

PROGRESSIVE POLARIZATION OF PHENANTHRIDINE WITH INCREASING HYDRATION DEGREE EVIDENCED BY QUADRUPOLE AND ITS COMPARISON WITH FORMAMIDE CLUSTERS

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The structure of the microsolvated complexes of phenanthridine (PAN) with up to three water molecules has been investigated previously using chirped pulse Fourier transform microwave (CP-FTMW) spectroscopy from 2-8 GHz. In this work, the effect of Resonance Assisted Hydrogen Bonding (RAHB), also called π -cooperativity, on those complexes has been studied. In the resonant forms, the increase of the electronic density around the nitrogen nucleus enhances its hydrogen acceptor capabilities. Thus, the main effects expected due to the resonance of the multiple conjugated π -bonds in the structure of the complexes are a strengthening of the hydrogen bonds and a lengthening of the N-C bonds. However, due to the subtle changes that occur on the molecular structure, the effect on the N-C distances could not be detected experimentally and only a shortening of the hydrogen bonds has been observed. Therefore, the use of the quadrupole coupling interactions as a probe for the polarization has been used to investigate these effects on the almost planar structures of PAN-(H₂O)_n n=1-3. This form of analysis has been shown to be effective in similar studies with formamide.^{a,b} The experimental quadrupole coupling constant χ_{cc} shows a clear trend from isolated PAN to complexes with higher hydration degree, illustrating how the electronic environment at the ¹⁴N nucleus is altered by microsolvation.

^aS. Blanco, P. Pinacho, J. C. López, *Angew. Chem. Int. Ed.*, 2016, **128**, 9477-9481.

^bS. Blanco, P. Pinacho, J. C. López, *J. Phys. Chem. Lett.*, 2017, **8**, 6060-6066.