Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives

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Abstract

The design of molecules with optimal properties is an important challenge in chemistry because of the astronomically large number of possible stable structures that is accessible in chemical space. This obstacle can be overcome through inverse molecular design. In inverse design, one uses the computation of certain indices to design molecules with an optimal target property. In this study, for the first time, inverse design was used to optimize reactivity properties of molecules. Specifically, we optimized the acidity of substituted 2-naphthols, both in the ground and the excited state. Substituted 2-naphthols belong to the class of photoacids, showing enhanced acidity when excited from the singlet ground state to the first singlet excited state. The focus of this work is the ground state. As a measure of acidity, three different properties are optimized: the charge on the hydroxyl hydrogen atom of the acid, the charge on the negatively charged oxygen atom of the conjugate base and the energy difference between acid and conjugate base. Both the practical use of the methodology and the results for ground and excited states are discussed.

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