Structural stability and vibrational analysis of dihalophosphoric acids HO-POX2 and aminophosponic dihalides NH2-POX2 (X = F, Cl). Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Canadian Journal of Analytical Sciences and Spectroscopy (2006), 51(4), 215-224.

Abstract

The structural stability of F2POOH and Cl2POOH acids and phosphoramidic dihalides F2PONH2 and Cl2PONH2 was investigated by DFT-B3LYP and MP2 methods using extended 6-311+G** basis set. Difluorophosphoric acid was calcd. to exist in planar structure (hydrogen eclipses P = O bond), while dichlorophosphoric exists as a nonplanar structure with OPOH torsional angle of about 14-30°. The P-O rotational barrier was calcd. to be about 2-3 kcal/mol for difluorophosphoric acid. Aminophosphonic difluoride and dichloride were predicted to have non-planar structure. The planar structure of the two amides was predicted to have an imaginary frequency by both levels of calcns. The vibrational frequencies were computed, normal coordinate analyses were carried out and potential energy distributions (PED) were calcd. for the four mols. in their low energy structures. On the basis of PED values and comparison with exptl. data of the acids reliable assignments were provided for the normal modes of the four mols.