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C~4~0, C~4~0^+, Nb@C~4~0^+, NbC~3~9^+, Nb@C~4~0H~4^+的 量子化学研究

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摘要

用量子化学从头计算方法研究了C~4~0,C~4~0^+,Nb@C~4~0^+,NbC~3~9^+,Nb@C~4~0H~4^+的几何构型、电子结构和C~2~8一样,C~4~0(T~d)基态也为^5A~2态,笼骨架上具有四个悬挂键。计算结果表明C~4~0和C~4~0^+比NbC~3~9^+和Nb@C~4~0^+稳定,与实验结果一致。

关键词 铌络合物 金属碳笼 碳笼 富勒烯 笼状结构 电子结构 构型 从头计算法

分类号 0641

Quantum chemical study of C~4~0, C~4~0^+, Nb@C~4~0^+, NbC~3~9^+, Nb@C~4~0H~4^+

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Abstract Ab initio Hartree-Fock calculations were performed on the equilibrium geometries and electronic structures of a series of endohedral, exohedral and endohedral-exohedral complexes of C~4~0. The C~4~0(T~d) cage is found to have four unpaired electrons with a ^5A~2 open-shell ground state and have four dangling bonds. C~4~0(T~d) behaves as a sort of hollow superatom with an effective valence of 4, both toward the outside and inside of the carbon cage, so it is possible to form the endohedral metallofullerene Nb@C~4~0, exohedral complex C~4~0H~4 and endohedral-exohedral complex Nb@C~4~0H~4 from C~4~0. From the values of binding energies per atom, it's found that C~4~0(T~d) is more stable than C~4~0(C~3~v), while C~4~0^+ (C~3~v) is more stable than C~4~0^+(T~d). In networked metallofullerenes NbC~3~9^+, Nb is connected directly with three carbon atom, forming three Nb-C single bonds with the Nb atom protruding from the surface of the carbon cage. Our calculated results show that C~4~0 and C~4~0^+ are more stable than NbC~3~9^+, and NbC~3~9^+ is more stable than Nb@C~4~0^+. The results are consistent with the experimental results. Through the comparison of the C~4~0 series clusters with the C~2~8 and related compounds, we have found that there are many similarities between C~4~0 and C~2~8. Our calculated results may shed light on other endohedral and exhedral complexes of fullerenes and networked type metallofullerenes in general.

Key words NIOBIUM COMPLEX FULLERENES CAGE STRUCTURE ELECTRONIC STRUCTURE CONFIGURATION AB INITIO CALCULATION

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