MICROWAVE SPECTRA, MOLECULAR GEOMETRIES AND BARRIERS TO INTERNAL ROTATION IN COMPLEXES OF Ar$\cdots C_5H_7N_2$ AND $H_2O\cdots C_5H_7N_2$ (WHERE $C_5H_7N_2$ IS 1-, 2-, 4- OR 5-METHYLIMIDAZOLE)

NICK WALKER, EVA GOUGOULA, *School of Natural and Environmental Sciences, Newcastle University, Newcastle-upon-Tyne, UK*; CHRIS MEDCRAFT, *School of Chemistry, UNSW, Sydney, NSW, Australia*; JULIANE HEITKÄMPER, *Institute of Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany*.

Experiments performed to observe the broadband microwave spectra of 1-methylimidazole, 2-methylimidazole, 4-methylimidazole and 5-methylimidazole also yielded the spectra of molecular complexes containing these molecules. The complexes were generated through laser vaporisation of a solid target rod in the presence of a gas sample undergoing supersonic expansion and containing Ar and H_2O precursors. Spectra have thus been recorded for a series of structural isomers of Ar$\cdots C_5H_7N_2$ and $H_2O\cdots C_5H_7N_2$ where $C_5H_7N_2$ is an isomer of methylimidazole. Rotational constants, B_0, centrifugal distortion constants, D_J, and nuclear quadrupole coupling constants, χ_{aa}(N) and χ_{bb}(N)-χ_{cc}(N) have been determined through assignment of the observed rotational spectra. For each of the structural isomers identified, it will be shown that the argon atom of Ar$\cdots C_5H_7N_2$ coordinates to π electrons of the aromatic ring of methylimidazole. The water molecule in $H_2O\cdots C_5H_7N_2$ binds to the pyridinic nitrogen atom of the methylimidazole sub-unit. For each complex, the barrier to internal rotation, V_3, of the methyl group has been determined.