Influence of substituents on the nature of sigma holes on Halogen Centers in Organic Compounds

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Halogen bonding is a weak sub-covalent interaction between a Lewis base and a region of positive electrostatic potential on the surface of a halogen atom that is bonded to an electron withdrawing group. New evidence has emerged that nature and size of the sigma-hole the stability of the halogen bonding interaction can be moderated by the identity of substituents that are adjacent to the halogen atom on the organic compound. We find most significantly that the sigma hole can in fact be quenched, and may even disappear due to charge redistribution to the sigma hole region in halogen if the adjacent substituents are electron rich – like other halogen atoms for example. All of our calculations have been carried out at the MP2(full) level theory using the cc-pVTZ quality basis set for all the elements.