# On the rotational isomerism of one rotor molecules. A comparative study of the HSSH and HXNX (X = O,S) series of molecules

Cárdenas-Jirón, Gloria I.

Cárdenas-Lailhacar, Cristián

Toro-Labbé, Alejandro

Ab initio torsional potential functions for a series of representative sulphur-containing molecules are presented. A few interesting parameters determining the relevant characteristics of the intermediate conformations were formulated and used to rationalize the isomerization processes. Although theoretical results concerning molecular structures and energies are in quite good agreement with the available experimental data, we show that a much better comparison of potential functions can be obtained when conveniently defined scaling factors are introduced. 