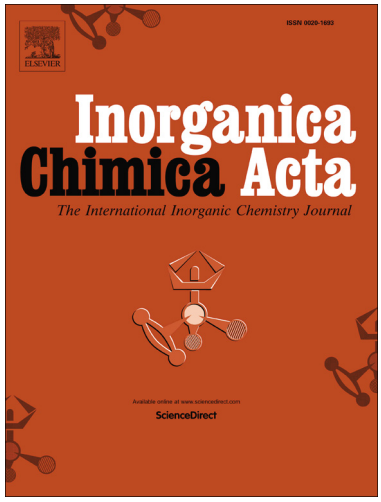

Research paper

Selective detection of Cu^{2+} and S^{2-} by a colorimetric chemosensor: Experimental and theoretical calculations

So Young Kim, Seong Youl Lee, Jae Min Jung, Min Seon Kim, Cheal Kim

PII: S0020-1693(17)31092-7
DOI: https://doi.org/10.1016/j.ica.2017.12.016
Reference: ICA 18050

To appear in: *Inorganica Chimica Acta*

Received Date: 13 July 2017
Revised Date: 6 December 2017
Accepted Date: 7 December 2017

Please cite this article as: S.Y. Kim, S.Y. Lee, J.M. Jung, M.S. Kim, C. Kim, Selective detection of Cu^{2+} and S^{2-} by a colorimetric chemosensor: Experimental and theoretical calculations, *Inorganica Chimica Acta* (2017), doi: https://doi.org/10.1016/j.ica.2017.12.016

Selective detection of Cu^{2+} and S^{2-} by a colorimetric chemosensor: Experimental and theoretical calculations

So Young Kim, Seong Youl Lee, Jae Min Jung, Min Seon Kim,* Cheal Kim*

Department of Fine Chemistry and Department of Interdisciplinary Bio IT Materials, Seoul National University of Science and Technology, Seoul 139-743, Korea. Fax: +82-2-973-9149; Tel: +82-2-970-6693; E-mail: dltmf2303@naver.com and chealkim@seoultech.ac.kr

Abstract

A multifunctional colorimetric chemosensor **1**, based on 4-(diethylamino)-2-hydroxybenzaldehyde and 2,3-diamino-5-bromopyridine, has been synthesized and characterized. Sensor **1** detected instantly both Cu^{2+} and S^{2-} by the color change from pale yellow to deep yellow. The binding modes of **1** with Cu^{2+} and S^{2-} were found to be the 1:1 stoichiometry through Job plot and ESI-mass spectrometry analysis, respectively. In addition, the detection limit of **1** for Cu^{2+} was found to be 68.6 nM, which was much lower than WHO guideline (31.5 μM) in drinking water. Importantly, sensor **1** could be used to quantify Cu^{2+} in water samples. Moreover, **1** exhibited a high selectivity for S^{2-} in the presence of other anions. The sensing mechanisms of Cu^{2+} and S^{2-} by **1** were explained by theoretical calculations.

Keywords: colorimetric chemosensor, naked-eye, copper ion, sulfide, theoretical calculations