Input Description

of

MOLFDIR

A relativistic Dirac-Fock-CI
program package
developed at the
University of Groningen

Contributors:
P.J.C. Aerts, O. Visser
L. Visscher, H. Merenga
W.A. de Jong, M. Pernpointer
W.C. Nieuwpoort

Department of Chemistry, Chemical Physics, Theoretical Chemistry Group
Nijenborgh 4, 9747 AG, GRONINGEN (The Netherlands)
E-Mail for information and questions: H.B.Broer-Braam@chem.rug.nl

Input description MOLFDIR

Task : Generation of double group symmetry adapted functions. Use of groupchain to make functions which are adapted to the appropriate pointgroup and to the highest abelian subgroup thereof. Pointgroups must be subgroups of O_h.

Necessary files : none
Optional files : none
Produces files : MFD1OUT, MFDSYMC, MFDHER, MOLECULE.INP, DIRAC.INP, MFDAREP
Scratch files : none

&GENERAL
TWOC: Use two-component formalism (F)

&MOLFDIR: Namelist used as keyword to find the formatted MOLFDIR input.
NAME: Comment line. ('No title given')
GROUPN: 1-3 Pointgroupnames (3A3) (' ',' ',' ')
(group 2,3 to designate the groupchain)

NEQNUC: Number of unique Nuclei (0)
IDEFNUC: Use the MOLFDIR (1) or the GRASP (2) model to calculate the exponent for the finite nucleus (2)
AUANG: Atomic Units or ANGstrom (AU)
IFRLC: Remove non Y_{lm} combinations : (0)
0 : Yes for Large Component; Small Component s-combination form g's only.
1 : Yes for Large and Small Component.
2 : Yes for Large; No for Small Component.
-1 : No for Large and Small Component.
PRNT Print option. (0)
0 : Default output
-1 : 0 minus spinor transformation table and list of exponents
-2 : only geometry and number of basisfunctions per symmetry repr.
1 : 0 plus form of the symmetry adapted spinors
2 : 1 plus unitary rotation matrices, plus group multiplication table, plus contraction coefficients (in GENBAS format), plus ....
SUPDCK Suppress Distance Check (F)
Use (at own risk) for calculations with R smaller than 0.1 Bohr.
AREP Perform 2-component calculation using ECP and spin-orbit potentials (F)
PROPERTY When computing properties, this sets some options similar to DIRAC (F)

Do i = 1, NeqNuc
Card 1 : CentrN, X, Y, Z, Charge, NucExp (A2, 5F12.8)

- CentrN : Chemical symbol of the atom.
- X, Y, Z : Coordinates of the atom.
- Charge : Charge of the atom
- NucExp : Nuclear exponent (Gaussian model for finite nuclei).

The default charge and nuclear exponent are read from the basis set files. If the basis is not read from file, CentrN will be used to look them up in a table. The default charges and exponents may be altered by specifying Charge and NucExp. Ghost bases are to be specified with CentrN "GH".

Enddo

Large Component :
Do i = 1, NeqNuc
Card 2 : Basfil (A80)

Options : 1) Basfil.eq.'UNCONTRACTED'

Card 3 : Type (i) (5(3x, A))
Card 4 : Ntype (i), NVprim(i) (10I4)

- Type (i) : L-Type functions (e.g. S P D).
- Ntype(i) : Number of exponents for each L-Type.
- NVprim (i) : Number of exponents designated valence.

Do j =1 , Ntype(i)

Card 5 : Alpha (j) (free format)

- Alpha : Exponent of the Gaussian.

Enddo

2) Basfil.eq.'CONTRACTED'

Card 3 :	Type (i)	(5(3x, A))
Card 4 :	Ntype (i), NVprim(i)	(10I4)
Card 5 :	Norb (i), NVcontr(i)	(5I4)

- Type (i) : L-Type functions (e.g. S P D).
- Ntype(i) : Number of exponents for each L-Type.
- NVprim (i): Number of exponents designated valence.
- Norb (i) : Number of contracted functions for each L-Type.
- NVcontr (i): Number of contracted functions designated valence.

Do j =1 , Ntype(i)

Card 6 : Alpha(j), (Coef(j,jc), jc = 1, Norb(i)) (F16.8, 5F11.8)

- Alpha : Exponent of the Gaussian.
- Coef : Coefficient of this gaussian in (general) contracted function jc

Enddo

3) Basfil is the name of a file which contains a bassisset, generated by the program GENBAS or GRASPG.

4) Basfil.eq.'EVEN'

Card 3 :	Type (i)	(5(3x, A))
Card 4 :	Ntype (i), NVprim(i)	(10I4)

- Type (i) : L-Type functions (e.g. S P D).
- Ntype(i) : Number of exponents for each L-Type.
- NVprim (i) : Number of exponents designated valence.

Do j =1 , Ntype(i)

Card 5 : Evenct, Evenrat (free format)

- Evenct : Center of even tempered set of exponents
- Evenrat : Ratio of expansion

Enddo

5) Basfil.eq.'EMPTY'. The number of functions in the large component basis of the atom is zero. No additional input is required.

Enddo

Small Component (for TWOC=T no input of small component basisset required):

Do i = 1, NeqNuc

Card 2 : Basfil (A80)

Options : 1) 2), 3), 4) and 5) have input similar as for large component

6) Basfil.eq.'KINETIC'. A kinetic balanced small component basisset is constructed from the large component basisset. This option can only be used when the large component basisset is given in a Basfil.eq.'UNCONTRACTED' form. An additional keyword after KINETIC ("KINETIC UNI") is optional:

Keyword: 'UNI' if the basisfunctions are different for each L-Type.
'SUB' if the d-type basisset is a subset of the s-type,
and the f-type basisset is a subset of the p-type, ect.

Default is 'UNI'.

Enddo

Preferable use of options :

- For small calculations : use uncontracted (non-relativistic) basis and option KINETIC.
- Use program GRASPG and option 3 to do calculations in a general contracted basis or use natural spinors from CI calculation in combination with GENBAS and option 3.

In PROPERTY is set to .TRUE. one can specify an input deck for the DIRAC code. For this define the card &DIRAC as a blank card. This card is then followed by the required DIRAC input.

Input description of GENBAS

Task : Generation of general contracted basis functions based on atomic spinors.

Necessary files : MFD1OUT, MFDVECA or MFDNAT_"ROOT"
Optional files : none
Produces files : BASIS_FILE
Scratch files : none

&GENBAS: Namelist, also used as keyword to find the remaining formatted GENBAS input.

NMO : Total number of M.O.'s to be used in the contraction.
NAMES (1) : Comment line. (Comment line of MFD1OUT calculation)
NAMES (2) : Basis file ('BASIS_FILE')
IPRINT : Print option (higher : more output). (2)
IPROF : Profile of the basis (0)
0 : No Profile
1 : Only profile, no basisgeneration.
2 : Profile and basisgeneration.
3 : Profile and basisgeneration plus profile of Gen. C. basis.
DEFSM : Default handling of Small part of MO's (KA)
K : Kinetic balance (e.g. d in large -> p and f in small)
L : Kinetic balance only upwards (e.g. d in large -> p in small)
M : Kinetic balance only downwards (e.g. d in large -> f in small)
A : Small part of MO (e.g.d in large -> p and f in small)
B : Small part of MO only downwards (e.g. d in large -> p in small)
C : Small part of MO only upwards (e.g. d in large -> f in small)
If (TWOC) no small parts (default XX)
TRSHLD(3) : Thresholds dealing with Non Orthogonality in selected MO parts
If (1 - (overlap of a function with all previous ones) .lt. Trsh)
then this function is disgarded.
Trsh (1) : Large component MO parts (1.D-5)
Trsh (2) : Small component MO parts (1.D-7)
Trsh (3) : Kinetic balance on previously generated Large Comp. function (1.D-7)

Formatted part of GENBAS input.

Card 1 (NMO times): IndMO, Type, SmPrt, Trsh (I4, 1X, A1, 2X, A2,3G10.4)
- IndMO : Index of MO to be used for contraction (see output)
- Type : Type of the large comp. function to be extracted from this MO.
- SmPrt : Specific handling of small part for this MO (K, A etc, see above)
- Trsh (1..3) : Specific handling of tresholds for this MO (see above)

Optional extra functions (repeat Card 2,3,4 for each extra l-type) :

Card 2 : LS, Lltyp, Nprim, Ncontr, Defsm, Trsh (I4,1X,A1,2I4, 2X, A2, 2G10.4)
- LS : 1 : Large (Default); 2 : Small
- Lltyp : Type of new functions (S, P, D, ...).
- Nprim : Number of primitives of this type.
- Ncontr : Number of contracted of this type.
- Defsm : Handling (K,L,M,X) of small part for this type of new functions.
- Trsh :Tresholds for this type of new functions (Trsh(1), Trsh (3)).

Card 3 En (free format)
- En : Primitive exponents of the extra functions

If (Ncontr.ne.Nprim) :

Card 4 Cn (free format)
- Cn : Contraction coefficients of the extra functions

&NATORB

USENAT:	Use natural spinors generated by Dirrci	(F)
FILENAM:	Name of file with natural spinors, that is for example "MFDNAT_1"	('MFDVECA ')

Input description of RELONEL

Task : Calculation of one-electron integrals. Nuclear model used is point charge or gaussian.

Necessary files : MFD1OUT, MFDSYMC
Optional files : MFDAREP, socints (from ARGOS)
Produces files : MFDONEE
Scratch files : fort.10, fort.11, fort.12

&GENERAL

TWOC:	Use two-component formalism	(F)

&RELONEL

DNORM :	"Distab" treshold.	(32.)
ENORM :	Integral value treshold.	(1.d-14)
OVLAPL :	Tolerance of linear dependence in Large Component basis.	(1.d-10)
OVLAPS :	Tolerance of linear dependence in Small Component basis.	(1.d-10)
GNUC :	Use Gaussian model to describe nuclei.	(T)
IEIGEN :	Print eigenvalues overlap matrix (0 : no; 1 : <OVLAP; 2 : all)	(1)
IKINBL :	Print kinetic balance per Large Component function	(1)
NAREP :	0 = No (A)REP, 1 = AREP, 2 = REP	(0)

When NAREP is set to 1 or 2 the namelist AREP will be expected.

&AREP

NUNIQATOM:	Number of unique atoms in the molecule	(1)

The AREP card has to be followed by some additional free-format cards of the form:

```
Do i = 1, NUNIQATOM
      Natoms , MaxAng
      Contr.(i), (i=1, MaxAng)
Enddo
```

Natoms :	Total number of atoms generated from this symmetry unique atom
MaxAng:	Maximum angular momentum of the basis set for this atom (s=0, p=1, ..)
Contr. (i):	Number of contracted functions for each angular momentum

Input description of RELTWEL

Task : Calculation of two-electron Coulomb and Gaunt integrals. Integral generation can be restricted to generation of specific types (LL,SL,SS,GAUNT)

Necessary files : MFD1OUT
Optional files : none
Produces files : When run in serial mode: SRTTWLL,SRTLBLL, SRTTWSL, SRTLBSL, SRTTWSS, SRTLBSS, SRTBREI, SRTBREL
When run in parallel mode: SRTPQIL, SRTPQLN
Scratch files : none

&GENERAL

TWOC:	Use two-component formalism	(F)

&RELTWEL

DNORM :	"Distab" treshold (Not used in this version).	(32.)
ENORM(1) :	Integral value treshold for the class (LL|LL),SL,SS and BR	(1.d-12)
ENORM(2) :	Integral value treshold for the class (SS|LL)	(1.d-12)
ENORM(3) :	Integral value treshold for the class (SS|SS)	(1.d-12)
ENORM(4) :	Integral value treshold for the class (SL|SL) or Breit	(1.d-12)
ICR :	Restart point indicator (file : LL = 1, SL = 2, SS =3, BR = 4).	
ICMX :	Last file to be calculated (see above).	(4)
COUNT :	Count only number of integrals (no calculation).	(F)
ONECEN :	Skip integrals with 2 or more small components basisfunctions on different centers.	(F)
ICORE :	0 : All integrals calculated	(0)
	1 : Discard (SS|SS) integrals with one or more valence functions	
	2 : Discard (SL|SL) and (SS|LL) ints with one or more valence functions	

Input description of MFDSCF

Task : Perform Fock-Dirac iterations and calculate Gaunt interaction perturbatively. Generate spinor set which can be used in CI calculations.

Necessary files :	MFD1OUT, MFDSYMC, MFDONEE, SRT *
Optional files :	MFDVECA,MFDVECB, DIISFIL, SELVECF
Produces files :	MFDVECA,MFDVECB
Scratch files :	MFDVECB, MFDOEMR, MFDOEMI, MFDENSM, DIISFIL

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used. Some of the namelists are alse used by other programs.

The SCF program will automatically restart when MFDVECA or MFDVECB is present. When both are present, the vectors from MFDVECA will be used.

When performing a four-component Fock-Dirac calculation and MFDVECA consists of two-component vectors, a four-component start will be generated. The detailed form of the operator used to generate the small component part of the four-component vectors is determined by SFrac. Use of SFrac = 0.0 is recommended.

The data on file SELVECF are used to select the occupied vectors: from the set of vectors which have at least a '&OSSEL SMALL' amount of the specified character, those corresponding to the lowest eigenvalues are used. The format of file SELVECF has been changed. First, a title card is expected. Next loop over irps: for each irp one textcard, followed by NOC(irp) sets of MO-data. One set of MO-data consists of one info card in the same format as found in MFDVECA, followed by cards with N, U (2I4) (N basisfunctions contribute to the character with weight U) until all basisfunctions have been assigned a weight. Only the first representation of degenerate representations should be specified.

&TITLE

SCFTXT:	Comment line	('NO TITLE SPECIFIED ON SCF - INPUT')

&SCF

NCYCLS:	Number of SCF iterations	(50)
MFIL:	Number of 2-electron integrals files to be used for Coulomb interaction	(3)
	If 1 : only (LL|LL) interaction	
	If 2 : (LL|LL) + (SS|LL) interaction	
	If 3 : complete interaction (LL|LL) + (SS|LL) + (SS|SS)	
CONVCRT:	Convergence (of density) criterion	(1.0D-10)
CLIGHT:	Speed of light	(137.0359895)
ONLYONE:	Only one-electron part (ignore two-electron interaction)	(F)

SELECT:	Select vectors by overlap with previous iterations; if vectors are given on MFDVECA then vector selection by character (using SELVECF) will be used for the first iteration; if the vectors are given on MFDVECB overlap selection will be used from the start	(F)
RSKINB	Apply restricted kinetic balance	(F)
BREIT:	Include Breit interaction variationally	(F)
ONLYBRT:	Calculate Breit interaction as perturbation after SCF run	
SFRAC:	Used when two-component start is being used	(0.0D0)
DEGEN:	if two eigenvalues are closer than this value, the corresponding eigenvectors are considered to be degenerate; this set will be rotated in order to maximize the overlap with the corresponding vectors of the previous iteration	(1.0D-8)

&GENERAL

TWOC:	Use two-component formalism	(F)

&XTRPOL

NDAMP:	Number of the iteration *in current run* during which damping is started; if very large, no damping	(very large)
DAMPFX:	Damping factor	(0.35)
NPOPLE	Number of the iteration *in current run* during which pople's extrapolation is started; if very large, no extrapolation	(very large)
NDIIS:	Number of the iteration *in current run* during which the DIIS procedure is started.	(very large)
CODIIS:	Convergence criterion for starting the DIIS procedure; if 0.0, no DIIS	(0.0)
	If both NDIIS and CODIIS are specified DIIS extrapolation will start when either the number of iterations exceeds NDIIS or when the convergence reaches CODIIS, whichever comes first.	
NSLOTI:	Number of iterations during which 2-el. interaction is gradually turned on	(0)
XORTHO	Perform orthogonalization after each iteration	(T)

&PRFLAG

PRTOD:	Print spinor differences	(F)
PRTRD:	Print differences per representation	(F)
PRTEW:	Print eigenvalues	(F)
PRTVC:	Print eigenvectors	(F)
PRTDM:	Print Dirac matrix	(F)
PRDINF	Print Diis information	(F)

&OSSEL

SMALL	Select only from vectors with char > SMALL	(0.01D0)
NOORTHO	No explicit orhogonalization from the set of selected vectors	(T)
DEBUG	Print reordering info	(F)
OSVIRT	Use Open Shell virtuals for CI.	(F)
HARDSEL	Fixed selection of occupied spinors	(F)

After &OSSEL with HARDSEL equals T formatted input as follows:

Do j =1 , Nsymrp

Index(i,j) i=1, Noc(j) 16I4

EndDo

&ORTHO

THRESH:	Threshold used for generating an non-linear dependent orthogonal basis	(1.D-12)

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

Input description of ROTRAN

Task : Transform 2-electron atomic scalar integrals to 4-component MO integrals
over the active spinors which are to be used in CI or CC calculations.

Necessary files : MFD1OUT, MFDSYMC, MFDVECA, SRT *
Optional files : none.
Produces files : MDCINT, MDBINT
Scratch files : INTSRT, INTTWO, INTSKEL

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used.
Some of the namelists are also used by other programs.

&ROTRAN

IPRNT:	Print flag. 0: Minimal output 1: Print number of reduced matrix elements. 2: Print transformed integrals (WARNING : very large output)	(0)
BREIT:	Transform Breit Interaction	(F)
DELSRT:	Delete SRT * files (F) after first half-transformation is done	
MFIL:	Number of Coulomb 2-e files to be transformed	(3)

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input for as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

This namelist is used to determine the number of vectors on MFDVECA and must have the same values as the one used with the scf-run which has generated the vectors on this file.

&EDIT

NMO:	Total number of MO's	(0)
DEFRAS:	Future use : Define RAS space for RASCI calculation	(F)

After &EDIT namelist formatted input as follows:

Nskip (I),	I=1, Nsymrp	16I4	(0)
Nmos (I),	I=1, Nsymrp	16I4	(Ncl (I) + Nop (I))

with

Nskip: number of vectors to skip on MFDVECA in this (sub)representation
Nmos: number of MO's taken from MFDVECA in this (sub)representation

&GENERAL

TWOC:	Use two-component formalism	(F)

&TRANTH

THRGEN :	General precision threshold for storing half-transformed integrals etc.	(1.E-16)
THROUT :	Threshold for writing transformed integrals	(1.E-16)

Input description of TMOONE

Task : Transform 1-electron and 2-electron atomic scalar integrals to effective 1-electron 4-component MO integrals over the active spinors which are to be used in CI calculations. Calculate core energy. Write abelian symmetry information necessary for CI.

Necessary files :	MFD1OUT, MFDSYMC, MFDVECA, MFDONEE, SRT *
Optional files :	none.
Produces files :	MRCONEE.
Scratch files :	MFDENSM, MFDOEMR, MFDOEMI, MFDVECB

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used. Some of the namelists are alse used by other programs.

&TMOONE

IPRNT:	Print flag. 0: Minimal output 1: Print effective one-electron MO integrals	(0)
BREIT:	Include Breit Interaction in MO integrals	(F)
ONLYBRT:	Transform Breit integrals only and add contribution to file MRCONEE.	(F)
MFIL:	Number of Coulomb 2-e files to be transformed	(3)

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

This namelist is used to determine the number of vectors on MFDVECA and must have the same values as the one used with the scf-run which has generated the vectors on MFDVECA.

&EDIT

NMO:	Total number of MO's		(0)

After &EDIT namelist formatted input as follows:

Nskip (I),	I=1, Nsymrp	16I4	(0)
Nmos (I),	I=1, Nsymrp	16I4	(Ncl (I) + Nop (I))

with

Nskip: number of vectors to skip on MFDVECA in this (sub)representation
Nmos: number of MO's taken from MFDVECA in this (sub)representation

&GENERAL

TWOC:	Use two-component formalism	(F)

Input description of GOSCIP

Task : Do Full CI within the active spinor set. Generate starting vectors for direct CI in a RASCI space with RAS2 exactly equal to the active set in this calculation.

Necessary files :	MRCONEE, MDCINT
Optional files :	none.
Produces files :	MDTRIV_"Representation name"
Scratch files :	none

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used. Some of the namelists are alse used by other programs.

&CI

NELEC:	Number of electrons in CI calculation	(0)
REFDET:	Decimal representation of the MO's to be frozen in the CI calculation	(0)
IREFE:	Number of electrons in frozen MO's	(# of frozen spinors)
IPRNT:	Print flag: = 5: gives population analysis, = 10: lists determinants	(0)

&POPAN

THRESH:	Print contributions of determinants only if the square of the coef is larger than THRESH	(1.0D-3)
DEGEN:	Eigenvalues seperated by less then DEGEN are considered to be degenerate (when preparing the output list of ew)	(1.0D-10)
SELPOP:	The population analysis is given only for the states with energy (relative to the ground state energy) less then SELPOP	(1.0D2)

&CIVEC

NVEC:	Number of CI-vectors written to files (like MDTRIV_1EG) for each representation	(5)

Input description of DIRRCI

Task : Do RASCI calculation. Uses Davidsons diagonalization algoritm.

Necessary files : MRCONEE, MDCINT, MFDVECA.
Optional files : MRCTWOE, MDTRIV_"IREPNA".
Produces files : MRCFINV, MFDNAT_"ROOT"
Scratch files : MRCTWOE, MRCEXCS, MRCVECS

Note : MDTRIV must contain vectors made in a COSCI calculation with the spinors now used as RAS2.

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used.

&RASORB

NELEC:	Number of electrons in CI calculation	(0)
NORBR(3):	Number of MO's in RAS1, RAS2 and RAS3	(0, total number of spinors, 0)
MAXH1:	Maximum number of holes in RAS1 spinors	(0)
MAXE3:	Maximum number of electrons in RAS3 spinors	(0)

&ORBDEL

NDELETE:	Number of spinors that are to be deleted	(0)

If the number of spinors that are to be deleted is larger then 0, an additional card is required with the indices of these spinors. The input is free format.

&DIRECT

MAXITER:	Maximum number of iterations	(10)
CPUMAX:	Maximum amount of CPU time to be used	(604800. seconds)
CONVERR :	Required convergence on residual vector	(1.d-10)
CONVERE :	Required energy convergence	(1.d-9)
RESTART :	Restart from file MRCFINV	(F)

&CIROOT

IREPNA :	Abelian symmetry character of the many-electron wavefunction	(First one in the list)
NROOTS :	Number of CI-vectors which are to be optimized	(1)
NSEL:	Rank number of CI-vectors on MDTRIV which are to be optimized	(1,2,3,4,..)

SELECT : Select wavefunctions on basis of largest overlap with the start wavefunction. (F)

ISTART : Start vector method. (1)

1. COSCI start vectors
2. Determinant with lowest eigenvalue
3. First (reference) determinant

If the COSCI start vectors are not available then the default will be 3.

&OPTIM

IGENEX : Writes 1-electron excitations to file (2) or calculates them when needed (1). (2)

&LEADDET

GETDET : Get the leading determinants. (T)

COMIN : Print contributions of determinants only if the square of the coeff. is larger then COMIN. (1.0D-1)

&NATURAL

MAKENAT: Construct vector files (MFDNAT_"ROOT") with natural spinors. (T)

Input description of RELCCSD

Task : The program is capable of doing energy calculations at the MP2, CCSD and CCSD(T) levels of theory, first order properties are available at the HF and MP2 level of theory (MP2 only in the serial code). An in-core RPA module makes it possible to run second order properties at the HF level of theory. Open shell states can be calculated via the Fock space Coupled Cluster method in which electrons are added to or subtracted from a closed shell core. Currently only the sectors (0,1) and (1,0) are available, they can be used to calculate electron affinities and ionization energies, respectively.

Necessary files : MRCONEE, MDCINT, MDBINT
Optional files : MDPROP
Produces files : none.
Scratch files : ft*

&RELCCSD :

NELEC:	Number of active electrons per symmetry representation	(0,0,0,..)
NFROZ:	Number of frozen spinors per symmetry representation	(0,0,0,..)
CARITH:	Use complex arithmetic (necessary for complex groups)	(T)
MWORD:	Memory used in calculation	(16)
IPRNT:	Print flag (Level 1 gives information in the convergence of the CCSD iterations)	(0)
DEBUG:	Produce debug information	(F)
TIMING:	Print out timing information	(F)
DOENER:	Perform energy calculations	(T)
DOFOPR:	Calculate the (relaxed) density matrix and first order properties	(F)
DOSOPR:	Calculate second order properties	(F)
DOEXC:	Calculate excitation energies	(F)
DOFSPC:	Perform Fock-space opens-shell energy calculations	(F)

&CCENER:

DOMP2:	Calculate the MP2 energy	(T)
DOCCSD:	Calculate the CCSD energy	(F)
DOCCSDT:	Calculate the CCSD plus non-iterative triples corrections	(F)
MAXIT:	Maximum number of iterations to solve the equations	(30)
MAXDIM:	Maximum dimension of DIIS matrix	(8)
NTOL:	Convergence tolerance (10**-NTOL)	(12)

&CCFOPR:

DOMP2G:	Calculate the MP2 gradient	(F)
NEOPER:	Number of first order property operators $\langle E \rangle$	(1)
NAMEE:	Names of E operators in $\langle E \rangle$	('ZDIPLEN')
MAXIT:	Maximum number of iterations to solve the equations	(30)
MAXDIM:	Maximum dimension of DIIS matrix	(8)
NTOL:	Convergence tolerance (10**-NTOL)	(12)

Note: CCFOPR requires the file MDPROP to be available. The PRTRAN module, which needs integrals from the DIRAC code, creates this file.

&CCSOPR:

NAOPER:	Number of A operators in $\langle\langle A;B \rangle\rangle_\omega$	(1)
NBOPER:	Number of B operators in $\langle\langle A;B \rangle\rangle_\omega$	(1)
NAMEA:	Names of A operators in $\langle\langle A;B \rangle\rangle_\omega$	('ZDIPLEN')
NAMEB:	Names of B operators in $\langle\langle A;B \rangle\rangle_\omega$	('ZDIPLEN')
NFREQ:	Number of frequencies to be calculated	(1)
EFREQ:	List of frequencies (au) in $\langle\langle A;B \rangle\rangle_\omega$	(0.0)
MAXIT:	Maximum number of iterations to solve the equations	(30)
MAXDIM:	Maximum dimension of DIIS matrix	(8)
NTOL:	Convergence tolerance (10**-NTOL)	(12)

Note: CCSOPR requires the file MDPROP to be available. The PRTRAN module, which needs integrals from the DIRAC code, creates this file.

&CCEXC:

NEXC:	Number of excitations energies in each irrep	(1,1,1,1…)
MAXIT:	Maximum number of iterations to solve the equations	(30)
MAXDIM:	Maximum dimension of DIIS matrix	(8)
NTOL:	Convergence tolerance (10**-NTOL)	(12)

&CCFSPC:

DOEA:	Calculate electron affinities (AF)	(F)
DOIE:	Calculate ionization energies (IE)	(F)
NACTP:	Number of active spinors in each irrep in which electrons may be put . There is no default. (determines the active space for the EA calculation and should be set when DOEA=.TRUE.)	(0,0,0,0…)
NACHTH:	Number of active spinors in each irrep in which holes can be created . There is no default. (determines the active space for the IE calculation and should be set when DOIE=.TRUE.)	(0,0,0,0…)
MAXIT:	Maximum number of iterations to solve the equations	(30)
MAXDIM:	Maximum dimension of DIIS matrix	(8)
NTOL:	Convergence tolerance (10**-NTOL)	(12)

Input description of PRTRAN

Task : Compute expectation values and/or transform property integrals to MO integrals for linear response code.

Necessary files : MFDSYMC, MFD1OUT, MFDHER, MFDVECA, AOPROPER
Optional files : none.
Produces files : MDPROP
Scratch files : none.

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used. Some of the namelists are also used by other programs.

&PRTRAN

IPRNT:	Print level	(1)

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input for as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

This namelist is used to determine the number of vectors on MFDVECA and must have the same values as the one used with the scf-run which has generated the vectors on this file.

&EDIT

NMO:	Total number of MO's	(0)
DEFRAS:	Future use : Define RAS space for RASCI calculation	(F)

After &EDIT namelist formatted input as follows:

Nskip (I),	I=1, Nsymrp	16I4	(0)
Nmos (I),	I=1, Nsymrp	16I4	(Ncl (I) + Nop (I))

with

Nskip: number of vectors to skip on MFDVECA in this (sub)representation
Nmos: number of MO's taken from MFDVECA in this (sub)representation

&GENERAL

TWOC:	Use two-component formalism	(F)

Input description of PROPAN

Task : Make population analysis of SCF spinors.

Necessary files : MFD1OUT, MFDSYMC, MFDONEE, MFDVECA or MFDNAT_"ROOT"
Optional files : none.
Produces files : none.
Scratch files : none.

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used.
Some of the namelists are alse used by other programs.

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

This namelist is used to determine the number of vectors on MFDVECA and must have the same values as the one used with the scf-run which has generated the vectors on MFDVECA.

&EDITPOP

NMO:	Total number of MO's	(0)

After &EDIT namelist formatted input as follows:

Nskip (I),	I=1, Nsymrp	16I4	(0)
Nmos (I),	I=1, Nsymrp	16I4	(Ncl (I) + Nop (I))

with

Nskip: number of vectors to skip on MFDVECA in this (sub)representation
Nmos: number of MO's taken from MFDVECA in this (sub)representation

&GENERAL

TWOC:	Use two-component formalism	(F)

&GRLABEL

NLABEL:	Number of labels used to identify functions	(0)

After &GRLABEL namelist NLABEL cards with formatted input:

Grlab, Ilab(I), I = 1, Nind (Nind < 25) A6, 24I3

Ilab refers to the numbers of the groups of symmetry related functions (printed in molfdir output).

&NATORB

USENAT:	Use natural spinors generated by Dirrci	(F)
FILENAM:	Name of file with natural spinors, that is for example "MFDNAT_1"	('MFDVECA ')

&PROPAN

PRTNET:	Print Overlap and Net populations	(F)
PRTOP:	Print populations for each spinor	(T)
PRTRP:	Print populations for each representation	(T)
PRTTP:	Print total populations	(T)

Input description of CALDENS

Task : Make data for density plots of SCF spinors. Output is to be used for processing with the AVS visualisation package.

Necessary files : MFD1OUT, MFDSYMC, MFDVECA or MFDNAT_"ROOT"
Optional files : none.
Produces files : AVS.fld, DENST.data, DENSL.data, DENSS.data, GRIDX.data, GRIDY.data, GRIDZ.data
Scratch files : none

Namelist input. Namelists can be given in any order. The first occurrence of a namelist is used. Some of the namelists are alse used by other programs.

&GRID

NDIM:	Number of dimensions of grid	(1)
X0:	Origin of grid	(0.0D0)
Y0:	id.	(0.0D0)
Z0:	id.	(0.0D0)

After &GRID namelist free format input as follows:

For Idim=1,NDIM
Rx (Idim), Ry (Idim), Rz (Idim), Af (Idim), Al (Idim), Na (Idim)
with
Rx, Ry, Rz: Direction of this grid-dimension (will be normalized)
Af: First distance in this direction
Al: Last distance in this direction
Na: Number of points in this direction

&OCCUP

TOTAL:	Total number of electrons	(0)
Nopen :	Number of open shells (maximally 2)	(0)

After &OCCUP namelist formatted input as follows:

Ncl (I),	I=1, Nsymrp	16I4	(0)

For each open shell :

Nop (I),	I=1, Nsymrp	16I4	(0)
Ocopn		F12.8	(0.0)

with

Ncl : Number of closed shells in this (sub)representation.
Nop: Number of open shells in this (sub)representation.
Ocopn : Occupation of the open shells in the (sub)representations.

This namelist is used to determine the number of vectors on MFDVECA and must have the same values as the one used with the scf-run which has generated the vectors on MFDVECA

&NATORB

USENAT:	Use natural spinors generated by Dirrci	(F)
FILENAM:	Name of file with natural spinors, that is for example "MFDNAT_1"	('MFDVECA ')

&EDITDENS

NMO:	Total number of MO's	(0)

After &EDITDENS namelist formatted input as follows:

Nskip (I),	I=1, Nsymrp	16I4	(0)
Nmos (I),	I=1, Nsymrp	16I4	(Ncl (I) + Nop (I))

with

Nskip: number of vectors to skip on MFDVECA in this (sub)representation
Nmos: number of MO's taken from MFDVECA in this (sub)representation

&GENERAL

TWOC:	Use two-component formalism	(F)

&CALDENS

FORMOUT:	Print formatted output instead of AVS data files	(F)
LOGSCL:	Use logarithmic scale for density plot	(F)