EVIDENCE FOR A STRONG INTERMOLECULAR BOND IN THE PHENOL·N_2 COMPLEX CATION

MARTIN C. R. COCKETT, DARREN M. CHAPMAN, CAROLINE E. H. DESSENT, WOLF D. GEPPERT, STEPHEN R. HAINES, KLAUS MÜLLER-DETHLEFS, and MARK J. WATKINS, *Department of Chemistry, University of York, Heslington, York, United Kingdom, YO1 5DD.*

The vibrational spectrum of the [phenol·N_2]$^+$ complex cation has been observed for the first time by high resolution two-colour threshold ionisation techniques (ZEKE-PFI spectroscopy and mass analysed threshold ionisation (MATI) spectroscopy). The spectra exhibit vibrational progressions in three modes, which have been assigned on the basis of *ab initio* calculations, to the three intermolecular modes (in-plane bend β' 35 cm^{-1}, wag γ' 113 cm^{-1} and stretch σ' 125 cm^{-1}). ZEKE and MATI spectra were acquired through different intermediate S_1 vibrational levels to aid the assignment of the vibrational structure in the cation spectra. Features were observed in the [phenol·N_2]$^+$ MATI channel up to an ion internal energy of 1400 cm^{-1} providing a lower bound for the dissociation energy of the cationic complex. Although the binding energy is weaker than the hydrogen bonded [phenol·water] cluster[a], it is considerably stronger than the van der Waals [phenol·Ar]$^+$ complex[b] suggesting an intermediate binding case characteristic of a combined charge-induced dipole / charge-quadrupole interaction.

[a] G. Reiser, O. Dopfer R. Lindner, G. Henri, K. Müller-Dethlefs, E. W. Schlag, and S. D. Colson, Chem. Phys. Lett. 181, 1 (1991).
[b] E. Beiske, M. W. Rainburn, I. M. Atkinson, and A. E. W. Knight, J. Chem. Phys. 91, 752 (1989).