

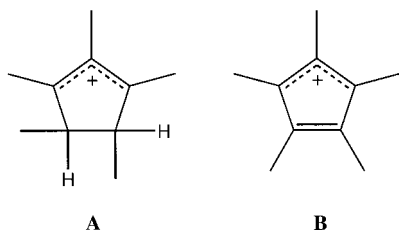
- [4] ^{13}C NMR data for allyl cations: a) G. A. Olah, G. Liang, *J. Am. Chem. Soc.* **1972**, *94*, 8071; b) H. Mayr, G. A. Olah, *J. Am. Chem. Soc.* **1977**, *99*, 510; c) G. A. Olah, H. Mayr, *J. Am. Chem. Soc.* **1976**, *98*, 7333; d) G. A. Olah, P. R. Clifford, Y. Halpern, R. G. Johanson, *J. Am. Chem. Soc.* **1971**, *93*, 4219; e) G. A. Olah, R. J. Spear, *J. Am. Chem. Soc.* **1975**, *97*, 1539.
- [5] All calculations were performed with Gaussian98 Revisions A3–A9, Gaussian, Inc., M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A.

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- [6] a) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098; b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.
- [7] a) R. Ditchfield, *Mol. Phys.* **1974**, *27*, 789; b) K. Wolinski, J. F. Hilton, P. Pulay, *J. Am. Chem. Soc.* **1982**, *104*, 5667; c) J. R. Cheeseman, G. W. Trucks, T. A. Keith, M. J. Frisch, *J. Chem. Phys.* **1996**, *104*, 5497.
- [8] For an introduction in the methodology see: W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, *Ab initio molecular orbital theory*, Wiley, New York, **1986**.
- [9] Calculated from single-point energies using the heavy-atom geometry of **1a** with all 15 hydrogen positions of **1** optimized at B3LYP/6–31G(d).
- [10] Calculated by using the heavy-atom geometry of **1a** with all 17 hydrogen positions of **2** optimized at B3LYP/6–31G(d).

Statement

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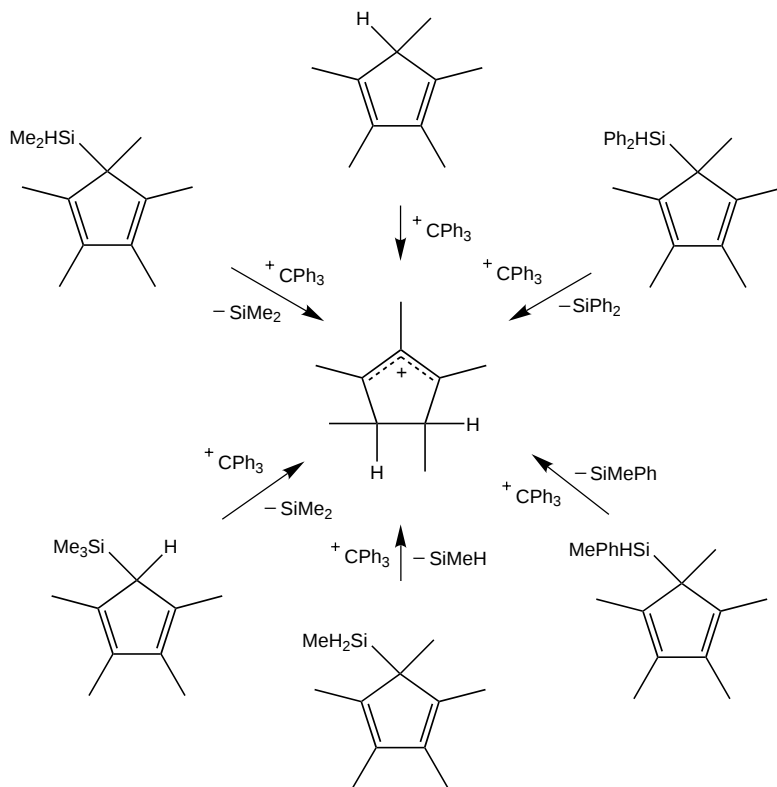
As we conclude in the accompanying Correspondence,^[1] the X-ray structure described recently^[2] is of the pentamethylcyclopentenyl cation (**A**) rather than the pentamethylcyclopentadienyl cation (**B**). The



key resonance of the CH protons in the NMR spectrum of **A** is broad and featureless, inexplicably lacking the expected quartet splitting. In the $^1\text{H}/^{13}\text{C}$ 2D spectrum, the CH group exhibits a weak to negligible cross peak, in contrast to the strong cross peaks for all the methyl groups. Consequently, the methine carbon appears to show no hydrogen connectivity.

In addition to the method of formation described in ref. [2], we previously prepared the same cation by five other methods (Scheme 1), all of which admit of logical pathways to **B** rather than to **A**. Triphenylcarbinol is not a product, only triphenylmethane in each case. We are currently exploring mechanistic pathways that can explain these unusual observations.

Because of the evidence presented in ref. [1], I am retracting the conclusions of ref. [2], which were entirely my



Scheme 1.

own and imply no reflection on the part of my co-workers (whose experimental and theoretical work is valid).

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- [2] J. B. Lambert, L. Lin, V. Rassolov, *Angew. Chem.* **2002**, *114*, 1487; *Angew. Chem. Int. Ed.* **2002**, *41*, 1429.