High Diastereoselectivity in Borohydride Reductions of Coordinated Imines

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ESI Figures

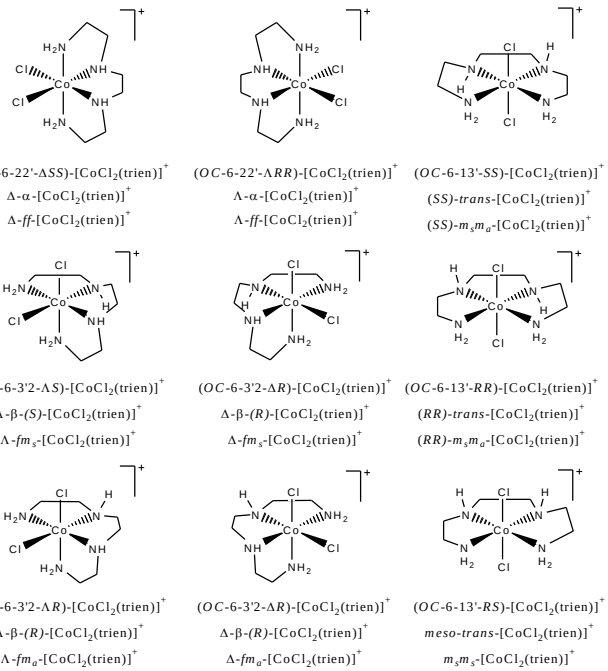

Figure S1: The nine stereoisomers of $[Co(trien)Cl_2]^+$. Isomers are labelled using IUPAC configuration indices (top), the classical α/β system, and the segment approach (see R. M. Hartshorn and D. A. House, *J. Chem. Soc., Dalton Trans.*, 1998, 2577).

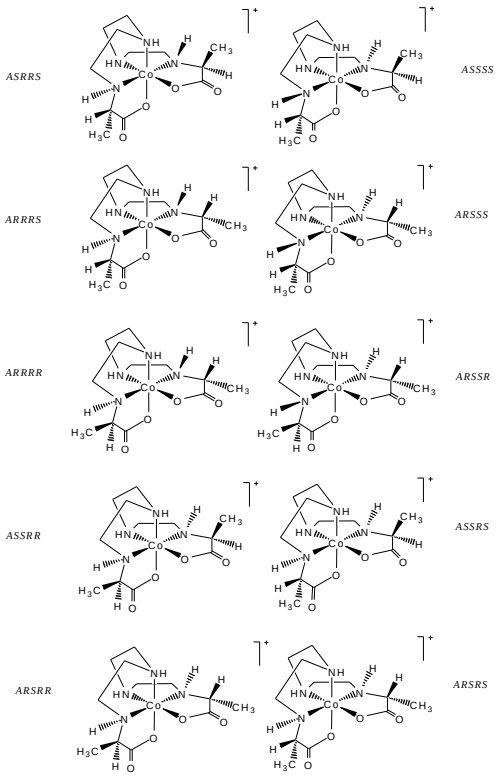

Figure S2: Ten of the 20 stereoisomers formed from the reduction reaction. The remaining ten stereoisomers are each an enantiomer of one of those shown. The configurations of stereogenic centres are indicated in the following order: cobalt (*C*/*A*), followed by α-C-H, NH, NH, α-C-H for the amino acid portions of the ligand, starting from the end of the ligand at the top or right of each drawn structure and working through the ligand

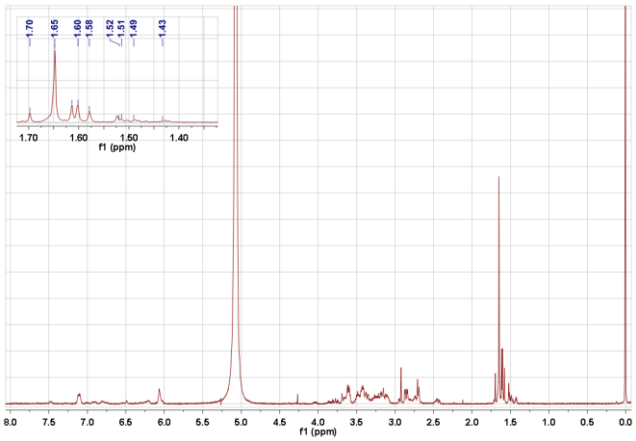

Figure S3 1H NMR spectrum of the crude reaction product from $NaBD_4$ reduction.

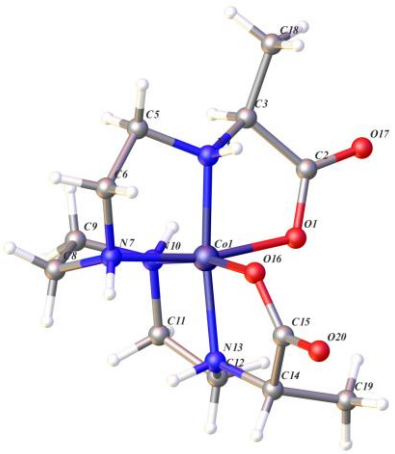

Figure S4: Complex **3**, a minor isomer isolated from the reduction product. The configurations at Co1, C3, C14, and N4 are the same as those found in the major isomer. The configuration at N13 is opposite.

Table S1 Crystallographic details for complex **3**

Empirical formula		$C_{12}H_{26}N_4O_4ClCo$
Formula weight		416.75
Temperature (K)		296(2)
Wavelength		0.71073
Crystal system		Monoclinic
Space group		$P2_1/n$
Unit cell dimensions:	a(Å)	7.5702(12)
	b(Å)	21.160(3)
	c(Å)	12.3205(19)
	α (°)	90
	β (°)	96.930(8)
	γ (°)	90
Volume ($Å^3$)		1959.1(5)
Z		4
Density (calculated) Mg/m^3		1.413
Absorption coefficient mm^{-1}		1.044
F(000)		872
Crystal size mm^3		0.36 × 0.28 × 0.04
Theta range for data collection (°)		1.92 to 24.99
Reflections collected		36332
Independent reflections [R(int)]		3430 [0.1258]
Completeness to theta = 25.05° (%)		0.999
Data / restraints / parameters		3430 / 0 / 246
Goodness-of-fit on F^2		1.083
Final R_1 indices [I>2sigma(I)]		0.1203
wR_2 (all data)		0.3425
Largest diff. peak and hole ($e.Å^{-3}$)		1.843 and -1.286

Notes

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