Determination of the Absolute Configuration of Bis(tetrahydropyran-2-yl)methane by Comparison of Measured and Calculated CD-spectra

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The absolute configuration of bis(tetrahydropyran-2-yl)methane (**1**) was determined by comparison of measured and calculated CD spectra.

The theoretical CD spectra were obtained by means of the CNDO/2S method. The five presumably lowest 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 the MM3 force field, the semiempirical AM1 method and one-determinant *ab initio* calculations employing the 6-31G* basis set. Boltzmann factors were then obtained using relative energies calculated with three different basis sets and including correlation- and zero point vibrational energy. Based on the sign of the observed and calculated longest wavelength Cotton effect we assign an absolute configuration to the compound which is in keeping with the chirality expected from the assumed reaction mechanism.

The results of force field and *ab initio* calculations converge to the point that the conformer equilibrium is dominated (85 - 96%) by one single conformer which is energetically separated from the other conformers by about 2 - 3 kcal/mol. This result agrees with previous experimental data.

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