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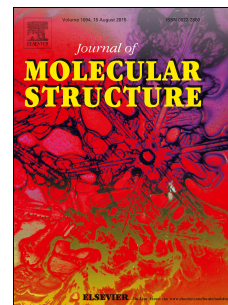
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Pyrrole Multimers and Pyrrole-Acetylene Hydrogen bonded Complexes Studied in N₂ and *para*-H₂ Matrixes using Matrix Isolation Infrared Spectroscopy and *ab initio* computations

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Abstract

Hydrogen bonded interaction of pyrrole multimer and acetylene-pyrrole complexes were studied in N₂ and *p*-H₂ matrixes. DFT computations showed T-shaped geometry for the pyrrole dimer and cyclic complex for the trimer and tetramer were the most stable structures, stabilized by N-H... π interactions. The experimental vibrational wavenumbers observed in N₂ and *p*-H₂ matrixes for the pyrrole multimers were correlated with the computed wavenumbers. Computations performed at MP2/aug-cc-pVDZ level of theory showed that C₂H₂ and C₄H₅N forms 1:1 hydrogen-bonded complexes stabilized by C-H... π interaction (Complex A), N-H... π interaction (Complex B) and π ... π interaction (Complex C), where the former complex is the global minimum and latter two complexes were the first and second local minima, respectively. Experimentally, 1:1 C₂H₂-C₄H₅N complexes A (global minimum) and B (first local minimum) were identified from the shifts in the N-H stretching, N-H bending, C-H bending region of pyrrole and C-H asymmetric stretching and bending region of C₂H₂ in N₂ and *p*-H₂ matrixes. Computations were also performed for the higher complexes and found two minima corresponding to the 1:2 C₂H₂-C₄H₅N and three minima for the 2:1 C₂H₂-C₄H₅N complexes. Experimentally the global minimum 1:2 and 2:1 C₂H₂-C₄H₅N complexes were identified in N₂ and *p*-H₂ matrixes.

Keywords: Hydrogen bonding, pyrrole, acetylene, matrix isolation, N-H... π complex

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