

EVIDENCE FOR A STRONG INTERMOLECULAR BOND IN THE PHENOL·N₂ COMPLEX CATION

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The vibrational spectrum of the [phenol·N₂]⁺ 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 S₁ vibrational levels to aid the assignment of the vibrational structure in the cation spectra. Features were observed in the [phenol·N₂]⁺ 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.

^aG. Reiser, O. Dopfer R. Lindner, G. Henri, K. Müller-Dethlefs, E. W. Schlag, and S. D. Colson, *Chem. Phys. Lett.* **181**, 1 (1991).

^bE. Beiske, M. W. Rainburn, I. M. Atkinson, and A. E. W. Knight, *J. Chem. Phys.* **91**, 752 (1989).