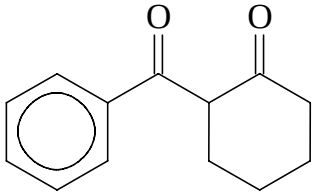
ROSKILDE UNIVERSITY
Department of Science, Systems and Models

22. August 2007

Project suggestion:

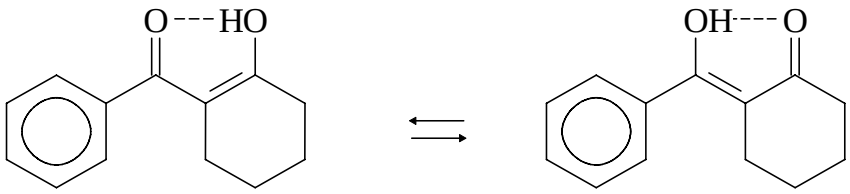
2-Benzoylcyclohexanone

Investigation of the preferred configuration(s) of a flexible molecule by spectroscopic and theoretical procedures



It is well known that molecular structure and shape are decisive factors in most aspects of Chemistry and Biochemistry. 2-Benzoylcyclohexanone (BCH) may seem to be a relatively simple organic compound, but the molecule actually displays a number of conformational and configurational degrees of freedom, in particular:

1) The benzene and cyclohexanone moieties may *rotate* around the formal single bonds to the central carbonyl group, giving rise to a variety of conformations.
2) The cyclohexanone ring may adopt a *chair*- or a *boat*-like conformation.
3) The benzoyl substituent may occupy different positions, e.g., *axial* or *equatorial*.
4) The compound may exist as an *enol* tautomer. Two tautomers, stabilized by intra-molecular H-bonding, are of particular interest:



How do we determine the preferred constitutions and configurations of BCH? Which spectroscopic and theoretical tools are available? These are some of the questions that may be addressed in this project.

Jens Spanget-Larsen, Associate Professor, dr.scient.
Roskilde University (RUC), Building 18.1, P. O. Box 260, DK-4000 Roskilde, Denmark
Phone: (+45) 4674 2710 *Fax*: (+45) 4674 3011 *E-mail*: spanget@ruc.dk *www*: http://www.ruc.dk/~spanget/