

Pyridinyloxazolidines: Versatile Scaffolds for Chiral Catalyst Construction

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SUPPLEMENTARY INFORMATION

1. Experimental Section

1.1 General considerations

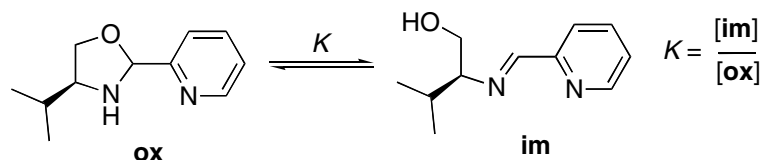
The metal precursor *trans*-PdCl₂(PhCN)₂ was made according to a literature procedure.¹ Simple amino alcohols were prepared by the reduction of the corresponding amino acids using NaBH₄/I₂ in THF solution.² (1*R*,2*S*)-(-)-ephedrine, (1*R*,2*R*)-(-)-pseudoephedrine and all other reagents were purchased from commercial sources and used as supplied. Drying and deoxygenation of solvents was not necessary for the synthesis of ligands or complexes; all syntheses were performed under air. All 1-D NMR spectra were obtained with a Varian Mercury 400 spectrometer (400.089 MHz for ¹H, 100.613 MHz for ¹³C) at room temperature (r.t.) using CDCl₃ solutions of the free ligands and DMSO-*d*₆ solutions of the metal complexes, unless otherwise noted. Spectra were referenced to residual ¹H or ¹³C in the deuterated solvent. All 2-D and variable temperature spectra were recorded using a Varian INOVA 400 spectrometer (399.762 MHz for ¹H) at r.t. and referenced to residual ¹H in the deuterated solvent. Downfield shifts are taken as positive. All coupling constants are given in Hertz; s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, p = pseudo, br = broad. Elemental analyses were performed by Guelph Chemical Laboratories LTD. Mass spectra were collected using a MASPEC II TOF ESI system by Mr. Douglas Hairsine at the University of Western Ontario.

1.2 Crystallography

Crystal structure data were collected using a Nonius Kappa-CCD area detector diffractometer running COLLECT software (Nonius B.V., 1997-2002). The unit cell parameters were calculated and refined from the full data set. Crystal cell refinement and data reduction were carried out using HKL2000 DENZO-SMN (Otwinowski & Minor, 1997) and absorption correction was applied using HKL2000 DENZO-SMN (SCALEPACK). The SHELXTL/PC V6.14 for Windows NT (Sheldrick, G.M., 2001) suite of programs was used to solve the structure by direct methods. Subsequent difference Fourier syntheses allowed the remaining atoms to be located. All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atom positions were calculated geometrically and were included as riding on their respective carbon atoms. The absolute structure parameters for **7^{ox}** and **11^{ox}**·CHCl₃ were -0.07(4) and -0.05(4), respectively, indicating that the correct diastereomers were refined and that there was no sign of racemic twinning. Full crystallographic data for **7^{ox}** (608170) and **11^{ox}**·CHCl₃ (608171) are available free of charge from the Cambridge Crystallographic Data Centre.

2 Variable temperature NMR spectroscopic study of $1^{ox/im}$

The equilibrium studied is shown in Scheme S1.



Scheme S1. The $1^{ox/im}$ equilibrium.

The protocol for determining K from NMR data is outlined in full in the main body of the paper. The resulting van't Hoff plot appears in Figure S1, below.

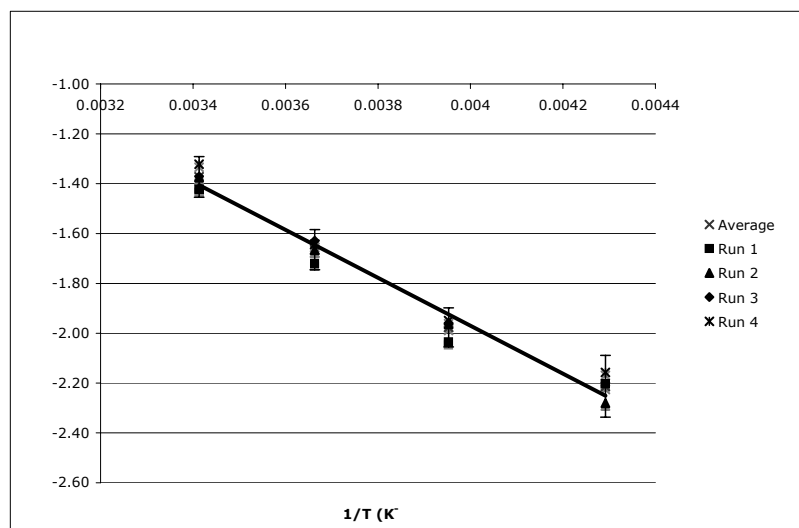


Figure S1. van't Hoff plot for the $1^{ox/im}$ equilibrium.

3 References

1. R. Ugo, F. Cariati and G. L. Monica, *Inorg. Synth.* 1968, **11**, 105.
2. M. J. McKennon and A. I. Meyers, *J. Org. Chem.* 1993, **58**, 3568