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HF,Ne等电子体系对内对间电子相关能的比较研究

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摘要 采用MELD程序ROHF－OPT1方法在MP2/6-311++G(d)水平上，计算了HF分子基态1^∑和Ne原子基态1^S的对内对间电子相关能，并对两等电子体系的对相关能进行了分析和比较，
深入研究两等电子体系对内对间相关能所具有的共同规律和存在的差异性，
通过比较说明分子内的化学键是影响电子相关能的重要因素之一。HF分子和Ne原子两体系三重激发和四重激发对体系电子相关能的贡献的计算结果表明高激发项对电子相关能的贡献在精确量子化学计算中是不可以忽略的。

关键词 氟化氢 氖 等电 等电子体系 对内电子相关 对间电子相关 电子相关能 量子化学

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Comparative study on the intrapair and interpair correlation energies of two isoelectronic systems HF and Ne

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Abstract The intrapair and interpair correlation energies of HF molecule and Ne atom are calculated at MP2/6-311 + + G(d) level by using ROHF-OPT1 method of MELD program. The pair correlation energies of these two isoelectronics systems are analyzed and compared. The generality and difference of intrapair and interpair correlation energies between these two isoelectronic system are investigated. One of the results of the comparison shows that the chemical bond of a molecule is one of the important factors to influence the electron correlation energy of the system. Our calculated results for the contribution of triple and quaduple excitations of these two systems indicate that the contribution of the higher-excitation termsis not negligible for the accurate calculations in quantum chemistry.

Key words HYDROGEN FLUORIDE NEON QUANTUM CHEMISTRY

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