Using Iso-density Contours to Visualize Atoms in Molecules: Both Noncovalent and Covalent Interactions

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The focus of this paper is on the utilization of varying iso-density contours to gauge the strengths of intermolecular and intramolecular noncovalent interactions, as well as covalent interactions. It is well documented that plotting properties such as the electrostatic potential on iso-density contours such as the 0.001 a.u to the 0.003 a.u. generally mask the presence of intramolecular and intermolecular interactions [1-5]. This poster will present illustrations of the usefulness of varying the contours of the electron density upon which to plot properties, such as the electrostatic potential, ranging from weak to stronger intermolecular and intramolecular interactions, and also including covalent interactions.

References

1. J. S. Murray and P. Politzer, WIREs Comput. Mol. Sci. 7, 2017, e1326.
2. J. S. Murray and P. Politzer, Mol. Phys. 116, 2018, 570.
3. J. S. Murray, D. H. Zadeh, P. Lane and P. Politzer, Mol. Phys. 117, 2019, 2260.
4. G. Roos and J. S. Murray, J. Phys. Chem. A 127, 2023, 8354.
5. J. S. Murray and G. Roos, Phys. Chem. Chem. Phys., 2023, submitted.