HIGH-LEVEL ROVIBRATIONAL CALCULATIONS ON KETENIMINE

MARTIN TSCHÖPE, BENJAMIN SCHRÖDER, SEBASTIAN ERFORT, GUNTRAM RAUHUT, *Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Baden-Württemberg, Germany*.

From an astrochemical point of view ketenimine (CH_2CNH) is a complex organic molecule (COM) and therefore likely to be a building block for biologically relevant molecules. Since it has been detected in the star-forming region Sagittarius B2(N), it is of high relevance in this field. Although experimental data are available for certain bands, for some energy ranges such as above $1200\,cm^{-1}$ reliable data virtually do not exist. In addition, high-level ab initio calculations are neither reported for ketenimine nor for one of its deuterated isotopologues. In this paper, we provide for the first time data from accurate quantum chemical calculations and a thorough analysis of the full rovibrational spectrum. Based on high-level potential energy surfaces obtained from explicitly correlated coupled-cluster calculations including up to 4-mode coupling terms, the (ro)vibrational spectrum of ketenimine has been studied in detail by variational calculations relying on rovibrational configuration interaction (RVCI) theory. Strong Fermi resonances were found for all isotopologues. Rovibrational infrared intensities have been obtained from dipole moment surfaces determined from the distinguishable cluster approximation. A comparison of the spectra of the CH_2CNH molecule with experimental data validates our results, but also reveals new insight about the system, which shows very strong Coriolis coupling effects.