化学学报 2002 60 (4): 681-686 ISSN: 0567-7351 CN: 31-1320/06

(RXNR)_4(X=B，Al，Ga)簇合物的结构与化学键性质

武海顺,张聪杰,许小红,张富强

山西师范大学化学系,临汾(041004)

收稿日期 修回日期 网络版发布日期 接受日期

摘要 用自洽场理论（HF）和密度泛函理论（DFT）的B3LYP方法，在6-311G~*水平上 ，首次从理论上研究了(RXNR)_4 (R = B，Al，Ga；R = H，CH_3，NH_2，OH)簇合 物及其先驱化合物（RXNR）_2的几何构型、电子结构和化学键性质，并与其异构体 及其等电子化合物进行了比较。结果表明，(RBNR)_4为环状骨架结构，(RAlNR)_4 和(RGaNR)_4为建立骨架结构。

关键词 自洽场 簇状化合物 化学键 构型

分类号 0641

Structure and Chemical Bonding Behavior of (RXNR)_4 (X = B, Al, Ga) Clusters

Wu Haishun,Zhang Congjie,Xu Xiaohong,Zhang Fuqiang

Department of Chemistry, Shanxi Normal University,Linfen(041004)

Abstract The optimized geometries, electron structure and bonding behavior of (RXNR)_4 (X = B, Al, Ga; R = H, CH_3, NH_2, OH) and their precursor fragments (RXNR)_2 were investigated by means of self-consistend field (SCF) theory at the HF/6-311G~* and density functional theory (DFT) at the B3LYP/6-311G~* level. Moreover, the comparison with their isoelectron compounds has been carried out. The results show that (RXNR)_4 has a ring-sketch structure, while both (RAlNR)_4 and (RGaNR) _4 have cube-sketch ones.

Key words SELF-CONSISTENT FIELD CLUSTER COMPOUND CHEMICAL BONDS CONFIGURATION

DOI:

通讯作者