C₂ Inclusion by C₆₀ Films

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The deposition of hyperthermal C₂⁻ anions onto C₆₀ films has been studied by means of mass spectrometry (MS), thermal desorption spectroscopy (TDS), ultraviolet photoionization spectroscopy (UPS), atomic force microscopy (AFM) and Raman spectroscopy. Covalent attachment of C₂ dimers to C₆₀ cages manifests itself by the sublimation of the C₆₂, C₆₄ and C₆₆ cages as well as by pronounced modifications of the thermal, electronic and vibronic properties of the C₆₀ films. The yield of volatile C₆₂ species formed depends on the deposition conditions, but was not greater than 10⁻² per C₂. UPS and Raman spectra of the C₂/C₆₀ layers supported by DFT calculations indicate the formation of polymeric network based on -C₆₀-C₂-C₆₀- chains as well as the prevailing inclusion channel. Thermal desorption spectra reveal correlated sublimation of C₆₀ and C₆₂ which implies that thermal decomposition of the -C₆₀-C₂-C₆₀- oligomeric chains is the common dissociative reaction step. In the temperature range 750 - 975 K the thermal decomposition of the -C₆₀-C₂-C₆₀- oligomeric chains may compete with the thermally activated C₂ incorporation by C₆₀ cages resulting in a semiconducting network of carbon oligomers. At higher temperatures the fullerene network becomes converted predominantly into a conducting phase.

Figure 1: The two lowest isomers as predicted by DFT calculations for the system consisting of C₂ and two C₆₀ cages