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Document Title : *A theoretical calculation of the hindering internal rotation of the methyl group in solid*

حساب نظري لحاجز الجهد الميعيق للحركة الدورانية لداخلية لمجموعة الميثيل في الجوامد

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Abstract : The reorientation of a methyl group about its axis in the solid state is hindering by a potential barrier. The magnitude and shape of this hindering barrier ref1ects the molecular and electronic structure of methyl group environment. The motional spectrum of the methyl group at low temperature is dominated by Quantum mechanical tunnelling through the barrier at a rate that is determined by the splitting of the ground torsional state, while at high temperature it is dominated by hopping motion characterised by the reorientation rate. We calculated the hindering potential of the rotation of the two methyl groups in Acetylacetone in the basis of pair potentials. The shape, the magnitude and the origin of the barrier are presented

Supervisor : د. علي محمد السنوسي

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