Features of IR bands of the $CD_3F\cdots HCl$ complex in liquid and solid noble gas solutions.

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Streszczenie

IR spectra of the CD3F. . .HCl complex have been studied in liquid and solid noble gas (Ar, Xe) solutions. It was found that solid xenon may be used for spectroscopic studies of weak simple complexes in thermodynamic equilibrium. All bands of the proton donor and acceptor reveal a sensitivity to complex formation. Extremely strong narrowing of the ν1 and 2ν 5 (A1) parallel bands in solid xenon is explained as a result of the freezing of the rotation defined by the highest moment of inertia. Observed changes of the CD3F spectrum in the ν4 region caused by complex formation are discussed taking into account vibrational resonance. Ab initio calculations on the 6-31G * * level suggest the nonlinear structure of the complex. Such symmetry lowering is consistent with experimentally observed transformations of the IR spectrum.

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