Gibbs energy treatment on a set of $C_{60}F_{36}$ isomers

Zdeněk Slanina,[1] Filip Uhlík[2] and Ludwik Adamowicz[3]

[1]Department of Theoretical Studies
Institute for Molecular Science
Myodaiji
Okazaki, J 444-8585
Japan

[2]Department of Physical and Macromolecular Chemistry
School of Science, Charles University
Albertov 6
Prague 2, CZ 128 43
Czech Republic

[3]Department of Chemistry
University of Arizona
1306 E. University Blvd.
Tucson, AZ 85721-0041
U. S. A.

$C_{60}F_{36}$ is know to be formed by several isomers. The computations show that the isomers are relatively close in potential energy. Moreover, the system is prepared at higher temperatures. In overall, $C_{60}F_{36}$ represents an interesting candidate for computational treatment not only in the terms of potential energy or heats of formation but also in the terms of Gibbs function. The treatment is reported, based on the PM3 semiempirical quantum-chemical method.