Determination of the Absolute Configuration of 1,5-Diaza-*cis*-decalin by Comparison of Measured and Calculated CD-Spectra

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The absolute configurations of both 1,5-diaza-*cis*-decalin enantiomers were determined by comparison of measured and calculated CD spectra.

CD spectra for both enantiomers were recorded. Theoretical CD spectra for one of the isomers were calculated by means of the semiempirical CNDO/2S method. Eight local minima on the energy hypersurface of the title compound were used to describe the conformer equilibrium mixture. The geometries of these conformers were calculated employing one-determinant *ab initio* calculations using the split valence 6-31G* basis set. Boltzmann factors were then obtained using relative energies calculated with three different basis sets and including correlation(MP2)- and zero point vibrational energy.

Comparing the sign of the observed and calculated longest wavelength Cotton effect, we assign an absolute configuration to the compound. This assignment was verified by means of X-ray structure determination of one of the enantiomers' α-methoxy-α-trifluoromethylphenyl aceticacid (MTPA, Mosher's reagent) derivative.

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