

It is difficult to quantify the electron withdrawing power of substituents. Like electronegativity, that phenomenon is hard to quantify in a transferrable way because it is sensitive to the local chemical environment. We assess in this work the electron-withdrawing power of common substituents on benzene, using (distances and binding energies) halogen bonding to an iodine substituent as a measure of the influence of substituents at the *meta* and *para* positions on the ring. The calculations reported herein have been performed at the M06-2X level of theory with the basis set cc-pVTZ using the Gaussian 09 suite of programs. The results show very good agreement so far with the basic qualitative ordering expected for substituents on benzene based on inductive effects. At both the meta and para positions, NO₂ induces the shortest I---N separation between the iodine center (the Lewis acid) and N in the Lewis base (NH₃). NHCH₃ appears at the opposite end of the scale as the least electron withdrawing in the list of 22 cases considered. The binding energies, in kilocalories per mole, agree very well with the distance data, with more negative binding energies corresponding with the shorter distances. The results that we have obtained so far suggest that a quantitative scale of the electron donating and withdrawing power of the substituents for benzene substitution at least may be practical and can be defined in a straight forward way based on halogen bonding.