Excited Electronic States and Stabilities of Isomeric Fullerenes

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Very high temperatures of fullerene synthesis do allow for a significant population of excited electronic states and thus for non-negligible electronic partition functions. This unique feature can have some interesting consequences for computed fullerene-related thermodynamics or kinetics. The excited electronic states can be evaluated by means of the (limited) configuration interaction (CI) approach. Numerical illustrations are served with C_{78} and $Mg@C_{72}$ isomeric systems. There are five isolated-pentagon-rule (IPR) satisfying isomers for C_{78}, but only three were originally observed in experiments. Only very recently, a fourth isomer has been observed, too. In this work we report calculated structural, spectral, and energetic data of the five IPR C_{78} fullerenes, and apply the data to evaluation of their relative concentrations. Similarly, relative concentrations of isomers of $Mg@C_{72}$ (a not yet isolated system) are studied, too. In both cases, the electronic partition functions are considered accordingly. The calculations supply a further interesting example of sometimes profound (nevertheless, frequently ignored) role of enthalpy-entropy interplay in stabilities of isomeric fullerenic structures, and in particular point out a possible significant role of excited electronic states.