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Calculation of core electron binding energies from structural formulas

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Abstract

We propose a simple algorithm that relates core ionization energy shifts to the expression $\sum_i N_c^i a_i$, where N_c^i is calculated from a structural formula. The constants a_i are considered typical for each element i and are determined by a least-squares fit to already available experimental data. A numerical demonstration is performed for the fluorine 1s core ionization energies of compounds with 2–10 atoms and for C1s core ionization energies of alkanes. Different formulas for expressing shifts in external polarizabilities are presented and discussed.

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