Computing Temperature Development of the Ca@C_{72} Isomeric System

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Temperature dependencies of the relative populations in a model isomeric system Mg@C_{72} (not isolated yet) were computed recently. It was the very first case when relative concentrations for an endohedral fullerene isomeric system were evaluated as before that time only pristine higher or lower isomeric fullerenes had been treated in the thermodynamically consistent way. The simulation has pointed out an interesting temperature development and thus, it has re-focused attention back to the original parent isomeric system of Ca@C_{72} (one isolated-pentagon-rule structure, two structures with a pair of adjacent pentagons, and one cage with a heptagon). In order to evaluate the entropy contributions, the molecular vibrations are to be computed and this task actually represents the most time consuming step. Once the task is mastered, the whole thermodynamic scheme can be completed.