Atoms Do Exist in Molecules: Analysis Using Electrostatic Potentials at Nuclei

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We have shown in the past that the electrostatic potential at the nucleus of a given atom A is relatively insensitive to that atom's molecular environment [1,2]. However, the separate nuclear and electronic contributions to it can be quite different. For a free atom, the electrostatic potential at the nucleus is due entirely to its electrons. If this were to be subtracted from the total electronic potential at the nucleus of a molecule or polyatomic ion, this would yield the potential due to the electrons in the remainder of the molecule or ion, not including those of the atom in question itself. In this presentation we will show results for ten atoms in a variety of molecules and polyatomic ions. We find that the potentials created by other electrons are almost identical in magnitude with the potentials due to the other nuclei. This is a significant finding because it demonstrates that an atom in a molecule or polyatomic ion is only very slightly affected by the nuclei and electrons of the other atoms. It supports the concept that there are individual atoms in molecules and ions [3].

References

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2. P. Politzer and J. S. Murray, Theoret. Chem. Accts., 140, 2021, 7.
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