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## **ACCEPTED MANUSCRIPT**

Preparation, characterization and molecular modeling studies of the beta-cyclodextrin inclusion complex with benzoguanamine and its analytical application as chemosensor for the selective sensing of  $\mathrm{Ce}^{4+}$ 

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#### **Abstract**

The inclusion complex of  $\beta$ -cyclodextrin ( $\beta$ -CD) with benzoguanamine (BGA) has been investigated in three states. UV-visible and fluorescence spectral techniques are used in liquid state. FTIR, NMR and MASS techniques are used in solid state and virtual state studies are done by molecular simulation work. The binding constants for the formation of 1:1 BGA:  $\beta$ -CD inclusion complex is estimated by UV-visible and fluorescence spectral techniques. The chemosensory ability of BGA:  $\beta$ -CD complex was investigated thoroughly for various metal cations and we found the emission of complex showed a linear increase in the intensity for Ce<sup>4+</sup> with the linearity range of 1000  $\mu$ M – 2000  $\mu$ M. Sensitivity analysis shows good sensing for Ce<sup>4+</sup> with the LOD of 671  $\mu$ M and LOQ of 2034  $\mu$ M. Our result suggests that the BGA:  $\beta$ -CD inclusion complex would be promising material for developing solid state sensory device for sensing Ce<sup>4+</sup>.

**Keywords:** β-cyclodextrin, benzoguanamine, fluorescence enhancement, chemosensor, cerium ion.

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