CONFORMATIONAL ANALYSIS OF METHYLBORONIC ACID AND ITS ACYCLIC ESTERS

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With the use of RHF/6-31G(*d*) and MP2/6-31G(*d*)//RHF/6-31G(*d*) semi-empirical (AM1) and non-empirical quantum chemical approximations conformational isomerization of methylboronic acid and its methyl, isopropyl, *tert*-butyl, and phenyl esters is studied. With the exception of the *tert*-butyl analogue, the potential energy surface of molecules in these compounds, is shown to contain three minima that correspond to planar and near-planar conformers: *cis–cis*, *trans–trans*, and *cis–trans*, with the latter being the main one. The minima are separated by two conformational isomerization barriers corresponding to the orthogonal arrangement of one of the OH(OR) groups.

Keywords: methylboronic acid, boric ester, conformer, quantum chemical calculations, potential energy surfaces, internal rotation barrier.