CORRELATION AND RELAXATION EFFECTS IN THE CALCULATION OF GENERALIZED AND OPTICAL OSCILLATOR STRENGTHS FOR INNER-SHELL EXCITATIONS OF MOLECULES

Carlos E. Bielschowsky

Instituto de Química, Departamento de Físico-Química, UFRJ
21910, Rio de Janeiro, Brazil

Relaxation effects are known to be important when an inner-shell electron is promoted to a valence-like orbital. In order to correctly consider this effect in the GOS and OOS calculations, non-orthogonal target wave functions should be used. In this work a biorthogonalization procedure is used to calculate the matrix elements between the non-orthogonal ground and excited target wave functions.

Another important effect in core electron excitations in molecules like N_2 and C_2H_2 is the description of the hole produced in this process. In the present work the excited state is constructed as a linear combination of wave-functions representing localized holes in each equivalent atom. They are calculated with the Generalized Multistructural Method (GMS). This description assures the proper symmetry of the molecule.

Other correlations may be important in the description of these processes , and are taken into account by the use of Configuration-Interaction (CI) wave-functions for both the ground and excited states (or each localized hole structure in the Multistructural case).

GOS and OOS results will be presented for several inner-shell discrete excitations in the N_2, C_2H_2 and CO_2 molecules.