PATHWAYS OF CONFORMATIONAL ISOMERIZATION OF 4-PHENYL-1,3-DIOXANE

V. V. Kuznetsov,[1,2] A. E. Kuramshina,[2] and S. A. Bochkor[2]

UDC 547.841:541.63

A study of the potential energy surface of 4-phenyl-1,3-dioxane by non-empirical quantum chemical RHF/STO-3G and 6-31G(*d*) approximations reveals six energetically inequivalent pathways of conformational isomerization of equatorial and axial *chair* forms.

Keywords: 4-phenyl-1,3-dioxane, conformer, minimum of the potential energy surface, *twist*-form, quantum chemistry.