Using MOPAC instead of extdh

(1) Prepare extdh.dat. Do not include S 3d orbitals.

(2) Run extdhg3.exe to make hdat.dat and hdat1.wob for MOPAC inputs in addition to the ordinary extdh results: hadt.d1 and (if designated) fort.10.

(3) Start MOPAC, read hdat.dat from [File][Open].

[Edit][Edit Z-Matrix] means the following indications:

AM1 Carry out AM1 calculation.

1SCF One SCF calculation. Geometry optimization is not done.

Vectors Molecular orbitals are stored in hdat.wob. ±16 Orbitals around the HOMO and LUMO.

XYZ Rectangular coordinates.

(4) [Calculation][Start] to do the MO calculation.

(5) Using [Properties][Molecular orbitals], you can see the molecular orbitals.

To store the molecular orbital image, push [PrtSc] bottom (print screen bottom at the right top of the keyboard), and start the [Paint] tool from the startup menu. Copy the image by using [ctrl]c. Select the necessary region, and copy it by [ctrl]c. Copy to a (for example) word file by [ctrl]v.

(6) It is recommended to compare the extdh MOs with MOPAC MOs. In order to do so,

Change hdat.wob to hdat2.wob.

Change hdat1.wob to hdat.wob.

Repeat [Properties][Molecular orbitals] from MOPAC.

(7) Run trpacg.exe, which read molecular orbitals from hdat.out to output them to fort.50.

(8) Usually trpacg coverts HOMO and LUMO to fort.50, so default run of scal reads the HOMO.

To use the LUMO, change the order of HOMO and LUMO in fort.50. trpacg1 converts from HOMO - 4 to LUMO + 4 into fort.50.