Atomic and Bond Topological Properties of Strained Carbon Ring and Cage Systems

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The discovery of the fullerenes in the 80ies brought a new class of carbons cage compounds with unusual structural properties into the scope of chemical research, similarly as happened with Cope systems in the 60ies, where, for example, bullvalene with its unique property to exist in more than 1.2 million isomers [1], raised considerable attention. Not only preparative chemists, but also nature was able to generate complicated oligocyclic carbon cages, as for example, for several opioide derivatives. They all have in common to contain carbon atoms in very unusual steric arrangements and to exhibit C-C bonds of unusual lengths. Distances far beyond normal single bond lengths are then in question whether or not a covalent bond exists. We have analyzed experimental and theoretical electron densities of a number of strained carbon cages from the compound classes mentioned above. We could derive quantitative atomic and bond topological properties making use of Bader's AIM formalism [2]. The existence/non existence of bond critical points and the analysis of the Laplacian function allowed also the characterization of bond/no bond regions in a [1.1.1]propellane and a related bicyclo [1.1.1]pentane derivative. Electron densities on bond critical points allowed bond orders to derive which were found remarkably smaller than one in several strained cages, for example in halogenated C_{60} derivatives.

[1] Doering W.E. von, Roth W.R., *Tetrahedron*, 1963, **19**, 715. [2] Bader R.F.W., *Atoms in Molecules*, Clarendon Press, Oxford, 1990.
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