## Documents

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**Influence of the protonation, deprotonation and transition metal ions on the fluorescence of 8-hydroxyquinoline: A computational study**

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**Abstract**
8-Hydroxyquinoline (8HyQ) and its derivatives are the important constituents in a variety of pharmaceutical compounds. The effect of protonation and deprotonation of 8HyQ on its electronic structure and fluorescence was investigated using B3LYP/6-311G** level of theory. We also investigated the interaction of chemosensor, 8HyQ, with different transition metals (Zn2+, Fe2+, Ni2+ and Co2+) at the same level. Our results revealed that 8HyQ displays an unusual fluorescence intensity-proton transfer relationship with diminished emission in a protonated form but enhanced emission in a deprotonated form. The Zn 2+, Fe2+, Ni2+ and Co2+ complexes of 8HyQ, which were investigated at the same level of theory, showed that the order of binding energies was 8HyQ-Ni2+>8HyQ-Zn 2+>8HyQ-Co2+>8HyQ-Fe2+. Time-dependent density functional theory calculations indicated that Zn ion enhances the fluorescence of 8HyQ as a consequence of the inhibition of the proton transfer. The results are in good agreement between the predicted properties of transition metal complexes of 8HyQ and previously published experimental and theoretical results. A natural bond orbital analysis was performed to understand the nature of hydrogen-bonding interaction in 8HyQ and also to reveal the inter-relations between electronic structure and other properties. © 2011 Taylor & Francis.

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8-hydroxyquinoline; fluorescence; HOMO-LUMO; NBO; TD-DFT

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