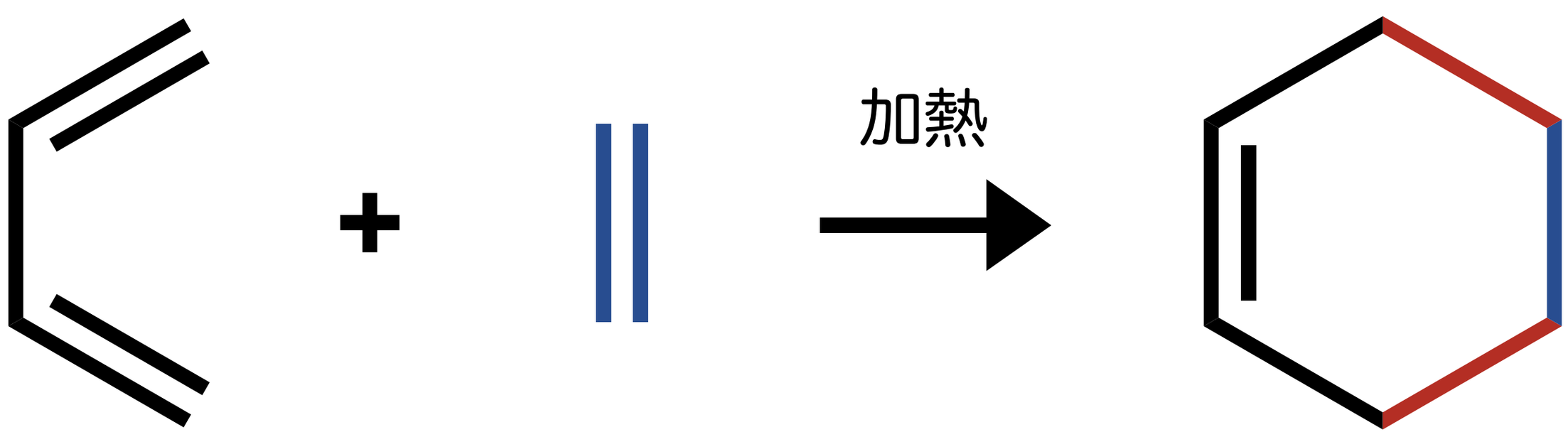
応用化学実験３：量子化学実験

Diels-Alder反応の解析

この実習で学ぶことは？

Diels-Alder反応とは？

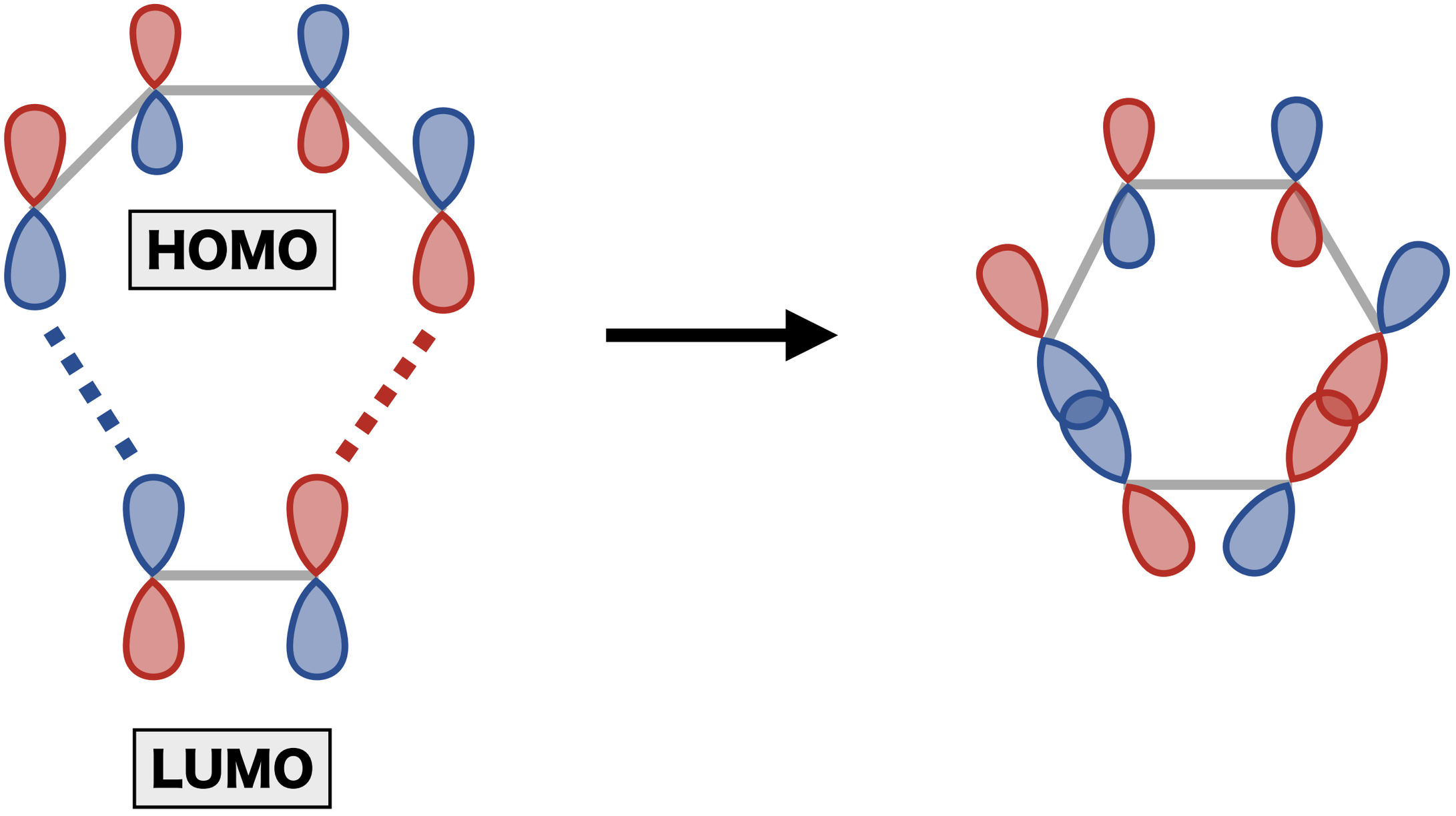
共役ジエンにアルケンが付加して６員環構造を
生成する [4+2] 環化付加反応の代表例



1,3-ブタジエン　　エチレン　　シクロヘキセン

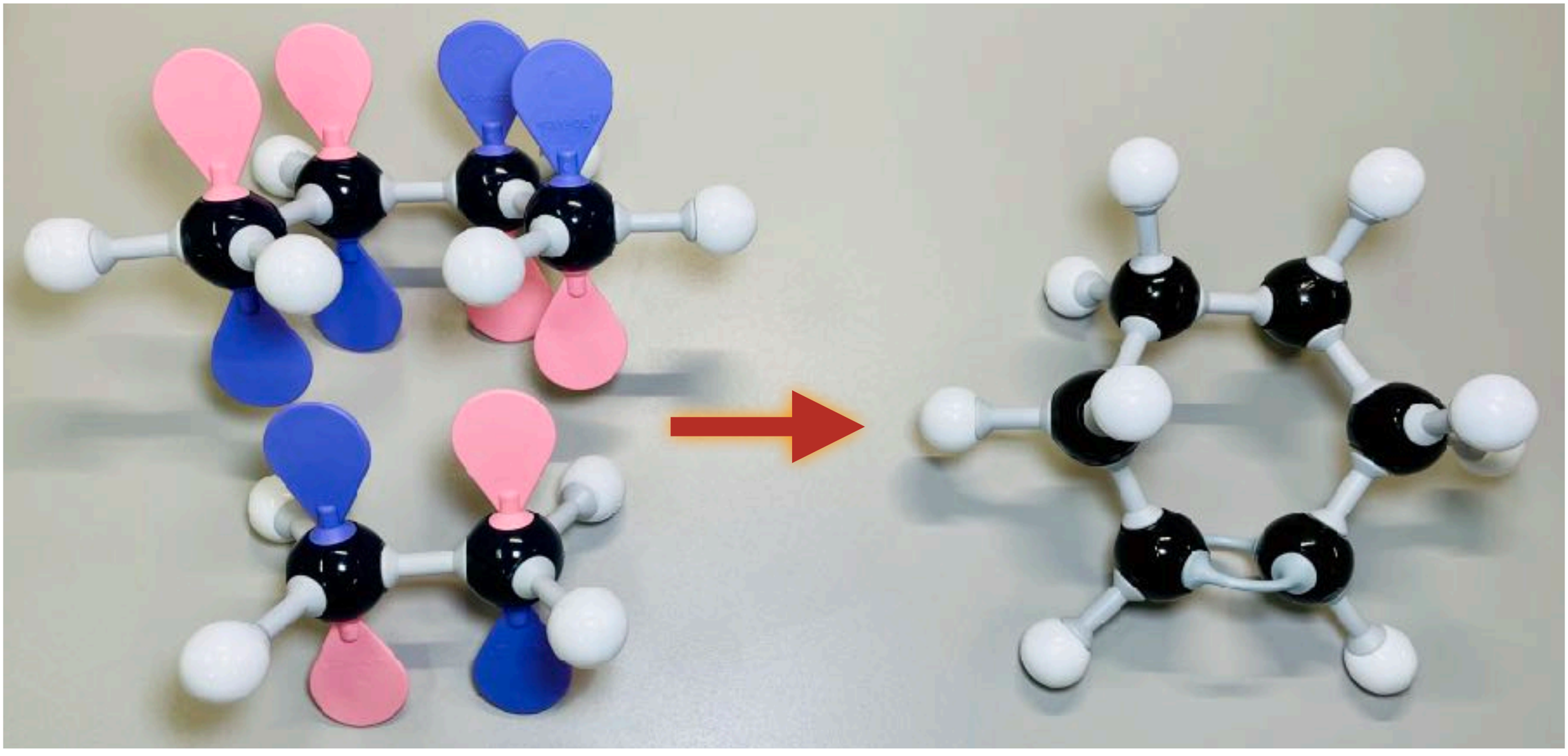
Diels-Alder反応を分子軌道で考える

ブタジエン の HOMO と エチレン の LUMO が
相互作用することで，環化（結合形成）が起こる



Diels-Alder反応を分子模型で考える

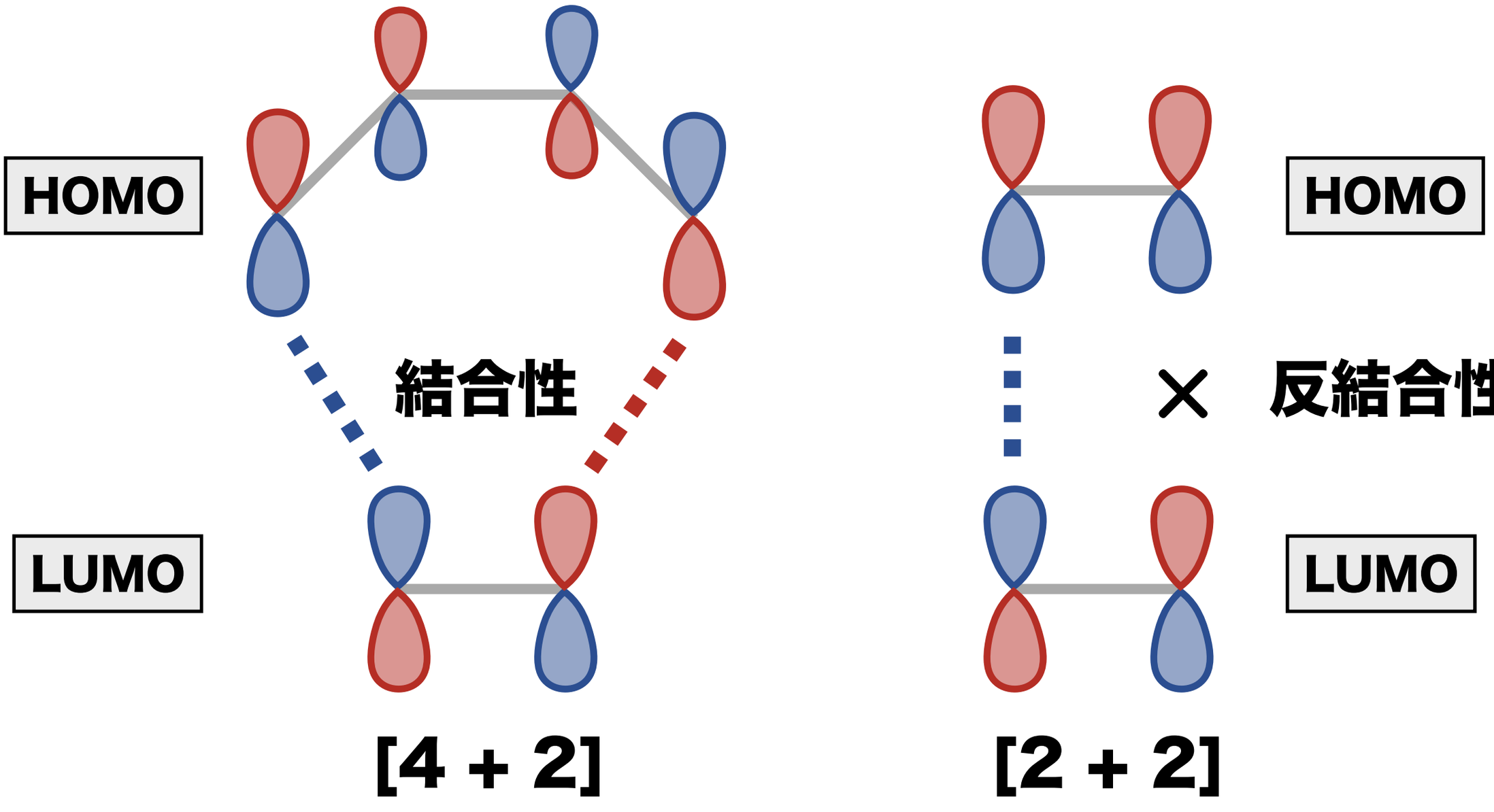
ブタジエン の HOMO と エチレン の LUMO が相互作用することで，環化（結合形成）が起こる



Diels-Alder反応を分子軌道で考える

エチレン同士の場合，HOMO と LUMO の

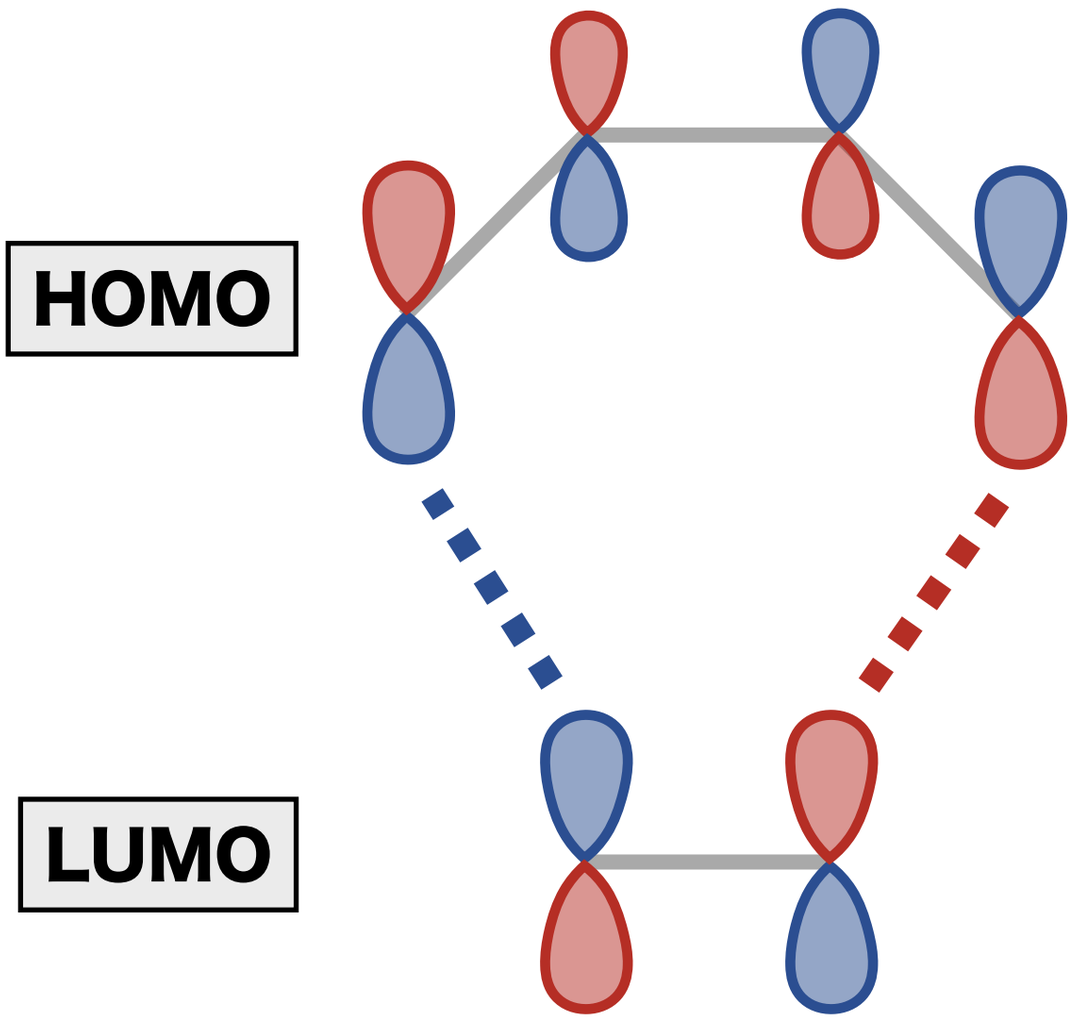
位相がそろわない ➡ 結合を形成しない



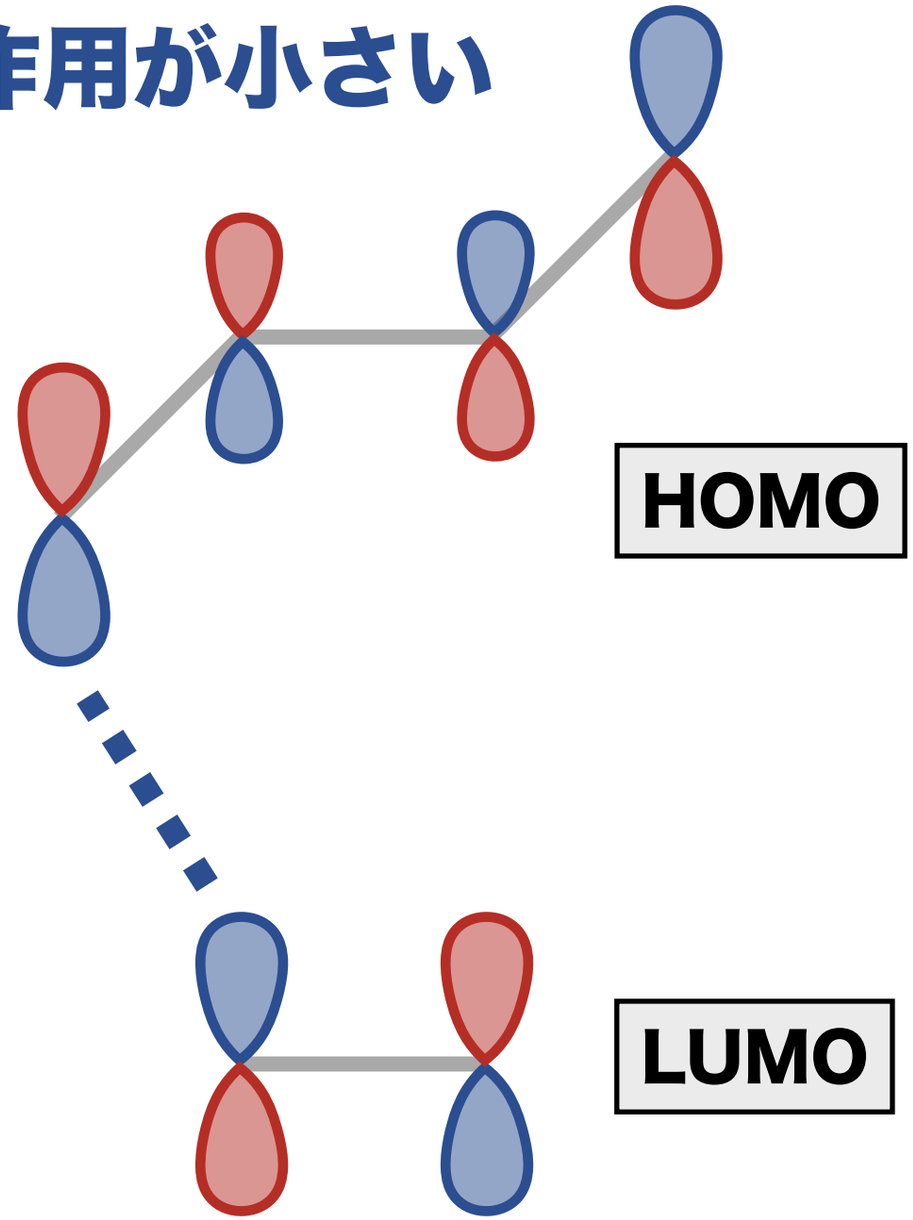
Diels-Alder反応を分子軌道で考える

トランス型の場合，HOMO と LUMO の

軌道の重なりが小さい ➡ 相互作用が小さい

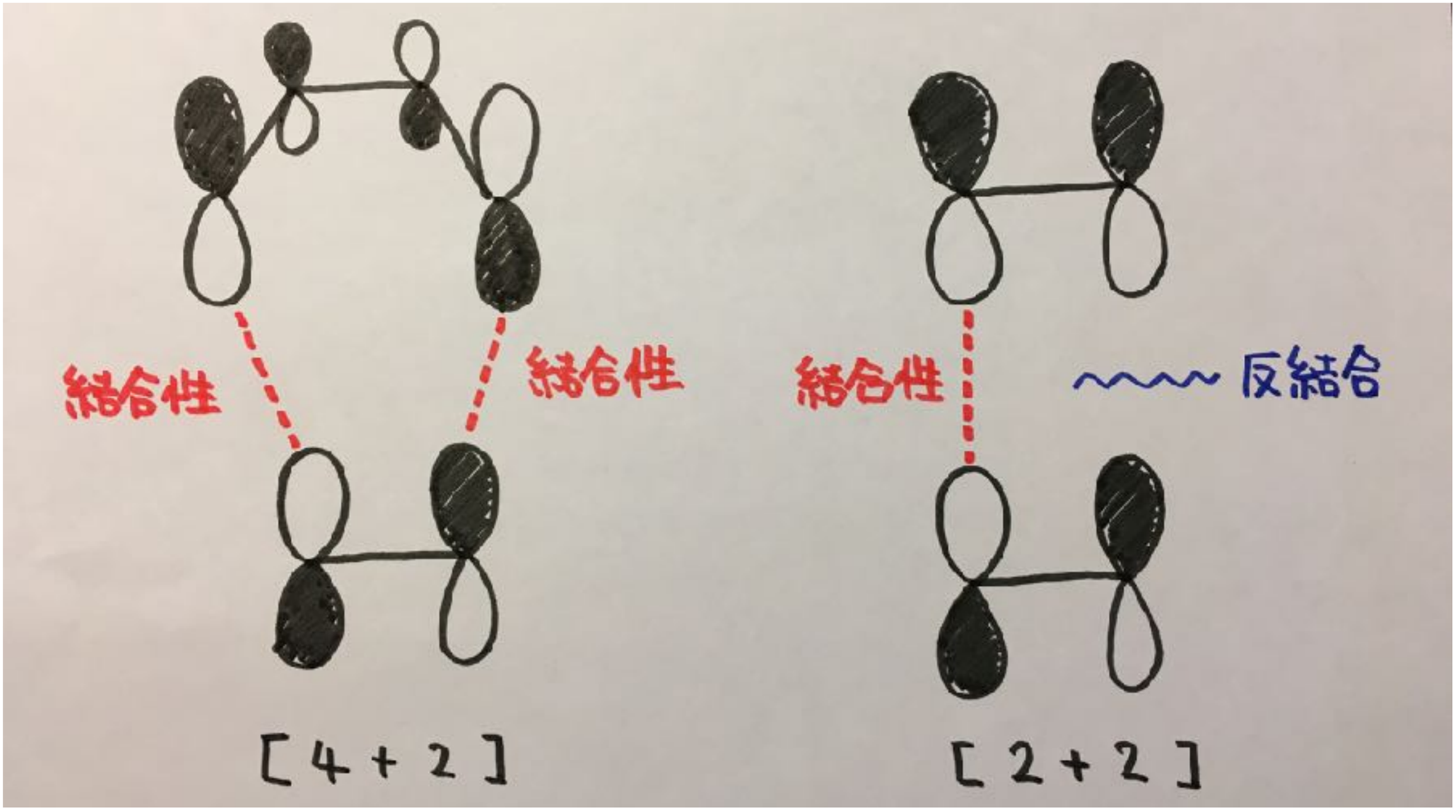


シス型



トランス型

できる化学者は 図 や 模型 で考えて、
量子化学計算 で 理論的に解析 する！

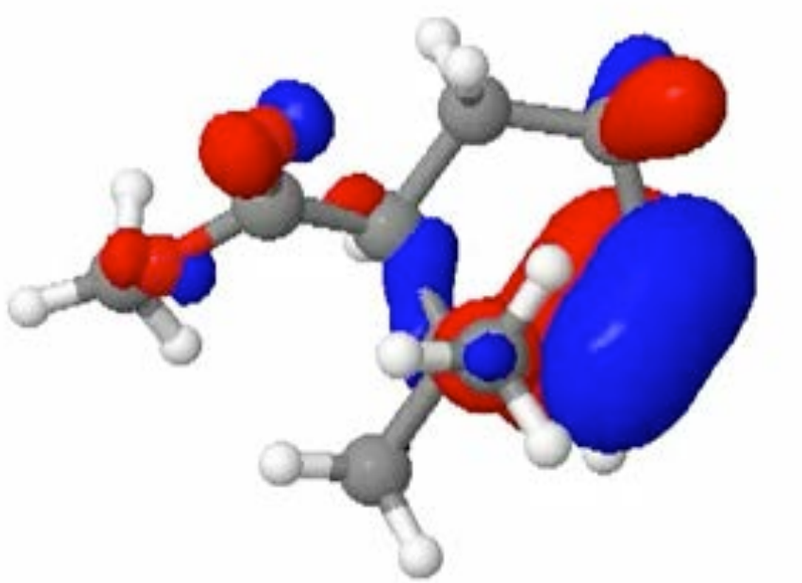


量子化学計算 とは？

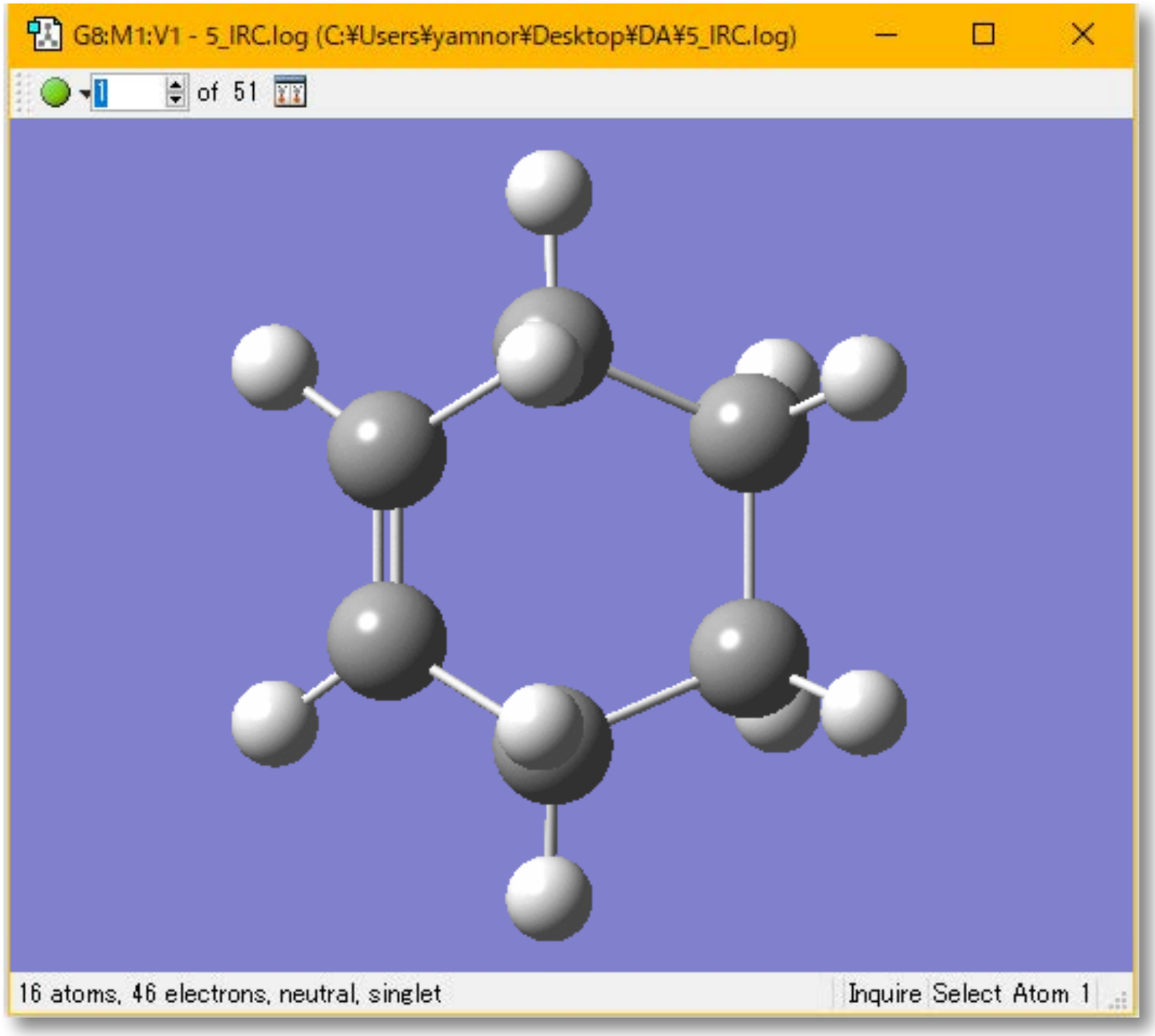
シュレディンガー方程式 を **コンピュータ** を用いて

まあまあ厳密 に解くことで、**定量的な精度** で、

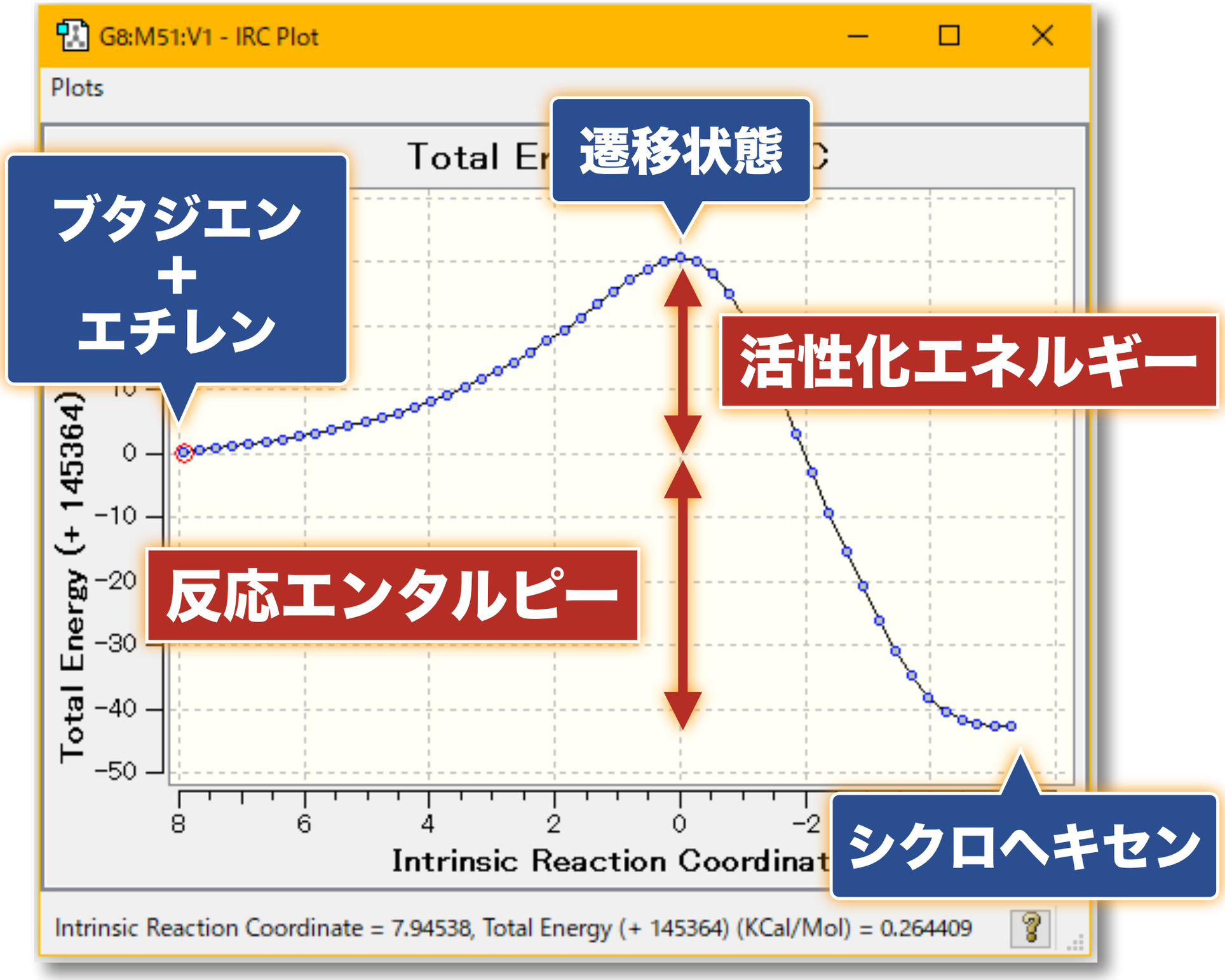
研究開発の実際的な問題解決 ができる強力な方法



Diels-Alder反応をシミュレーション



Diels-Alder反応のエネルギー曲線



今日の課題

- ブタジエンを計算する
- エチレンを計算する

分子構造を自分で作る

- 遷移状態を計算する
- シクロヘキセンを計算する

入力ファイルを利用する

- 反応経路を解析する

出力ファイルを利用する

実習の準備

デスクトップにファイルを展開する

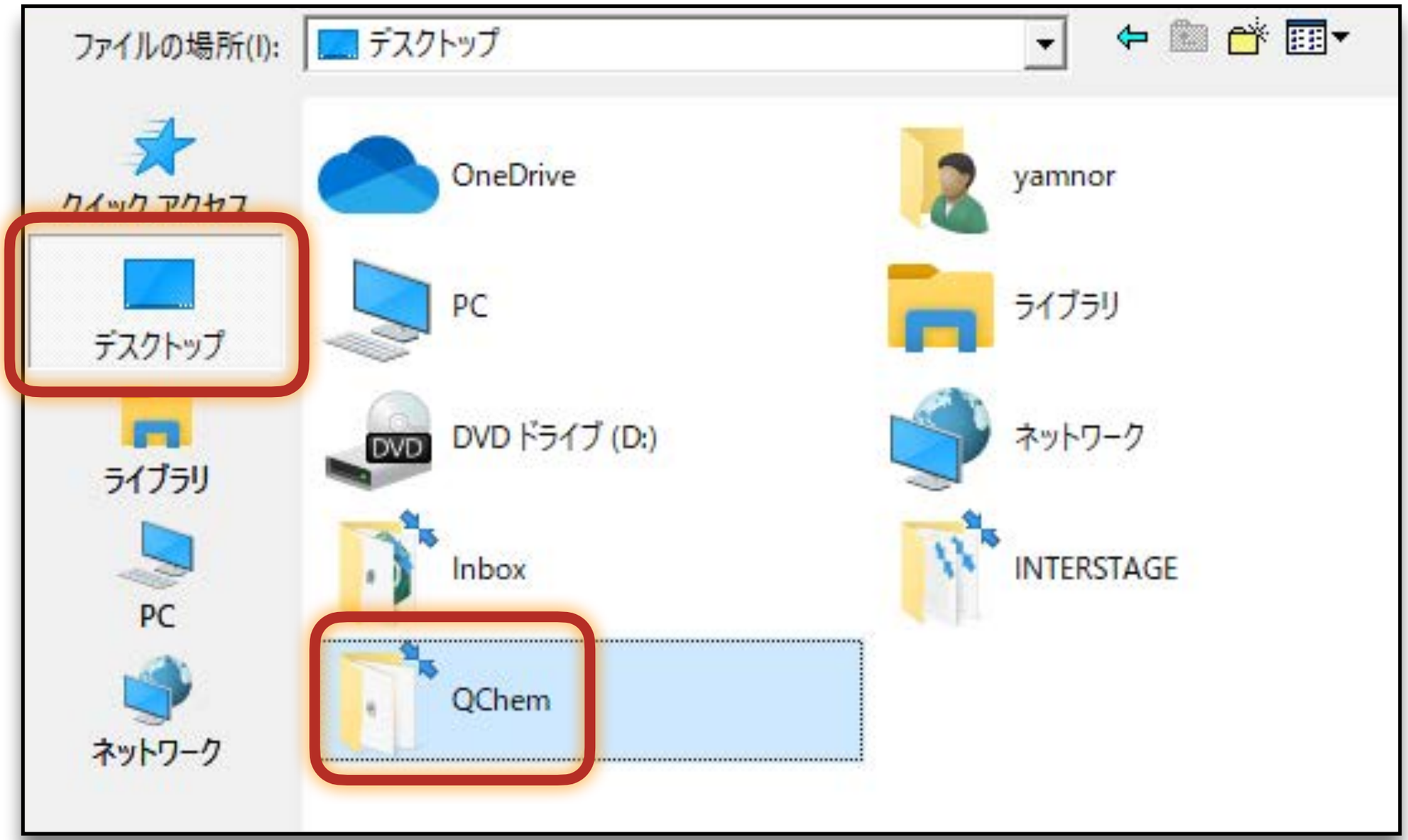
QChem.zip をダウンロード

➡ 右クリック

➡ すべて展開（保存先を**デスクトップ**に指定する）

全てのファイルの保存先

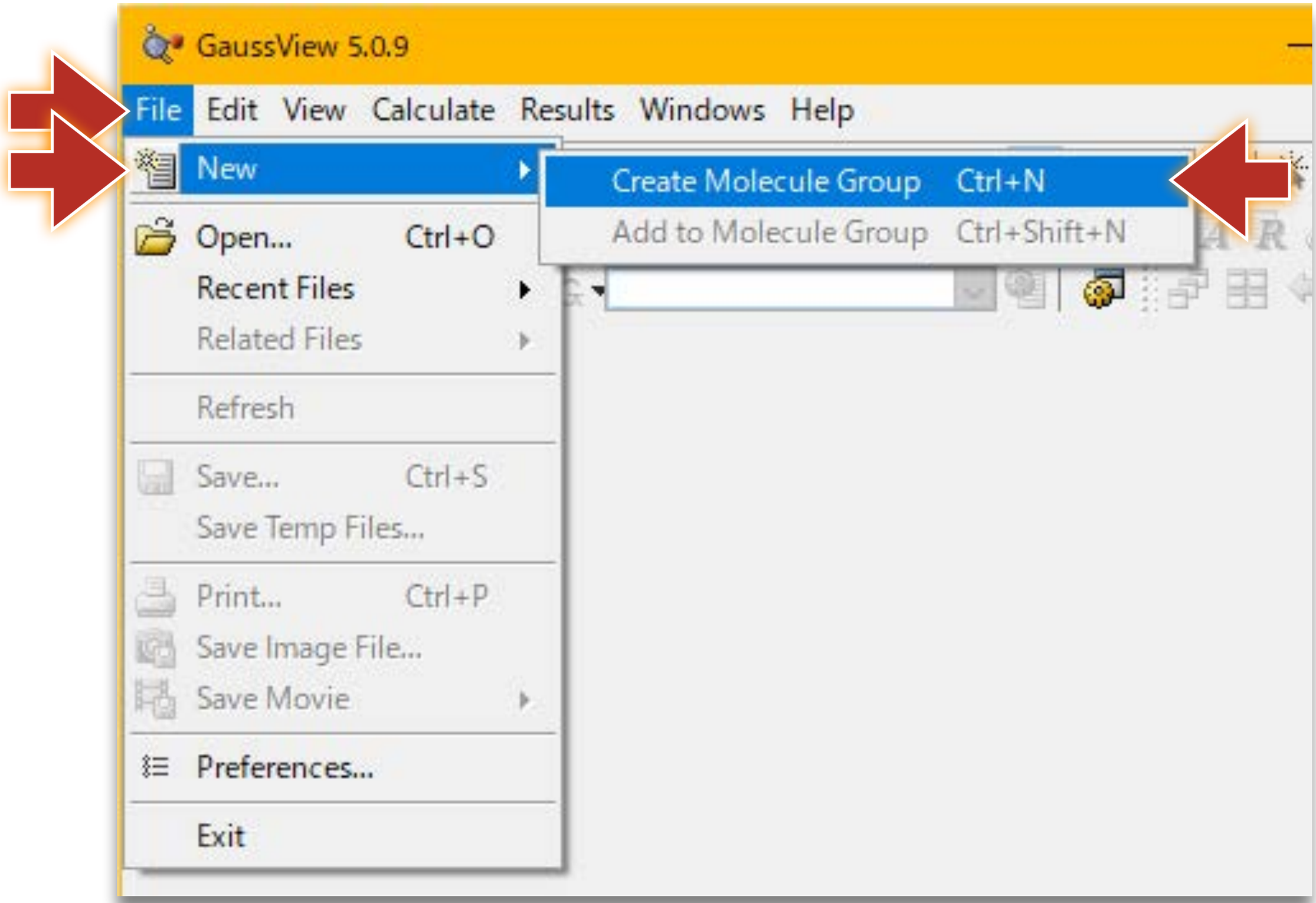
今日作成する全てのファイルは、
デスクトップ の **QChem フォルダ** に保存する



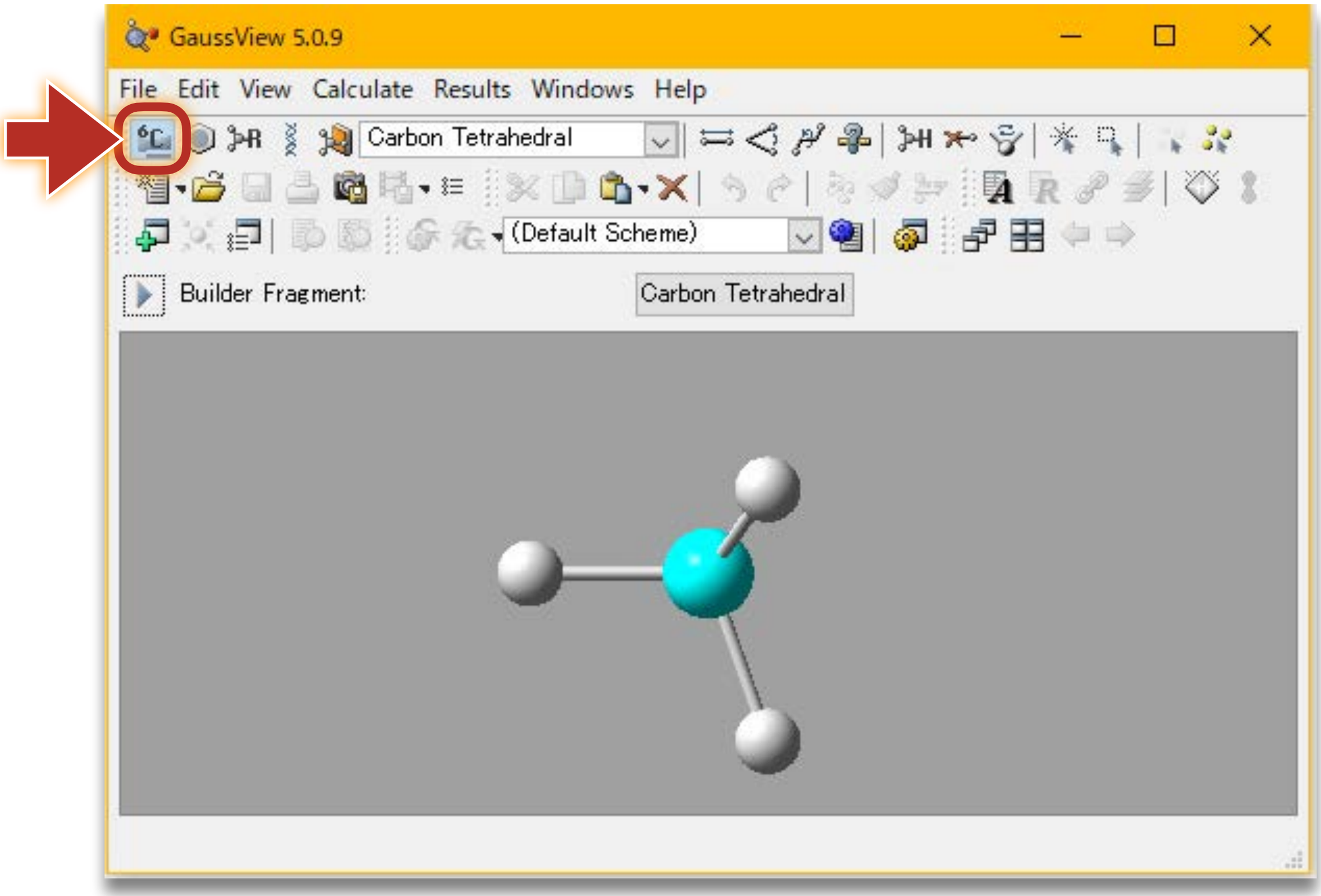
休憩時間：5分

ブタジエンの量子化学計算

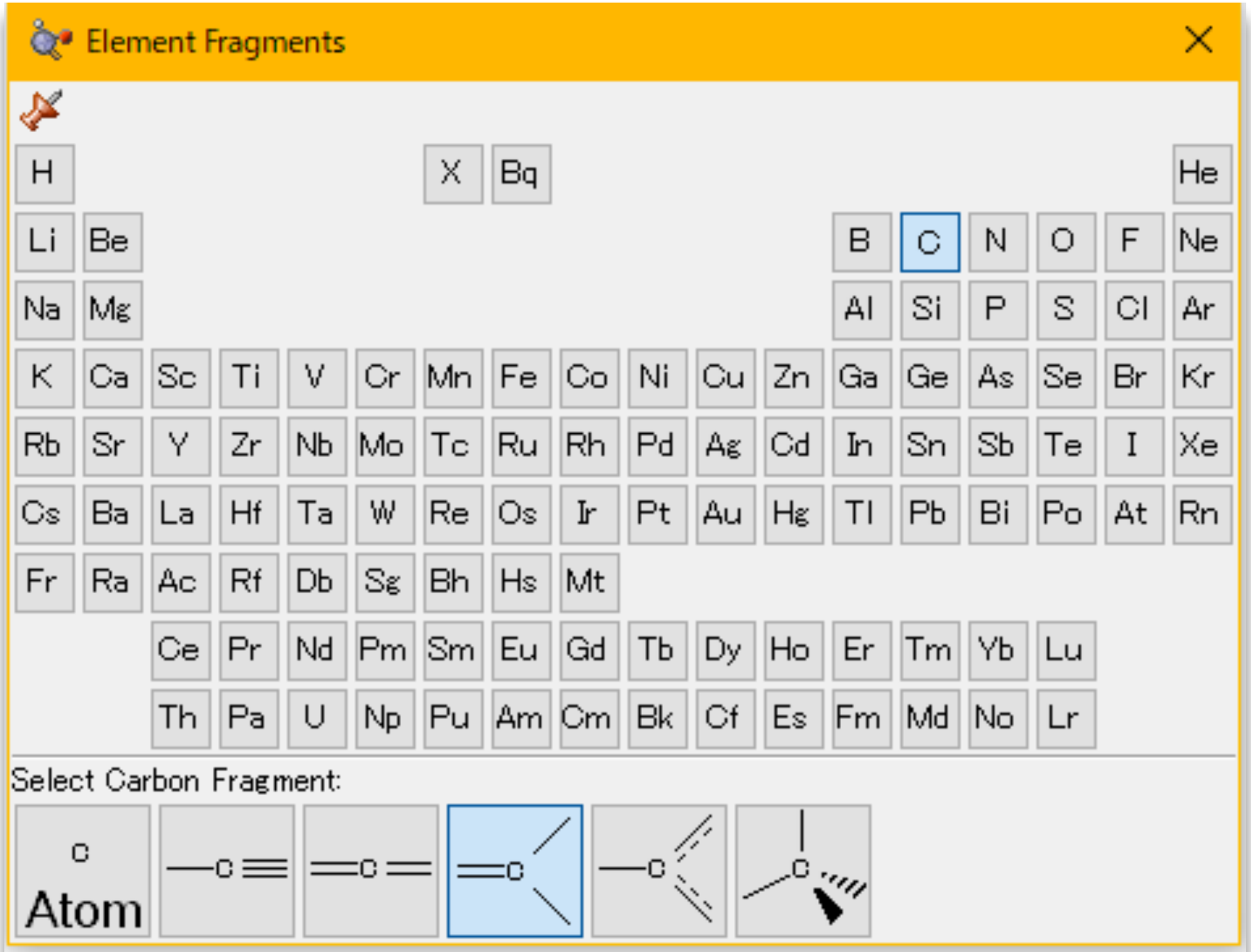
分子構造を作成する


GaussView 5.0.9
File
Edit
View
Calculate
Results
Windows
Help
New
Open... Ctrl+O
Recent Files
Related Files
Refresh
Save... Ctrl+S
Save Temp Files...
Print... Ctrl+P
Save Image File...
Save Movie
Preferences...
Exit
Create Molecule Group Ctrl+N
Add to Molecule Group Ctrl+Shift+N

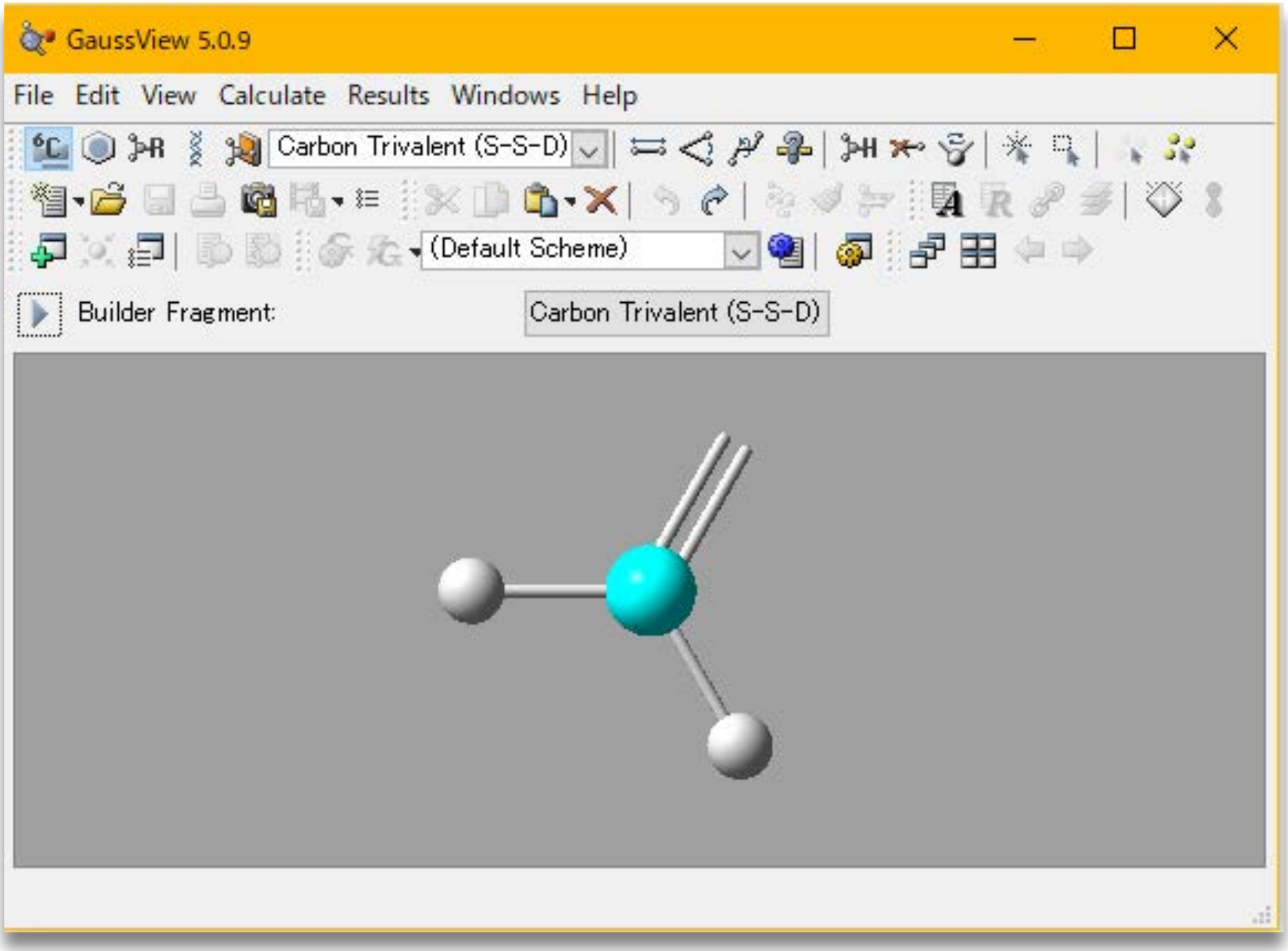
分子構造を作成する


GaussView 5.0.9
File Edit View Calculate Results Windows Help
Carbon Tetrahedral
(Default Scheme)
Builder Fragment:
Carbon Tetrahedral

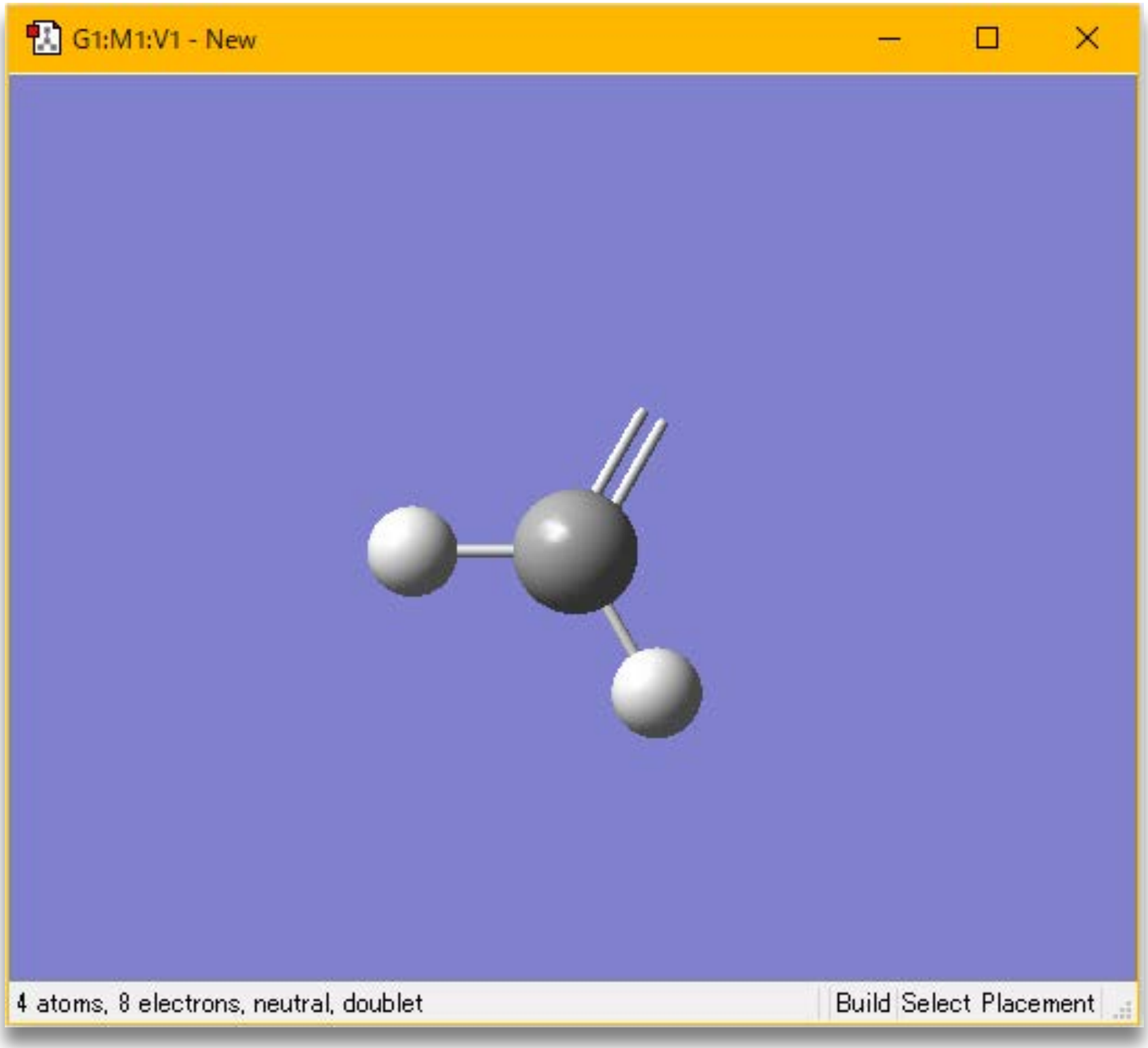
分子構造を作成する


Element Fragments
H
X
Bq
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
La
Hf
Ta
W
Re
Os
Ir
Pt
Au
Hg
Tl
Pb
Bi
Po
At
Rn
Fr
Ra
Ac
Rf
Db
Sg
Bh
Hs
Mt
Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Th
Pa
U
Np
Pu
Am
Cm
Bk
Cf
Es
Fm
Md
No
Lr
Select Carbon Fragment:
C
Atom

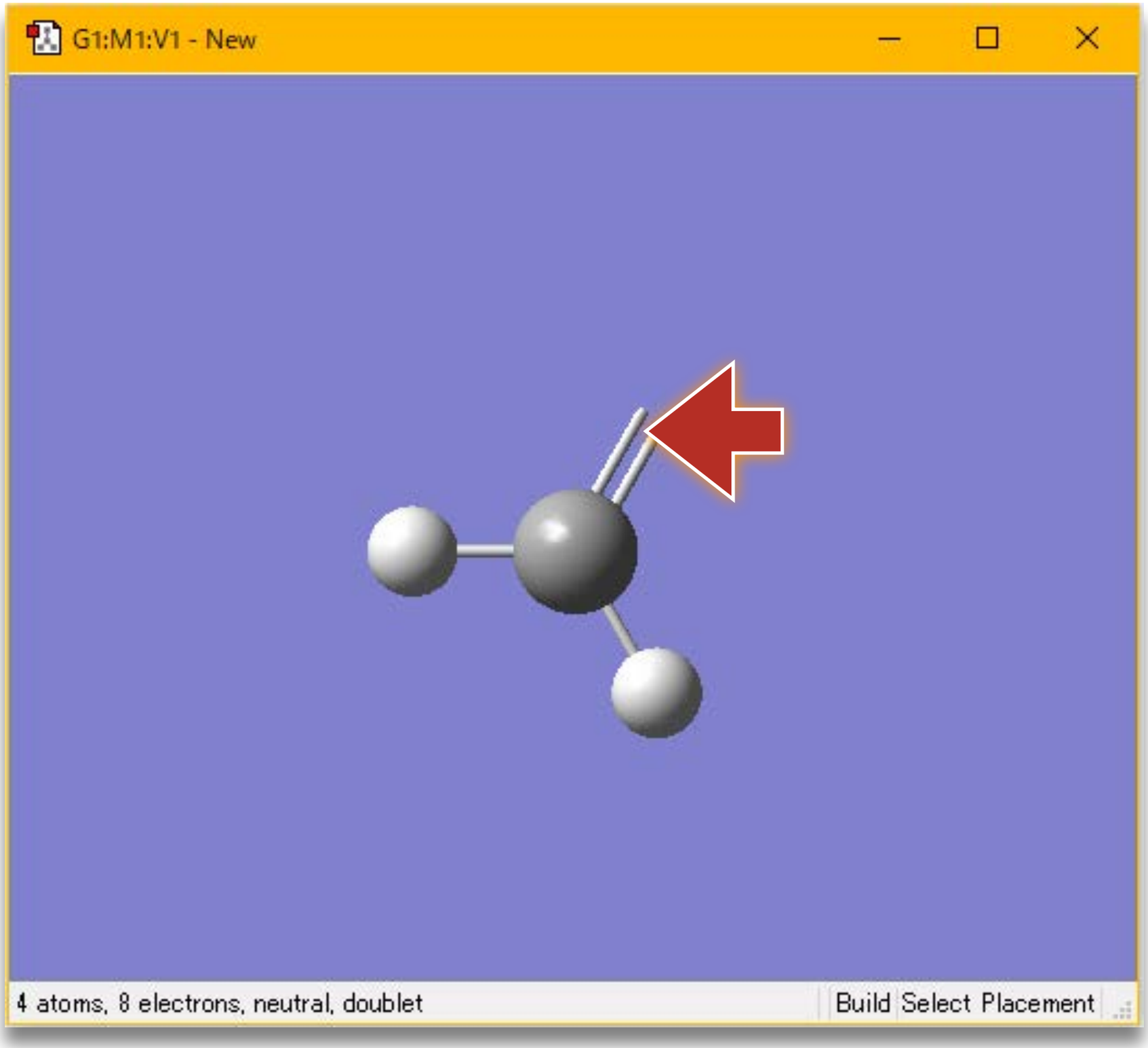
分子構造を作成する


GaussView 5.0.9
File Edit View Calculate Results Windows Help
Carbon Trivalent (S-S-D)
(Default Scheme)
Builder Fragment:
Carbon Trivalent (S-S-D)

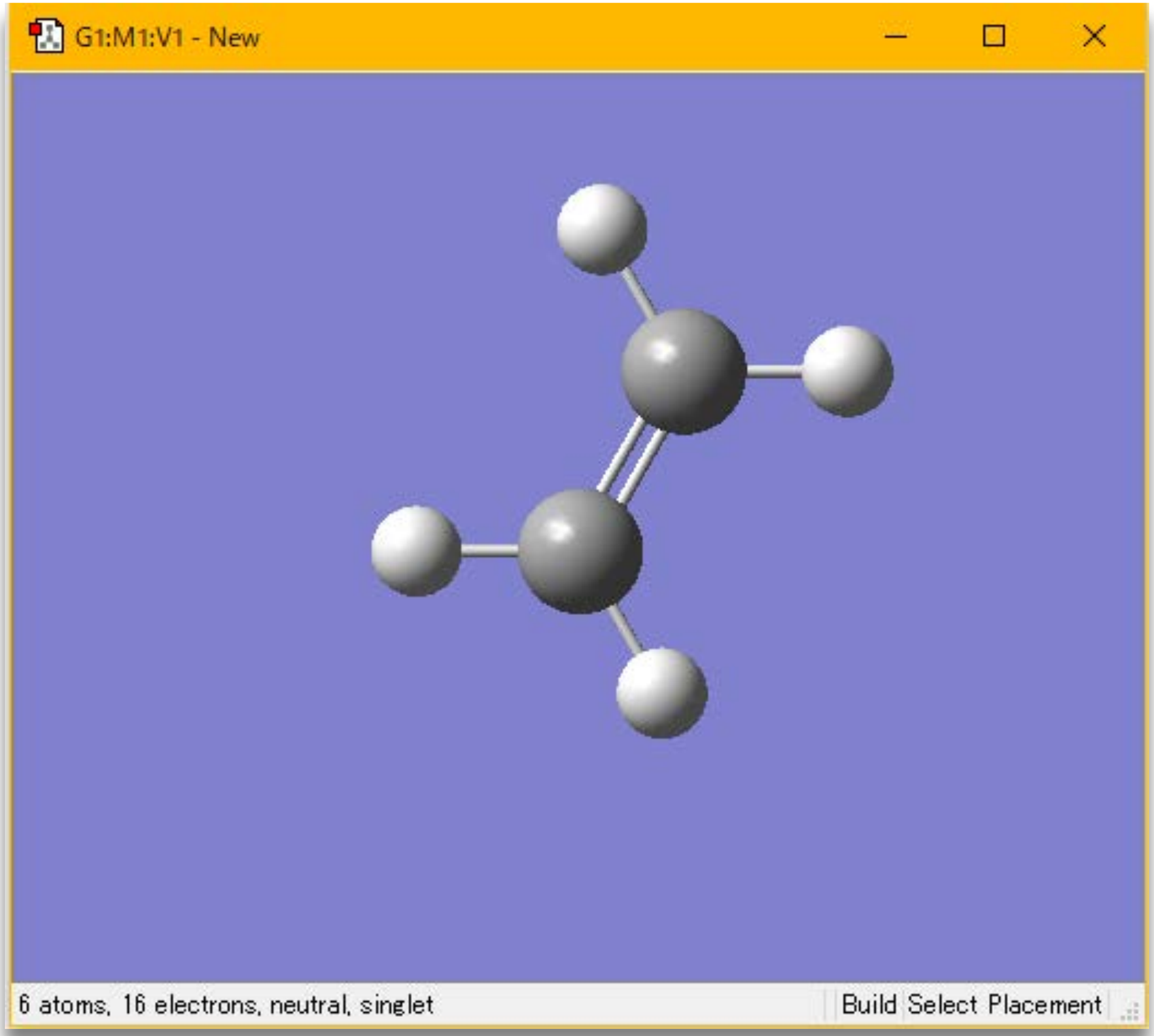
分子構造を作成する


G1:M1:V1 - New
4 atoms, 8 electrons, neutral, doublet
Build Select Placement

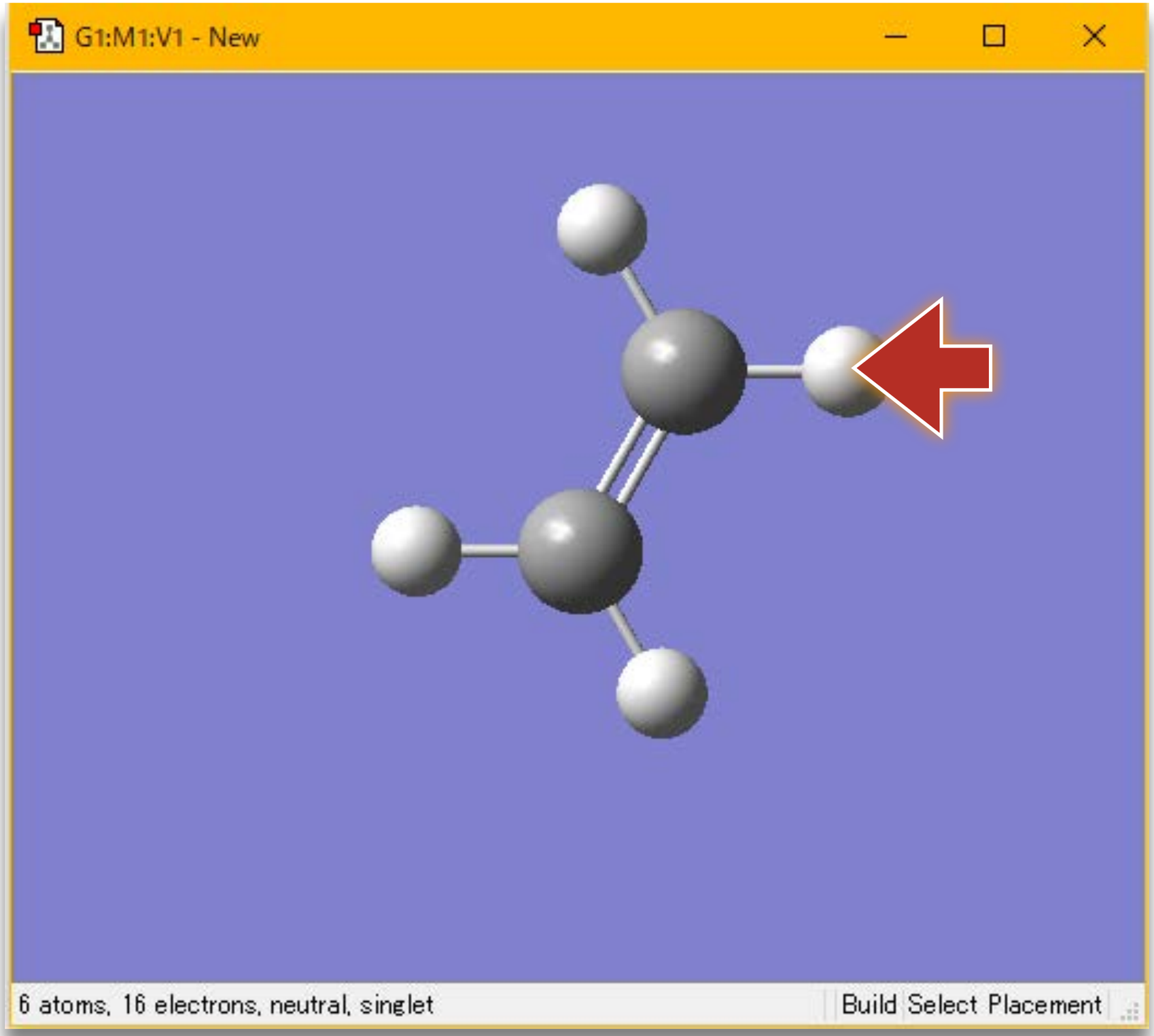
分子構造を作成する


G1:M1:V1 - New
4 atoms, 8 electrons, neutral, doublet
Build Select Placement

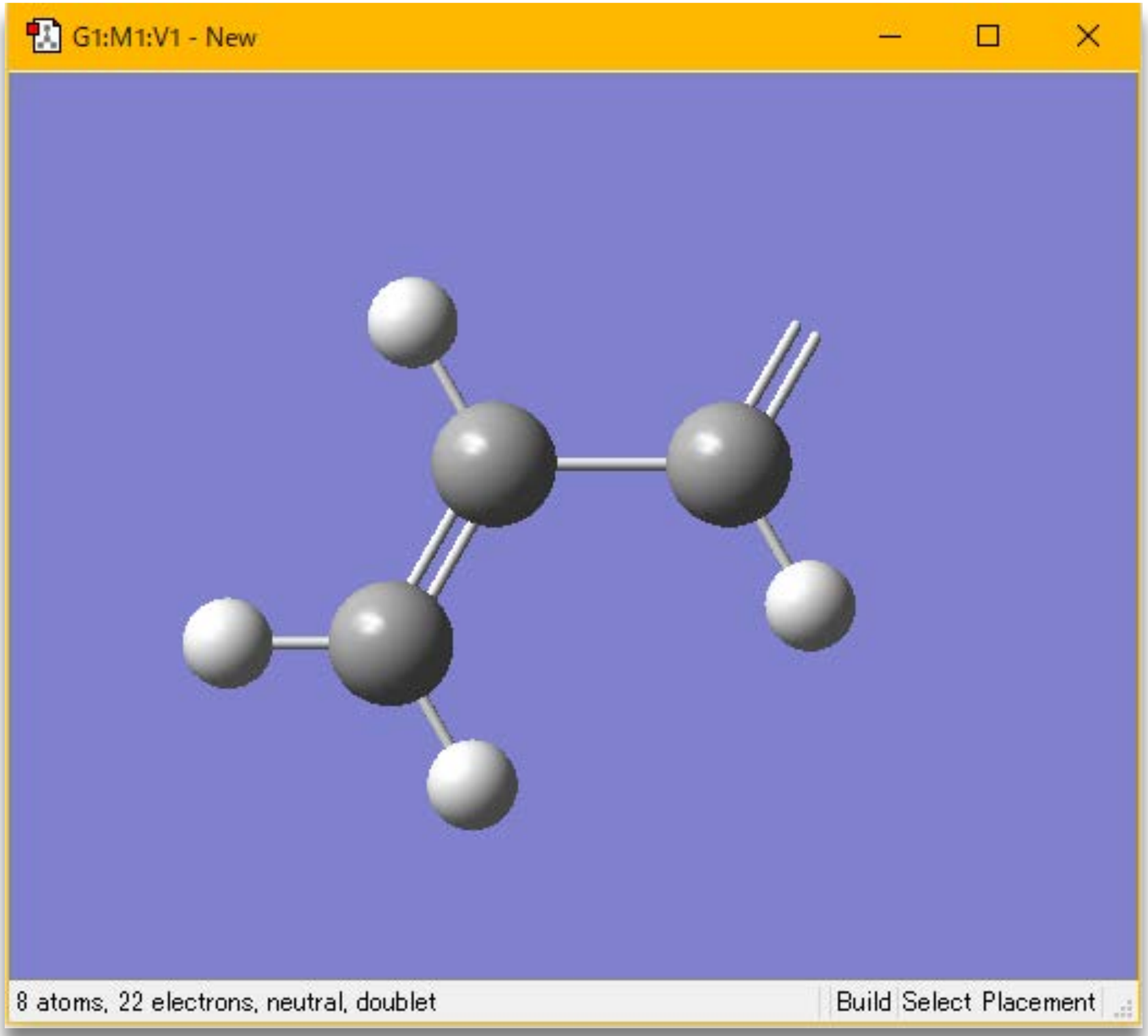
分子構造を作成する


G1:M1:V1 - New
6 atoms, 16 electrons, neutral, singlet
Build Select Placement

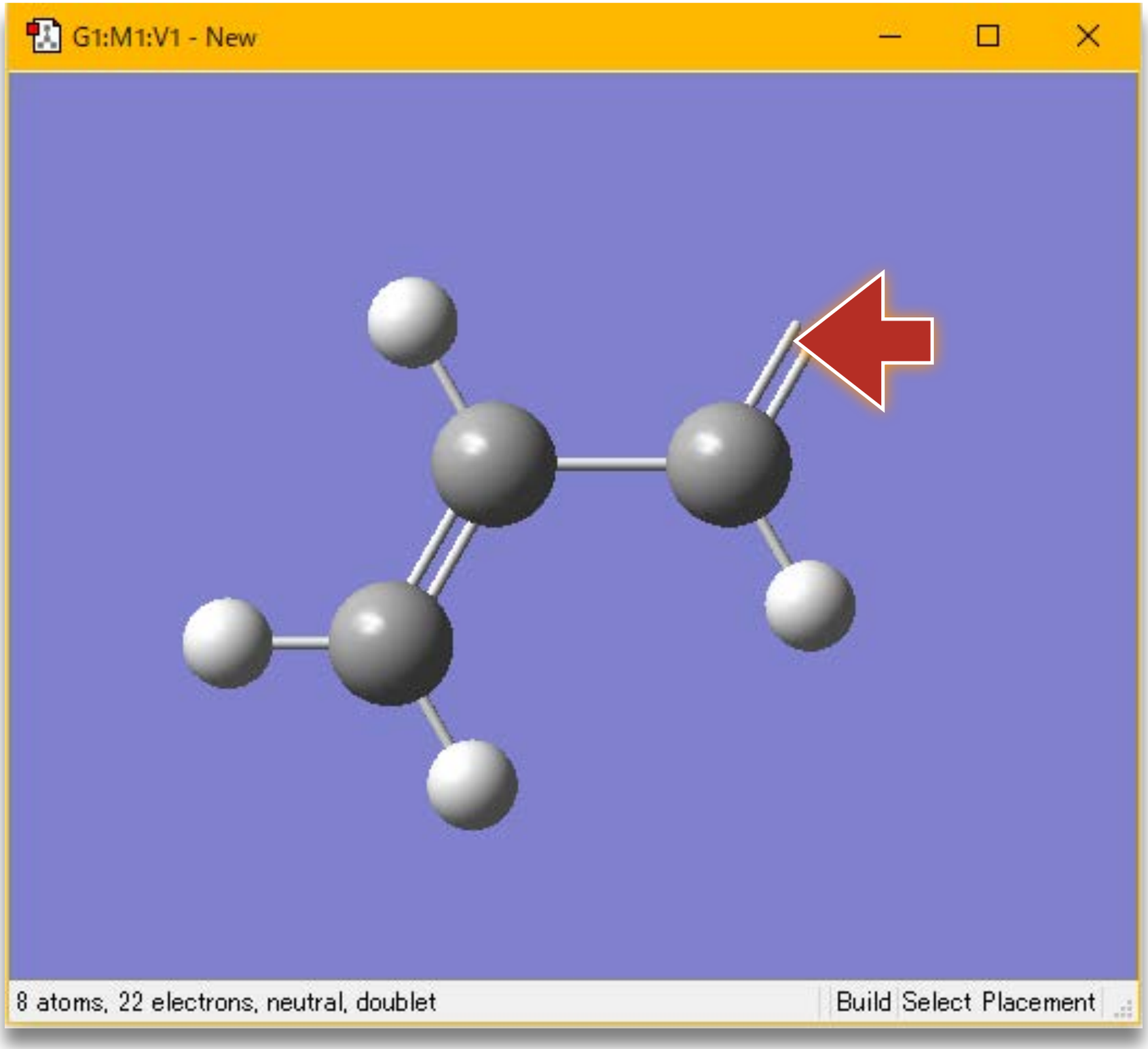
分子構造を作成する


G1:M1:V1 - New
6 atoms, 16 electrons, neutral, singlet
Build Select Placement

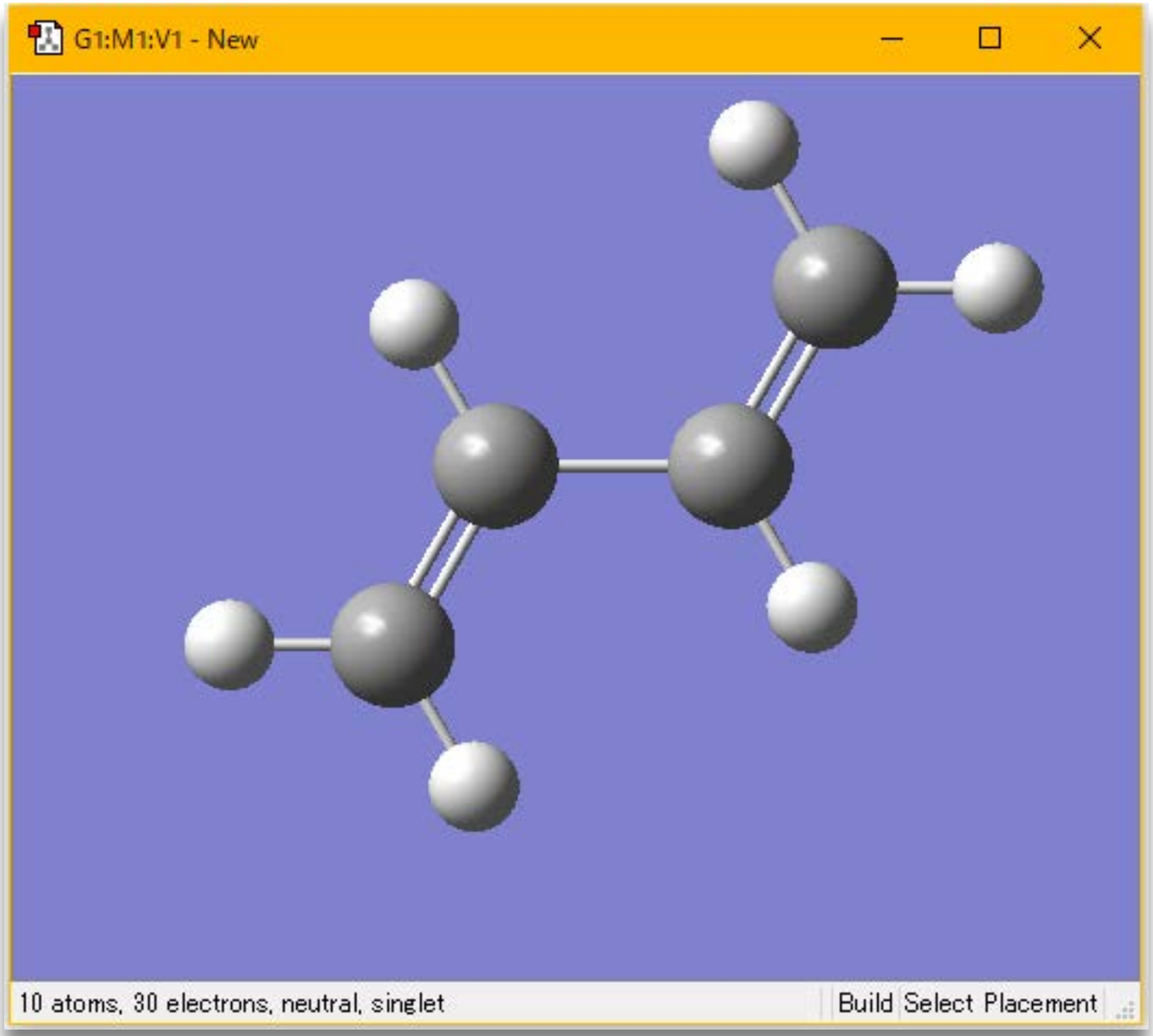
分子構造を作成する


G1:M1:V1 - New
8 atoms, 22 electrons, neutral, doublet
Build
Select
Placement

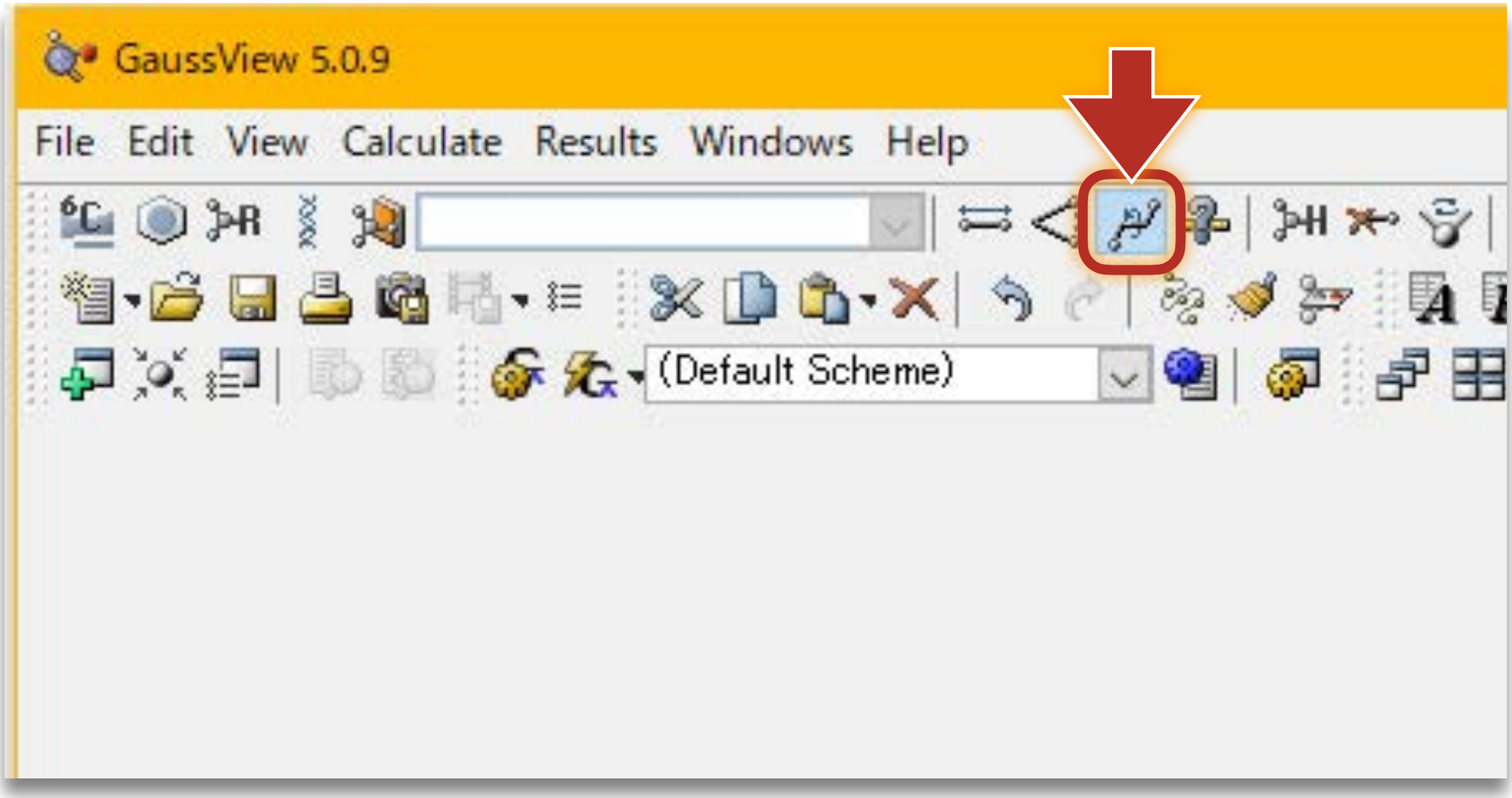
分子構造を作成する


G1:M1:V1 - New
8 atoms, 22 electrons, neutral, doublet
Build
Select
Placement

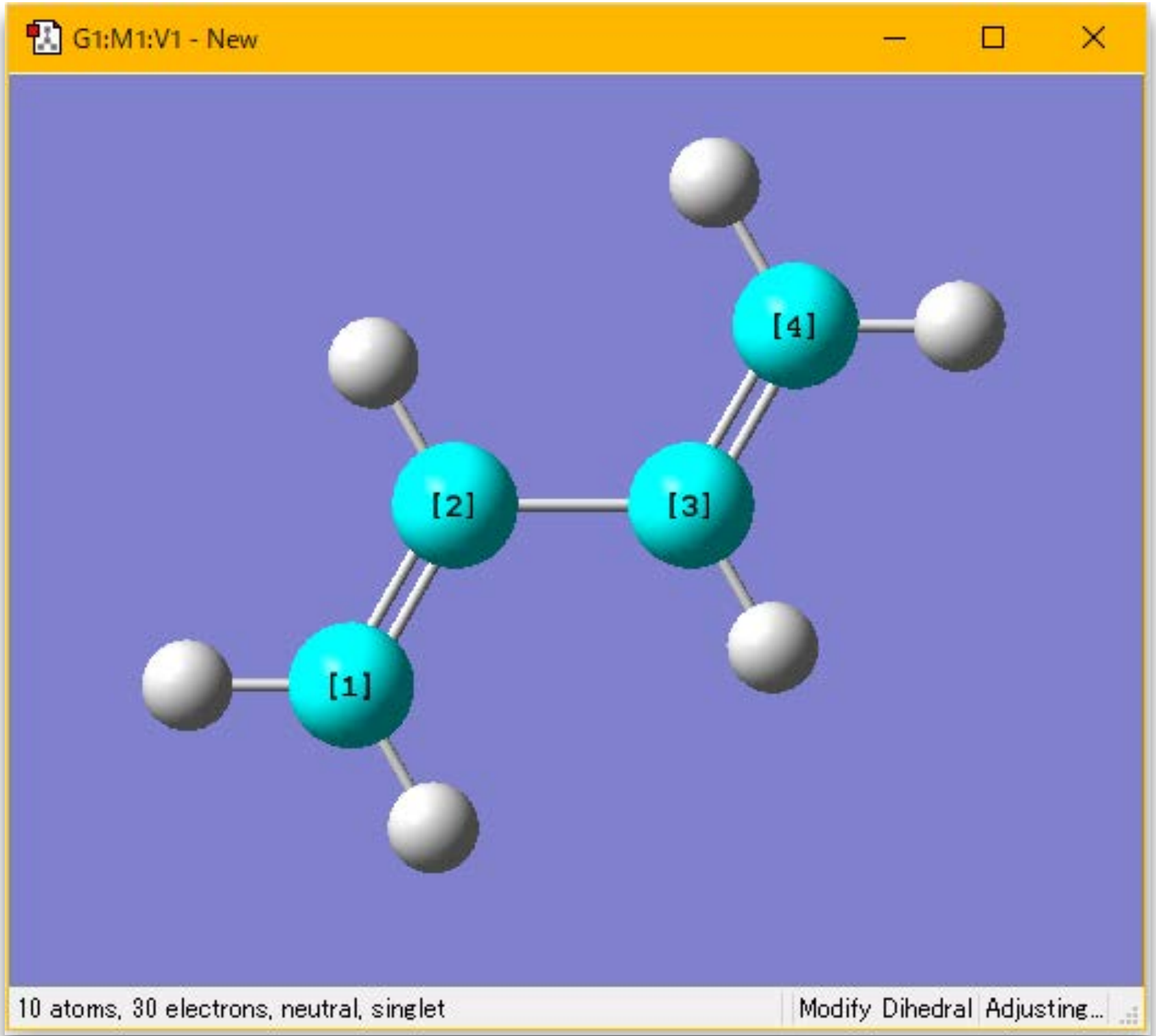
分子構造を作成する


G1:M1:V1 - New
10 atoms, 30 electrons, neutral, singlet
Build
Select
Placement

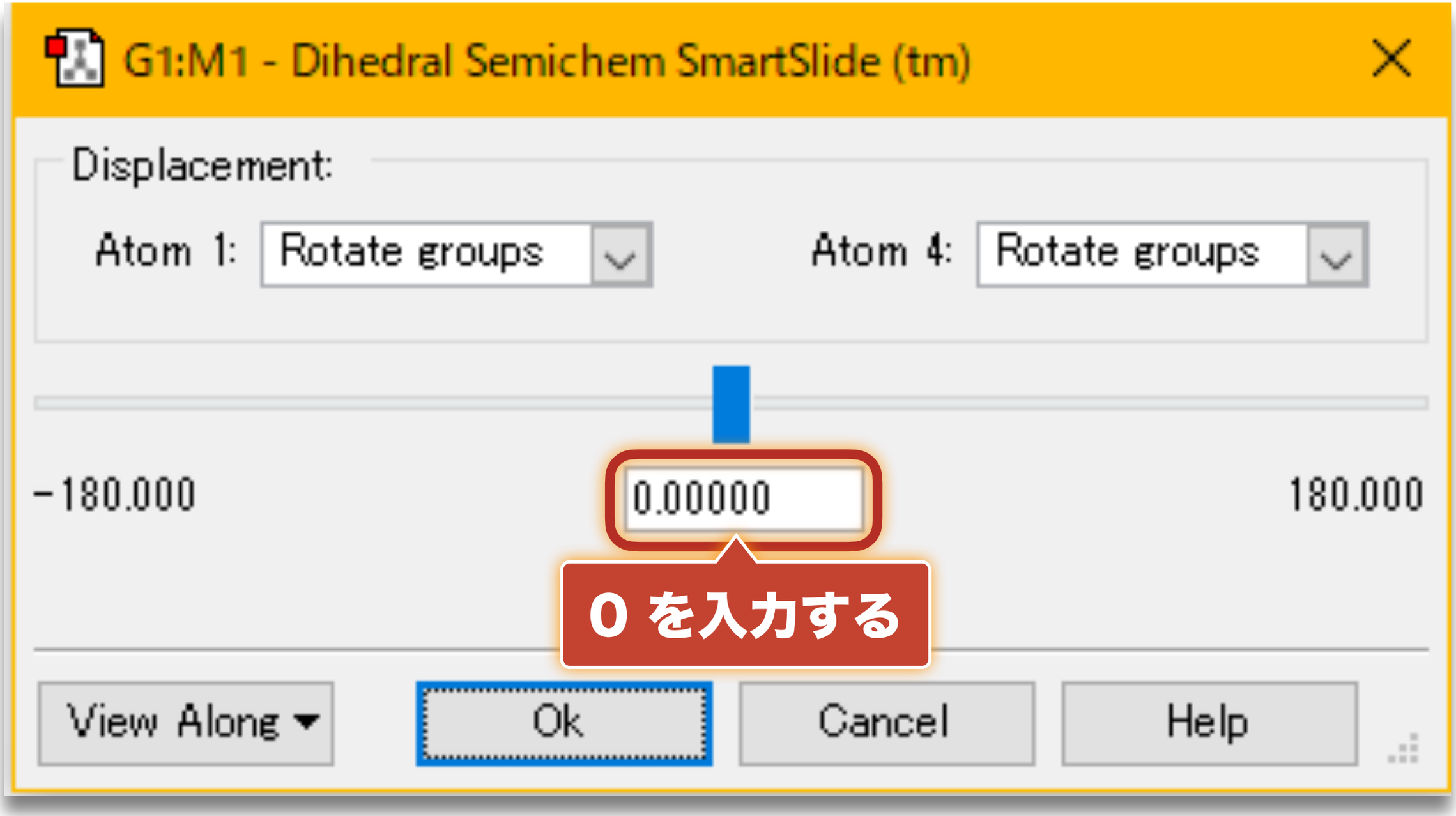
分子構造を作成する


GaussView 5.0.9
File Edit View Calculate Results Windows Help
(Default Scheme)

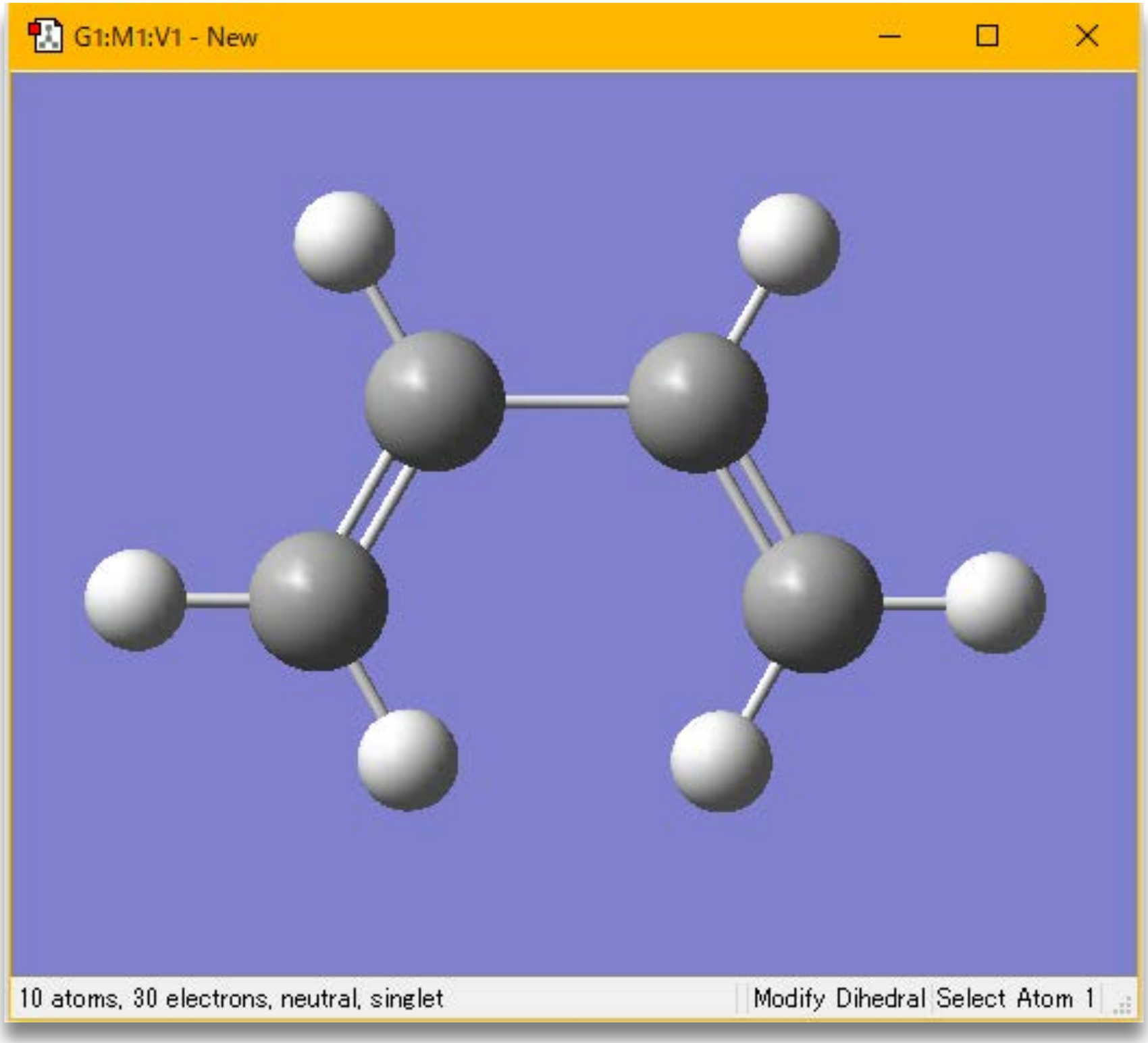
分子構造を作成する


G1:M1:V1 - New
[4]
[2]
[3]
[1]
10 atoms, 30 electrons, neutral, singlet
Modify Dihedral
Adjusting...

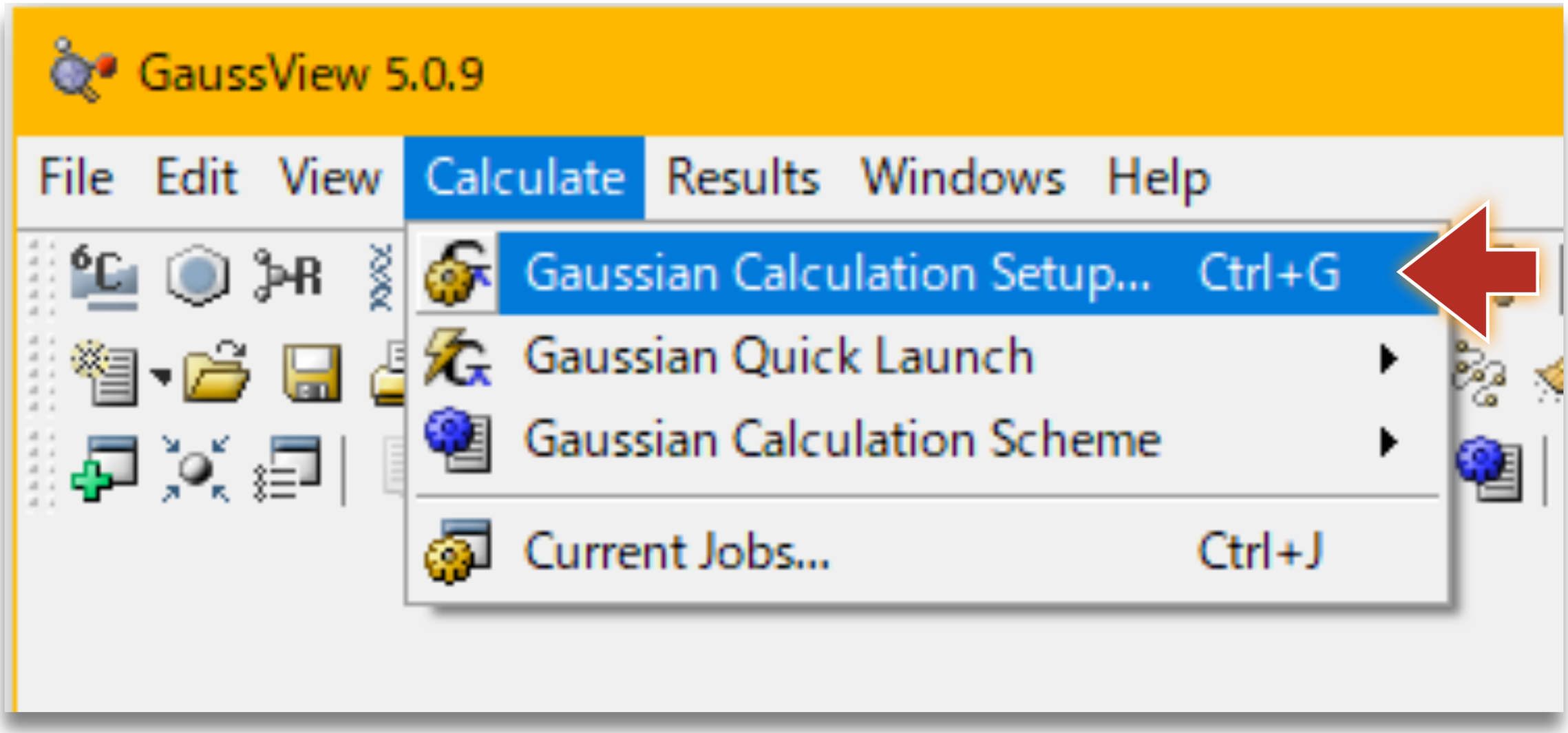
分子構造を作成する


G1:M1 - Dihedral Semichem SmartSlide (tm)
Displacement:
Atom 1:
Rotate groups
Atom 4:
Rotate groups
-180.000
0.00000
180.000
0 を入力する
View Along
Ok
Cancel
Help

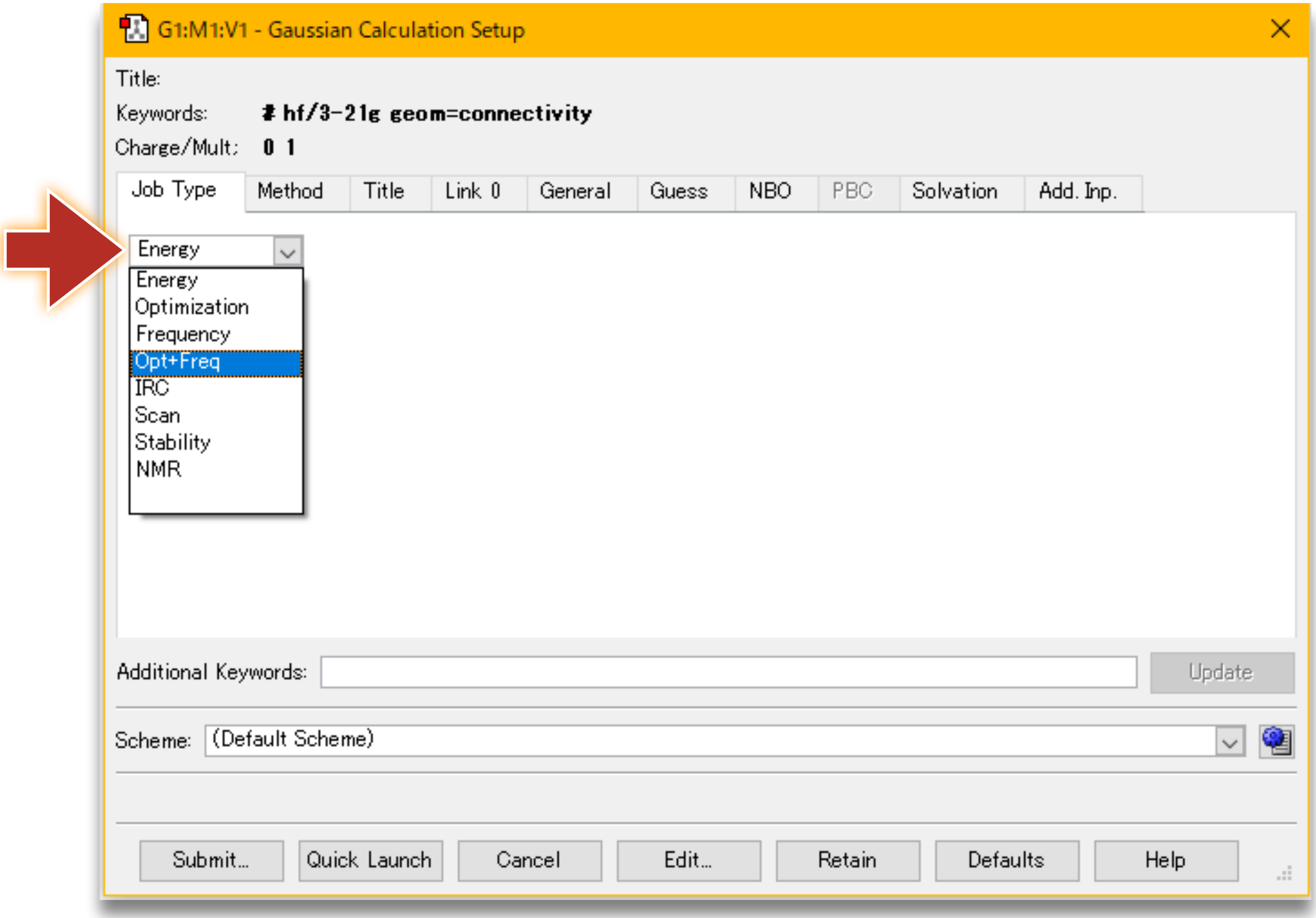
分子構造を作成する


G1:M1:V1 - New
10 atoms, 30 electrons, neutral, singlet
Modify Dihedral
Select Atom 1

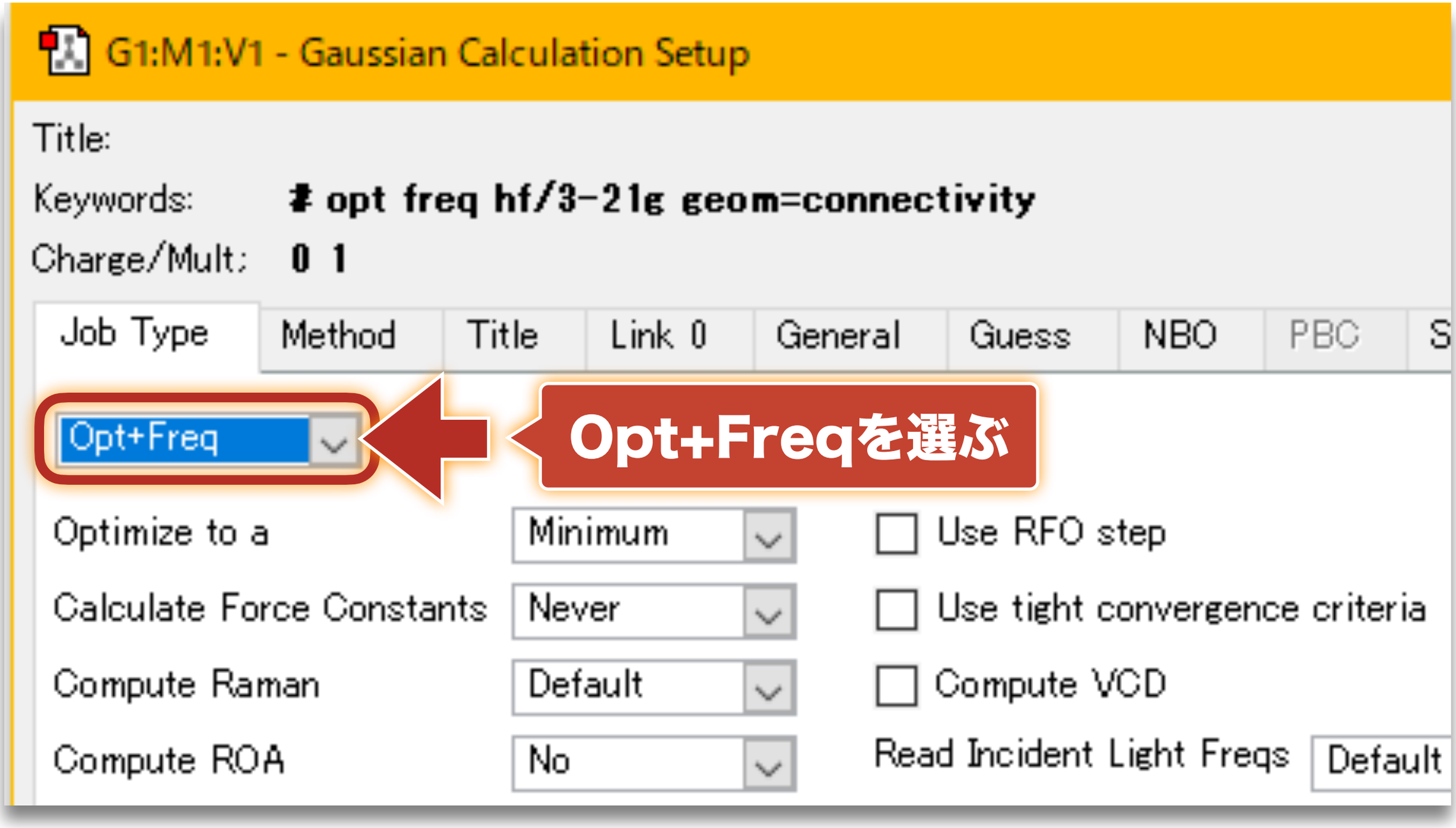
構造最適化


GaussView 5.0.9
File
Edit
View
Calculate
Results
Windows
Help
Gaussian Calculation Setup... Ctrl+G
Gaussian Quick Launch
Gaussian Calculation Scheme
Current Jobs... Ctrl+J

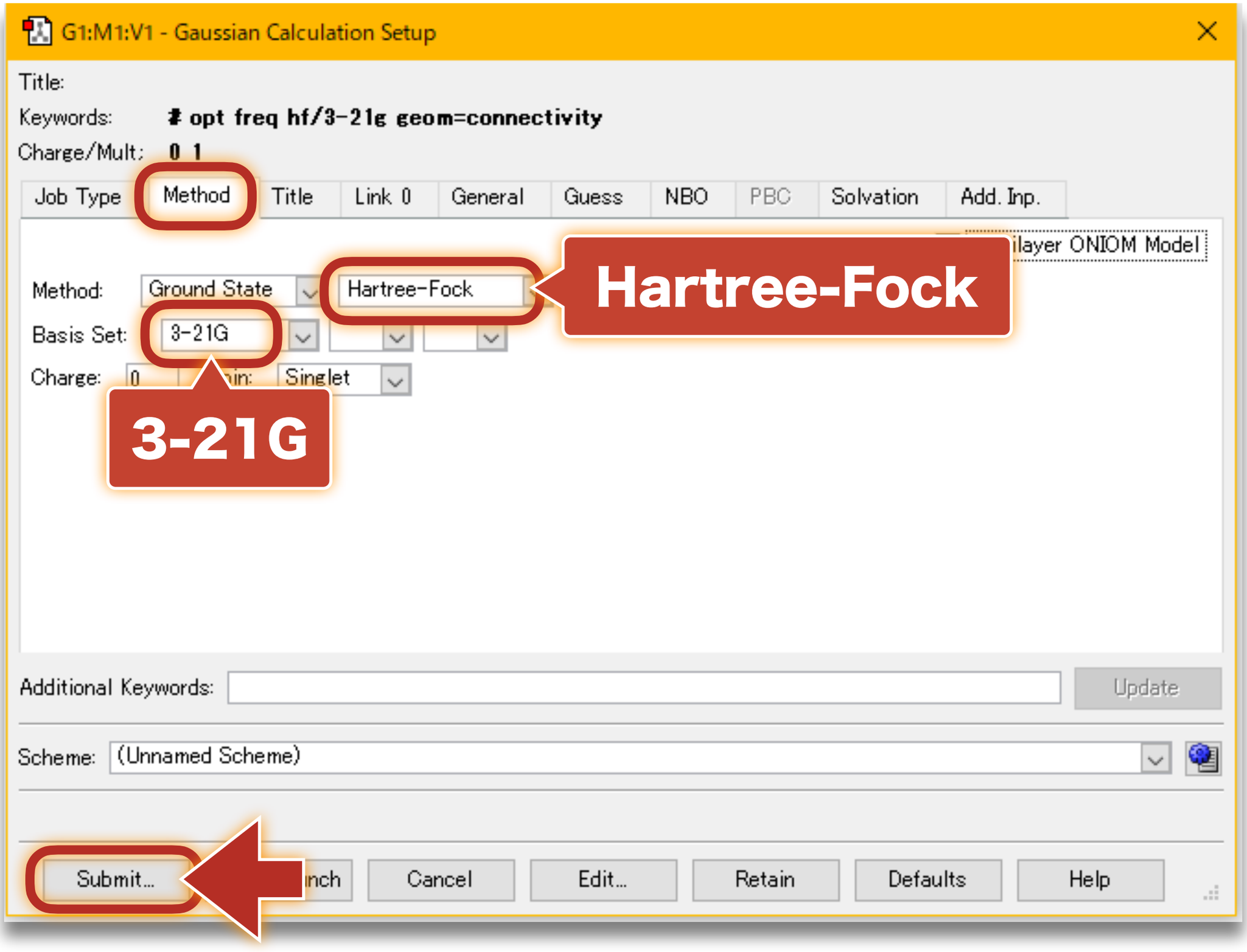
構造最適化


G1:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # hf/3-21g geom=connectivity
Charge/Mult: 0 1
Job Type
Method
Title
Link 0
General
Guess
NBO
PBC
Solvation
Add. Inp.
Energy
Energy
Optimization
Frequency
Opt+Freq
IRC
Scan
Stability
NMR
Additional Keywords:
Update
Scheme: (Default Scheme)
Submit...
Quick Launch
Cancel
Edit...
Retain
Defaults
Help

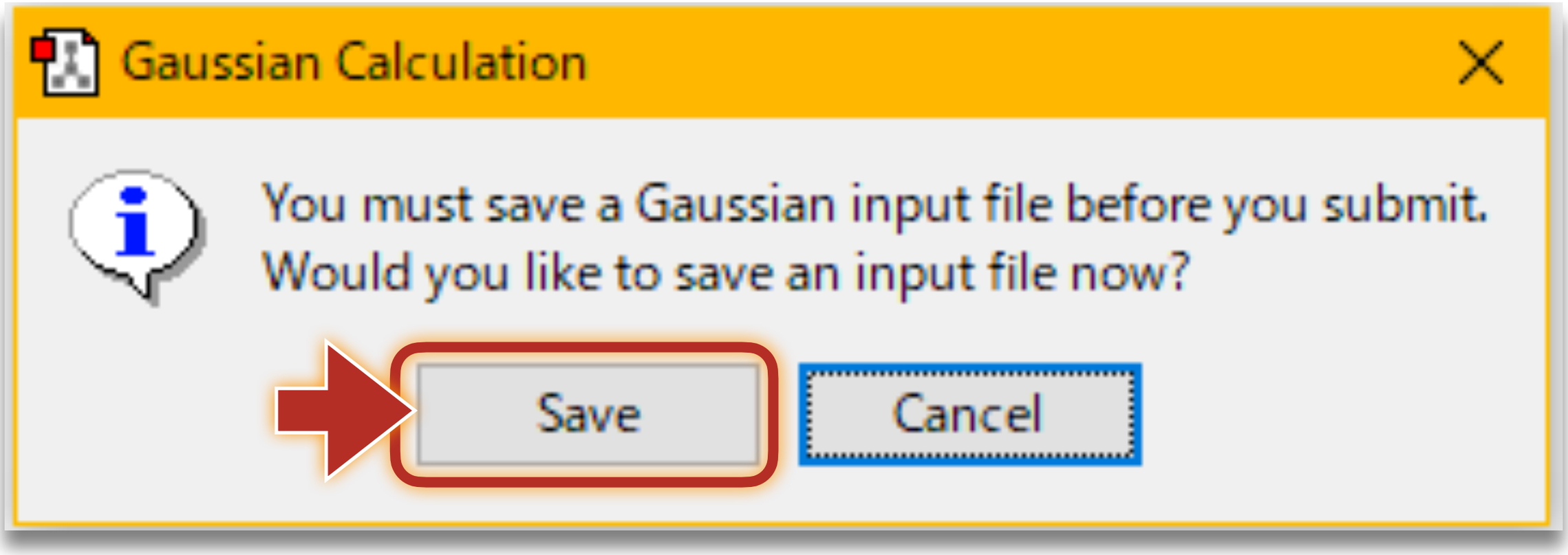
構造最適化


G1:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # opt freq hf/3-21g geom=connectivity
Charge/Mult: 0 1
Job Type
Method
Title
Link 0
General
Guess
NBO
PBC
S
Opt+Freq
Opt+Freqを選ぶ
Optimize to a
Minimum
Use RFO step
Calculate Force Constants
Never
Use tight convergence criteria
Compute Raman
Default
Compute VCD
Compute ROA
No
Read Incident Light Freqs
Default

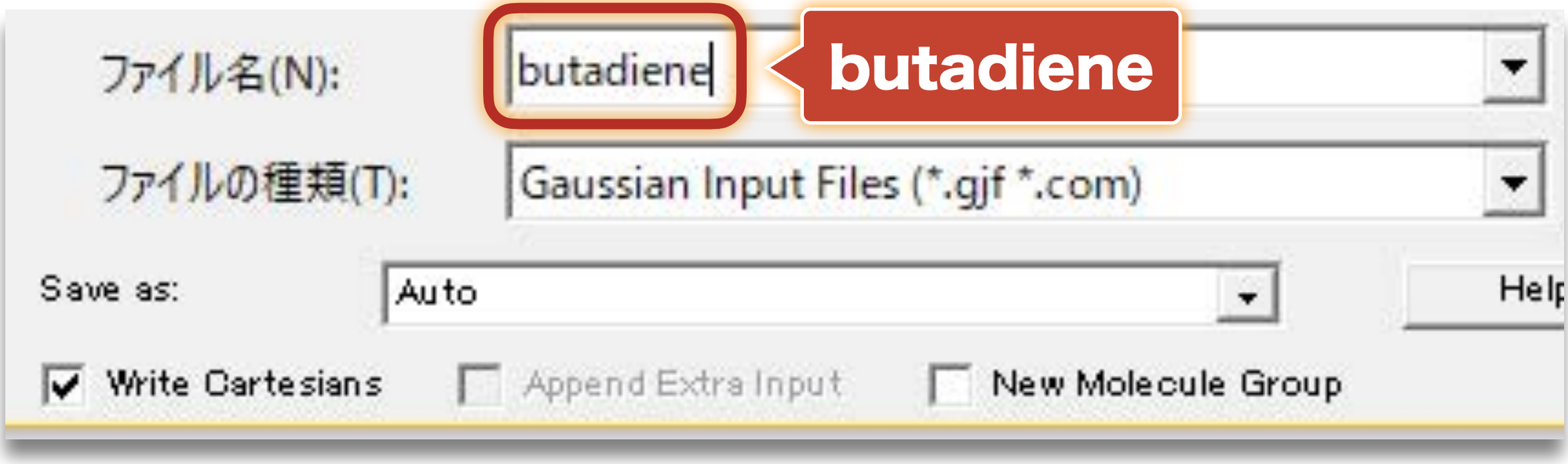
構造最適化


G1:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # opt freq hf/3-21g geom=connectivity
Charge/Mult: 0 1
Job Type
Method
Title
Link 0
General
Guess
NBO
PBC
Solvation
Add. Inp.
ilayer ONIOM Model
Method:
Ground State
Hartree-Fock
Basis Set:
3-21G
Charge:
0
Singlet
Hartree-Fock
3-21G
Additional Keywords:
Update
Scheme:
(Unnamed Scheme)
Submit...
Cancel
Edit...
Retain
Defaults
Help

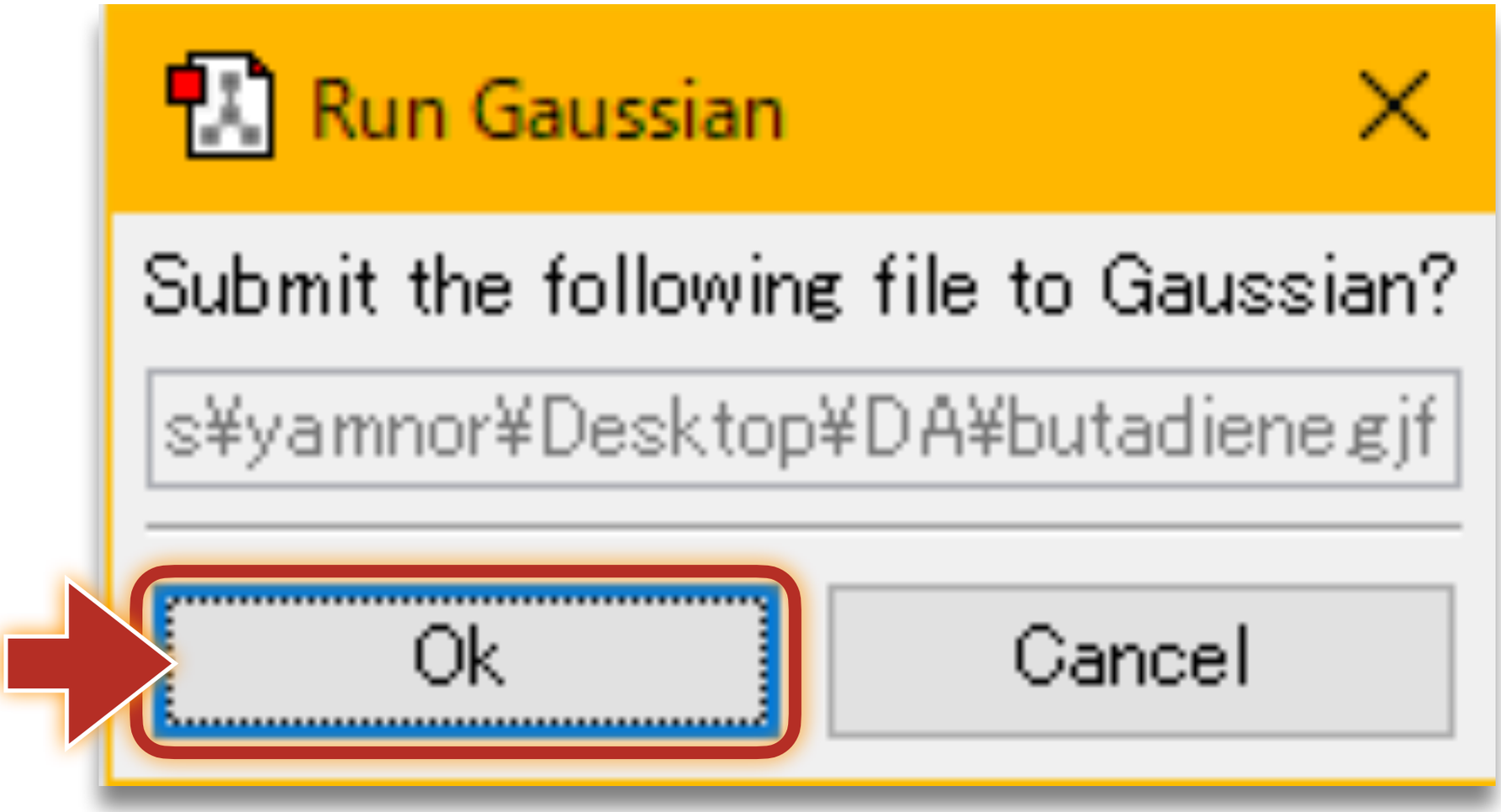
構造最適化


Gaussian Calculation
You must save a Gaussian input file before you submit.
Would you like to save an input file now?
Save
Cancel

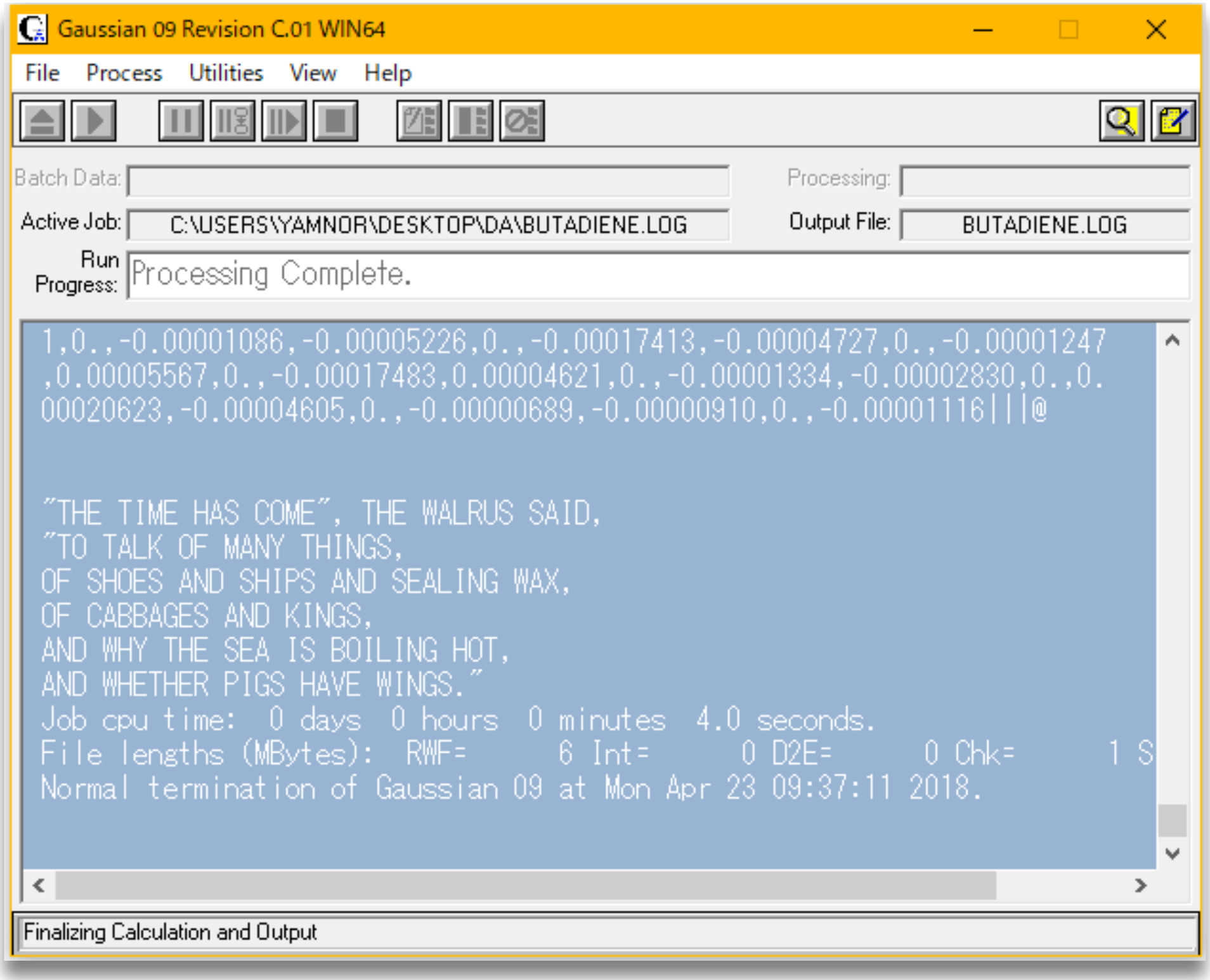
構造最適化


ファイル名(N):
butadiene
butadiene
ファイルの種類(T):
Gaussian Input Files (*.gjf *.com)
Save as:
Auto
Help
Write Cartesians
Append Extra Input
New Molecule Group

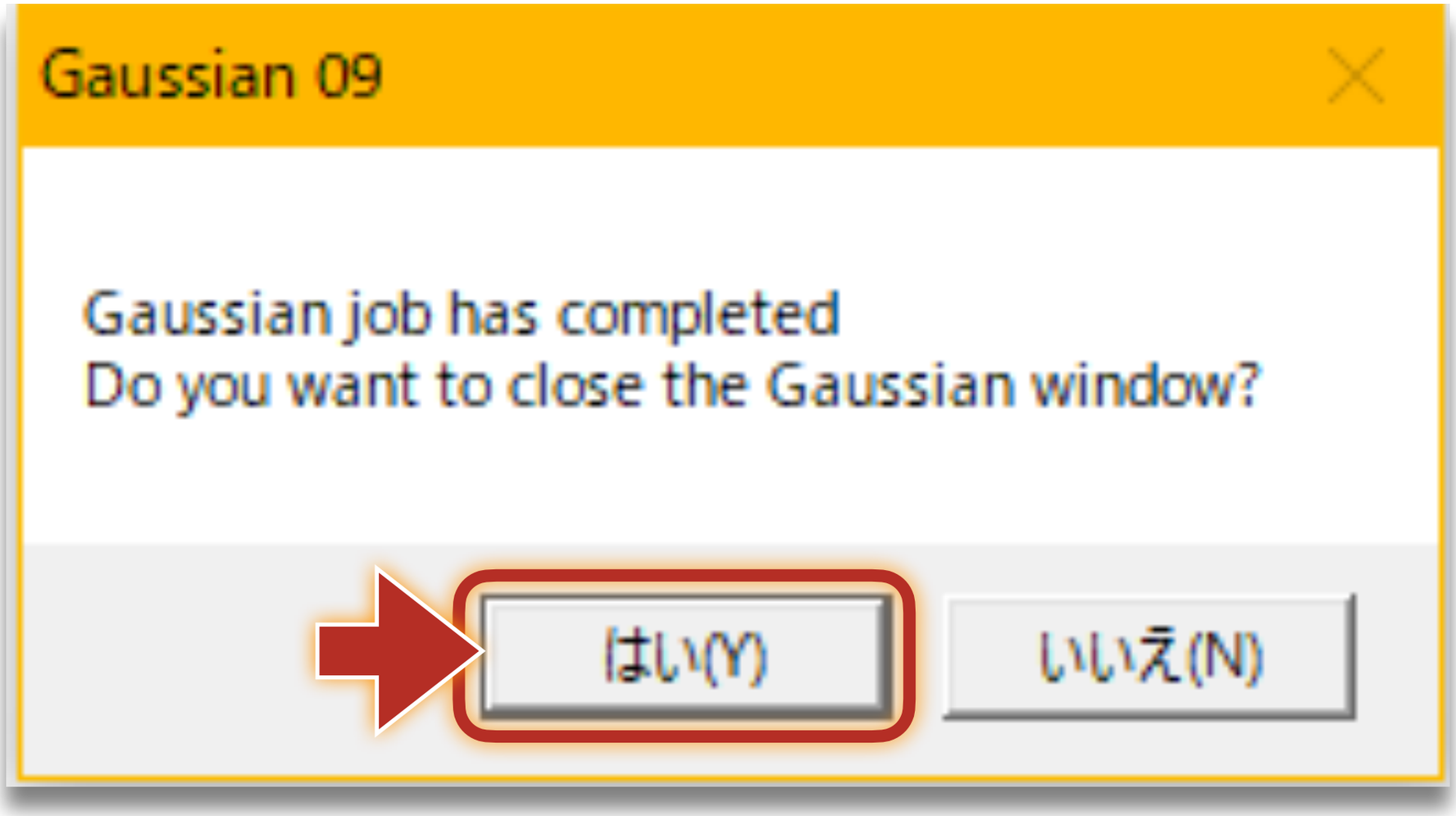
構造最適化


Run Gaussian
Submit the following file to Gaussian?
s¥yamnor¥Desktop¥DA¥butadiene.gjf
Ok
Cancel

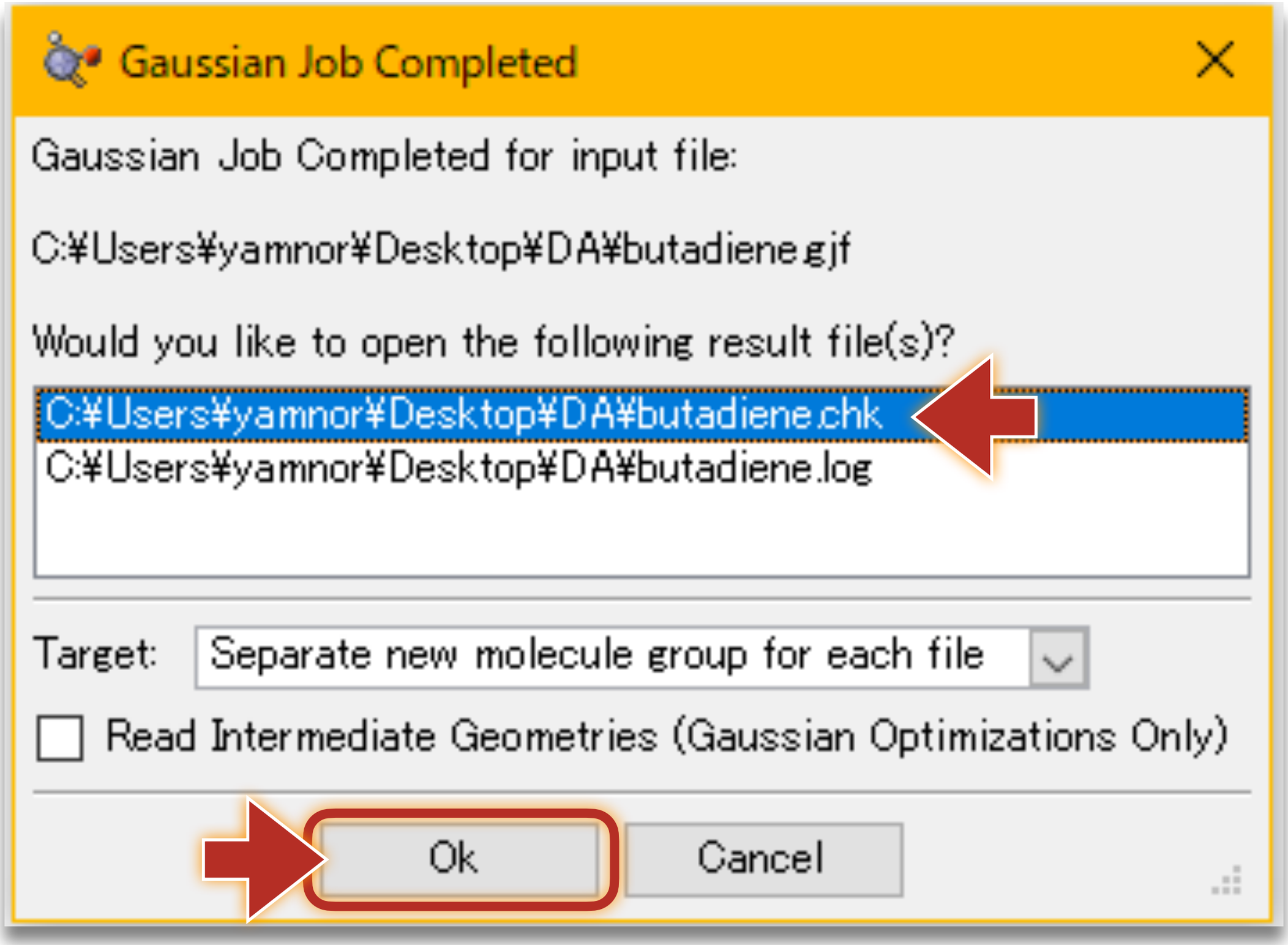
構造最適化


Gaussian 09 Revision C.01 WIN64
File Process Utilities View Help
Batch Data:
Processing:
Active Job: C:\USERS\YAMNOR\DESKTOP\DA\BUTADIENE.LOG
Output File: BUTADIENE.LOG
Run Progress: Processing Complete.
1,0.,-0.00001086,-0.00005226,0.,-0.00017413,-0.00004727,0.,-0.00001247
,0.00005567,0.,-0.00017483,0.00004621,0.,-0.00001334,-0.00002830,0.,0.
00020623,-0.00004605,0.,-0.00000689,-0.00000910,0.,-0.00001116|||@
"THE TIME HAS COME", THE WALRUS SAID,
"TO TALK OF MANY THINGS,
OF SHOES AND SHIPS AND SEALING WAX,
OF CABBAGES AND KINGS,
AND WHY THE SEA IS BOILING HOT,
AND WHETHER PIGS HAVE WINGS."
Job cpu time: 0 days 0 hours 0 minutes 4.0 seconds.
File lengths (MBytes): RWF= 6 Int= 0 D2E= 0 Chk= 1 S
Normal termination of Gaussian 09 at Mon Apr 23 09:37:11 2018.
Finalizing Calculation and Output

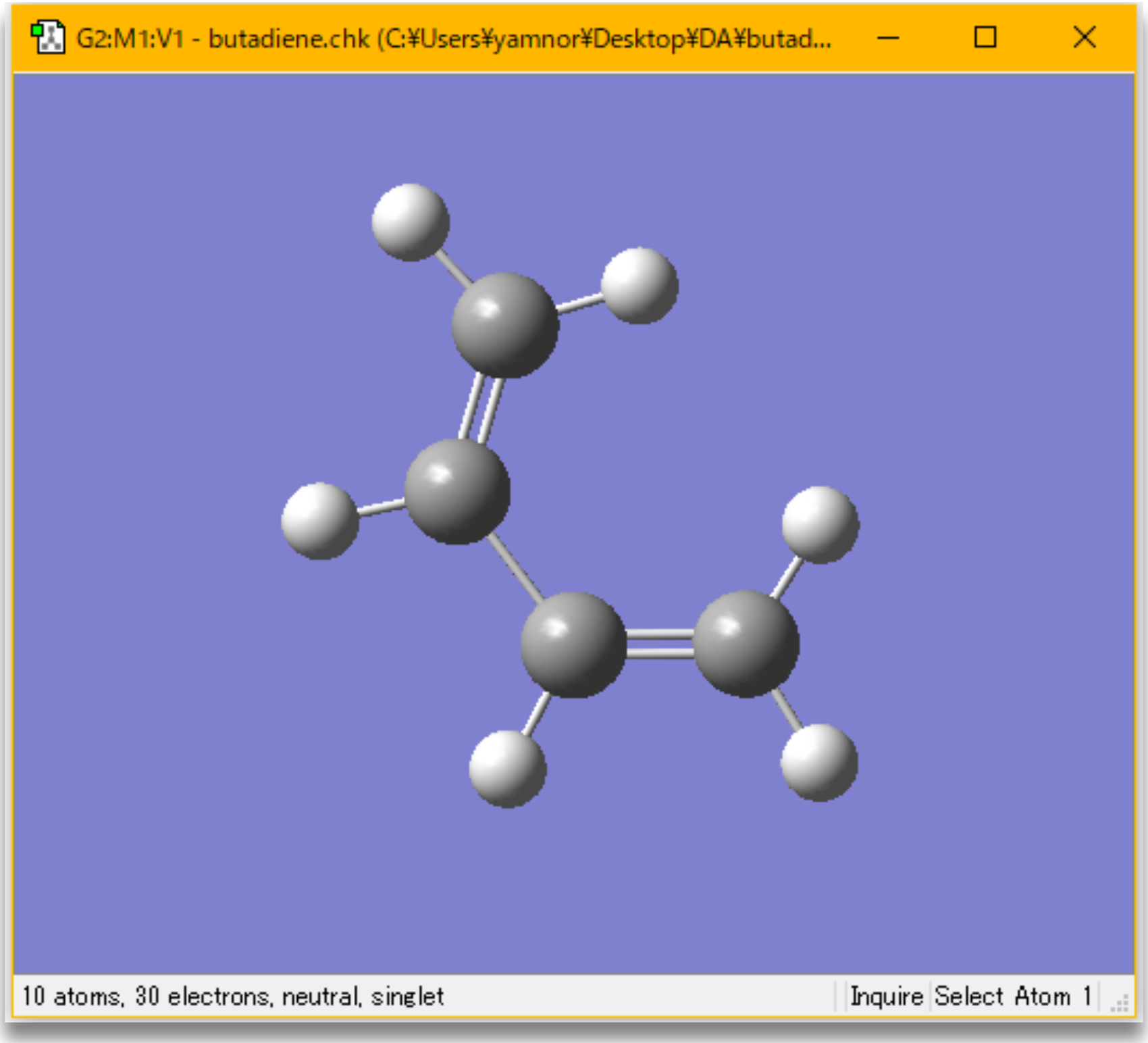
構造最適化


Gaussian 09
Gaussian job has completed
Do you want to close the Gaussian window?
はい(Y)
いいえ(N)

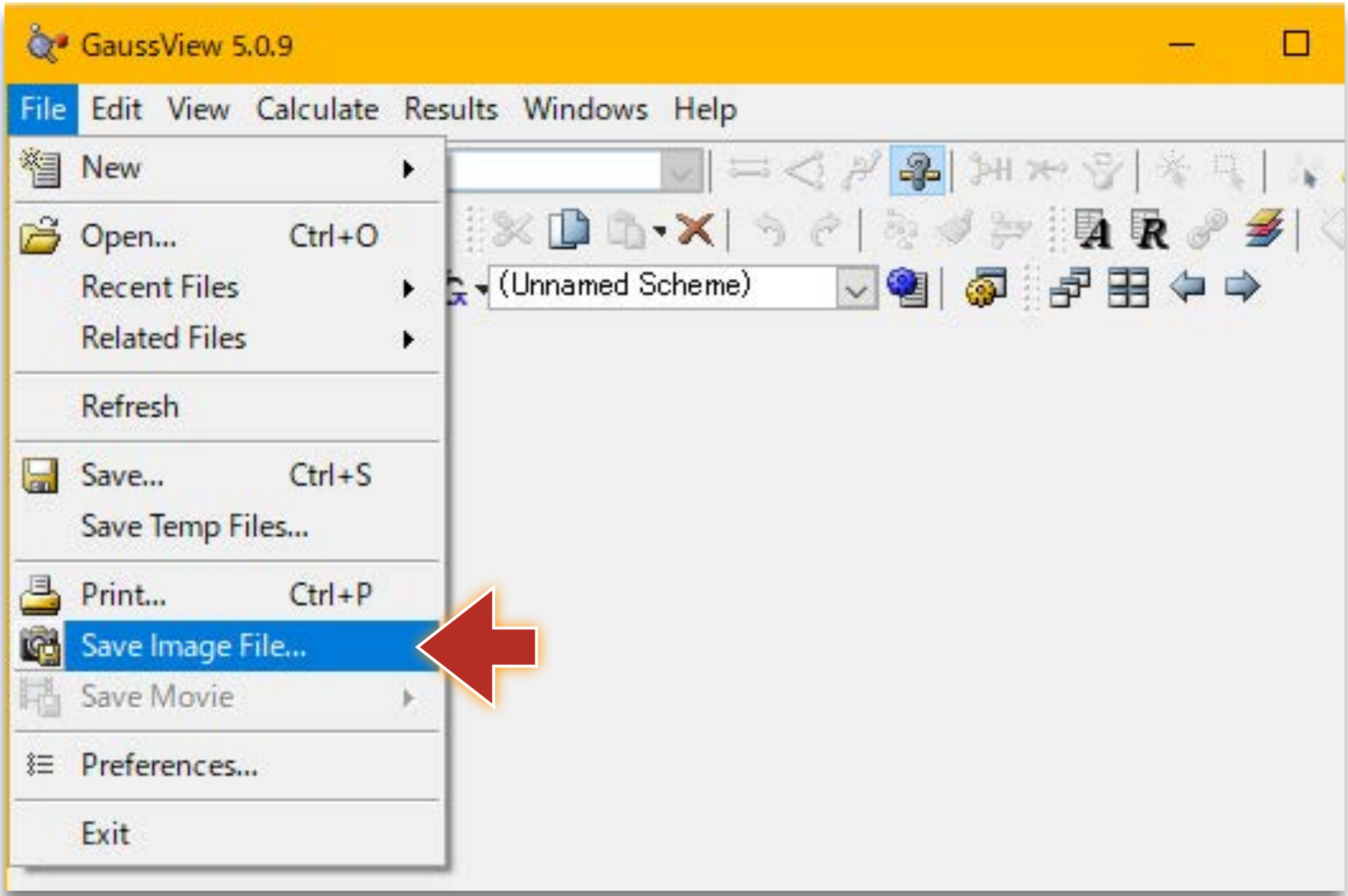
構造最適化


Gaussian Job Completed
Gaussian Job Completed for input file:
C:¥Users¥yamnor¥Desktop¥DA¥butadiene.gjf
Would you like to open the following result file(s)?
C:¥Users¥yamnor¥Desktop¥DA¥butadiene.chk
C:¥Users¥yamnor¥Desktop¥DA¥butadiene.log
Target:
Separate new molecule group for each file
Read Intermediate Geometries (Gaussian Optimizations Only)
Ok
Cancel

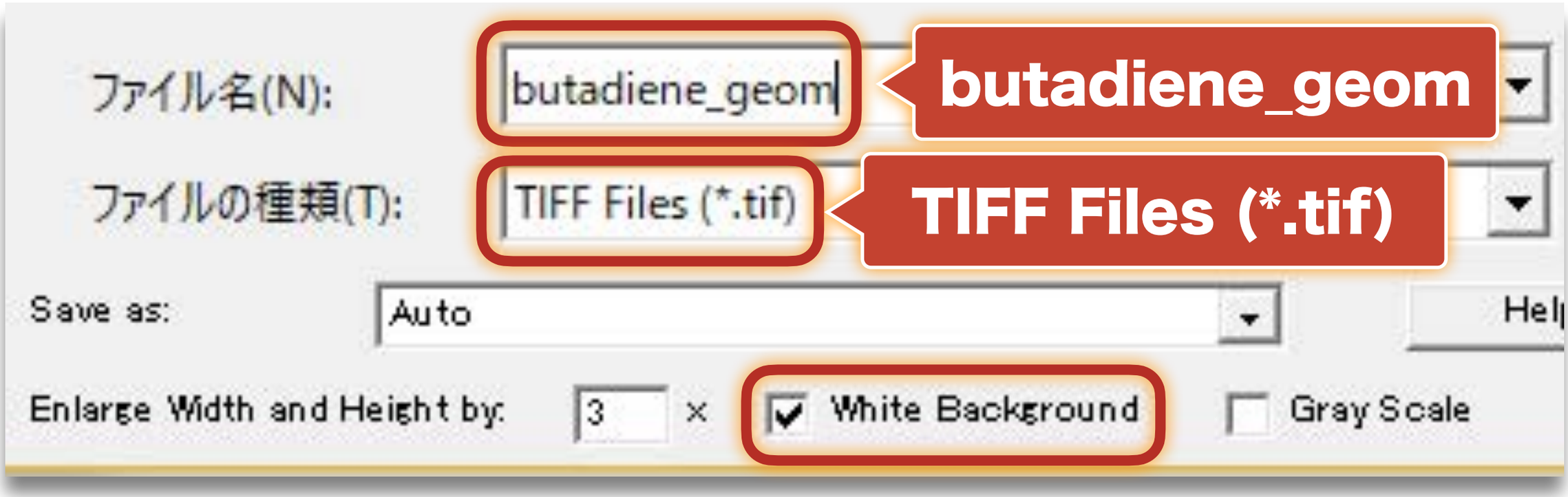
構造最適化


G2:M1:V1 - butadiene.chk (C:¥Users¥yamnor¥Desktop¥DA¥butad...
10 atoms, 30 electrons, neutral, singlet
Inquire
Select Atom 1

画像を保存する（分子構造）

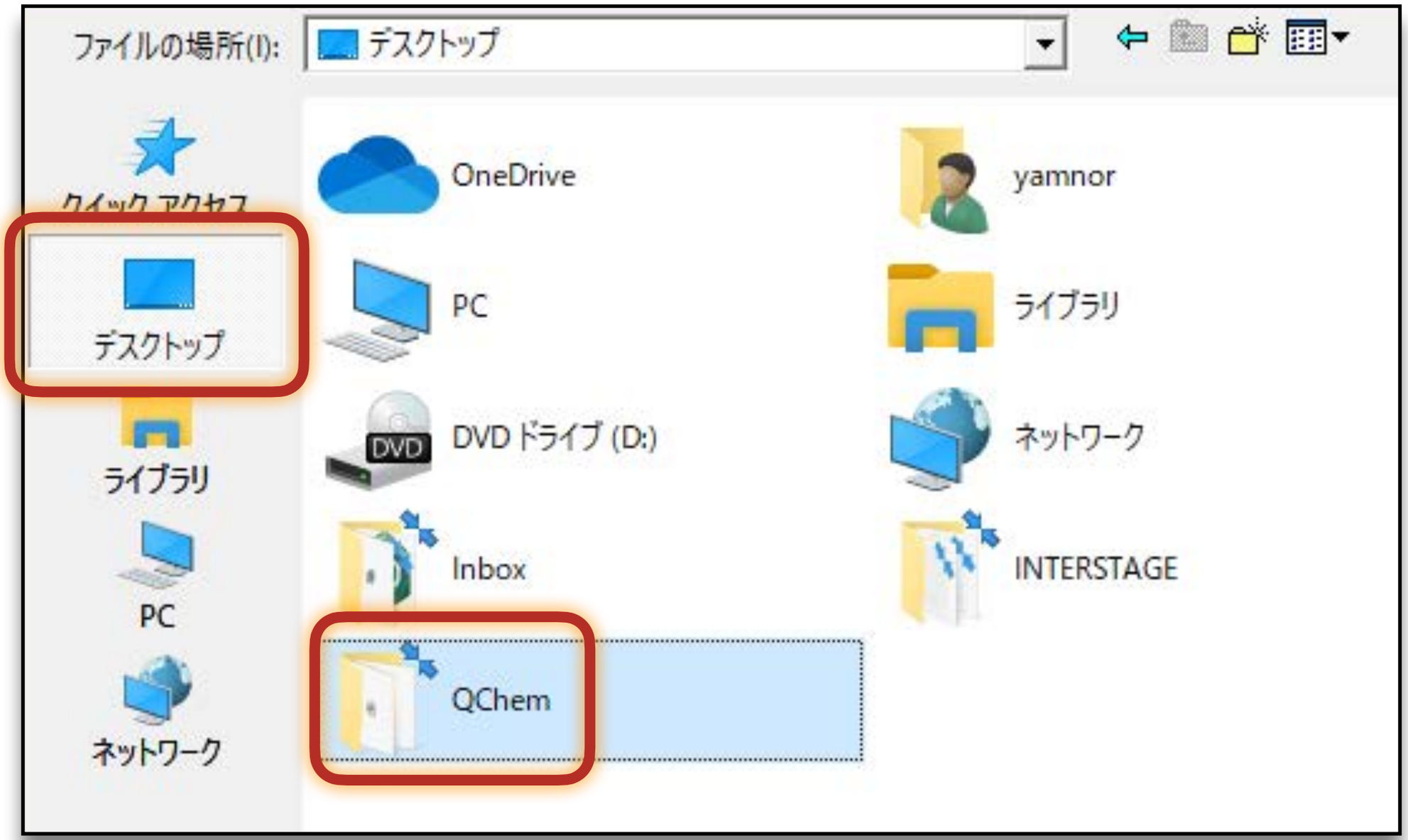


画像を保存する（分子構造）

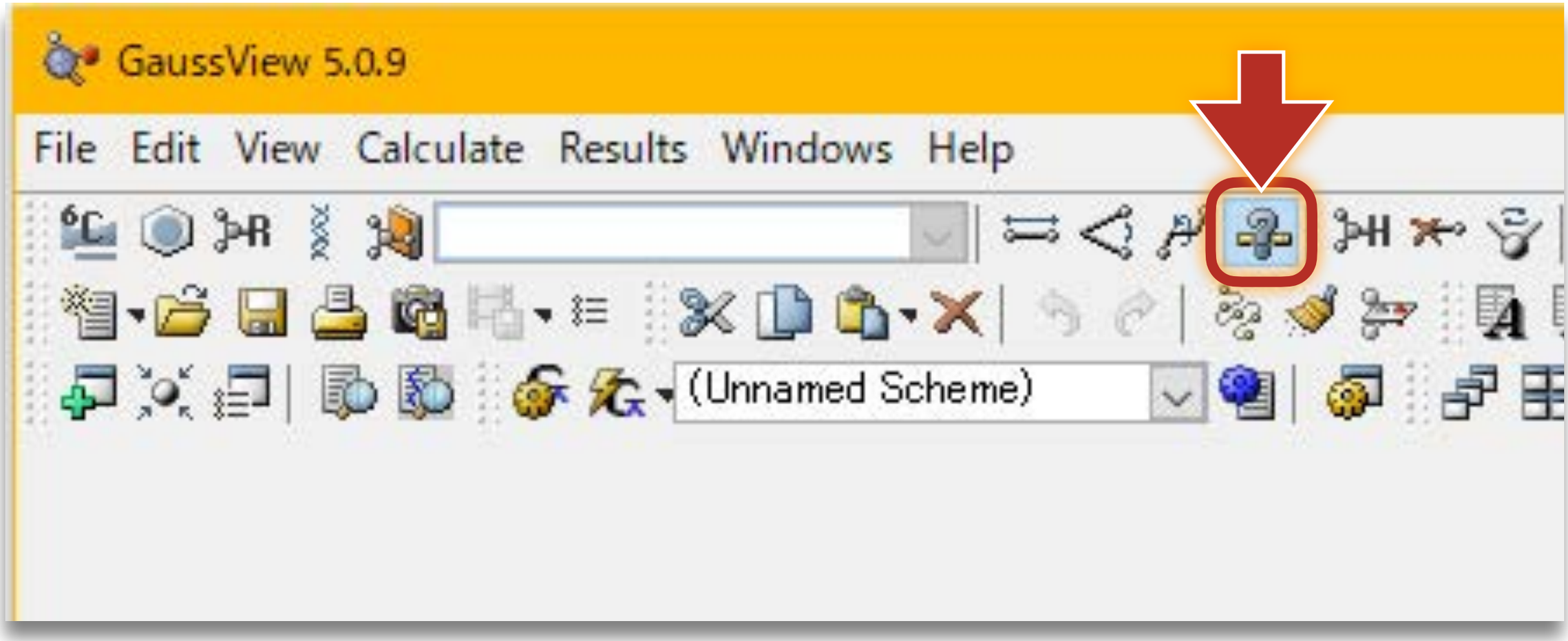


全てのファイルの保存先

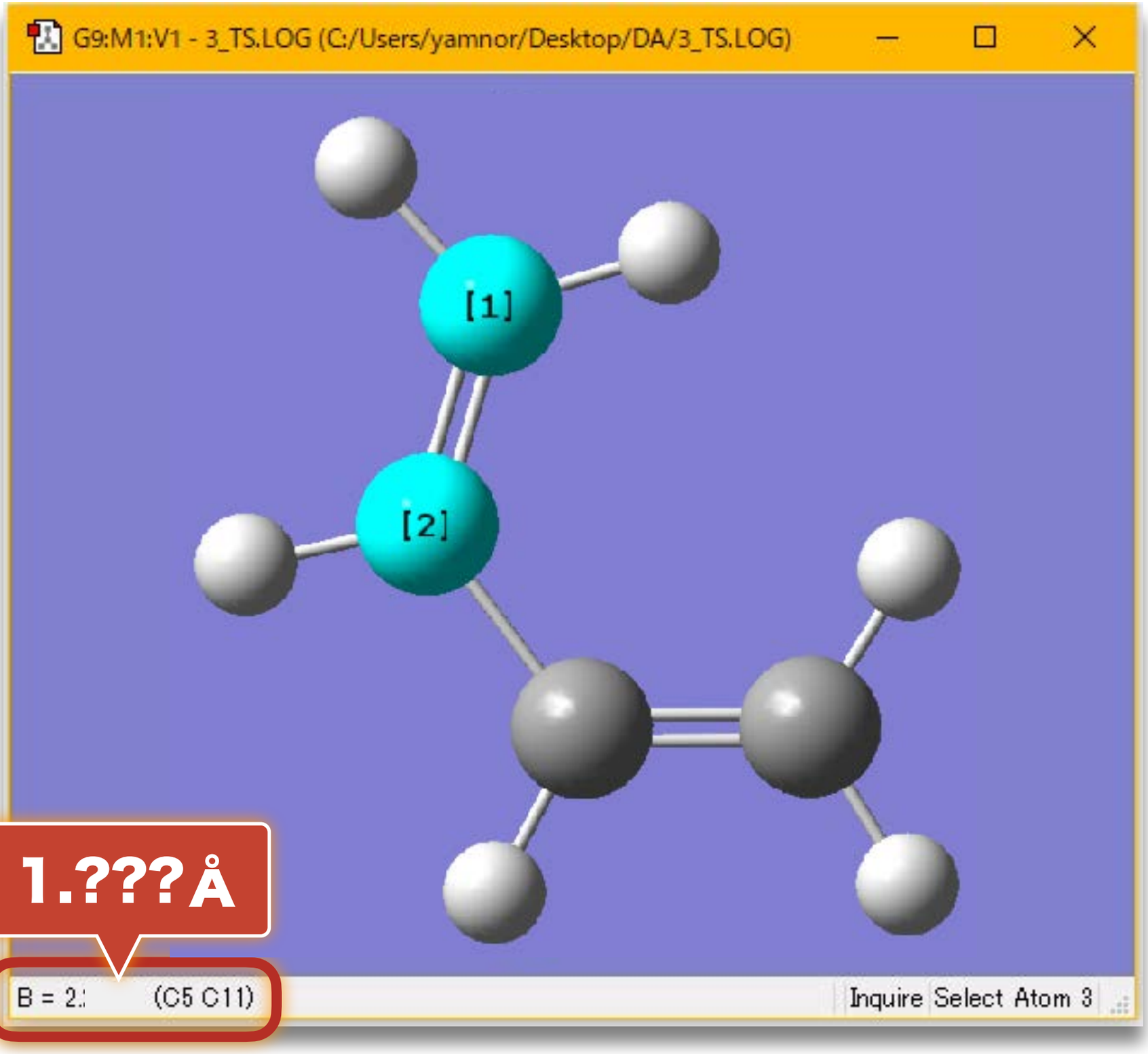
今日作成する全てのファイルは、
デスクトップ の **QChem フォルダ** に保存する



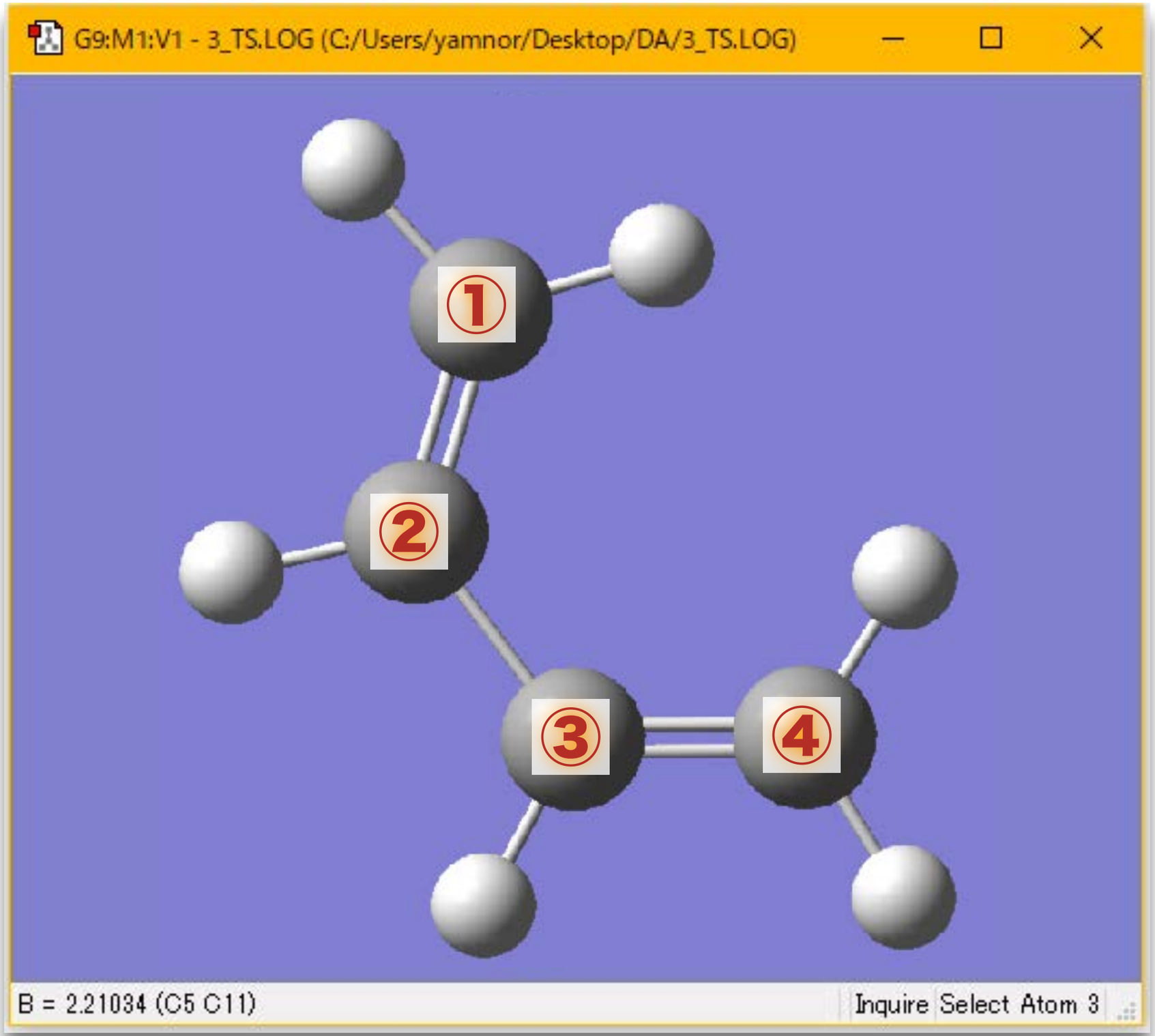
原子間距離を調べる


GaussView 5.0.9
File Edit View Calculate Results Windows Help
(Unnamed Scheme)

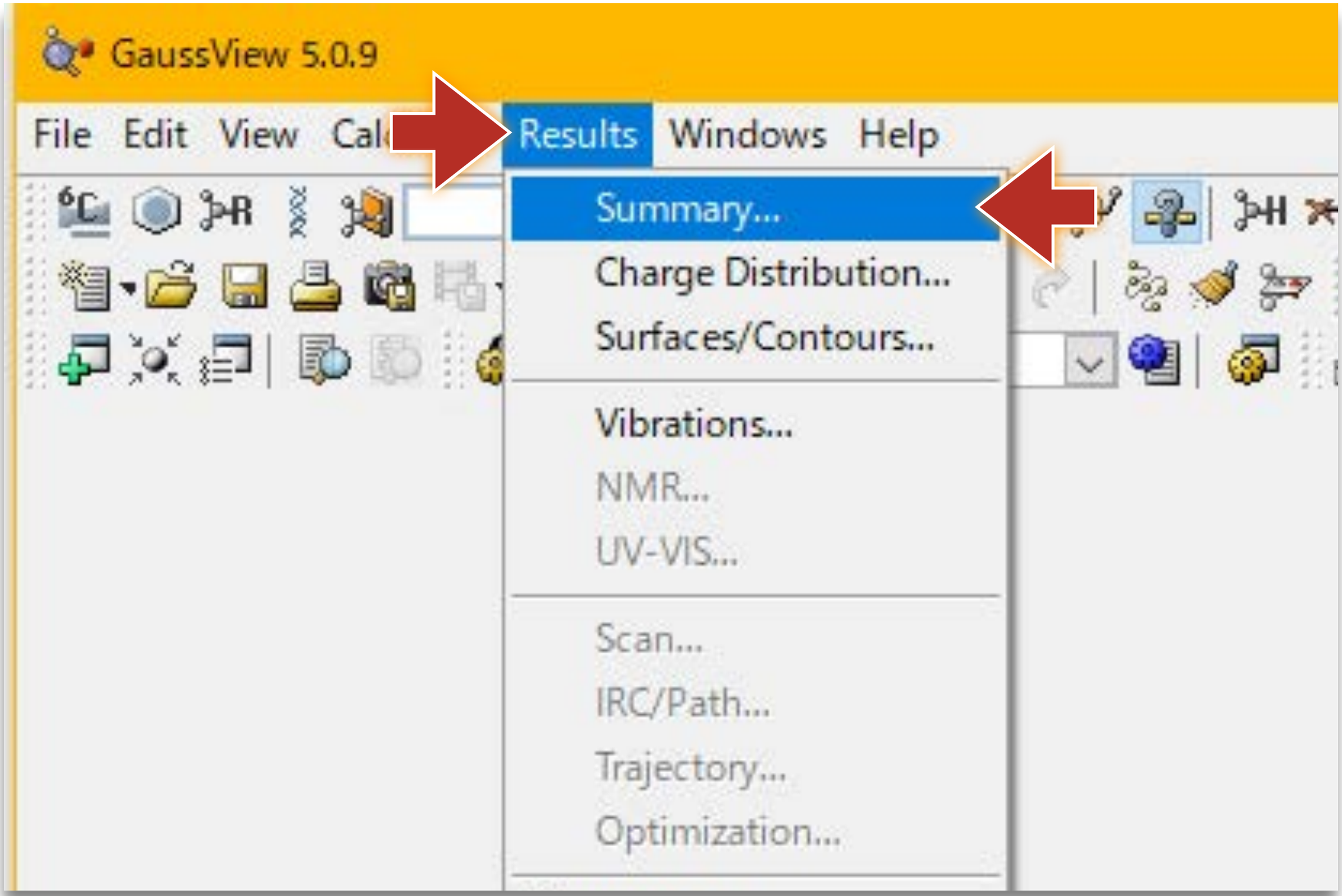
原子間距離を調べる


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
[1]
[2]
1.???Å
B = 2.
(C5 C11)
Inquire Select Atom 3

各原子の番号（ラベル）


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
①
②
③
④
B = 2.21034 (C5 C11)
Inquire Select Atom 3

全エネルギーを調べる


GaussView 5.0.9
File Edit View Cal
Results
Windows
Help
Summary...
Charge Distribution...
Surfaces/Contours...
Vibrations...
NMR...
UV-VIS...
Scan...
IRC/Path...
Trajectory...
Optimization...

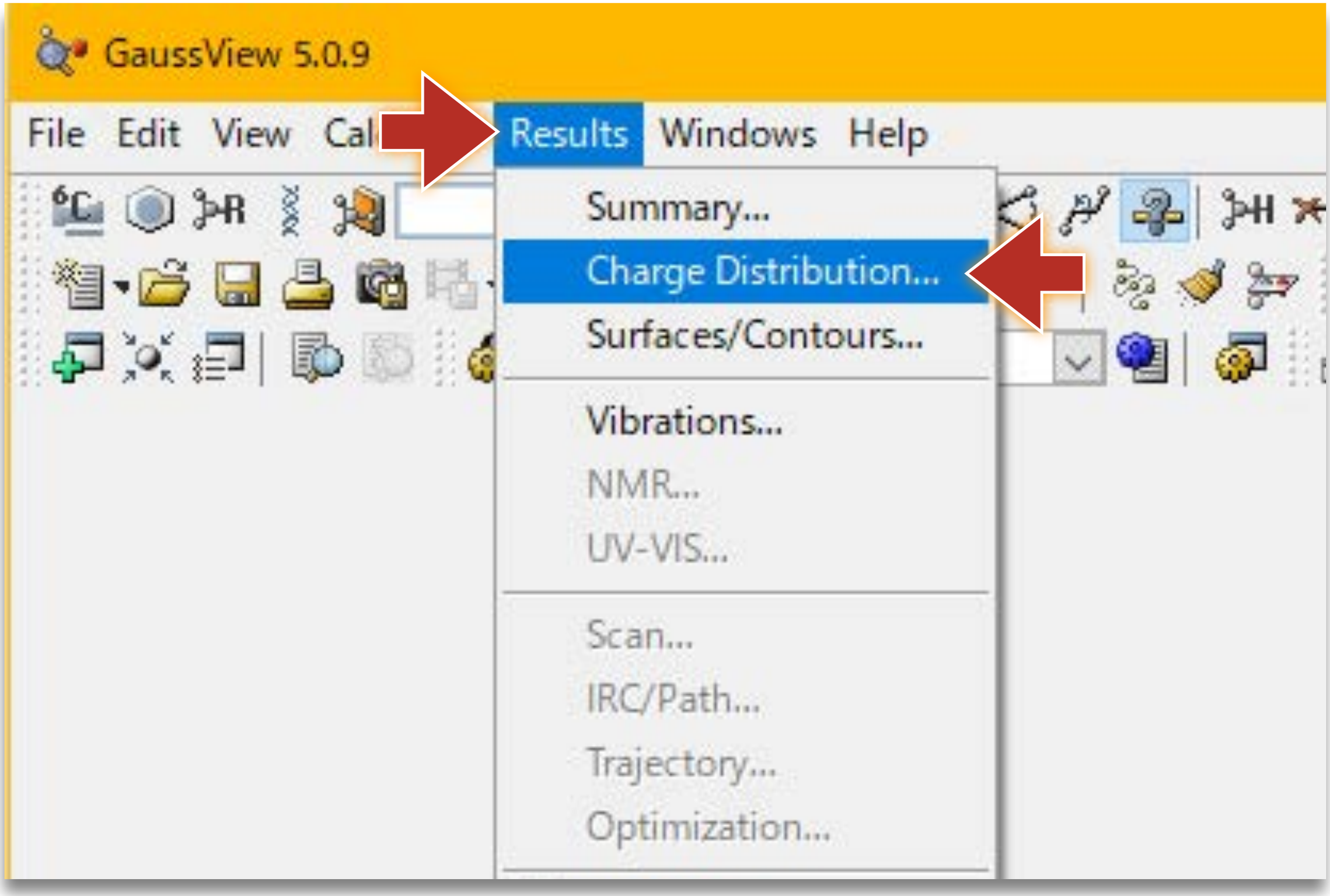
全エネルギーを調べる

G2:M1:V1 - Gaussian Calculation Summary

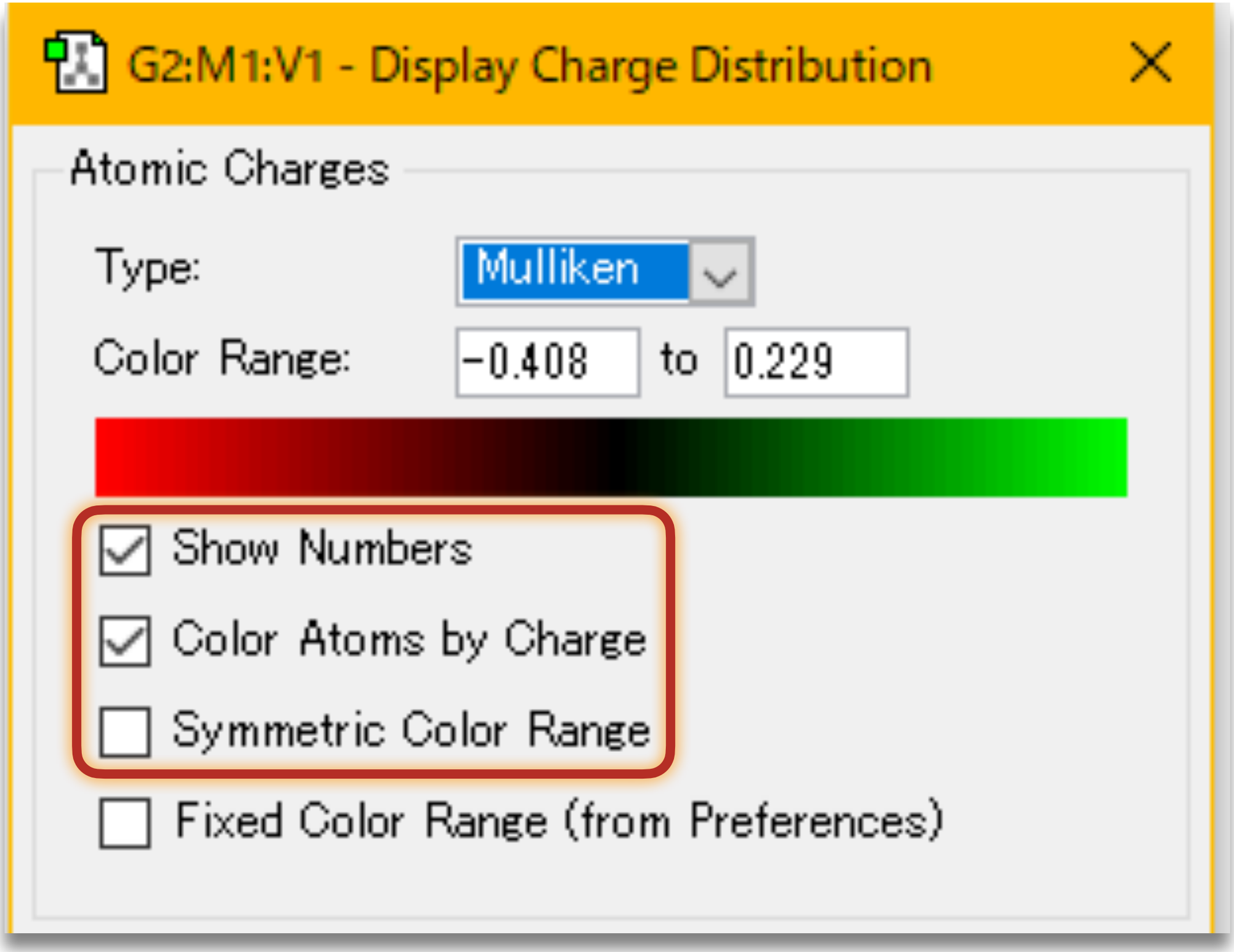
Title Card Required		
File Name	butadiene	
File Type	.chk	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	3-21G	
Charge	0	
Spin	Singlet	
Total Energy	-154.	a.u.
RMS Gradient Norm	0.00007352	a.u.
Imaginary Freq		
Dipole Moment	0.0342	Debye
Point Group		

Ok　View File　Save Data

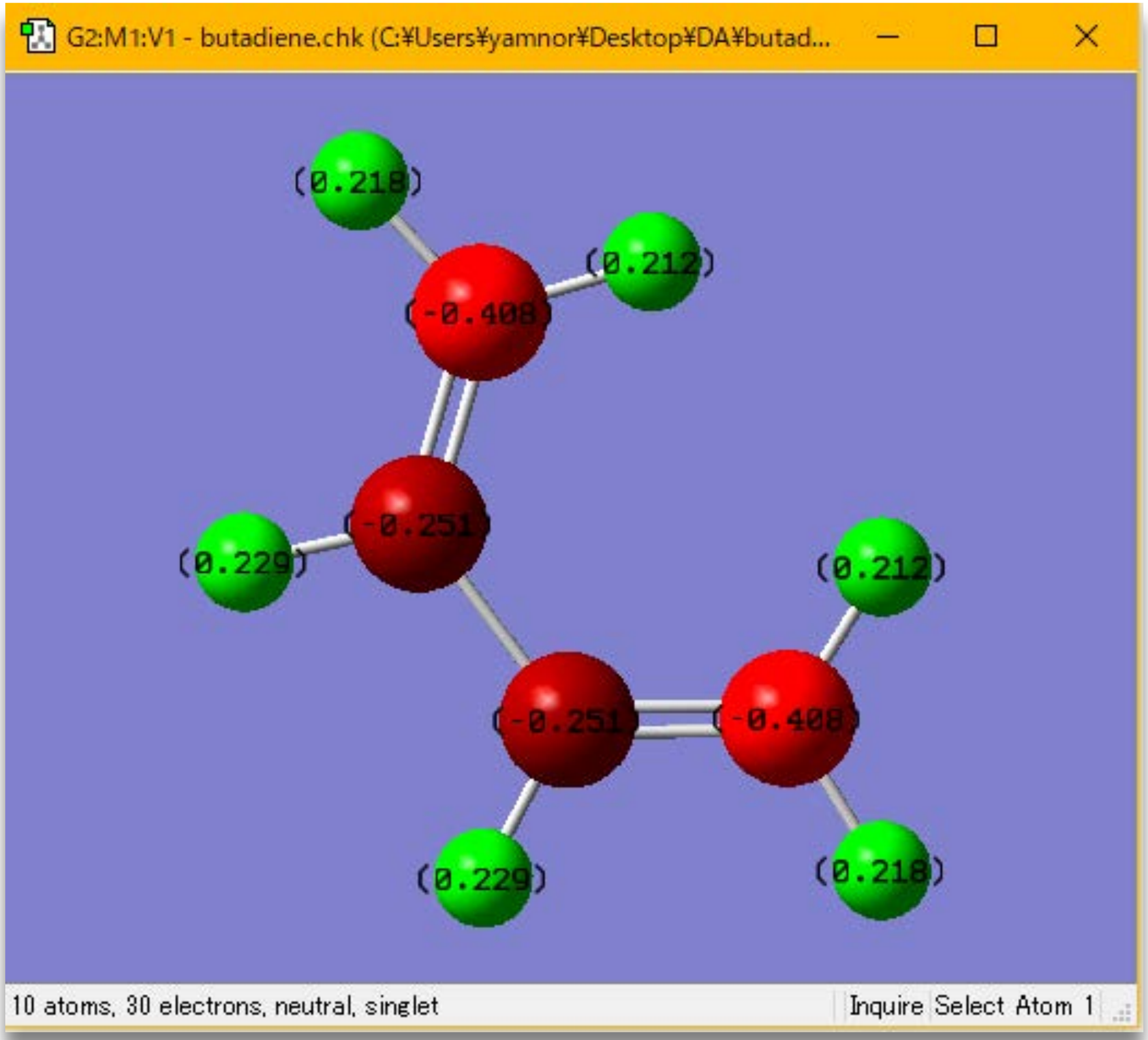
電荷分布を調べる


GaussView 5.0.9
File Edit View Cal
Results
Windows
Help
Summary...
Charge Distribution...
Surfaces/Contours...
Vibrations...
NMR...
UV-VIS...
Scan...
IRC/Path...
Trajectory...
Optimization...

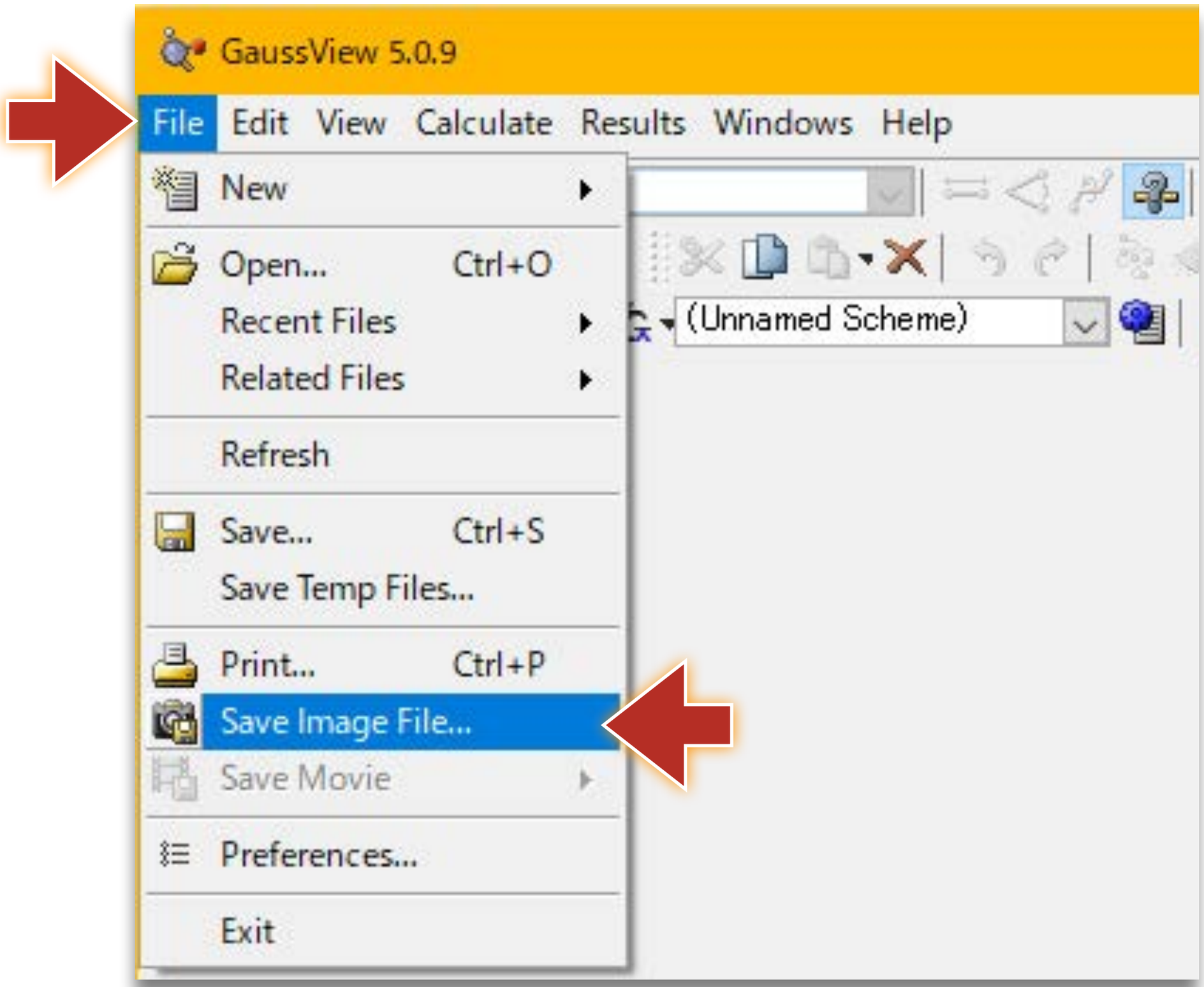
電荷分布を調べる


G2:M1:V1 - Display Charge Distribution
Atomic Charges
Type:
Mulliken
Color Range:
-0.408
to
0.229
Show Numbers
Color Atoms by Charge
Symmetric Color Range
Fixed Color Range (from Preferences)

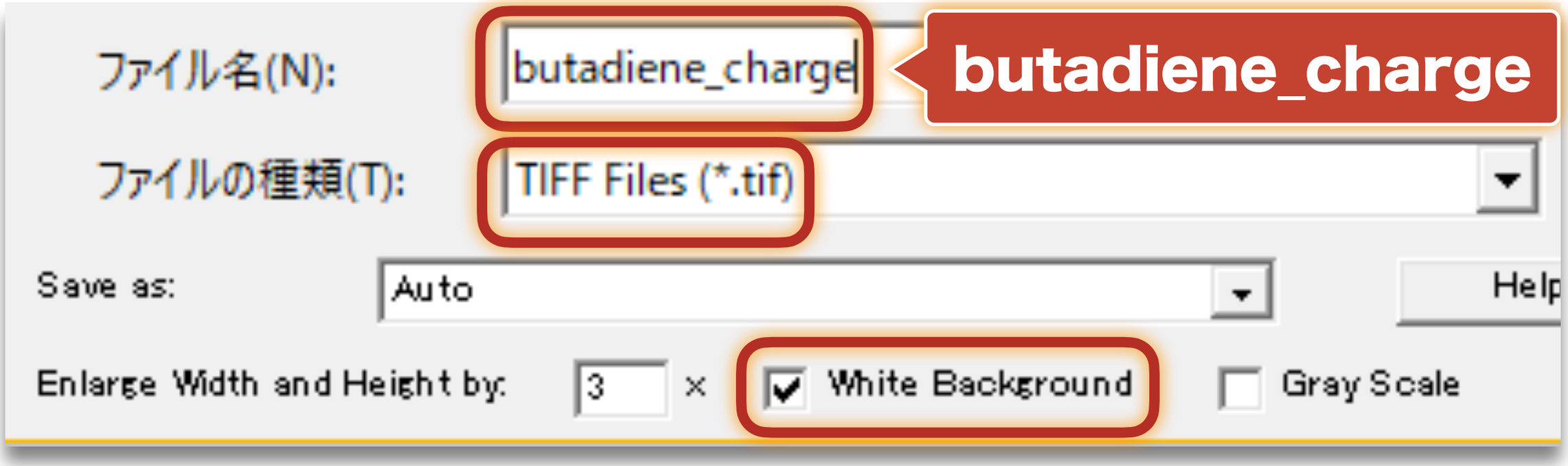
電荷分布を調べる


G2:M1:V1 - butadiene.chk (C:¥Users¥yamnor¥Desktop¥DA¥butad...
(0.218)
(0.212)
(-0.408)
(-0.251)
(0.229)
(0.212)
(-0.251)
(-0.408)
(0.229)
(0.218)
10 atoms, 30 electrons, neutral, singlet
Inquire
Select Atom 1

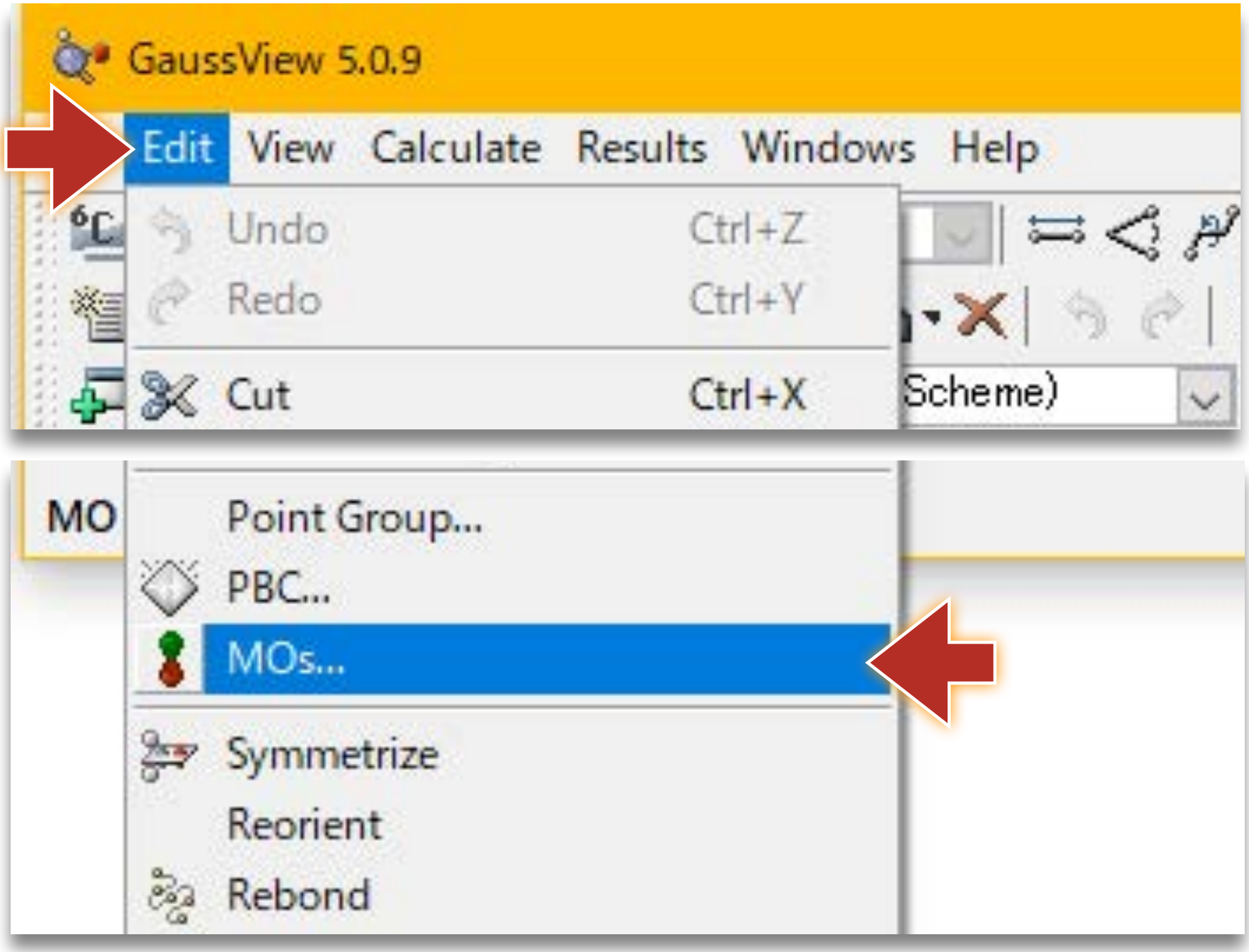
画像を保存する（電荷分布）



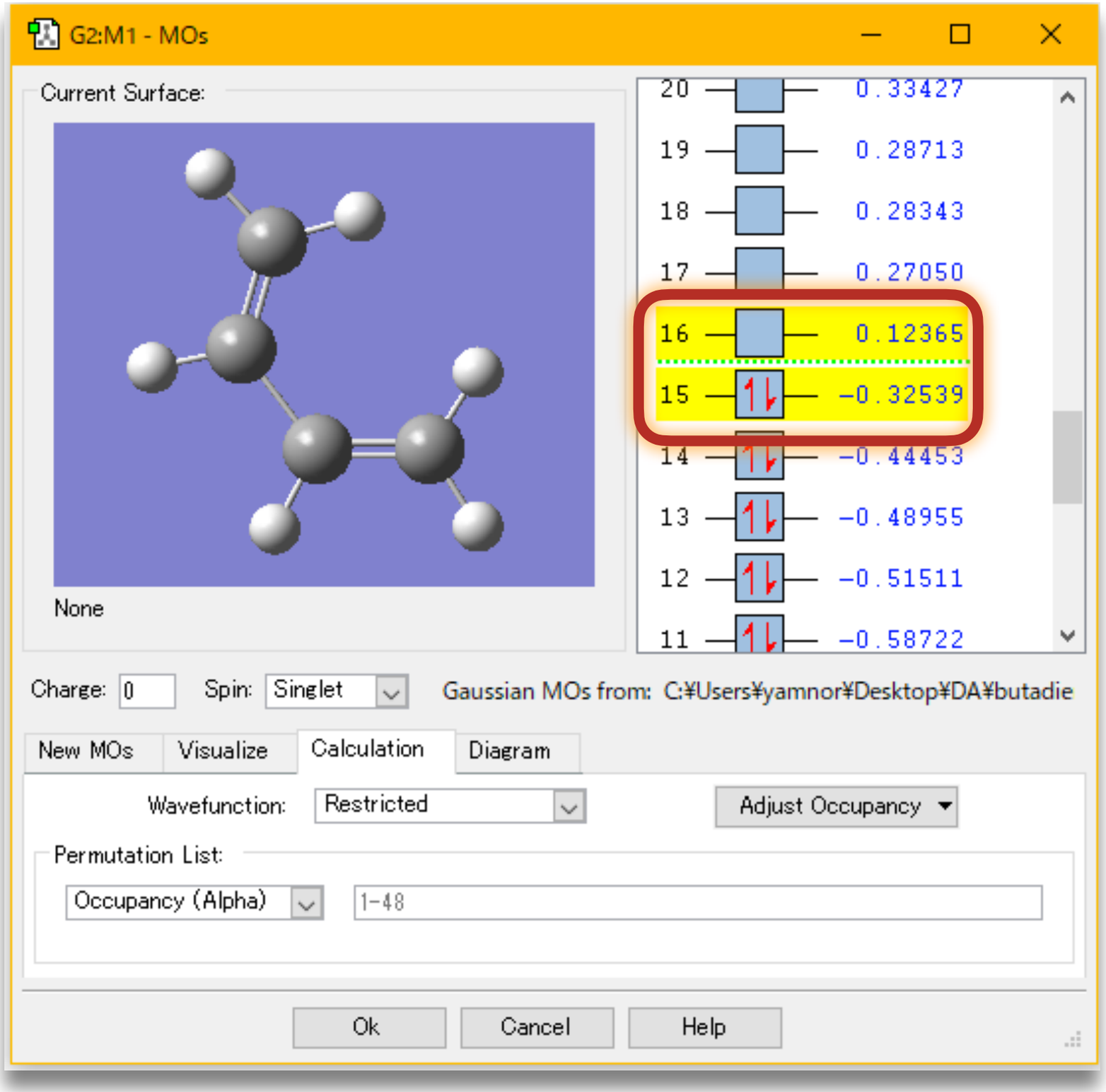
画像を保存する（電荷分布）



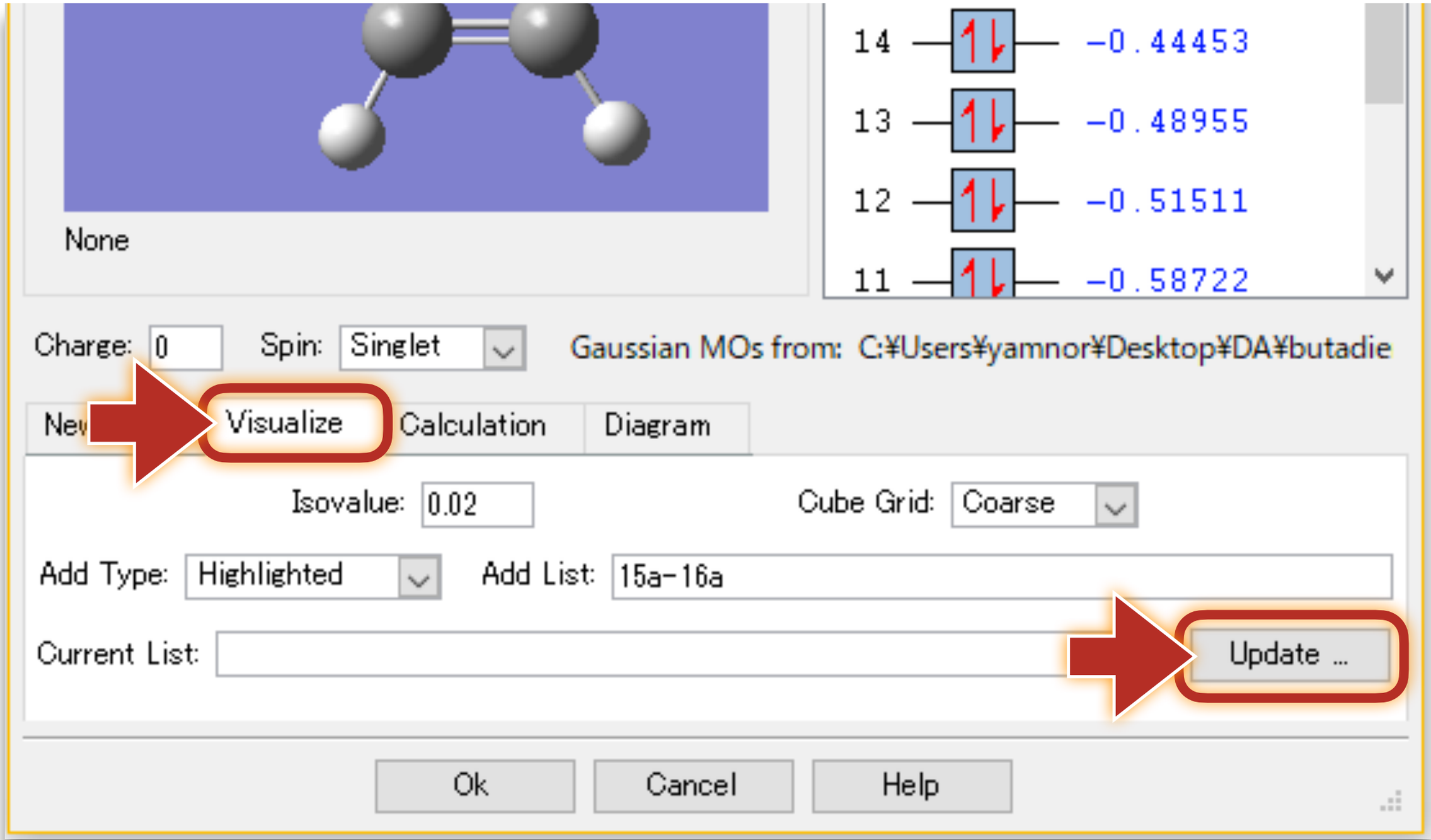
分子軌道を調べる


GaussView 5.0.9
Edit
View
Calculate
Results
Windows
Help
Undo Ctrl+Z
Redo Ctrl+Y
Cut Ctrl+X
Scheme)
MO
Point Group...
PBC...
MOs...
Symmetrize
Reorient
Rebond

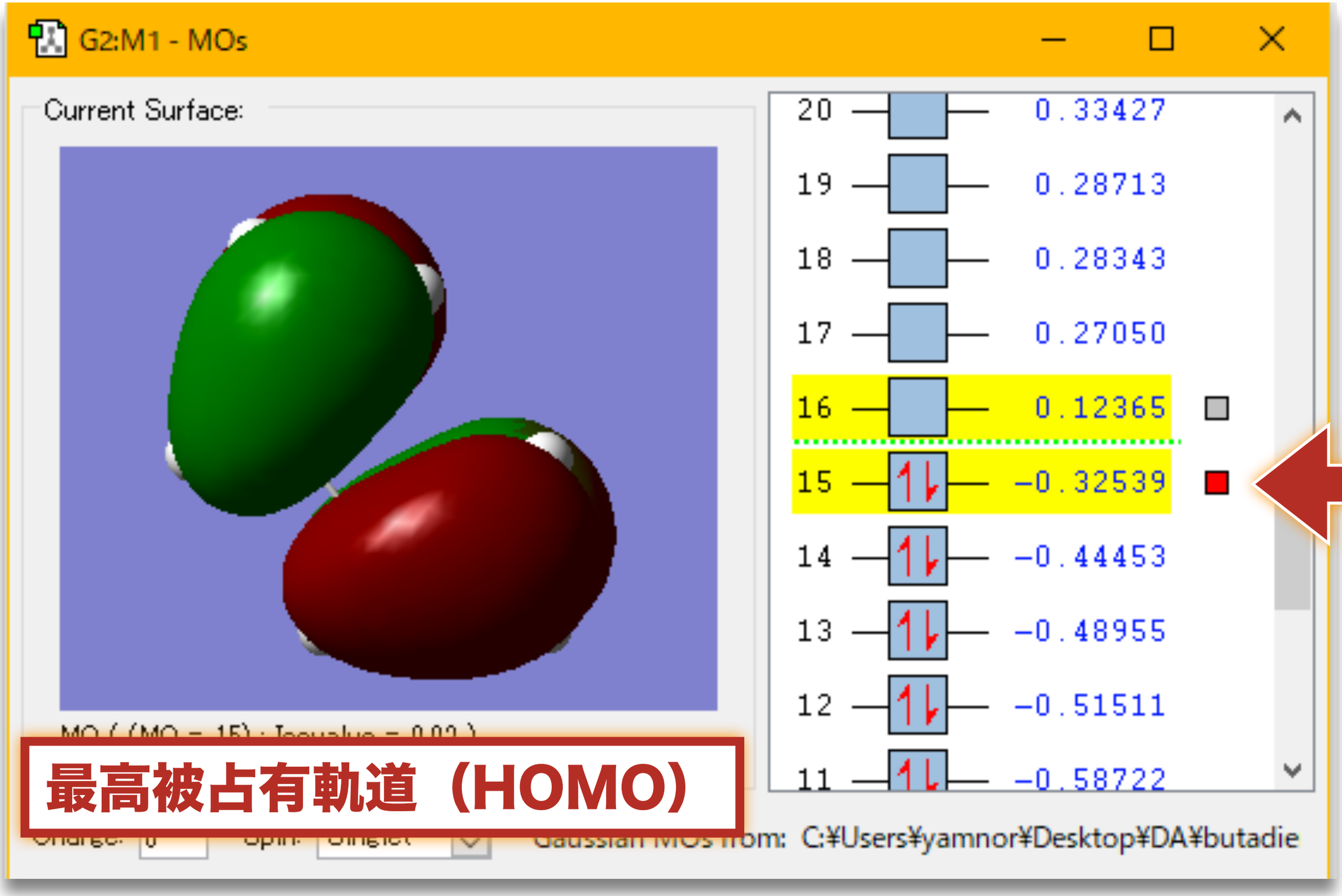
分子軌道を調べる


G2:M1 - MOs
Current Surface:
None
20 0.33427
19 0.28713
18 0.28343
17 0.27050
16 0.12365
15 −0.32539
14 −0.44453
13 −0.48955
12 −0.51511
11 −0.58722
Charge: 0
Spin: Singlet
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥butadie
New MOs
Visualize
Calculation
Diagram
Wavefunction: Restricted
Adjust Occupancy
Permutation List:
Occupancy (Alpha)
1-48
Ok
Cancel
Help

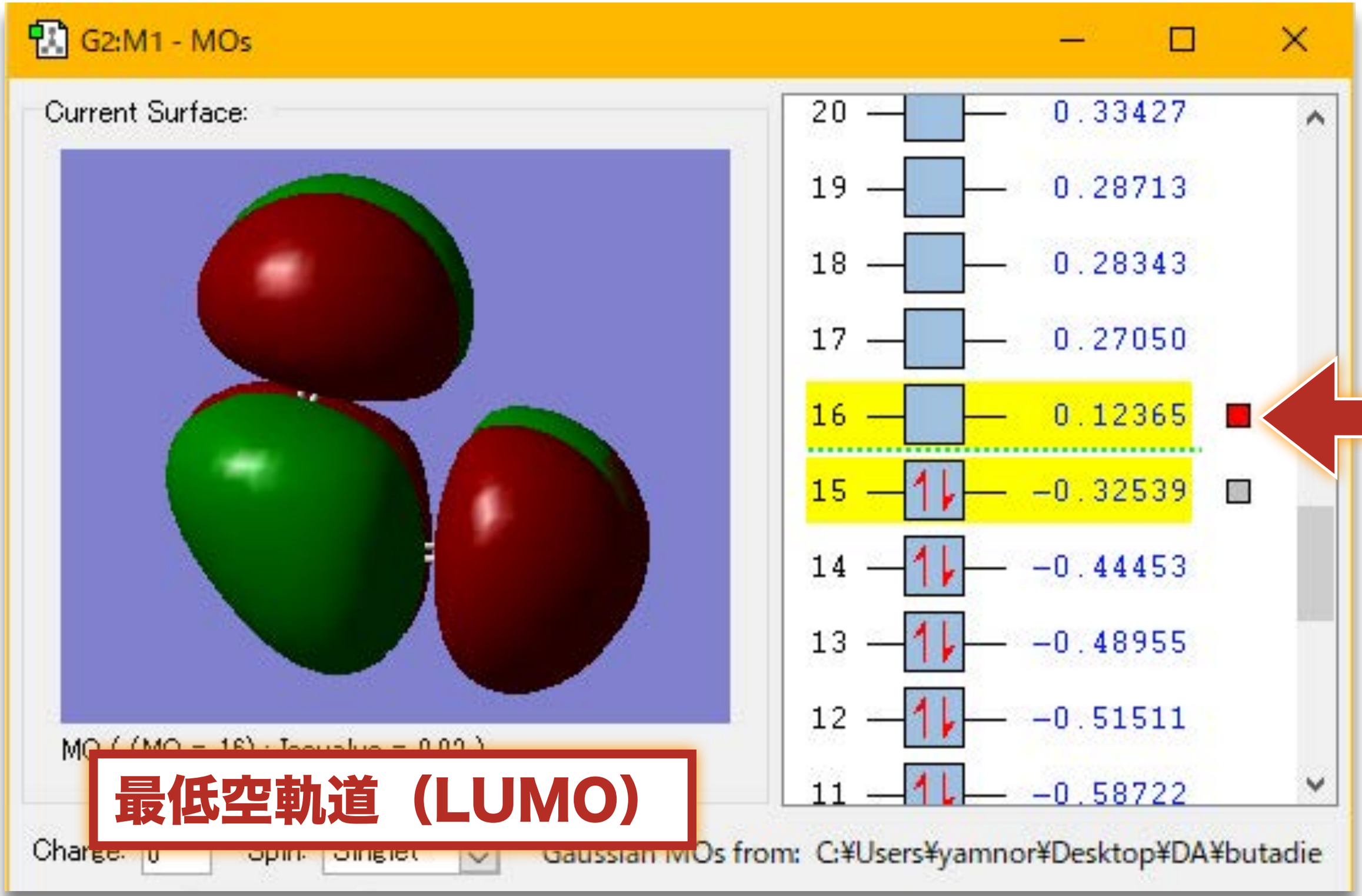
分子軌道を調べる


None
14 −0.44453
13 −0.48955
12 −0.51511
11 −0.58722
Charge: 0
Spin: Singlet
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥butadie
New
Visualize
Calculation
Diagram
Isovalue: 0.02
Cube Grid: Coarse
Add Type: Highlighted
Add List: 15a-16a
Current List:
Update ...
Ok
Cancel
Help

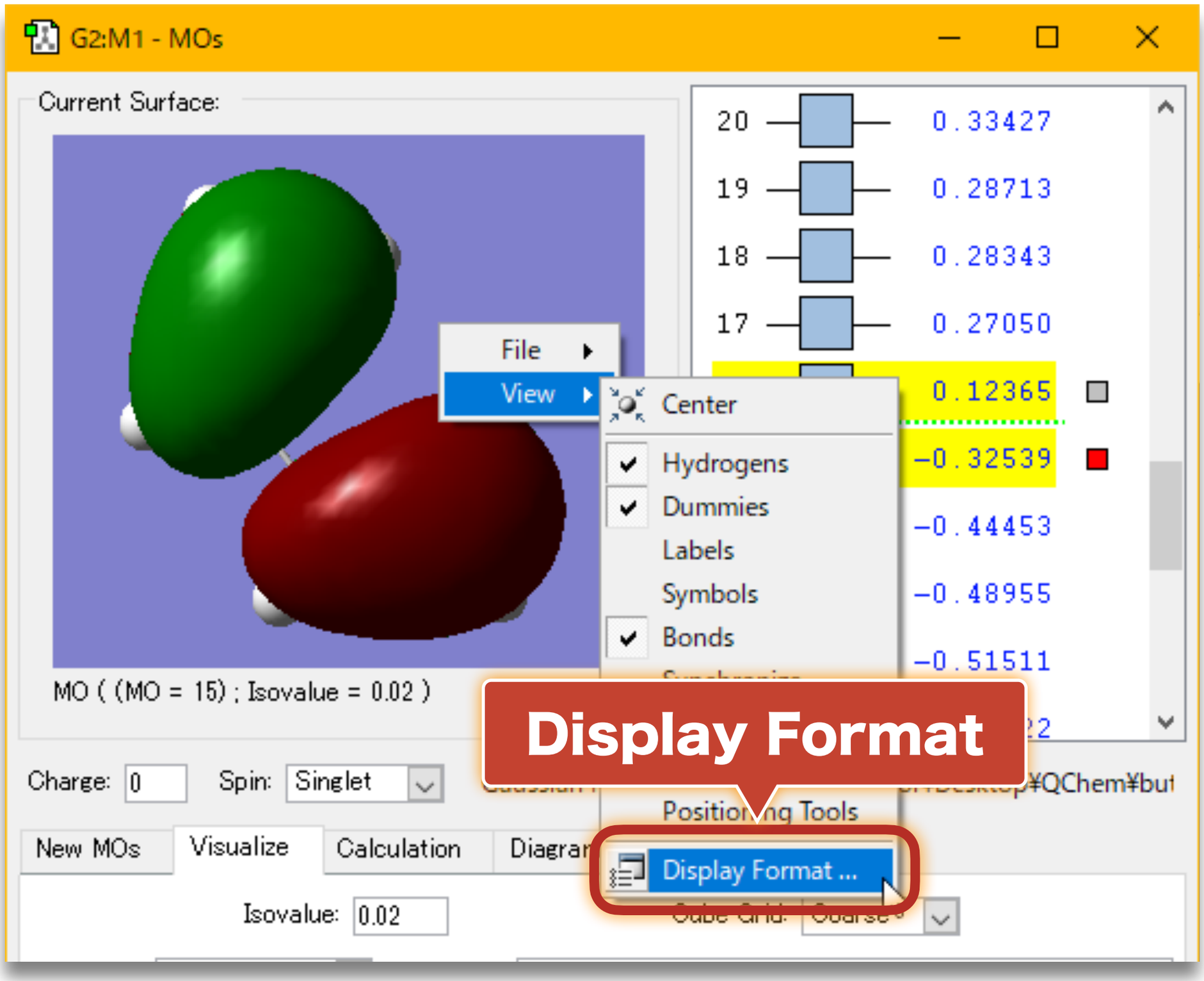
分子軌道を調べる


G2:M1 - MOs
Current Surface:
20 0.33427
19 0.28713
18 0.28343
17 0.27050
16 0.12365
15 −0.32539
14 −0.44453
13 −0.48955
12 −0.51511
11 −0.58722
最高被占有軌道（HOMO）
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥butadie

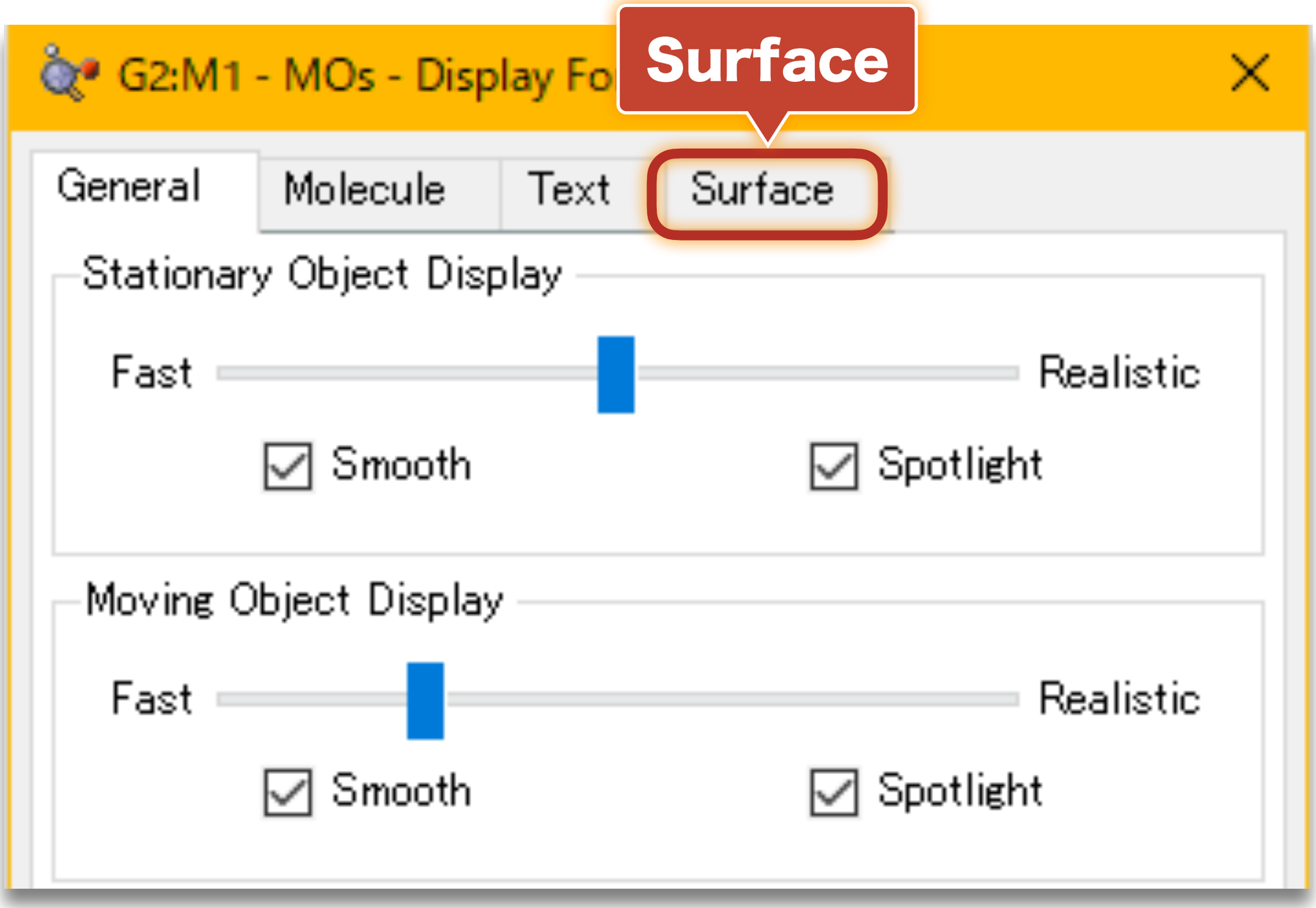
分子軌道を調べる


G2:M1 - MOs
Current Surface:
20 0.33427
19 0.28713
18 0.28343
17 0.27050
16 0.12365
15 -0.32539
14 -0.44453
13 -0.48955
12 -0.51511
11 -0.58722
最低空軌道（LUMO）
Charge:
Spin:
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥butadie

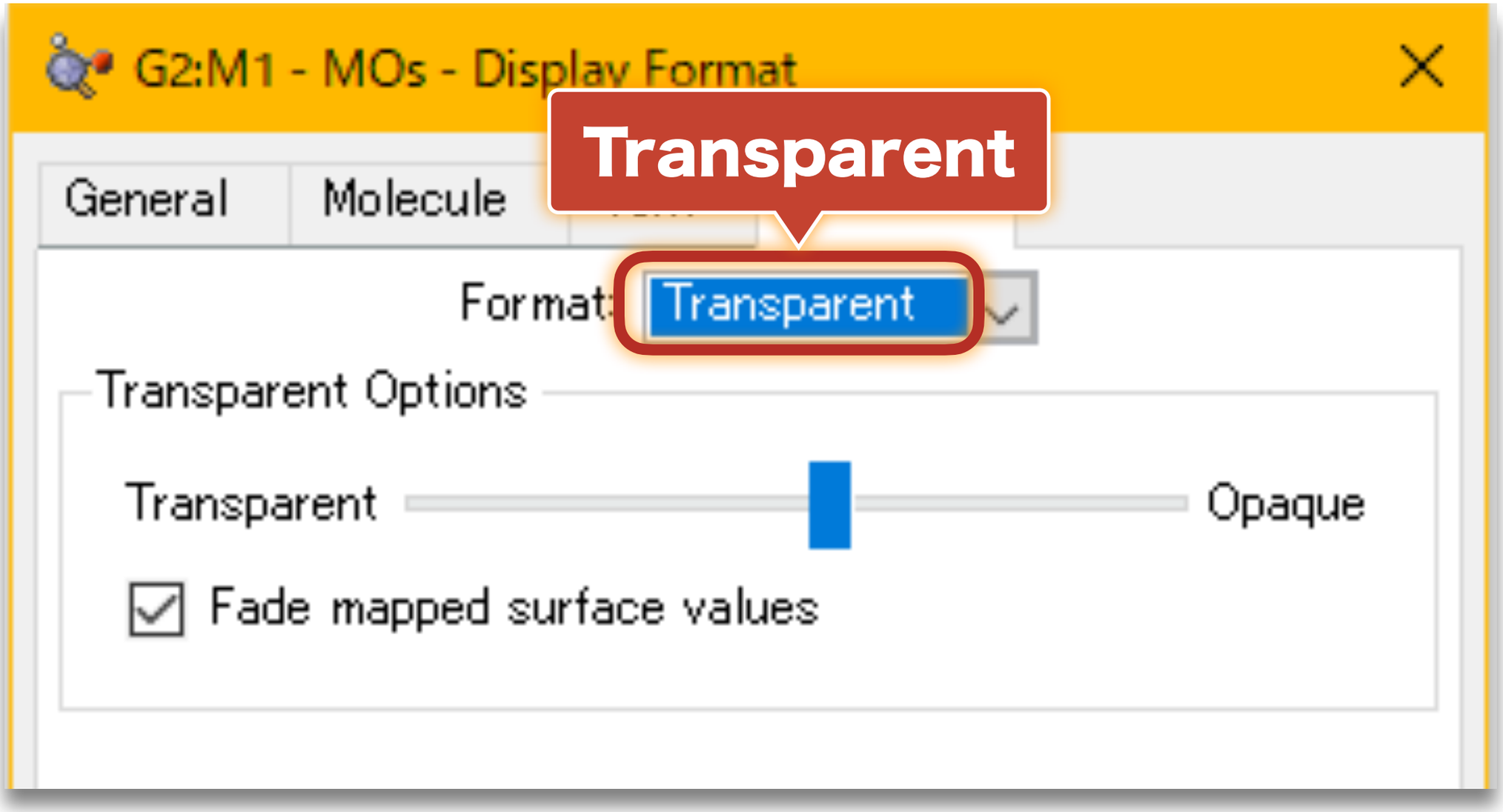
分子軌道の表示方法を変更する



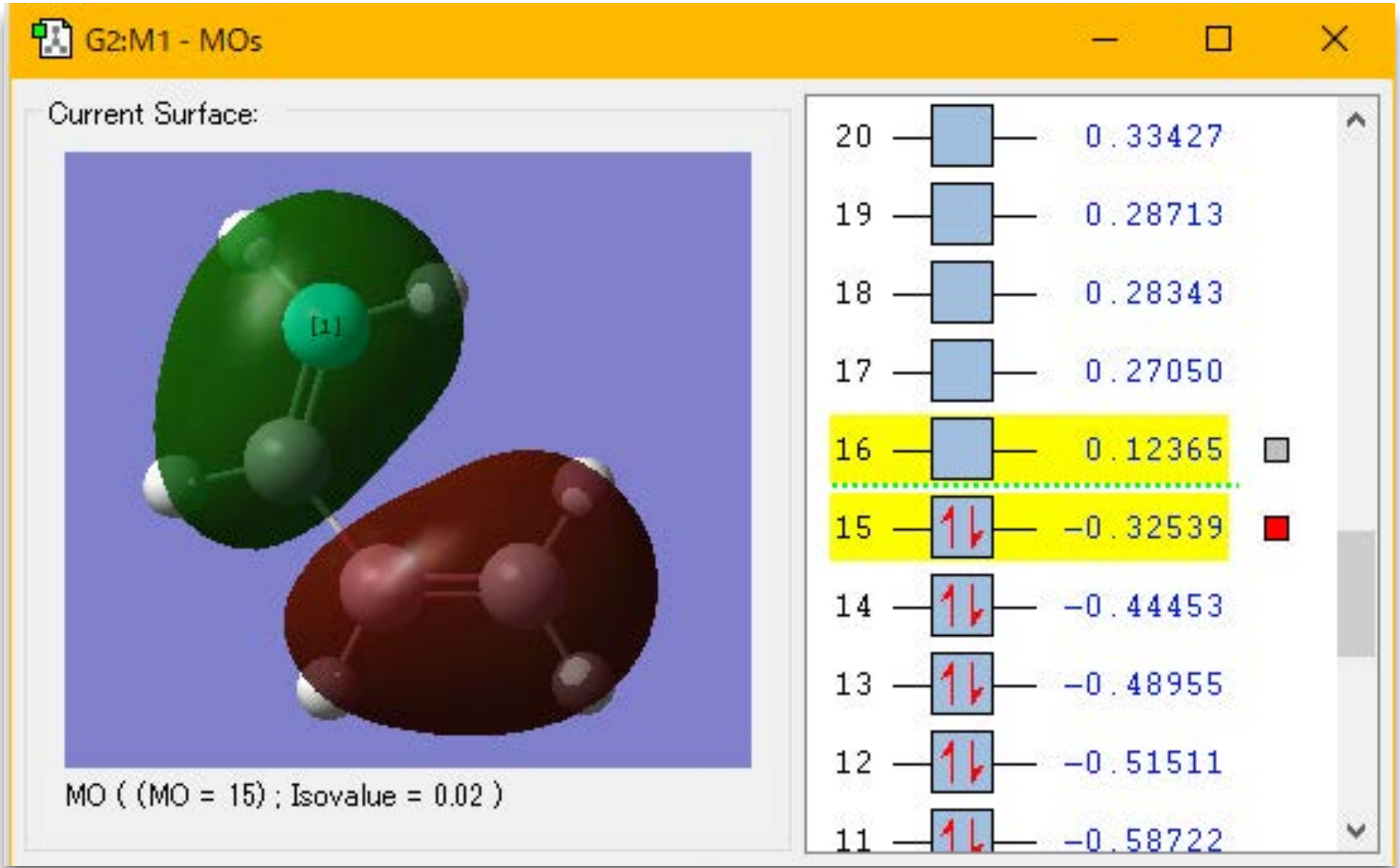
分子軌道の表示方法を変更する



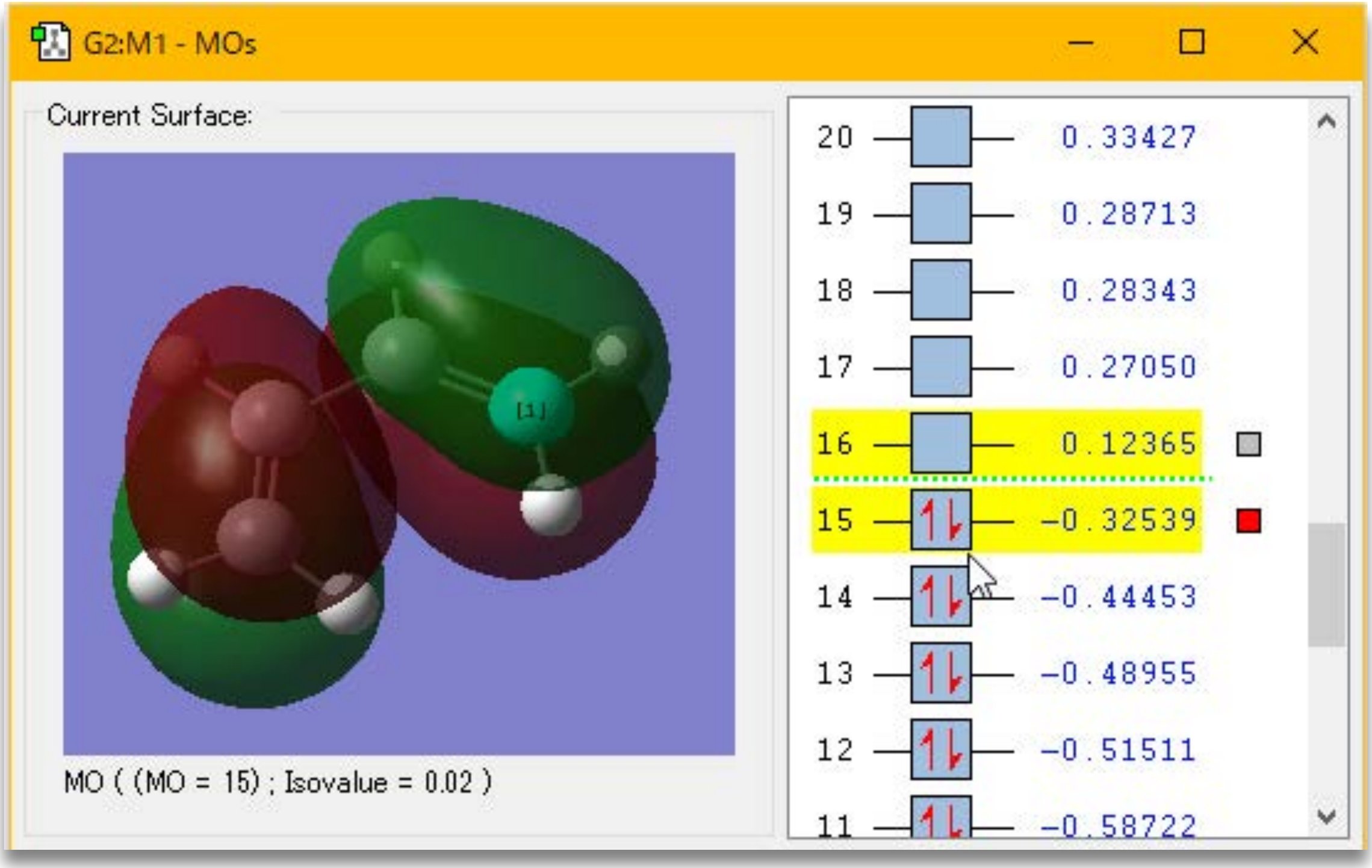
分子軌道の表示方法を変更する



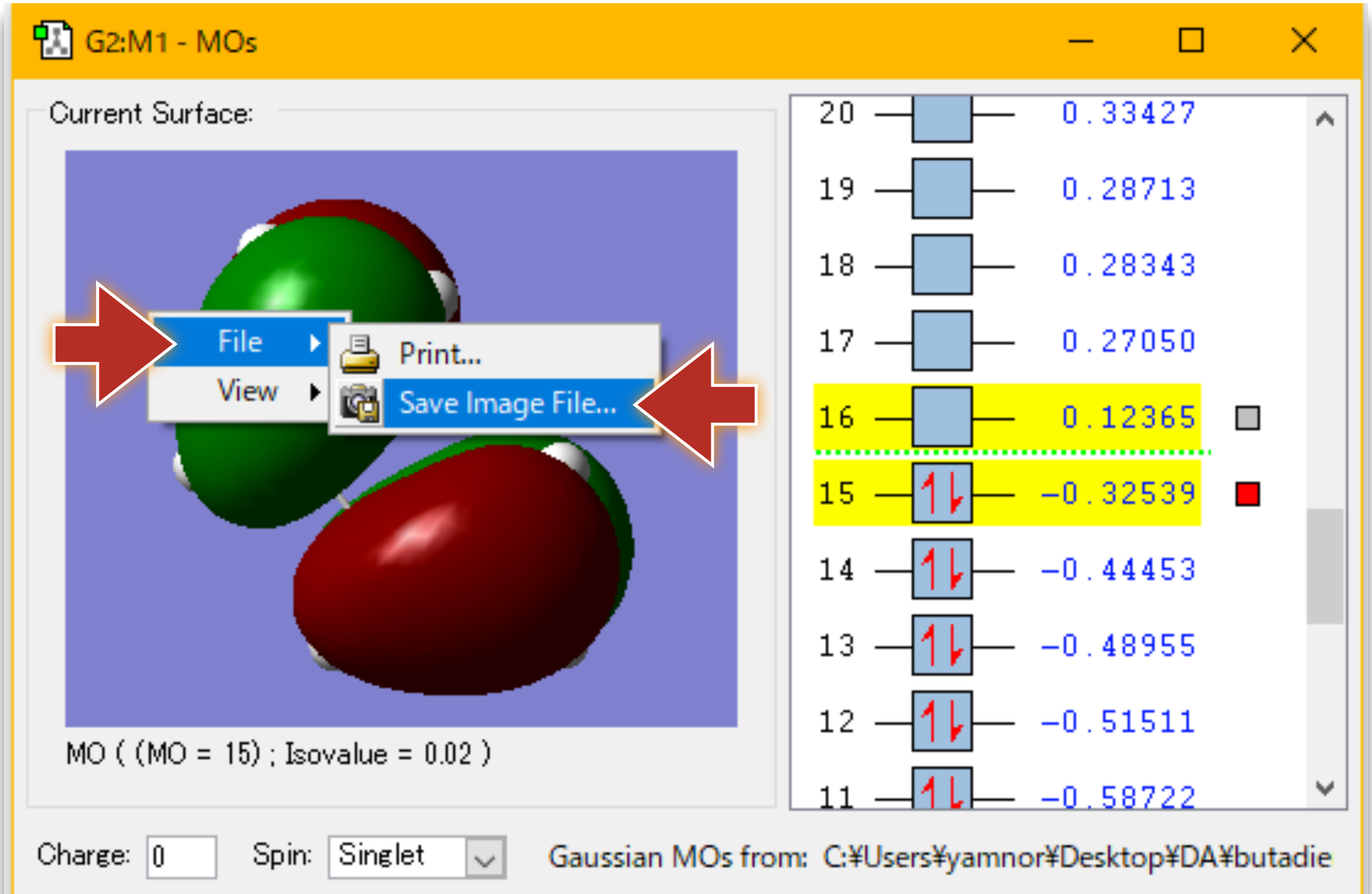
分子軌道の表示方法を変更する



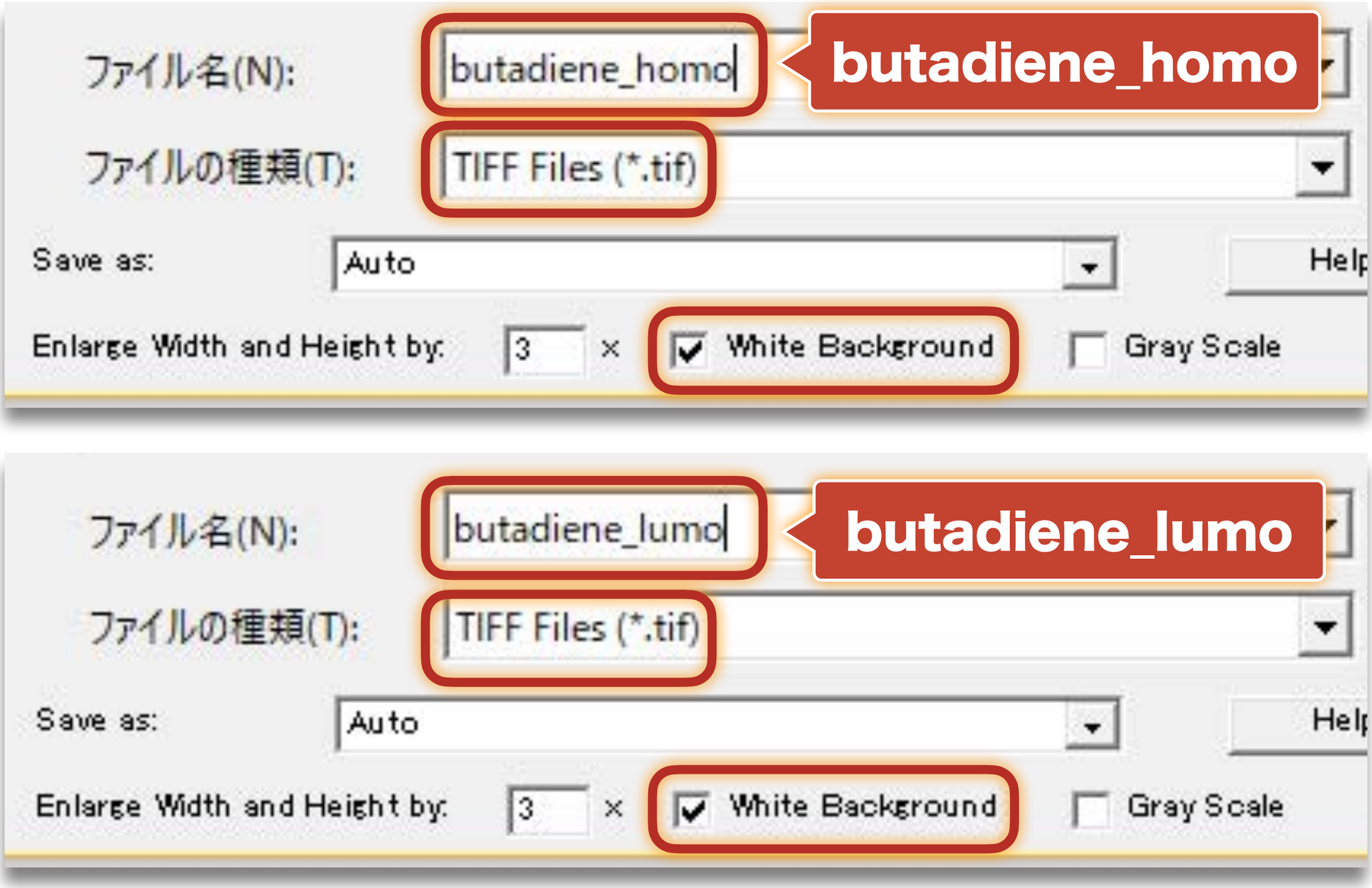
分子軌道の表示方法を変更する



画像を保存する（分子軌道）

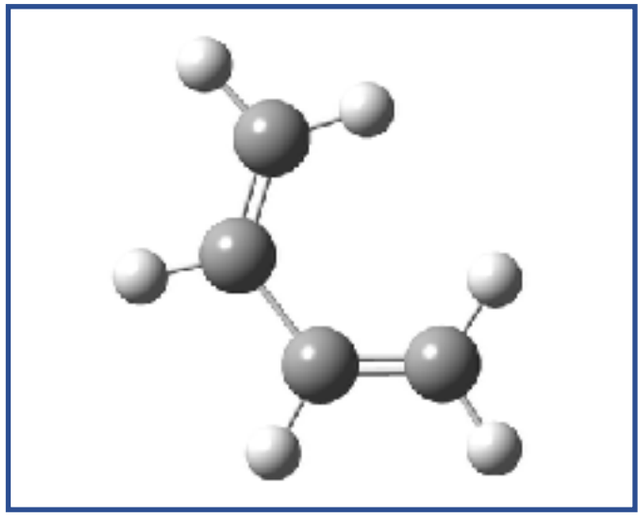


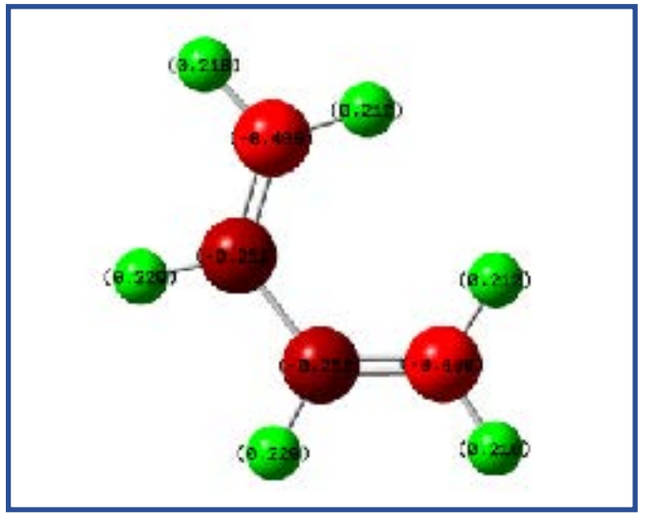
画像を保存する（分子軌道）

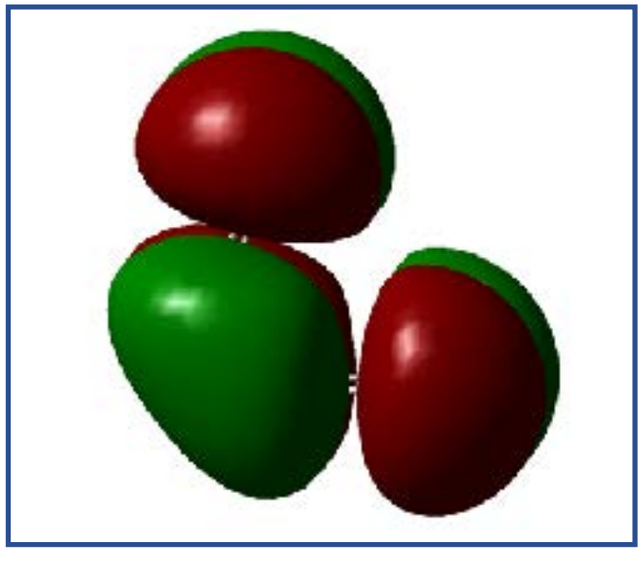


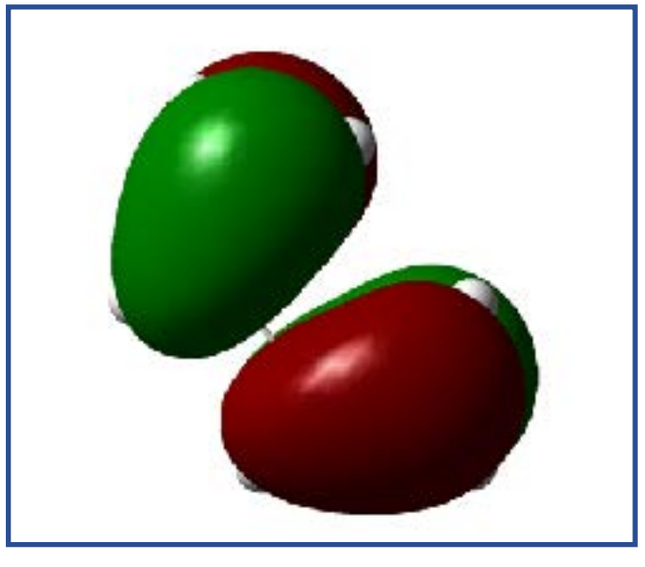
計算結果をまとめる（ブタジエン）

- 全エネルギーの値：＿＿＿＿＿＿ a.u.
- 炭素・炭素間距離：＿＿＿＿＿＿ Å
- 分子構造の図
- 電荷分布の図
- 分子軌道の図





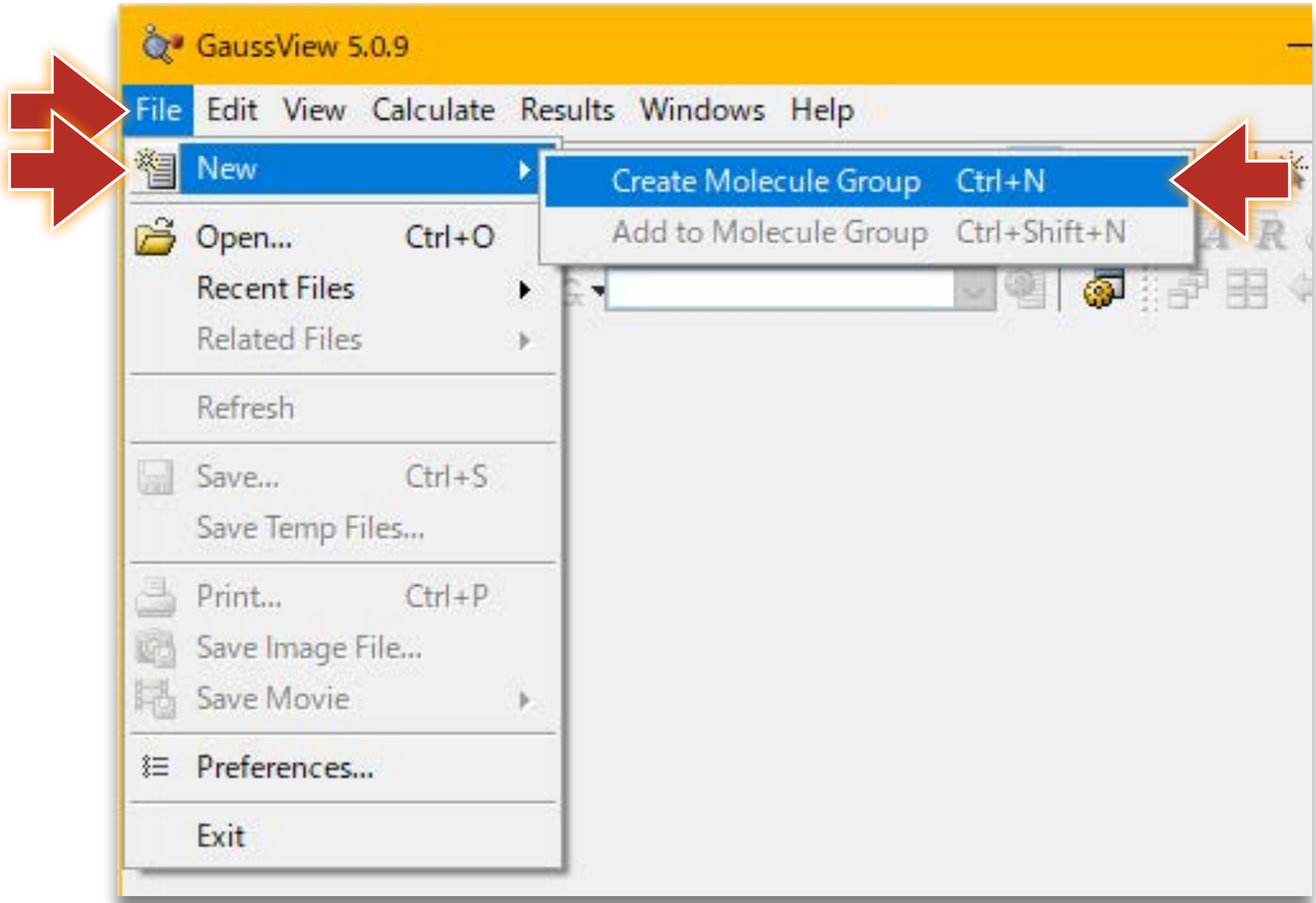




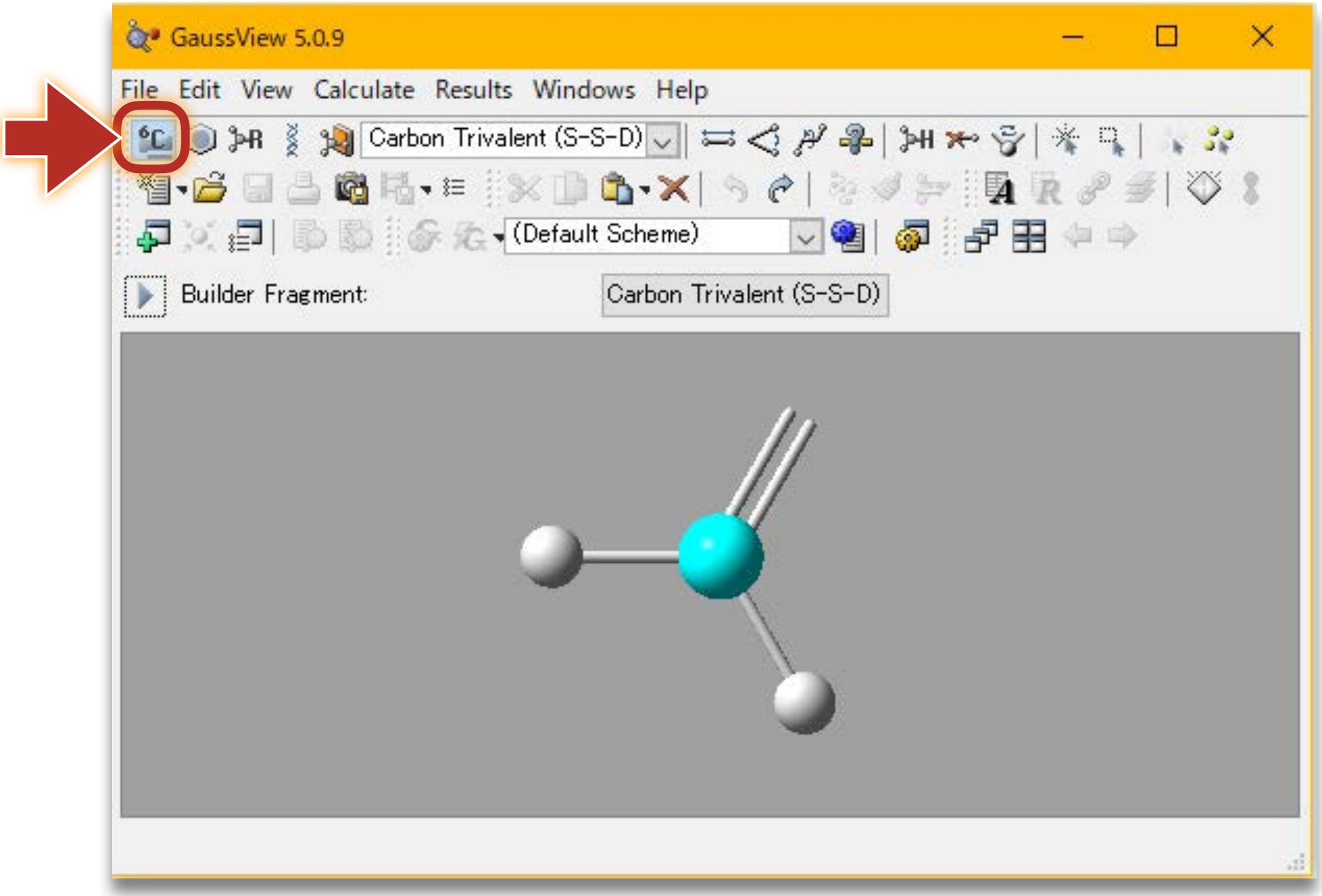
休憩時間：5分

エチレンの量子化学計算

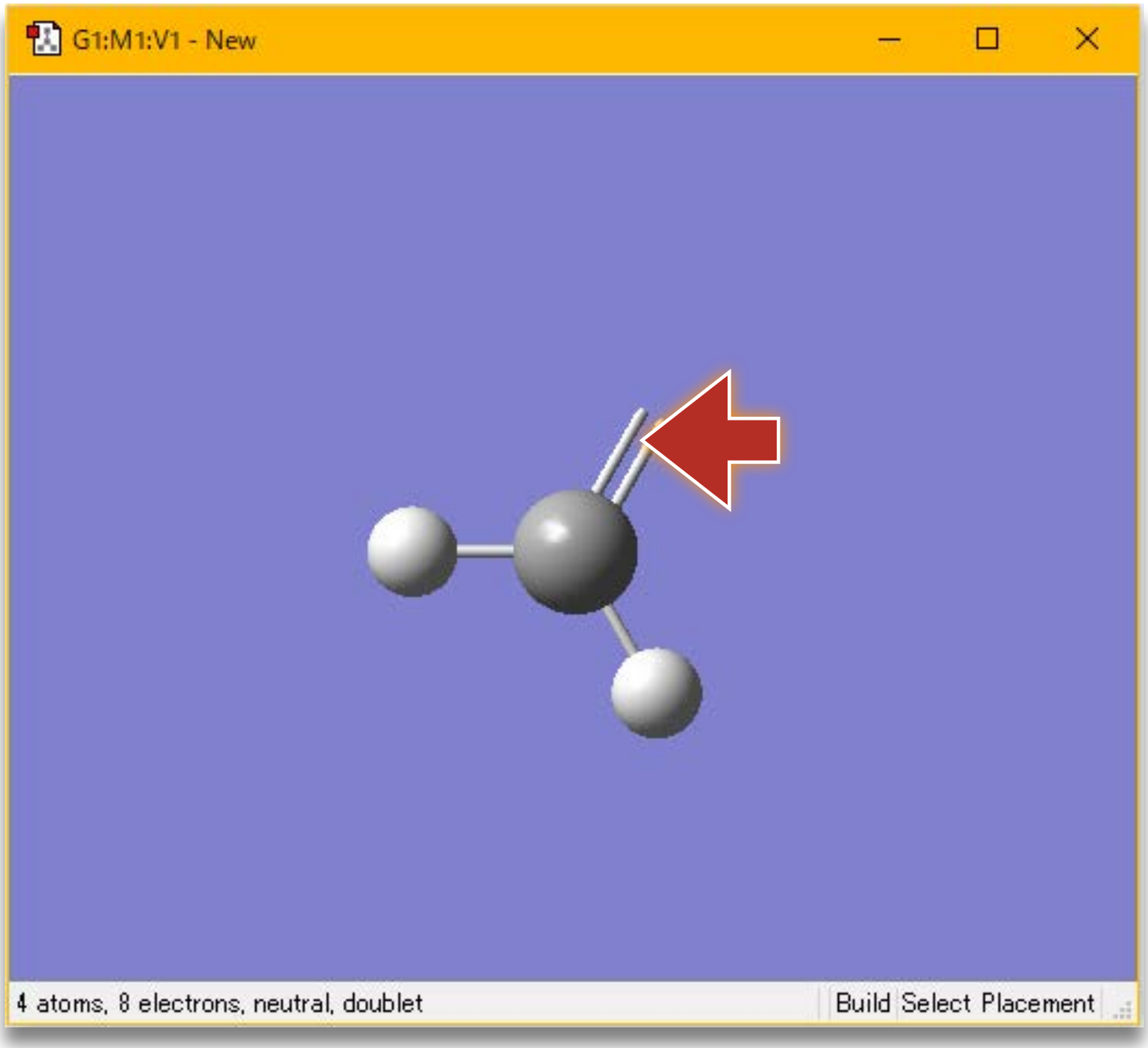
分子構造を作成する


GaussView 5.0.9
File
Edit
View
Calculate
Results
Windows
Help
New
Open... Ctrl+O
Recent Files
Related Files
Refresh
Save... Ctrl+S
Save Temp Files...
Print... Ctrl+P
Save Image File...
Save Movie
Preferences...
Exit
Create Molecule Group Ctrl+N
Add to Molecule Group Ctrl+Shift+N

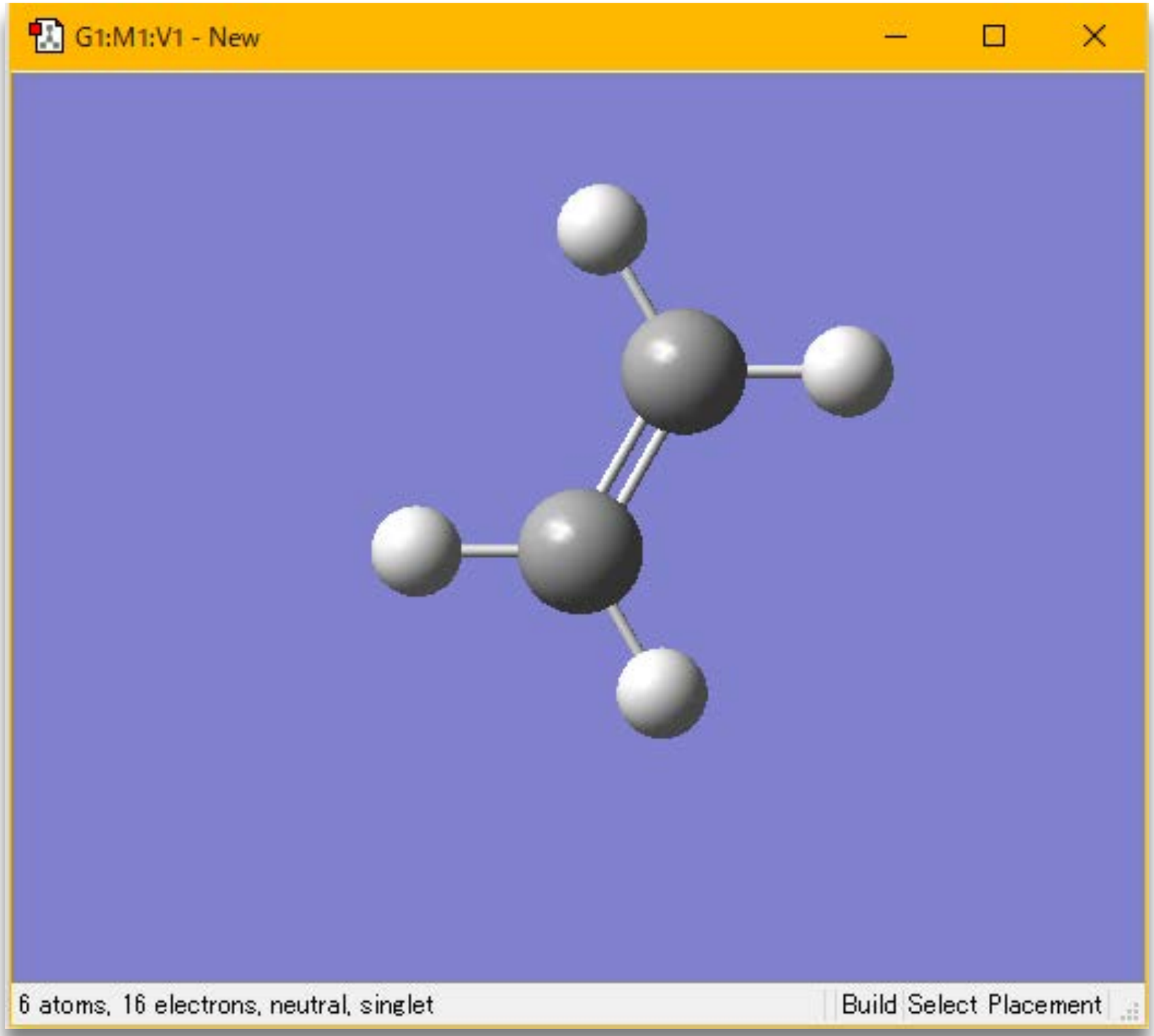
分子構造を作成する


GaussView 5.0.9
File Edit View Calculate Results Windows Help
Carbon Trivalent (S-S-D)
(Default Scheme)
Builder Fragment:
Carbon Trivalent (S-S-D)

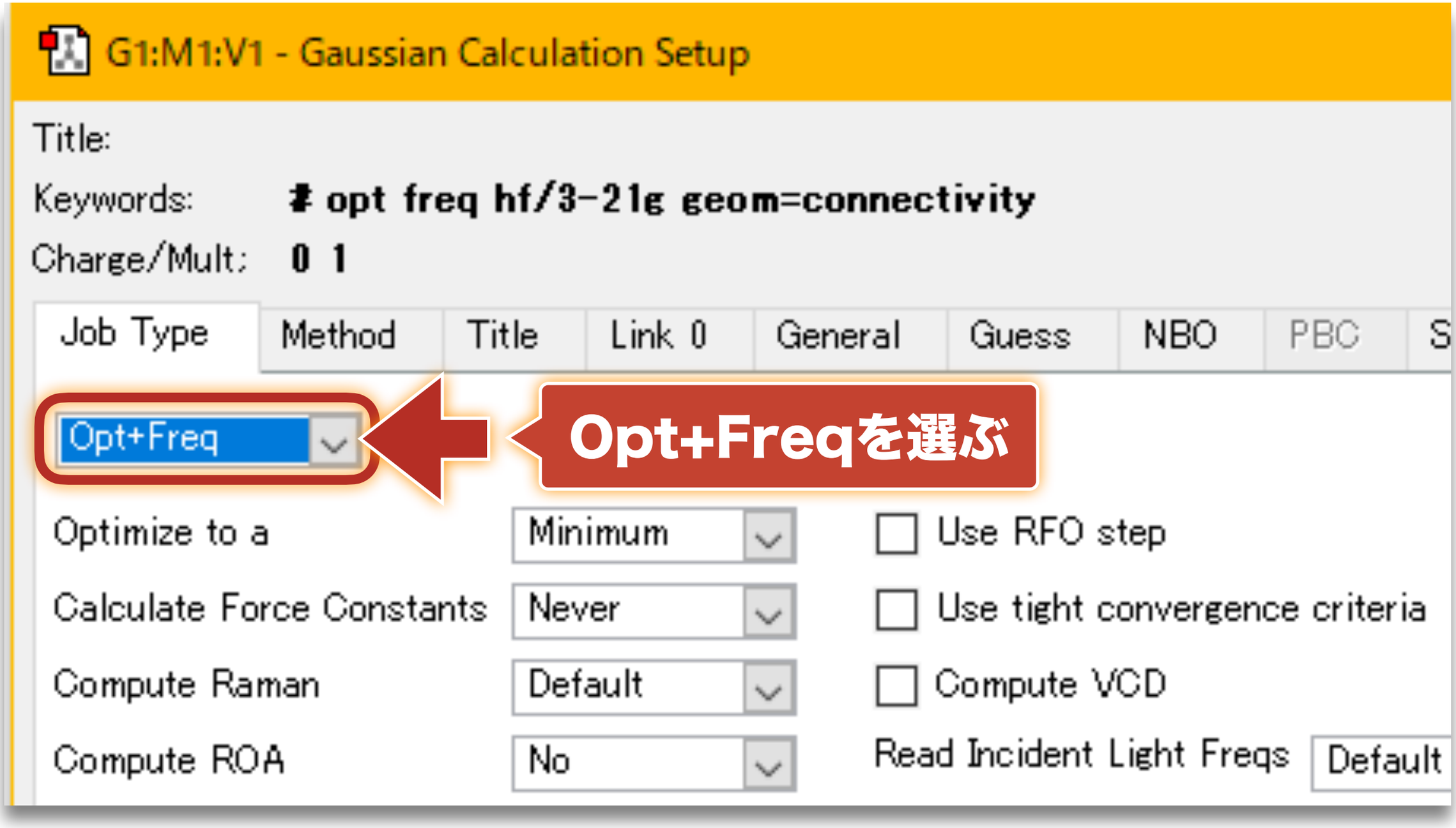
分子構造を作成する


G1:M1:V1 - New
4 atoms, 8 electrons, neutral, doublet
Build Select Placement

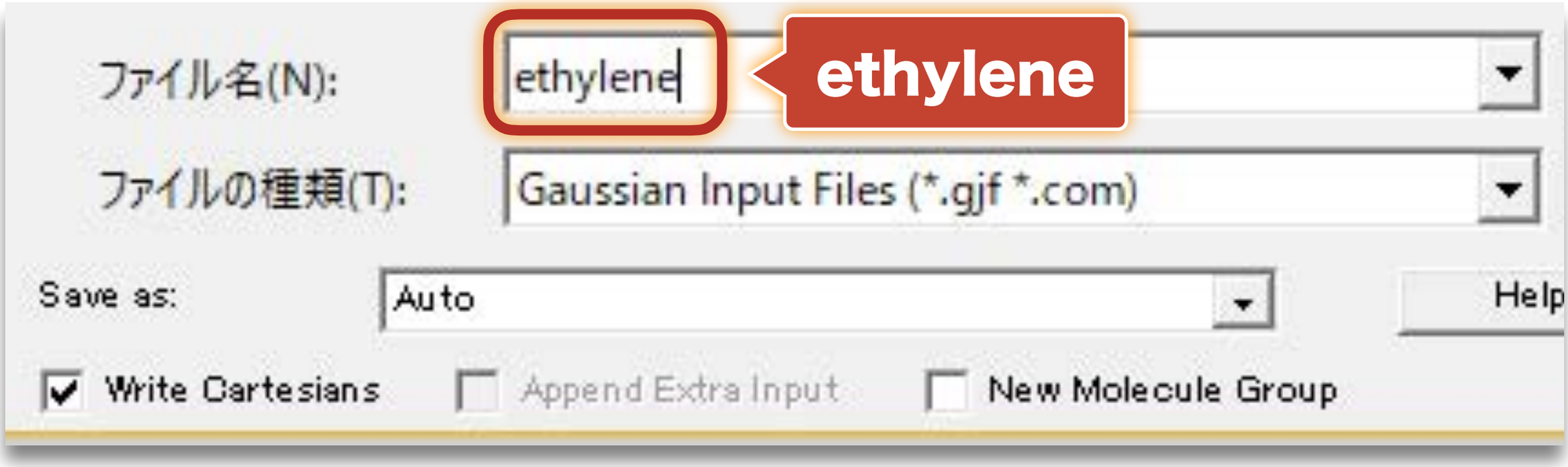
分子構造を作成する


G1:M1:V1 - New
6 atoms, 16 electrons, neutral, singlet
Build Select Placement

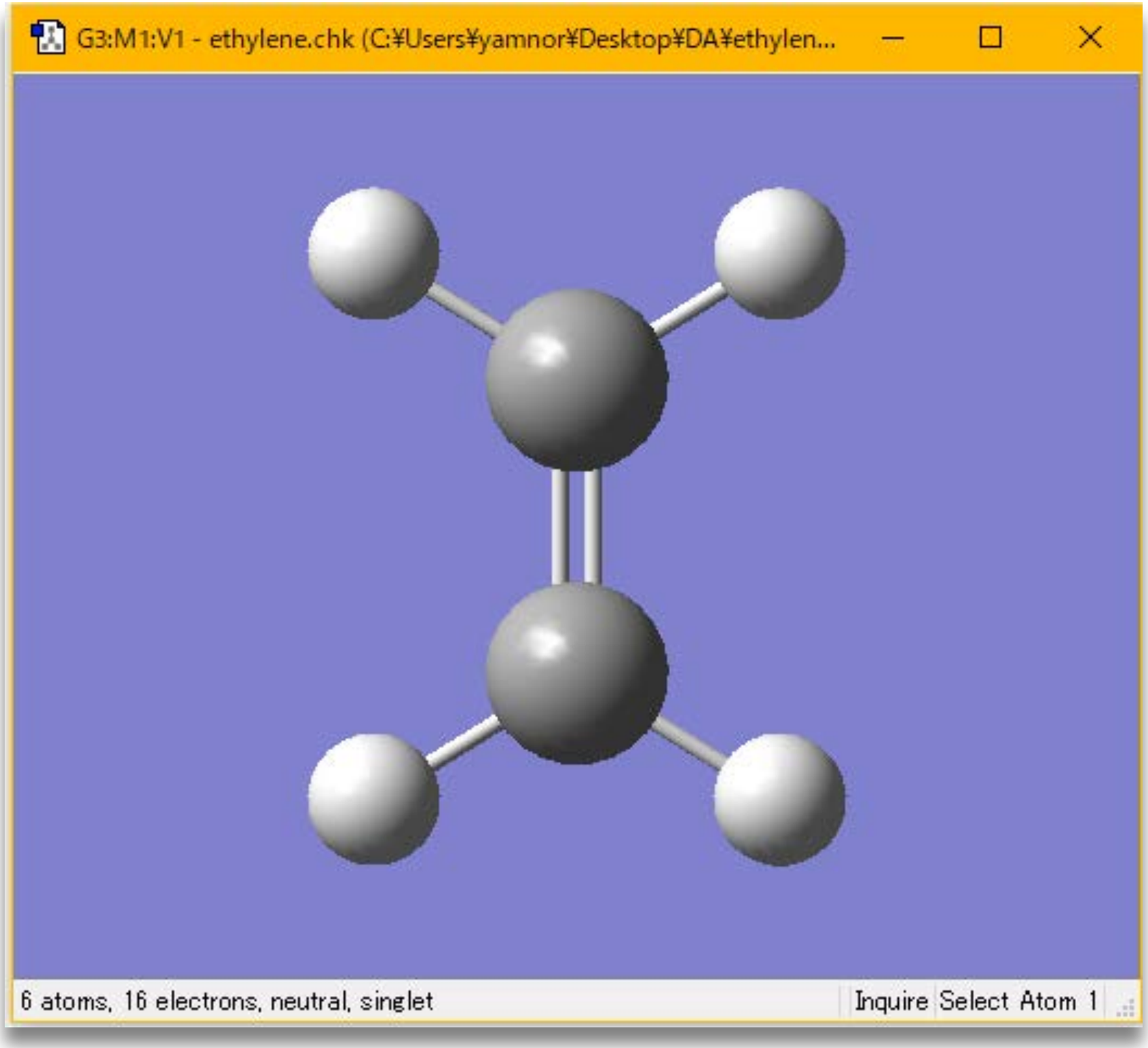
構造最適化


G1:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # opt freq hf/3-21g geom=connectivity
Charge/Mult: 0 1
Job Type
Method
Title
Link 0
General
Guess
NBO
PBC
S
Opt+Freq
Opt+Freqを選ぶ
Optimize to a
Minimum
Use RFO step
Calculate Force Constants
Never
Use tight convergence criteria
Compute Raman
Default
Compute VCD
Compute ROA
No
Read Incident Light Freqs
Default

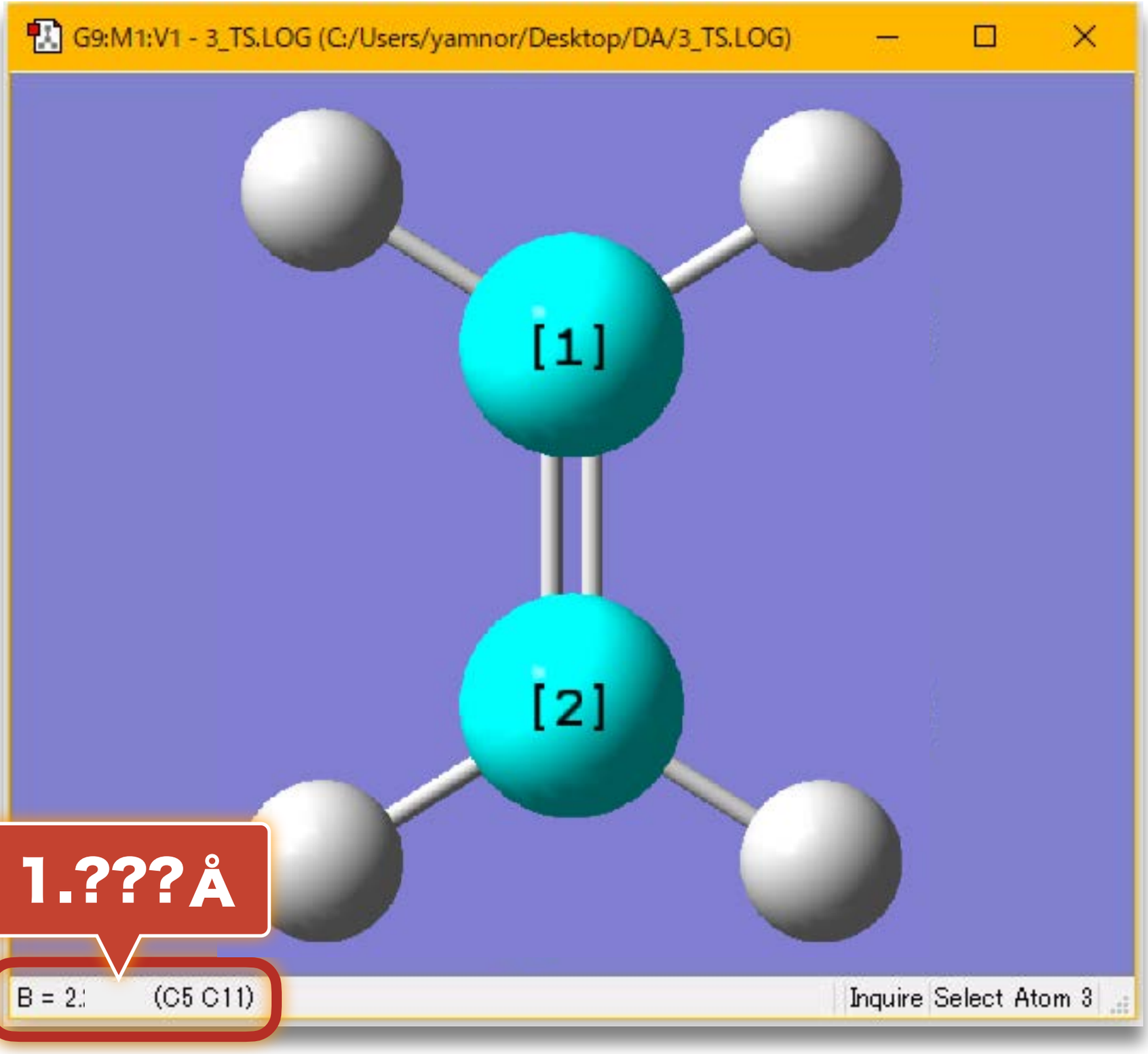
構造最適化


ファイル名(N):
ethylene
ethylene
ファイルの種類(T):
Gaussian Input Files (*.gjf *.com)
Save as:
Auto
Help
Write Cartesians
Append Extra Input
New Molecule Group

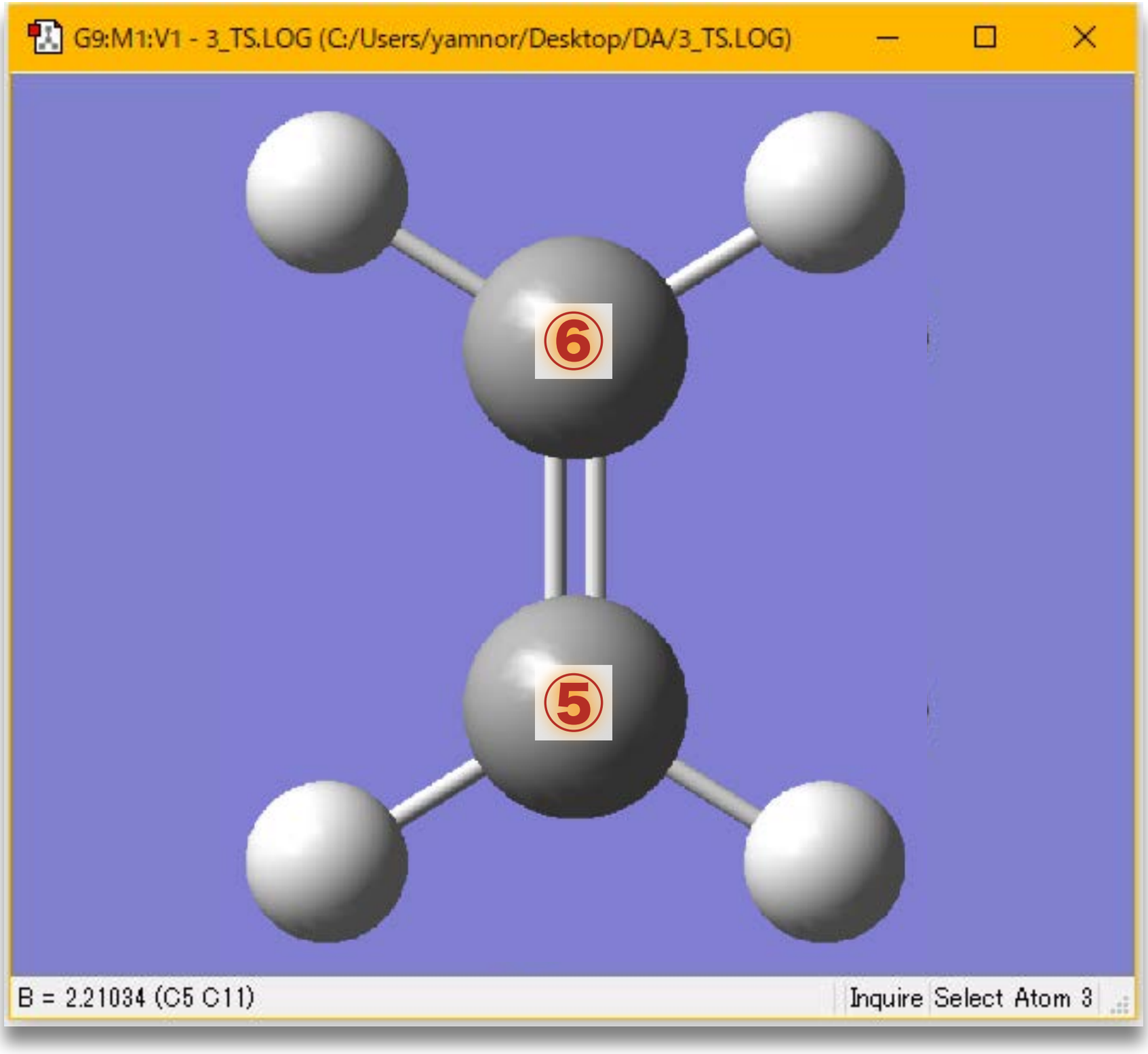
構造最適化


G3:M1:V1 - ethylene.chk (C:¥Users¥yamnor¥Desktop¥DA¥ethylen...
6 atoms, 16 electrons, neutral, singlet
Inquire
Select Atom 1

原子間距離を調べる


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
[1]
[2]
1.???Å
B = 2.
(C5 C11)
Inquire
Select Atom 3

原子の番号（ラベル）


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
⑥
⑤
B = 2.21034 (C5 C11)
Inquire Select Atom 3

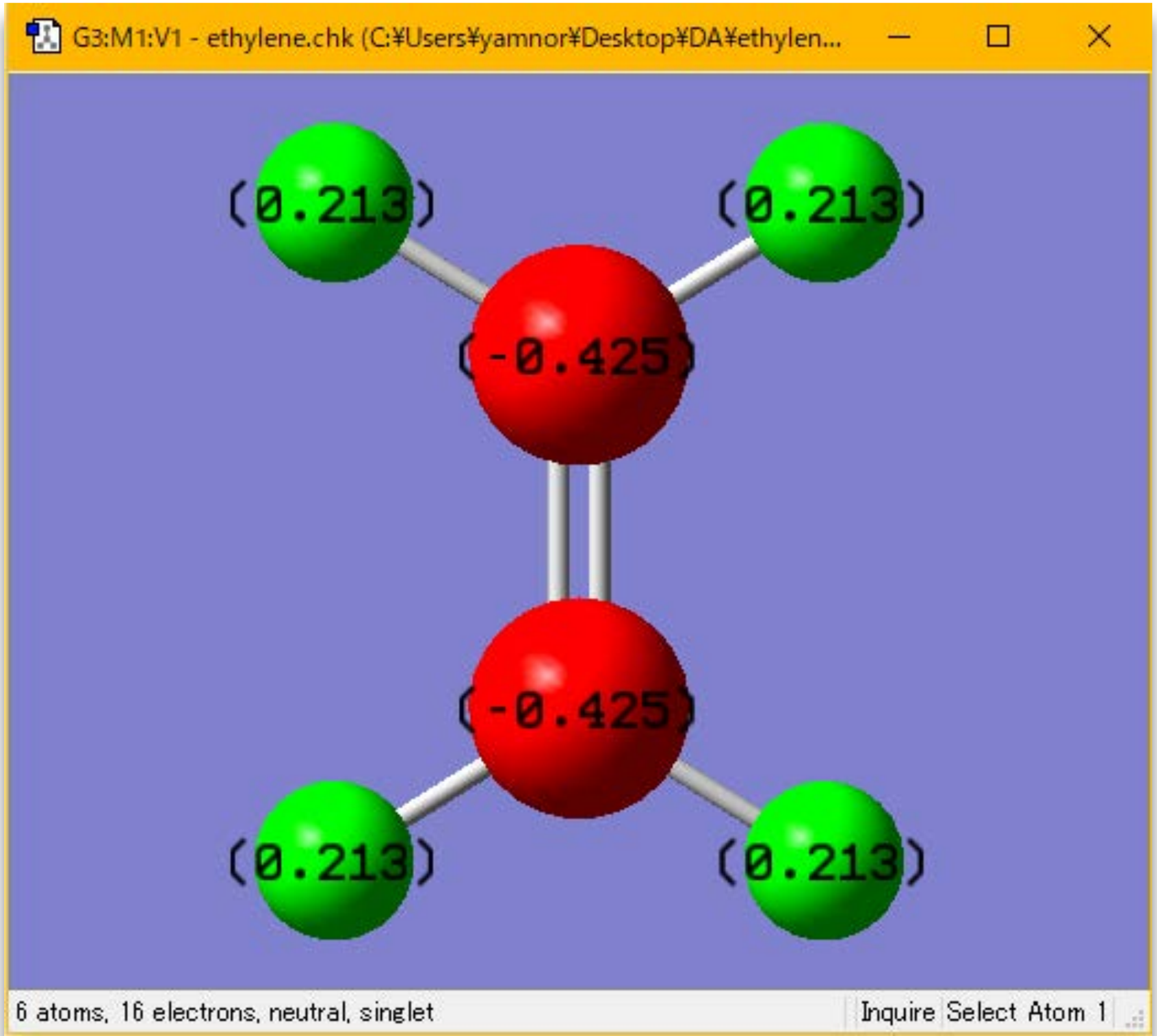
全エネルギーを調べる

G3:M1:V1 - Gaussian Calculation Summary

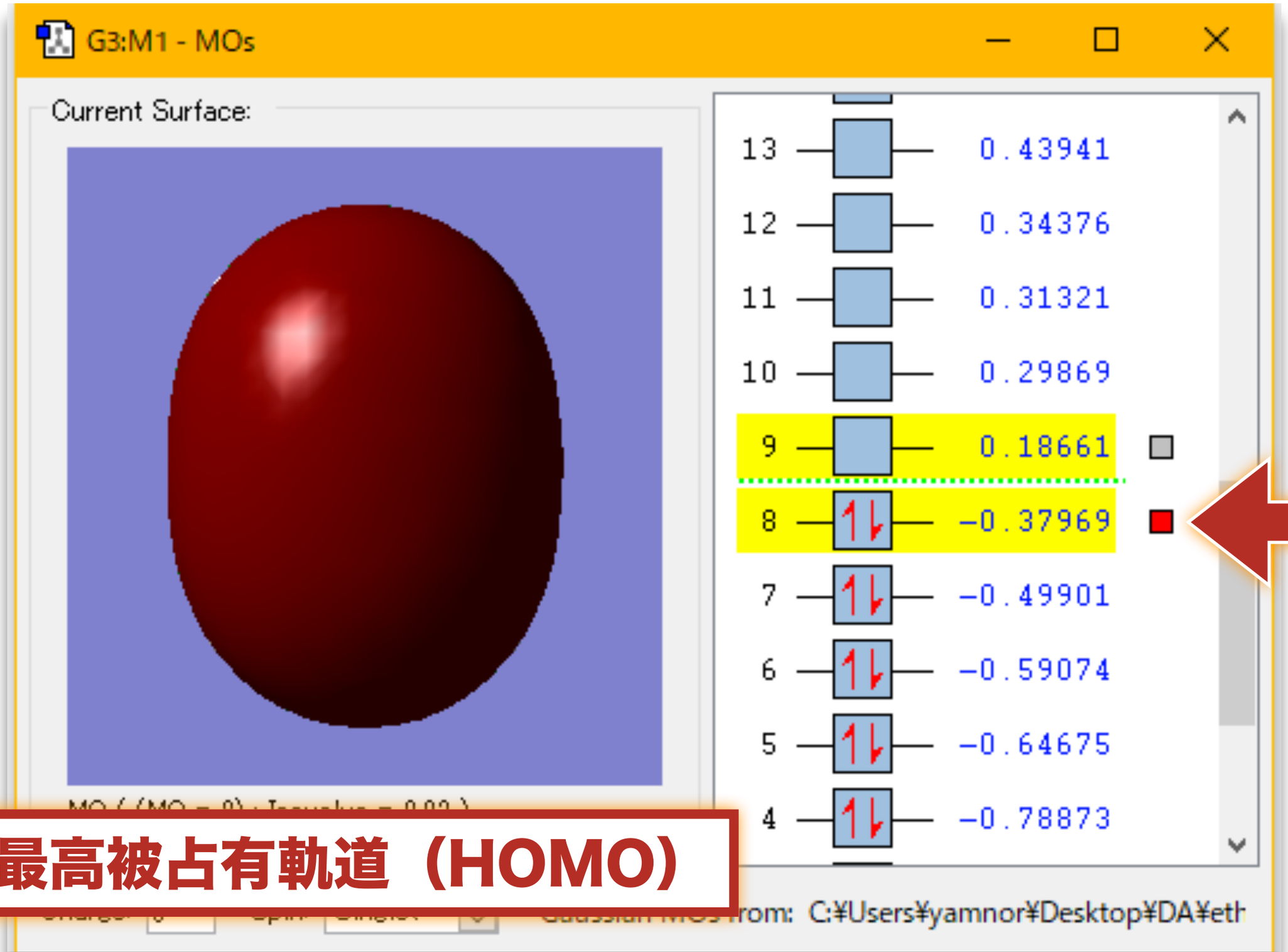
Title Card Required		
File Name	ethylene	
File Type	.chk	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	3-21G	
Charge	0	
Spin	Singlet	
Total Energy	-77.	a.u.
RMS Gradient Norm	0.00009216	a.u.
Imaginary Freq		
Dipole Moment	0.0000	Debye
Point Group		

Ok　View File　Save Data

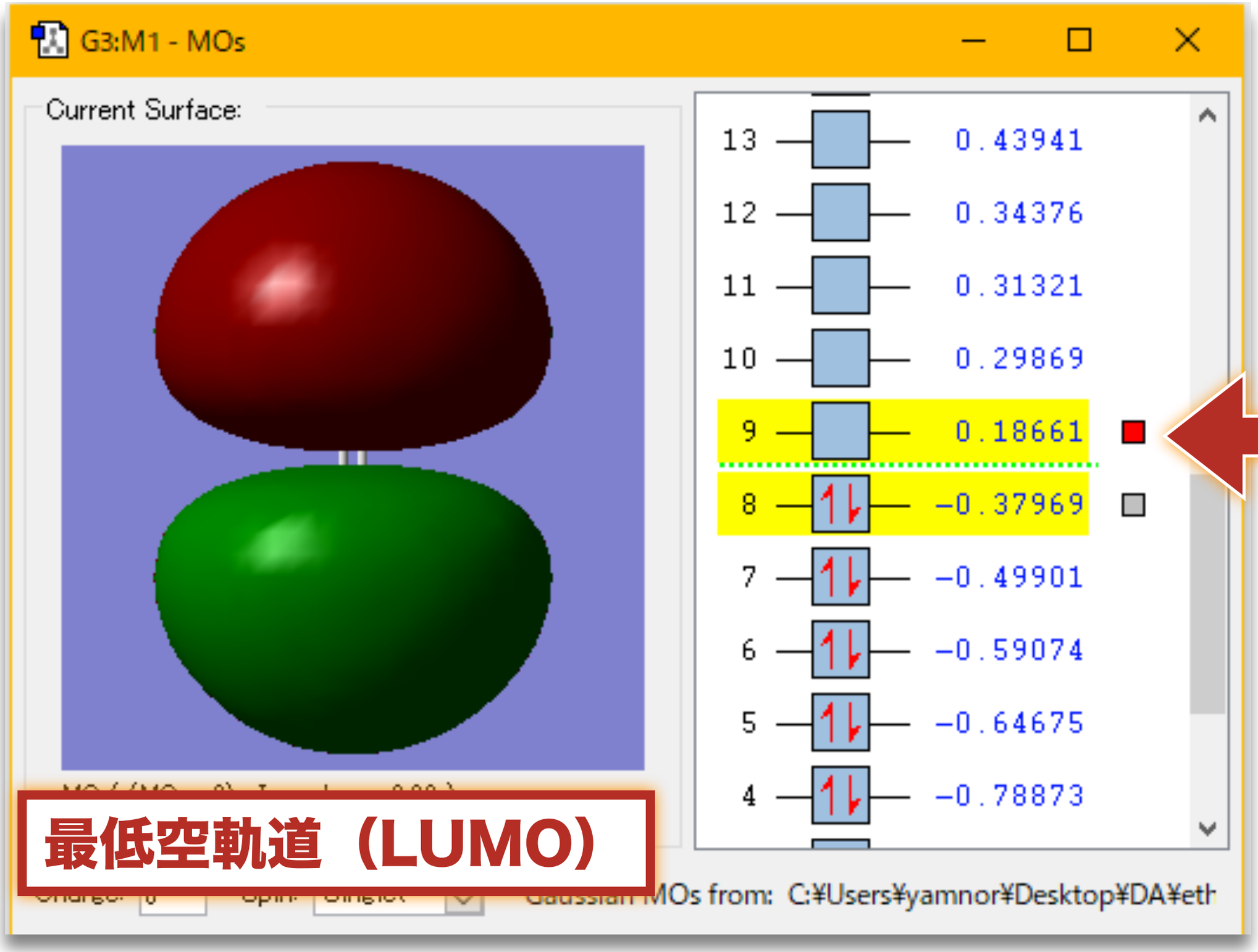
電荷分布を調べる


G3:M1:V1 - ethylene.chk (C:¥Users¥yamnor¥Desktop¥DA¥ethylen...
(0.213)
(0.213)
(-0.425)
(-0.425)
(0.213)
(0.213)
6 atoms, 16 electrons, neutral, singlet
Inquire
Select Atom 1

分子軌道を調べる

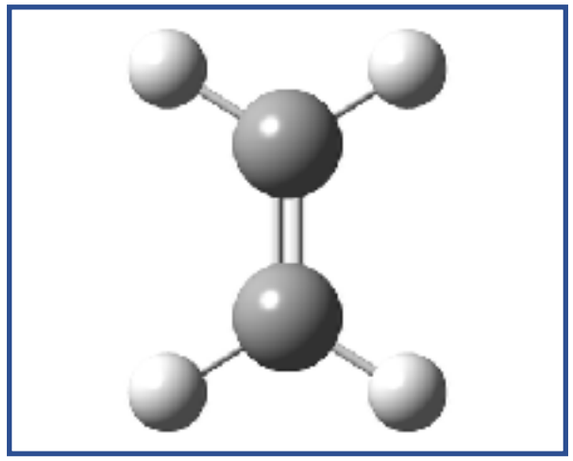

G3:M1 - MOs
Current Surface:
13 0.43941
12 0.34376
11 0.31321
10 0.29869
9 0.18661
8 -0.37969
7 -0.49901
6 -0.59074
5 -0.64675
4 -0.78873
最高被占有軌道（HOMO）

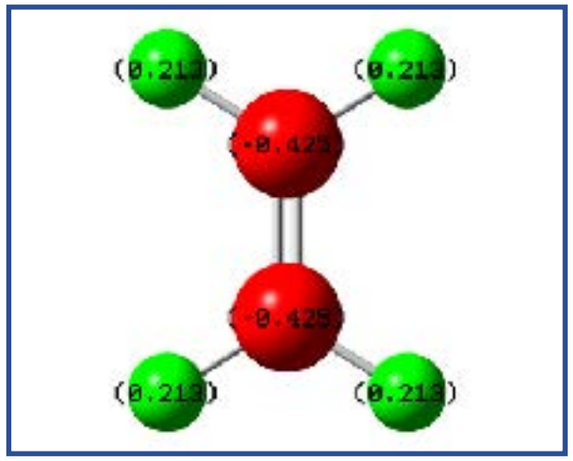
分子軌道を調べる

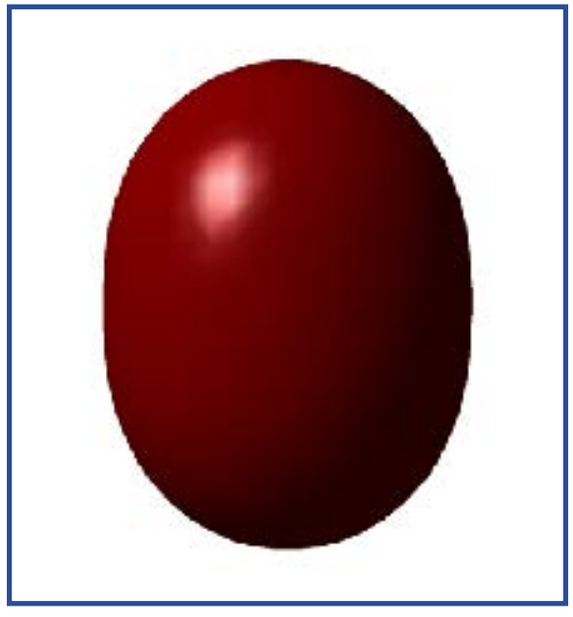

G3:M1 - MOs
Current Surface:
13 0.43941
12 0.34376
11 0.31321
10 0.29869
9 0.18661
8 -0.37969
7 -0.49901
6 -0.59074
5 -0.64675
4 -0.78873
最低空軌道（LUMO）
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥eth

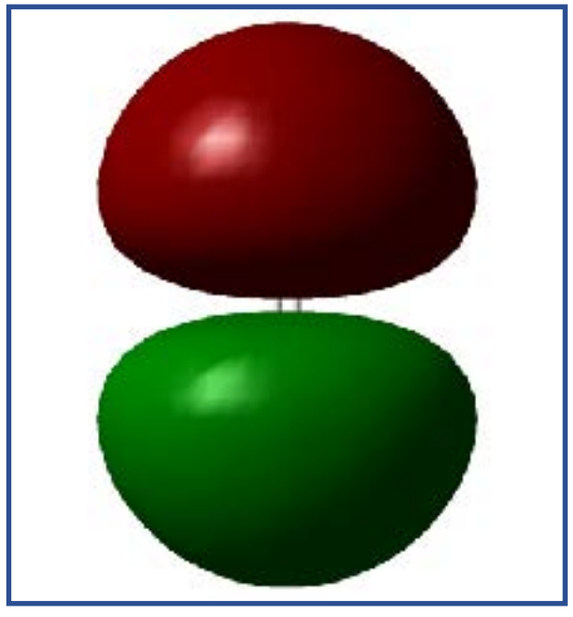
計算結果をまとめる（エチレン）

- 全エネルギーの値：＿＿＿＿＿＿ a.u.
- 炭素・炭素間距離：＿＿＿＿＿＿ Å
- 分子構造の図
- 電荷分布の図
- 分子軌道の図



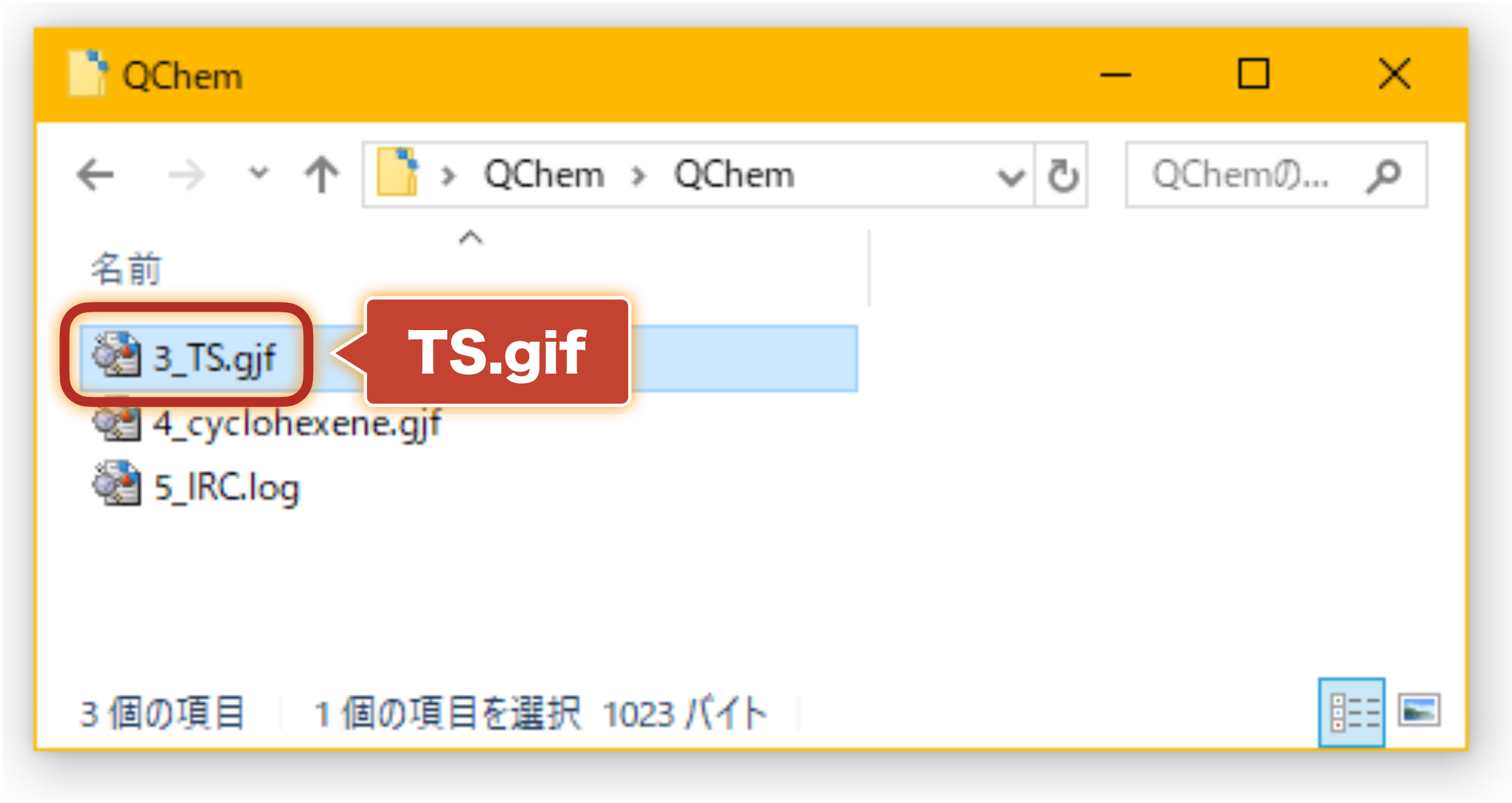




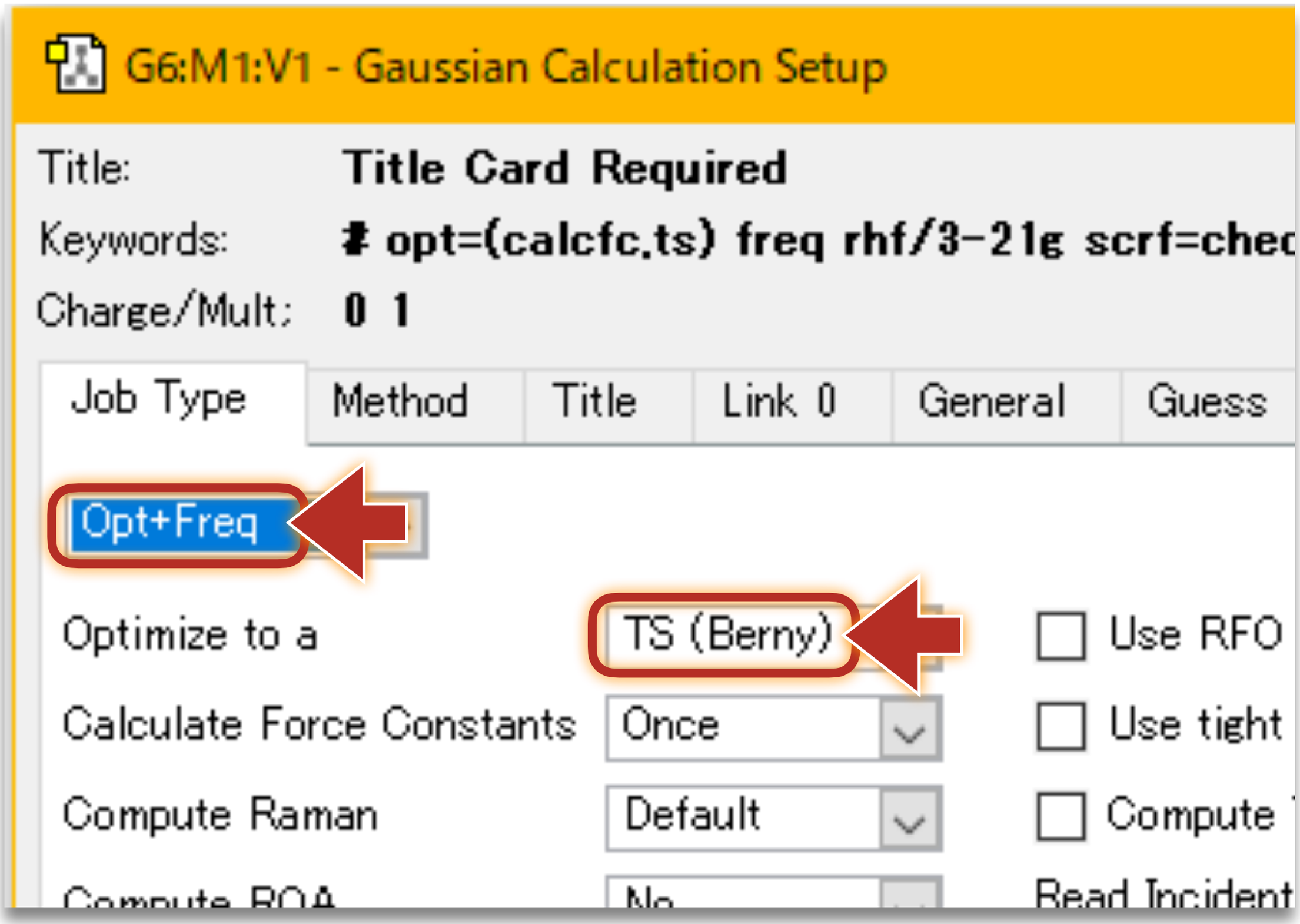


遷移状態を探索する

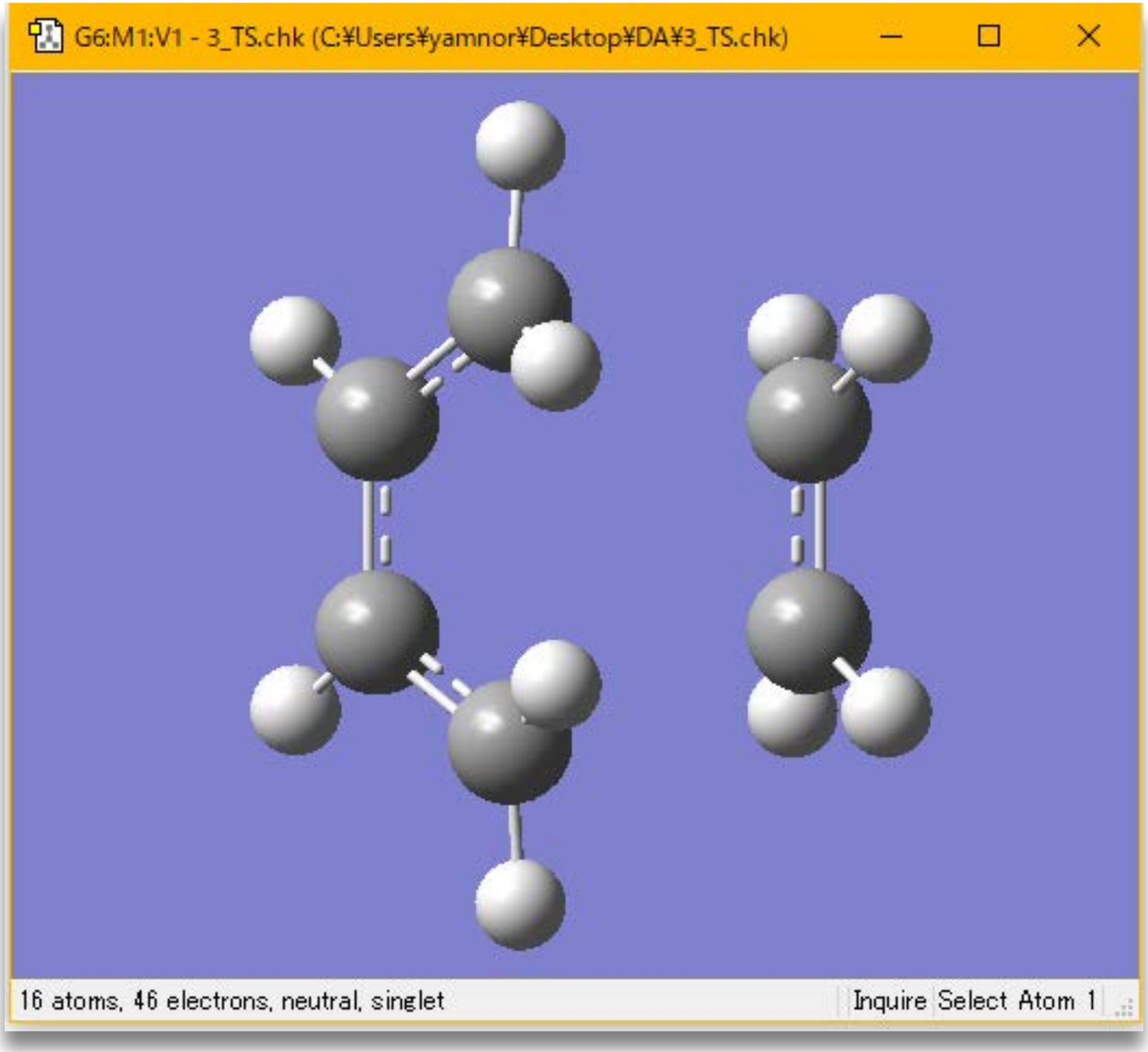
入力ファイルを開く


QChem
QChem › QChem
QChemの...
名前
3_TS.gjf
TS.gif
4_cyclohexene.gjf
5_IRC.log
3 個の項目
1 個の項目を選択 1023 バイト

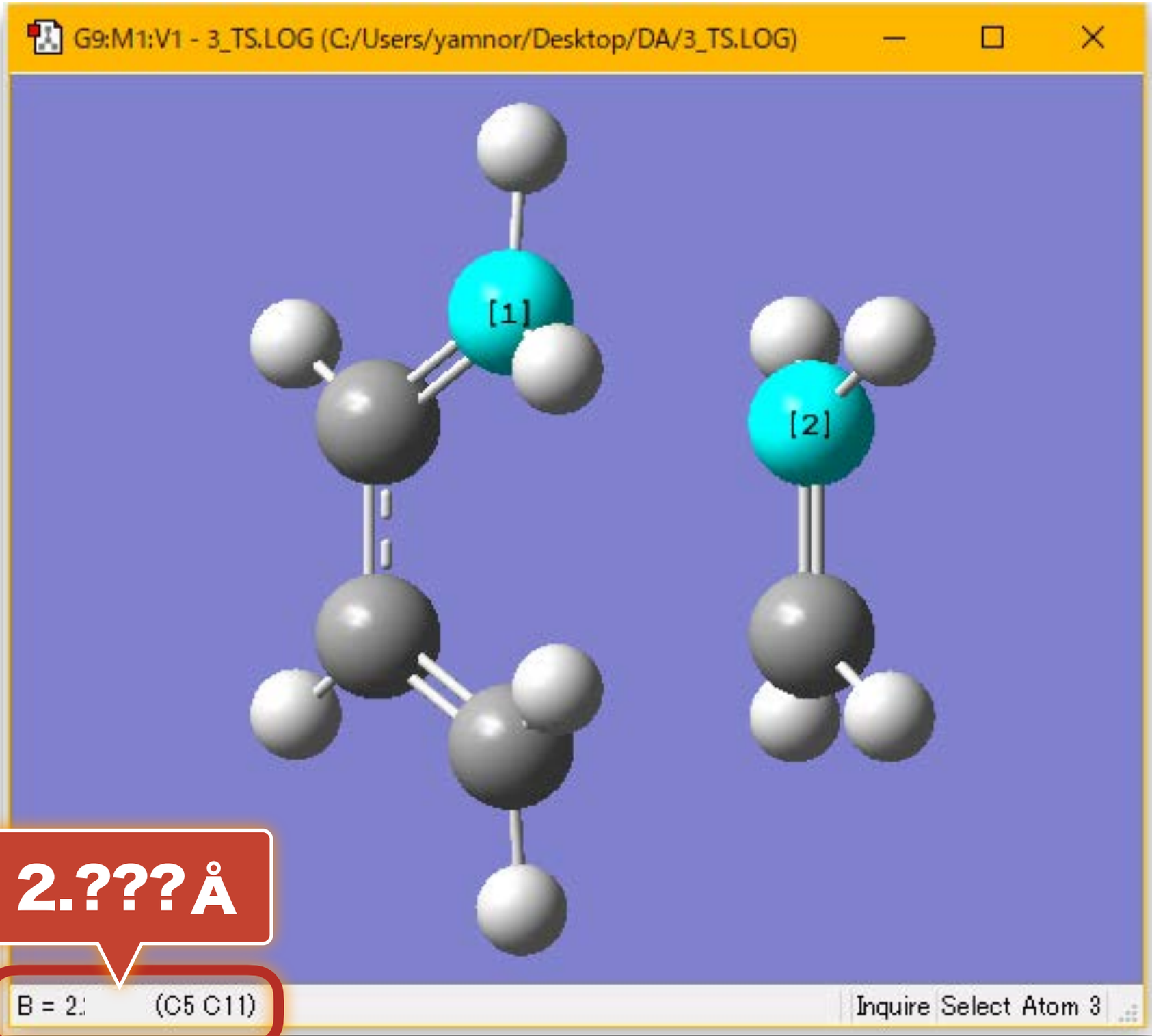
構造最適化


G6:M1:V1 - Gaussian Calculation Setup
Title:
Title Card Required
Keywords:
opt=(calcfc,ts) freq rhf/3-21g scrf=chec
Charge/Mult:
0 1
Job Type
Method
Title
Link 0
General
Guess
Opt+Freq
Optimize to a
TS (Berny)
Use RFO
Calculate Force Constants
Once
Use tight
Compute Raman
Default
Compute
Compute ROA
No
Read Incident

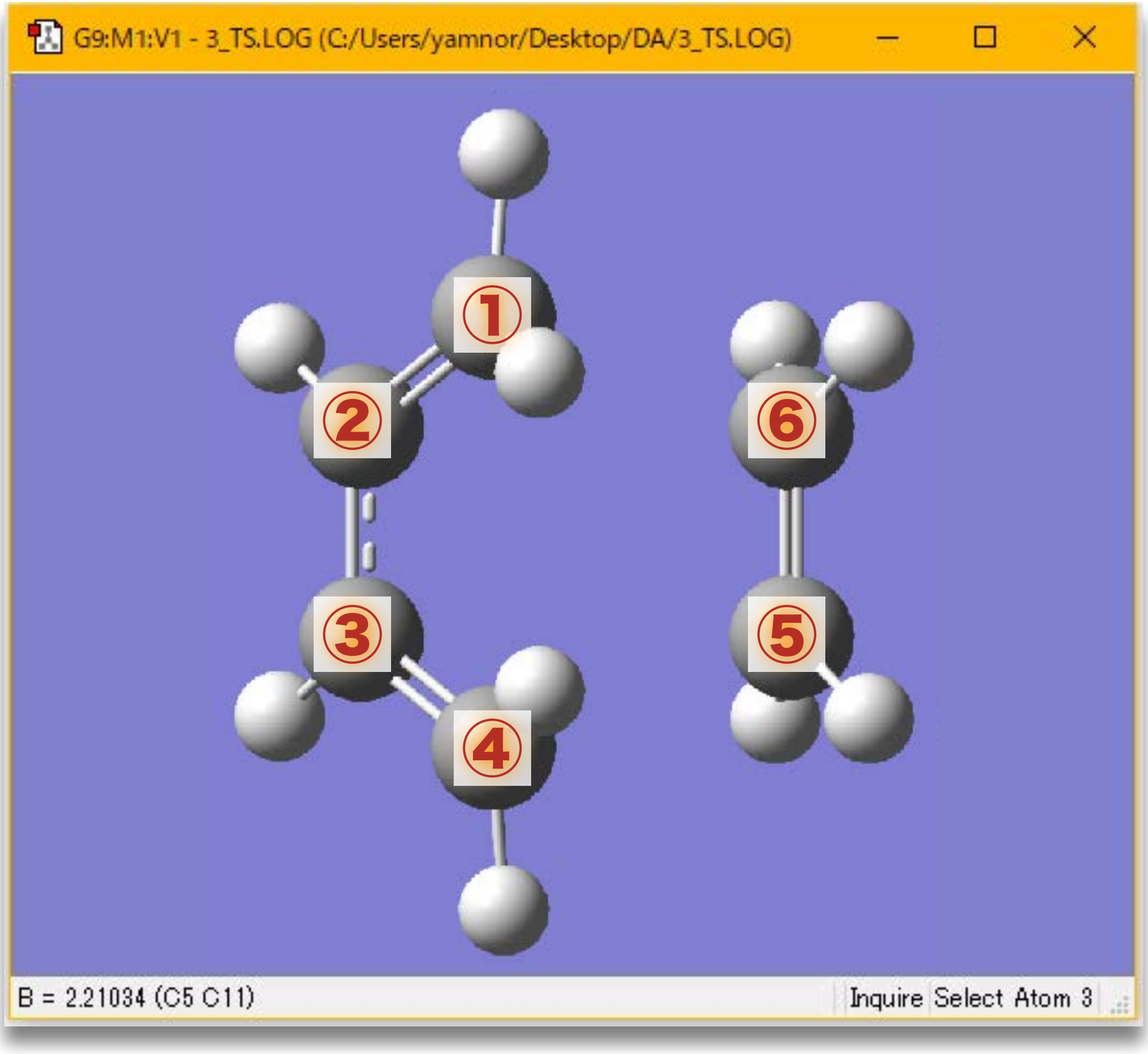
構造最適化


G6:M1:V1 - 3_TS.chk (C:¥Users¥yamnor¥Desktop¥DA¥3_TS.chk)
16 atoms, 46 electrons, neutral, singlet
Inquire
Select Atom 1

原子間距離を調べる


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
[1]
[2]
2.??? Å
B = 2.
(C5 C11)
Inquire Select Atom 3

原子の番号（ラベル）


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
①
②
③
④
⑤
⑥
B = 2.21034 (C5 C11)
Inquire Select Atom 3

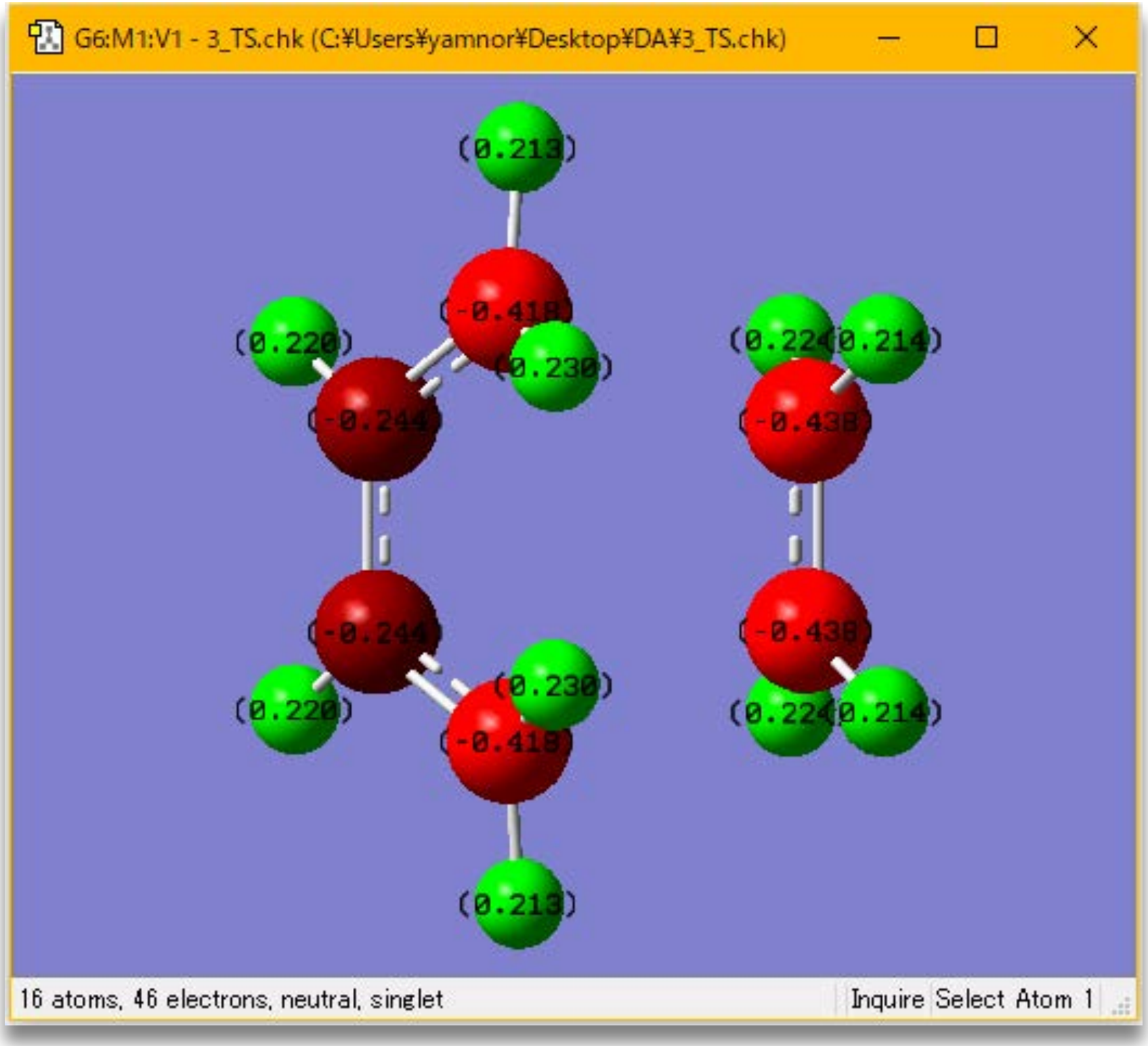
全エネルギーを調べる

G6:M1:V1 - Gaussian Calculation Summary

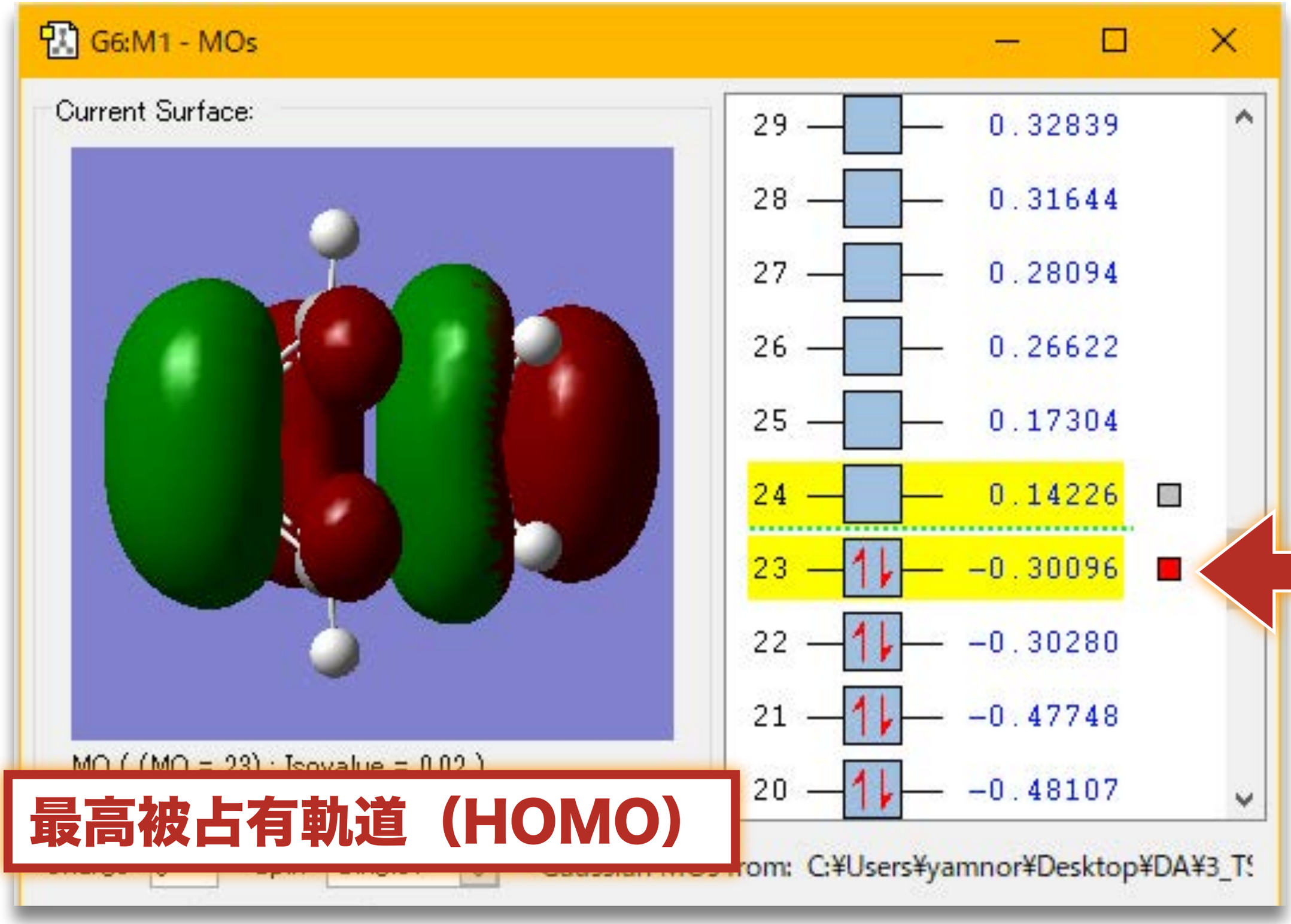
Title Card Required		
File Name	3_TS	
File Type	.chk	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	3-21G	
Charge	0	
Spin	Singlet	
Total Energy	-231.	a.u.
RMS Gradient Norm	0.00014630	a.u.
Imaginary Freq		
Dipole Moment	0.5748	Debye
Point Group		

Ok　View File　Save Data

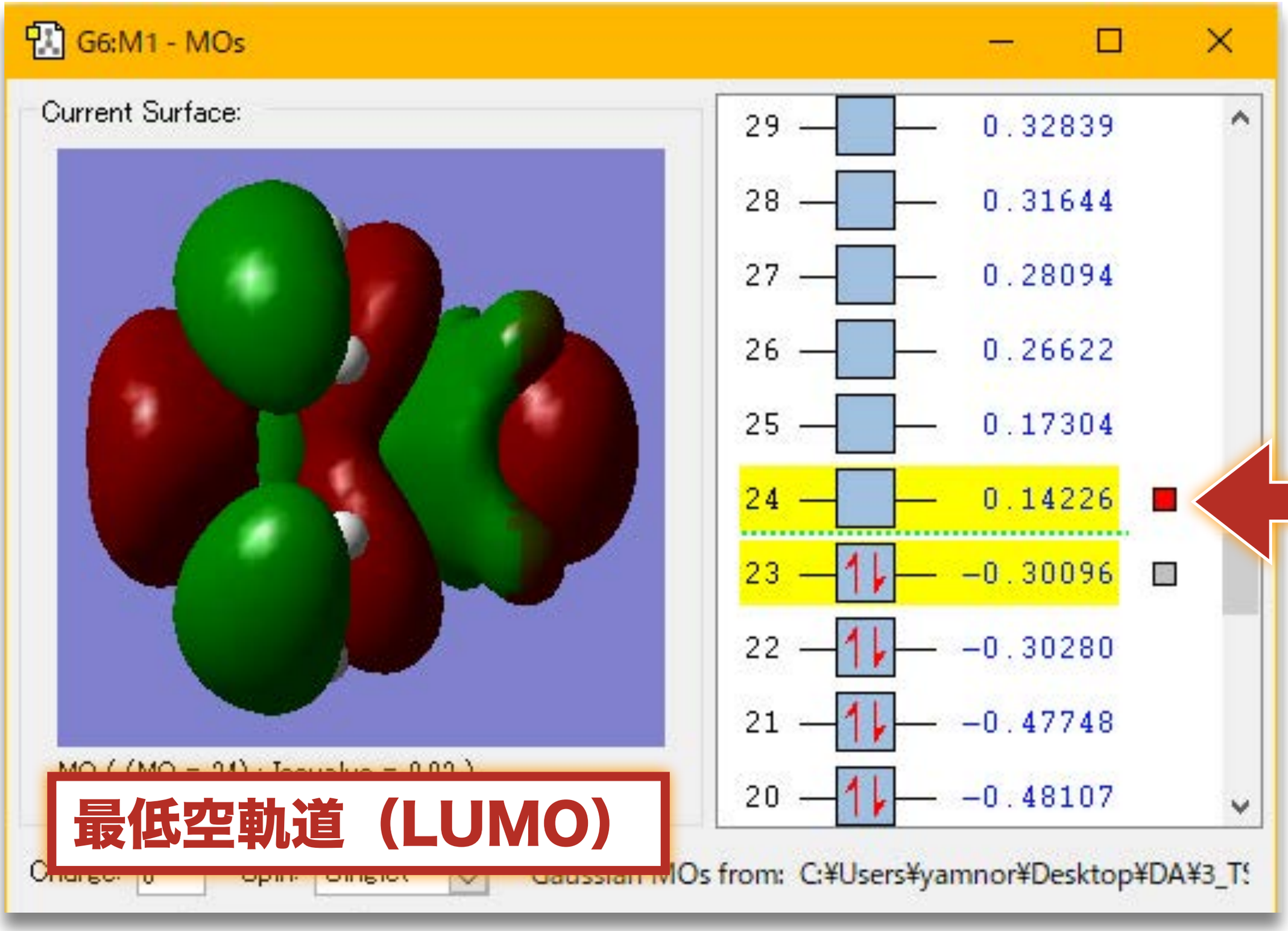
電荷分布を調べる


G6:M1:V1 - 3_TS.chk (C:¥Users¥yamnor¥Desktop¥DA¥3_TS.chk)
(0.213)
(-0.418)
(0.220)
(0.230)
(-0.244)
(0.224)
(0.214)
(-0.438)
(-0.244)
(0.230)
(0.220)
(-0.418)
(0.224)
(0.214)
(0.213)
16 atoms, 46 electrons, neutral, singlet
Inquire
Select Atom 1

分子軌道を調べる

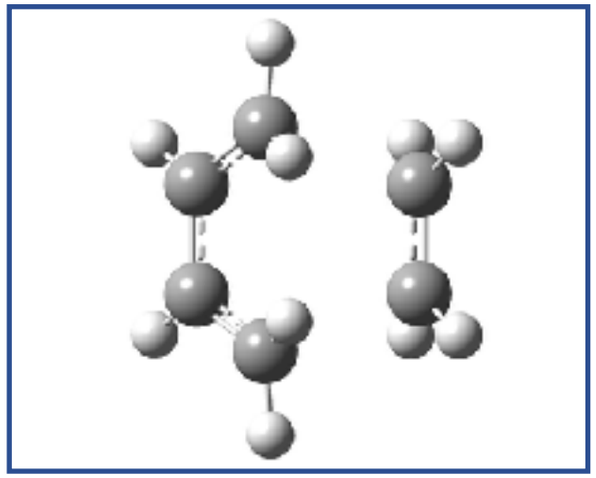

G6:M1 - MOs
Current Surface:
29 0.32839
28 0.31644
27 0.28094
26 0.26622
25 0.17304
24 0.14226
23 -0.30096
22 -0.30280
21 -0.47748
20 -0.48107
最高被占有軌道（HOMO）

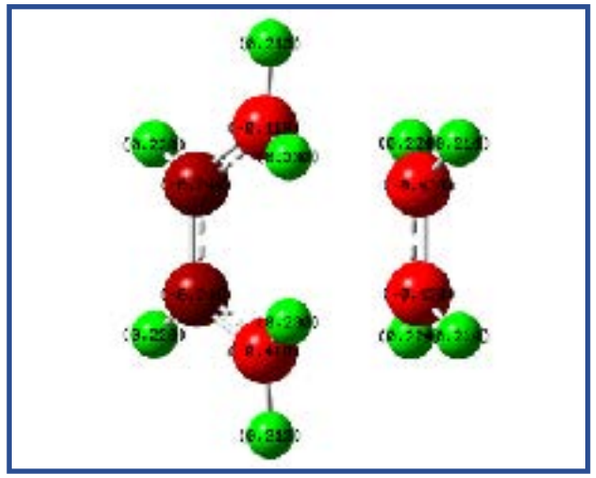
分子軌道を調べる


G6:M1 - MOs
Current Surface:
29 0.32839
28 0.31644
27 0.28094
26 0.26622
25 0.17304
24 0.14226
23 -0.30096
22 -0.30280
21 -0.47748
20 -0.48107
最低空軌道（LUMO）
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥3_T

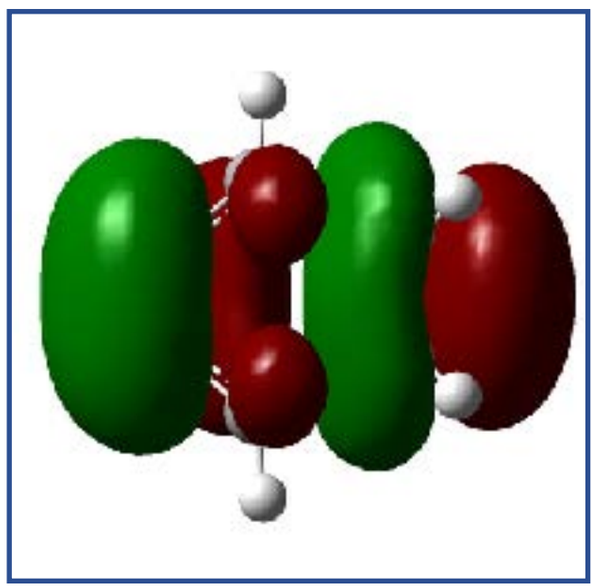
計算結果をまとめる（遷移状態）

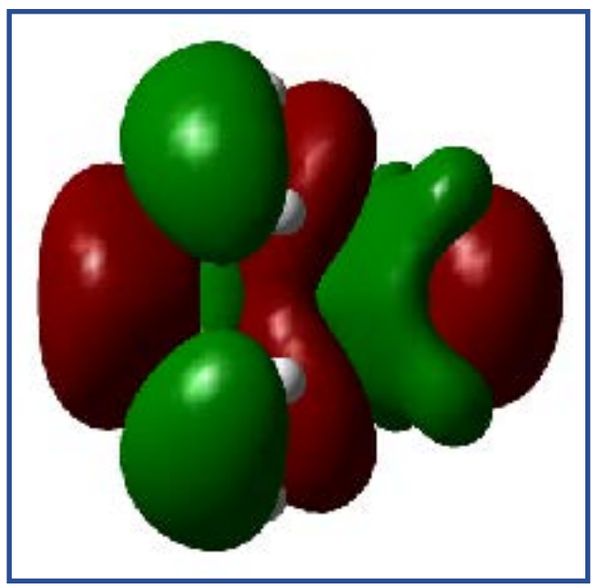
- 全エネルギーの値：＿＿＿＿＿＿ a.u.
- 炭素・炭素間距離：＿＿＿＿＿＿ Å
- 分子構造の図





- 電荷分布の図
- 分子軌道の図



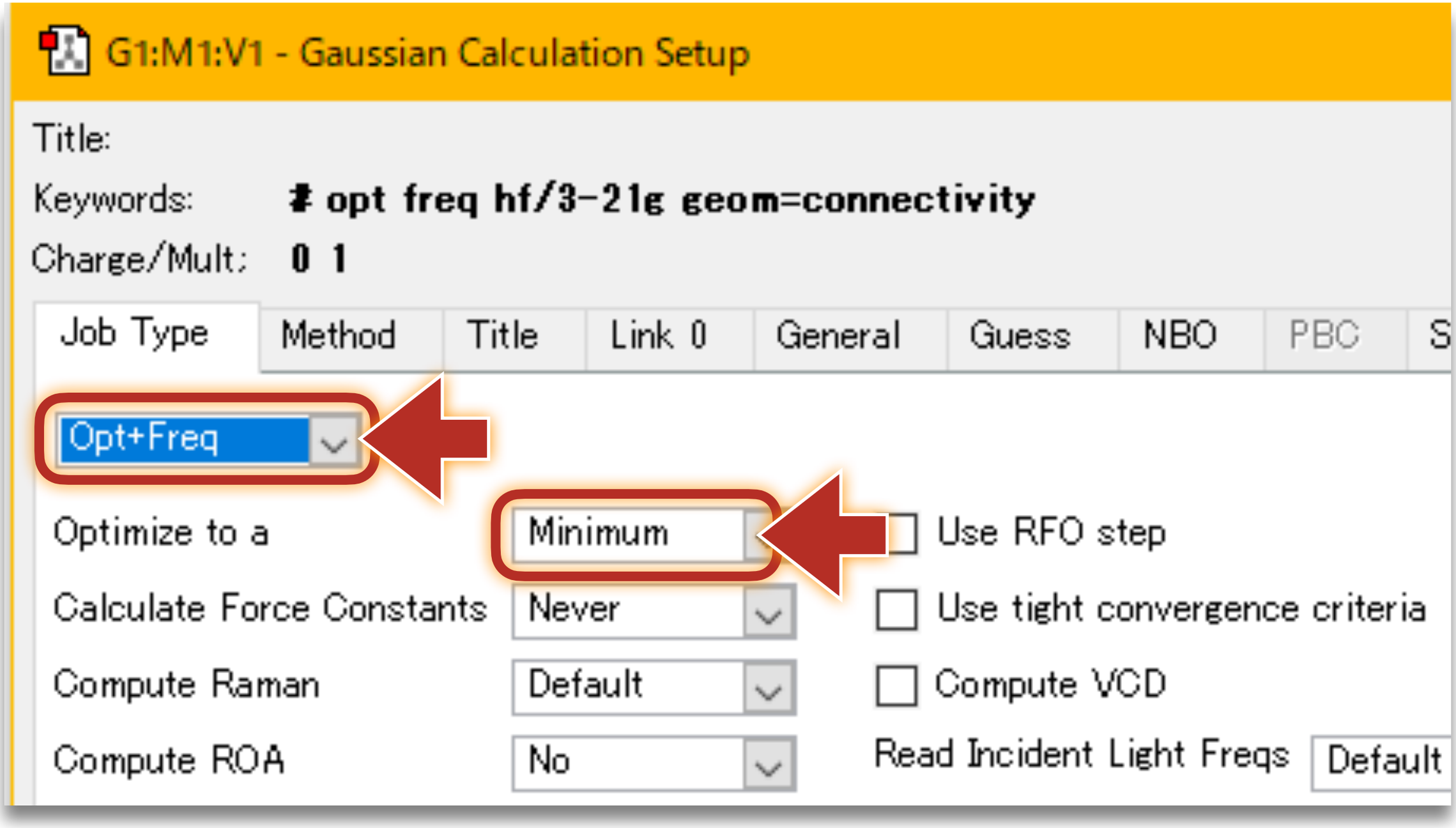


シクロヘキセンの量子化学計算

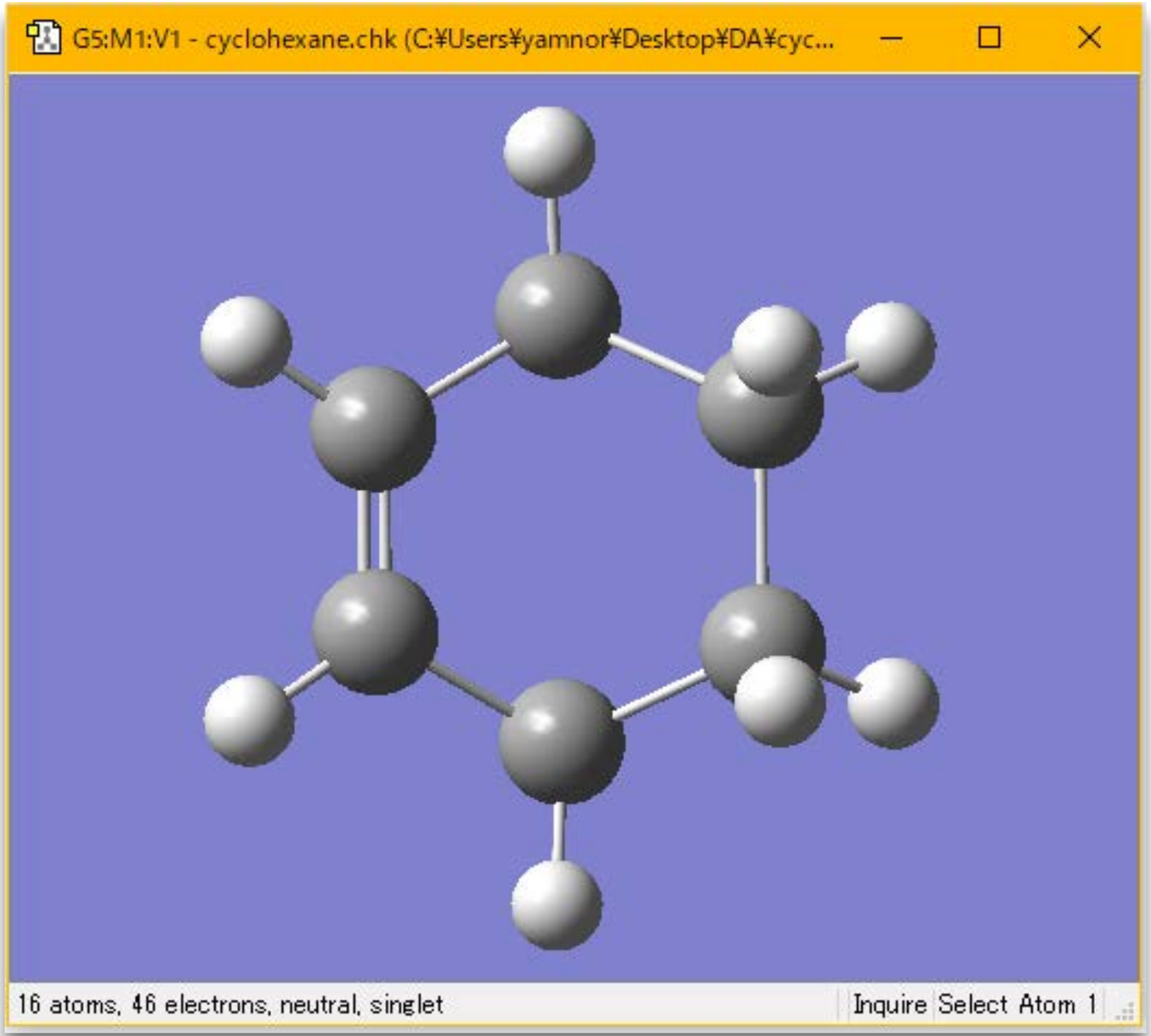
入力ファイルを開く


QChem
QChem › QChem
QChemの...
名前
3_TS.gjf
4_cyclohexene.gjf
5_IRC.log
cyclohexene.gjf
3 個の項目
1 個の項目を選択 1.01 KB

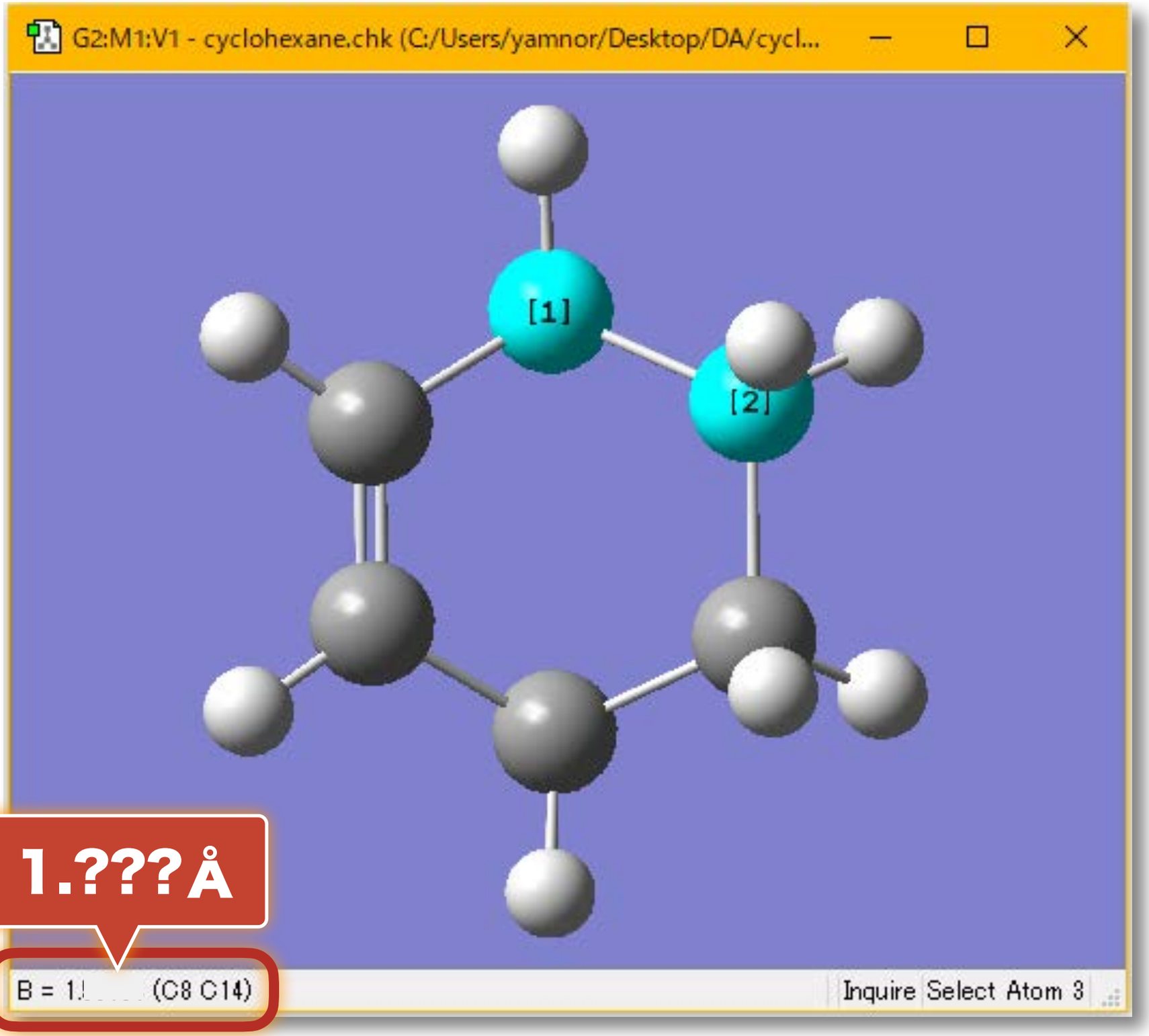
構造最適化


G1:M1:V1 - Gaussian Calculation Setup
Title:
Keywords: # opt freq hf/3-21g geom=connectivity
Charge/Mult: 0 1
Job Type
Method
Title
Link 0
General
Guess
NBO
PBC
S
Opt+Freq
Optimize to a
Minimum
Use RFO step
Calculate Force Constants
Never
Use tight convergence criteria
Compute Raman
Default
Compute VCD
Compute ROA
No
Read Incident Light Freqs
Default

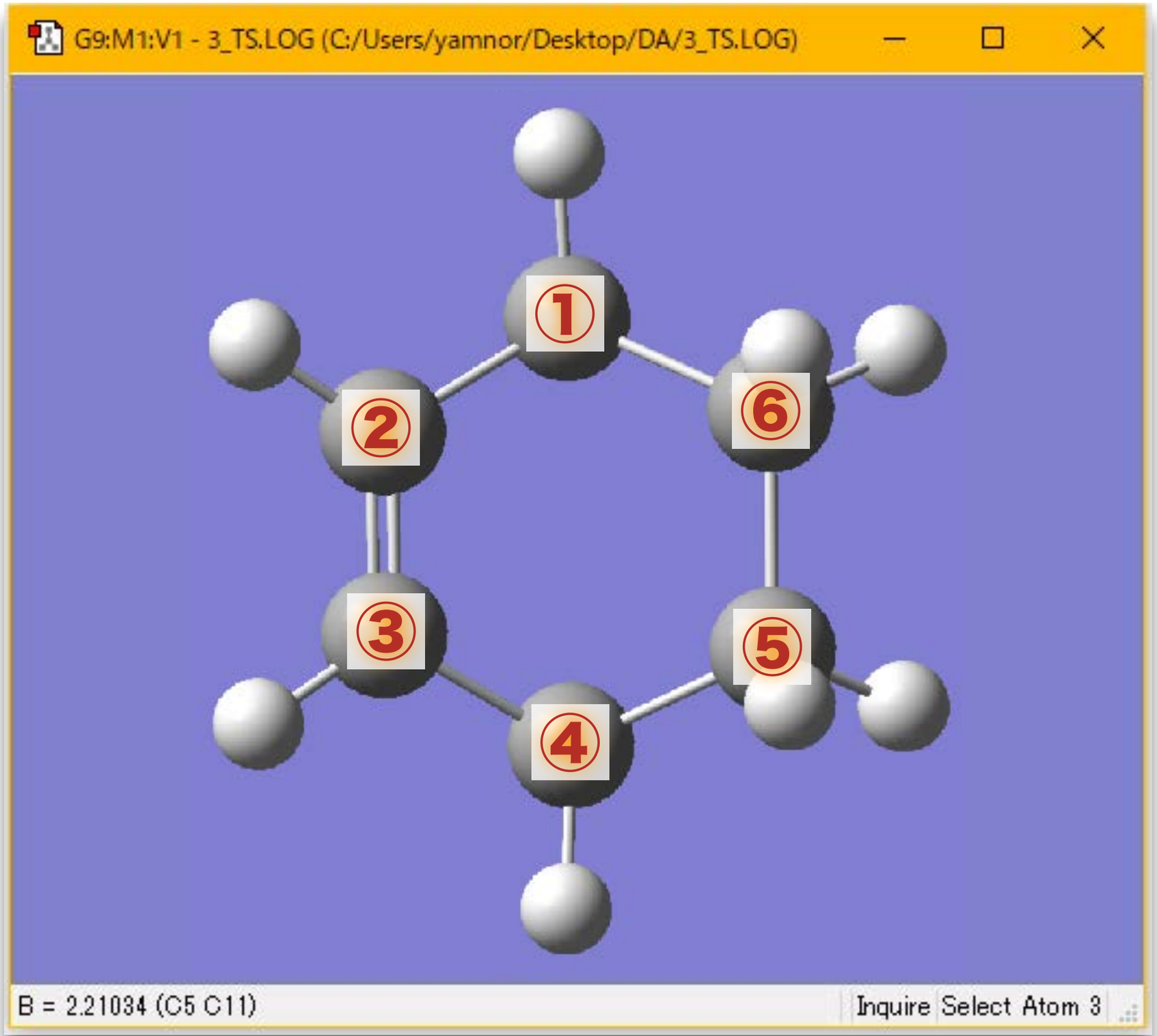
構造最適化


G5:M1:V1 - cyclohexane.chk (C:¥Users¥yamnor¥Desktop¥DA¥cyc...
16 atoms, 46 electrons, neutral, singlet
Inquire Select Atom 1

原子間距離を調べる


G2:M1:V1 - cyclohexane.chk (C:/Users/yamnor/Desktop/DA/cycl...
[1]
[2]
1.???Å
B = 1.[illegible] (C8 C14)
Inquire Select Atom 3

原子の番号（ラベル）


G9:M1:V1 - 3_TS.LOG (C:/Users/yamnor/Desktop/DA/3_TS.LOG)
①
②
③
④
⑤
⑥
B = 2.21034 (C5 C11)
Inquire Select Atom 3

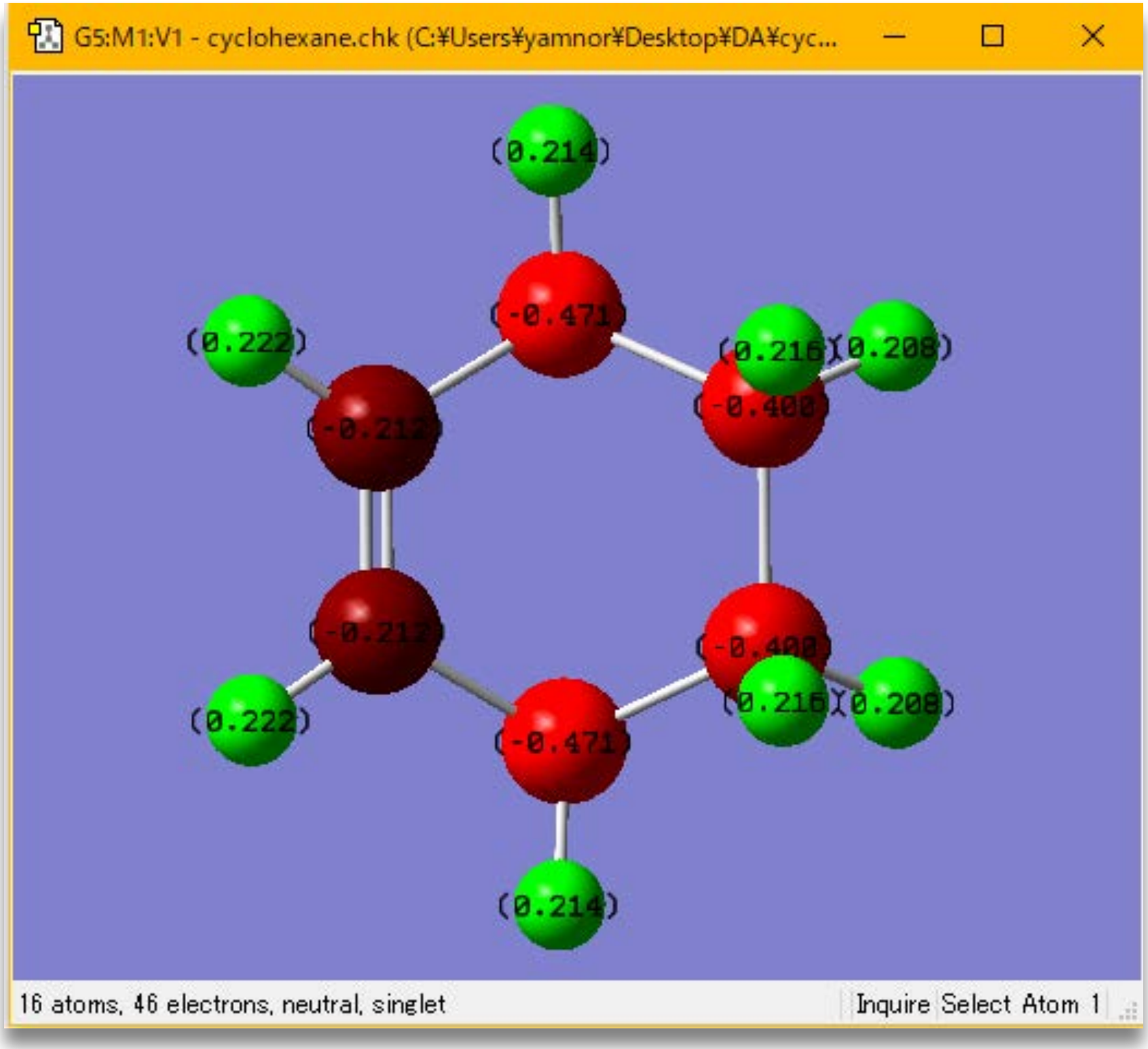
全エネルギーを調べる

G5:M1:V1 - Gaussian Calculation Summary

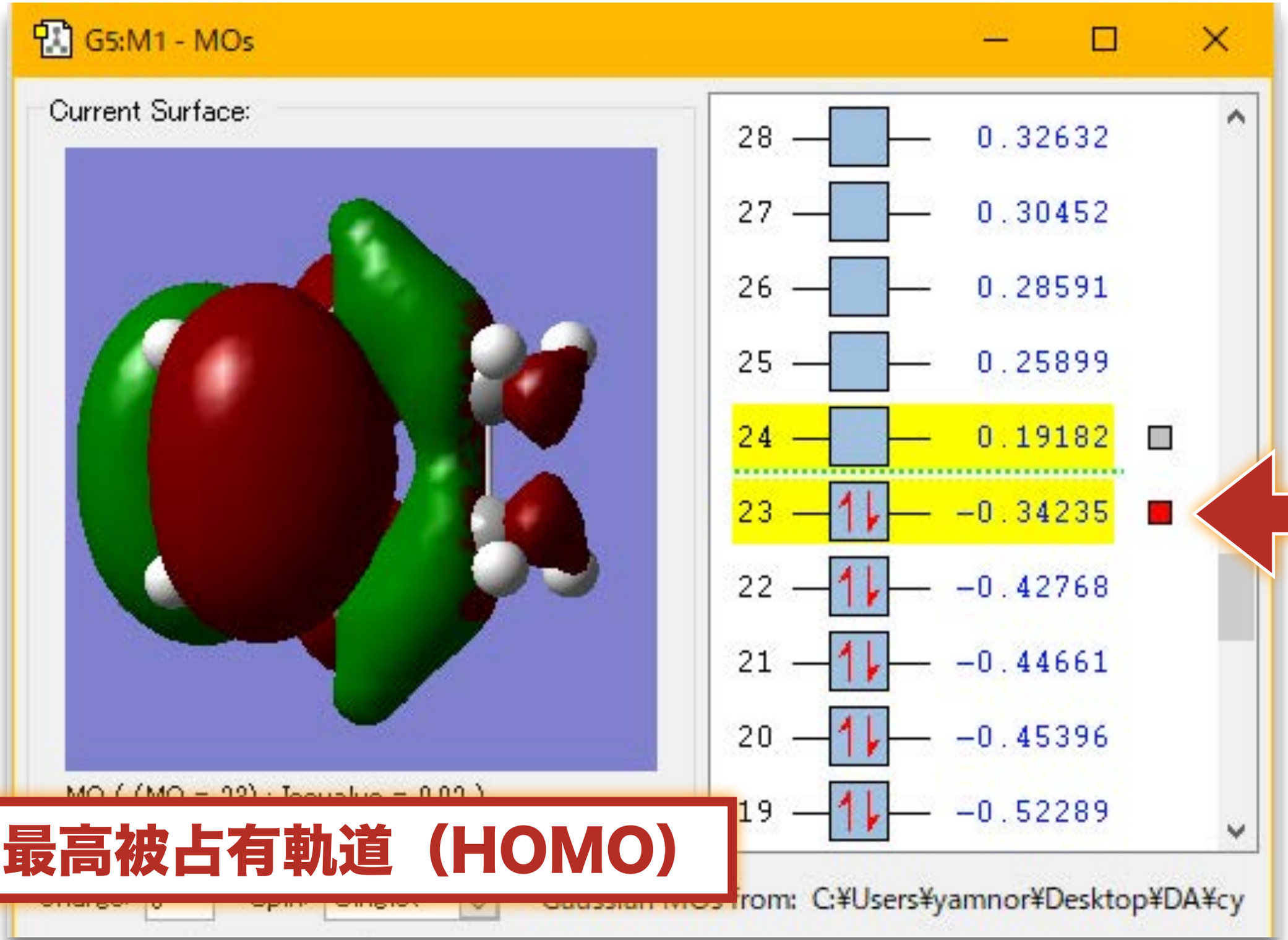
Title Card Required		
File Name	cyclohexane	
File Type	.chk	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	3-21G	
Charge	0	
Spin	Singlet	
Total Energy	-231.	a.u.
RMS Gradient Norm	0.00000071	a.u.
Imaginary Freq		
Dipole Moment	0.2259	Debye
Point Group		

Ok　View File　Save Data

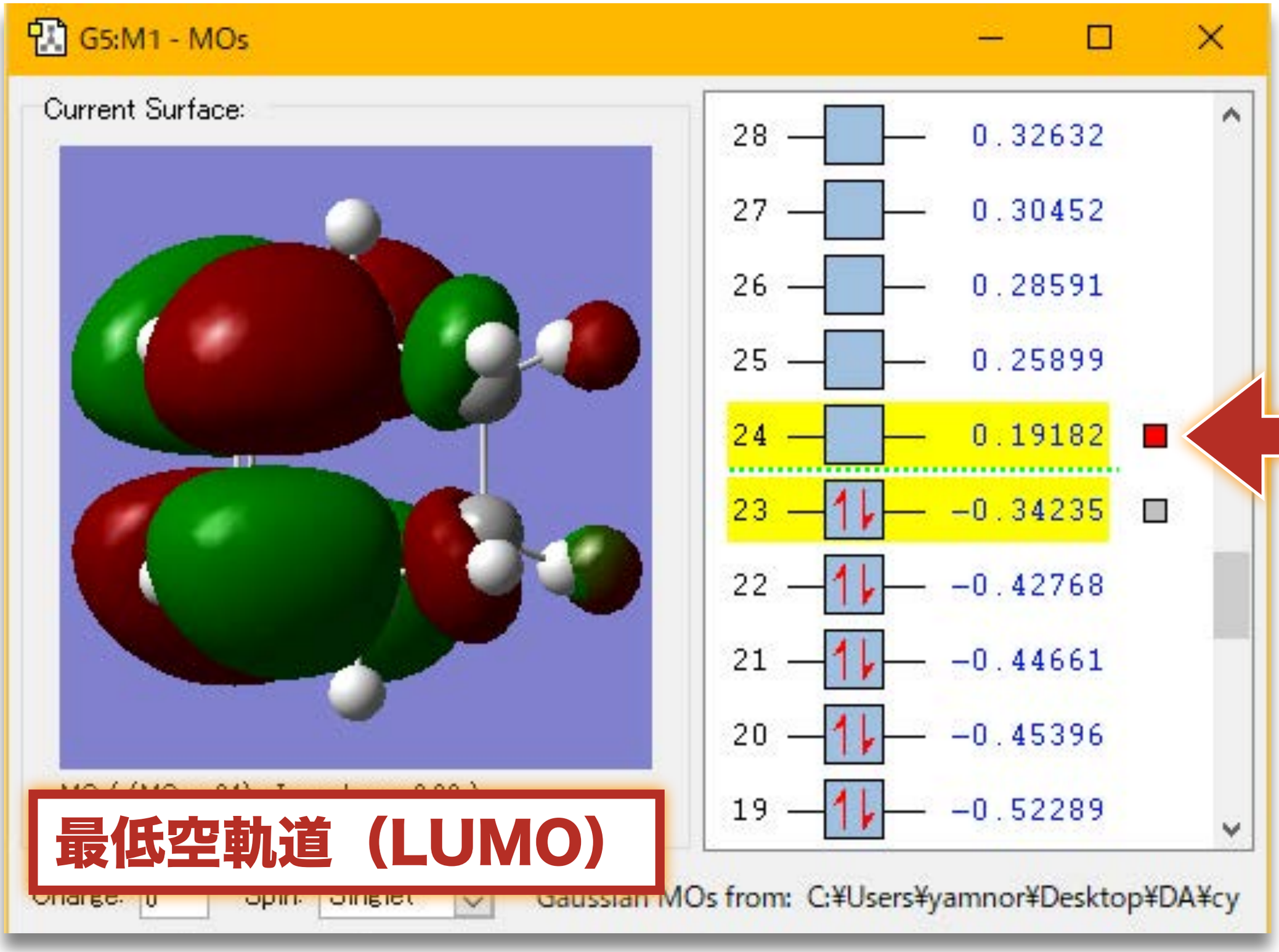
電荷分布を調べる


G5:M1:V1 - cyclohexane.chk (C:¥Users¥yamnor¥Desktop¥DA¥cyc...
(0.214)
(-0.471)
(0.222)
(0.216)(0.208)
(-0.212)
(-0.400)
(-0.212)
(-0.400)
(0.216)(0.208)
(0.222)
(-0.471)
(0.214)
16 atoms, 46 electrons, neutral, singlet
Inquire Select Atom 1

分子軌道を調べる

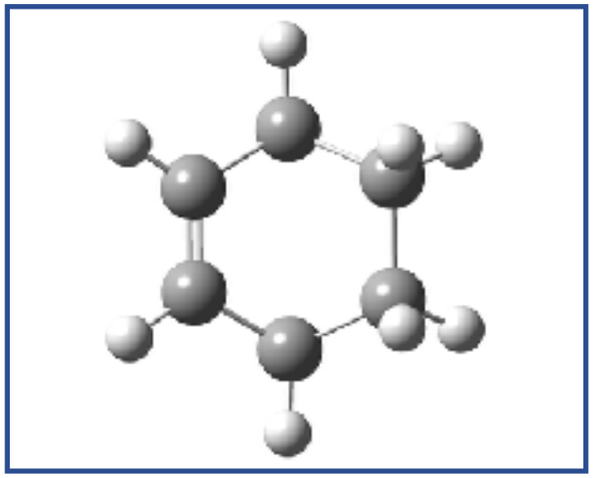

G5:M1 - MOs
Current Surface:
28 0.32632
27 0.30452
26 0.28591
25 0.25899
24 0.19182
23 -0.34235
22 -0.42768
21 -0.44661
20 -0.45396
19 -0.52289
C:¥Users¥yamnor¥Desktop¥DA¥cy
最高被占有軌道（HOMO）

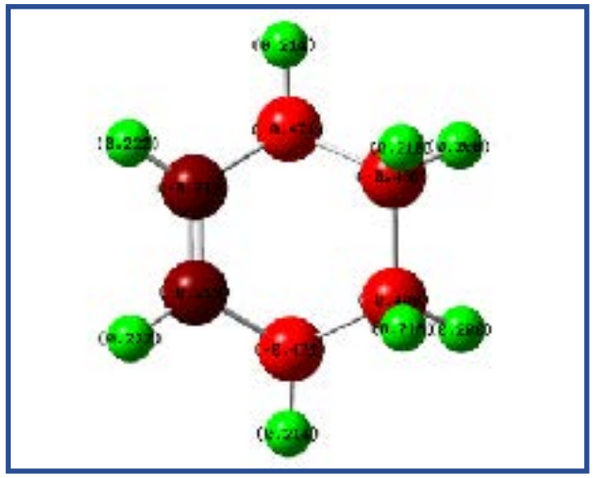
分子軌道を調べる


G5:M1 - MOs
Current Surface:
28 0.32632
27 0.30452
26 0.28591
25 0.25899
24 0.19182
23 -0.34235
22 -0.42768
21 -0.44661
20 -0.45396
19 -0.52289
最低空軌道（LUMO）
Gaussian MOs from: C:¥Users¥yamnor¥Desktop¥DA¥cy

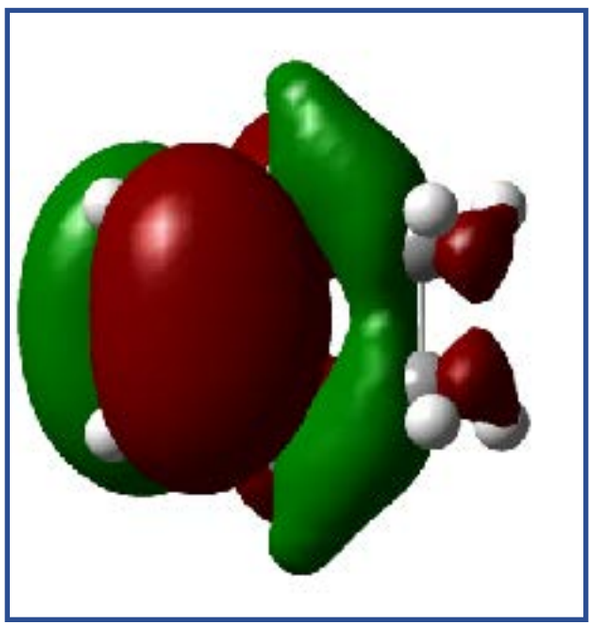
計算結果をまとめる（シクロヘキセン）

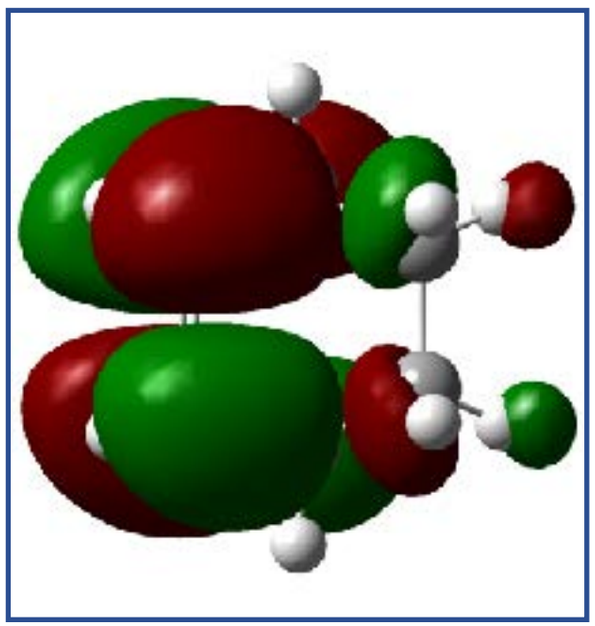
- 全エネルギーの値：＿＿＿＿＿＿ a.u.
- 炭素・炭素間距離：＿＿＿＿＿＿ Å
- 分子構造の図





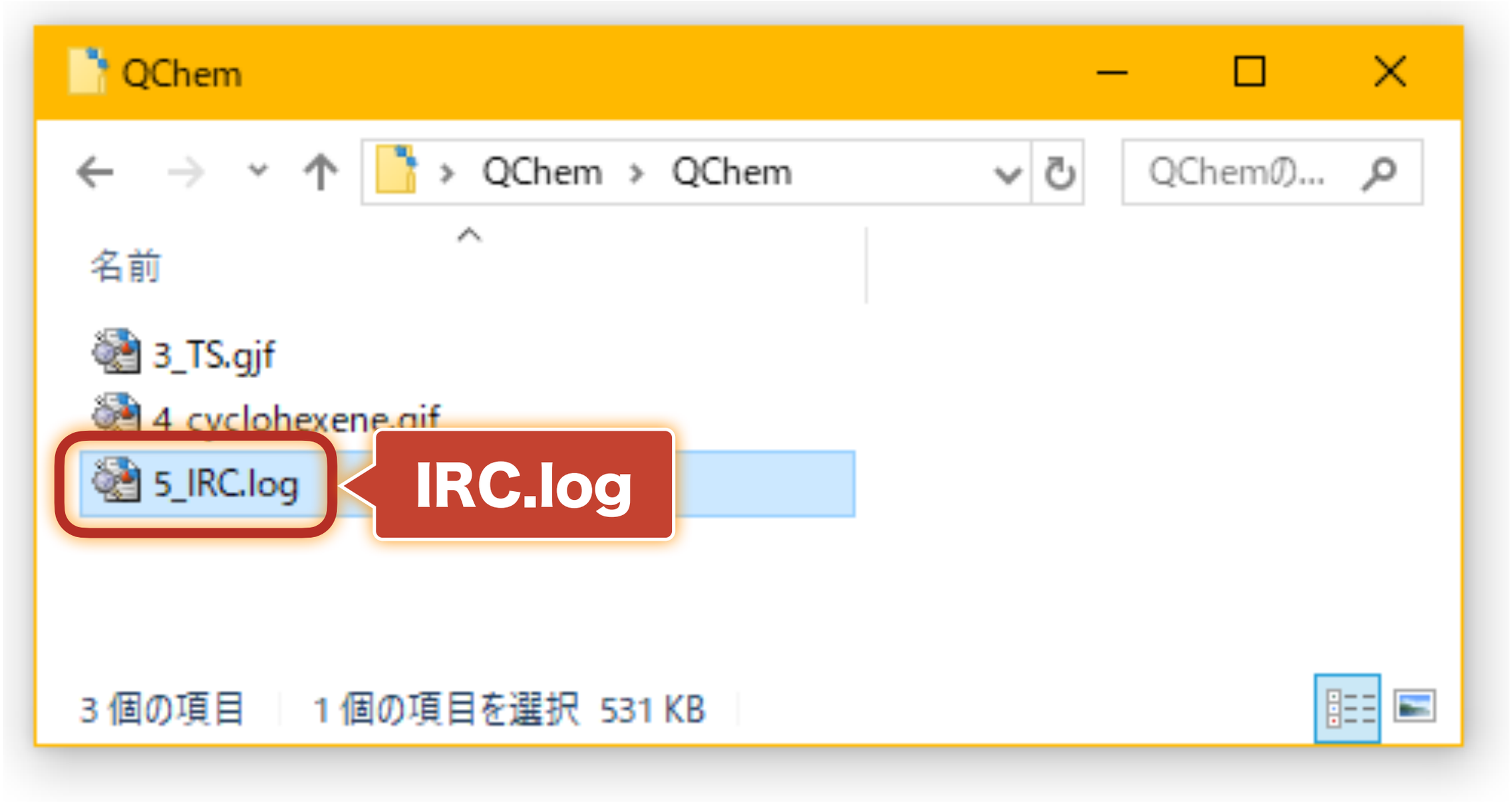
- 電荷分布の図
- 分子軌道の図



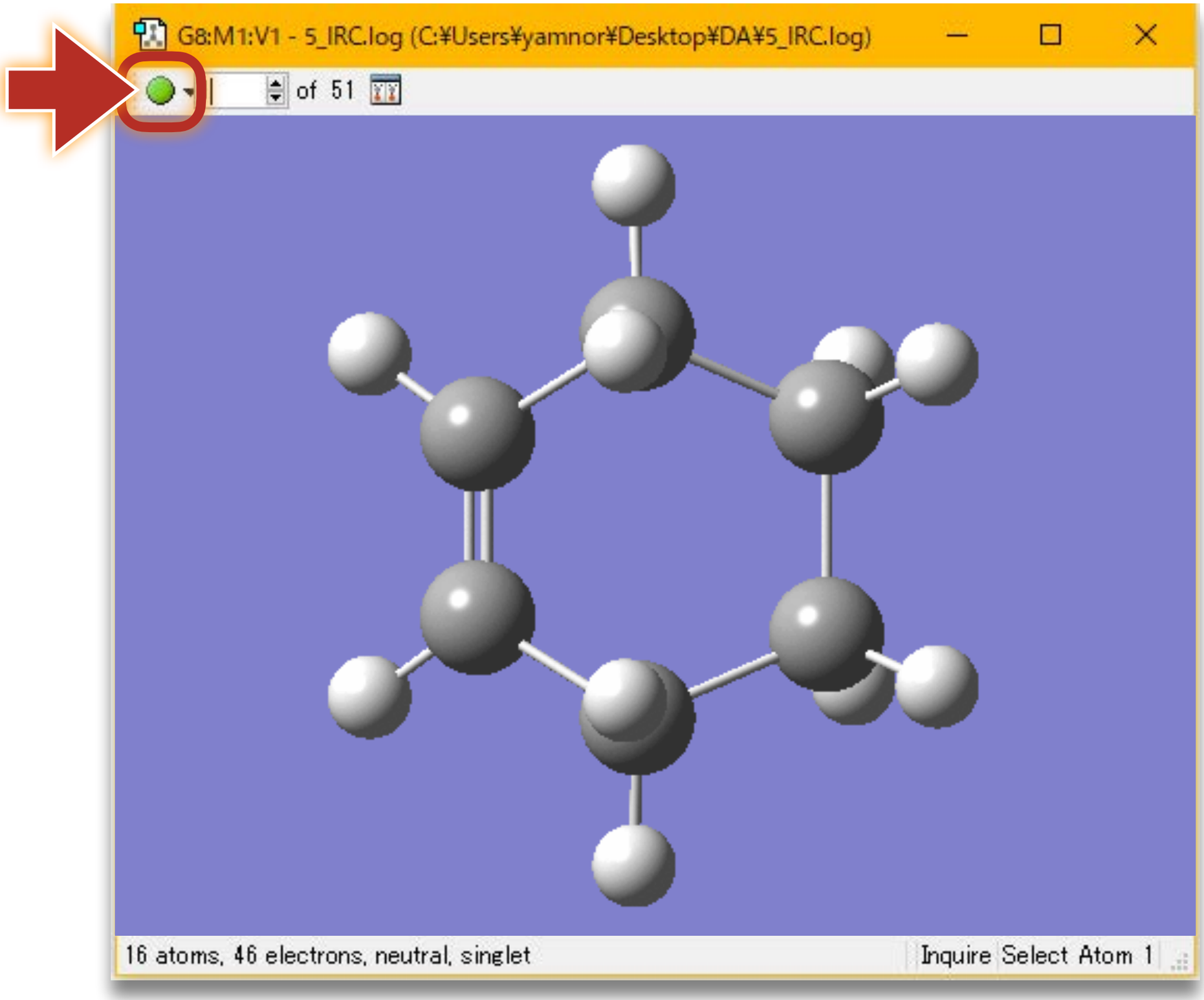


反応経路の解析

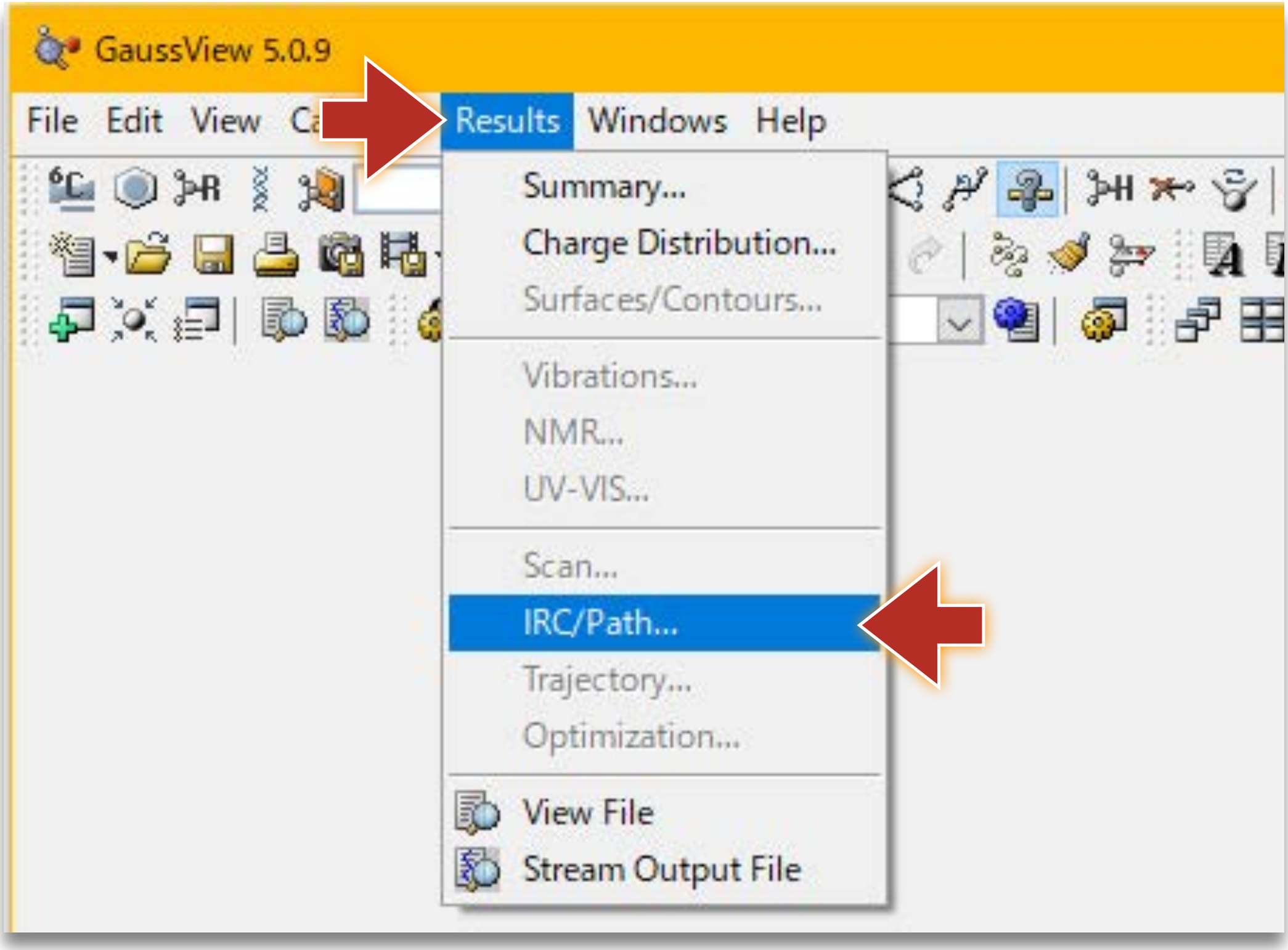
出力ファイルを開く


QChem
QChem › QChem
QChemの...
名前
3_TS.gjf
4_cyclohexene.gif
5_IRC.log
IRC.log
3 個の項目
1 個の項目を選択 531 KB

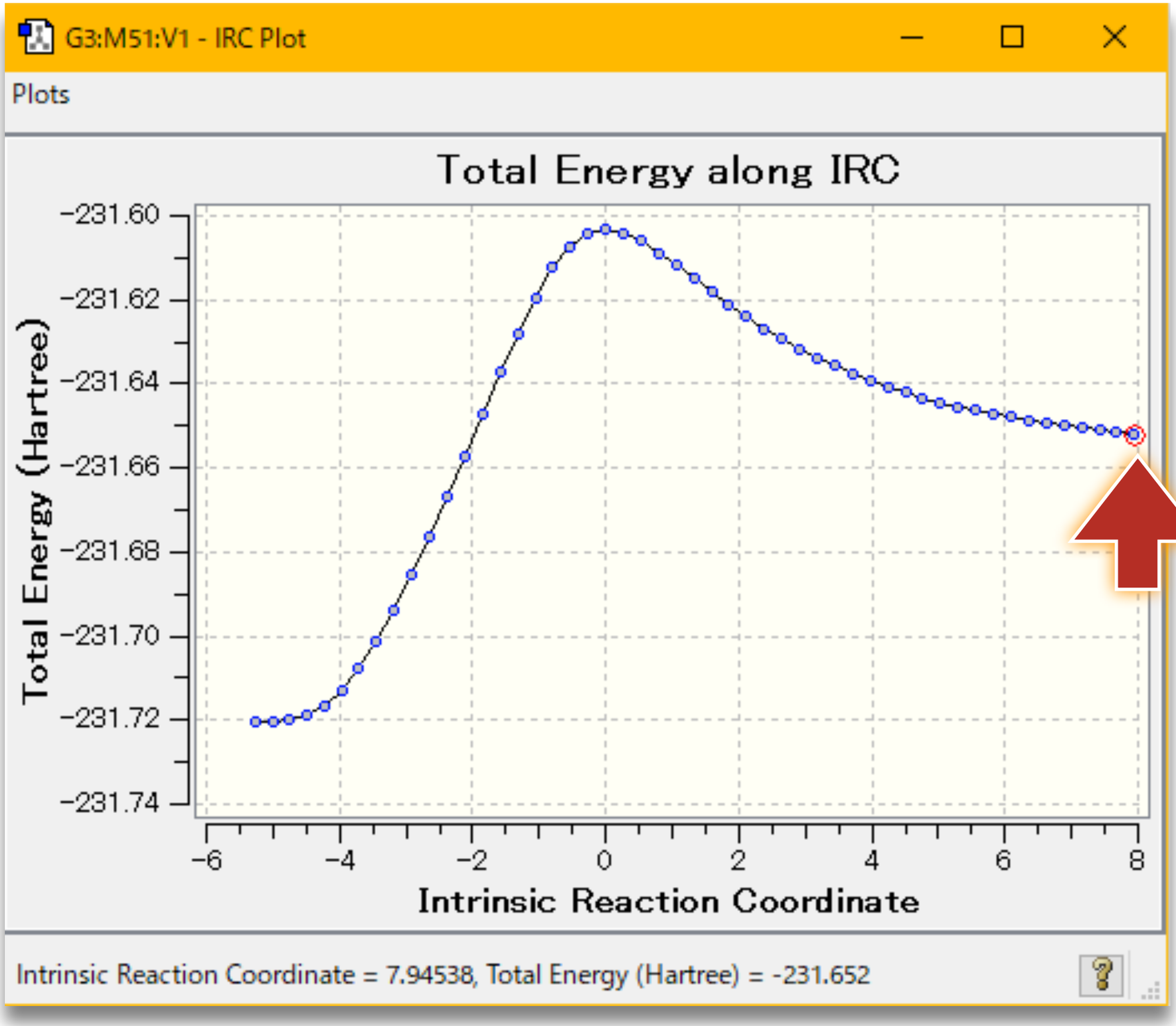
反応経路を調べる


G8:M1:V1 - 5_IRC.log (C:¥Users¥yamnor¥Desktop¥DA¥5_IRC.log)
of 51
16 atoms, 46 electrons, neutral, singlet
Inquire
Select Atom 1

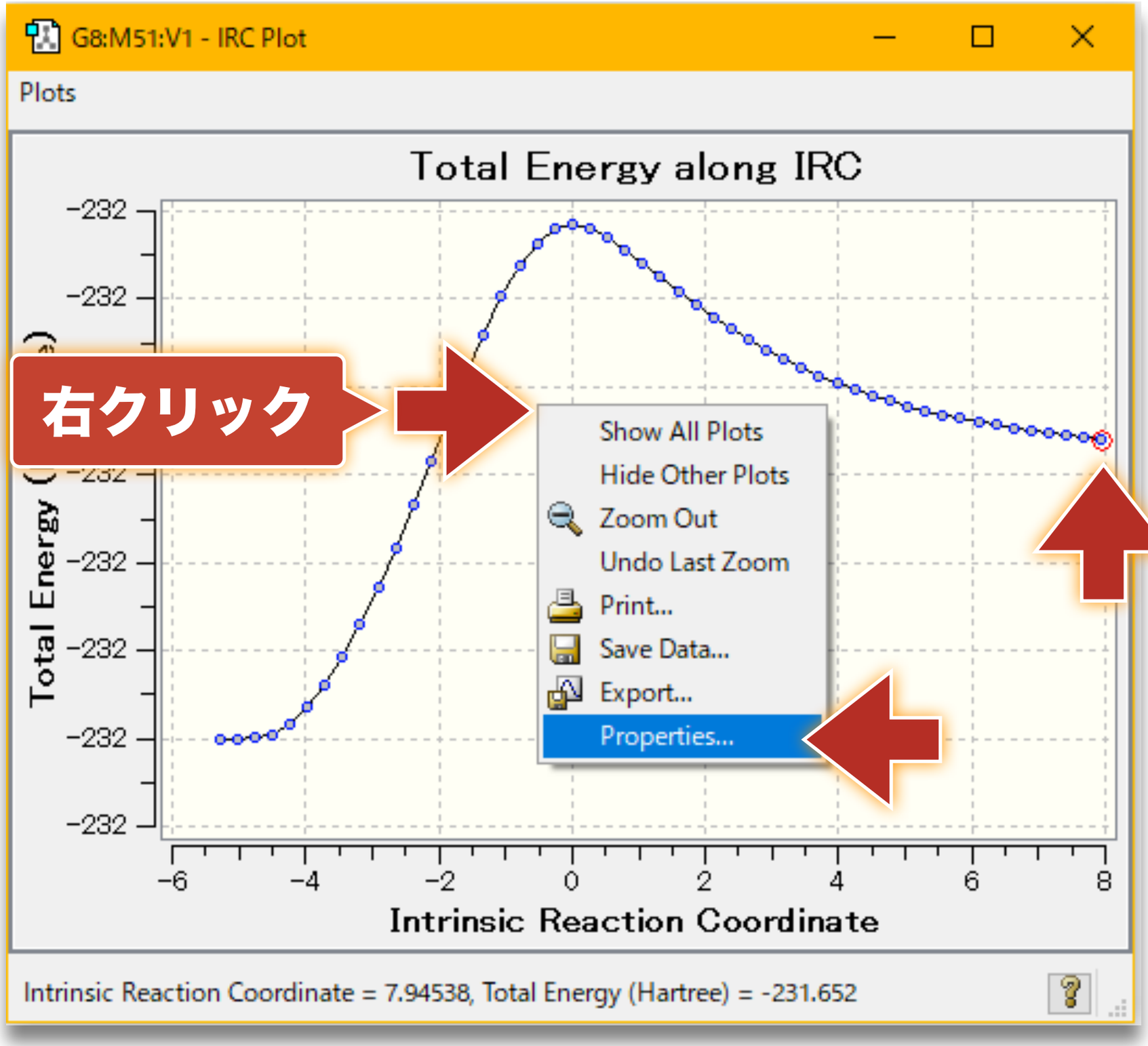
反応経路を調べる


GaussView 5.0.9
File Edit View Ca
Results
Windows
Help
Summary...
Charge Distribution...
Surfaces/Contours...
Vibrations...
NMR...
UV-VIS...
Scan...
IRC/Path...
Trajectory...
Optimization...
View File
Stream Output File

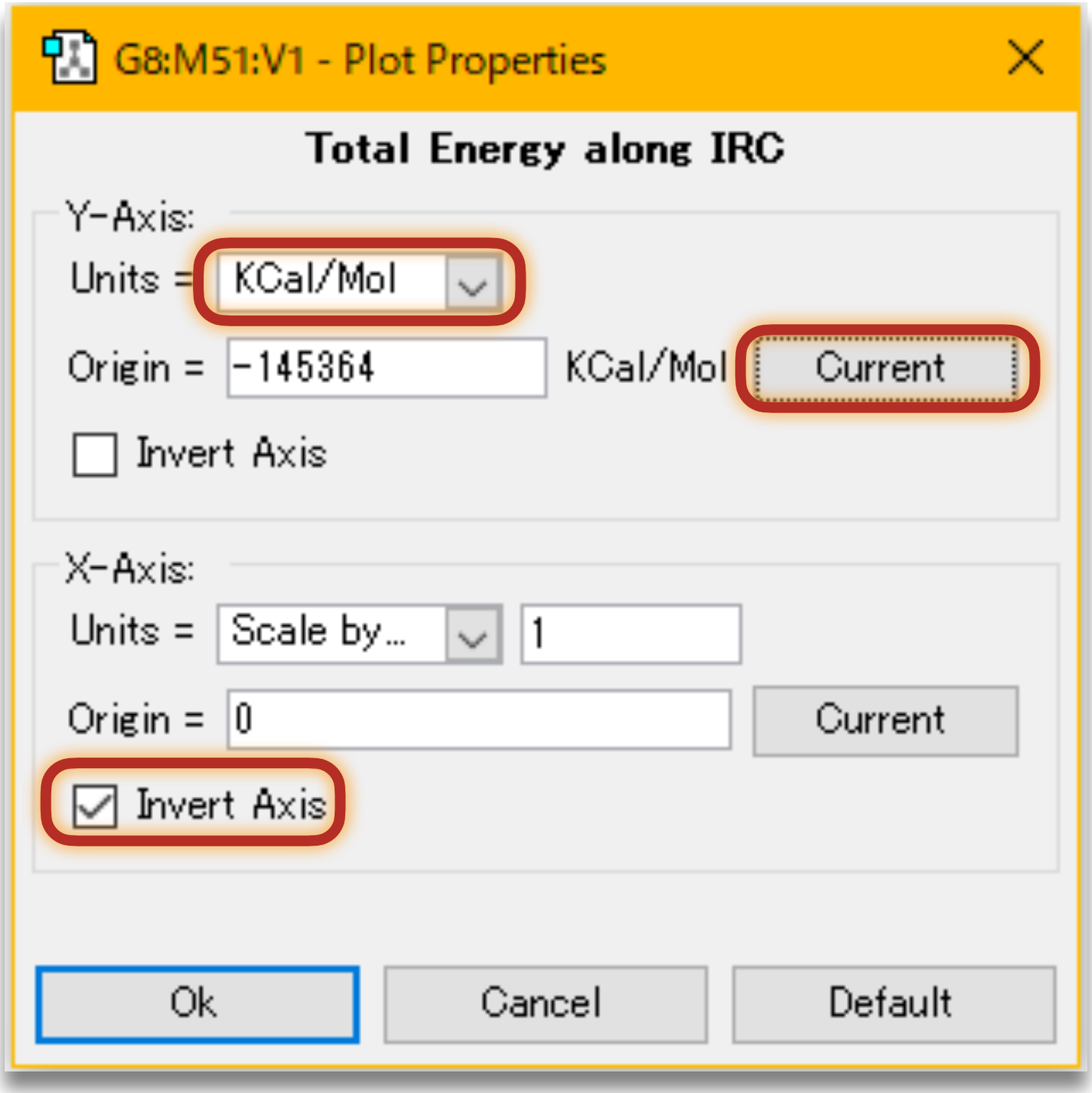
反応経路を調べる


G3:M51:V1 - IRC Plot
Plots
Total Energy along IRC
Total Energy (Hartree)
−231.60
−231.62
−231.64
−231.66
−231.68
−231.70
−231.72
−231.74
−6
−4
−2
0
2
4
6
8
Intrinsic Reaction Coordinate
Intrinsic Reaction Coordinate = 7.94538, Total Energy (Hartree) = -231.652

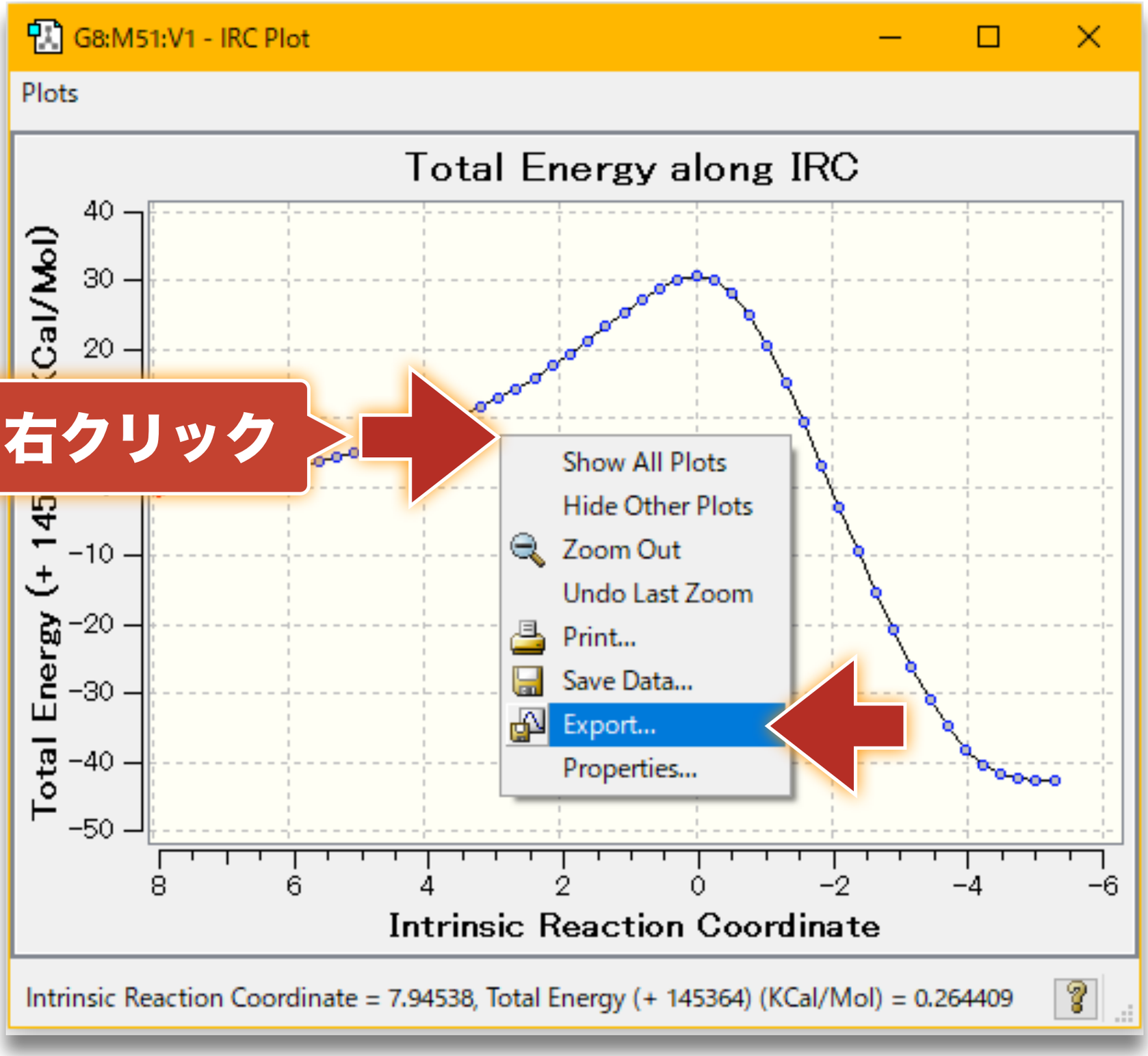
反応経路を調べる


G8:M51:V1 - IRC Plot
Plots
Total Energy along IRC
Total Energy
-232
-232
-232
-232
-232
-6
-4
-2
0
2
4
6
8
Intrinsic Reaction Coordinate
右クリック
Show All Plots
Hide Other Plots
Zoom Out
Undo Last Zoom
Print...
Save Data...
Export...
Properties...
Intrinsic Reaction Coordinate = 7.94538, Total Energy (Hartree) = -231.652

反応経路を調べる


G8:M51:V1 - Plot Properties
Total Energy along IRC
Y-Axis:
Units =
KCal/Mol
Origin =
-145364
KCal/Mol
Current
Invert Axis
X-Axis:
Units =
Scale by...
1
Origin =
0
Current
Invert Axis
Ok
Cancel
Default

画像を保存する（反応経路）



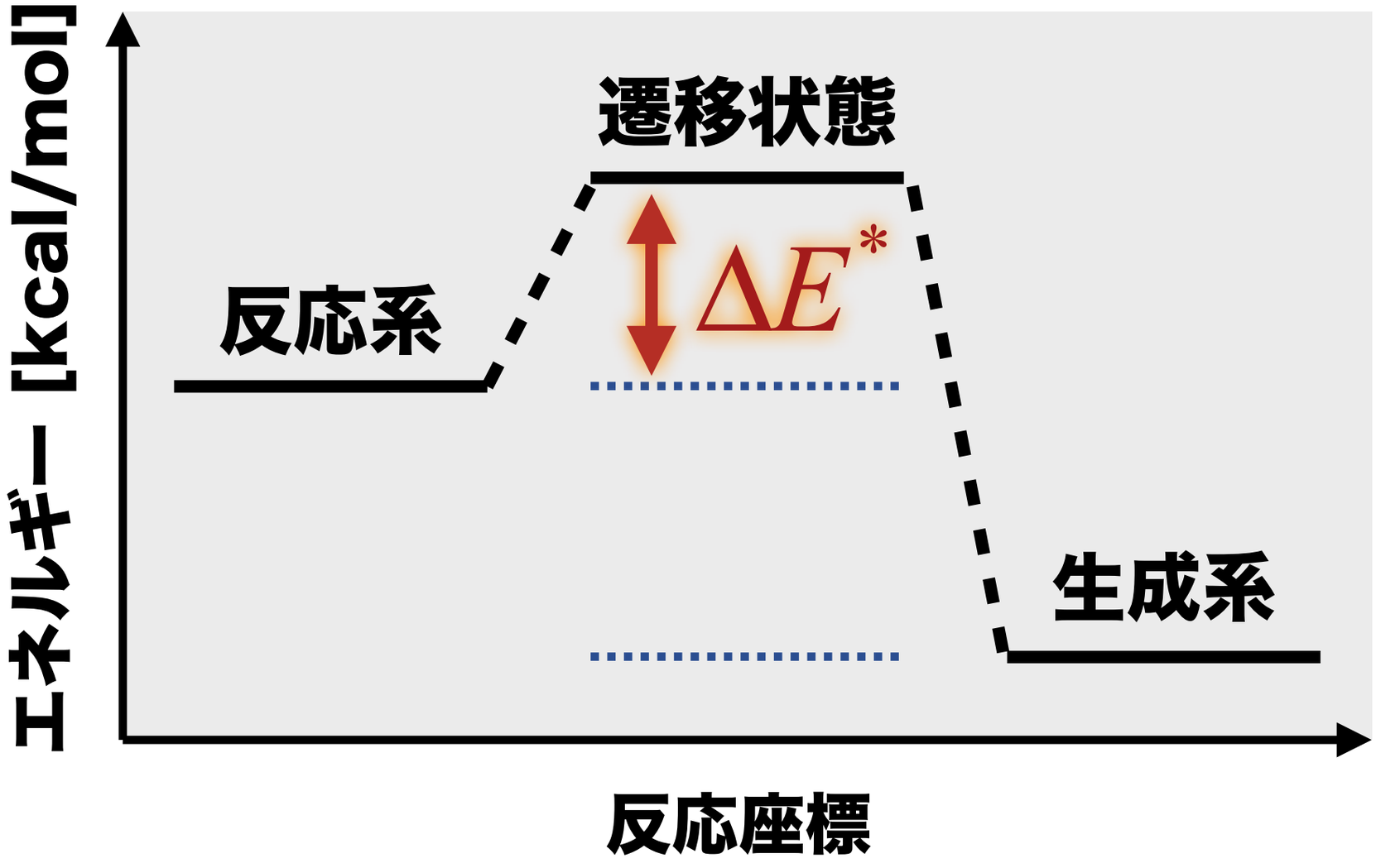
画像を保存する（反応経路）

計算結果のまとめ

活性化エネルギーの計算

a.u. ➡ kcal/mol

$$\Delta E^{*} = \left[E_{\mathrm{TS}} - \left(E_{\mathrm{butadiene}} + E_{\mathrm{ethylene}} \right) \right] \times 627.5095$$



反応エンタルピーの計算

a.u. ➡ kcal/mol

$$\Delta H = \left[E_{\text{cyclohexene}} - \left(E_{\text{butadiene}} + E_{\text{ethylene}} \right) \right] \times 627.5095$$