Structure and Stability of Molecular Carbon: Importance of Electron Correlation [Phys. Rev. Lett. 75, 3870 (1995)]

Jeffrey C. Grossman, Lubos Mitas, and Krishnan Raghavachari

An early version of Fig. 2 was inadvertently printed. The correct Fig. 2 appears below.

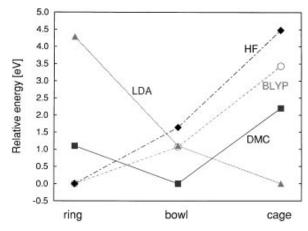


FIG. 2. The relative energy differences for the ring, bowl, and cage C_{20} isomers (DMC error bars are 0.2 eV). For each theory the lowest energy structure is taken as a reference. BLYP refers to calculations done with the Becke-Lee-Yang-Parr functional.