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How to improve the optical properties of a pyridinium luminophore: Theoretical study

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In recent decades, sensors have become valuable tools in our lives. The application of sensors is broad, ranging from measuring temperature to alarming the presence of harmful materials in the environment. These different applications lead to a variety of sensors occurring due to their advantages in certain situations. For example, in a harsh environment, non-contact high-precision measurements are performed mostly by optical sensors, where the luminophore is a critical component, as it directly affects the sensor's ability to detect target analytes or environmental changes.

Recently, we obtained that the KL 1421 luminophore exhibits selective sensing behavior toward acetic acid vapors, as no significant photoluminescence response was observed for other tested substances. Hence, we concluded that the incorporation of carotenoids could lead to an increase in the molar absorptivity of the luminophore, which leads to an increase in its absorption efficiency and improving the sensitivity of the optical sensor, provided that photoluminescence quantum yield and other photophysical properties remain favorable.

The geometry, its change, and the charge redistribution in KL 1421 when the molecule interacts with carotenoids and/or sensed molecules such as NH_3 and acetic acid were studied by the B3LYP/cc-pVTZ approach. The orbital diagrams were used to illustrate the excitations and their variations resulting from the formation of the above complexes. The increase in molar absorptivity is observed in compounds with carotenoids, leading to higher absorbance of KL 1421. The results of our investigations exhibit that conjugated double-bond number influences charge redistribution in the KL 1421 & carotenoid & sensed molecule compounds. The strong interactions of KL 1421 and carotenoids, and KL 1421 & carotenoids with sensed molecules were observed. The results of our investigation prove that NH_3 could not be sensed by KL 1421, although it could be possible by KL 1421 & carotenoid due to the energy level variations and the shifts of the peaks corresponding to the excitations due to charge transfer from the sensed molecule. We also found that in the KL 1421 & carotenoids & sensed molecule, the triplet state is closer to the singlet one. Hence, the singlet-triplet transfer in the compounds with carotenoids will be faster than that in the KL 1421 & sensed molecule, while the transfer from the triple state to the ground one is longer and more efficient. The molar absorptivity indicates higher absorbance of the compound under study with carotenoids than without them. Additionally, the analysis of oscillator strength reveals that the strong interaction among species in KL 1421 & carotenoids could facilitate radiation emission.

In conclusion, the carotenoids are a good choice to improve the sensory properties of KL 1421 - novel organic luminophores.