# Comparison between experimental and theoretical scales of electrophilicity based on reactivity indexes

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A comparative study between a relative experimental scale of electrophilicity and a theoretical absolute scale based on electronic reactivity indexes is presented. The theoretical scale correctly predicts the experimental electrophilicity within the dihalogen and inter-halogen subseries (XY) including F2, Cl2, Br2, BrCl, and ClF and the HX (X = F, Cl, Br) series. It is shown that the best correlation is obtained for the local electrophilic index that encompasses the global electrophilicity power weighted by a local factor described by the electrophilic Fukui function. This result is in agreement with the electrostatic model of Legon (Angew. Chem., Int. Ed. Engl. 1999, 38, 2686), as the electrophilic power of molecules is mainly determined by the local properties of the electrophilic ends of HX and XY species. We also evaluated the electrophilicity of Li2, LiH, LiF, and LiCl species for which experimental data are not available. Whereas LiH is predicted to have an electrophilic potentia