

SUPPORTING INFORMATION

Stepwise Cyclopalladation of 2- Phenacylthiopyridine to Give *C,C,N-pincer* Complexes

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Table 1 Crystal data and structure refinement of compounds **1·Br·CHCl₃**, **1·OAc** and **7c**

Compound	1·Br·CHCl₃	1·OAc	7c
Chemical formula	C ₁₄ H ₁₁ BrCl ₃ NOPdS	C ₁₅ H ₁₃ NO ₃ PdS	C ₂₂ H ₁₈ N ₂ OPdS
Formula Mass	533.96	393.72	464.84
Crystal system	Monoclinic	Monoclinic	Triclinic
<i>a</i> /Å	5.7973(6)	33.973(3)	9.018(5)
<i>b</i> /Å	16.3154(17)	11.7646(11)	10.724(5)
<i>c</i> /Å	18.2287(18)	15.7365(14)	11.165(5)
α /°	90.00	90.00	110.244(5)
β /°	93.927(4)	109.394(3)	105.196(5)
γ /°	90.00	90.00	101.431(5)
Unit cell volume/Å ³	1720.1(3)	5932.6(10)	926.5(8)
Temperature/K	100(2)	100(2)	100(2)
Space group	<i>P</i> 2(1)/ <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
No. formula units per unit cell, <i>Z</i>	4	16	2
No. of reflections measured	72896	81719	28993
No. of independent reflections	3803	7352	4635
<i>R</i> _{int}	0.0426	0.0540	0.0253
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2σ(<i>I</i>))	0.0463	0.0337	0.0186
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.1136	0.0711	0.0459
Final <i>R</i> _{<i>I</i>} values (all data)	0.0477	0.0458	0.0206
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.1143	0.0744	0.0467
Goodness of fit on <i>F</i> ²	1.182	1.197	1.113