IMPACT: International Journal of Research in Applied, Natural and Social Sciences (IMPACT: IJRANSS)
ISSN(E): 2321-8851; ISSN(P): 2347-4580
Vol. 2, Issue 4, Apr 2014, 179-184

CONFORMATION DEPENDENT VIBRATIONAL MODES IN 2-(2-HYDROXYPHENYL) BENZOTHIAZOLE MOLECULE

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ABSTRACT

Optimized structures for all the four possible conformers of 2-(2-hydroxyphenyl) benzothiazole have been computed using the DFT method at the B3LYP/6-311++G** level. With these optimized structures vibrational parameters have also been computed. Comparative studies of conformer dependent vibrational fundamentals have been carried out.

KEYWORDS: Conformational Study, Vibrational Study, 2-(2-Hydroxyphenyl) Benzothiazole