

Accepted Manuscript

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PII: S1386-1425(15)00508-9
DOI: <http://dx.doi.org/10.1016/j.saa.2015.04.036>
Reference: SAA 13587

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received Date: 10 December 2014
Revised Date: 8 March 2015
Accepted Date: 16 April 2015



Please cite this article as: G-Y. Li, D. Liu, H. Zhang, W-W. Li, F. Wang, Y-H. Liang, TDDFT Study on the Sensing Mechanism of a Fluorescent Sensor for Fluoride Anion: Inhibition of the ESPT process, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2015), doi: <http://dx.doi.org/10.1016/j.saa.2015.04.036>

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TDDFT Study on the Sensing Mechanism of a Fluorescent Sensor for Fluoride Anion: Inhibition of the ESPT process

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Abstract: The fluoride-sensing mechanism of a reported salicylaldehyde-based sensor (*J. Photochem. Photobiol. B* 2014, 138, 75) has been investigated by the TDDFT method. The present theoretical study indicates that there is an excited-state proton transfer (ESPT) process from the phenolic O–H moiety to the neighbor N atom in the sensor. The added fluoride anion could capture the proton in the O–H moiety and the corresponding phenolic anion is formed, which could inhibit the ESPT process. The experimental UV/Vis and fluorescence spectra are well reproduced by the calculated vertical excitation energies. Frontier molecular orbital analysis indicates that the local excited state of phenolic anion is responsible for its enhanced fluorescence. Due to this reason, the sensor can be used to sense fluoride anion by monitoring the fluorescent change.

Keywords: Fluorescence, Sensor, Fluoride, TDDFT, ESPT

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