ANALYSIS OF THE MICROWAVE SPECTRUM, STRUCTURE AND INTERNAL ROTATION OF THE CH_3 GROUP IN *N*-METHYLIMIDAZOLE...H_2O AND 2-METHYLIMIDAZOLE...H_2O COMPLEXES

CHARLOTTE NICOLE CUMMINGS, *School of Chemistry, Newcastle University, Newcastle-upon-Tyne, United Kingdom*; EVA GOUGOULA, *Photon Science - Spectroscopy of Molecular Processes, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*; CHRIS MEDCRAFT, *School of Chemistry, UNSW, Sydney, NSW, Australia*; JULIANE HEITKÄMPER, *Institute of Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany*; NICK WALKER, *School of Natural and Environmental Sciences, Newcastle University, Newcastle-upon-Tyne, UK*.

The broadband rotational spectra of *N*-methylimidazole...H_2O and 2-methylimidazole...H_2O have been recorded by Chirped Pulse Fourier Transform Microwave (CP-FTMW) spectroscopy in the frequency range 6.5-18.5 GHz. Each complex was generated by the co-expansion of the methylimidazole isomer and water in an argon backing gas. The spectra of five isotopologues of each complex have been assigned, allowing rotational constants (A_0, B_0 and C_0), centrifugal distortion constants (D_J and D_{JK}), nuclear quadrupole coupling constants (χ_{aa} and χ_{bb-cc}) and internal rotation parameters (V_3, $\angle(i, b)$) to be determined. In both *N*-methylimidazole...H_2O and 2-methylimidazole...H_2O, a hydrogen bond forms between H_2O acting as a hydrogen bond donor and the pyridinic nitrogen of the methylimidazole ring which is the hydrogen bond acceptor. In addition, there is a weak electrostatic interaction between the oxygen atom of H_2O and the hydrogen or CH_3 group attached to the C2 carbon of the methylimidazole ring. The (V_3) barrier to internal rotation of the CH_3 group has been determined for each complex. For *N*-methylimidazole...H_2O, the V_3 barrier is essentially unchanged from the monomer. For 2-methylimidazole...H_2O, there is a large increase in the barrier height (relative to the V_3 of CH_3 in the 2-methylimdizole monomer) which results from the interaction between the oxygen atom of H_2O and the CH_3 group.