

SUPPORTING INFORMATION

Reductive Labilization of a Cyclometalating Ligand Applied to Auxiliary-Mediated Asymmetric Coordination Chemistry

Marianne Kraack,[†] Klaus Harms,[†] and Eric Meggers^{*,†,‡}

[†]Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Strasse, 35043 Marburg,
Germany

[‡]College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's
Republic of China

*E-mail: meggers@chemie.uni-marburg.de

Table S1. Crystallographic Data and Structure Refinement for (S)-2, (S)-5, and Λ -(S)-7.

	(S)-2	(S)-5	Λ -(S)-7
Chemical formula	C ₂₀ H ₂₅ F ₆ N ₆ O ₃ PRu, 0.5(CH ₃ CN)	C ₃₆ H ₃₇ F ₆ N ₅ O ₃ P ₂ Ru, CH ₂ Cl ₂	C ₆₄ H ₅₇ BN ₆ O ₃ Ru, Et ₂ O
M_r	664.03	949.64	1144.15
Crystal system	orthorhombic	orthorhombic	orthorhombic
Space group	$P2_12_12$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	13.6445(5)	10.124(2)	13.6846(14)
b (Å)	24.8208(7)	17.374(3)	14.8157(18)
c (Å)	8.2145(3)	22.971(5)	28.691(4)
V (Å ³)	2781.98(16)	4040.4(14)	5817.0(13)
Z	4	4	4
μ (mm ⁻¹)	0.70	0.67	0.32
Crystal size (mm)	0.38 × 0.10 × 0.08	0.15 × 0.15 × 0.05	0.41 × 0.04 × 0.03
$T_{\min}$, $T_{\max}$	0.928, 0.990	0.92, 0.97	0.888, 1.136
No. of measured, independent and observed [I > 2 $\sigma(I)$] reflections	23795, 5886, 5146	23033, 9203, 7823	30855, 10543, 2506
R_{int}	0.054	0.058	0.306
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.048, 0.88	0.035, 0.063, 1.00	0.057, 0.142, 0.59
No. of reflections	5886	9203	10543
No. of parameters	356	520	729
No. of restraints	0	0	558
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.57, -0.52	0.37, -0.39	0.72, -0.63
Flack parameter ^{S1}	-0.045(19)	-0.049(17)	0.02(8)
CCDC number	947534	947535	947536

Reference

(S1) Flack, H. D. *Acta Cryst.* **1983**, A39, 876–881.