Reply to "Comment on 'Theoretical Investigation of the Formation Mechanism of Metallofullerene $Y@C_{82}$'"

Li-Hua Gan and Chun-Ru Wang*

Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, China

Received: January 16, 2006

Fullerenes and endohedral metallofullerenes are formed in high-temperature plasma by laser ablating or arc-discharging graphite. As simulated by Yamaguchi et al.[1] with a molecular dynamics theory, metallofullerenes are formed in a timescale at >4000 ps under a high temperature (3000 K). Obviously, various unstable and quasi-stable clusters will be generated continuously in the high-temperature plasma, and afterward they can either react with other clusters to form new stable molecules, for example, fullerenes, metallofullerenes, and nanotubes, and so forth, or transform to some more stable structural isomers of the clusters finally. In our recent paper,[2] we have suggested that the formation mechanism of $Y@C_{82}$ is via a reaction between two clusters, that is, C_{76} and YC_6, in which the YC_6 owns a nonplanar ring structure. In allusion to this mechanism, Strout presented an interesting proposal that the nonplanar isomer YC_6 may transform to its more stable structures, such as the planar or fan isomers.[4] In fact, the two reaction models of YC_6 proposed by us[2] and Strout[4] represent just the two possible reaction routes for an unstable cluster as mentioned above.

We consider a typical $Y@C_{82}$ production process by arc-discharging yttrium/graphite rods. In the high-temperature plasma, C_6 rings would be generated in a large amount as one of the main graphite fragments and yttrium atoms/ions are also evaporated at the high-temperature plasma. They should have good probability to collide with each other in high-temperature plasma and form various isomers of YC_6, including the nonplanar ring isomer. Once this nonplanar ring isomer of YC_6 is formed, due to the unstable property of this isomer as calculated by Strout,[4] it must either react with other unstable clusters to form stable molecules, for example, $YC_6 + C_{76} \rightarrow Y@C_{76}$, as we suggested in the previous paper,[2] or transform to some more stable structures of YC_6, for example, the planar or fan isomers, as suggested by Strout.[4]

* To whom correspondence should be addressed. E-mail: crwang@iccas.ac.cn.

References and Notes

(1) Yamaguchi, Y.; Maruyama, S. *Eur. Phys. J. D* **1999**, *9*, 385.
(2) Gan, L. H.; Wang, C. R. *J. Phys. Chem. A* **2005**, *109*, 3980.
(3) Shinohara, H. *Rep. Prog. Phys.* **2000**, *63*, 843.
(4) Strout, D. L. *J. Phys. Chem. A* **2006**, *110*, 4285.

10.1021/jp068009w CCC: $33.50
Published on Web 03/07/2006