A theoretical study on the relationship between nucleophilicity and ionization potentials in solution phase

Contreras, R.

Andres, J.

Safont, V. S.

Campodonico, P.

Santos, J. G.

In this paper we describe a method to obtain estimates of the relative nucleophilicity for a series of neutral and charged electron donors from their solution phase ionization potential (Is). The relationship between nucleophilicity and the solution phase ionization potentials is first tested for experimental Is values in aqueous solution. On the basis of the meaningful relationship found, the method is then applied to the theoretical solution phase Is obtained at the IPCM-MP2/6-311G(2d,p) level of theory. The comparison between the experimental nucleophilicity as given by Ritchie's N+ scale and the solution phase ionization energy for a series electron donors split out into two families: a first group of marginal and moderate nucleophiles that mainly contains atoms of the first row (H2O, NH2CONHNH2, CF3CH2NH2, NH3, CH3ONH2, NH2OH and CH3O-), with nucleophilicity number N+ < 6.0; a second group of strong nucleophiles, mainly including second-row sulfur atom (CH3CH2S-, CH3CH2CH2S-, OHCH