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键能的分子轨道理论研究2: 键能与Mulliken布居对键强度的 判断的比较

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摘要 用键能E~A~B和Mulliken布居对化学键强度的判别进行了分析比较。结果表明,
键能判据比Mulliken布居判据所得结论更符合实际情况。作为衡量原子间化学键强度的尺度,
不仅应考虑原子轨道间的布居因素,还应考虑分子轨道(或原子轨道)的能量因素。

关键词 键能 分子轨道理论 Mulliken布局 键强度

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Molecular orbital theory studies on bond energy 2: The comparison of the judgment of bond strength by bond energy and Mulliken's overlap population

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Abstract The comparison of the judgment of chemical bond strength by means of bond energy (E~A~B) and Mulliken's overlap population (M~A~B), has been discussed in this paper. The result shows that in most cases both E~A~B and M~A~B are consistent with experimental data qualitatively, with E~A~B being better than M~A~B on a quantitativebasis. In some cases, M~A~B is not compartible with experimental data even on a qualitative basis, whereas E~A~B is, both qualitatively and quatifatively. As a criterion for the character and the strength of chemical bond between atoms in a molecule, E~A~B is better than M~A~B, because both the overlap population factor between atomic orbitals and the energy factor of molecular or atomic orbitals are included in E~A~B.

Key words BOND ENERGY MOLECULAR ORBITAL THEORY

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