

Table SI-1. Selected X-ray Crystallographic Data for Complexes *all-cis-2*·1.5CH₂Cl₂, *3*·3CH₂Cl₂·H₂O, *cis-7*.

	<i>all-cis-2</i> ·1.5CH ₂ Cl ₂	<i>3</i> ·3CH ₂ Cl ₂ ·H ₂ O	<i>cis-7</i>
formula	C ₄₁ H ₃₉ N ₃ P ₂ Pd ₂ Br ₄ ·1.5CH ₂ Cl ₂	C ₅₉ H ₆₁ N ₃ P ₄ Pd ₂ Br ₄ ·3CH ₂ Cl ₂ ·H ₂ O	C ₂₂ H ₂₂ Br ₂ N ₃ PPd
fw	1295.52	1741.22	625.62
cryst size (mm)	0.50 x 0.30 x 0.26	0.40 x 0.36 x 0.36	0.20 x 0.18 x 0.03
temp (K)	100(2)	100(2)	100(2)
cryst syst	Monoclinic	Monoclinic	Monoclinic
space group	<i>P2(1)/c</i>	<i>P2(1)/n</i>	<i>P2(1)/c</i>
<i>a</i> (Å)	14.6313(12)	16.0280(13)	7.8629(8)
<i>b</i> (Å)	19.8067(17)	14.1822(12)	7.5919(8)
<i>c</i> (Å)	16.2085(14)	30.130(3)	37.124(4)
α (deg)	90	90	90
β (deg)	99.723(2)	91.669(2)	92.747(3)
γ (deg)	90	90	90
<i>V</i> (Å ³)	4629.7(7)	6846.0(10)	2213.6(4)
<i>Z</i>	4	4	4
<i>D</i> _c (g cm ⁻³)	1.859	1.689	1.877
μ (mm ⁻¹)	4.505	3.230	4.535
θ range (deg)	2.42–27.84	1.46–27.50	2.20–27.50
no. of unique data	6301	15728	15300
max, min transmission	0.3871, 0.2116	0.9051, 0.6765	0.7898, 0.5652
final <i>R</i> indices (<i>I</i> > 2 σ (<i>I</i>))	<i>R</i> ₁ = 0.0416, <i>wR</i> ₂ = 0.1056	<i>R</i> ₁ = 0.0536, <i>wR</i> ₂ = 0.1262	<i>R</i> ₁ = 0.0494, <i>wR</i> ₂ = 0.0922
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0553, <i>wR</i> ₂ = 0.1113	<i>R</i> ₁ = 0.0721, <i>wR</i> ₂ = 0.1331	<i>R</i> ₁ = 0.0745, <i>wR</i> ₂ = 0.1001
goodness of fit on <i>F</i> ²	1.047	1.046	1.051
peak/ hole (e Å ⁻³)	1.205/-1.109	2.979/-1.893	0.951 /-0.685