Formation of Heterofullerenes by Direct Exposure of C_{60} to Boron Vapor

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Results and Discussion

An intriguing way to modify the properties of fullerenes is to replace a carbon atom in the caged network with a heteroatom. Boron-doped nanocarbon structures have important potential for use in materials science and electronics. However, heterofullerenes that incorporate boron have scarcely been studied due to lack of a strategy to form borafullerenes from C_{60}. Here, we report facile gas-phase formation of $C_{59}B$ by atom exchange reactions resulting from exposure of C_{60} to boron vapor. The processes are elucidated by means of a pulsed laser vaporization cluster source and analyzed by 9.4 T Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. This procedure, or other vaporization setups, such as arc discharge, for $C_{59}B$ formation may be scaled up to preparative level. Further, the technique is convenient because synthetic preparation of boron-containing C_{60} derivative precursors is not necessary; it is the first report of borafullerene formation directly from pristine C_{60}. The method is also applicable to other fullerenes; e.e., $C_{69}B$ can be generated directly from C_{70}. Thus, many new borafullerenes and endohedral borafullerenes may be synthesized by exposure of various pre-existing fullerenes to boron vapor. The atom exchange process is efficient even with low-cost, commercially available grades of boron (90%B).

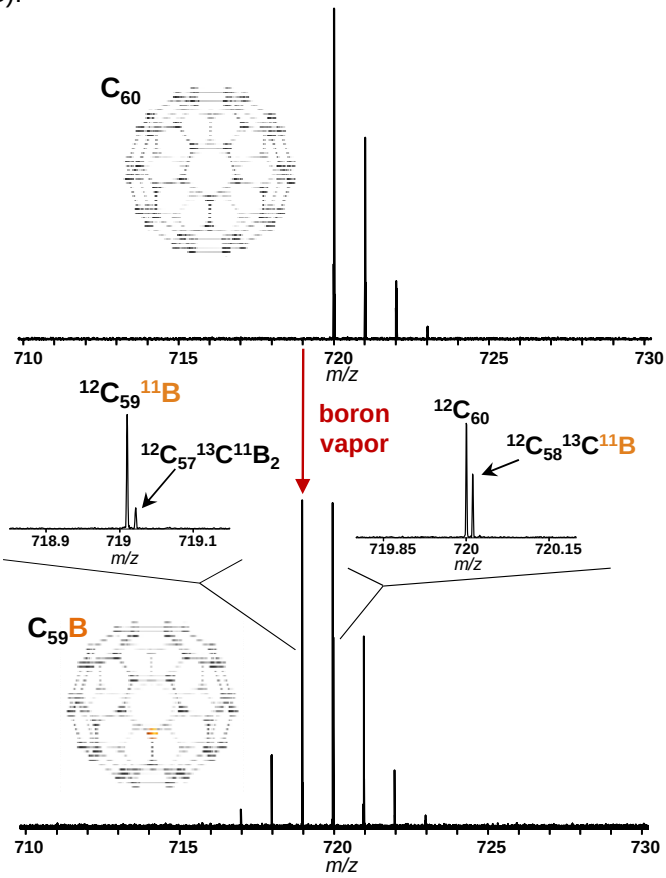

Figure 1. Negative ion 9.4 T FT-ICR mass spectra of C_{60} without boron vapor (top), and after exposure to boron vapor (bottom). The heterofullerene, $C_{59}B$, was directly generated from pristine C_{60} by atom exchange reactions.

Acknowledgments

Work supported by the Florida State U. Research Foundation, NSF DMR-06-54118, Spanish Ministry of Science and Innovation (CTQ2011-29054-C02-01 and Generalitat de Catalunya (2009SGR462 and XRQTC).

References

[1] Dunk, P.W. *et al*., Angewandte Chemie International Edition, **52**, 315-319 (2013).