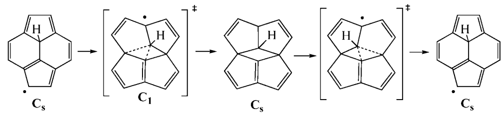
# ADDITIONS AND CORRECTIONS

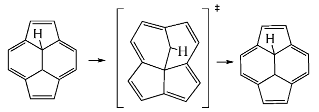
## 2005, Volume 109A

**Mark R. Nimlos,* Jonathan Filley, and J. Thomas McKinnon:** Hydrogen Atom Mediated Stone−Wales Rearrangement of Pyracyclene: A Model for Annealing in Fullerene Formation

Page 9896. We regret that we did not acknowledge the relevant and insightful work of Alder and Harvey.[1] We originally released our work almost simultaneously with Alder and Harvey as part of a conference proceedings[2] but failed to sufficiently upgrade our literature search before publication of our paper. In our paper we considered two mechanisms for the enhancement of Stone−Wales rearrangement in pyracyclene upon addition of a hydrogen atom. These mechanisms are shown in reactions 1 and 2. Reaction 1 contains a stable cyclobutyl intermediate and reaction 2 is a mechanism proposed by Scuseria et al.[3,4]

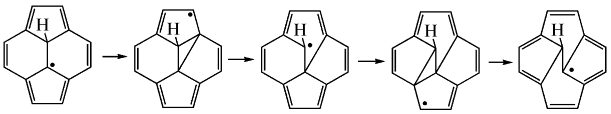


(1)



(2)

Alder and Harvey proposed a mechanism that contained homoallyl-cyclopropylcarbinyl intermediates and conducted calculations on several other molecules, including chrysene. Their mechanism applied to pyracyclene is shown in reaction 3. We were unable to locate the cyclopropylcarbinyl intermediate for pyracyclene in our studies. This starting geometry converged to the cyclobutyl intermediate shown in reaction 1. Perhaps these mechanisms converge as a result of the strain imposed by the rigid pyracyclene structure.



(3)

## References and Notes

(1) Alder, R. W.; Harvey, J. N. *J. Ame. Chem. Soc.* **2004**, *126*, 2490.
(2) Nimlos, M.; Filley, J.; McKinnon, J. T. *Abstr. Pap. .Am. Chem. Soc.* **2004**, *227*, U1100.
(3) Bettinger, H. F.; Yakobson, B. I.; Scuseria, G. E. *J. Am. Chem. Soc.* **2003**, *125*, 5572.
(4) Murry, R. L.; Strout, D. L.; Odom, G. K.; Scuseria, G. E. *Nature* **1993**, *366*, 665.

10.1021/jp061383b
Published on Web 03/16/2006