#### Accepted Manuscript

Title: A Recognition Mechanism Study: Luminescent Metal-Organic Framework for the Detection of Nitro-explosives

Authors: Zhengyan Zhao, Xuedan Song, Lei Liu, Guanglan Li, Shaheen Shah, Ce Hao



Please cite this article as: Zhengyan Zhao, Xuedan Song, Lei Liu, Guanglan Li, Shaheen Shah, Ce Hao, A Recognition Mechanism Study: Luminescent Metal-Organic Framework for the Detection of Nitro-explosives, Journal of Molecular Graphics and Modelling https://doi.org/10.1016/j.jmgm.2017.12.024

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# ACCEPTED MANUSCRIPT

## A Recognition Mechanism Study: Luminescent Metal-Organic

## Framework for the Detection of Nitro-explosives

Zhengyan Zhao<sup>a</sup>, Xuedan Song<sup>a</sup>, Lei Liu<sup>b</sup>, Guanglan Li<sup>a</sup>, Shaheen Shah<sup>c</sup>, Ce Hao<sup>a,\*</sup>

- <sup>a</sup> State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, China
- <sup>b</sup> College of Chemical and Materials Engineering, Anhui Science and Technology University, Fengyang 233100, China
- <sup>c</sup> Department of Chemistry, Karakorum International University, Gilgit-Baltistan 15100, Pakistan \* Corresponding author. *E-mail address: haoce@dlut.edu.cn (C. Hao)*.

#### **Graphical abstract**



#### Highlights

- TDDFT method is utilized to study the hydrogen bond in the excited state.
- 2. The presence of nitrobenzene causes the change of luminescence mechanism of LMOF-1.
- 3. The increased of hydrogen bond can largely facilitated the fluorescence quenching.
- 4. LMOF-1 can be used as a fluorescent probe for the detection of nitrobenzene.
- 5. A recognition mechanism for nitro-explosives by LMOF-1 is studied.

#### Abstract

Download English Version:

# https://daneshyari.com/en/article/6877462

Download Persian Version:

https://daneshyari.com/article/6877462

Daneshyari.com