Understanding the selective-sensing mechanism of Al^{3+} cation by a chemical sensor based on Schiff-base. A novel theoretical methodology

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Abstract

A methodology that allows to explain 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 Al^{3+} cations. This sensor increases its emission when interacting with ion upon excitation at 442 nm, which is denoted as the chelation-enhanced fluorescence (CHEF) effect. The PET is responsible for the fluorescence quenching in L1 at 335 nm, in Ni^{2+}/L1 at 385 nm and in Zn^{2+}/L1 at 378 nm. In the Ni^{2+}/L, The LMCT, from the molecular orbital of the ligand to the Ni $3d_{x2-y2}$ orbital, can contributed to the quenching of fluorescence. Based on oscillator strength, the highest luminescent intensity the L1 at 401 nm and the Al^{3+}/L1 at 494 nm in relation to the others is evidenced. The consideration of the relative energies of the excited states, the calculation the rate and lifetime of the electron transfer deactivation is necessary to get a good description of the sensor.

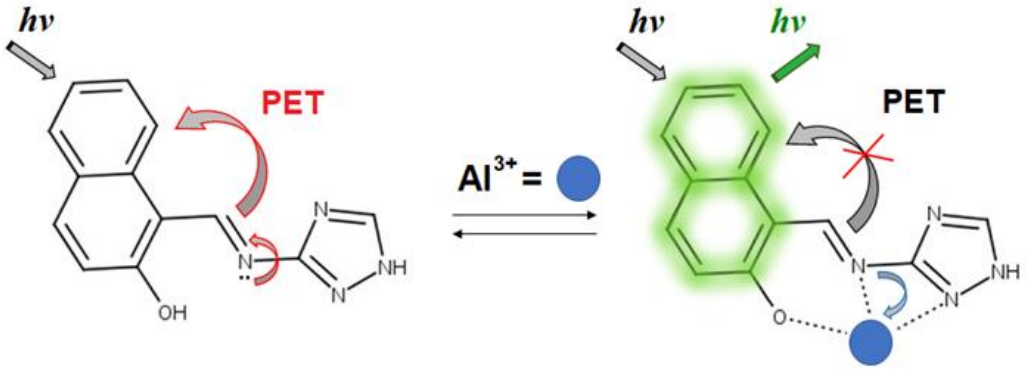

Figure. Sensing of Al^{3+} cations, due to the CHEF effect that produce in L1 when is excited at 442 nm