

## **P26: DBM molecular conformation: Comparison of DFT calculations with that found by neutron diffraction at 14 K**

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### **Abstract:**

Many works have been done on the methyl rotation barriers and molecular conformation in substituted benzenes by correlated quantum chemistry methods [1,2]. In studies of the molecular conformation and spectroscopic properties of the tribromo- (TBM) and triodo-mesitylene (TIM), it has been demonstrated [3,4] that DFT calculations using B3LYP or MPW1PW91 functionals and LanL2DZ(d,p) or 6-311+G(d,p) basis sets, not only allow a precise prediction of the molecular conformation in good agreement with that observed by neutron diffraction, in the crystal at low temperature (14K) [5], but that they also give with a precision better than a few % all the internal frequencies modes. It is why we have done DFT computations (MPW and B3) for this study of the DBM conformation and of the rotation barriers of its Me groups: MPW computations were done using the MPW1PW91 functional and B3 computations by B3LYP, the bases set used being the LANLD2Z(d,p) and 6-311+G(d,p). The difference between the angles calculated by these two functionals was always smaller than 0.1°. For two third of the DBM molecule, DFT and neutron diffraction results are almost in perfect agreement, they have found that C<sub>2v</sub> molecular symmetry is respected in a limit of 2x10<sup>-3</sup> for the angles and also the bond lengths; A discrepancy occurs for the environment of Me<sub>2</sub>, conformation found by ND at 14 K is quasi symmetrical, contrary to that calculated by DFT calculations which are "obliged" to optimize the position of three protons on a quasi equilateral triangle, because they admit that the Born-Oppenheimer approximation (BOa) is valuable for all nuclei, even the protons of Me<sub>2</sub>, and at last they do not take in account the spin states.

**Key words:** Molecular conformation, DFT, neutron diffraction; 1,3-dibromo-2,4,6-trimethylbenzene (DBM)

**References:**

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