Blue shifts and unusual intensity changes in the infrared spectra of the enflurane···acetone complexes : spectroscopic and theoretical studies.

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Streszczenie

Blue-shifting C-H···O hydrogen-bonded complexes between enflurane (CHFCl-CF(2)-O-CHF(2)) and deuterated acetone have been identified in CCl(4) solution by FT-IR spectroscopy. For the two ν(C-H) stretching vibrations of enflurane the observed blue shifts are +17 and +11 cm(-1). The corresponding two infrared ν(C-H) bands show the opposite changes of their intensity, one is decreasing, and the other is significantly increasing, upon formation of the hydrogen bonding. The structures, binding energies, and theoretical infrared spectra of the enflurane-acetone complexes were calculated by MP2 and B3LYP methods using the 6-311++G(d,p) basis set. The interaction energies were evaluated by the complete basis set limit (CBS) calculations at the HF, MP2, and CCSD(T) levels of theory. Although the MP2 method slightly overestimates the blue shifts, the MP2 predicted frequency difference and the relative IR intensities of two ν(C-H) stretching bands for the enflurane-acetone complexes show good agreement with experiment. Unfortunately, the B3LYP method predicts incorrect IR intensities of these hydrogen-bonded systems. The NBO analysis was performed to unravel the origin of the unusual intensity changes of two ν(C-H) stretching bands, in enflurane complexes.

Adres publiczny

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https://www.acs.org/content/acs/en.html