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密度泛函理论下的分子电负性Ⅲ: 分子总能量的直接计算

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摘要 本文根据密度泛函理论, 在分子基态总能量表达式中, 考虑了组成原子的内在能量、电负性和硬度的价态特征, 并引入协调原子间相互作用能项的k因子,不仅使处理和解释更为合理, 而且大大提高了计算精度和适用范围。据此, 我们提出和设计了一个直接计算体系基态总能量的新方案, 可广泛应用于各类分子和基团, 同时给出了一套较为普遍的实用参数, 通过上百个大小分子或基团的实际计算, 结果与从头计算结果符合相当好, 相对误差不到千分之一。此外, 该方案具有简单快速、易于执行等优点, 为大分子体系的能量计算提供了一个切实有效的方法。

关键词 电负性 密度泛函理论 STO-3G从头计算 基态总能量

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Molecular electronegativity in density functional theoryⅢ: Direct calculation of total molecular energy

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Abstract On the basis of density functional theory, we have investigated the intraatomic energy, electronegativity and hardness of an atom in a molecule and introduced the adjusting factor k for interatomic interactive energy terms in the total molecular energy expression. This allows not only to explain and treat more reasonably some problems but also increase greatly the computed precision and the applied areas. On these grounds, we have developed a new scheme of direct calculation of total molecular energy and applied it to calculations of about 100 molecules or groups of different sizes, The results obtained are in good agreement with those from ab initio calculations at the same level, The relative deviation of the two results is less than one thousandth. In addition, the new method presented here is advantage of simplicity, rapidness and easy perform as well. So that it provides an efficent and practical method for the energy calculations of macromolecular system.

Key words ELECTRONEGATIVITY

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