Computational Insight into Fullerene Stabilities

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Stabilities in fullerene systems, both the relative and absolute stabilities, are predetermined by the original high formation temperatures. However, after condensation to room temperature, the stabilities can sometimes be modified further. In the original high-temperature regime several scenarios can come into action like partial thermodynamic equilibrium, pressure modulation, kinetic control, catalysis and autocatalysis. Computational treatments have supplied illustrations for any of the partial situations and thus clarified conditions in numerous fullerenic system - pristine cages, their derivatives, and cages with encapsulates.