Theoretical analysis of torsional potential functions. Part II. The rotational isomerization of glyoxal and related molecules

Bock, Charles W.

Toro-Labbé, Alejandro

A systematic investigation of the international rotation of glyoxal (OHC-CHO), fluoroglyoxal (OHC - CFO), chloroglyoxal (OHC-CClO), oxalylfluoride (OFC-CFO) and oxalyl chloride (OClC-CClO) is presented. A new partition for torsional potential functions is shown to be useful in identifying the specific contributions that determine the shape of the resulting curves. SCF-MO theory was used together with gradient techniques and a 6-31G basis set to perform full structural optimizations of trans- and cis-OXC-CXO and for the transition states connecting them. Our results show that all the molecules except oxalyl chloride appear to exist as the trans and cis conform; we present evidence that (OClC-CClO) exists in a trans and a gauche form. © 1991.