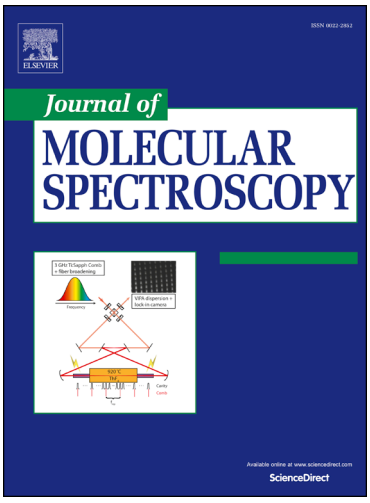

Influence of inert matrixes on the conformational switching of trimethyl phosphate at low temperatures through thermal effects

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Influence of inert matrixes on the conformational switching of trimethyl phosphate at low temperatures through thermal effects

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Abstract

The conformational switching of trimethyl phosphate (TMP) in Ne, Ar, Kr and Xe matrixes was studied using infrared spectroscopy under isolated conditions at low temperatures. In all the inert matrixes, the vapor phase population of ground state $C_3(G^{\pm}G^{\pm}G^{\pm})$ and the higher energy $C_1(TG^{\pm}G^{\pm})$ conformers of TMP is preserved during the initial deposition. However, on annealing the inert Ar/Kr/Xe matrixes, the conformational composition of TMP was irreversibly altered. In Ar and Kr matrixes, an interconversion from ground state $C_3(G^{\pm}G^{\pm}G^{\pm})$ to higher energy $C_1(TG^{\pm}G^{\pm})$ conformer was observed whereas Xe presents an interesting variation. In Xe matrix, the higher energy $C_1(TG^{\pm}G^{\pm})$ conformer completely depopulated with a concomitant increase in the population of the ground state $C_3(G^{\pm}G^{\pm}G^{\pm})$ conformer. In Ne matrix notably, no conformational interconversion was observed. Computations on the conformers of TMP were performed using B3LYP and M06-2X levels of theory with 6-311++G(d,p) and aug-cc-pVDZ basis sets. The effect of inert matrixes was modeled using Self-Consistent Reaction Field (SCRF) methods.

Keywords: Conformations, trimethyl phosphate, matrix isolation, infrared, *DFT*, SCRF methods

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