

## Accepted Manuscript

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PII: S0009-2614(13)00162-0  
DOI: <http://dx.doi.org/10.1016/j.cplett.2013.01.057>  
Reference: CPLETT 30976

To appear in: *Chemical Physics Letters*

Received Date: 7 July 2012  
Accepted Date: 29 January 2013

Please cite this article as: V. Enchev, N. Markova, M. Stoyanova, P. Petrov, M. Rogozherov, N. Kuchukova, I. Timtcheva, V. Monev, S. Angelova, M. Spassova, Excited state proton transfer in 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol, *Chemical Physics Letters* (2013), doi: <http://dx.doi.org/10.1016/j.cplett.2013.01.057>

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**Excited state proton transfer in 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol**

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**Abstract**

A theoretical and experimental study on the absorption and fluorescence properties of a newly synthesized compound 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol in ethanol is reported. Evidence suggesting intramolecular proton transfer in the excited singlet state is presented. All possible tautomeric forms are studied by means of TDDFT B3LYP/6-31G(d,p) in both the ground and the first excited singlet state. On the basis of the results obtained excited state double proton transfer in the title compound is proposed.

**Keywords:** proton transfer, excited state, catechol, phototautomerism, TDDFT

**Highlights**

- Synthesis of 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol.
- Excited state intramolecular double proton transfer.
- Tautomerism in excited state.

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