Table 1. X-ray Crystal Data

Compound	*rac*-4	6Pd	7Rh
Molecular formula	$C_{42}H_{40}O_2P_2$	$C_{64}H_{70}Cl_6N_2P_2Pd_2$	$C_{50}H_{50}F_6P_3Rh$
Molecular weight	638.68	1354.66	960.72
Crystal habit	colorless plate	pale yellow needle	orange plate
Crystal dimensions(mm)	0.22x0.10x0.10	0.20x0.16x0.16	0.22x0.12x0.08
Crystal system	triclinic	orthorhombic	orthorhombic
Space group	Pbar1	P212121	P212121
a(Å)	10.572(1)	17.660(5)	12.737(5)
b(Å)	13.172(1)	18.503(5)	16.766(5)
c(Å)	13.501(1)	19.066(5)	20.593(5)
α(°)	86.396(1)		
β(°)	67.056(1)		
γ(°)	87.169(1)		
V(Å^3)	1727.3(2)	6230(3)	4398(2)
Z	2	4	4
d(g-cm^{-3})	1.228	1.444	1.451
F(000)	676	2768	1976
μ(cm^{-1})	0.161	0.926	0.558
Absorption corrections	multi-scan ; 0.9654 min, 0.9841 max	multi-scan; 0.8364 min, 0.8659 max	multi-scan; 0.8871 min, 0.9567 max
Diffractometer	KappaCCD	KappaCCD	KappaCCD
X-ray source	MoKα	MoKα	MoKα
λ(Å)	0.71069	0.71069	0.71069
Monochromator	graphite	graphite	graphite
T (K)	150.0(1)	150.0(1)	150.0(1)
Scan mode	phi and omega scans	phi and omega scans	phi and omega scans
Maximum θ	30.03	27.47	27.47
HKL ranges	-14 14 ; -18 18 ; -18 19	-18 21 ; -15 24 ; -17 16	-16 16 ; -21 21 ; -26 26
Reflections measured	15587	8497	9997
Unique data	10014	7242	9997
Rint	0.0156	0.0310	0.0000
Reflections used	7955	6267	9101
Criterion	I > 2σI)	I > 2σI)	I > 2σI)
Refinement type	Fsqd	Fsqd	Fsqd
Hydrogen atoms	mixed	mixed	mixed
Parameters refined	419	695	557
Reflections / parameter	18	9	16
wR2	0.1455	0.1694	0.1293
R1	0.0461	0.0601	0.0490
Flack's parameter		-0.01(5)	-0.04(3)
Weights a, b	0.0812 ; 0.3234	0.1012; 13.888	0.0750 ; 6.5391
GoF	1.074	1.034	1.004
difference peak / hole (e Å^{-3})	1.328(0.054) / -0.606(0.054)	0.805(0.108) / -0.920(0.108)	2.599(.095) / -1.316(.09