

CUBIC POLYMERIC STRUCTURES ON THE BASIS OF SMALL FULLERENES C_{20} , C_{24} , C_{28} , C_{32}

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Introduction

In previous paper [1] we considered the equilibrium configurations of fullerenes' molecule C_{28} , dimer $(C_{28})_2$ and also high symmetry clusters $(C_{28})_4$ and $(C_{28})_8$. In this work we continue earlier started researches.

Results and discussions

In the frames of semiempirical method PM3 [2,3] geometrical parameters of equilibrium configurations of small fullerenes' molecules C_n , their dimers $(C_n)_2$, square $(C_n)_4$ and cubic $(C_n)_8$ clusters for $n=20, 24, 28, 32$, are defined. In the Fig.1-4 below equilibrium configurations of cubic clusters, which can be considered as fragments of polymeric crystal structures having simple cubic symmetry, are shown.

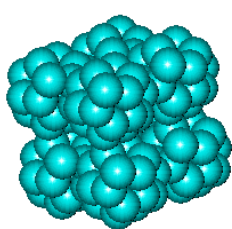


Fig.1. Cluster $(C_{20})_8$

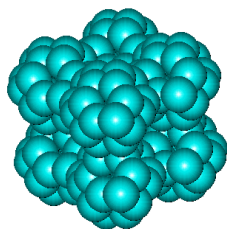


Fig.2. Cluster $(C_{24})_8$

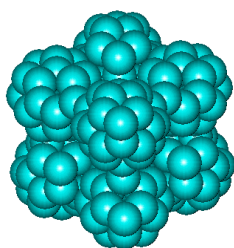


Fig.3. Cluster $(C_{28})_8$

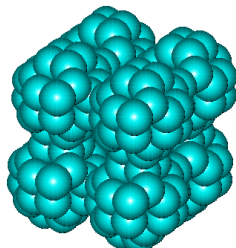


Fig.4. Cluster $(C_{32})_8$

The results of our calculations of geometrical parameters of equilibrium configurations of small fullerenes' clusters and their electronic structure

too, are in reasonable agreement with data of early researches [4-6].

The interest on polymeric structures on the basis of small fullerenes isn't casual and it's connected with high chemical activity of small fullerenes' molecules. It leads in particular to formation of more rigid (then in case of classic fullerene C_{60}) polymerized structures that have the whole number of unusual physical and chemical properties [4-5].

The stimulating influence of a prominent work [6] (in which on the basis of quantum chemistry calculations the structure of cubic graphite was correctly defined for the first time) should be especially pointed out.

Conclusions

On the basis of semi-empirical calculations of equilibrium configurations and electronic structures of small fullerenes' clusters the conclusion about the possibility of existence of polymerized cubic crystal structures of small fullerenes is done.

References

1. Popov A.P., Bazjin I.V., NATO Science Series, 2004, v. 172, 239.
2. Stewart J.J.P., J. Comput. Chem., 1989, v. 10, p. 209.
3. Stewart J.J.P., J. Comput. Chem., 1989, v. 10, p.221.
4. Kim J., Galli G., Wilkins J.W., Canning A., J. Chem. Phys., 1998, v. 108, 2631.
5. Grossman J.C., Piscoti C., Louie S.G., Cohen M.L., Zettl A., in Fullerenes Chemistry, Physics and Technology, 887-916, N.Y., 2000.
6. Покропивный В.В., Покропивный А.В., ФТТ, 2004, v. 46, 380.