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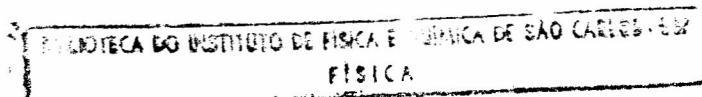
COMMUNICATED ABSTRACTS

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09.4-9 CRYSTALLINE AND MOLECULAR STRUCTURE OF (2-MERCAPTOBENZOXALATE) METHYLMERCURY(II) AND (2-MERCAPTOBENZOXALATE) PHENYLMERCURY(II). By Y.P. Mascarenhas, IFQSC/USP, C.P. 369, 13560, São Carlos, S.P., Brazil; K. Tomita, IQ-Araraquara, C.P. 174, 14800, Araraquara, S.P., Brazil; C.O.P. Santos, UNESP - Presidente Prudente, 19100, Presidente Prudente, S.P., Brazil; J.S. Casas, Dept. of Inorganic Chemistry, School of Pharmacy, U. of Santiago, Galicia, Spain.

The X-ray structure determinations were performed with the purpose of elucidate if the intramolecular secondary bond of Hg involved either the endocyclic nitrogen or oxygen. Furthermore, it is also of interest, to consider the role of these complexes in agricultural environments if we recall that the ligand itself is a fungicide, has bacteriostatic activity and is a regulator of plants growth. (Preti, C., Tosi, G. - J. Inorg. Nucl. Chem., 18, 1125 (1976)). Thus, it is quite possible that the organometallic contaminant of the environment and this ligand used in agriculture may naturally interact.

Crystal data for the phenyl Hg(II) complexes (A): $C_{13}H_{10}NOHg$, M.W. = 411.34, triclinic, $P\bar{1}$, $a = 10.677(2)$, $b = 11.176(6)$, $c = 11.445(3)$ Å, $\alpha = 66.67(3)^\circ$, $\beta = 86.55(2)^\circ$, $\gamma = 78.69(3)^\circ$, $V = 1229.4(9)$ Å³, $Z = 4$, $D = 2.22$ g/cm³, $\lambda(MoK\alpha) = 0.71073$ Å, $\mu = 122$ cm, $F(000) = 792$, $T = ca 293^\circ K$, $R = 0.075$ for 2297 observed reflections ($I > 3\sigma(I)$), unit weights.

Crystal data for the methyl-Hg(II) complex (B): C_8H_8NOSHg , M.W. = 345.74, monoclinic, $P2_1$, $a = 10.601(1)$, $b = 8.164(3)$, $c = 10.876(2)$ Å, $\beta = 103.87(1)^\circ$, $V = 913.83$ Å³, $Z = 4$, $D = 2.51$ g/cm³, $\mu = 163.86$, $\lambda(MoK\alpha) = 0.71073$ Å, $F(000) = 664$, $T = ca 293^\circ K$, $R = 0.077$, $R_w = 0.076$ for 1247 observed reflections ($I > 3\sigma(I)$), $w = (\sigma(F) + 0.003 F)^{-1}$. Both structures were solved by Patterson and difference Fourier methods and refined by blocked L.S. method. An intramolecular secondary bond between Hg and the endocyclic nitrogen was found for both complexes. For complex A the crystal packing may be described as discrete sets of dimerized molecules via Hg and S interactions between the two independent molecules present in assymetric unit with $Hg-S' = 3.33$ Å and $Hg'-S = 3.47$. For complex B we have a much more complex network of intermolecular interactions involving Hg, S and O with $Hg-S'(1) = 3.75$ Å, $Hg-O'(2) = 2.90$ Å, $Hg'-S(3) = 3.47$ and $Hg'-O(4) = 2.86$ Å where the primed and unprimed atom's names stand for the two independent molecules in the assymetric unit and the number in parenthesis for the following symmetry operations: (1) = $x, 1.0-y, z$; (2) = $-x, 0.5+y, -z$; (3) = $x, 1.0+y, z$; (4) = $1-x, 1.5+y, -z$.

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