POSSIBLE SUPERFINE AND HYPERFINE ROVIBRATIONAL STRUCTURES FOR FULLERENE ISOTOPOMERS AND DOPANTS: EXTREME SYMMETRY BREAKING EFFECTS

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The possible point symmetries of the various fullerene molecular structures range from icosahedral symmetry, which is the highest molecular point symmetry possible, through a multitude of lower symmetries including (most often) none at all. One per-cent natural abundance of Carbon-13 means about half the sixty-Carbon fullerenes have completely lost their extraordinary rotational symmetry. Also, since Carbon-12 nuclei are spin-0 a sixty-Carbon-12 fullerene is a perfect 'Bose-Einstein ball' which excludes all but scalar rovibronic symmetry states, but even one extra Carbon-13 completely breaks the Bose exclusion. The effects of isotopic and other types of doping on fullerene rovibrational levels is explored. A tensor model for centrifugal distortion is used to see the effects of doping on the rotational level fine structure. In spite of the extreme symmetry breaking there is still considerable order and near-degeneracy in the rotational spectrum. A semi-classical rotational energy surface picture helps to explain the structure. At the other extreme is the sixty-Carbon-13 molecule, a monstrous 'Fermi-Dirac ball' which is compared to sulfur hexafluoride. However, the hyperfine structure of the latter is dwarfed by the former which has over an octillion of nuclear spin states[a]. Perhaps they might be considered in the search for quantum computing elements.

[a] W. G. Harter and T. C. Reimer *Chem. Phys. Lett.* **194** 230(1992).