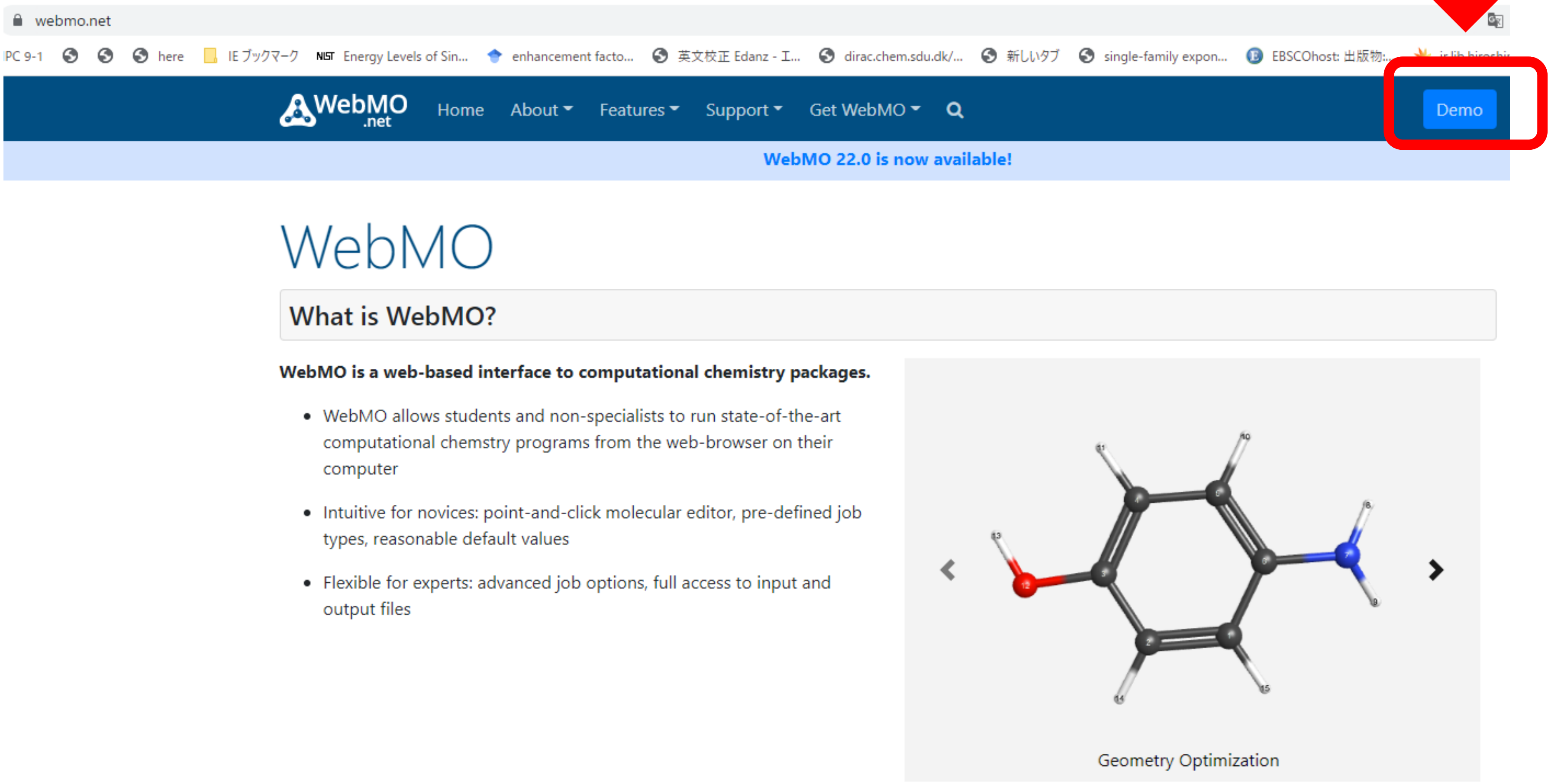
WebMOで検索

Click


webmo.net
PC 9-1
here
IE ブックマーク
Energy Levels of Sin...
enhancement facto...
英文校正 Edanz - エ...
dirac.chem.sdu.dk/...
新しいタブ
single-family expon...
EBSCOhost: 出版物:...
WebMO .net
Home
About
Features
Support
Get WebMO
Demo

WebMO 22.0 is now available!

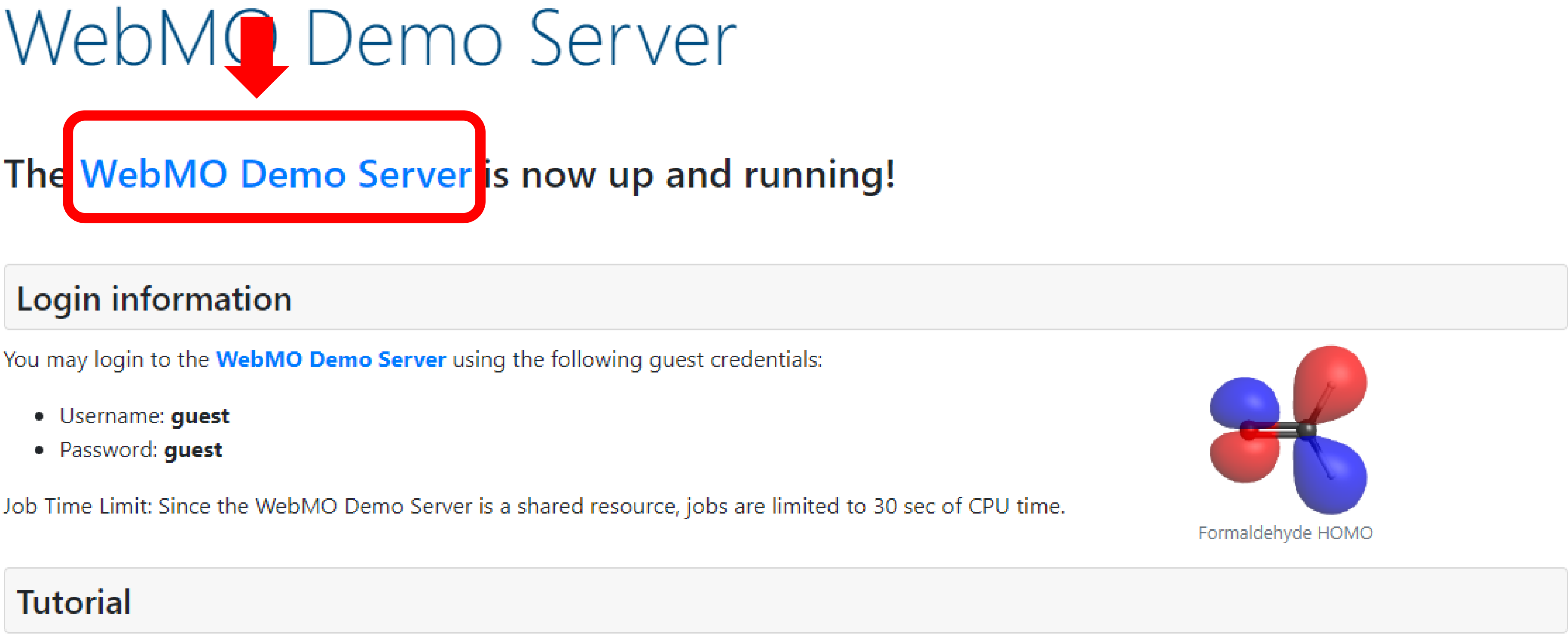
WebMO

What is WebMO?

WebMO is a web-based interface to computational chemistry packages.

- WebMO allows students and non-specialists to run state-of-the-art computational chemstry programs from the web-browser on their computer
- Intuitive for novices: point-and-click molecular editor, pre-defined job types, reasonable default values
- Flexible for experts: advanced job options, full access to input and output files

Geometry Optimization



Click

WebMO Demo Server

The WebMO Demo Server is now up and running!

Login information

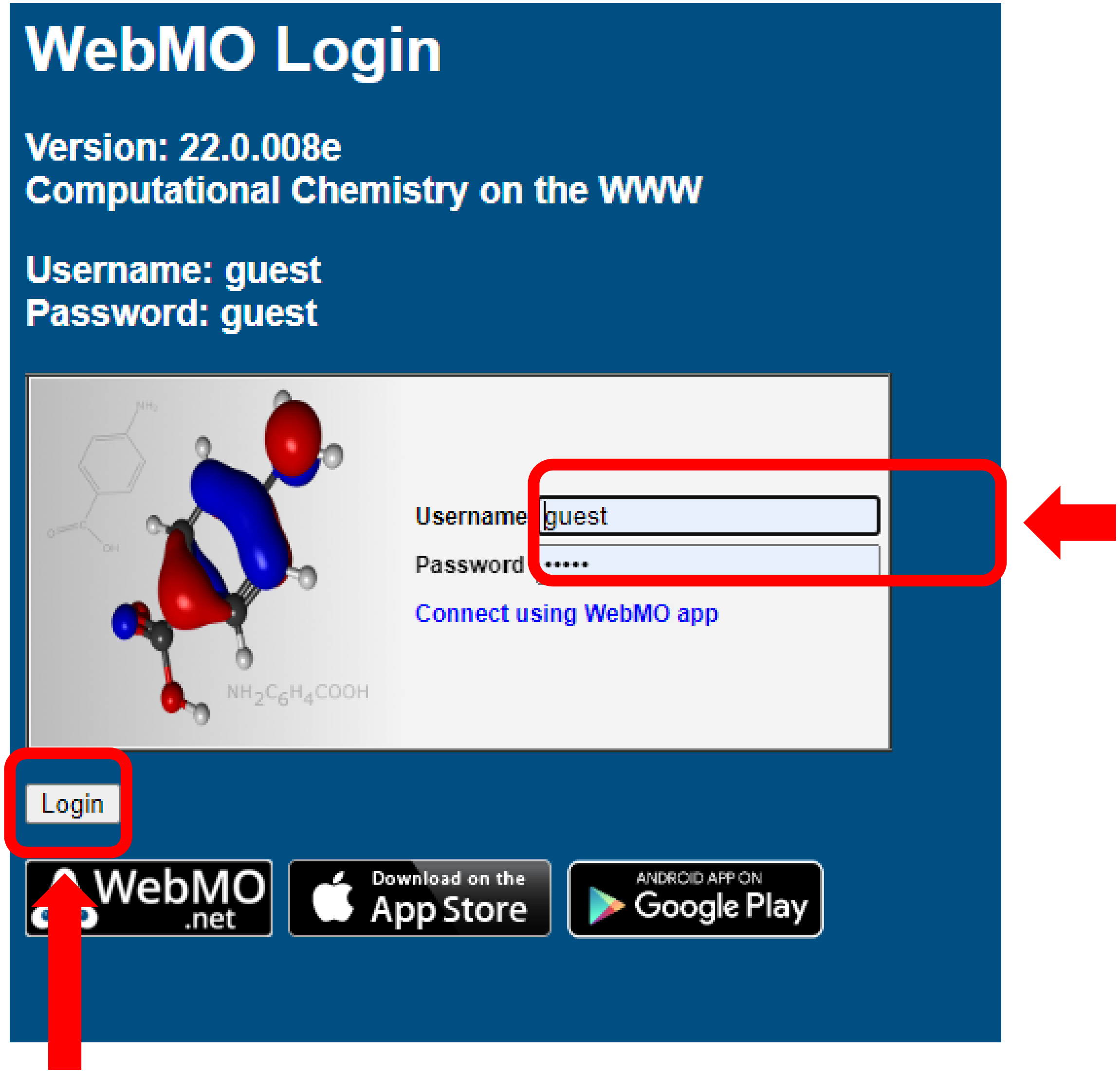
You may login to the **WebMO Demo Server** using the following guest credentials:

- Username: **guest**
- Password: **guest**

Job Time Limit: Since the WebMO Demo Server is a shared resource, jobs are limited to 30 sec of CPU time.

Formaldehyde HOMO

Tutorial



WebMO Login

Version: 22.0.008e
Computational Chemistry on the WWW

Username: guest
Password: guest

Username: guest
Password: •••••

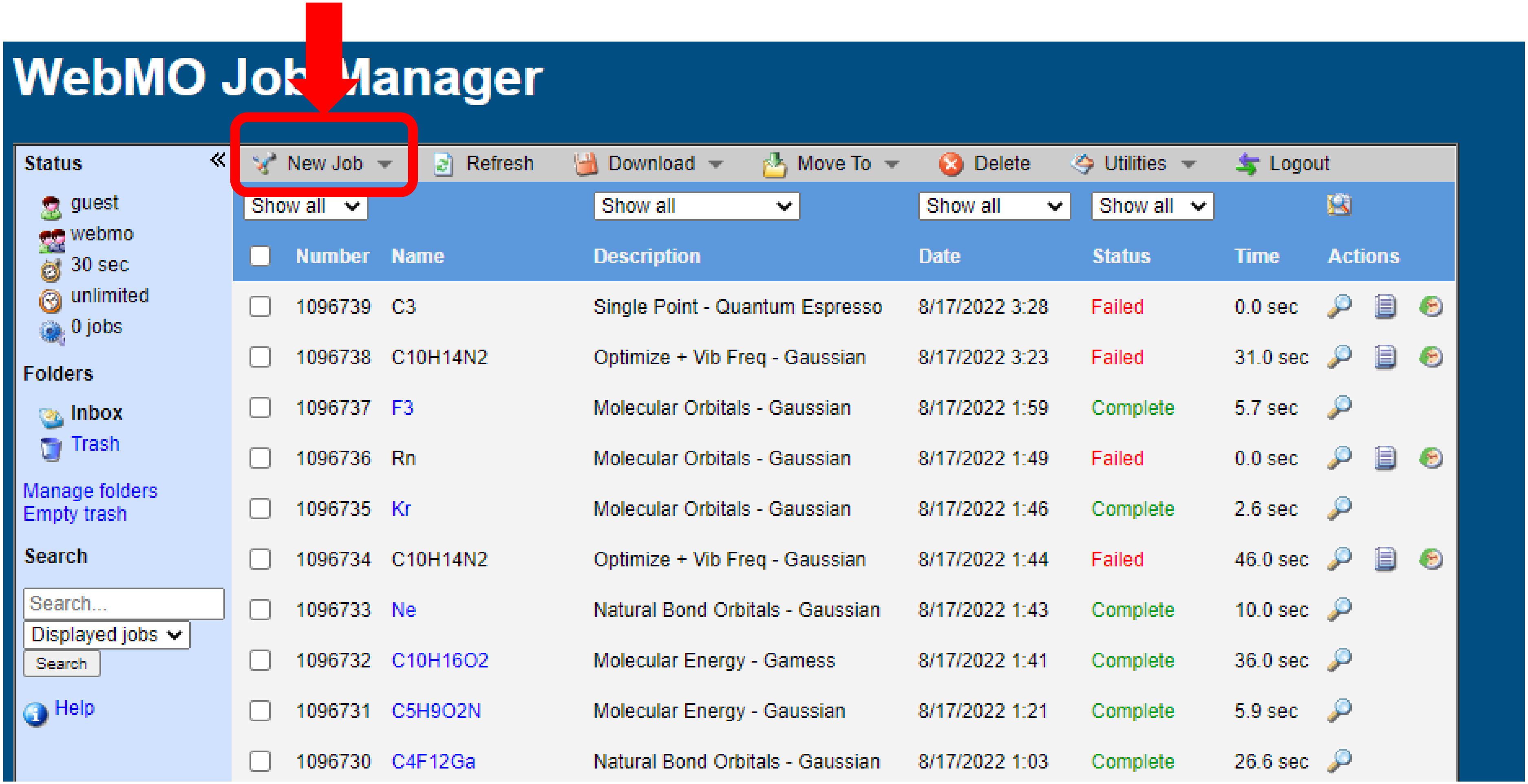
Connect using WebMO app

NH₂C₆H₄COOH
Login
WebMO .net
Download on the App Store
ANDROID APP ON Google Play

① どちらも
guest
と入力

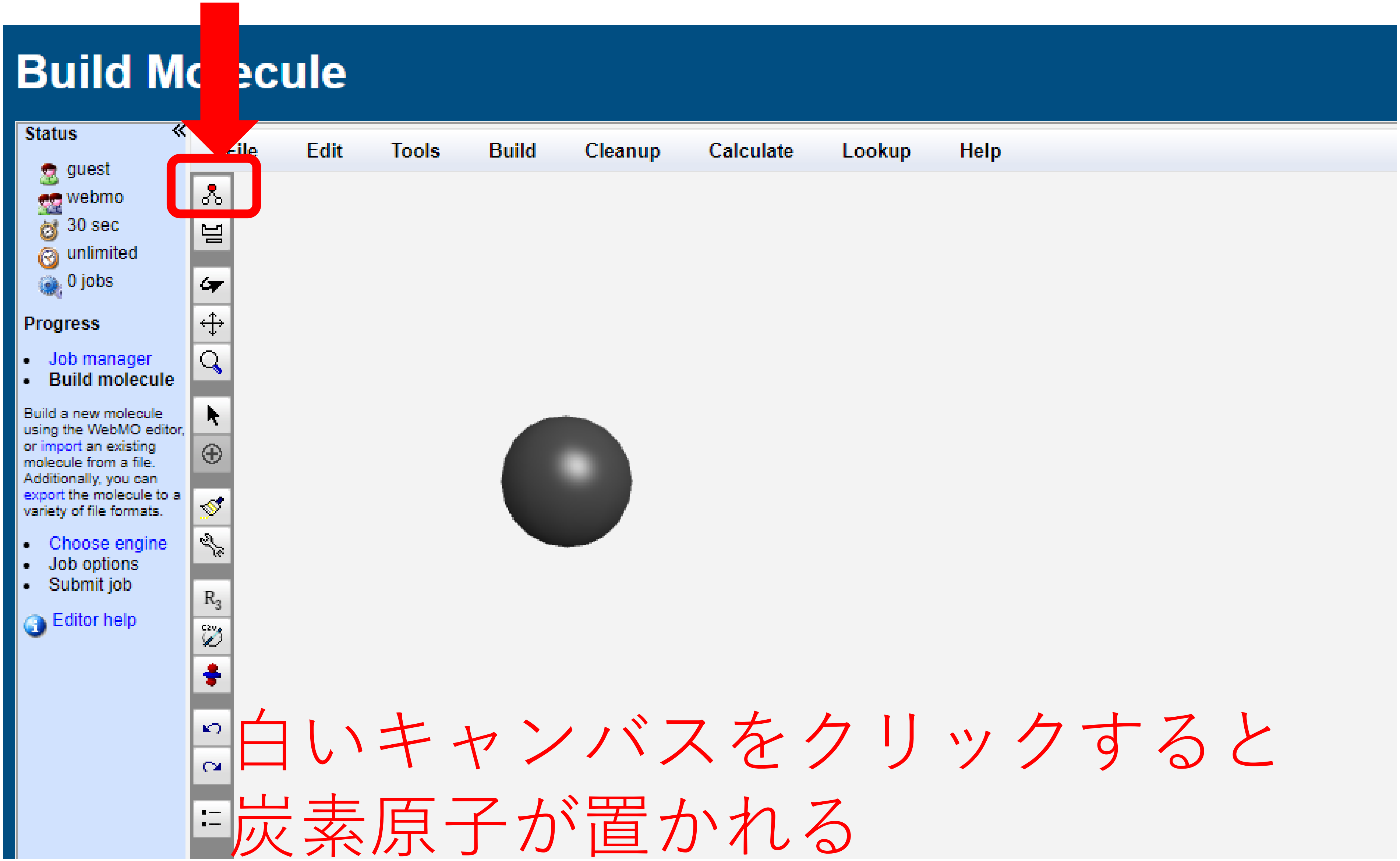
② Click

New Jobタブから Create new jobsを選択


WebMO Job Manager
New Job
Refresh
Download
Move To
Delete
Utilities
Logout
Status
guest
webmo
30 sec
unlimited
0 jobs
Folders
Inbox
Trash
Manage folders
Empty trash
Search
Search...
Displayed jobs
Search
Help
Show all
Show all
Show all
Show all

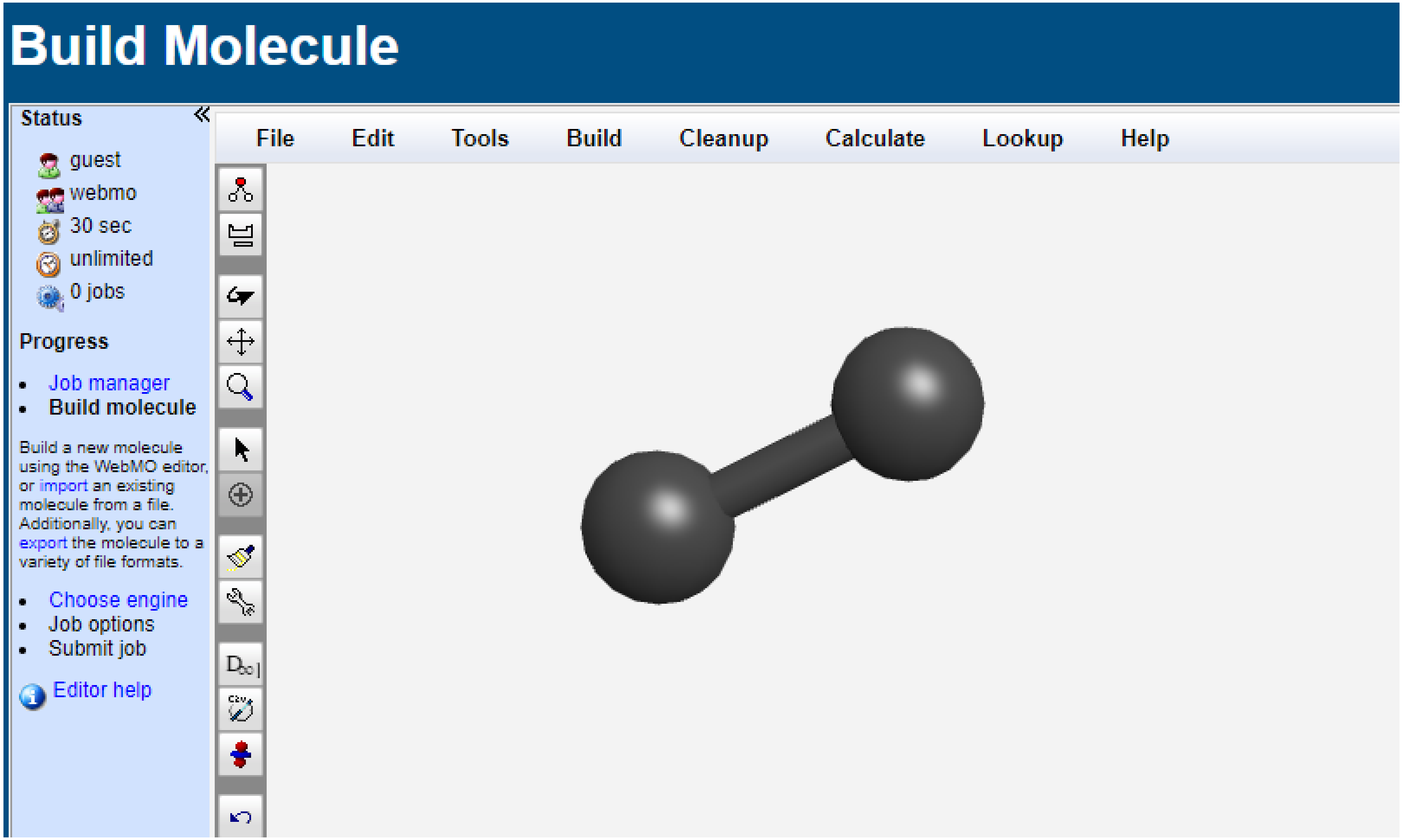
☐	Number	Name	Description	Date	Status	Time	Actions
☐	1096739	C3	Single Point - Quantum Espresso	8/17/2022 3:28	Failed	0.0 sec	
☐	1096738	C10H14N2	Optimize + Vib Freq - Gaussian	8/17/2022 3:23	Failed	31.0 sec	
☐	1096737	F3	Molecular Orbitals - Gaussian	8/17/2022 1:59	Complete	5.7 sec	
☐	1096736	Rn	Molecular Orbitals - Gaussian	8/17/2022 1:49	Failed	0.0 sec	
☐	1096735	Kr	Molecular Orbitals - Gaussian	8/17/2022 1:46	Complete	2.6 sec	
☐	1096734	C10H14N2	Optimize + Vib Freq - Gaussian	8/17/2022 1:44	Failed	46.0 sec	
☐	1096733	Ne	Natural Bond Orbitals - Gaussian	8/17/2022 1:43	Complete	10.0 sec	
☐	1096732	C10H16O2	Molecular Energy - Gamess	8/17/2022 1:41	Complete	36.0 sec	
☐	1096731	C5H9O2N	Molecular Energy - Gaussian	8/17/2022 1:21	Complete	5.9 sec	
☐	1096730	C4F12Ga	Natural Bond Orbitals - Gaussian	8/17/2022 1:03	Complete	26.6 sec	

分子構造を作るボタン


Build Mo ecule
Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Submit job
Editor help
ile
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

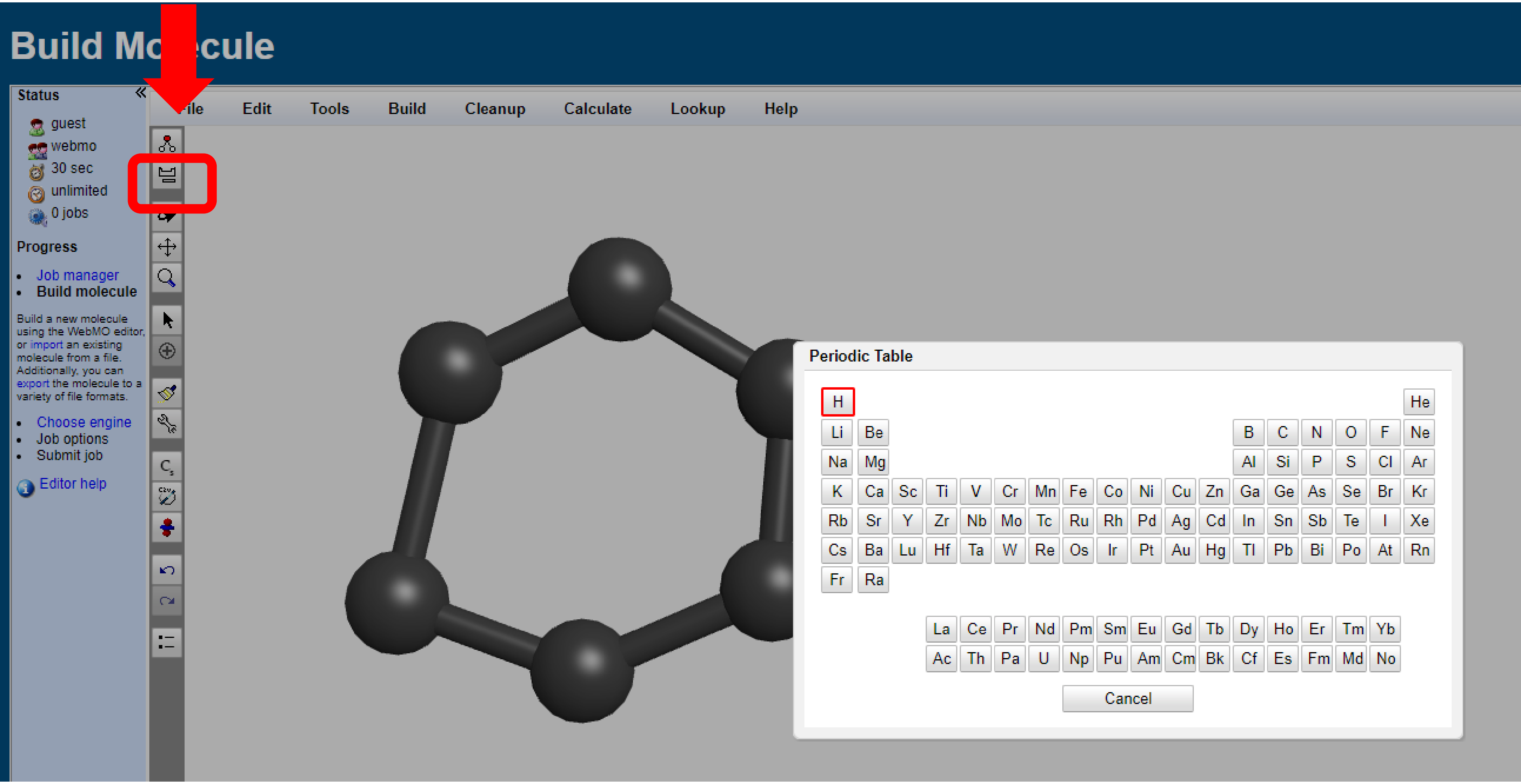
白いキャンバスをクリックすると
炭素原子が置かれる


Build Molecule
Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Submit job
Editor help
File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

すでに存在する原子からドラッグすると結合を作ってもう一つ炭素ができる。炭素で六角形を作ってみよう。

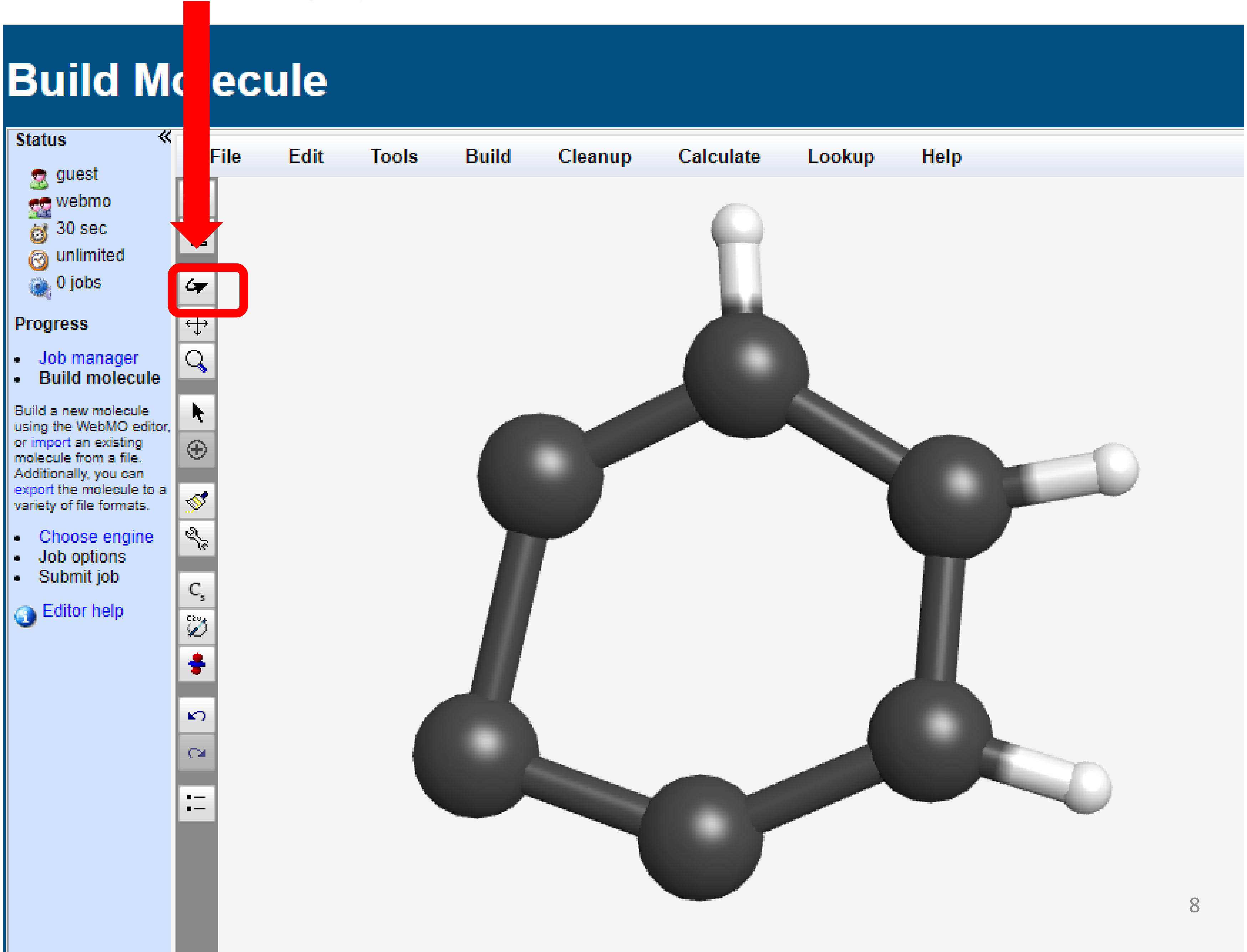
原子を変更するボタン


Build Molecule
Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Submit job
Editor help
File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help
Periodic Table
H 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 Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No
Cancel

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

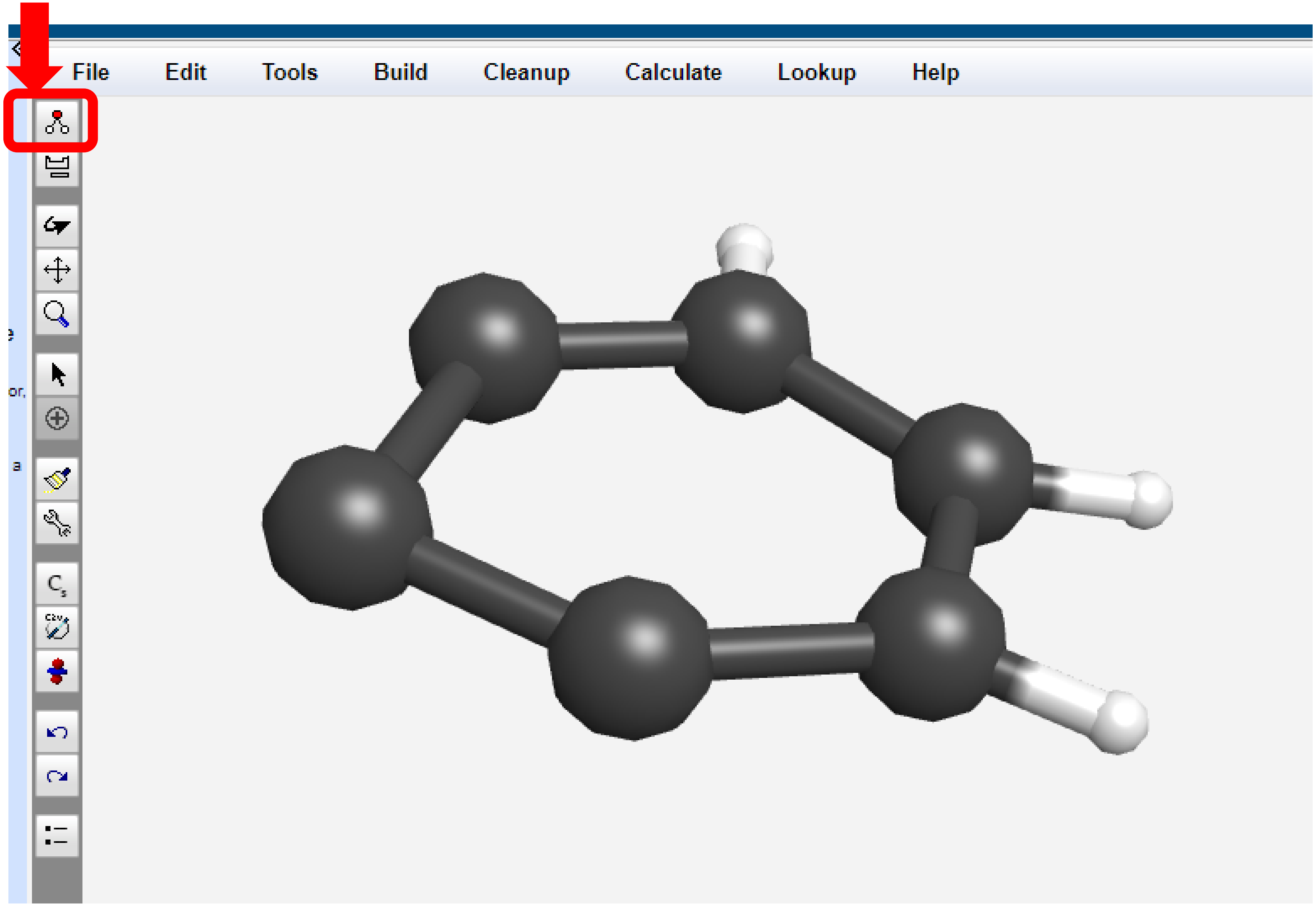
周期表からHを選び、ベンゼンを作る

分子を回転するボタン

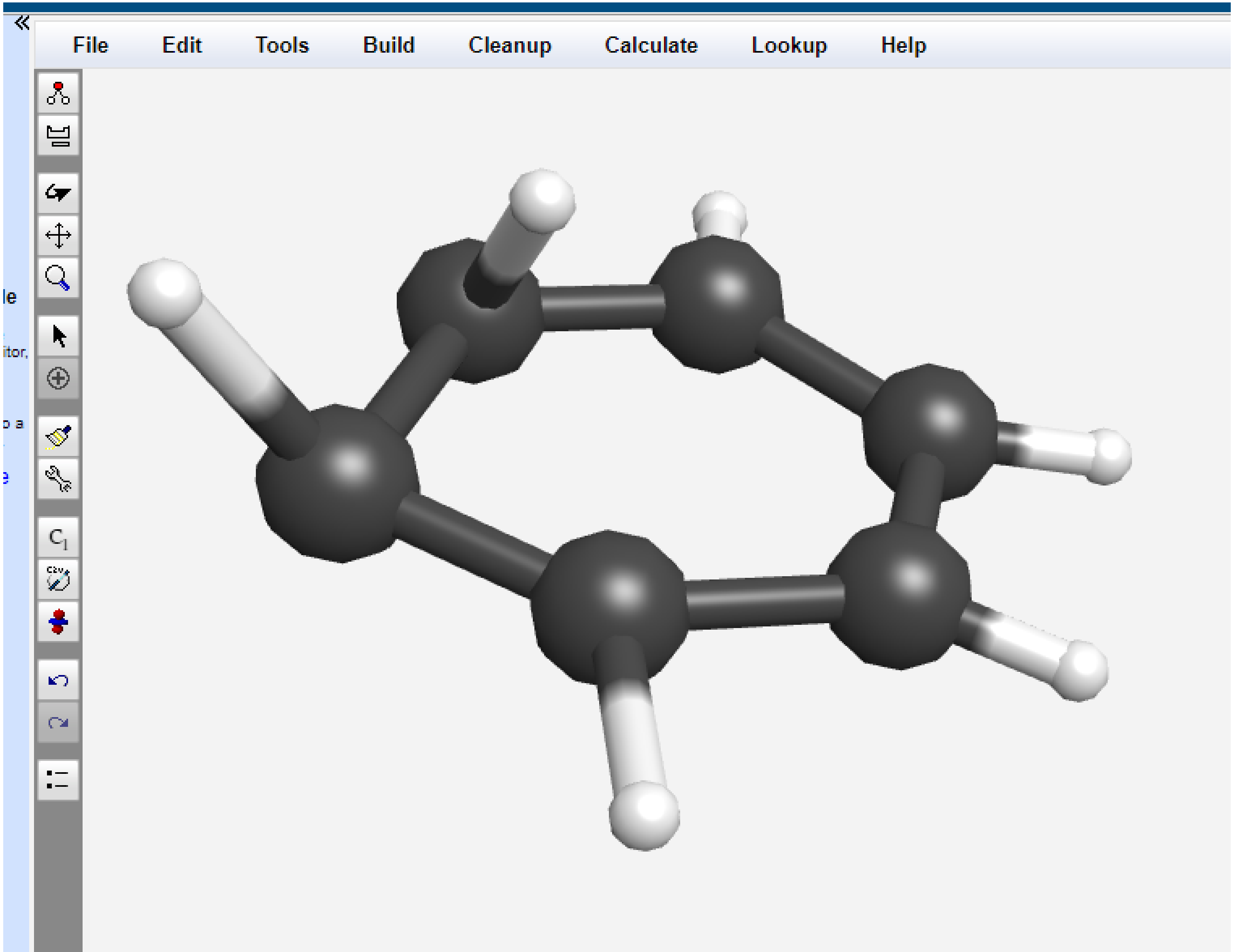

Build Molecule
Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Submit job
Editor help
File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

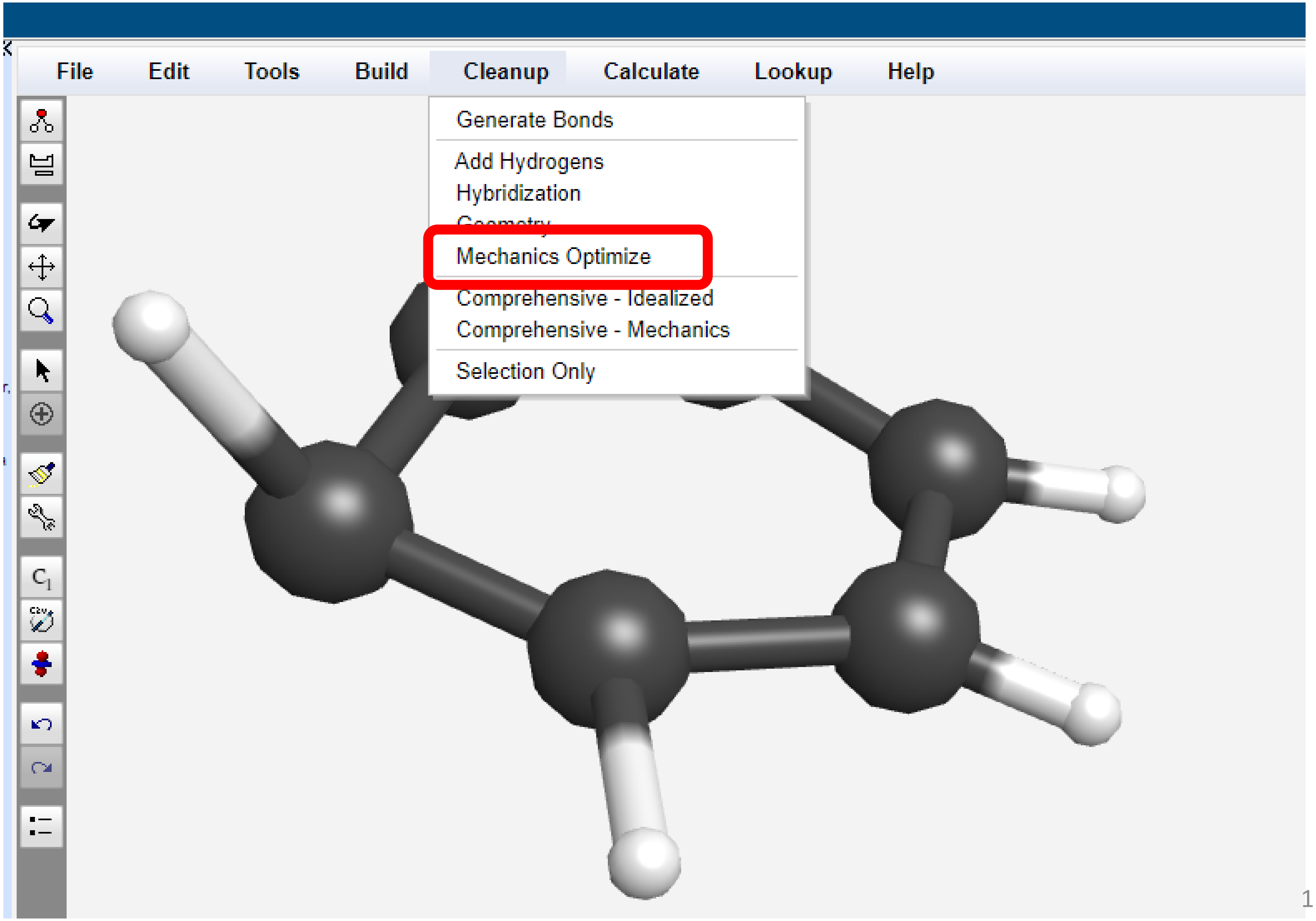
回転後、分子構造の編集を開始


File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help

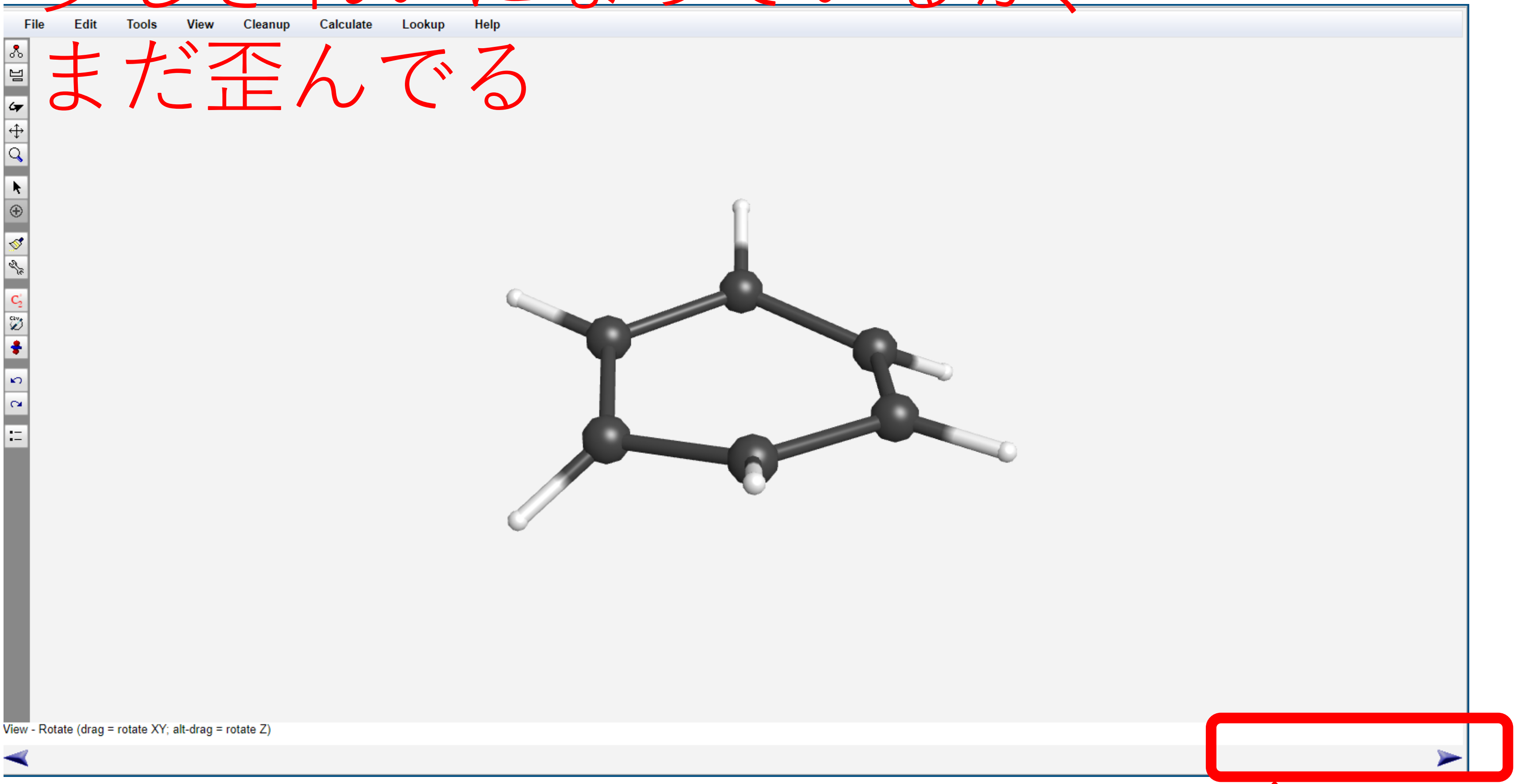
あえて水素を変な向きに付けてみる


File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help
C1
C2v
le
itor,
o a
e

CleanupのMechanics Optimizationで簡易的な分子構造最適化を行う


File
Edit
Tools
Build
Cleanup
Calculate
Lookup
Help
Generate Bonds
Add Hydrogens
Hybridization
Geometry
Mechanics Optimize
Comprehensive - Idealized
Comprehensive - Mechanics
Selection Only

回転してみると
少しきれいになっているが、
まだ歪んでる

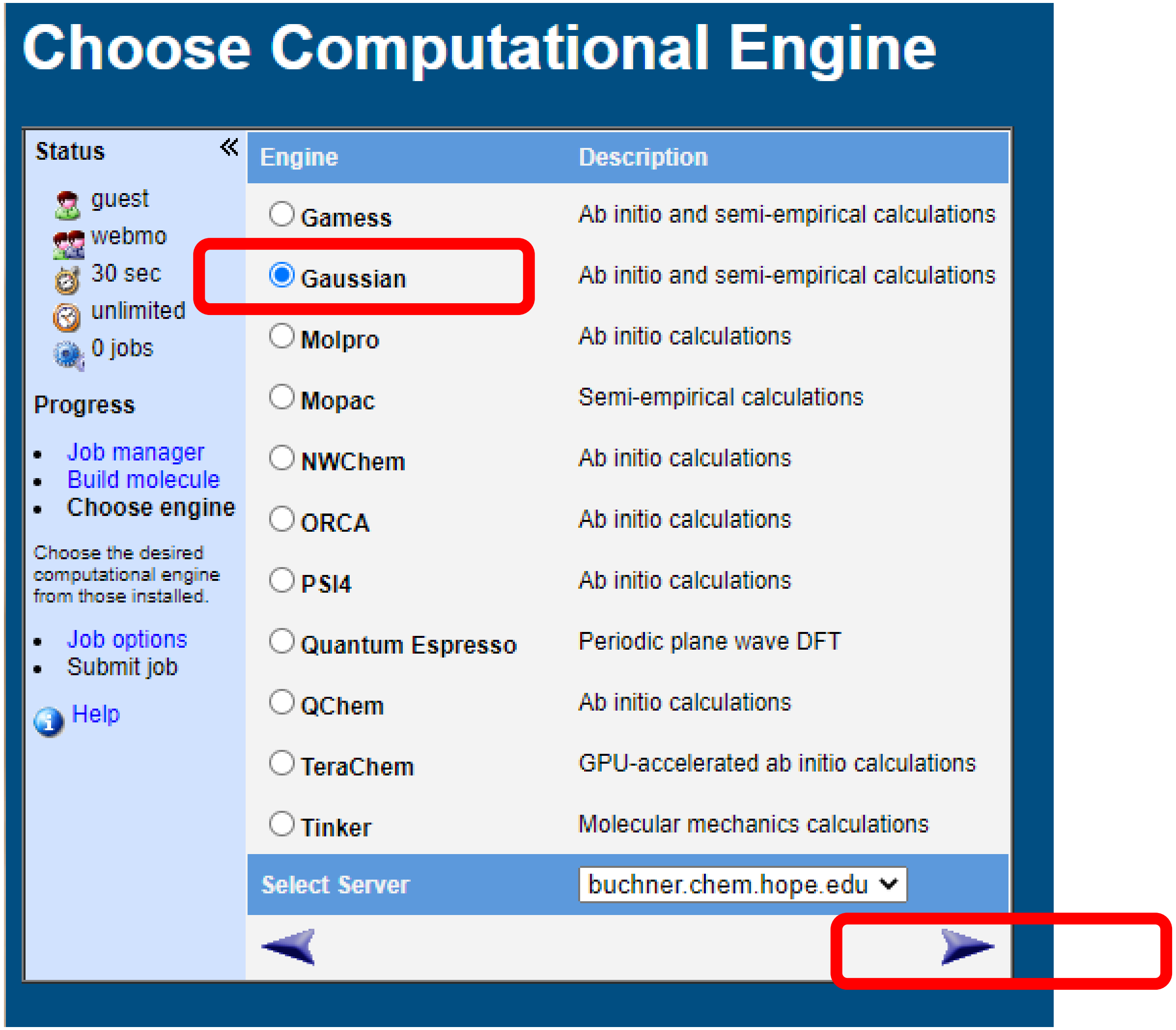

File
Edit
Tools
View
Cleanup
Calculate
Lookup
Help

View - Rotate (drag = rotate XY; alt-drag = rotate Z)

Click

量子化学計算を行う

①Gaussian
を選択



Choose Computational Engine

Status

guest
webmo
30 sec
unlimited
0 jobs

Progress

- Job manager
- Build molecule
- Choose engine

Choose the desired computational engine from those installed.

- Job options
- Submit job

Help

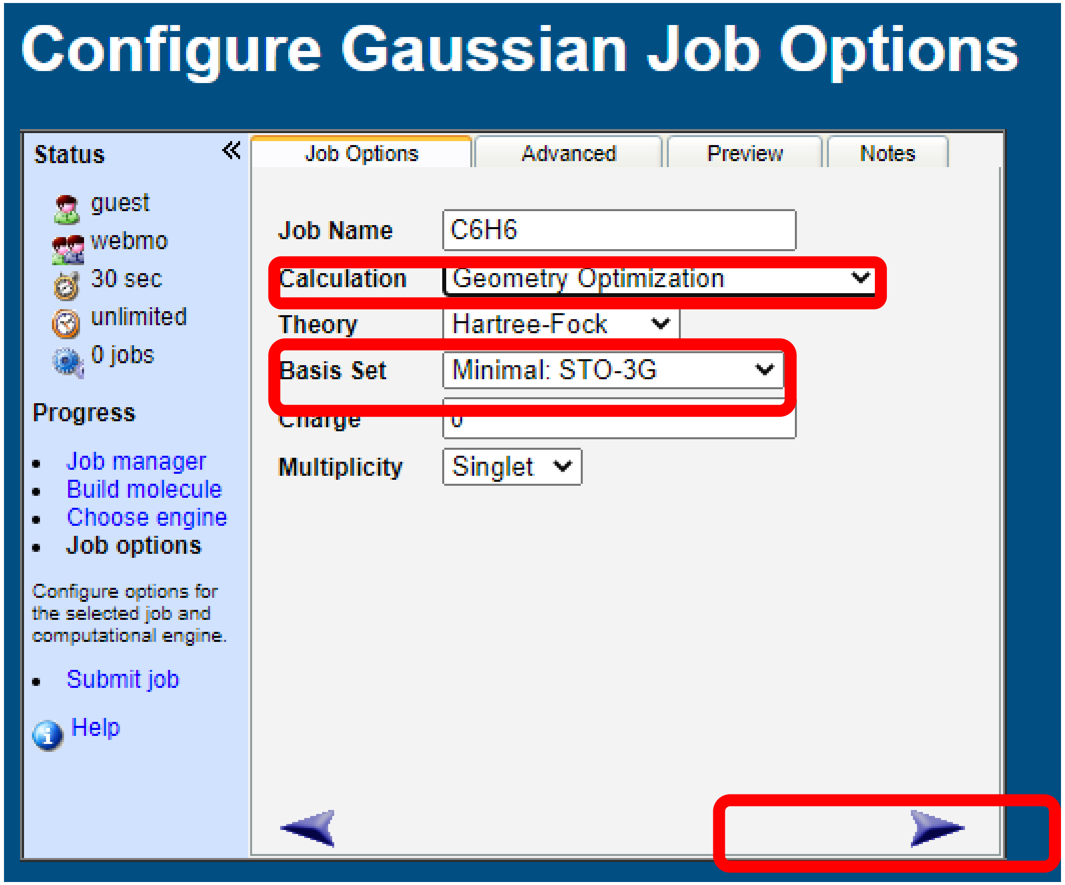
Engine	Description
○ Gamess	Ab initio and semi-empirical calculations
● Gaussian	Ab initio and semi-empirical calculations
○ Molpro	Ab initio calculations
○ Mopac	Semi-empirical calculations
○ NWChem	Ab initio calculations
○ ORCA	Ab initio calculations
○ PSI4	Ab initio calculations
○ Quantum Espresso	Periodic plane wave DFT
○ QChem	Ab initio calculations
○ TeraChem	GPU-accelerated ab initio calculations
○ Tinker	Molecular mechanics calculations
Select Server	buchner.chem.hope.edu

②Click

①

Calculationは Geometry Optimization

Basis setは Minimalを選ぶ



Configure Gaussian Job Options

Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Job Options
Advanced
Preview
Notes
Help
Submit job

Configure options for the selected job and computational engine.

Job Name: C6H6

Calculation: Geometry Optimization

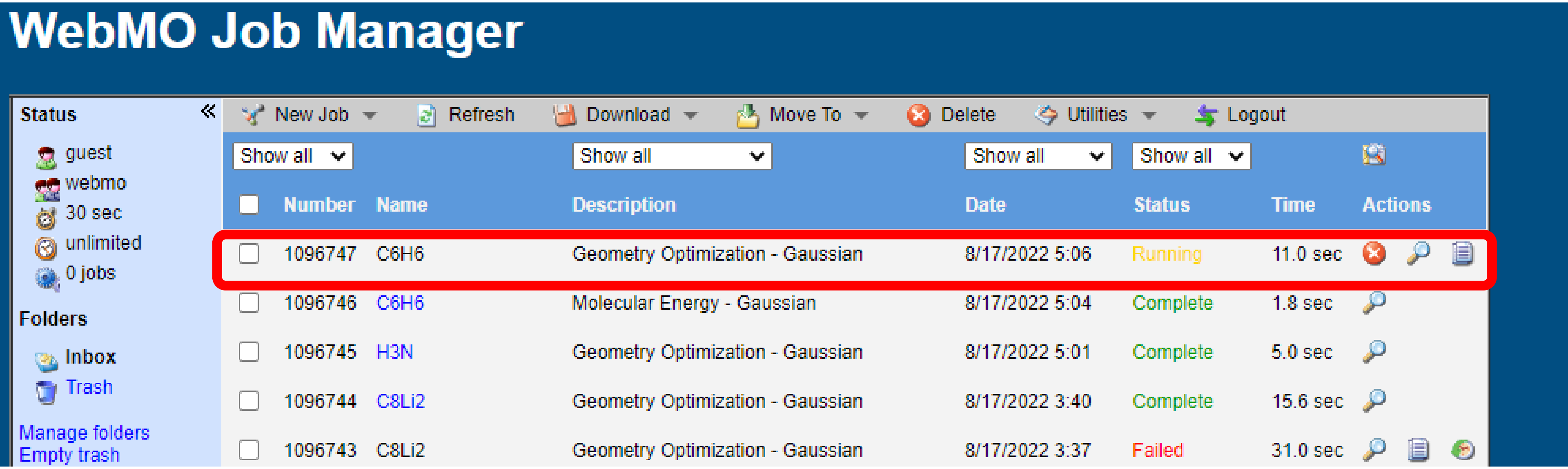
Theory: Hartree-Fock

Basis Set: Minimal: STO-3G

Charge: 0

Multiplicity: Singlet

②Click


New Job
Refresh
Download
Move To
Delete
Utilities
Logout
Show all
Show all
Show all
Show all

WebMO Job Manager

Status

guest
webmo
30 sec
unlimited
0 jobs

Folders

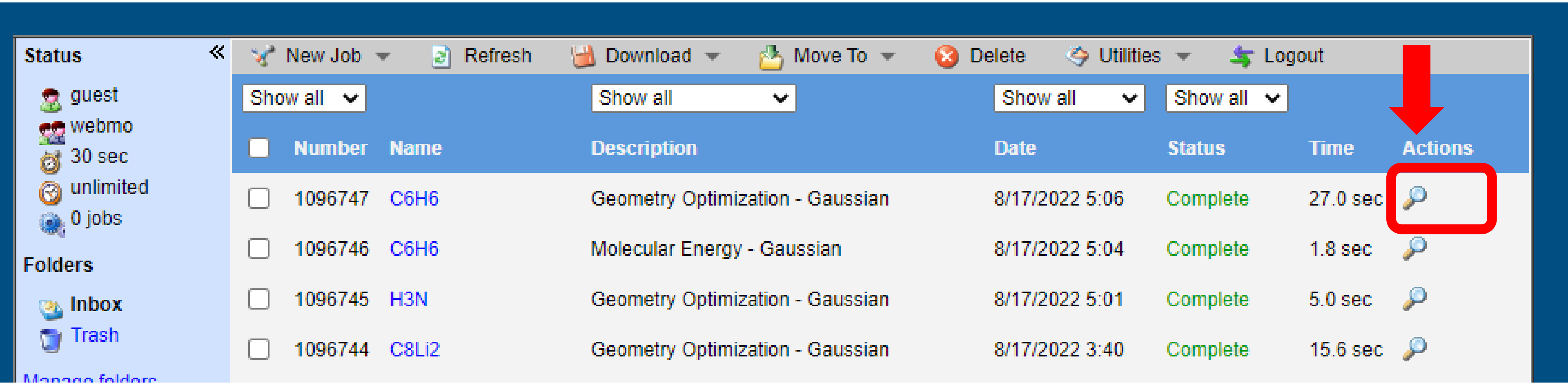
Inbox
Trash

Manage folders
Empty trash

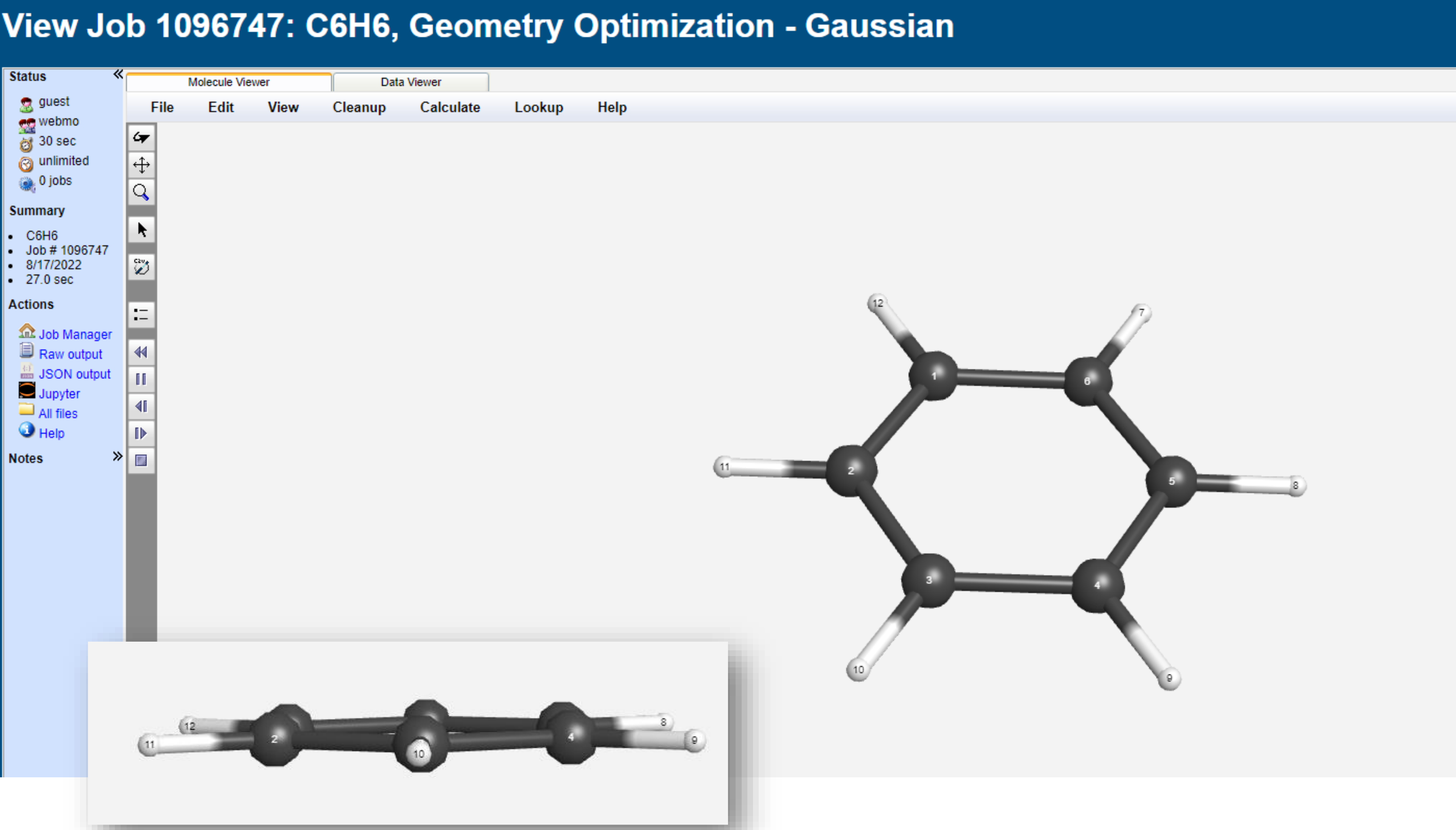
☐	Number	Name	Description	Date	Status	Time	Actions
☐	1096747	C6H6	Geometry Optimization - Gaussian	8/17/2022 5:06	Running	11.0 sec	
☐	1096746	C6H6	Molecular Energy - Gaussian	8/17/2022 5:04	Complete	1.8 sec	
☐	1096745	H3N	Geometry Optimization - Gaussian	8/17/2022 5:01	Complete	5.0 sec	
☐	1096744	C8Li2	Geometry Optimization - Gaussian	8/17/2022 3:40	Complete	15.6 sec	
☐	1096743	C8Li2	Geometry Optimization - Gaussian	8/17/2022 3:37	Failed	31.0 sec	

計算状況が示される
（いろんな人が流している）
StatusのRunningがCompleteになれば終了

Clickして結果を確認


Status
guest
webmo
30 sec
unlimited
0 jobs
Folders
Inbox
Trash
Manage folders
New Job
Refresh
Download
Move To
Delete
Utilities
Logout
Show all
Show all
Show all
Show all

☐	Number	Name	Description	Date	Status	Time	Actions
☐	1096747	C6H6	Geometry Optimization - Gaussian	8/17/2022 5:06	Complete	27.0 sec	🔍
☐	1096746	C6H6	Molecular Energy - Gaussian	8/17/2022 5:04	Complete	1.8 sec	🔍
☐	1096745	H3N	Geometry Optimization - Gaussian	8/17/2022 5:01	Complete	5.0 sec	🔍
☐	1096744	C8Li2	Geometry Optimization - Gaussian	8/17/2022 3:40	Complete	15.6 sec	🔍



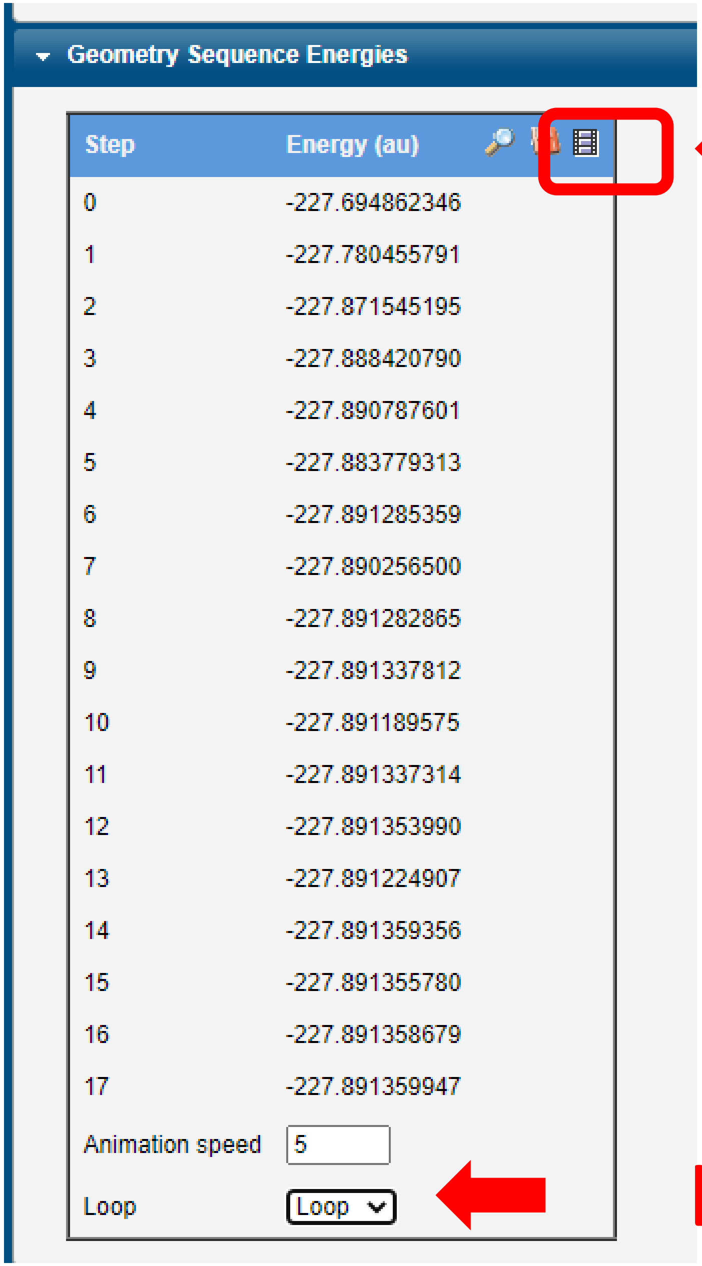
View Job 1096747: C6H6, Geometry Optimization - Gaussian

Status
- guest
- webmo
- 30 sec
- unlimited
- 0 jobs

Summary
- C6H6
- Job # 1096747
- 8/17/2022
- 27.0 sec

Actions
Job Manager
Raw output
JSON output
Jupyter
All files
Help
Notes
Molecule Viewer
Data Viewer
File
Edit
View
Cleanup
Calculate
Lookup
Help
1
2
3
4
5
6
7
8
9
10
11
12

①回転などして
きれいになったか確認
②下にスクロール



Geometry Sequence Energies

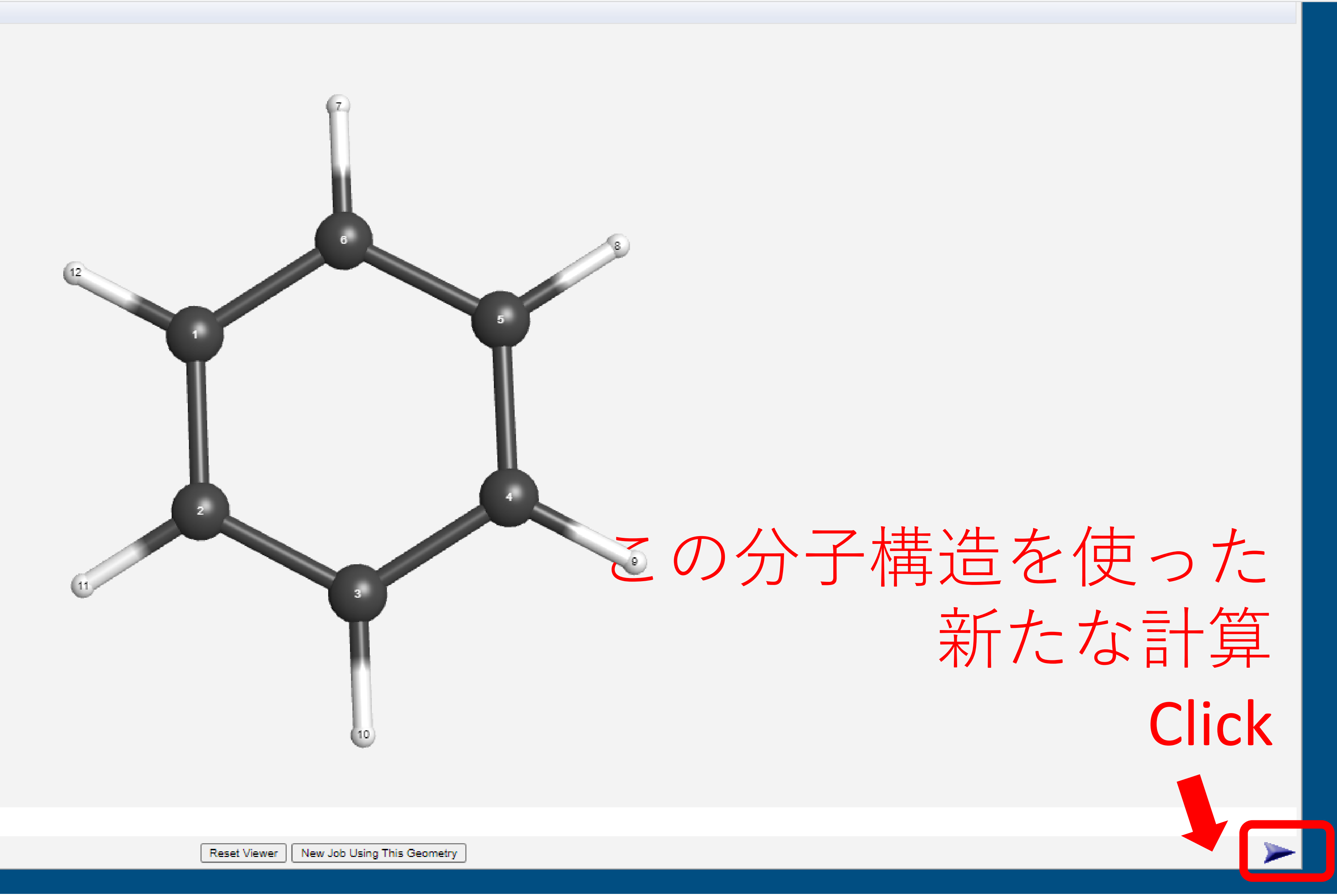
Step	Energy (au)
0	-227.694862346
1	-227.780455791
2	-227.871545195
3	-227.888420790
4	-227.890787601
5	-227.883779313
6	-227.891285359
7	-227.890256500
8	-227.891282865
9	-227.891337812
10	-227.891189575
11	-227.891337314
12	-227.891353990
13	-227.891224907
14	-227.891359356
15	-227.891355780
16	-227.891358679
17	-227.891359947

Animation speed: 5

Loop: Loop

構造最適化の結果が
動画で見られる

Loop再生（お好みで）

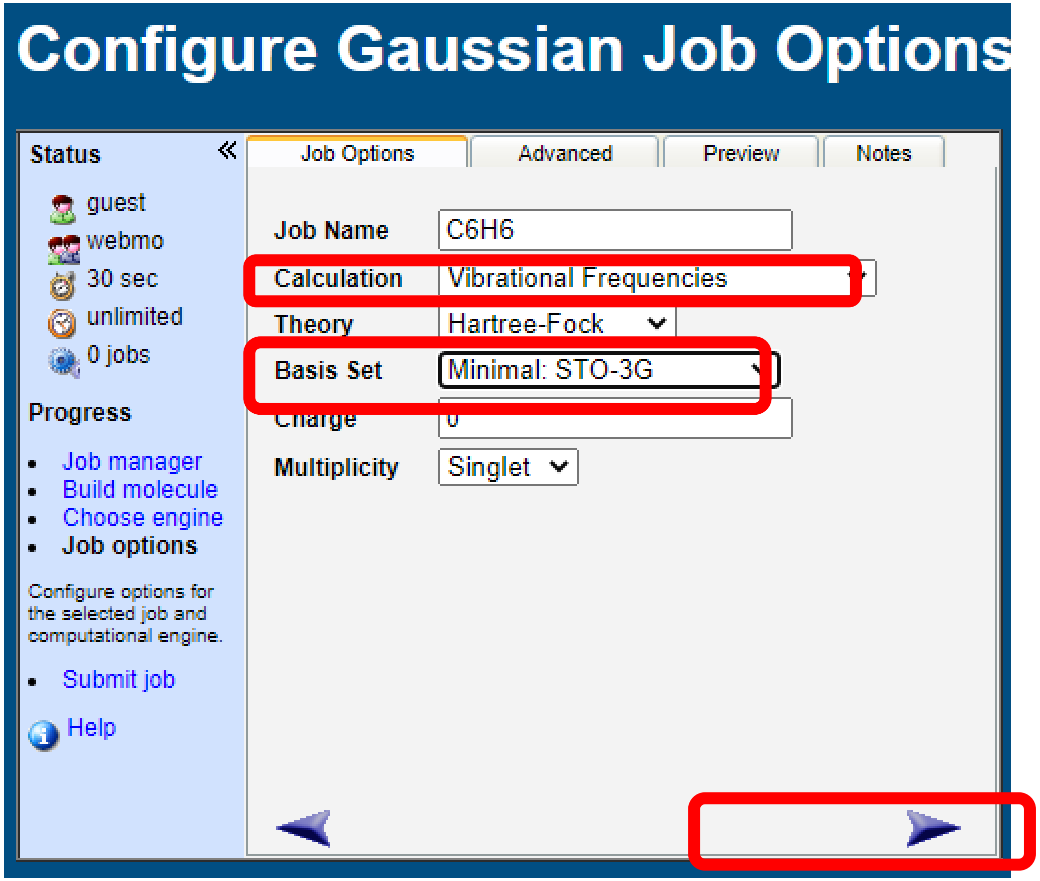

7
6
8
12
5
1
4
2
9
11
3
10
Reset Viewer
New Job Using This Geometry

この分子構造を使った
新たな計算

Click

⓪前の画面でGaussianを選択後

①
Calculationは
Vibrational
Frequencies
Basis setは
Minimalを
選ぶ



Configure Gaussian Job Options

Status
guest
webmo
30 sec
unlimited
0 jobs
Progress
Job manager
Build molecule
Choose engine
Job options
Submit job
Help
Job Options
Advanced
Preview
Notes

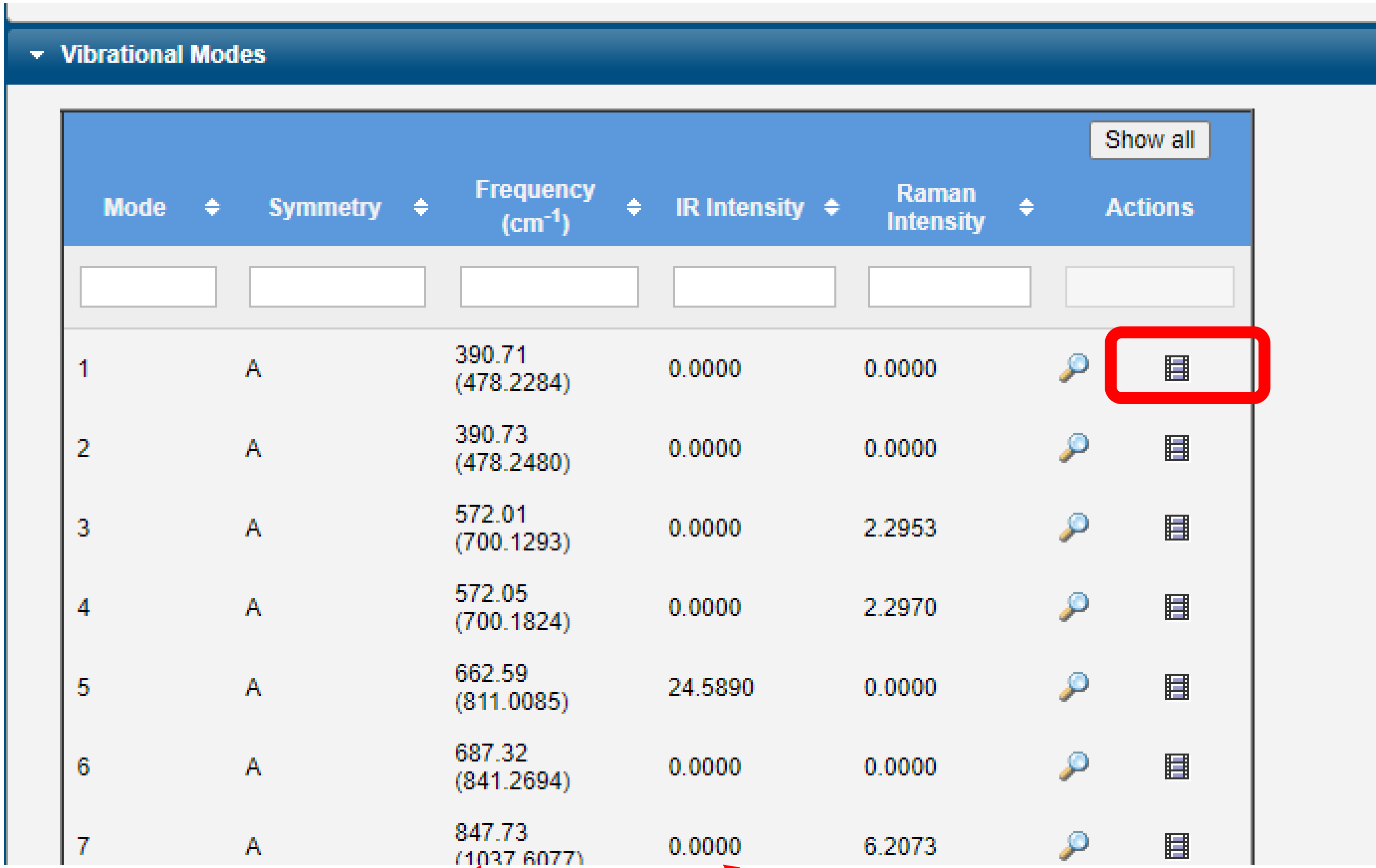
Configure options for the selected job and computational engine.

Job Name C6H6
Calculation Vibrational Frequencies
Theory Hartree-Fock
Basis Set Minimal: STO-3G
Charge 0
Multiplicity Singlet

②Click
計算を進める

計算がうまくいったら分子の図の下の方にスクロール

Vibrational Modes



Mode	Symmetry	Frequency (cm^{-1})	IR Intensity	Raman Intensity	Actions
1	A	390.71 (478.2284)	0.0000	0.0000	🔍 ▤
2	A	390.73 (478.2480)	0.0000	0.0000	🔍 ▤
3	A	572.01 (700.1293)	0.0000	2.2953	🔍 ▤
4	A	572.05 (700.1824)	0.0000	2.2970	🔍 ▤
5	A	662.59 (811.0085)	24.5890	0.0000	🔍 ▤
6	A	687.32 (841.2694)	0.0000	0.0000	🔍 ▤
7	A	847.73 (1037.6077)	0.0000	6.2073	🔍 ▤

動画ボタンを押すと分子振動が見られる！

Frequencies
振動数
(必要なエネルギー)

Intensities
振動の
起こりやすさ

振動数は分子に固有、
振動数は実験で得られた分子が何かを知るのに重要