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Halogen bonded complexes between volatile anaesthetics (chloroform, halothane, enflurane, isoflurane) and formaldehyde: a theoretical study.

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Streszczenie

The structures and intermolecular interactions in the halogen bonded complexes of anaesthetics (chloroform, halothane, enflurane and isoflurane) with formaldehyde were studied by *ab initio* MP2 and CCSD(T) methods. The CCSD(T)/CBS calculated binding energies of these complexes are between −2.83 and −4.21 kcal mol^{-1}. The largest stabilization energy has been found for the C–Br···O bonded halothane···OCH_2 complex. In all complexes the C–X bond length (where X = Cl, Br) is slightly shortened, in comparison to a free compound, and an increase of the C–X stretching frequency is observed. The electrostatic interaction was excluded as being responsible for the C–X bond contraction. It is suggested that contraction of the C–X bond length can be explained in terms of the Pauli repulsion (the exchange overlap) between the electron pairs of oxygen and halogen atoms in the investigated complexes. This is supported by the DFT-SAPT results, which indicate that the repulsive exchange energy overcompensates the electrostatic one. Moreover, the dispersion and electrostatic contributions cover about 95% of the total attraction forces, in these complexes.

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