

Research into the structure of 2-phenyl-4*H*-1,3,4-oxa- and thiadiazine-5,6-diones

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Abstract

2-phenyl-4*H*-1,3,4-oxa(thia)diazine-5,6-diones theoretically may exist in various tautomeric forms. It has been shown with the methods of NMR and IR spectroscopy that in solid state and DMSO solutions these substances exist mainly in 5,6-dioxoform, and in gaseous phase, as it has been demonstrated by thermochemical calculations with CBS-4*M* method, equilibrium mixture of 5,6-dioxo- and 6-oxo-4-th-5-olate tautomers can exist.