11.S: Evaluating the Matrix Elements of N-electron Wavefunctions (Summary)

In all of the examples in Chapter 11, the Slater-Condon rules were used to reduce matrix elements of one- or two- electron operators between determinental functions to one- or two- electron integrals over the orbitals which appear in the determinants. In any **ab initio** electronic structure computer program there must exist the capability to form symmetry-adapted CSFs and to evaluate, using these SC rules, the Hamiltonian and other operators' matrix elements among these CSFs in terms of integrals over the Molecular Orbitals that appear in the CSFs. The Slater-Condon rules provide not only the tools to compute quantitative matrix elements; they allow one to understand in qualitative terms the strengths of interactions among CSFs. In the following section, the SC rules are used to explain why chemical reactions in which the reactants and products have dominant CSFs that differ by two spin-orbital occupancies often display activation energies that exceed the reaction endoergicity.