Electronic Supplementary Material (ESI) for Catalysis Science & Technology

Unsymmetrical α-diiminonickel bromide complexes: Synthesis, characterization and investigation of their catalytic behavior toward ethylene

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Table S Crystal data and structure refinement for **Ni4** and **Ni5**

	Ni4	**Ni5**
Empirical formula	$C_{45}H_{41}Br_2ClN_2Ni$	$C_{47}H_{45}Br_2ClN_2Ni$
fw	863.78	891.83
T/K	173(2)	173(2)
λ/ Å	0.71073	0.71073
Cryst. syst.	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/c
a/ Å	9.6013(19)	9.922(2)
b/ Å	16.927(3)	16.840(3)
c/ Å	24.799(5)	24.975(5)
α (o)	90	90
β (o)	100.77(3)	98.41(3)
γ (o)	90	90
V ($Å^3$)	3959.4(14)	4128.3(14)
Z	4	4
Dcalcd. (gcm^{-3})	1.449	1.435
μ/ mm^{-1}	2.610	2.505
F(000)	1760	1824
Cryst. size / mm	0.54×0.22×0.19	0.20×0.13×0.08
θ range (o)	2.41 - 27.48	1.46 - 27.46
Limiting indices	$-12 \le h \le 10$ $-21 \le k \le 21$ $-32 \le l \le 29$	$-12 \le h \le 11$ $-20 \le k \le 21$ $-32 \le l \le 29$
No. of rflns collected	26497	27562
No. unique rflns [R(int)]	9040 (0.0594)	9393(0.0702)
Completeness to θ (%)	99.4%	99.4 %
Abs corr	none	none
Data / restraints / params	9040 / 0/ 460	9393 / 0 / 478
Goodness of fit on F^2	1.079	1.193
Final R indices[$I > 2\sigma(I)$]	R1 = 0.0668 wR2 = 0.1943	R1 = 0.0979 wR2 = 0.2363
R indices (all data)	R1 = 0.0818 wR2 = 0.2163	R1 = 0.1333 wR2 = 0.2722
Largest diff. peak and hole (e $Å^{-3}$)	0.612 and -0.574	1.364 and -0.989