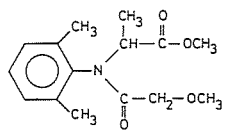
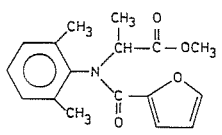
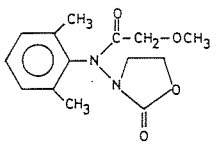
The molecular conformations of metalaxyl and furalaxyl are similar with the dimethylphenyl ring being almost perpendicular to the amidic plane of the molecule, as is also the case for the two isostructural compounds with the oxazolidinone and butyrolactone rings. The amidic nitrogen atom is sp^2 hybridized. As in most N-substituted anilides, metalaxyl and furalaxyl exist preferentially in the exo isomeric form with the phenyl ring trans with respect to the carbonyl group. The oxazolidinone ring is in a half chair form and the butyrolactone ring in a typical envelope conformation.

Metalaxyl

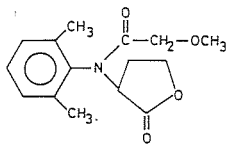


Furalaxyl





Oxazolidinone derivative



Butyrolactone derivative

03. 5–23 LOW TEMPERATURE STUDIES OF CHOLINE ESTERS

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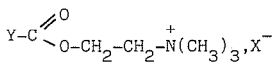
The crystal structures of many salts of choline esters are known.



Strong thermal motion or disorders are often observed in these salts, and the accuracy of the structures is generally rather low. A survey of the known structures has disclosed a strong correlation between the magnitude of some bond angles and the actual conformation. Many types of theoretical studies of molecular flexibility still make use of crystallographically observed geometry, and it was found worth while to collect low temperature data for a selection of choline ester salts, in order to get more precise knowledge about the correct values of bond lengths and angles. Results will be presented for methoxycarbonylcholine iodide, carbamoylcholine chloride and bromide, acetylcholine chloride, and succinylcholine iodide, representing the three known conformers *trans-trans*, *trans-gauche* and *gauche-gauche*.