ALL-ELECTRON CI VALENCE-BOND CALCULATION OF CARBIDE TRANSITION METAL MOLECULE: PdC

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All electron *ab initio* configuration interaction valence-bond (CIVB) calculations have been performed for the ground and first excited states of the PdC molecule. Equilibrium geometries, dissociation energies, rotational and vibrational constants, and potential energy surfaces are computed. The properties of the metal-carbon bond as a function of internuclear separation are investigated with an electron population analysis. The hyperfine structure constant, the Fermi contact term, is derived using electron spin densities at the nuclear sites. Our version of the CIVB method is based on the Hartree-Fock and Sturm's type nonorthogonal basis functions of each atom. Molecular wave functions consist of a large number of determinants constructed from these atomic orbitals. Reexpansion of atomic orbitals from one nuclear center to another is used to simplify many-center integral calculations.