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A new 3D grid method for accurate electronic structure calculation of polyatomic molecules: The Voronoi-cell finite difference method[1] SANG-KIL SON, SHIH-I CHU, Department of Chemistry, University of Kansas — We introduce a new computational method on *unstructured* grids in the three-dimensional (3D) spaces to investigate the electronic structure of polyatomic molecules. The Voronoi-cell finite difference (VFD) method realizes a simple discrete Laplacian operator on *unstructured* grids based on Voronoi cells and their natural neighbors. The feature of *unstructured* grids enables us to choose intuitive pictures for an optimal molecular grid system. The new VFD method achieves highly adaptability by the Voronoi-cell diagram and yet simplicity by the finite difference scheme. It has no limitation in local refinement of grids in the vicinity of nuclear positions and provides an explicit expression at each grid without any integration. This method augmented by *unstructured* molecular grids is suitable for solving the Schrödinger equation with the realistic 3D Coulomb potentials regardless of symmetry of molecules. For numerical examples, we test accuracies for electronic structures of one-electron polyatomic systems: linear H_2^+ and triangular H_3^{++}. We also extend VFD to the density functional theory (DFT) for many-electron polyatomic molecules.

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