

A C_3 SYMMETRIC SULFATE COMPLEX: SELECTIVE RECOGNITION OF SULFATE WITH AN *M*-NITROPHENYL-FUNCTIONALIZED HEXAUREA RECEPTOR

Bobby Portis¹, Maryam Emami Khansari¹, Corey R. Johnson¹, Douglas R. Powell² and Md. Alamgir Hossain¹

¹*Department of Chemistry, physics and Atmospheric Sciences, Jackson State University, Jackson, MS, USA*

²*Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK 73019, USA*

Abstract: Anion binding properties of atripodal-based hexaurea appended with *m*-nitrophenyl group has been studied, showing strong affinities for sulfate over other oxoanions such as hydrogen sulfate, dihydrogen phosphate, bicarbonate, nitrate and perchlorate. Structural analysis of the sulfate complex reveals that the receptor organizes all urea-binding sites toward the cavity at precise orientations around a tetrahedral sulfate anion to form a perfect C_3 symmetric encapsulated sulfate complex that is stabilized from optimal interactions with all hydrogen bonding sites in a single molecule. The receptor and the encapsulated sulfate are located on the three-fold axis passing through the bridgehead nitrogen of the receptor and the sulfur atom of the anionic guest.

Acknowledgements: The project described was supported by Grant Number G12MD007581 from the National Institutes of Health.