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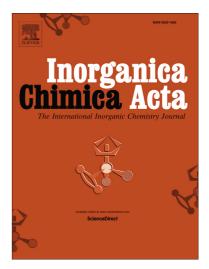
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Selective detection of Cu²⁺ and S²⁻ by a colorimetric chemosensor: Experimental and theoretical calculations

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Abstract

A multifunctional colorimetric chemosensor **1**, based on 4-(diethylamino)-2hydroxybenzaldehyde 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 μ M) in drinking water. Importantly, sensor **1** could be used to quantify Cu^{2+} in water samples. Moreover, **1** exhibited a high selectivity for S²⁻ in the presence of other anions. The sensing mechanisms of Cu^{2+} and S²⁻ by **1** were explained by theoretical calculations.

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

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