 14)	
Unit cell dimensions	a = 12.0451(14) Å	$\alpha = 90°$
	b = 15.1265(14) Å	$\beta = 110.467(12)°$
	c = 14.382(3) Å	$\gamma = 90°$
Volume	2455.0(6) Å^3	
Z	4	
D_{calc}	1.274 Mg · m^{-3}	
Absorption coefficient	0.889 mm^{-1}	
F(000)	984 e	
Crystal size	0.32 x 0.53 x 0.53 mm	
θ range for data collection	2.69 to 27.44°	
Index ranges	$-15 \le h \le 14, -19 \le k \le 0, 0 \le l \le 18$	
Reflections collected	5807	
Independent reflections	5593 [R_{int} = 0.0173]	
Absorption correction	none	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5592 / 0 / 238	
Goodness-of-fit on F^2	1.040	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0375$	$wR^2 = 0.0891$
R indices (all data)	$R_1 = 0.0985$	$wR^2 = 0.1107$
Largest diff. peak and hole	0.383 and –0.354 e · Å^{-3}	

Table 5. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a.[a]

	x	y	z	U_{eq}
Pd	2071(1)	1697(1)	2445(1)	66(1)
P(1)	3660(1)	2389(1)	2233(1)	80(1)
P(2)	2554(1)	2434(1)	3932(1)	80(1)
C(1)	1127(4)	865(3)	1349(4)	81(1)
C(2)	649(3)	842(3)	1989(3)	69(1)
C(3)	–313(3)	461(3)	2230(4)	78(1)
C(4)	–1272(4)	95(3)	1505(4)	103(2)
C(5)	–2189(5)	–284(4)	1746(7)	146(3)
C(6)	–2148(7)	–301(5)	2704(9)	161(4)
C(7)	–1227(7)	53(5)	3419(6)	154(3)
C(8)	–285(5)	427(4)	3195(5)	117(2)
C(9)	4263(5)	3191(4)	3249(4)	116(2)
C(10)	3964(5)	3024(4)	4130(4)	121(2)
C(11)	4926(4)	1671(4)	2266(5)	115(2)
C(12)	5220(6)	1038(5)	3087(6)	171(3)
C(13)	6034(5)	2150(5)	2243(5)	152(3)
C(14)	3445(5)	3075(4)	1126(5)	117(2)
C(15)	2486(7)	3764(5)	1027(6)	174(3)
C(16)	3069(7)	2498(6)	220(5)	175(3)
C(17)	2909(5)	1796(3)	5095(4)	101(2)
C(18)	3664(6)	1017(4)	5068(5)	145(2)
C(19)	3436(6)	2311(5)	6057(4)	139(2)
C(20)	1551(7)	3292(4)	4075(6)	134(2)
C(21)	404(6)	2903(5)	4025(6)	163(3)
C(22)	1313(8)	3989(5)	3258(7)	199(4)

[a] U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 6. Bond Lengths [Å] and Angles [°] for 3a.

Pd–P(1)	2.294(1)	Pd–P(2)	2.301(1)
Pd–C(1)	2.028(5)	Pd–C(2)	2.062(4)
P(1)–C(9)	1.842(6)	P(1)–C(11)	1.861(5)
P(1)–C(14)	1.841(7)	P(2)–C(10)	1.851(6)
P(2)–C(17)	1.848(5)	P(2)–C(20)	1.834(7)
C(1)–C(2)	1.246(7)	C(1)–H(1)	0.82(5)
C(2)–C(3)	1.441(6)	C(3)–C(4)	1.374(7)
C(3)–C(8)	1.379(9)	C(4)–C(5)	1.392(8)
C(5)–C(6)	1.36(2)	C(6)–C(7)	1.33(1)
C(7)–C(8)	1.40(1)	C(9)–C(10)	1.455(9)
C(11)–C(12)	1.46(1)	C(11)–C(13)	1.530(8)
C(14)–C(15)	1.53(1)	C(14)–C(16)	1.50(1)
C(17)–C(18)	1.498(9)	C(17)–C(19)	1.520(8)
C(20)–C(21)	1.48(1)	C(20)–C(22)	1.53(1)

C(2)–Pd–C(1)	35.4(2)	C(2)–Pd–P(2)	120.8(1)
C(2)–Pd–P(1)	152.1(1)	C(1)–Pd–P(2)	156.2(1)
C(1)–Pd–P(1)	116.6(1)	P(2)–Pd–P(1)	87.2(1)
C(14)–P(1)–C(11)	102.5(3)	C(14)–P(1)–C(9)	102.3(3)
C(14)–P(1)–Pd	120.0(2)	C(11)–P(1)–C(9)	105.8(3)
C(11)–P(1)–Pd	116.4(2)	C(9)–P(1)–Pd	108.2(2)
C(20)–P(2)–C(17)	102.8(3)	C(20)–P(2)–C(10)	104.3(3)
C(20)–P(2)–Pd	119.1(3)	C(17)–P(2)–C(10)	101.7(3)
C(17)–P(2)–Pd	119.5(2)	C(10)–P(2)–Pd	107.2(2)
H(1)–C(1)–C(2)	149(3)	H(1)–C(1)–Pd	137(3)
C(2)–C(1)–Pd	73.8(3)	C(3)–C(2)–C(1)	143.8(5)
C(3)–C(2)–Pd	145.4(3)	C(1)–C(2)–Pd	70.8(3)
C(8)–C(3)–C(4)	117.9(4)	C(8)–C(3)–C(2)	121.2(4)
C(4)–C(3)–C(2)	120.9(5)	C(5)–C(4)–C(3)	120.5(7)
C(6)–C(5)–C(4)	120.6(7)	C(7)–C(6)–C(5)	119.9(8)
C(8) - C(7)–C(6)	120.5(8)	C(7)–C(8)–C(3)	120.6(6)
C(10)–C(9)–P(1)	115.3(4)	C(9)–C(10)–P(2)	116.3(4)
C(13)–C(11)–C(12)	111.1(5)	C(13)–C(11)–P(1)	115.9(4)
C(12)–C(11)–P(1)	111.5(4)	C(16)–C(14)–C(15)	109.1(6)
C(16)–C(14)–P(1)	109.4(5)	C(15)–C(14)–P(1)	109.8(5)
C(19)–C(17)–C(18)	111.3(5)	C(19)–C(17)–P(2)	116.5(4)
C(18)–C(17)–P(2)	109.8(4)	C(22)–C(20)–C(21)	108.4(7)
C(22)–C(20)–P(2)	110.8(6)	C(21)–C(20)–P(2)	110.7(5)

Table 7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a.[a]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd	60(1)	63(1)	70(1)	3(1)	18(1)	-6(1)
P(1)	69(1)	83(1)	84(1)	14(1)	24(1)	-12(1)
P(2)	81(1)	78(1)	77(1)	-7(1)	23(1)	-19(1)
C(1)	80(3)	79(3)	77(3)	-10(3)	19(2)	-7(2)
C(2)	60(2)	67(2)	74(2)	-3(2)	15(2)	-5(2)
C(3)	61(2)	60(2)	110(3)	0(2)	26(2)	1(2)
C(4)	75(3)	80(3)	146(4)	-16(3)	30(3)	-10(2)
C(5)	77(3)	99(4)	256(10)	-21(6)	52(5)	-23(3)
C(6)	113(6)	108(5)	297(12)	14(7)	115(8)	-17(4)
C(7)	141(5)	161(6)	197(8)	33(6)	105(6)	-16(5)
C(8)	105(4)	120(4)	138(5)	0(4)	57(4)	-20(3)
C(9)	108(4)	115(4)	123(4)	-13(3)	39(3)	-50(3)
C(10)	130(4)	127(4)	107(4)	-24(3)	41(3)	-65(4)
C(11)	80(3)	142(5)	132(5)	37(4)	47(3)	5(3)
C(12)	137(5)	160(7)	230(9)	77(7)	83(6)	49(5)
C(13)	102(4)	192(7)	173(7)	38(6)	61(4)	2(4)
C(14)	96(4)	129(5)	119(5)	42(4)	29(3)	-8(3)
C(15)	177(7)	141(6)	176(7)	72(6)	28(6)	30(6)
C(16)	154(6)	255(10)	113(5)	48(6)	42(5)	-7(6)
C(17)	104(3)	107(4)	83(3)	-3(3)	21(3)	-28(3)
C(18)	187(6)	120(5)	106(4)	26(4)	24(4)	3(5)
C(19)	158(5)	168(6)	84(4)	-13(4)	33(4)	-47(5)
C(20)	141(5)	127(5)	134(5)	-35(4)	46(4)	13(4)
C(21)	122(5)	186(7)	208(8)	-7(6)	90(5)	26(5)
C(22)	203(8)	118(6)	272(11)	50(7)	76(8)	41(6)

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