

EFFECT OF OXYGEN-BY-SULFUR EXCHANGE ON DESEXCITATION PATHWAYS IN FLAVONOLS

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The substitution of atoms by their heavier counterparts in the periodic table is an interesting way to modulate the properties of some molecules. This has been studied intensively in some families such as alkalis (group 1) or halogens (group 17). Chalcogen family (group 16) is formed by oxygen, sulfur, selenium, tellurium, polonium and, incidentally, livermorium. The first four elements are quite common in molecular chemistry and some reagents have been developed to favor their interconversion.

The substitution of oxygen by another chalcogen is a common phenomenon in the environment, often driven by microorganisms, that is worth studying for the consequences it has on several properties. Structural parameters are always modified, but other properties such as photophysics are also altered [1]. The difference between oxygen and sulfur has been especially studied [2] owing to the omnipresence of these elements. For these studies, many molecular frameworks have been used, but among them, the nucleobases are predominant, especially guanine and uracil [3]. Indeed, the increase of the quantum yield from the lowest triplet state, that is attributed to a heavy-atom effect [4], enables its use as a probe in biological tissues.

In this study [5], we focus on another family of molecules widely present in the vegetable kingdom: the flavonols. The 3-hydroxyflavone was chosen as a representative of this family, along with its chalcogen derivatives. This study involves both electronic spectra measurements and quantum chemistry computations, whose association leads to a good confidence in the proposed interpretations. Moreover, the quantum chemistry tools deepen this study by exploring non-measurable quantities and by extending the oxygen/sulfur series to selenium and tellurium that would have been quite tough to use experimentally. Then, the structure, the intramolecular bonding, the electronic spectra and the excited states properties were studied and will be presented on this poster. The main feature, quenching of fluorescence when sulfur replace oxygen, is explained in terms of excited states crossing.

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