

MOLECULAR STRUCTURE OF 4-(PHOSPHONOMETHYL)-
2-HYDROXY-2-OXO-1,4,2-OXAZAPHOSPHORINANE

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The phosphorylation of ethanoldiamine under the reaction conditions described by Moedritzer and Irani [1] gave a Complexone with an unusual structure as shown by x-ray diffraction structure analysis. The product, 4-(phosphonomethyl)-2-hydroxy-2-oxo-1,4,2-oxazaphosphorinane contains an ester ring $O^6P^2C^2NC^3C^4$ (see figure) formed as a result of intermolecular esterification of the alcoholic group of ethanoldiaminedimethyl-ene phosphonic acid acid with one of the phosphonic groups. The monoclinic crystals contained a phosphone group. The space group was $P2_1/n$. The unit cell parameters are: $a = 8.959(4)$, $b = 8.979(4)$, and $c = 11.710(5)$ Å, $\beta = 100.36(3)^\circ$, $Z = 4$, $R = 0.040$.

This study showed that the complexone has a zwitter-ionic structure, i.e., one of the hydrogen atoms is bound to the nitrogen atom. The phosphonic group, whose oxygen atom is in the ester ring, is protonated while the remaining two protons are on the two oxygen atoms of the second phosphone group. Thus, this complexone is a tribasic acid and has two phosphone groups differing in their structural functions. The ester ring of the complexone has chair conformation with intracyclic angles in the range from 101.2° to 116.1° . The bond lengths are shown in the figure.

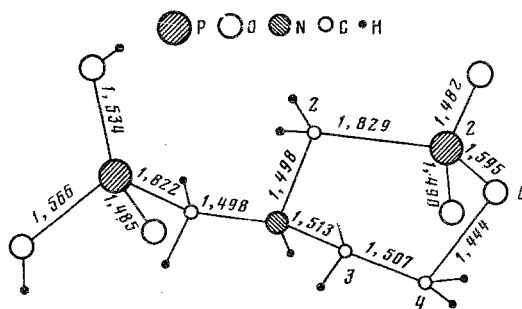


Fig. 1

LITERATURE CITED

1. K. Moedritzer and R. R. Irani, *J. Org. Chem.*, **31**, 1603 (1966).

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