Title:	Interplay between C–H···O, O–H···X (X = C, F, Cl) and H–O···Y (C, Cl, F) interactions in methane–water and halogen substituted methane–water complexes: Theoretical investigations of structure and energy
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Abstract:	MP2/6-311++G(d,p), DFT/B3LYP/6-311++G(d,p), and DFT-D/ωB97XD/6-311++G(d,p) levels of theory have been used to investigate the structure, interaction energy and vibrational frequency of a series of 1:1 complexes of halogen (Cl/F) substituted methane with water. More than one stationary point is found on the potential energy surface for a majority of the complexes. Energy decomposition analysis (EDA) was performed on the optimized geometries to understand the contributions of the various components of intermolecular interactions to the stability of the complexes. An increase in dimer interaction energy with increasing chlorination in methane has been observed in case of chloromethane–water complex. No such gradual change is observed in case of fluoro substitution on methane. The bond path for all the complexes was obtained by performing an atoms-in-molecule (AIM) analysis on optimized geometries. NBO analysis performed using MP2/6-311++G(d,p) level of theory shows that the hyperconjugation interaction has a major role in stabilizing the complexes. The blue shift in vC–H fundamental vibration has been discussed in the light of hyperconjugation and rehybridyzation mechanism.
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