

#### 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 its 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<sup>a</sup>. 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.

---

<sup>a</sup>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.