SYMMETRT DILEMMA APPLIED TO THE BIACETYL

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The symmetry of certain molecules may be destroyed in an ab-initio calculation, due to the full optimization of the molecular geometry. Such an example to be studied in this work is trans-dimethylglioxal (byacetil) which represents a fully symmetric double-rotor system. The indistingishability of the hydrogen atoms (dynamical symmetry) must be in agreement with the results obtained by ab-initio calculations (symmetry dilemma). Several approaches are proposed to overcome the dilemma mentioned above. It is seen that the method which averages the energy of the energetically equivalent conformations furnish the closest solutions to those of the dynamical symmetric approach. The lowest levels of the torsional far-infrared spectrum are calculated and compared to experimental results.