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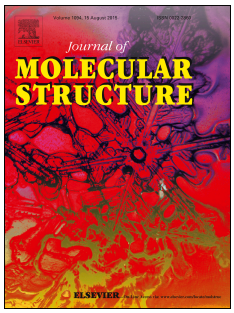

Pyrrole multimers and pyrrole-acetylene hydrogen bonded complexes studied in N_2 and *para*-H_2 matrixes using matrix isolation infrared spectroscopy and *ab initio* computations

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Pyrrole Multimers and Pyrrole-Acetylene Hydrogen bonded Complexes Studied in N_2 and *para*-H_2 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 N_2 and *p*-H_2 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 N_2 and *p*-H_2 matrixes for the pyrrole multimers were correlated with the computed wavenumbers. Computations performed at MP2/aug-cc-pVDZ level of theory showed that C_2H_2 and C_4H_5N 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 C_2H_2-C_4H_5N 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 C_2H_2 in N_2 and *p*-H_2 matrixes. Computations were also performed for the higher complexes and found two minima corresponding to the 1:2 C_2H_2-C_4H_5N and three minima for the 2:1 C_2H_2-C_4H_5N complexes. Experimentally the global minimum 1:2 and 2:1 C_2H_2-C_4H_5N complexes were identified in N_2 and *p*-H_2 matrixes.

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

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