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1-[5-(Hydrazidomethylsulfinyl)pentyl]-3,5-dimethylisocyanurate: Protolytic properties and complexation reactions

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Abstract

© 2014 Springer Science+Business Media New York. The compound with antituberculosis activity, 1-[5-(hydrazidomethylsulfinyl)pentyl]-3,5-dimethylisocyanurate, was studied in aqueous dimethyl sulfoxide by potentiometric titration, spectrophotometry, and mathematical simulation of equilibria in solution (the CPESSP program). The protolytic properties of the compound were examined. The compositions and stability constants of its complexes with copper(II) were determined. The geometries of the isocyanurate and its complexes were optimized by molecular mechanics computations.

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Keywords

1-[5-(hydrazidomethylsulfinyl)pentyl]-3,5-dimethylisocyanurate, acid-base properties, complexation, copper(II), mathematical modeling of equilibria