交叉学科

关于量子化学从头计算法及高斯98程序包计算结果的精度评述

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摘要

利用Gaussian98程序HF，MP2和G2方法和除cc-pVQZ外基组对大量分子进行了几何优化和单点能计算，并将结果与实验数据进行了比较。

The structure geometry and single point energy of small molecule are calculated by HF, MP2 and G2 methods and all base sets （except cc-pVQZ）available in Gaussian98 program software package. All these results are compared with the experimental data. It indicates that the molecule geometries optimized by G2 method in Gaussian98 are always in good accordance with experimental results, but the single point energy calculated by MP2 or G2 method differs some much from the experimental data. It is unsuitable to calculate the heat of formation through the single point energy of reactant calculated by methods and base sets provided by Gaussian98.

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