

Phenylmercury Chloride: Its Single-Crystal X-Ray Structure and Some Aspects of its Biological Chemistry

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A single crystal of phenylmercury chloride (PhHgCl) was obtained by serendipity from a solution of diphenylmercury (HgPh₂) and dihydrolipoic acid in tetrahydrofuran / carbon tetrachloride. The crystal structure of PhHgCl is pseudotetragonal. It is best described in the orthorhombic space group *Cmma* with $a = 6.856(1)$, $b = 6.882(1)$, $c = 14.309(2)$ Å (at 193 K), and $Z = 4$. The Cl-Hg-C moiety of the PhHgCl molecule is exactly linear. The bond lengths at the Hg atom are Hg-Cl 2.345(2) and Hg-C 2.044(9) Å. In the crystal, the molecules are arranged in double layers parallel to the a,b plane.

In a model medium for the gastric juice (0.1 M DCl in D₂O / [D₈]dioxan, 37 °C), HgPh₂ reacts to form PhHgCl. HgCl₂, which would result from complete dearylation, cannot be isolated from the reaction mixture. However, it appears that a small equilibrium concentration of HgCl₂ may be present, because on addition of 1,4,7-trithiacyclononane (ttcn) and diethyl ether, the dichloride can be trapped as solid [Hg(ttcn)₂][HgCl₄]. We estimate that after oral uptake of HgPh₂ 20 - 90% are transformed into PhHgCl in the stomach after 30 min.