

ABSTRACT

A Revised Lewis-Langmuir Atomic Charge Equation:
A quick calculation of atomic charges and some applications.

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The original Lewis-Langmuir Atomic Charge Equation is used to calculate atomic charge in a simple and straightforward manner, relying only on the Lewis dot structure of a molecule and the mathematical solution of a set of linear equations.

Without compromising its simplicity and ease of calculation, the Lewis-Langmuir Atomic Charge Equation is modified in this thesis to discount the influence of the atom under consideration when calculating its atomic charge. We therefore introduce the notion of fractional bond weighting into the equation.

When fractional bond weighting is considered, the chemical results are not only intuitively more acceptable but also demonstrate improved correlation with the results of *ab initio* methods for polyatomic molecules, resonance hybrids, hypervalent molecules and polymers. In the case of hypervalent molecules, an alternative method of calculation is presented which conforms to the octet rule.

In order to apply the revised Lewis-Langmuir Atomic Charge Equation to some ions, we introduce the device of a "phantom atom" which has either an infinitely large or zero electronegativity. The results are again plausible.

Finally, expressions for group electronegativity are derived from the revised Lewis-Langmuir Atomic Charge Equation. These expressions are used to calculate the electronegativities of twenty-nine functional groups. Again, the results correlate well with those of *ab initio* methods.

Keywords: atomic charge; electronegativity; group electronegativity.