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An experimental and quantum-chemical study of the Raman spectra and rotational isomerism of thiophosphites (RS) n PCl3 - N (R = Me, Et; N = 1, 2)

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Abstract

The Raman spectra of different conformations of CH3SPCl 2, C2H5SPCl2, and (C 2H5S)2PCl are studied within the framework of the density functional theory (B3LYP/6-31G*and B3LYP/6-31+G*) using the method of scaling of force fields. Comparison of the calculated and experimental spectra makes it possible to interpret the latter and to establish the existence of trans and gauche conformers of these molecules, which are formed due to internal rotation about the P-S and S-C bonds. This comparison also shows that, for the prediction of the degrees of depolarization of Raman lines to be correct, it is necessary to introduce diffuse functions into the basis set. © Nauka/Interperiodica 2006.

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