Quantum Chemistry Simulation of 60-Fullerene Interaction under External Pressure

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The results of the interaction of two 60-fullerene molecules interaction under external pressure, studied by a semi-empirical PM3 quantum chemical method, are reported. A set of 15 space structures of 60-fullerene dimers from the simplest one up to partially graphitized material has been simulated. Calculated pressures referring to the dimers' formation reproduce the experimental order of magnitude rather well. The dependences of the heat of formation and the force ballancing the applied pressure versus compression have been determined. A mechanism of the dimerization is proposed.

Key words: Quantum Chemistry; Semi-empirical Method; 60-Fullerene Dimers; High Pressure; High Temperature; PM3.