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A COMPUTATIONAL STUDY OF KETO-ENOL EQUILIBRIA OF CATECHOL



A Computational Study of
Keto-Enol Equilibria of
Catechol

In Gas and Aqueous Solution Phase



Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | In Gas and Aqueous Solution Phase | Keto-enol equilibria in catechol have been studied using ab initio methods and first principle density functional theory. Six structural isomers of CHO were fully optimized in gas phase at HF and B3LYP levels of theory in combination with the 6-311++G basis set. Self-Consistent Reaction Field Polarizable Continuum Model (SCRF-PCM) was used to investigate the effect of an aqueous solvent on the extent of tautomerisation at...

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