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Study of the spatial structure of the chloroanhydride of dichloromethylphosphonic acid by a combination of various physical methods

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Abstract

1. In the liquid state, in solution, and in one of its crystalline modifications, the chlorohydrate of dichloromethylphosphonic acid exists as a mixture of two nonrotating isomers of Cs and C1 symmetries (gauche-gauche and gauche-trans orientation of the two CHCl₂ group chlorines with respect to the P=O bond). The conformers are individually stabilized in the other crystalline modifications. 2. It is assumed that weak intramolecular bonds of the C-H...O=P type play a role in the stabilizing the conformer with the chlorine in the gauche-trans orientation. © 1977 Plenum Publishing Corporation.

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