Infrared studies of acetylene dissolved in liquefied Ar, Kr, N_2, CO, and CO_2.

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Streszczenie

FTIR spectra of acetylene have been studied in liquefied Ar, Kr, N_2, CO and CO_2 in the range ~1000–9000 cm^{-1}. Width, position and absolute integral intensity of a set of fundamental and combination bands were determined. In the case of ν_3 band an effect of vibrational resonance interaction of Fermi-type has been taken into account and the position of non-perturbed ν_3^0 and $(\nu_2+\nu_4+\nu_5)^0$ bands were evaluated in the solutions studied. Liquid to crystal state phase transition experiments, performed in Kr solutions, show reversible growth of self-associates when going to lower temperatures of C_2H_2 doped solid Kr. The $\nu_3(\Sigma_u^+)$ C–H stretch band exhibits weak side shoulders in the case of CO and CO_2 solvents. New combination bands, attributed to $\nu_2(C_2H_2)+\nu_3(CO_2)$, $\nu_3(C_2H_2)+\nu_3(CO_2)$ and $\nu_1(C_2H_2)+\nu_3(CO_2)$ simultaneous transitions due to vibrational excitation of both the interacting partners have been revealed in the region of ~4000–6000 cm^{-1}. Detecting the $\nu_3(C_2H_2)+\nu_3(CO_2)$ combination band, which is forbidden in the frame of dipole approximation, suggests an appreciable role of mutual polarization due to dipole–quadrupole polarizability of molecular partners. The observed spectroscopic features are compared with the results of theoretical DFT/B3LYP and ab initio MP2 calculations utilizing the 6-311++G(3df,3pd) basis set, which predict weak heterodimer formation, with linear H–C≡C–H···C=O and slipped parallel
H-C C-HO-C-Ostructures being favored.

Słowa kluczowe

C2H2, Weak interactions, Vibrational spectra, Simultaneous transitions, Noble gas solutions

Adres publiczny

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