Synthesis and Structural Characterization of N-[4-(2-Hydroxyethyl)-1,2,4-oxathiazinan-3-ylidene]-benzamide and its Mercury(II) Chloride Adduct

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The synthesis of N-[4-(2-hydroxyethyl)-1,2,4-oxathiazinan-3-ylidene]-benzamide (**2a**) and N-[4-(2-hydroxyethyl)-1,2,4-oxathiazinan-3-ylidene]-2-fluorobenzamide (**2b**) by oxidation of the corresponding 1,1-bis(2-hydroxyethyl)-3-aroylthioureas with potassium iodate in aqueous solution is reported. Variable temperature ^{1}H NMR spectra of **2a** prove that the heterocyclic 1,2,4-(O, S,N) six-membered ring is involved in a dynamic chair-boat conformational interconversion. Molecular mechanic calculations show that the chair conformation is more stable than the boat conformation by 3.0 kcal/mol. The synthesis of the adduct [(**2a**)·0.5 $HgCl_2$] **3** as well as the X-ray structural characterization of **2a** and **3** are also reported.

Key words: Oxathiazinanes, Mercury(II) Chloride Adduct, Synthesis, Crystal Structure, NMR Data