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Chemical Physics

Volume 176, Issue 1, 1 October 1993, Pages 61-66

Jahn-Teller distortions in solid C₂₀ and other fullerene structures

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[https://doi.org/10.1016/0301-0104\(93\)85007-U](https://doi.org/10.1016/0301-0104(93)85007-U)

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Abstract

We have used first principles molecular dynamics to determine the energies of Jahn-Teller distortions in a variety of neutral and negatively charged fullerene structures. We find that smaller structures have larger Jahn-Teller distortion energies. Solid C₂₈ and solid C₂₀, which have covalent bonds connecting the individual fullerene balls, are found to have energies which are much lower than the energies of their molecular components. The charged state of solid C₂₀ is found to have a total distortion energy which is about six times larger than that of C^{âˆ—}₆₀.



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