Bulletin of the Academy of Sciences of the USSR Division of Chemical Science 1984 vol.33 N10, pages 2079-2083

Conformations and electronic structure of cyclic sulfites and quantum-chemical calculations, ab initio and in the CNDO/2 approximation

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Abstract

Ab initio quantum-chemical calculations transmit satisfactorily the conformational and electronic properties of cyclic esters of sulfurous acid, whereas calculations in the CNDO/2 approximation gives a satisfactory description of only the features of electronic structures of this class of compounds. © 1985 Plenum Publishing Corporation.

http://dx.doi.org/10.1007/BF00954086