Excited Electronic States and Relative Stabilities of C_{80} Isomers

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Very high temperatures of fullerene synthesis allow for a significant population of excited electronic states and thus for non-negligible electronic partition functions. This feature can have some interesting consequences for computed fullerene-related thermodynamics or kinetics. The excited electronic states can be evaluated by means of the configuration interaction (CI) approach. An illustration is served with the C_{80} isomeric systems. C_{80} consists of seven IPR isomers (the structures are sometimes coded **A-G**). The SAM1 computations predict the **C** isomer (D_{5d} symmetry) as the system ground state, being followed by the **A** species of a D_2 symmetry. At very low temperatures the ground-state structure, **C**, has to be prevailing. At a temperature of 1178 K the **A** species reaches equimolarity with the **C** species, and also other species become gradually significant. These SAM1 results without inclusion of the electronic partition function are now complemented with the values corrected for the ZINDO electronic excitations. Interestingly enough, the computed effects of the electronic excited states are still larger than in the previously tested C_{78} and $Mg@C_{72}$ cases.