

Energy, chemical potential and hardness profiles for the rotational isomerization of HOOH, HSOH and HSSH

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A theoretical study is reported of the mechanisms for internal rotation of hydrogen peroxide (HOOH), hydrogen thioperoxide (HSOH) and hydrogen persulphide (HSSH). Calculations at the ab initio HF//6-311G** and MP2//6-311G** levels show that these are gauche molecules presenting double-barrier torsional potentials. Important results have been obtained: two different isomerization mechanisms (trans and cis) have been characterized in terms of specific local interactions; the corresponding energy barriers have been classified according to through bond and through space interactions; and the principle of maximum hardness is qualitatively verified in all three molecules. © 1999 Taylor & Francis Group, LLC.