

Solvent effects on electrophilicity

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Continuum solvent effect on the electrophilicity index recently proposed by Parr and co-workers (Parr, R. G.; von Szentpaly, L.; Liu, S. J. *Am. Chem. Soc.* 1999, 121, 1922) is discussed in detail. Solvent effect is introduced using the self-consistent isodensity polarized continuum model (SCI-PCM). A linear relationship is found between the change in electrophilicity index and the solvation energy as represented in the frame of the reaction field theory. The effect of a polarizable environment on the global electrophilicity is examined for a series of 18 well-known electrophiles presenting a wide diversity in structure and bonding properties. It is found that solvation enhances the electrophilicity power of neutral electrophilic ligands but attenuates this power in charged and ionic electrophiles.