

Understanding the Selective-Sensing Mechanism of Al³⁺ Cation by a Chemical Sensor Based on Schiff Base: A Theoretical Approach

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A methodology that allows us to explain the experimental behavior of a turn-on luminescent chemosensor is proposed and verified in 1-[(1H-1,2,4-triazole-3-ylimino)-methyl]-naphthalene-2-ol] (L1), selective to Al³⁺ cations. This sensor increases its emission when interacting with ions upon excitation at 442 nm, which is denoted as the chelation-enhanced fluorescence effect. Photoinduced electron transfer is responsible for the fluorescence quenching in L1 at 335 nm, in Ni²⁺/L1 at 385 nm, and in Zn²⁺/L1 at 378 nm. In Ni²⁺/L, ligand-to-metal charge transfer (LMCT), from the molecular orbital of the ligand to the Ni 3d_{x²-y²} orbital, can contribute to the quenching of fluorescence. Based on oscillator strength, the highest luminescence intensity of L1 at 401 nm and that of Al³⁺/L1 at 494 nm in relation to the others is evidenced. The consideration of the relative energies of the excited states and the calculation of the rate and lifetime of the electron transfer deactivation are necessary to get a good description of the sensor. Copyright © 2019 American Chemical Society.