

Bonding in hypohalous acids HOX (X = F, Cl, Br, and I) from the topological analysis of the electron localization function (ELF).

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Streszczenie

The bonding in hypohalous acids has been investigated from the topological analysis of the electronlocalization function~ELF!at the Becke3LYP and Hartree–Fock levels. The interaction betweenhalogen and oxygen atoms has been characterized by the presence of bonding, disynaptic attractorsV~O,X!X5F, Cl, Br, and I with the mean electron populationN⁻of 0.32, 0.61, 0.45, and 0.35e,respectively. In the case of HOBr, the possibility of a strong contribution of 3dbromine coreelectrons to the valence shell has been observed. On the base of the bonding evolution theory~BET!,the O–F bond has been recognized as a covalent, polarized one whereas, the bonding between O andCl, Br, and I atoms is of the electron donor–acceptor-type with halogen donating the electrodensity to valence shell of oxygen. The observed difference between HO1F2and HO2X1(X5Cl,Br, and I!polarizations is reflected in topology of ELF maps with a large localization domainsurrounding the V~F!and V~F,O!attractors in HOF and a common superbasin encompassing theV~O,H!,V~O!, and V~X,O!attractors in HOCl, HOBr, and HOI. The very large values of therelative quantum fluctuation~I!, above 0.8, found for V~O,X!suggest that the covalent electrodensity is almost entirely delocalized over other basins. The comparison of the mean electronpopulation (N⁻) of the V~H,X!and V~H,O!basins computed for hydrohalic~HX!and hypohalousacids~HOX!has revealed that the population alters in line with values ofDEacid, therefore can beused as a approximate measure of acidic properties of molecules. The topological analysis of theELF function supports the concept of probonded electronegativity and its usefulness as a tool forprediction of the nature of the oxygen–halogen linkage.

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