

Al₂F₂分子结构与稳定性的ab initio计算研究

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摘要 用abinitio方法在UMP2/6-311G(d)水平下计算了Al₂F₂分子可能的异构体构型和AlF二聚化成Al₂F₂分子的反应能。UMP2/6-311G(d)和UQCISD(T)/6-311+G(3df)//UMP2/6-311G(d)

水平下的能量值均说明具有D_{2h}对称性、1^{Ag}电子态的异构是Al₂F₂分子的最稳定构型,其Al-F键长为0.19074nm,键角Al-F-Al和F-Al-F分别为104.62°和75.38°,以及两个强振动,441.27cm⁻¹和401.93cm⁻¹,均与实验结果相符合。电子结构分析表明,具有D_{2h}对称性的异构体的活性中心在2个Al原子上,在形成衍生物时是主要的反应加成位置。在UMP2/6-311G(d)和UQCISD(T)/6-311+G(3df)//UMP2/6-311G(d)水平下得到了AlF二聚化能量分别为-75.01kJ/mol和-66.07kJ/mol,与文献估计计算基本一致,说明AlF二聚化反应能量上是有利的。

关键词 [分子结构](#) [氟化铝](#) [异构化反应](#) [二聚作用](#) [电子结构](#) [稳定性](#) [从头计算法](#)

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An ab initio study of structure and stability of Al₂F₂ molecule

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Abstract Possible isomers of Al₂F₂ molecule are shown to exist by ab initio molecular orbital calculations at UMP2/6-311G(d) level. The values of energy at UMP2/6-311G(d) and UQCISD(T)/6-311+G(3df)//UMP2/6-311G(d) level of the theory show that the isomer that has D_{2h} symmetry and 1^{Ag} electronic state is the most stable equilibrium geometry. In the isomer, the Al-F bond length is 0.19074 nm, and the bond angles Al-F-Al and F-Al-F are 104.62° and 75.38°, respectively. Two strong vibrations have been found at 441.27 cm⁻¹ and 401.93 cm⁻¹. These results are in agreement with experimental ones. Analyses of electronic structure show that the active positions are on the Al atoms, and are main additive areas where it reacts with other compounds. The dimerization energies at UMP2/6-311G(d) and UQCISD(T)/6-311+G(3df)//UMP2/6-311G(d) levels are -75.01 kJ/mol and -66.13 kJ/mol, respectively, and are in agreement with those in the literature. The results show that the dimerization of AlF is thermodynamically favored.

Key words [MOLECULAR STRUCTURE](#) [ALUMINIUM FLUORIDE](#) [ISOMERIZATION REACTION](#) [DIMERIZATION](#) [ELECTRONIC STRUCTURE](#) [STABILITY](#) [AB INITIO CALCULATION](#)

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