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Higher Electric Multipole Moments for Some Polyatomic Molecules from Accurate SCF Calculations

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Abstract: Higher electric multipole moments for the ground-state electronic configuration of some polyatomic molecules, i.e. CH_4, NH_3, H_2O, were calculated from SCF-HFR wavefunctions using Slater-type orbital basis sets. The calculated results for electric multipole moments of these molecules are in good agreement with the theoretical and experimental ones.

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Key words: electric multipole moments, Slater-type orbitals, HFR approximation

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