Structure, spectra and stability of a tetrafluoromethane-water complex.

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The complex formed between water and tetrafluoromethane has been studied by infrared matrix isolation spectroscopy and *ab initio* calculations. The geometries of the CF_4–H_2O complexes were optimized in two steps at the MP2/aug-cc-pVTZ level of theory. The structure found at this level was reoptimized on the CP-corrected potential energy surface. The interaction energy was partitioned according to the SAPT scheme and the topological analysis of the electron density was performed. The optimized structure corresponds to the nonhydrogen bonded complex with an oxygen atom of water oriented toward the carbon atom of CF_4. The infrared spectra of CF_4/H_2O/Ne(Ar) matrices demonstrate the presence of a well defined CF_4–H_2O structure in accord with theoretical prediction. Two complex vibrations were identified in the spectra of neon matrices and four vibrations were observed in the spectra of argon matrices. The available experimental data are in accord with the CP-corrected calculated data.

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