Building Carbon Bridges on and between Fullerenes in Helium Nanodroplets

S. A. Krasnokutski[†1], J. Postler[*], M. Goulart[*], M. Kuhn[*], A. Kaiser[*], A. Mauracher[*], M. Renzler[*], D. K. Bohme[‡], P. Scheier[*2]

[*] Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, A-6020 Innsbruck, Austria,
[†] Laboratory Astrophysics Group of the Max Planck Institute for Astronomy, University of Jena, 07743 Jena, Germany,
‡ Department of Chemistry, York University 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3.

Synopsis: We report mass spectrometric investigations and the observation of sequential encounters of fullerenes with C atoms in helium nanodroplets. Density functional theory calculations were also performed to interpret the experimental results.

Ever since the discovery of fullerenes by Kroto et al. [1] and even more since the recent laboratory confirmation of fullerene presence in the interstellar medium [2], fullerene formation and reaction schemes have been subject of a lively debate. Here we report the observation of sequential encounters of fullerenes with C atoms in an extremely cold environment. The experiments were performed with helium nanodroplets at 0.37 K doped with C_{60} molecules and C atoms derived from a pure source of C atoms. They were subsequently exposed to electrons at a controlled energy and investigated using a high-resolution time-of-flight mass spectrometer. The mass spectra revealed the formation of carbenes of the type $C_{60}(C:)_n$ with n up to 6. Bridge-type bonding of the C adatoms to form the known dumbbell $C_{60}{=}C{=}C_{60}$ was also observed.

To interprete the experimental findings, we employed density functional theory calculations at the B3LYP/6-31g(d) level that elucidated the carbene character of the $C_{60}(C:)_n$ species and their structures.

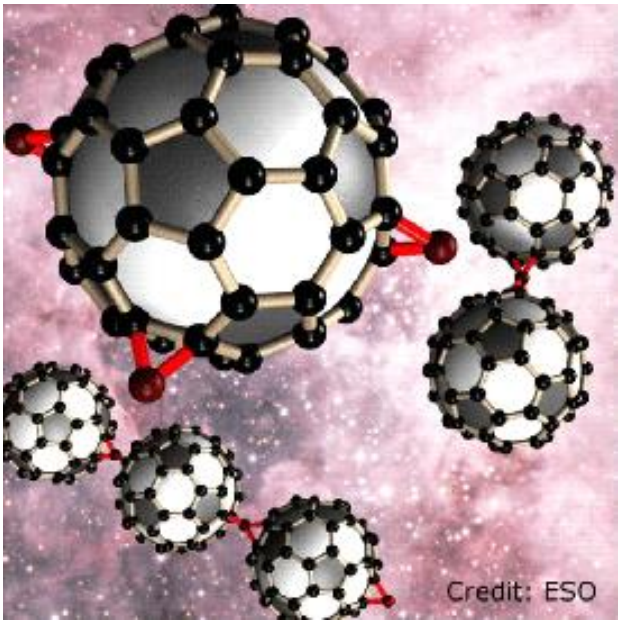

Figure 1. Graphic representation of molecular structures formed by single carbon addition in He clusters doped with fullerene molecules.

References

[1] Kroto, H. W. *et al.* 1985 *Nature* **318** 162;
[2] Campbell, E. K. *et al.* 2015 *Nature* **523** 322.

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