Electronic Cigarettes Flavoring Chemicals: Theoretical Insights on Reactivities, Bond Dissociation Energy and Photophysical Characteristics

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Abstract

We investigated the molecular electronic structure characteristics of flavoring chemicals 2,3-butanedione (1) and the analog 2,3-pentanedione (2) and its reduced form acetoin (3) within DFT. The study includes estimating essential issues of their interactions such as the chemical reactivity, bond dissociation energy (BDE), and potential energy curves (PES) of COCO homolytic bond rupture. Relaxed scanning of the ground state geometry at different theory levels generated PES for S0, S1, S2, T1and T2 states. Based on the excited state dynamic (ESD) module of the ORCA package, we predicted the excited states' radiative (fluorescence and phosphorescence) and non-radiative (intersystem crossing (ISC)) emission rates to provide a detailed picture of the considered flavors' photophysical characteristics. The information gained could be helpful for ongoing investigations on the toxicity, health, and environmental impact of the vaporizations and free-radical formation of foods and E-cigarettes' flavors. It may represent a practical orientation for assessing the effectiveness of flavorsô safety for the health and the atmosphere and predicting more stable candidates.

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