

# deh266\_sq

**Table 1 Crystal data and structure refinement for deh266\_sq.**

Identification code	deh266_sq
Empirical formula	C <sub>53.19</sub> H <sub>42.37</sub> Cl <sub>4.37</sub> N <sub>2</sub> P <sub>2</sub> Ru
Formula weight	1027.51
Temperature/K	150.0
Crystal system	orthorhombic
Space group	Pccn
a/Å	33.4946(15)
b/Å	14.0731(7)
c/Å	23.4674(11)
α/°	90
β/°	90
γ/°	90
Volume/Å <sup>3</sup>	11061.9(9)
Z	8
ρ <sub>calc</sub> /cm <sup>3</sup>	1.234
μ/mm <sup>-1</sup>	0.586
F(000)	4191.0
Crystal size/mm <sup>3</sup>	0.33 × 0.11 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.52 to 55.16
Index ranges	-43 ≤ h ≤ 43, -18 ≤ k ≤ 18, -30 ≤ l ≤ 30
Reflections collected	295194
Independent reflections	12779 [R <sub>int</sub> = 0.1153, R <sub>sigma</sub> = 0.0349]
Data/restraints/parameters	12779/0/589
Goodness-of-fit on F <sup>2</sup>	1.085
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0485, wR <sub>2</sub> = 0.1166
Final R indexes [all data]	R <sub>1</sub> = 0.0755, wR <sub>2</sub> = 0.1294
Largest diff. peak/hole / e Å <sup>-3</sup>	0.98/-0.57

**Table 2 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh266\_sq.  $U_{\text{eq}}$  is defined as 1/3 of of the trace of the orthogonalised  $U_{\text{IJ}}$  tensor.**

Atom	x	y	z	U(eq)
C1	3272.2(10)	3673(3)	4677.1(15)	39.0(8)
C2	2867.1(11)	3742(3)	4868.6(15)	44.7(10)
C3	2781.1(13)	3767(4)	5456.8(18)	69.8(16)
C4	2391.9(14)	3794(5)	5632(2)	89(2)
C5	2082.0(13)	3804(5)	5233(2)	75.1(17)
C6	2160.5(12)	3782(4)	4661.4(18)	53.9(11)
C7	2558.1(10)	3758(3)	4465.1(15)	39.1(8)
C8	2671.1(9)	3753(2)	3870.4(14)	31.2(7)
C9	3080.1(9)	3721(2)	3728.8(13)	26.2(7)
C10	3200.8(9)	3762(2)	3156.3(13)	27.0(7)
C11	2915.4(10)	3812(3)	2734.0(15)	34.4(8)
C12	2509.4(10)	3825(3)	2859.3(15)	37.8(8)
C13	2391.1(10)	3796(3)	3423.1(16)	38.4(8)
C14	2206.2(12)	3872(4)	2385.2(18)	58.8(13)
C15	3774.4(9)	3302(2)	2320.5(12)	26.9(7)
C16	3691.5(10)	2343(3)	2255.8(14)	33.3(7)
C17	3683.5(12)	1933(3)	1719.6(16)	44.0(9)
C18	3767.6(11)	2466(3)	1243.3(14)	43.6(10)
C19	3854.8(12)	3408(3)	1303.4(15)	46.0(10)
C20	3856.6(11)	3838(3)	1835.3(14)	39.4(9)
C21	3818.2(10)	5086(2)	2904.5(14)	31.8(7)
C22	4210.2(10)	5393(3)	2812.1(14)	33.8(8)
C23	4296.3(13)	6342(3)	2732.1(17)	47.9(10)
C24	3997.9(17)	6993(3)	2748(3)	80.0(18)
C25	3609.1(17)	6709(3)	2853(4)	101(3)
C26	3520.2(13)	5747(3)	2930(2)	65.1(14)
C27	4036.7(10)	5290(2)	4227.0(14)	32.3(7)
C28	4200.6(11)	6165(2)	4427.6(14)	34.3(8)
C29	3952.6(13)	6928(3)	4581.0(19)	50.7(10)
C30	4113.9(14)	7735(3)	4810.8(18)	50.7(10)
C31	4524.4(13)	7792(3)	4899.7(15)	40.2(9)
C32	4774.4(12)	7066(2)	4746.2(13)	34.5(8)
C33	4616.8(10)	6235(2)	4500.1(13)	28.8(7)
C34	4855.5(10)	5442(2)	4314.0(12)	26.1(7)
C35	4664.1(9)	4618(2)	4099.7(12)	24.0(6)
C36	4893.6(9)	3849(2)	3895.0(12)	23.3(6)
C37	5304.4(9)	3901(2)	3918.2(13)	28.7(7)
C38	5501.5(10)	4699(3)	4136.9(14)	31.9(7)

C39	5275.2(10)	5450(2)	4331.2(13)	31.0(7)
C40	5950.9(10)	4732(3)	4156.3(17)	44.6(9)
C41	4751.3(9)	2879(3)	2835.3(13)	33.7(8)
C42	4621.6(11)	2122(3)	2505.8(16)	47.5(10)
C43	4708.2(14)	2102(5)	1924.8(19)	69.9(17)
C44	4917.2(15)	2821(5)	1675.8(17)	77(2)
C45	5048.1(13)	3564(4)	1996.6(18)	66.2(15)
C46	4968.0(11)	3602(3)	2581.6(14)	42.7(9)
C47	4843.0(10)	1767(2)	3812.4(13)	29.5(7)
C48	5227.8(11)	1530(3)	3628.4(16)	39.1(8)
C49	5407.7(13)	696(3)	3798.3(17)	49.1(10)
C50	5202.2(13)	66(3)	4144.2(18)	49.8(11)
C51	4819.1(13)	277(3)	4313.7(17)	45.0(9)
C52	4640.4(11)	1127(2)	4153.0(14)	34.9(8)
Cl1	3686.2(2)	1720.9(6)	3686.7(3)	29.34(17)
Cl2	4148.2(2)	2797.5(6)	4841.2(3)	30.79(18)
N1	3380.9(7)	3646(2)	4144.2(11)	27.1(6)
N2	4245.8(8)	4551(2)	4075.7(10)	26.6(6)
P1	4604.7(2)	2880.1(6)	3585.9(3)	24.10(17)
P2	3735.1(2)	3818.7(6)	3031.7(3)	24.01(17)
Ru1	3982.5(2)	3267.0(2)	3854.5(2)	22.70(8)
C53	3874(2)	-662(6)	3426(4)	129(4)
Cl3	3384.0(8)	-896.0(17)	3546.8(18)	164.6(16)
Cl4	3927.1(9)	-340.5(13)	2638.0(10)	130.4(12)
C54	2662(7)	6272(11)	4735(11)	110(8)
Cl5	2820.2(18)	6222(4)	4156(3)	117(2)
Cl6	2955(2)	6459(7)	5366(5)	189(4)

**Table 3 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh266\_sq. The Anisotropic displacement factor exponent takes the form:**

$$-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...].$$

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
C1	28.7(17)	61(2)	27.1(17)	-8.1(17)	2.5(14)	0.2(17)
C2	33.3(19)	73(3)	28.2(18)	-2.7(19)	10.3(15)	3.7(19)
C3	39(2)	137(5)	33(2)	-4(3)	9.5(18)	14(3)
C4	48(3)	182(7)	36(2)	3(3)	19(2)	20(3)
C5	37(2)	140(5)	49(3)	3(3)	20(2)	9(3)
C6	30.5(19)	89(3)	42(2)	4(2)	10.8(17)	1(2)
C7	25.4(17)	58(2)	34.3(19)	-2.2(17)	7.8(14)	-1.4(17)
C8	23.9(15)	38.2(19)	31.6(17)	-2.8(15)	5.8(13)	-5.8(14)
C9	23.0(15)	30.6(17)	25.0(16)	-2.4(13)	2.7(12)	-4.4(13)
C10	21.2(14)	34.4(18)	25.5(16)	-1.2(14)	2.3(12)	-3.7(13)
C11	26.2(16)	49(2)	28.4(17)	-0.9(16)	1.1(13)	-4.0(15)
C12	24.6(16)	52(2)	37.4(19)	-0.7(17)	-3.2(15)	-4.2(16)
C13	19.6(16)	53(2)	43(2)	0.0(18)	2.2(14)	-4.5(16)
C14	29(2)	106(4)	41(2)	2(2)	-7.2(17)	-2(2)
C15	20.2(14)	41.9(18)	18.6(14)	-2.7(14)	1.5(11)	-4.0(14)
C16	36.0(18)	41.1(19)	22.6(16)	-3.0(14)	2.1(14)	-3.2(16)
C17	51(2)	51(2)	30.4(18)	-14.0(17)	-0.6(17)	-7.7(19)
C18	38(2)	74(3)	18.7(16)	-11.9(17)	0.7(14)	-11(2)
C19	44(2)	74(3)	20.6(16)	4.2(18)	3.4(15)	-17(2)
C20	38.2(19)	54(2)	26.5(17)	1.9(16)	2.1(14)	-16.3(18)
C21	29.9(17)	32.6(18)	32.8(17)	-2.8(14)	4.7(14)	-7.4(14)
C22	33.1(18)	37.8(19)	30.6(17)	-0.9(15)	4.6(14)	-9.4(15)
C23	51(2)	45(2)	47(2)	-6.9(19)	11.2(19)	-20(2)
C24	77(4)	32(2)	131(5)	-3(3)	28(4)	-13(2)
C25	64(3)	34(2)	204(8)	2(4)	31(4)	5(2)
C26	40(2)	37(2)	119(4)	-3(3)	21(3)	1.6(19)
C27	27.2(17)	37.6(19)	32.1(17)	-12.5(15)	5.1(13)	-1.2(15)
C28	40.9(19)	34.4(19)	27.4(17)	-7.9(14)	4.5(15)	-4.8(16)
C29	47(2)	51(2)	54(3)	-17(2)	4.6(19)	2.1(19)
C30	68(3)	34(2)	50(2)	-12.6(18)	10(2)	0(2)
C31	64(3)	31.4(19)	25.5(17)	-2.4(15)	-3.7(17)	-13.9(18)
C32	51(2)	31.8(17)	20.5(15)	4.7(14)	-3.4(15)	-11.2(16)
C33	38.4(18)	31.8(17)	16.3(14)	1.9(13)	-0.4(13)	-10.1(15)
C34	35.5(17)	29.7(16)	13.1(13)	4.7(12)	-0.1(12)	-7.9(14)
C35	26.7(15)	33.1(17)	12.2(13)	0.2(12)	-0.5(11)	-7.9(13)
C36	26.4(15)	29.2(16)	14.3(13)	3.0(12)	0.3(11)	-5.0(12)
C37	25.5(15)	37.6(18)	23.1(15)	6.8(14)	0.2(12)	-2.7(14)
C38	28.3(16)	42.3(19)	25.0(16)	11.4(15)	-4.5(13)	-9.8(15)

C39	33.2(17)	38.0(19)	21.7(15)	9.7(14)	-7.5(13)	-16.6(15)
C40	28.2(19)	60(3)	46(2)	5.4(19)	-6.5(16)	-10.6(18)
C41	22.1(15)	63(2)	16.3(14)	-7.3(15)	0.9(12)	10.5(16)
C42	34.2(19)	79(3)	29.5(18)	-21.1(19)	-3.6(15)	13(2)
C43	55(3)	123(5)	32(2)	-35(3)	-13(2)	44(3)
C44	62(3)	155(6)	14.9(18)	-5(3)	3.8(19)	60(4)
C45	46(2)	123(4)	30(2)	26(3)	15.3(18)	32(3)
C46	30.3(18)	75(3)	22.4(17)	12.0(18)	4.7(14)	12.0(18)
C47	30.3(16)	35.0(17)	23.2(15)	-8.9(14)	-5.8(13)	0.9(14)
C48	41(2)	45(2)	31.5(18)	-15.3(16)	1.8(15)	4.9(17)
C49	49(2)	52(2)	47(2)	-20(2)	-3.4(19)	19(2)
C50	62(3)	37(2)	50(2)	-15.1(19)	-16(2)	16(2)
C51	59(3)	36(2)	39(2)	-4.1(17)	-10.1(18)	-4.2(19)
C52	40.5(19)	35.3(19)	29.0(17)	-5.5(15)	-4.8(15)	-2.6(16)
Cl1	28.2(4)	33.7(4)	26.1(4)	-3.2(3)	0.1(3)	-9.4(3)
Cl2	29.9(4)	44.0(5)	18.5(3)	-4.6(3)	1.0(3)	-6.0(3)
N1	22.4(13)	36.5(15)	22.2(13)	-5.8(11)	3.5(10)	-2.9(11)
N2	23.7(13)	37.9(15)	18.1(12)	-6.0(11)	3.1(10)	-4.3(12)
P1	22.5(4)	33.7(4)	16.1(3)	-5.6(3)	1.7(3)	-3.2(3)
P2	19.9(4)	31.6(4)	20.5(4)	-3.1(3)	2.8(3)	-5.8(3)
Ru1	19.79(12)	31.63(14)	16.68(12)	-5.81(10)	3.00(9)	-5.90(10)
C53	76(5)	124(7)	188(10)	-117(7)	17(5)	-7(5)
Cl3	103.9(18)	75.5(14)	315(5)	-47(2)	-5(2)	8.5(13)
Cl4	222(3)	59.5(11)	109.3(17)	-8.5(11)	-36.1(17)	57.8(14)
C54	124(18)	26(8)	180(20)	-28(11)	9(17)	21(9)
Cl5	110(4)	77(3)	164(6)	-35(4)	27(4)	-23(3)
Cl6	85(4)	218(9)	262(11)	-66(8)	45(6)	-8(5)

**Table 4 Bond Lengths for deh266\_sq.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.433(5)	C30	C31	1.393(6)
C1	N1	1.303(4)	C31	C32	1.369(5)
C2	C3	1.410(5)	C32	C33	1.408(5)
C2	C7	1.403(5)	C33	C34	1.440(5)
C3	C4	1.368(6)	C34	C35	1.417(4)
C4	C5	1.397(7)	C34	C39	1.406(5)
C5	C6	1.368(6)	C35	C36	1.412(4)
C6	C7	1.409(5)	C35	N2	1.406(4)
C7	C8	1.446(5)	C36	C37	1.379(4)
C8	C9	1.410(4)	C36	P1	1.822(3)
C8	C13	1.409(5)	C37	C38	1.400(5)
C9	C10	1.404(4)	C38	C39	1.379(5)
C9	N1	1.406(4)	C38	C40	1.506(5)
C10	C11	1.379(4)	C41	C42	1.386(5)
C10	P2	1.815(3)	C41	C46	1.384(6)
C11	C12	1.391(5)	C41	P1	1.829(3)
C12	C13	1.382(5)	C42	C43	1.394(6)
C12	C14	1.508(5)	C43	C44	1.362(8)
C15	C16	1.386(5)	C44	C45	1.361(8)
C15	C20	1.393(5)	C45	C46	1.400(5)
C15	P2	1.825(3)	C47	C48	1.400(5)
C16	C17	1.385(5)	C47	C52	1.383(5)
C17	C18	1.376(5)	C47	P1	1.837(3)
C18	C19	1.364(6)	C48	C49	1.379(6)
C19	C20	1.387(5)	C49	C50	1.385(6)
C21	C22	1.399(5)	C50	C51	1.376(6)
C21	C26	1.365(5)	C51	C52	1.390(5)
C21	P2	1.830(3)	Cl1	Ru1	2.4238(8)
C22	C23	1.380(5)	Cl2	Ru1	2.4712(8)
C23	C24	1.356(7)	N1	Ru1	2.193(3)
C24	C25	1.385(7)	N2	Ru1	2.076(3)
C25	C26	1.398(6)	P1	Ru1	2.2442(8)
C27	C28	1.427(5)	P2	Ru1	2.2401(8)
C27	N2	1.304(4)	C53	Cl3	1.696(8)
C28	C29	1.405(5)	C53	Cl4	1.911(11)
C28	C33	1.408(5)	C54	Cl5	1.46(2)
C29	C30	1.369(6)	C54	Cl6	1.79(2)

**Table 5 Bond Angles for deh266\_sq.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	124.6(3)	C37	C36	C35	119.3(3)
C3	C2	C1	120.1(4)	C37	C36	P1	125.8(3)
C7	C2	C1	119.2(3)	C36	C37	C38	121.8(3)
C7	C2	C3	120.6(3)	C37	C38	C40	120.5(3)
C4	C3	C2	119.3(4)	C39	C38	C37	118.5(3)
C3	C4	C5	120.4(4)	C39	C38	C40	121.1(3)
C6	C5	C4	120.9(4)	C38	C39	C34	122.3(3)
C5	C6	C7	120.2(4)	C42	C41	P1	117.0(3)
C2	C7	C6	118.5(3)	C46	C41	C42	119.3(3)
C2	C7	C8	117.3(3)	C46	C41	P1	123.7(3)
C6	C7	C8	124.3(3)	C41	C42	C43	119.7(5)
C9	C8	C7	118.8(3)	C44	C43	C42	120.7(5)
C13	C8	C7	123.0(3)	C45	C44	C43	119.9(4)
C13	C8	C9	118.2(3)	C44	C45	C46	120.6(5)
C10	C9	C8	120.2(3)	C41	C46	C45	119.6(4)
C10	C9	N1	117.4(3)	C48	C47	P1	120.9(3)
N1	C9	C8	122.3(3)	C52	C47	C48	118.4(3)
C9	C10	P2	116.1(2)	C52	C47	P1	120.7(3)
C11	C10	C9	119.4(3)	C49	C48	C47	121.1(4)
C11	C10	P2	124.4(2)	C48	C49	C50	119.8(4)
C10	C11	C12	121.8(3)	C51	C50	C49	119.7(4)
C11	C12	C14	120.2(3)	C50	C51	C52	120.6(4)
C13	C12	C11	118.8(3)	C47	C52	C51	120.4(4)
C13	C12	C14	121.0(3)	C1	N1	C9	117.6(3)
C12	C13	C8	121.6(3)	C1	N1	Ru1	124.2(2)
C16	C15	C20	118.5(3)	C9	N1	Ru1	117.50(19)
C16	C15	P2	118.3(2)	C27	N2	C35	118.1(3)
C20	C15	P2	123.1(3)	C27	N2	Ru1	122.3(2)
C17	C16	C15	120.6(3)	C35	N2	Ru1	119.5(2)
C18	C17	C16	120.5(4)	C36	P1	C41	103.98(15)
C19	C18	C17	119.3(3)	C36	P1	C47	106.98(14)
C18	C19	C20	121.2(3)	C36	P1	Ru1	101.52(10)
C19	C20	C15	119.9(4)	C41	P1	C47	99.28(16)
C22	C21	P2	118.0(3)	C41	P1	Ru1	121.35(11)
C26	C21	C22	118.9(3)	C47	P1	Ru1	121.95(11)
C26	C21	P2	123.1(3)	C10	P2	C15	101.59(14)
C23	C22	C21	121.1(4)	C10	P2	C21	102.67(16)
C24	C23	C22	119.7(4)	C10	P2	Ru1	102.15(11)
C23	C24	C25	120.2(4)	C15	P2	C21	103.20(15)
C24	C25	C26	120.2(5)	C15	P2	Ru1	128.57(11)
C21	C26	C25	119.9(4)	C21	P2	Ru1	114.97(11)

N2	C27	C28	124.9(3)	Cl1	Ru1	Cl2	90.24(3)
C29	C28	C27	121.1(3)	N1	Ru1	Cl1	83.82(7)
C29	C28	C33	120.1(3)	N1	Ru1	Cl2	88.90(7)
C33	C28	C27	118.8(3)	N1	Ru1	P1	178.24(7)
C30	C29	C28	120.1(4)	N1	Ru1	P2	80.97(7)
C29	C30	C31	119.7(4)	N2	Ru1	Cl1	174.66(7)
C32	C31	C30	121.4(3)	N2	Ru1	Cl2	84.43(7)
C31	C32	C33	119.9(3)	N2	Ru1	N1	95.81(10)
C28	C33	C34	117.3(3)	N2	Ru1	P1	83.51(7)
C32	C33	C28	118.6(3)	N2	Ru1	P2	94.08(8)
C32	C33	C34	124.1(3)	P1	Ru1	Cl1	96.71(3)
C35	C34	C33	119.4(3)	P1	Ru1	Cl2	89.42(3)
C39	C34	C33	122.7(3)	P2	Ru1	Cl1	91.12(3)
C39	C34	C35	118.0(3)	P2	Ru1	Cl2	169.57(3)
C36	C35	C34	120.1(3)	P2	Ru1	P1	100.69(3)
N2	C35	C34	121.4(3)	Cl3	C53	Cl4	107.4(5)
N2	C35	C36	118.5(3)	Cl5	C54	Cl6	125.2(15)
C35	C36	P1	114.8(2)				



**Table 6 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for deh266\_sq.**

Atom	x	y	z	U(eq)
H1	3475.86	3644.31	4958.35	47
H3	2991.41	3764.52	5728.35	84
H4	2331.79	3806.2	6027.78	106
H5	1813.11	3825.17	5361.4	90
H6	1946.48	3784.35	4395.85	65
H11	2998.12	3838.08	2347.12	41
H13	2114.32	3806.65	3511.22	46
H14A	2306.41	4284.97	2080.85	88
H14B	1954.9	4129.76	2533.26	88
H14C	2160.16	3232.75	2233.51	88
H16	3639.61	1963.86	2582.4	40
H17	3619.54	1278.71	1680.45	53
H18	3765.02	2181.9	876.2	52
H19	3915.37	3775.94	975.18	55
H20	3913.8	4496.72	1868.68	47
H22	4420.46	4939.98	2804.23	41
H23	4563.62	6539.14	2666.28	58
H24	4055.81	7645.46	2685.83	96
H25	3402.18	7169.1	2874.08	121
H26	3252.88	5552.8	2999.43	78
H27	3754.26	5243.95	4201.92	39
H29	3672.27	6883.82	4525.25	61
H30	3946.55	8255.21	4909.18	61
H31	4633.32	8346.63	5070.5	48
H32	5053.86	7123.84	4805.81	41
H37	5458	3380.77	3782	34
H39	5407.32	5991.75	4482.02	37
H40A	6051.23	4179.29	4366.3	67
H40B	6036.88	5315.52	4348.04	67
H40C	6056.87	4721.95	3767.08	67
H42	4474.11	1619.36	2675.06	57
H43	4620.5	1580.69	1700.09	84
H44	4971.63	2803.84	1278.63	93
H45	5195.19	4062.47	1821.82	79
H46	5061.74	4120.72	2803.33	51
H48	5367.31	1951.57	3382.57	47
H49	5671.88	553.01	3678.34	59
H50	5325.22	-508.5	4263.87	60

H51	4675.51	-162.45	4542.7	54
H52	4377.27	1268.59	4278	42
H53A	4037.94	-1226.88	3516.35	155
H53B	3963.61	-127.29	3667.54	155
H54A	2514.79	5671.19	4796.77	132
H54B	2459.18	6783.76	4731.05	132

**Table 7 Atomic Occupancy for deh266\_sq.**

<b>Atom</b>	<b><i>Occupancy</i></b>	<b>Atom</b>	<b><i>Occupancy</i></b>	<b>Atom</b>	<b><i>Occupancy</i></b>
C53	0.853(4)	H53A	0.853(4)	H53B	0.853(4)
Cl3	0.853(4)	Cl4	0.853(4)	C54	0.3333
H54A	0.3333	H54B	0.3333	Cl5	0.3333
Cl6	0.3333				

**Table 8 Solvent masks information for deh266\_sq.**

Number	X	Y	Z	Volume	Electron count Content
1	0.250	-0.250	0.136	463	59
2	0.250	-0.250	0.636	463	59
3	0.750	0.250	0.364	463	58
4	0.750	0.250	0.864	463	58

## deh266\_sq

**Table 1 Crystal data and structure refinement for deh266\_sq.**

Identification code	deh266_sq
Empirical formula	C <sub>53.19</sub> H <sub>42.37</sub> Cl <sub>4.37</sub> N <sub>2</sub> P <sub>2</sub> Ru
Formula weight	1027.51
Temperature/K	150.0
Crystal system	orthorhombic
Space group	Pccn
a/Å	33.4946(15)
b/Å	14.0731(7)
c/Å	23.4674(11)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	11061.9(9)
Z	8
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.234
$\mu/\text{mm}^{-1}$	0.586
F(000)	4191.0
Crystal size/mm <sup>3</sup>	0.33 × 0.11 × 0.07
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)
2 $\Theta$ range for data collection/ $^\circ$	4.52 to 55.16
Index ranges	-43 ≤ h ≤ 43, -18 ≤ k ≤ 18, -30 ≤ l ≤ 30
Reflections collected	295194
Independent reflections	12779 [ $R_{\text{int}}$ = 0.1153, $R_{\text{sigma}}$ = 0.0349]
Data/restraints/parameters	12779/0/589
Goodness-of-fit on $F^2$	1.085
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.0485, $wR_2$ = 0.1166
Final R indexes [all data]	$R_1$ = 0.0755, $wR_2$ = 0.1294
Largest diff. peak/hole / e Å <sup>-3</sup>	0.98/-0.57