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- This file should help in the friendly user input maker of COLUMBUS.
- The basis set used for carbon and hydrogen atoms is the aug-cc-pVDZ.
- The point group used is the D_{2h} .
- For more details, please see the file “tutorial.pdf” on the folder “tutorial_and_hands_on_columbus”.

In the inputs, we will use the following informations:

		IRREP							
		ag	b3u	b2u	b1g	b1u	b2g	b3g	au
SCF	DOCC	6	5	4	3	1	1	1	0
	OPSH	0	0	0	0	0	0	0	0
MCSCF	DOCC	6	5	4	3	0	0	0	0
	RAS	0	0	0	0	0	0	0	0
	CAS	0	0	0	0	3	1	1	1
	AUX	0	0	0	0	0	0	0	0
MRCI	FC	2	2	1	1	0	0	0	0
	FV	0	0	0	0	0	0	0	0
-----		-----							
		DOCC	4	3	3	2	0	0	0
		ACT	0	0	0	0	3	1	1
		AUX	0	0	0	0	0	0	0
-----		-----							
		INT	4	3	3	2	3	1	1

State	Multiplicity	N. electrons	Symmetry
1	1	42	Ag
2	1	42	B2u
3	3	42	B3u

Number of distinct rows (DRTs):	3
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CASSCF calculation

Step 1. Integrals

I) Enter in the folder “C6H6_CAS_6-6_d2h_SP” and extract the files in the folder inputs with:

```
tar -xjf inputs-and-logs.tar
```

II) Make sure of copy the save_geom2etry file (unique atoms in the COLUMBUS format) to geom file:

```
cp save_geometry geom
```

III) Then run the following line:

```
$COLUMBUS/colinp
```

IV) Follow the steps:

COLUMBUS INPUT FACILITY

main menu options

- > 1) Integral program input (for argos/dalton/turbocol/molcas) → press enter
 2) SCF input
 3) MCSCF input
 4) CI input
 5) Set up job control
 6) Utilities
 7) Exit the input facility

Run the preparation program (prepin)? (y|n) y

Input for DALTON (1) or MOLCAS (2): 1

File inpcol exists. Do you want to overwrite it? y

Enter the point group symmetry: d2h

Name of the file containing the cartesian coordinates
 of the unique atoms (COLUMBUS format): geom

Number of atoms = 4

Sum formula: H2 C2

Show only basis sets containing the following string:
 (e.g. 6-31g, cc-pv - leave empty to show all basis sets)

cc-pv and press enter

-- Set basis set --

- 1: cc-pvdz (4s,1p)->[2s,1p]
- 3: aug-cc-pvdz
- 4: aug'-cc-pvdz (without p function in aug-set)
- 5: d'-aug-cc-pvdz (without p function in d-set)
- 6: d-aug-cc-pvdz
- 7: cc-pvtz(5s,2p,1d)->[3s,2p,1d]
- 8: aug'-cc-pvtz (without d function in aug-set)
- 9: aug-cc-pvtz
- 10: d'-aug'-cc-pvtz (without d function in aug- and d-set)
- 11: d''-aug'-cc-pvtz (without d in aug-set and without p and d in d-set)
- 12: aug-cc-pvtz(-d) (without any d functions)
- 13: cc-pvqz(6s,3p,2d,1f)->[4s,3p,2d,1f]
- 14: cc-pv5z(8s,4p,3d,2f,1g)->[5s,4p,3d,2f,1g]
- 15: diffuse functions for cc-pvdz(1s,1p)
- 16: diffuse functions for cc-pvtz(1s,1p,1d)
- 17: diffuse functions for cc-pvqz(1s,1p,1d,1f)
- 18: diffuse functions for cc-pv5z(1s,1p,1d,1f,1g)
- 0: Other library

Select the basis set for atom H: 3

Until now you've set the following basis sets:

H :: aug-cc-pvdz

- 1: cc-pvdz(9s,4p,1d)->[3s,2p,1d]
- 2: aug-cc-pvdz
- 3: aug'-cc-pvdz (without d function in aug-set)
- 4: d'-aug-cc-pvdz (without d function in d-set)
- 5: d-aug-cc-pvdz
- 6: cc-pvtz(10s,5p,2d,1f)->[4s,3p,2d,1f]
- 7: aug'-cc-pvtz (without f function in aug-set)
- 8: aug-cc-pvtz
- 9: d'-aug'-cc-pvtz (without f function in aug- and d-set)
- 10: d''-aug'-cc-pvtz (without f in aug-set and without f and d in d-set)
- 11: cc-pvqz(12s,6p,3d,2f,1g)->[5s,4p,3d,2f,1g]
- 12: cc-pv5z(14s,8p,4d,3f,2g,1h)->[6s,5p,4d,3f,2g,1h]
- 13: diffuse functions for cc-pvdz(1s,1p,1d)
- 14: diffuse functions for cc-pvtz(1s,1p,1d,1f)
- 15: diffuse functions for cc-pvqz(1s,1p,1d,1f,1g)
- 16: diffuse functions for cc-pv5z(1s,1p,1d,1f,1g,1h)
- 38: PAC-ECP basis; Pitzer group; cc-pvdz (4s4p1d)/[3s3p1d]/[2s2p1d]
- 0: Other library

Select the basis set for atom C: 2

Reorder geom file for geometry optimization and orbital print out? (y) **press enter**

Normal termination of prepinp. See result in inpcol.

Program Iargos
Argos and Dalton Input Program
version date 03-oct-01

```
*****
**  PROGRAM:          IARGOS      **
**  PROGRAM VERSION:   5.8        **
**  DISTRIBUTION VERSION: 5.9.a    **
*****
```

Defaults are in angle brackets <like this>.
Alphabetic responses may be abbreviated to as few letters
as desired, as long as the choice is still unique.
Whenever "PROCEED" is offered as an option,
it means to continue to the next item.

Would you like to do an interactive input? <NO> **press enter**

Do you want to adjust the remaining input files for the new basis set? (y|n) **y**

Adjusting Files for the new basis set:

Beware that this may not work in complicated cases!
In particular frozen virtual orbitals are not supported.

Files adjusted:

Files removed:

Finished!

Press return to continue. **press enter**

Step 2. SCF calculation

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
 -> 2) SCF input → [press enter](#)
 3) MCSCF input
 4) CI input
 5) Set up job control
 6) Utilities
 7) Exit the input facility

Found file makscfky. Use it for an automatic input? (y/n) [n](#)

```
*****
**  PROGRAM:      MAKSCF      **
**  PROGRAM VERSION:  5.5.1    **
**  DISTRIBUTION VERSION: 5.9.a  **
*****
```

Symmetry orbital summary:

Molecular symmetry group: d2h

Symm.blocks:	1	2	3	4	5	6	7	8
Symm.labels:	ag	b3u	b2u	b1g	b1u	b2g	b3g	au
Number of basis functions:	39	39	30	30	16	16	11	11

Do you want a closed shell calculation ? <YES> [press enter](#)

Input the no. of doubly occupied orbitals for each irrep, DOCC:
[6 5 4 3 1 1 1 0](#)

The orbital occupation is:

	ag	b3u	b2u	b1g	b1u	b2g	b3g	au
DOCC	6	5	4	3	1	1	1	0
OPSH	0	0	0	0	0	0	0	0

Is this correct? <YES> [press enter](#)

Would you like to change the default program parameters? <NO> [press enter](#)

Would you like to change the default program parameters? <NO>

Input a title: <Default SCF Title>

-->[press enter](#)

Step 3. MCSCF

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- > 3) MCSCF input press enter
- 4) CI input
- 5) Set up job control
- 6) Utilities
- 7) Exit the input facility

MCSCF WAVE FUNCTION DEFINITION

=====

(for an explanation see the COLUMBUS documentation and tutorial)

Freeze orbitals prior to MCSCF (no gradients available) [y|n] nprepare input for no(0), CI(1), MCSCF(2), SA-MCSCF(3) analytical gradient 0Skip DRT input (y|n) nEnter number of DRTS [1-8] 3number of electrons for DRT #1 (nucl. Charge: 42) 42multiplicity for DRT #1 1spatial symmetry for DRT #1 1excitation level (cas,ras)->aux 0excitation level ras->(cas,aux) 0number of electrons for DRT #2 (nucl. Charge: 42) 42multiplicity for DRT #2 1spatial symmetry for DRT #2 3excitation level (cas,ras)->aux 0excitation level ras->(cas,aux) 0number of electrons for DRT #2 (nucl. Charge: 42) 42multiplicity for DRT #3 3

spatial symmetry for DRT #3 2

excitation level (cas,ras)->aux 0

excitation level ras->(cas,aux) 0

count order (bottom to top): DOCC - RAS - CAS - AUX

irreps ag b3u b2u b1g b1u b2g b3g au

basis fcts 39 39 30 30 16 16 11 11

number of doubly occupied orbitals per irrep 6 5 4 3 0 0 0 0

number of CAS orbitals per irrep 0 0 0 0 3 1 1 1

Apply add. group restrictions for DRT 1 [y|n] n

Apply add. group restrictions for DRT 2 [y|n] n

Apply add. group restrictions for DRT 3 [y|n] n

Convergence

1. Iterations #iter [100] #miter [50] #ciiter [300]
2. Thresholds knorm [1.e-4] wnorm [1.e-4] DE [1.e-8]
3. HMC-matrix build explicitly [n]
diagonalize iteratively [y]
4. Miscellaneous quadratic cnvg. [y] from #iter [5]
... only with wnorm < [1.e-3]

Resolution (none|NO|QAA|FAA) RAS [QAA] CAS [QAA] AUX [QAA]

State-averaging

DRT 1: #states [1] weights[1]
 DRT 2: #states [2] weights[1]
 DRT 3: #states [2] weights[1]
 transition moments / non-adiabatic couplings [N]

FINISHED [y]

Editing: left/right, 'delete'; Switching fields: 'Tab', up/down

Help is available through selecting a field and pressing 'return'.

Indicate completion by selecting 'Finished' and pressing 'return'.

Step 4. Setting the job control

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- 4) CI input
- > 5) Set up job control press enter
- 6) Utilities
- 7) Exit the input facility

COLUMBUS INPUT FACILITY

submenu 1: type of calculation

- > 1) Job control for single point or gradient calculation press enter
- 2) Potential energy curve for one int. coordinate
- 3) Vibrational frequencies and force constants
- 4) Exit

You have an existing job control file. Discard it? (y|n) y

COLUMBUS INPUT FACILITY

submenu 1.1: job control setup

- > 1) single point calculation press enter
- 2) geometry optimization with GDIIS
- 3) geometry optimization with SLAPAF
- 4) saddle point calculation (local search - GDIIS)
- 5) stationary point calculation (global search - RGF)
- 6) optimization on the crossing seam or ISC (GDIIS)
- 7) optimization on the crossing seam (POLYHES)
- 8) Exit

COLUMBUS INPUT FACILITY

submenu 1.1.1: single point calculations

- > 1) (Done with selections)
- 2) [X] SCF
- 3) [X] MCSCF

- 4) ☐ transition moments for MCSCF
- 5) ☐ MR-CISD (serial operation)
- 6) ☐ MR-CISD (parallel operation)
- 7) ☐ SO-CI coupled to non-rel. CI
- 8) ☐ one-electron properties for all methods
- 9) ☐ transition moments for MR-CISD
- 10) ☐ single point gradient
- 11) ☐ nonadiabatic couplings (and/or gradients)
- 12) ☐ $\langle L \rangle$ value calculation for MR-CISD
- 13) ☒ convert MOs into molden format
- 14) ☐ get starting MOs from a higher symmetry
- 15) ☐ finite field calculation for all methods
- 16) ☐ include point charges
- 17) ☐ extended MOLCAS interface

In the next panels, select “Exit” until finishing COLINP execution.

Step 5. Run COLUMBUS

[runc -m 20000 > runls](#)

Run directly or use a submission file (highly recommended).

Step 6. Check the results

To check the results, go to the folder LISTINGS and follow the “tutorial.pdf”.

MRCISD calculation (Ground State: 1A_g)

Step 1. Prepare the files

I) Go to the folder “C6H6_MRCISD_6-6_d2h_SP/singlet_Ag/inputs” and extract the file “inputs-and-logs.tar”:

```
tar -xjf inputs-and-logs.tar
```

II) Then run the colinp file and follow the steps bellow

```
$COLUMBUS/colinp
```

Step 2. MRCI input

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- > 4) CI input press enter
- 5) Set up job control
- 6) Utilities
- 7) Exit the input facility

CI WAVE FUNCTION DEFINITION

=====

In the Distinct Row Table(s) (DRT) the wave functions for the electronic states to be calculated are defined. The CI wave function is defined in terms of single- and double excitations with respect to a set of reference configurations. Use one DRT for each class of states (e.g. one DRT for each symmetry). In the multiple-DRT case one unified DRT is constructed for the computation of transition moments. For more information on DRTs and the Graphical Unitary Group Approach (GUGA)

see the COLUMBUS Program Documentation and references therein.

Orbital classification scheme:

fc: frozen core (not correlated)

docc: reference doubly-occupied

active: variable occupation in the reference configurations

auxiliary: limited reference occupation

external: reference-unoccupied

fv: frozen virtual

internal = docc + active + auxiliary

Note: additional group restrictions available (see COLUMBUS documentation)

press return to continue press enter

CIDRT INPUT FACILITY
Version 0.992 - mar 2016

- > 1) Def. of CI wave function - one-DRT case press enter
 2) Def. of CI wave function - multiple-DRT case (transition moments)
 3) Def. of CI wave function - independent multiple-DRTs (intersystem crossings)
 4) Skip DRT input (old input files in the current directory)

Do you want to compute gradients or non-adiabatic couplings? [y|n] n

count order (bottom to top): fc-docc-active-aux-extern-fv
 irreps ag b3u b2u b1g b1u b2g b3g au
 # basis fcts 39 39 30 30 16 16 11 11
 Spin-Orbit CI [y|n] n

Enter the multiplicity 1

Enter the number of electrons 42

Enter the molec. spatial symmetry 1

number of frozen core orbitals per irrep 2 2 1 1 0 0 0 0

number of frozen virt. orbitals per irrep 0 0 0 0 0 0 0 0

number of internal(=docc+active+aux) orbitals per irrep 4 3 3 2 3 1 1 1

ref doubly occ orbitals per irrep 4 3 3 2 0 0 0 0

auxiliary internal orbitals per irrep 0 0 0 0 0 0 0 0

Enter the excitation level (0,1,2) 2

exc.level:2

Generalized interacting space restrictions [y|n] y

exc.level:2 gen.space:y

Enter the allowed reference symmetries 1

exc.level:2 gen.space:y allowed ref. syms:1

Apply additional group restrictions for DRT [y|n] n

Choose CI program: sequential ciudg [1]; parallel ciudg[2] 1

CIUDGIN INPUT MENU DRT# 1

Type of calculation: CI [Y] AQCC [N] AQCC-LRT [N]
 LRT shift: LRTSHIFT [0]
 State(s) to be optimized NROOT [1] ROOT TO FOLLOW [0]
 Reference space diagonalization INCORE[Y] NITER []
 RTOL []
 Bk-procedure: NITER [1] MINSUB [1] MAXSUB [6]
 RTOL [1e-3]
 CI/AQCC procedure: NITER [20] MINSUB [1] MAXSUB [6]
 RTOL [1e-3]
 FINISHED [y]

Editing: left/right, "delete"; Switching fields: "Tab", up/down
 Help is available through selecting a field and pressing "return".
 Indicate completion by selecting "Finished" and pressing "Return".

Step 3. Setting the job control

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- 4) CI input
- > 5) Set up job control press enter
- 6) Utilities
- 7) Exit the input facility

COLUMBUS INPUT FACILITY

submenu 1: type of calculation

- > 1) Job control for single point or gradient calculation press enter
- 2) Potential energy curve for one int. coordinate
- 3) Vibrational frequencies and force constants
- 4) Exit

You have an existing job control file. Discard it? (y|n) y

COLUMBUS INPUT FACILITY

submenu 1.1: job control setup

- > 1) single point calculation press enter
- 2) geometry optimization with GDIIS
- 3) geometry optimization with SLAPAF
- 4) saddle point calculation (local search - GDIIS)
- 5) stationary point calculation (global search - RGF)
- 6) optimization on the crossing seam or ISC (GDIIS)
- 7) optimization on the crossing seam (POLYHES)
- 8) Exit

COLUMBUS INPUT FACILITY

submenu 1.1.1: single point calculations

- > 1) (Done with selections)
- 2) ☐ SCF
- 3) ☒ MCSCF
- 4) ☐ transition moments for MCSCF
- 5) ☒ MR-CISD (serial operation)
- 6) ☐ MR-CISD (parallel operation)
- 7) ☐ SO-CI coupled to non-rel. CI
- 8) ☐ one-electron properties for all methods
- 9) ☐ transition moments for MR-CISD
- 10) ☐ single point gradient
- 11) ☐ nonadiabatic couplings (and/or gradients)
- 12) ☐ <L> value calculation for MR-CISD
- 13) ☒ convert MOs into molden format
- 14) ☐ get starting MOs from a higher symmetry
- 15) ☐ finite field calculation for all methods
- 16) ☐ include point charges
- 17) ☐ extended MOLCAS interface

In the next panels, select “Exit” until finishing COLINP execution.

Step 4. Run COLUMBUS

runc -m 20000 > runls

Run directly or use a submission file (highly recommended).

MRCISD calculation (2 Singlets $^1B_{2u}$)

Step 1. Prepare the files

I) Go to the folder “C6H6_MRCISD_6-6_d2h_SP/singlet_Ag/inputs” and extract the file “inputs-and-logs.tar”:

```
tar -xjf inputs-and-logs.tar
```

II) Then run the colinp file and follow the steps bellow

```
$COLUMBUS/colinp
```

Step 2. MRCI input

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- > 4) CI input press enter
- 5) Set up job control
- 6) Utilities
- 7) Exit the input facility

CI WAVE FUNCTION DEFINITION

=====

In the Distinct Row Table(s) (DRT) the wave functions for the electronic states to be calculated are defined. The CI wave function is defined in terms of single- and double excitations with respect to a set of reference configurations. Use one DRT for each class of states (e.g. one DRT for each symmetry). In the multiple-DRT case one unified DRT is constructed for the computation of transition moments. For more information on DRTs and the Graphical Unitary Group Approach (GUGA)

see the COLUMBUS Program Documentation and references therein.

Orbital classification scheme:

fc: frozen core (not correlated)

docc: reference doubly-occupied

active: variable occupation in the reference configurations

auxiliary: limited reference occupation

external: reference-unoccupied

fv: frozen virtual

internal = docc + active + auxiliary

Note: additional group restrictions available (see COLUMBUS documentation)

press return to continue press enter

CIDRT INPUT FACILITY
Version 0.992 - mar 2016

- > 1) Def. of CI wave function - one-DRT case press enter
 2) Def. of CI wave function - multiple-DRT case (transition moments)
 3) Def. of CI wave function - independent multiple-DRTs (intersystem crossings)
 4) Skip DRT input (old input files in the current directory)

Do you want to compute gradients or non-adiabatic couplings? [y|n] n

count order (bottom to top): fc-docc-active-aux-extern-fv
 irreps ag b3u b2u b1g b1u b2g b3g au
 # basis fcts 39 39 30 30 16 16 11 11
 Spin-Orbit CI [y|n] n

Enter the multiplicity 1

Enter the number of electrons 42

Enter the molec. spatial symmetry 3

number of frozen core orbitals per irrep 2 2 1 1 0 0 0 0

number of frozen virt. orbitals per irrep 0 0 0 0 0 0 0 0

number of internal(=docc+active+aux) orbitals per irrep 4 3 3 2 3 1 1 1

ref doubly occ orbitals per irrep 4 3 3 2 0 0 0 0

auxiliary internal orbitals per irrep 0 0 0 0 0 0 0 0

Enter the excitation level (0,1,2) 2

exc.level:2

Generalized interacting space restrictions [y|n] y

exc.level:2 gen.space:y

Enter the allowed reference symmetries 3

exc.level:2 gen.space:y allowed ref. syms:3

Apply additional group restrictions for DRT [y|n] n

Choose CI program: sequential ciudg [1]; parallel ciudg[2] 1

CIUDGIN INPUT MENU DRT# 1

Type of calculation: CI [Y] AQCC [N] AQCC-LRT [N]
 LRT shift: LRTSHIFT [0]
 State(s) to be optimized NROOT [2] ROOT TO FOLLOW [0]
 Reference space diagonalization INCORE[Y] NITER []
 RTOL [1e-3,1e-3,]
 Bk-procedure: NITER [1] MINSUB [2] MAXSUB [7]
 RTOL [1e-3,1e-3,]
 CI/AQCC procedure: NITER [40] MINSUB [4] MAXSUB [7]
 RTOL [1e-3,1e-3,]
 FINISHED [y]

Editing: left/right, "delete"; Switching fields: "Tab", up/down
 Help is available through selecting a field and pressing "return".
 Indicate completion by selecting "Finished" and pressing "Return".

Do not select any transition moments for this moment.

Step 3. Setting the job control

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- 4) CI input
- > 5) Set up job control press enter
- 6) Utilities
- 7) Exit the input facility

COLUMBUS INPUT FACILITY

submenu 1: type of calculation

- > 1) Job control for single point or gradient calculation press enter
- 2) Potential energy curve for one int. coordinate
- 3) Vibrational frequencies and force constants
- 4) Exit

You have an existing job control file. Discard it? (y/n) **y**

COLUMBUS INPUT FACILITY

submenu 1.1: job control setup

- > 1) single point calculation **press enter**
- 2) geometry optimization with GDIIS
- 3) geometry optimization with SLAPAF
- 4) saddle point calculation (local search - GDIIS)
- 5) stationary point calculation (global search - RGF)
- 6) optimization on the crossing seam or ISC (GDIIS)
- 7) optimization on the crossing seam (POLYHES)
- 8) Exit

COLUMBUS INPUT FACILITY

submenu 1.1.1: single point calculations

- > 1) (Done with selections)
- 2) ☐ SCF
- 3) ☒ MCSCF
- 4) ☐ transition moments for MCSCF
- 5) ☒ MR-CISD (serial operation)
- 6) ☐ MR-CISD (parallel operation)
- 7) ☐ SO-CI coupled to non-rel. CI
- 8) ☐ one-electron properties for all methods
- 9) ☐ transition moments for MR-CISD
- 10) ☐ single point gradient
- 11) ☐ nonadiabatic couplings (and/or gradients)
- 12) ☐ <L> value calculation for MR-CISD
- 13) ☒ convert MOs into molden format
- 14) ☐ get starting MOs from a higher symmetry
- 15) ☐ finite field calculation for all methods
- 16) ☐ include point charges
- 17) ☐ extended MOLCAS interface

In the next panels, select “Exit” until finishing COLINP execution.

Step 4. Run COLUMBUS

runc -m 20000 > runls

Run directly or use a submission file (highly recommended).

MRCISD calculation (2 Triplets $^3B_{3u}$)

Step 1. Prepare the files

I) Go to the folder “C6H6_MRCISD_6-6_d2h_SP/singlet_Ag/inputs” and extract the file “inputs-and-logs.tar”:

```
tar -xjf inputs-and-logs.tar
```

II) Then run the colinp file and follow the steps bellow

```
$COLUMBUS/colinp
```

Step 2. MRCI input

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- > 4) CI input press enter
- 5) Set up job control
- 6) Utilities
- 7) Exit the input facility

CI WAVE FUNCTION DEFINITION

=====

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see the COLUMBUS Program Documentation and references therein.

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fc: frozen core (not correlated)

docc: reference doubly-occupied

active: variable occupation in the reference configurations

auxiliary: limited reference occupation

external: reference-unoccupied

fv: frozen virtual

internal = docc + active + auxiliary

Note: additional group restrictions available (see COLUMBUS documentation)

press return to continue press enter

CIDRT INPUT FACILITY
Version 0.992 - mar 2016

- > 1) Def. of CI wave function - one-DRT case press enter
 2) Def. of CI wave function - multiple-DRT case (transition moments)
 3) Def. of CI wave function - independent multiple-DRTs (intersystem crossings)
 4) Skip DRT input (old input files in the current directory)

Do you want to compute gradients or non-adiabatic couplings? [y|n] n

count order (bottom to top): fc-docc-active-aux-extern-fv
 irreps ag b3u b2u b1g b1u b2g b3g au
 # basis fcts 39 39 30 30 16 16 11 11
 Spin-Orbit CI [y|n] n

Enter the multiplicity 3

Enter the number of electrons 42

Enter the molec. spatial symmetry 2

number of frozen core orbitals per irrep 2 2 1 1 0 0 0 0

number of frozen virt. orbitals per irrep 0 0 0 0 0 0 0 0

number of internal(=docc+active+aux) orbitals per irrep 4 3 3 2 3 1 1 1

ref doubly occ orbitals per irrep 4 3 3 2 0 0 0 0

auxiliary internal orbitals per irrep 0 0 0 0 0 0 0 0

Enter the excitation level (0,1,2) 2

exc.level:2

Generalized interacting space restrictions [y|n] y

exc.level:2 gen.space:y

Enter the allowed reference symmetries 2

exc.level:2 gen.space:y allowed ref. syms:3

Apply additional group restrictions for DRT [y|n] n

Choose CI program: sequential ciudg [1]; parallel ciudg[2] 1

CIUDGIN INPUT MENU DRT# 1

Type of calculation: CI [Y] AQCC [N] AQCC-LRT [N]
 LRT shift: LRTSHIFT [0]
 State(s) to be optimized NROOT [2] ROOT TO FOLLOW [0]
 Reference space diagonalization INCORE[Y] NITER []
 RTOL [1e-3,1e-3,]
 Bk-procedure: NITER [1] MINSUB [2] MAXSUB [7]
 RTOL [1e-3,1e-3,]
 CI/AQCC procedure: NITER [40] MINSUB [4] MAXSUB [7]
 RTOL [1e-3,1e-3,]
 FINISHED [y]

Editing: left/right, "delete"; Switching fields: "Tab", up/down
 Help is available through selecting a field and pressing "return".
 Indicate completion by selecting "Finished" and pressing "Return".

Do not select any transition moments for this moment.

Step 3. Setting the job control

COLUMBUS INPUT FACILITY

main menu options

- 1) Integral program input (for argos/dalton/turbocol/molcas)
- 2) SCF input
- 3) MCSCF input
- 4) CI input
- > 5) Set up job control press enter
- 6) Utilities
- 7) Exit the input facility

COLUMBUS INPUT FACILITY

submenu 1: type of calculation

- > 1) Job control for single point or gradient calculation press enter
- 2) Potential energy curve for one int. coordinate
- 3) Vibrational frequencies and force constants
- 4) Exit

You have an existing job control file. Discard it? (y/n) **y**

COLUMBUS INPUT FACILITY

submenu 1.1: job control setup

- > 1) single point calculation **press enter**
- 2) geometry optimization with GDIIS
- 3) geometry optimization with SLAPAF
- 4) saddle point calculation (local search - GDIIS)
- 5) stationary point calculation (global search - RGF)
- 6) optimization on the crossing seam or ISC (GDIIS)
- 7) optimization on the crossing seam (POLYHES)
- 8) Exit

COLUMBUS INPUT FACILITY

submenu 1.1.1: single point calculations

- > 1) (Done with selections)
- 2) ☐ SCF
- 3) ☒ MCSCF
- 4) ☐ transition moments for MCSCF
- 5) ☒ MR-CISD (serial operation)
- 6) ☐ MR-CISD (parallel operation)
- 7) ☐ SO-CI coupled to non-rel. CI
- 8) ☐ one-electron properties for all methods
- 9) ☐ transition moments for MR-CISD
- 10) ☐ single point gradient
- 11) ☐ nonadiabatic couplings (and/or gradients)
- 12) ☐ <L> value calculation for MR-CISD
- 13) ☒ convert MOs into molden format
- 14) ☐ get starting MOs from a higher symmetry
- 15) ☐ finite field calculation for all methods
- 16) ☐ include point charges
- 17) ☐ extended MOLCAS interface

In the next panels, select “Exit” until finishing COLINP execution.

Step 4. Run COLUMBUS

runc -m 20000 > runls

Run directly or use a submission file (highly recommended).