

Electronic Structure and Bonding in the Metallocarbohedrene Ti_8C_{12} [Phys. Rev. Lett. 70, 29 (1993)]

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The original paper presented a calculated geometry of the Ti_8C_{12} cluster, as obtained by means of energy minimization using a cluster full-potential linear muffin-tin orbital method. This geometry does not minimize the total energy correctly. The figure shows an alternate geometry, calculated using the same method, for which the forces are zero and the total energy is lower by 15.5 eV. The previously found structure is not a local minimum of the total energy, but is found to lie in a very flat part of the energy surface. The previous calculation used a starting geometry close to that of an ideal dodecahedron, and had omitted following the distortion path to sufficiently large distortions for which the forces and energy gain become relevant.

We thank H. Chen and co-workers for supplying us with their results prior to publication.

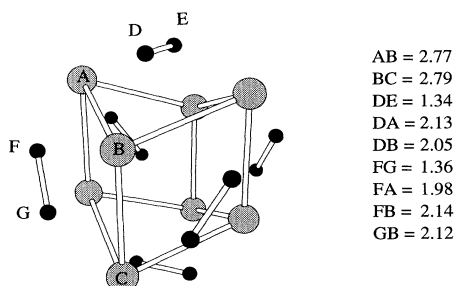


FIG. 1. Equilibrium structure and bond lengths of Ti_8C_{12} as obtained in the new calculation. Large and small spheres are Ti and C atoms, respectively. Bond lengths in Å.

0031-9007/93/71(1)/209(1)\$06.00

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Nonlinear Optics of Bessel Beams [Phys. Rev. Lett. 70, 1401 (1993)]

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We credited Durnin, Miceli, and Eberly [1] for the first experimental realization of a Bessel beam. S. L. McCall now brought to our attention some earlier papers on this topic, which we gratefully acknowledge. McLeod [2,3] worked on optical elements producing extended foci and developed a number of creative ideas for possible applications. However, he did not elaborate on the details of their transverse profile. Kelly pointed out later [4] that the transverse intensity profiles produced by axicons are described by J_0 , the zero-order Bessel function, and thus the term “Bessel beam” could have been applied to extended-focus axicon beams as early as 1963, although the term was not used by Kelly. The work of Durnin, Miceli, and Eberly appears to have prompted the term Bessel beam, and it also provided the theory, as well as the first measurements [1,5], of the “nondiffracting” subclass of Bessel beams, those for which the J_0 function is ideally independent of the longitudinal coordinate.

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