CH···B interactions in acetylene containing solutions: experimental and theoretical DFT studies.

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Streszczenie

Weak to medium H-bonded interactions of the CH···B type (B=CS_2 and $N(CD)_5$) have been studied in C_2H_2/B mixtures. The spectral characteristics (frequency, width, and absolute integral intensity) of the CH asymmetric stretching band of acetylene were determined. Analogously to C_2H_2/CO_2 system studied earlier, in the case of CS_2 solutions, the combination bands ascribed to simultaneous excitations of vibrations of interacted CS_2 and C_2H_2 molecular partners have been found. The observed spectroscopic features have been compared with the results of theoretical DFT/B3LYP calculations utilizing the 6-311++G(3df, 3pd) basis set. They predict 1:1 and 1:2 complex formations with the linear H-bonded structure in the case of $N(CD)_5$ and nonlinear weakly bounded structures in the case of CS_2. The results obtained suggest predomination of 1:1 complexes of acetylene with pyridine in Xe and CS_2 solutions at conditions studied.

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