

Supporting Information

Bis(imino)aryl NCN Pincer Cobalt Complexes: Synthesis and Disproportionation

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Table S1. Summary of crystallographic data for complexes **1d-LiBr**, **1d-CoCl₂**, **2b**, **2d**, **3a**, and **4d**.

	1d-LiBr	1d-CoCl₂	2b	2d	3a	4d
Formula	C ₄₈ H ₇₁ Br ₂ CoLiN ₂ O ₄	C ₆₄ H ₇₈ Br _{0.59} Cl _{3.41} Co ₃ N ₄	C ₅₆ H ₆₂ Br ₄ Co ₄ N ₄	C ₄₈ H ₇₁ Cl ₃ Co ₂ LiN ₂ O ₄	C ₃₀ H ₄₁ BrCoN ₂ P ₂	C ₆₇ H ₈₇ CoN ₄ P
<i>F_w</i>	965.75	1248.34	1346.46	971.21	630.43	1038.30
cryst syst	Orthorhombic	Triclinic	Monoclinic	Triclinic	Orthorhombic	Triclinic
space group	Pnma	P-1	P2(1)/n	P-1	Pbcn	P-1
<i>a</i> (Å)	21.7144(7)	11.4692(8)	11.0834(4)	11.2848(7)	16.5905(7)	11.4966(12)
<i>b</i> (Å)	21.1790(7)	15.6632(11)	13.2980(4)	13.9972(9)	23.4842(10)	13.3441(13)
<i>c</i> (Å)	10.5333(3)	21.5144(15)	18.3364(7)	18.1516(12)	15.8812(6)	22.168(2)
<i>α</i> (deg)	90	70.3670(10)	90	101.3510(10)	90	76.217(2)
<i>β</i> (deg)	90	80.8620(10)	94.5840(10)	105.3260(10)	90	82.452(2)
<i>γ</i> (deg)	90	69.8850(10)	90	109.0460(10)	90	76.299(2)
<i>v</i> (Å ³)	4844.2(3)	3414.1(4)	2693.90(16)	2484.6(3)	6187.5(4)	3198.8(6)
<i>Z</i>	4	2	2	2	8	2
<i>D_{calcd}</i> (gcm ⁻³)	1.324	1.214	1.660	1.298	1.353	1.078
<i>μ</i> (mm ⁻¹)	2.046	1.239	4.217	0.871	1.970	0.333
<i>F</i> (000)	2020	1299	1348	1026	2616	1118
<i>θ_{max}</i> (deg)	25.15	26.05	25.03	25.03	25.36	26.03
collected reflns	74553	21693	29328	12989	33881	16589
Uniq reflns	4445	13146	4754	8651	5610	12220
<i>R_{int}</i>	0.1056	0.0265	0.0302	0.0189	0.0256	0.0602
GOF	1.063	0.981	1.053	1.018	1.105	1.004
<i>R</i> 1	0.0486	0.0431	0.0420	0.0413	0.0657	0.0883
<i>wR</i> 2	0.1157	0.1126	0.1052	0.0969	0.2125	0.1881
Largest diff peak, hole (e Å ⁻³)	0.75, -0.68	0.47, -0.36	1.07, -1.15	0.50, -0.28	1.09, -2.59	0.59, -0.47