SUPPLEMENTARY DATA

Chelating and 'pincer' dicarbene complexes of palladium; synthesis and structural studies

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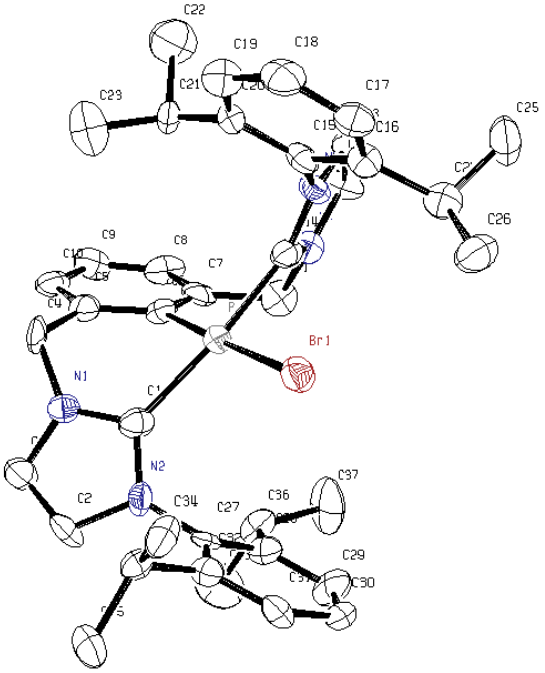

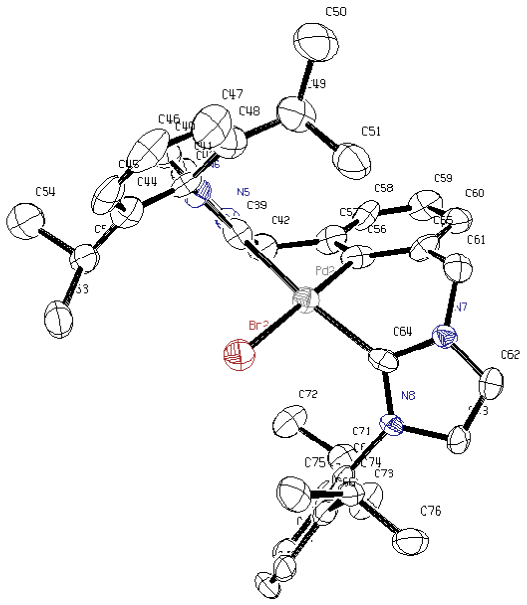

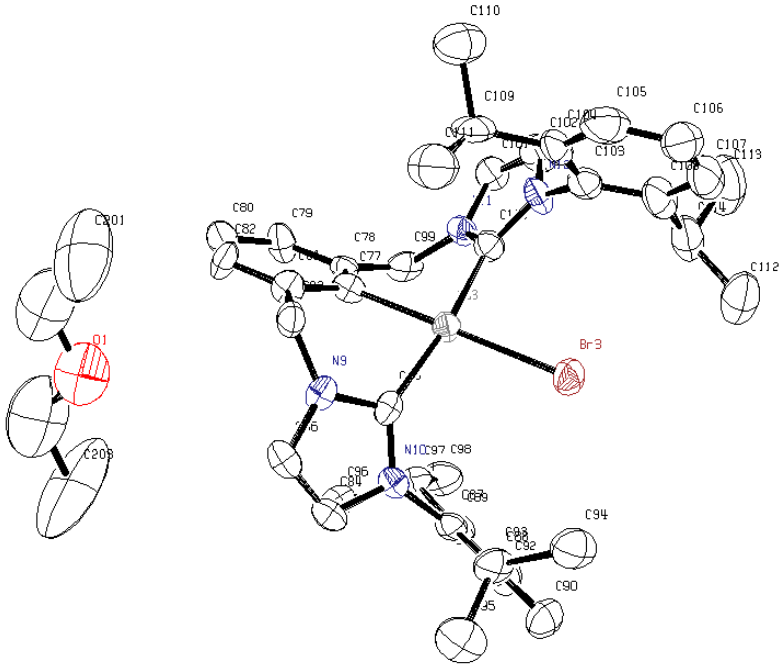

Table 1. Crystal data and structure refinement for 01sw049.

Identification code	s92	
Empirical formula	C118 H145 Br3 N12 O Pd3	
Formula weight	2306.39	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.0118(6) Å	α= 110.001(2)°.
	b = 16.4652(6) Å	β= 96.4400(10)°.
	c = 23.5036(10) Å	γ = 93.111(2)°.
Volume	5757.4(4) $Å^3$	
Z	2	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	1.556 mm^{-1}	
F(000)	2376	
Crystal size	0.03 x 0.03 x 0.01 mm^3	
Theta range for data collection	1.87 to 30.43°.	
Index ranges	-20<=h<=22, -22<=k<=19, -32<=l<=31	
Reflections collected	75784	
Independent reflections	25601 [R(int) = 0.2463]	
Completeness to theta = 30.43°	73.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9846 and 0.9548	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	25601 / 0 / 1234	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2sigma(I)]	R1 = 0.0922, wR2 = 0.1513	
R indices (all data)	R1 = 0.2882, wR2 = 0.2074	
Largest diff. peak and hole	0.917 and -1.113 e.$Å^{-3}$	