Paths Through The Fullerene-Derivative Jungle: How Theory Can Help

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The nature of the fullerene molecule, with its large sets of chemically equivalent or near equivalent sites, can make the experimental characterisation of fullerene derivatives a challenging problem. From the point of view of the theoretical chemist, the problem is also very challenging. The number of isomers and size of individual molecules make brute-force calculation an unattractive possibility, but leave room for more qualitative applications of theory, which may in the long run be more informative. In fullerene chemistry, theory has proved useful in helping to map out sets of possibilities, test and establish empirical rules, and compare energetics of isomeric possibilities. This contribution will discuss the successes and limitations of an approach where clues from experiment are combined with mathematically complete enumeration techniques from group theory, addition games based on simple rule sets from classical valence theory, qualitative energetics from semi-empirical models and, where necessary, full ab initio calculation.