REGULARITIES IN FULLERENE C_{60} FRAGMENTATION ACCORDING TO LASER-DESORPTION MASS-SPECTROMETRIC AND QUANTUM CHEMICAL DATA

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S u m m a r y

Experimental and theoretical results concerning the regularities in the fullerene C_{60} fragmentation are reported. The destruction of C_{60} thermally deposited onto a silicon substrate is studied with the use of laser-desorption mass spectrometry and provided various values of laser radiation power. The intensity of $[C_{60}]^+$ ions in the mass spectrum is shown to increase linearly, when the laser radiation power grows from 30 to 70% of its maximum. At the same time, the relative degree of C_{60} fragmentation first increases and then saturates at 50% of the laser power maximum. Two possible mechanisms of fullerene ionization are proposed. The electron structures of molecular, C_{60-2n}, and cationic, $[C_{60-2n}]^+$, fullerene forms, where the parameter $n = 0$ to 4 indicates the number of lost C_2 fragments, are calculated within the quantum chemistry method. The boundary molecular orbitals (EHOMO and ELUMO), adiabatic ionization potentials, and electron affinities are calculated.