Erratum: B_{80} Fullerene: An *Ab Initio* Prediction of Geometry, Stability, and Electronic Structure [Phys. Rev. Lett. 98, 166804 (2007)]

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In our recent Letter, the predicted spheroid molecule B_{80} was described as preserving the I_h symmetry, since the found true local minimum configuration does display recognizable icosahedral proportions. The reported values of the energy, bond lengths, and the HOMO-LUMO degeneracy and gap refer to the true local minimum structure. It should be clarified, however, that the geometry in this true minimum was slightly off from precise I_h, as the added boron atoms were not exactly in the centers of the corresponding hexagons, with the dihedral angle for these B atoms measuring between 0 to 5° with respect to six-member rings. Small deviation from I_h symmetry was also reflected by the splitting of the fivefold degenerate HOMO energy level into a **3** + **2** representation. In fact, more careful analysis reveals a number of local minima isomers, with the formal symmetries such as I_h for some, T_h for others, or yet a lower C_1. This has been verified by using more reliable functionals such as B3LYP. Although these distortions and their dissimilarities are not visually striking (Fig. 1), this points to a possibility of isomerization changes among the multiple local minima. The energy differences (10 to 100 meV depending on the method) between these structures, as well as the potential barriers separating them from each other, are rather small, ensuring frequent thermally activated transitions or possibly even tunneling.

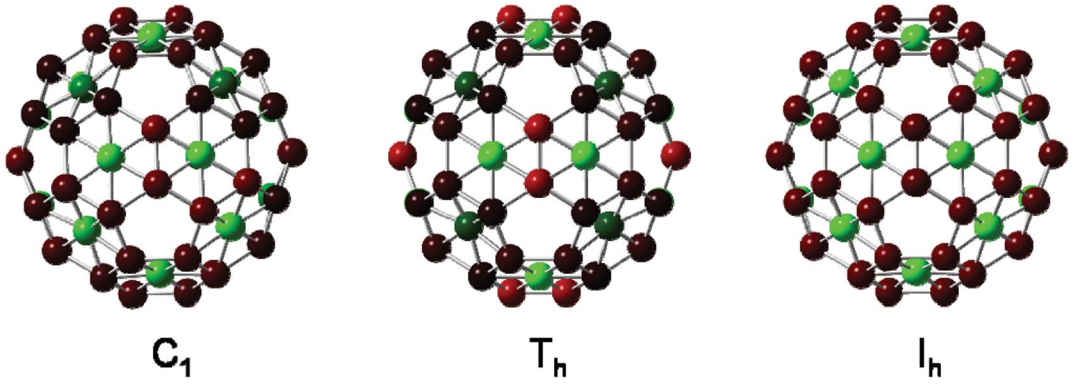

FIG. 1 (color). Visually the geometries of the structures are almost identical, yet one can see different symmetries from the charge redistribution. Mulliken charges are shown for the three isomers C_1, T_h, and I_h. Green (red) shows positive (negative) atomic charges. The brighter green corresponds to more positive charge and smaller dihedral angle.

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