4-HYDROXY PHENYL ETHANOL (P-TYROSOL) AND ITS SINGLY HYDRATED COMPLEX

JUNE MCCOMBIE and MELINDA. WALKER, *School of Chemistry, University of Nottingham, University Park, Nottingham, UK NG7 2RD*; MATTHEW. R. HOCKRIDGE, SARAH. M. KNIGHT, EVAN G. ROBERTSON and JOHN P. SIMONS, *Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford, UK OX1 3QZ.*

The conformational structures of 4-hydroxy phenol ethanol (p-tyrosol) and it's 1:1 hydrated cluster, have been characterised in a free jet expansion through a combination of mass-selected, resonantly enhanced two-photon ionisation (MS-R2PI), fluorescence excitation and ultra-violet 'hole-burning' spectroscopy, together with rotational contour analysis and $ab\ initio$ computation [a]. It has been possible to assign the structures of both the $gauche\ cis$ and $gauche\ trans$ OH rotamers, as well as the extended $anti$ conformer, and their 1:1 hydrated clusters. The 'tagging' of the phenolic OH group by the hydrogen-bonded water molecule also allows unambiguous assignment of the cis and $trans\ gauche$ conformers through rotational band contour analysis.

[a] M. R. Hockridge, S. M. Knight, E. G. Robertson, J. P. Simons, J. McCombie and M. Walker *Phys. Chem. Chem. Phys.* **1**, 407-413 1999.