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Colorimetric Cyanide Chemosensor Based on an Amide- π -Pyrene Moiety: Experimental and Theoretical Studies

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First published: 01 October 2015

<https://doi.org/10.1002/bkcs.10534>

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Abstract

A new simple colorimetric sensor **1** based on amide-*o*-pyrene moiety was designed and synthesized for cyanide (CN⁻) in aqueous solution. The sensor **1** showed high selectivity toward CN⁻, which induces an immediate color change from colorless to yellow for cyanide over other anions. Moreover, the sensor **1** could be used efficiently in a wide pH range (7–10) with no interference from other anions. The sensing of CN⁻ was found to be reversible with a proper reagent such as HCl. Additionally, the sensing mechanism for CN⁻ was theoretically supported by density functional theory and time-dependent density functional theory calculations. Therefore, sensor **1** can serve as a practical chemosensor for cyanide in aqueous solution.

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- Wan Zhang, Kaixiang Xu, Liangxu Yue, Zonglong Shao, Yan Feng and Min Fang, Two-dimensional carbazole-based derivatives as versatile chemosensors for colorimetric detection of cyanide and two-photon fluorescence imaging of viscosity *in vitro* *Dyes and Pigments*, **137**, (560), (2017).

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