

Structural features of 1-furoylthioureas 3-monosubstituted and 3,3-disubstituted: coordination to cadmium and analytical applications

O. Estévez-Hernández^{a,b*}, J. Duque^a and E. Reguera^{a,b}

^a*Instituto de Ciencia y Tecnología de Materiales (IMRE), Universidad de La Habana, Havana, Cuba;*

^b*Centro de Investigación en Ciencia Aplicada y Tecnología de Avanzada, Mexico City, México*

(Received 2 December 2010; final version received 19 January 2011)

The structural features of two series of 1-furoylthioureas 3-monosubstituted (Series 1) and 3,3-disubstituted (Series 2) 1-furoylthioureas and their CdCl_2 complexes are discussed. The coordination strength through the sulfur atom is determined by the ligand structure. In Series 1 ligands, the carbonyl group and the proton on N_2 are engaged in a strong hydrogen bond interaction. This leads to an “S”-shaped conformation type of the $\text{C}=\text{O}$ and $\text{C}=\text{S}$ groups where these donor sites reach a maximum separation. In the absence of that hydrogen bridge in 3,3-disubstituted derivatives, the $\text{C}=\text{O}$ and $\text{C}=\text{S}$ groups can adopt a “U”-shaped conformation type. This feature is also observed for two novel crystal structures of 1-(2-furoyl)-3-(2-hydroxyethyl)thiourea and 1-furoyl-3-ethyl-3-phenylthiourea, as determined by X-ray diffractometry and reported here. Emphasis is placed on the relationship between structural features of these ligands and their behavior as cadmium ionophores in potentiometric and amperometric sensors.

