PROGRAM LCOAO300

The directory includes the following files:

Howto.pdf:	This file
LCOAO300demo.exe:	Executable
Salflibc.dll:	A dynamic link library (needed by LCOAO300demo.exe)
Demo1inp.txt	Sample input file: Full $\pi-\pi*$ CIS calculation on the $C_{30}H_{16}$ PAH terrylene).
Demo1out.txt	Corresponding output file.
Demo2inp.txt	Sample input file: Canonical Ensemble $\pi-\pi*$ CIS calculation on the cyclopenta[*ef,kl*]heptalene radical cation).
Demo2out.txt	Corresponding output file.
LCOAO300.for	FORTRAN source code.
LCOAOpublications	A list of publications with applications of the LCOAO procedure

Description of the LCOAO procedure:

Jens Spanget-Larsen: ''The alternant hydrocarbon pairing theorem and all-valence electrons theory. An approximate LCOAO theory for the electronic absorption and MCD spectra of conjugated organic compound''

Part 1. *Croat. Chem. Acta* **59**, 711-717 (1986).

Part 2. *Theor. Chem. Acc.* **98**, 137-153 (1997).

Features:

Restricted Open Shell Formalism

Grand Canonical/Canonical mono-excited CI for open shell systems

MCD B-terms for π-π* transitions in planar compounds

This version of the program is a 100 atoms and 300 orbitals development version. It is not particularly user friendly!

System requirements

The LCOAO300 program was tested on a single computer running Windows 98 on which it was compiled, but it should run on any MS Windows, which can handle 32-bit. The present version of the LCOAO program was compiled by Bjarke K. V. Hansen, Dec. 2005.

Running the program

Run LCOAO300demo.exe and it will ask for the names of an input file (see below) and an output file (the output file must not previously exist).

Note: Input and output filenames should at a maximum contain 8+3 characters (F8.3)

Input file:

First Line: Text heading (a maximum of 72 characters including spaces)

Second line: 6 integers (each integer read as 3 characters [I3]):

a. Charge of the molecule

b. Number of electrons in partly occupied MOs (defaults: 0 for even and 1 for odd number of electrons).

c. Number of partly occupied MOs (defaults: 0 for even and 1 for odd number of electrons).

d. If this integer is above 0, only π-π^* configurations are included in CI. The molecular plane assumed to be X,Y.

e. A print code: 0 to 4 generates minimum to maximum printout.

f. Number of HOMOs and number of LUMOs printed (0 = default of 32)

Following lines (one line per atom) contain atomic numbers and coordinates:

a. Atomic number (two characters [I2])

b. X coordinate (13 characters with decimal point at the 7th positions [F13.6])

c. Y coordinate (15 characters with decimal point at the 9th position [F15.6])

d. Z coordinate (15 characters with decimal point at the 9th position [F15.6])

One blank line terminates the input of atomic coordinates.

Final line: 6 integers (each read as 3 characters [I3]) and one real number (read as 10 characters with decimal point at the 5th position [F10.5]).

a. CI calculation is performed if this integer is equal to 1, otherwise not.

b. N_A, the number of highest occupied valence MOs considered in CI (default 10).

c. N_B, the number of lowest unoccupied valence MOs considered in CI (default 10).

Note: The number of lowest unoccupied and highest occupied MO's define an all-valence MO 'window'. In general, the number of singly excited configurations generated are equal to the product of the number of lowest unoccupied and highest occupied MO's ($N_A* N_B$).

If only π-π^* configurations are included in the CI (see above), the number of configurations is the number of π's among the N_A's times the number of π's among the N_B's.

d. Dummy.

e. Dummy.

f. MCD B-terms for π-π^* states are computed if this integer is above zero and if only π-π^* configurations are included in CI. Integers 1-5 generate min-max MCD printout. The MCD calculation is truncated to a 100×100 matrix.

g. Cut-off limit in eV for the excited cfg. energy (default 15).