

Correlation effects in small carbon rings

Peter R. Taylor

*Department of Chemistry and
Centre for Scientific Computing
University of Warwick
Coventry, CV4 7AL, UK*

Abstract

Ten years ago small carbon rings such as C_6 were considered figments of the theoretician's imagination, but they were eventually synthesized and identified with the aid of computed vibrational spectra. In general these rings, which have even numbers of carbon atoms and can thus be represented as C_{2n} , are planar with an n -fold (but not a $2n$ -fold) axis of rotation. There are differences between the additional symmetry present when n is odd or even, resulting from whether bond angles alternate or bond lengths and angles alternate, and there is disagreement about the lowest value of n for which different types of alternations arise. Although the equilibrium geometries of these rings appear to be well described by coupled-cluster methods such as CCSD(T), a detailed examination reveals a number of subtle effects that mandate a multiconfigurational reference description. We shall discuss these issues, presenting results for selected systems.