

Catalytic Asymmetric Mannich Reactions of Glycine Derivatives with Imines – A new Approach to Optically Active α,β -Diamino Acid Derivatives

*Luca Bernardi, Aase S. Gothelf, Rita G. Hazell and Karl Anker Jørgensen**

Danish National Research Foundation: Center for Catalysis, Department of Chemistry,

Aarhus University, DK-8000 Aarhus C, Denmark

kaj@chem.au.dk

Supporting Information

X-ray Structure of 4b

X-ray work: Crystals of **4b** are triclinic, space group P1, with unit cell at 120K: $a = 11.099(1)\text{\AA}$, $b = 15.508(2)\text{\AA}$, $c = 16.210(2)\text{\AA}$, $\alpha = 91.344(2)^\circ$, $\beta = 100.149(2)^\circ$, $\gamma = 92.319(2)^\circ$, $V = 2743(1)\text{\AA}^3$, $Z = 4$, $\rho_{\text{calcd}} = 1.27$, $\mu = 1.57\text{cm}^{-1}$ (MoK α radiation, $\lambda = 0.71073\text{\AA}$), $F(000) = 1104$, $T = 120\text{K}$. 21712 reflections collected on a SMART diffractometer, 18255 independent, 15695 significant ($I > 3\sigma(I)$). Structure solved by means of the SIR97 program system.²⁴ Least squares refinement according to Rogers²⁵ included a parameter which is supposed to be 1.0 if the chirality is correct, -1.0 if it is wrong; the result is 1.16(17). The 15695 reflections used included 7355 Bijvoet pairs, 1368 parameters were refined, final $R = 0.071$, $R_w = 0.086$. All 4 independent molecules have the same absolute configuration; they differ in the torsion angles around the central single bonds.



