

Reference manuals

Gaussian

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Gaussian

<http://www.gaussian.com>

Help:

Support -> Gaussian 16 Documentation:

- Gaussian 16 Users Reference
- Keyword List

!!! All outputs below are only examples !!!

Their content is not related to the solved tasks.

Input file

Link0 commands are optional commands introduced after "%". They can specify the archive name (checkpoint), amount of memory, number of processors, etc.

Command line is specified after # (see Route (#)). It specifies QM **method and type of calculation**.

```
%Chk=h2o.chk
# RHF/cc-pVDZ Opt
optimization of water molecule geometry
0 1
O 0.000000 0.000000 -0.154167
H 0.000000 0.854766 0.538096
H 0.000000 -0.854766 0.538096
```

charge

multiplicity
 $M = 2S + 1$

total spin of electrons

QM method

basis set

geometry optimization

blank line

comment

blank line

blank line

system geometry specification (Cartesian coordinates in Å)
terminated by a blank line

How to run calculations (tests only)

It is strictly prohibited to run calculations in Gaussian directly in home directories. All Gaussian jobs need to be submitted to a batch system (see next page).

For testing in the scratch directory only:

```
$ module add gaussian
$ g16 job.com
```

← activate gaussian module
(only once in a terminal)

← name of input file

← name of gaussian program

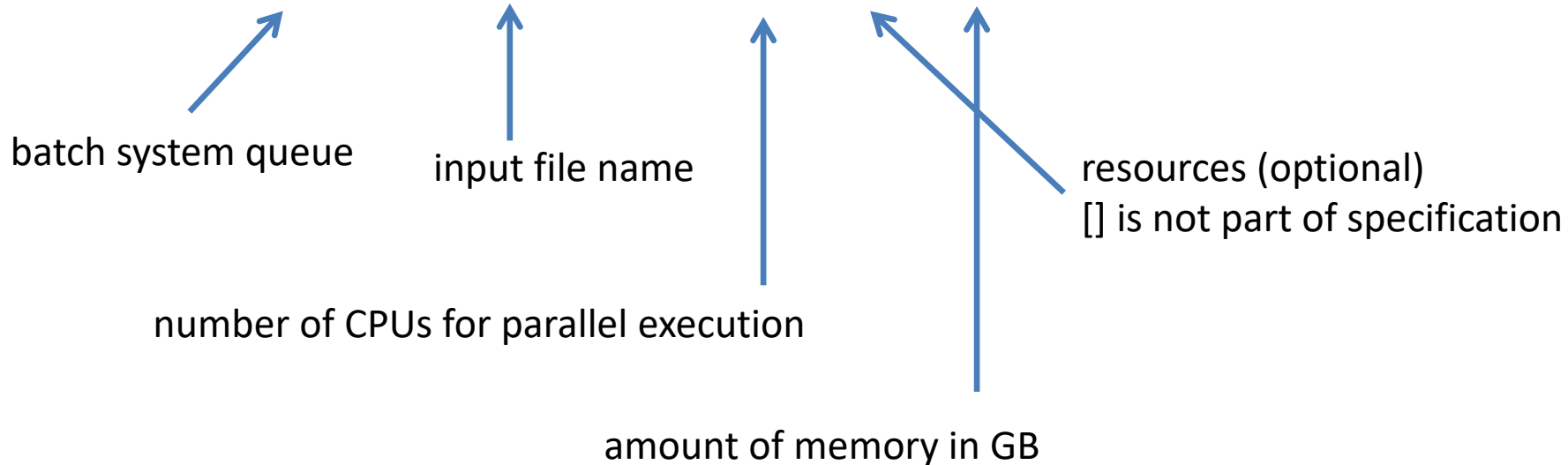
After completing the task, the result of the calculation will be saved in the **job.log** file, the last line of the file must state:

```
Normal termination of Gaussian 09 at Sun Oct 26 20:20:09 2014.
```

otherwise, the calculation is unsuccessful. The reason for premature termination of the calculation must be found in the output file.

How to run calculations on WOLF

```
$ psubmit default job.com [ncpus=N] [mem=XXg]
```



Example:

```
$ psubmit default job.com ncpus=2 mem=20g
```

**Energy calculation
(Single-point calculation)**

Geometry optimization

Energy calculation and optimization

```
%Chk=h2o.chk
# RHF/cc-pVDZ

energy calculation (water molecule)

0 1
O 0.000000 0.000000 -0.154167
H 0.000000 0.854766 0.538096
H 0.000000 -0.854766 0.538096
```

without the **Opt** keyword,
only energy and WF are
calculated including system
properties
(single point calculation)

←
←
terminated by a blank line

```
%Chk=h2o.chk
# RHF/cc-pVDZ Opt

geometry optimization (water molecule)

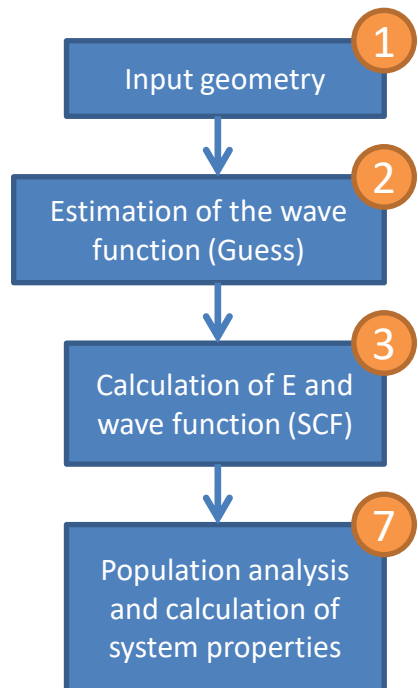
0 1
O 0.000000 0.000000 -0.154167
H 0.000000 0.854766 0.538096
H 0.000000 -0.854766 0.538096
```

←
request geometry optimization

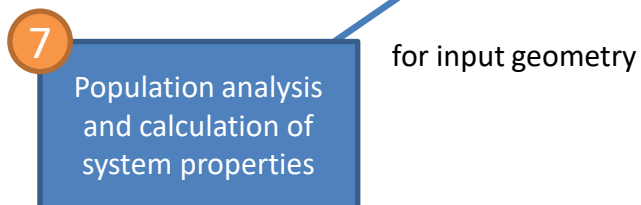
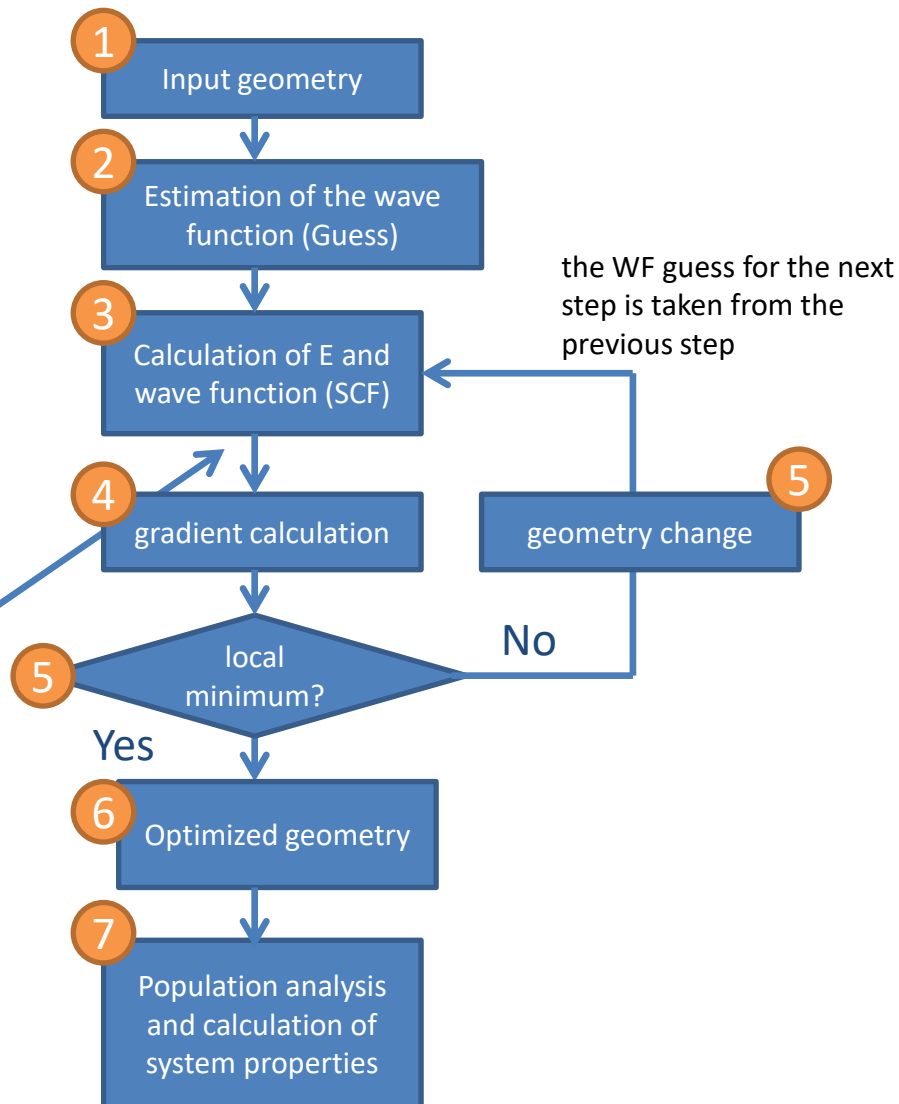
←
terminated by a blank line

Calculation progress

Single-point calculation



Geometry optimization



Data extraction in CLI

Geometry optimization

1) Module activation:

```
$ module add qmutil
```

only once in a given terminal

2) Optimization process (energy):

```
$ extract-gopt-ene job.log
```

It is advisable to analyze the course of optimization, in the GUI programs such as **vmd** or **Avogadro**

3) Optimization process (all geometries):

```
$ extract-gopt-xyz job.log > opt.xyz
```

4) Obtaining optimized geometry (last = optimized geometry):

```
$ extract-xyz-str opt.xyz last > last.xyz
```



Data extraction in CLI

Geometry optimization process (energy):

```
$ extract-gopt-ene job.log
# Coordinate:
# Step          Energy [kcal/mol]   Energy [au]
# -----
#              1          0.000          -0.028650961
#              2         -0.171          -0.028922822
#              3         -0.188          -0.028950914
#              4         -0.190          -0.028953934
```

optimization step
number

relative energy to the
first geometry

absolute energy in Hartree

The energy (in a.u.) of the optimized structure, i.e., the geometry contained in **opt.xyz**.
The opt.xyz geometry **can be visualised** in the programs: **Avogadro, Nemesis, vmd**.

Vibrational analysis

Vibrational analysis

```
%chk=h2o.chk
# RHF/cc-pVDZ Freq
vibrational analysis

0 1
O 0.0000000 0.0000000 -0.0780430
H 0.0000000 0.7492420 0.5000340
H 0.0000000 -0.7492420 0.5000340
```

request vibrational
frequency calculation

terminated by a blank line

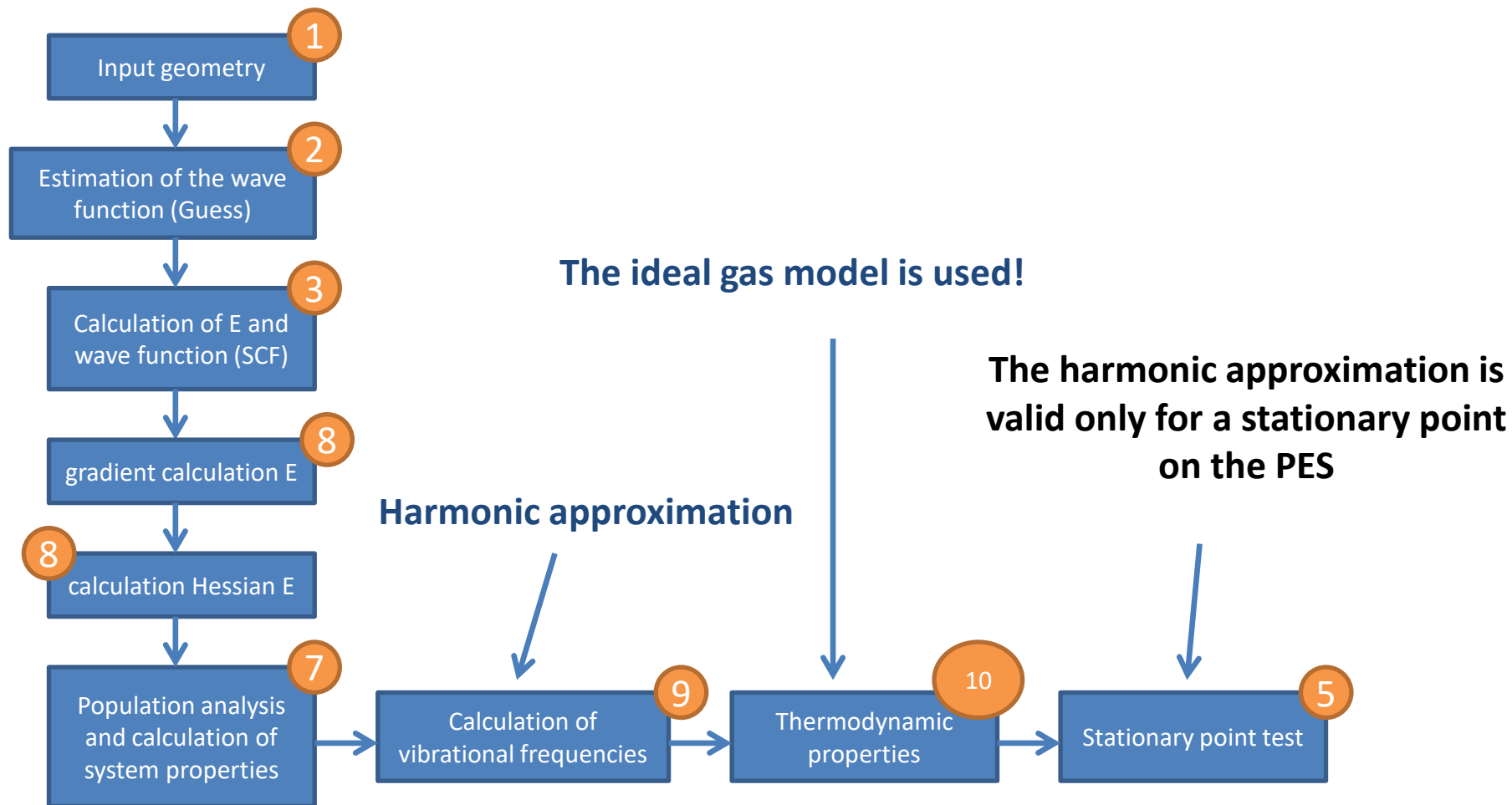
For optimized geometry (stationary point on PES), the type of stationary point can be determined from the number of imaginary frequencies of normal vibrations:

- 0 imaginary frequencies -> **local minimum**
- 1 imaginary (negative) frequency -> **first order transition state**

Vibrational analysis requires Hessian calculation, which can be very computationally intensive.

Calculation progress

Single-point calculation on optimized geometry



BSSE

CP correction for BSSE

```
%Chk=ene.chk
# RHF/cc-pVDZ Counterpoise=2

SP calculation with BSSE correction

0 1
O(Fragment=1) 0.231135 0.063539 0.203312
H(Fragment=1) 0.374693 0.253491 1.116647
H(Fragment=1) 0.074728 -0.864502 0.130817
O(Fragment=2) -1.648273 1.893276 -1.229780
H(Fragment=2) -1.166742 2.355543 -1.894982
H(Fragment=2) -1.036494 1.311764 -0.798971
```

request energy
calculation with
BSSE correction

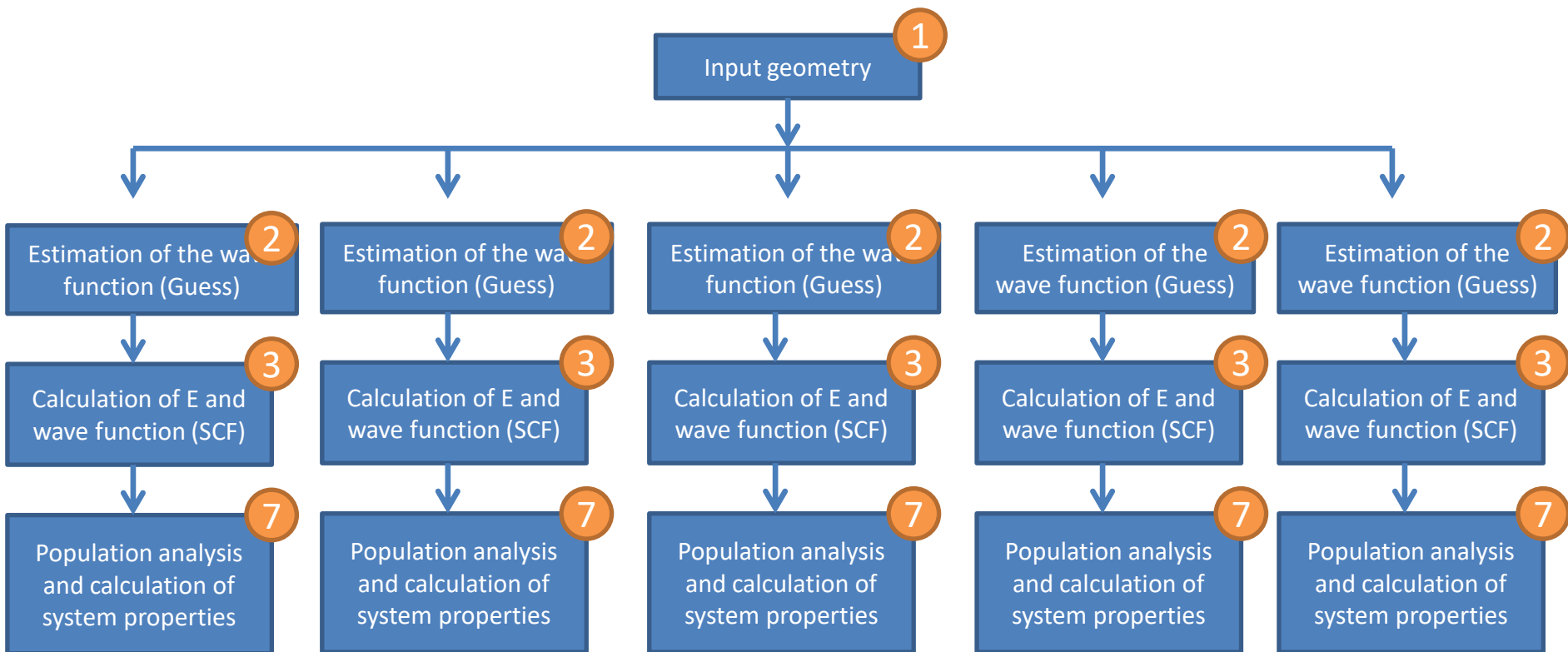
← terminated by a blank line

← Fragments representing interacting molecules.

Counterpoise correction of BSSE requires 5 energy calculations (AB, A(B), (A)B, A, and B), which are performed by Gaussian automatically.

This correction can be used during geometry optimization.

Calculation progress



AB

A(B)

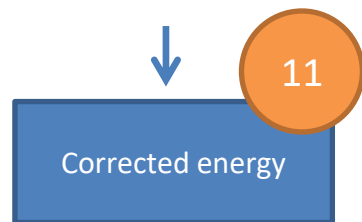
(A)B

A

B

$$E_{CP} = E_{AB} + \underbrace{(E_A - E_{A(B)}) + (E_B - E_{(A)B})}_{BSSE}$$

BSSE



Corrected energy

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Finding a reaction path

SCD

Single Coordinate Driving

Driving, strategy

The goal of SCD is to find an **estimate of transition state**. The driving is performed by changing the selected geometric parameter and optimizing all other degrees of freedom. The parameter can be, for example, a shortening of the length between the atoms between which a bond is formed during the reaction.

Selection of a suitable reaction coordinate describing the course of the reaction:

- The reaction coordinate is usually very complicated.
- It is necessary to use a simplified coordinate that best captures the intended change.
- The coordinate is chosen from simple geometric parameters (length, angle, torsion angle, etc.)
- The distances are natural choice in reactions, usually between atoms where bonds are formed or broken.
- Torsional angles are usually used for conformational transitions.
- The best choice for the starting geometry is to select a state with the smallest number of conformational degrees of freedom. Thus, driving need not to be necessary always performed from reactants to products.

Driving, input

```
%Chk=driving.chk  
# PM3 Opt=ModRedundant NoSymm
```

```
single coordinate driving
```

```
XX  
X .....  
X .....  
X .....
```

```
B A1 A2 S NStep StepSize
```

request driving

charge and multiplicity
geometry

terminated by a blank line

terminated by a blank line

distance

step size (positive or negative number), the number must contain a decimal point (for distance the optimal step length is about 0.1 Å)

number of steps (integer)

SCD

indexes of atoms between which we will change the distance (indexed from one)

Driving, example

```
.....  
H -7.27527 1.28418 0.56205
```

```
B 4 11 S 15 -0.1
```

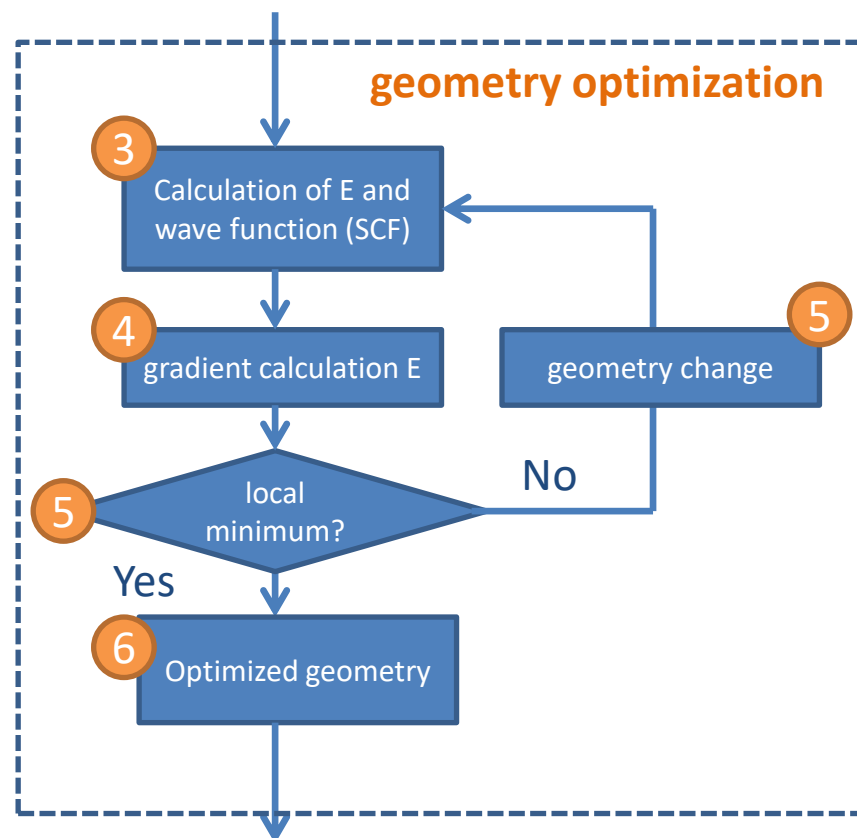
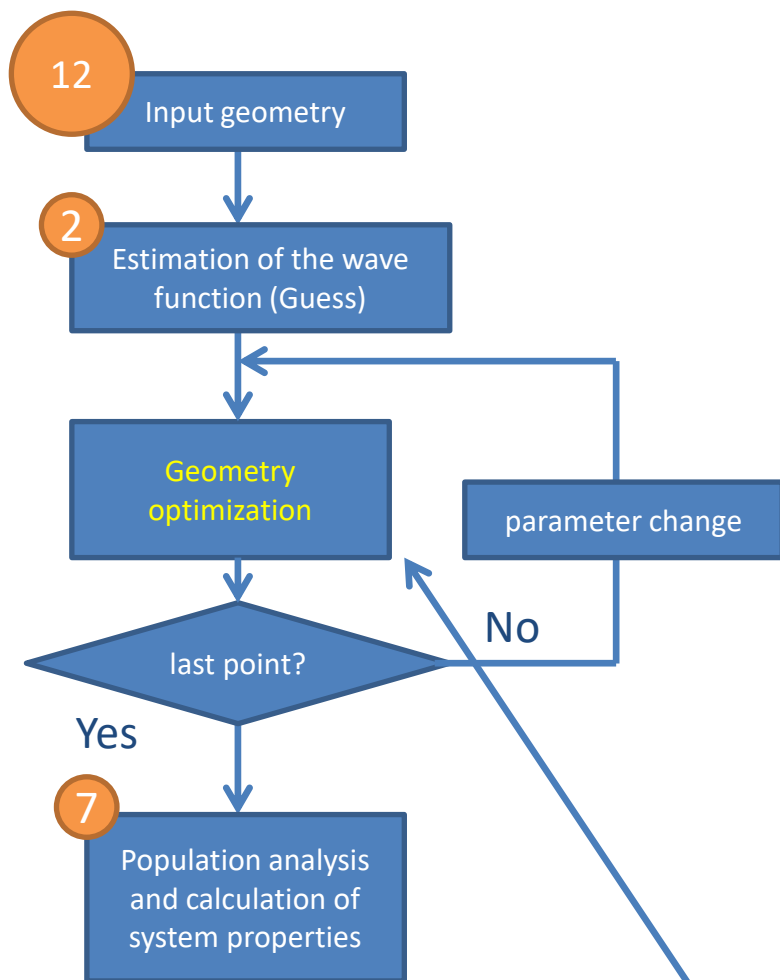
blank lines

We shorten the length (B) between atoms 4 and 11 in fifteen steps, always by 0.1 Å.

Detailed documentation:

<http://gaussian.com/opt/> - section Options/ModRedundant

Calculation progress



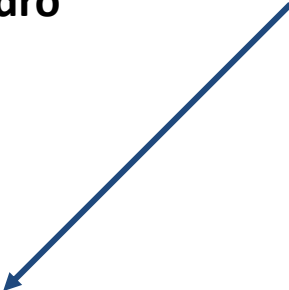
During optimization, the value of the SCD parameter is set a constant.

Data extraction in CLI

1) qmutil module activation:

```
$ module add qmutil
```

It is advisable to analyze the course of SCD, in the GUI programs such as **vmd** or **Avogadro**



2) Display the course of SCD (energy):

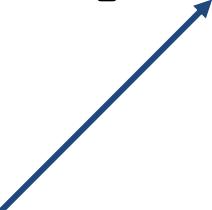
```
$ extract-gdrv-ene job.log
```

3) Display the course of SCD (all geometries):

```
$ extract-gdrv-xyz job.log > drv.xyz
```

4) Extract given geometry (geometry with index N):

```
$ extract-xyz-p drv.xyz N > TS_guess.xyz
```



The number of the structure we want to extract from the drv.xyz file.

Driving, results

Example: Diels-Alder cycloaddition reaction

Coordinate: R(4,7)

#	Step	Value	Energy [kcal/mol]	S	Energy [au]
	1	1.5380	0.000	-	0.002554791
	2	1.6380	2.648	/	0.006774307
	3	1.7380	8.526	/	0.016141320
	4	1.8380	15.826	/	0.027774776
	5	1.9380	23.919	/	0.040672342
	6	2.0380	32.626	/	0.054548199
	7	2.1380	41.714	/	0.069029627
	8	2.2380	50.746	/	0.083423613
	9	2.3380	59.194	/	0.096886686
	10	2.4380	66.597	/	0.108683559
	11	2.5380	72.657	/	0.118340986
	12	2.6380	77.257	/	0.125671188
	13	2.7380	80.400	/	0.130680500
	14	2.8380	36.191	\	0.060228061
	15	2.9380	35.376	\	0.058929736
	16	3.0380	34.774	\	0.057970622

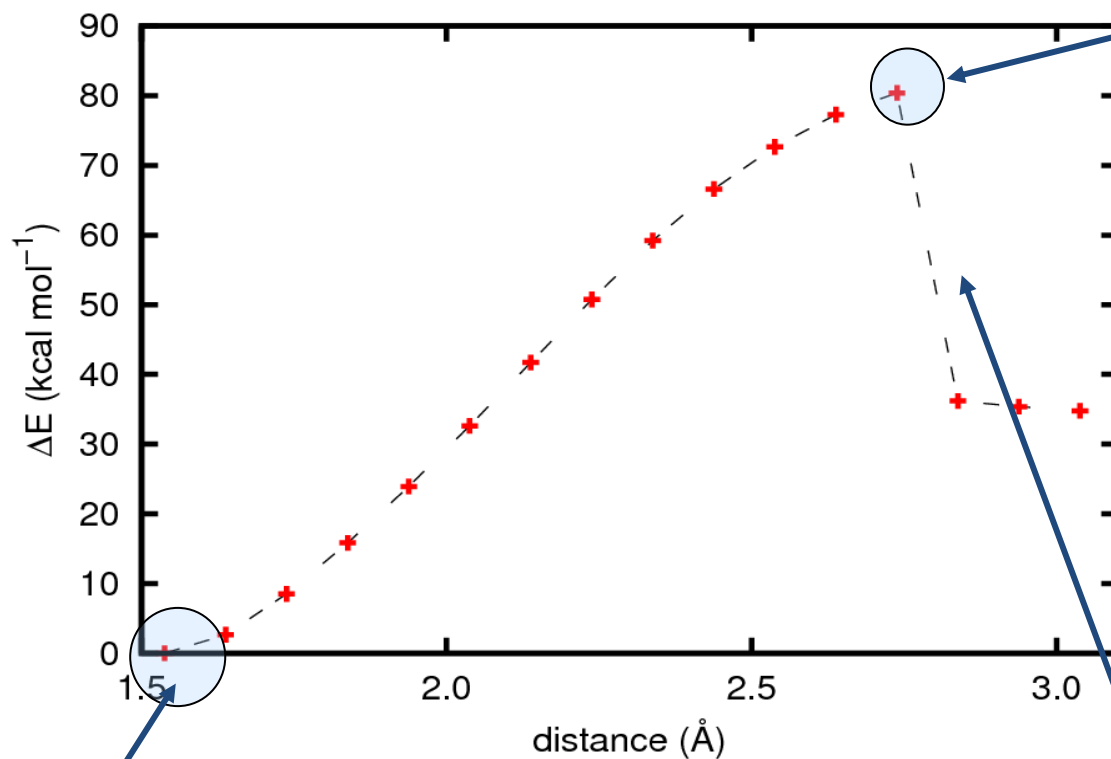
Structure number

Structure with maximum energy on the reaction path =>
estimate of transition state

Driving, results

Example: Diels-Alder cycloaddition reaction

coordinate driving



Structure with maximum energy on the reaction path
=>
estimate of transition state

product
(input state for driving)

bond breaking

The break indicates that the coordinate does not correctly describe the course of the reaction.

Geometry optimization of transition state

TS optimization, input

request optimization of the transition state

```
%Chk=ts.chk
# PM3 Opt( CalcFC, TS, NoEigenTest, MaxCycle=25)

transition state optimization

XX
X .....
X .....
X .....
```

terminated by a blank line

CalcFC

force constants (Hessian) are calculated on the input geometry

CalcAll

force constants (Hessian) are calculated on each geometry during optimization (Newton-Raphson method)

TS optimization, output

The output is processed in the same way as a regular geometry optimization.

- If the maximum number of steps is exceeded, you can try to continue the optimization (extract the last coordinates and perform the optimization again). The second option is to switch from **CalcFC** to **CalcAll**.
- If the TS is not found within about 30 optimization steps, it is necessary to find a better TS estimate.
- The TS must have only one imaginary ("negative") frequency.
- The vibrational motion corresponding to an imaginary frequency must follow the formation and termination of the bonds corresponding to the reaction step.

Output file

Output file: sections 1 and 2

1. Input geometry in internal coordinates

```
-----  
!      Initial Parameters      !  
! (Angstroms and Degrees)    !  
-----  
! Name  Definition              Value          Derivative Info.      !  
-----  
! R1    R(1,2)                  1.0999        estimate D2E/DX2      !  
! R2    R(1,3)                  1.0999        estimate D2E/DX2      !  
! A1    A(2,1,3)                101.9929      estimate D2E/DX2      !  
-----
```

2. WF initial guess

number of base siset functions = number of **c** coefficients,
which need to be found during SCF

```
Two-electron integral symmetry is turned off.  
 24 basis functions,      47 primitive gaussians,      25 cartesian basis functions  
 5 alpha electrons       5 beta electrons  
 nuclear repulsion energy      8.0071357792 Hartrees.  
NAtoms=    3 NActive=    3 NUniq=    3 SFac= 1.00D+00 NAtFMM=    60 NAOKFM=F Big=F  
One-electron integrals computed using PRISM.  
NBasis=    24 RedAO= T   NBF=    24  
NBsUse=    24 1.00D-06 NBFU=    24  
Harris functional with IExCor= 205 diagonalized for initial guess.
```

← initial guess of WF

Output file: section 3

3. Energy and WF calculations

```
SCF Done:  E(RHF) = -75.9901319773  
           Convg = 0.5258D-08
```

total energy

Energy change in the last cycle of SCF

```
A.U. after 10 cycles
```

Number of SCF cycles needed to find E and WF

virial theorem

```
-V/T = 2.0057
```

Energy is in a.u. (Hartree)

Full SFC progress is printed, if #P is specified in the input file.

Output file: section 3, cont.

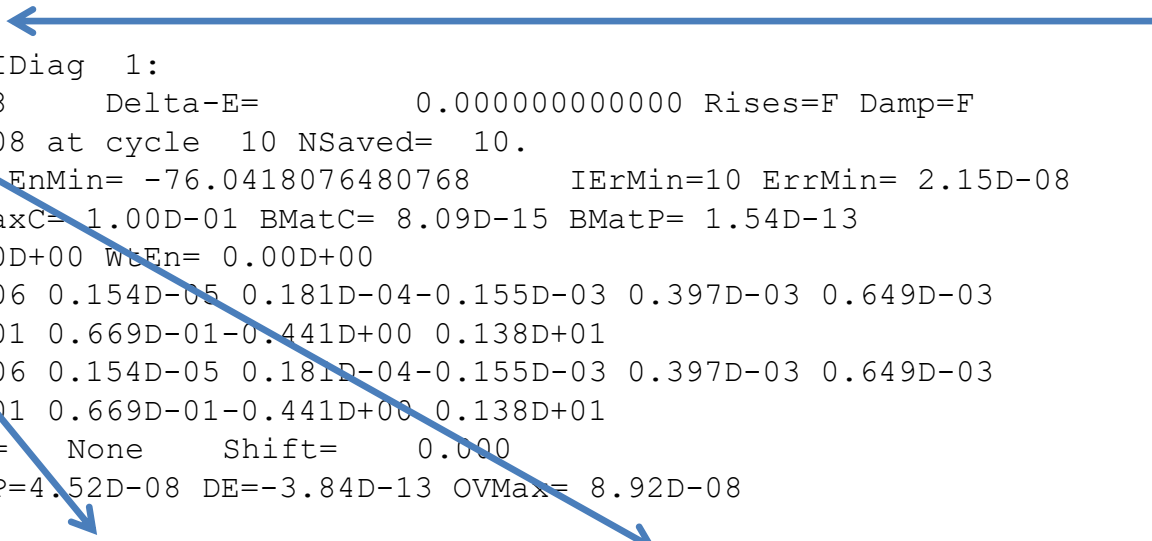
```
Cycle 1 Pass 1 IDiag 1:
E= -75.9710832672194
DIIS: error= 4.94D-02 at cycle 1 NSaved= 1.
NSaved= 1 IEnMin= 1 EnMin= -75.9710832672194 IErMin= 1 ErrMin= 4.94D-02
ErrMax= 4.94D-02 EMaxC= 1.00D-01 BMatC= 1.08D-01 BMatP= 1.08D-01
IDIUse=3 WtCom= 5.06D-01 WtEn= 4.94D-01
Coeff-Com: 0.100D+01
Coeff-En: 0.100D+01
Coeff: 0.100D+01
Gap= 0.463 Goal= None Shift= 0.000
GapD= 0.463 DampG=2.000 DampE=0.500 DampFc=1.0000 IDamp=-1.
RMSDP=6.04D-03 MaxDP=1.13D-01 OVMaX= 1.12D-01
```

.....

```
Cycle 10 Pass 1 IDiag 1:
E= -76.0418076480768 Delta-E= 0.00000000000000 Rises=F Damp=F
DIIS: error= 2.15D-08 at cycle 10 NSaved= 10.
NSaved=10 IEnMin=10 EnMin= -76.0418076480768 IErMin=10 ErrMin= 2.15D-08
ErrMax= 2.15D-08 EMaxC= 1.00D-01 BMatC= 8.09D-15 BMatP= 1.54D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.199D-06 0.154D-05 0.181D-04-0.155D-03 0.397D-03 0.649D-03
Coeff-Com: -0.110D-01 0.669D-01-0.441D+00 0.138D+01
Coeff: -0.199D-06 0.154D-05 0.181D-04-0.155D-03 0.397D-03 0.649D-03
Coeff: -0.110D-01 0.669D-01-0.441D+00 0.138D+01
Gap= 0.546 Goal= None Shift= 0.000
RMSDP=4.57D-09 MaxDP=4.52D-08 DE=-3.84D-13 OVMaX= 8.92D-08
```

```
SCF Done: E(RHF) = -76.0418076481 A.U. after 10 cycles
Conv g = 0.4573D-08 -V/T = 2.0008
```

shortened



Output file: section 4

4. Gradient calculation

forces = negative energy gradient (in atomic units)



Center	Atomic	Forces (Hartrees/Bohr)		
Number	Number	X	Y	Z

1	8	0.000000000	0.000000000	0.131133317
2	1	0.000000000	-0.085534245	-0.065566658
3	1	0.000000000	0.085534245	-0.065566658

Cartesian Forces:	Max	0.131133317	RMS	0.067020838

Output file: section 5

5. Geometry optimization

Grad

Berny optimization.

Internal Forces: Max 0.107734851 RMS 0.088033019

...

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.07857	-0.10773	0.00000	-0.21160	-0.21160	1.86697
R2	2.07857	-0.10773	0.00000	-0.21160	-0.21160	1.86697
A1	1.78011	-0.00599	0.00000	-0.02126	-0.02126	1.75885

shortened

Item	Value	Threshold	Converged?
Maximum Force	0.107735	0.000450	NO
RMS Force	0.088033	0.000300	NO
Maximum Displacement	0.177009	0.001800	NO
RMS Displacement	0.154831	0.001200	NO

Predicted change in Energy -3.060008D-02

Grad

convergence criteria for geometry optimization termination

planned geometry change

Output file: section 6

6. Optimized geometry

```
Item                Value          Threshold  Converged?
Maximum Force       0.000267      0.000450   YES
RMS      Force      0.000172      0.000300   YES
Maximum Displacement 0.000999      0.001800   YES
RMS      Displacement 0.000967      0.001200   YES
Predicted change in Energy=-2.315429D-07
Optimization completed.
```

-- Stationary point found.

```
-----
!   Optimized Parameters   !
! (Angstroms and Degrees)  !
```

```
-----
! Name  Definition                Value          Derivative Info.          !
-----
! R1    R(1,2)                    0.9463         -DE/DX =  -0.0001         !
! R2    R(1,3)                    0.9463         -DE/DX =  -0.0001         !
! A1    A(2,1,3)                  104.696        -DE/DX =  -0.0003         !
-----
```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Output file: section 7

7. Population analysis and system property calculations (shortened)

```
Alpha occ. eigenvalues -- -20.54839 -1.34218 -0.70556 -0.56822 -0.49389
Alpha virt. eigenvalues --  0.18742  0.25779  0.79793  0.86396  1.16257
```

energy of molecular orbitals

virtual orbitals

occupied orbitals

Mulliken atomic charges:

```
      1
  1  O  -0.292462
  2  H   0.146231
  3  H   0.146231
```

Mulliken atomic (point) charges

Sum of Mulliken atomic charges = 0.00000

Dipole moment (field-independent basis, Debye):

```
  X=          0.0000    Y=          0.0000    Z=          2.0430    Tot= 2.0430
```

Quadrupole moment (field-independent basis, Debye-Ang):

```
  XX=         -7.0085    YY=         -4.1369    ZZ=         -5.7327
  XY=          0.0000    XZ=          0.0000    YZ=          0.0000
```

dipol and quadrupole electrostatic moments

Type of population analysis can be selected the **pop** keyword.

Output file: section 8

```
Differentiating once with respect to electric field.
      with respect to dipole field.
      Electric field/nuclear overlap derivatives assumed to be zero.
      Keep R1 ints in memory in canonical form, NReq=873499.
      There are      3 degrees of freedom in the 1st order CPHF.  IDoFFX=0.
      3 vectors produced by pass  0 Test12= 3.17D-15 3.33D-08 XBig12= 1.15D+00 6.84D-01.
AX will form      3 AO Fock derivatives at one time.
      3 vectors produced by pass  1 Test12= 3.17D-15 3.33D-08 XBig12= 5.63D-02 1.22D-01.
      3 vectors produced by pass  2 Test12= 3.17D-15 3.33D-08 XBig12= 7.24D-03 3.79D-02.
      3 vectors produced by pass  3 Test12= 3.17D-15 3.33D-08 XBig12= 2.25D-04 7.06D-03.
      3 vectors produced by pass  4 Test12= 3.17D-15 3.33D-08 XBig12= 4.04D-06 8.17D-04.
      3 vectors produced by pass  5 Test12= 3.17D-15 3.33D-08 XBig12= 2.96D-08 7.41D-05.
      3 vectors produced by pass  6 Test12= 3.17D-15 3.33D-08 XBig12= 3.37D-10 9.10D-06.
      2 vectors produced by pass  7 Test12= 3.17D-15 3.33D-08 XBig12= 1.95D-12 5.99D-07.
      1 vectors produced by pass  8 Test12= 3.17D-15 3.33D-08 XBig12= 9.82D-15 4.57D-08.
Inverted reduced A of dimension      24 with in-core refinement.
End of Minotr Frequency-dependent properties file      721 does not exist.
End of Minotr Frequency-dependent properties file      722 does not exist.
Symmetrizing basis deriv contribution to polar:
IMax=3 JMax=2 DiffMx= 0.00D+00
G2DrvN: will do      4 centers at a time, making      1 passes doing MaxLOS=2.
Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
FoFDir/FoFCou used for L=0 through L=2.
End of G2Drv Frequency-dependent properties file      721 does not exist.
End of G2Drv Frequency-dependent properties file      722 does not exist.
```

Output file: section 9

6(5) vibrací musí mít nízké frekvence (ideálně nulové) – 3 translační a 3 rotační stupně volnosti systému

Full mass-weighted force constant matrix:

```
Low frequencies --- -40.7995 -0.0019 -0.0015 0.0005 37.6815 55.2358
```

```
Low frequencies --- 1774.9584 4112.7795 4211.8138
```

Harmonic frequencies (cm⁻¹), IR intensities (KM/Mole), Raman scattering activities (A⁴/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A1	A1	B2
Frequencies --	1774.9584	4112.7795	4211.8137
Red. masses --	1.0818	1.0460	1.0821
Frc consts --	2.0080	10.4246	11.3093
IR Inten --	80.8414	21.1644	60.8089
Raman Activ --	4.7861	68.9225	34.7495
Depolar (P) --	0.5271	0.1703	0.7500
Depolar (U) --	0.6903	0.2910	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	8	0.00	0.00	0.07	0.00	0.00	0.05	0.00	0.07	0.00
2	1	0.00	-0.43	-0.56	0.00	0.58	-0.40	0.00	-0.56	0.43
3	1	0.00	0.43	-0.56	0.00	-0.58	-0.40	0.00	-0.56	-0.43

frequencies of normal vibrational modes

direction of atom movements during the normal mode vibration

Output file: section 10

E(RHF) = -76.0270533118

IDEAL GAS MODEL

$$E_k = E_m(R_{opt,m}) + E_{VRT,l}$$

```
-----
- Thermochemistry -
-----
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
....
```

```
Zero-point correction= 0.023008 (Hartree/Particle)
Thermal correction to Energy= 0.025843
Thermal correction to Enthalpy= 0.026787
Thermal correction to Gibbs Free Energy= 0.005411
Sum of electronic and zero-point Energies= -76.004045
Sum of electronic and thermal Energies= -76.001211
Sum of electronic and thermal Enthalpies= -76.000267
Sum of electronic and thermal Free Energies= -76.021642
```

conditions

kráceno

zero-point vibrational energy

Gibbs energy

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	16.216	5.989	44.988
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	34.608
Rotational	0.889	2.981	10.376
Vibrational	14.439	0.028	0.004

http://gaussian.com/g_whitepap/thermo.htm

Output file: section 11

7. Calculations with BSSE corrections

```
Counterpoise: corrected energy = -152.060077655641  
Counterpoise: BSSE energy = 0.002829142358
```

BSSE correction



final interaction energy with **BSSE correction**

Output file: section 12

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.4982	estimate D2E/DX2	!
! R2	R(1,6)	1.3351	estimate D2E/DX2	!
! R3	R(1,17)	1.0954	estimate D2E/DX2	!
! R4	R(2,3)	1.4982	estimate D2E/DX2	!
! R5	R(2,7)	1.6028	estimate D2E/DX2	!
! R6	R(2,13)	1.5363	estimate D2E/DX2	!
! R7	R(3,4)	1.3351	estimate D2E/DX2	!
! R8	R(3,18)	1.0954	estimate D2E/DX2	!
! R9	R(4,5)	1.5075	estimate D2E/DX2	!
! R10	R(4,11)	3.7721	Scan	!
! R11	R(4,19)	1.0924	estimate D2E/DX2	!

R – distance between
atoms 4 and 11

initial value

indicates that the coordinate is subject of SCD