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

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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)Å, b = 15.508(2)Å, c = 16.210(2)Å, $\alpha = 91.344(2)^{\circ}$, $\beta = 100.149(2)^{\circ}$, $\gamma = 92.319(2)^{\circ}$, $V = 2743(1)\text{Å}^3$, Z = 4, $\rho_{calcd} = 1.27$, $\mu = 1.57\text{cm}^{-1}$ (MoK α radiation, $\lambda = 0.71073\text{Å}$), F(000) = 1104, T = 120K. 21712 reflections collected on a SMART diffractometer, 18255 independent, 15695 significant (I> $3\sigma(I)$). Structure solved by means of the SIR97 program system. 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.

