winmostar tutorial

GAMESS
Basis Set and ECP Settings for Each Element

V11.6.5

16 April 2024 X-Ability Co., Ltd.

About This Manual

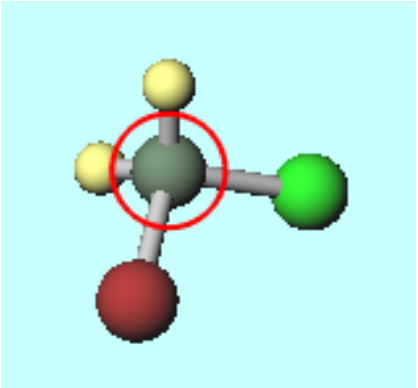
- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
-

Overview

Set the basis functions for each element of bromochloromethane (CH_2BrCl), and configure the basis sets and ECPs (Effective Core Potentials).

Basis set configuration only: C, Cl, Br: 6-31G*, H: STO-3G

Configuration of basis sets and ECPs: C, H: 6-31G*, Cl, Br: LANL2DZ (both basis set and ECP).

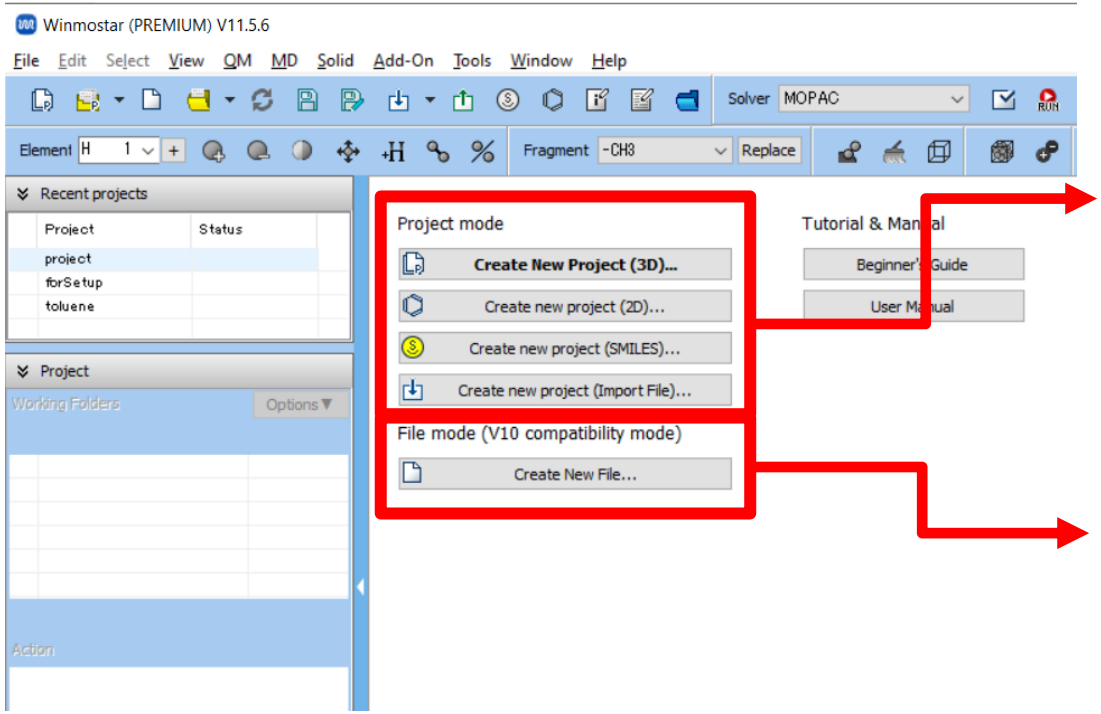


Preference of Operating Environment

- For GAMESS:
  - Please install GAMESS according to GAMESS Installation Manual available at https://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en_win.pdf

Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to tutorial for version 10.



Project Mode **New Features in V11**

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

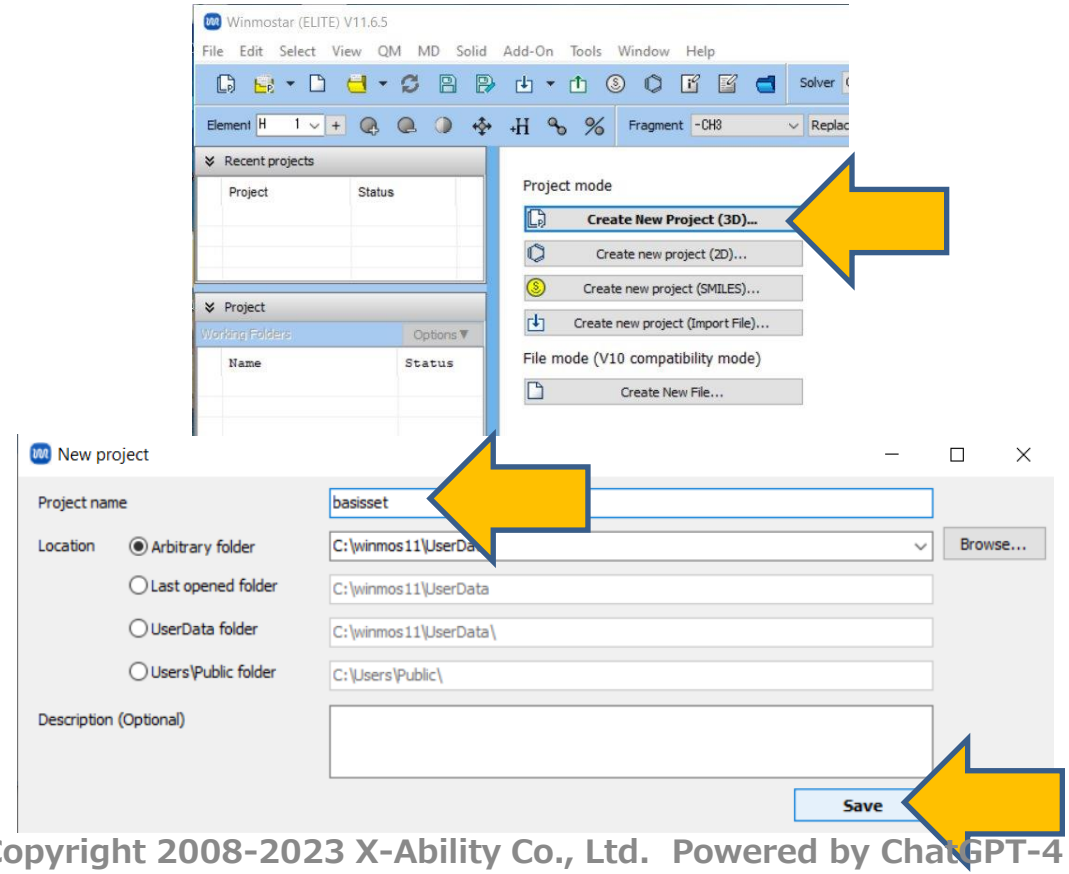
When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. Modeling of the System

For the basic operation methods, please refer to GAMESS Foundation Tutorial.

A. Launch Winmostar and click on **Create New Project (3D)**. If Winmostar is already running, click **File | Close** first.

B. Enter 'basisset' in **Project name** and click **Save**.

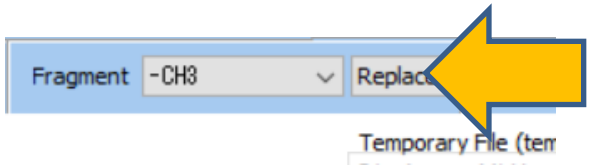


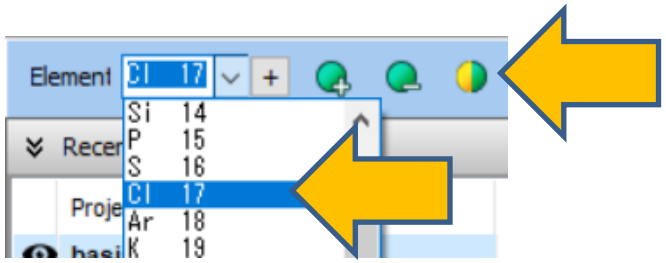
A. Modeling of the System

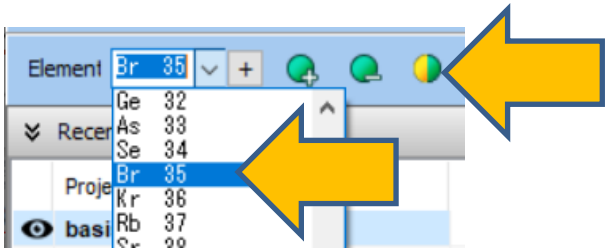
A. With **Fragment** set to **-CH3**, click **Replace** on the right once to create methane.

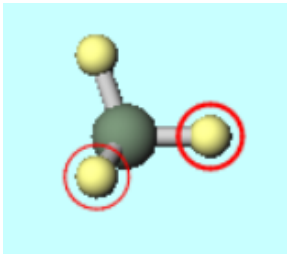
B. With a hydrogen atom selected (highlighted with a thick red circle), select **Cl 17** from **Element of Toolbar** at the top of Main Window and click **Change Element** to create chloromethane.

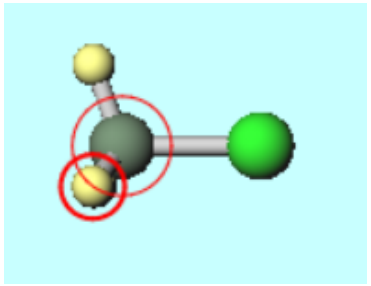
C. With another hydrogen atom selected (highlighted with a thick red circle), select **Br 35** from **Element of Toolbar** and click **Change Element** to create bromochloromethane.

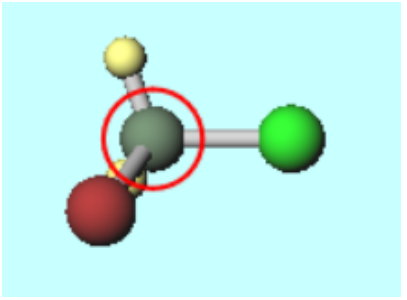










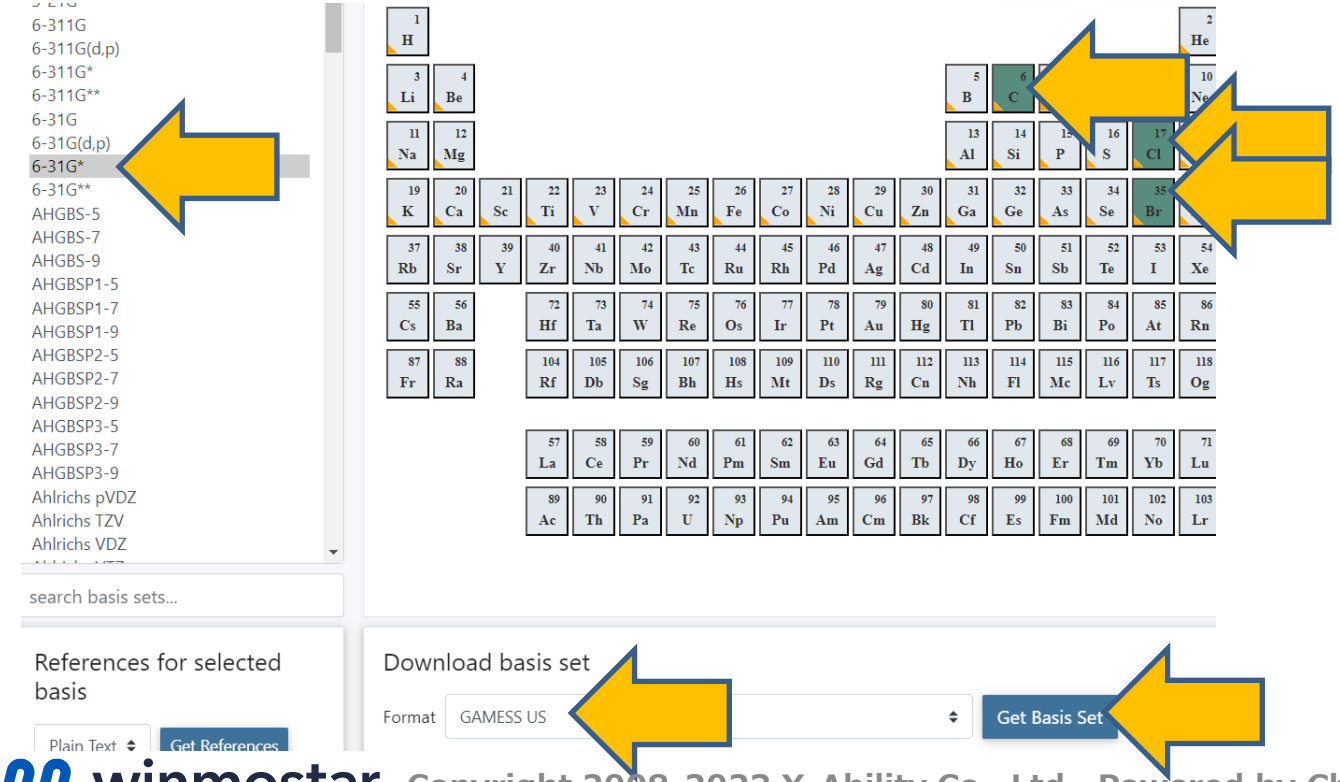


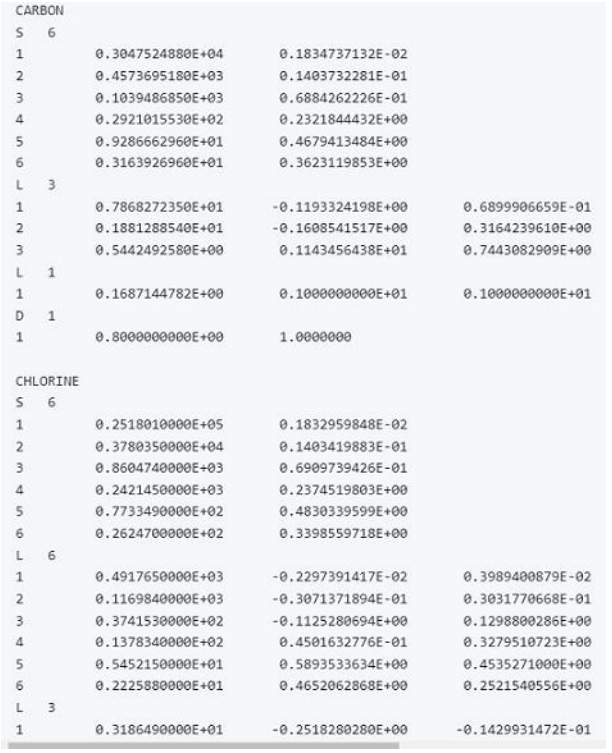
B. Execution of Calculate (Basis Set Only Configuration)

Retrieve the basis set data from Basis Set Exchange website.
(https://www.basissetexchange.org/)

A. Select 6-31G* for the basis set, and choose C, Cl, and Br for the elements. Select GAMESS US as Format, and click Get Basis Set.

B. Take notes of the basis set information displayed in the newly opened window.

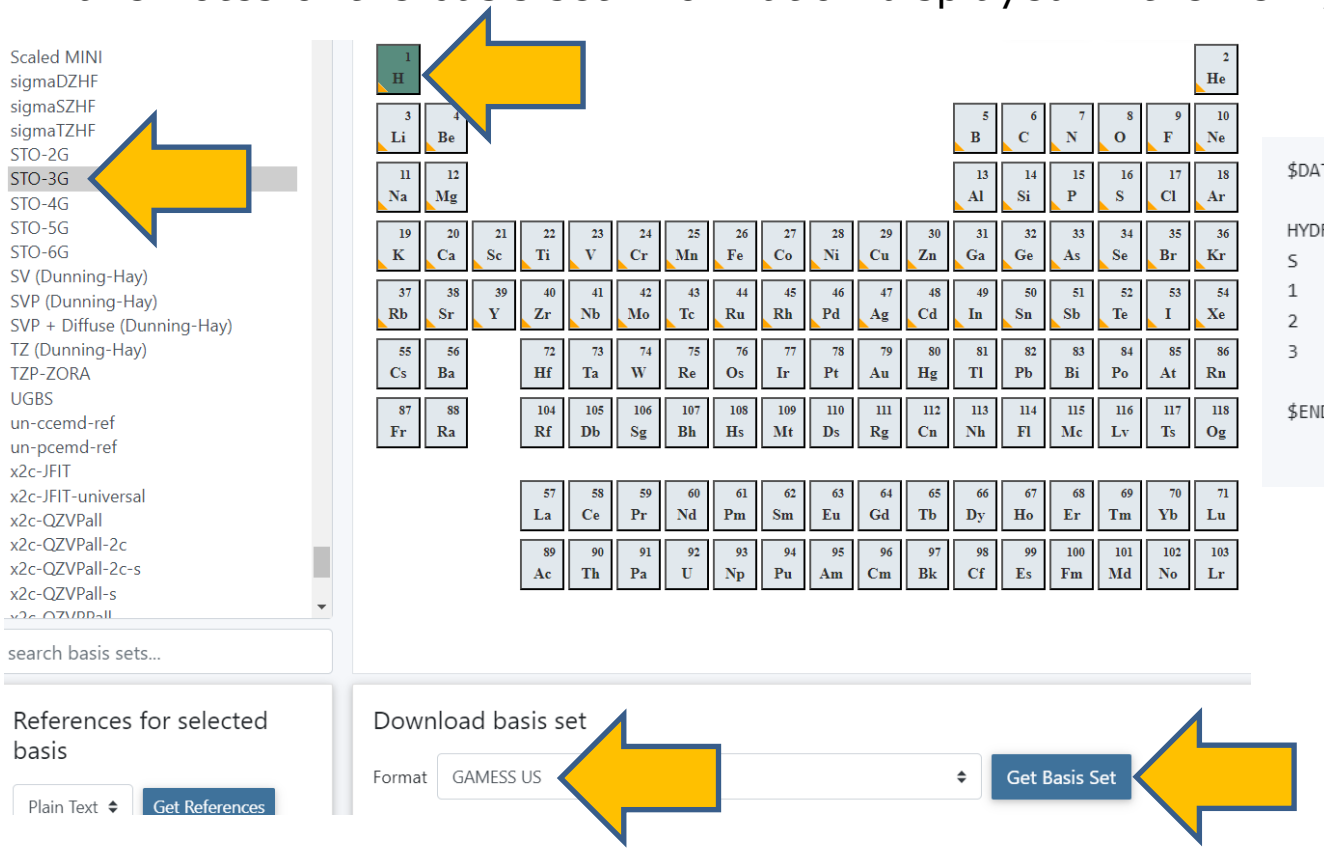




B. Execution of Calculate (Basis Set Only Configuration)

A. Select STO-3G for the basis set/ECP, choose H for the element, and select GAMESS US as Format, then click Get Basis Set.

B. Take notes of the basis set information displayed in the newly opened window.




```
$DATA

HYDROGEN
S   3
1          0.3425250914E+01        0.1543289673E+00
2          0.6239137298E+00        0.5353281423E+00
3          0.1688554040E+00        0.4446345422E+00

$END
```

B. Execution of Calculate (Basis Set Only Configuration)

Modify the basis set data for all elements to fit the input format based on the data obtained from Basis Set Exchange website. Here, we use the data for carbon (from 'CARBON' to the blank line) as an example.

A. Change the element name 'CARBON' to ' `$C`' and be sure to include one space at the beginning. The character following the $ is the keyword for the basis set of each element, and the keyword name can be arbitrary. In this tutorial, to keep it short, we have used the element symbols as keywords.

B. After the last blank line (leave the blank line), add ' `$END`'. Similarly, ensure to include one space at the beginning. Note that case distinction does not matter in GAMESS inputs.

```
CARBON
S  6
1      0.3047524880E+04     0.1834737132E-02
2      0.4573695180E+03     0.1403732281E-01
3      0.1039486850E+03     0.6884262226E-01
4      0.2921015530E+02     0.2321844432E+00
5      0.9286662960E+01     0.4679413484E+00
6      0.3163926960E+01     0.3623119853E+00
L  3
1      0.7868272350E+01    -0.1193324198E+00     0.6899906659E-01
2      0.1881288540E+01    -0.1608541517E+00     0.3164239610E+00
3      0.5442492580E+00     0.1143456438E+01     0.7443082909E+00
L  1
1      0.1687144782E+00     0.1000000000E+01     0.1000000000E+01
D  1
1      0.8000000000E+00     1.0000000
```

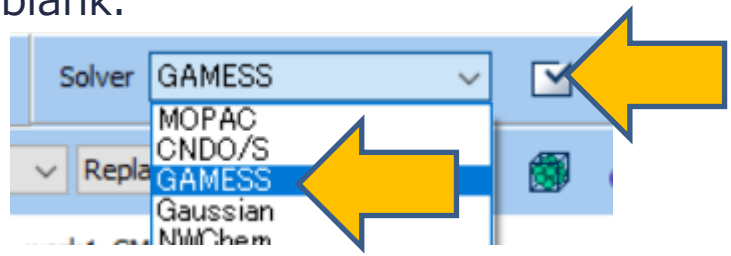
```
 $C
S  6
1      0.3047524880E+04     0.1834737132E-02
2      0.4573695180E+03     0.1403732281E-01
3      0.1039486850E+03     0.6884262226E-01
4      0.2921015530E+02     0.2321844432E+00
5      0.9286662960E+01     0.4679413484E+00
6      0.3163926960E+01     0.3623119853E+00
L  3
1      0.7868272350E+01    -0.1193324198E+00     0.6899906659E-01
2      0.1881288540E+01    -0.1608541517E+00     0.3164239610E+00
3      0.5442492580E+00     0.1143456438E+01     0.7443082909E+00
L  1
1      0.1687144782E+00     0.1000000000E+01     0.1000000000E+01
D  1
1      0.8000000000E+00     1.0000000

 $END
```

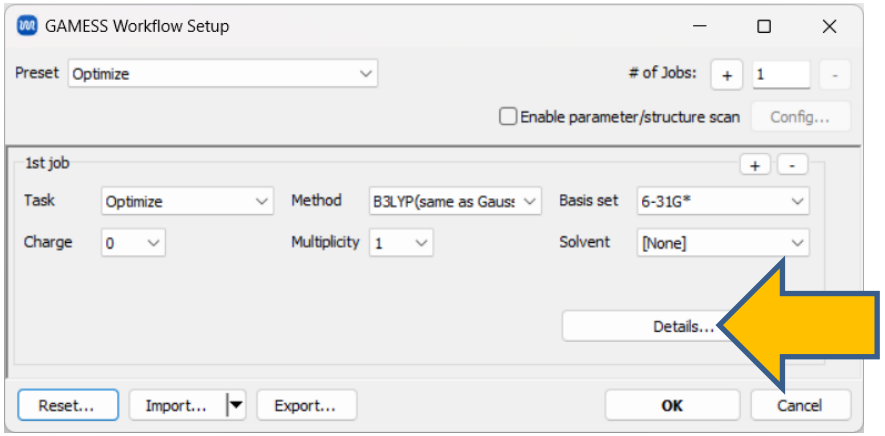
B. Execution of Calculate (Basis Set Only Configuration)

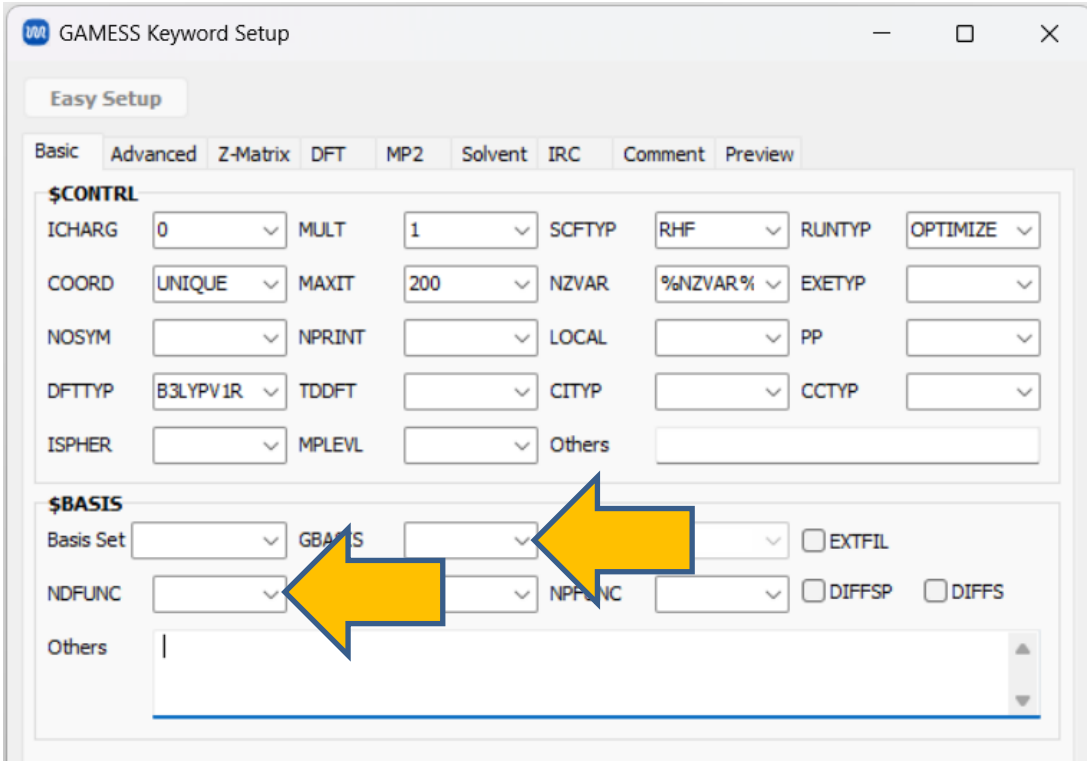
A. Select **GAMESS** from **Solver** and click **Workflow Setup**.

B. In **GAMESS Workflow Setup** window, click **Details**.

C. In **GAMESS Keyword Setup** window, leave **GBASIS** and **NDFUNC** under **$BASIS** blank.

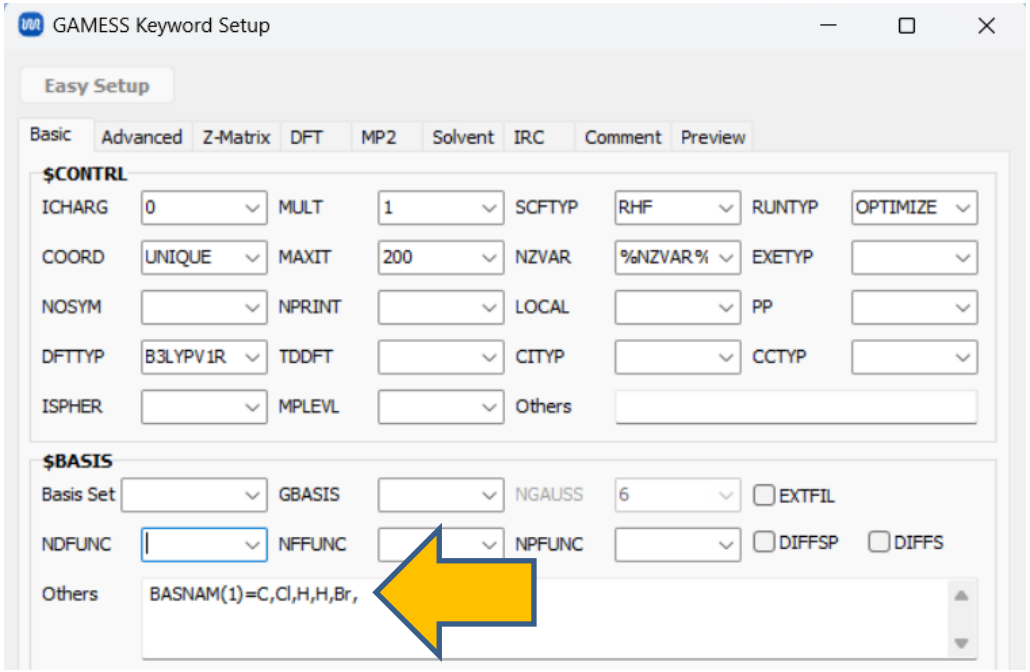


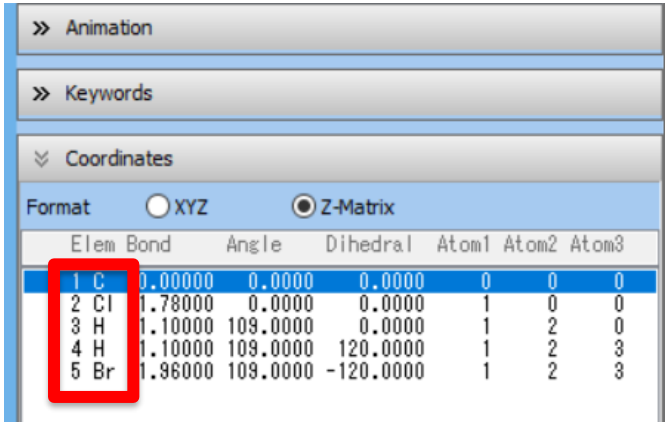




B. Execution of Calculate (Basis Set Only Configuration)

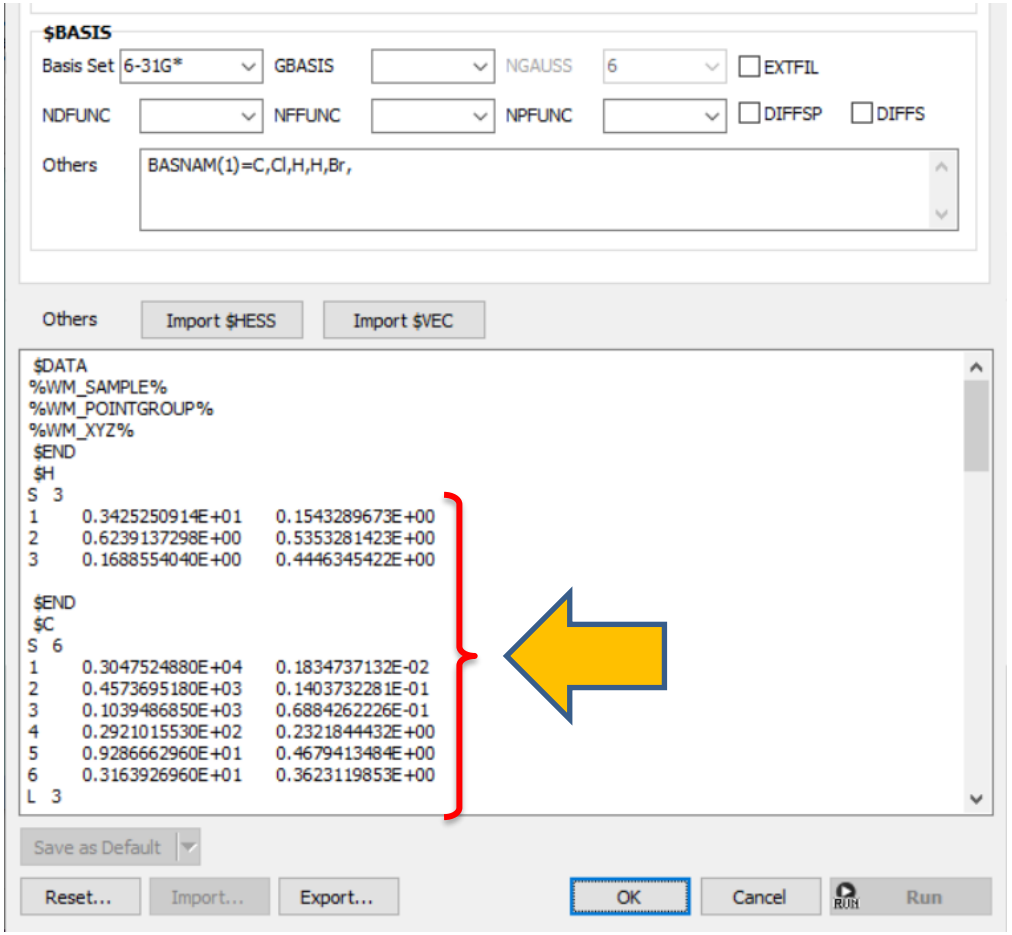
A. In **$BASIS** section's **Others**, enter '`BASNAM(1)=C,Cl,H,H,Br,`'. After BASNAM(1)=, list the basis set keywords for each atom starting from the first, as determined on p.10. Due to GAMESS specifications, a line of computational conditions can only read up to 80 characters, so in this tutorial, we use element symbols as keywords because they are shorter. If the molecular size is large and exceeds 80 characters, please divide the information into multiple lines. Verify the arrangement of atoms in Coordinate Viewer on the right of Main Window.





B. Execution of Calculate (Basis Set Only Configuration)

A. In **GAMESS Keyword Setup** window, add the basis set information for each element, as modified on page 10, below $END on the fifth line in **Others** section.



B. Execution of Calculate (Basis Set Only Configuration)

A. In **GAMESS Keyword Setup** window, click **OK**.
B. In **GAMESS Workflow Setup** window, click **OK**.
C. In **Job Setting** window, click **Run** to start the calculation.

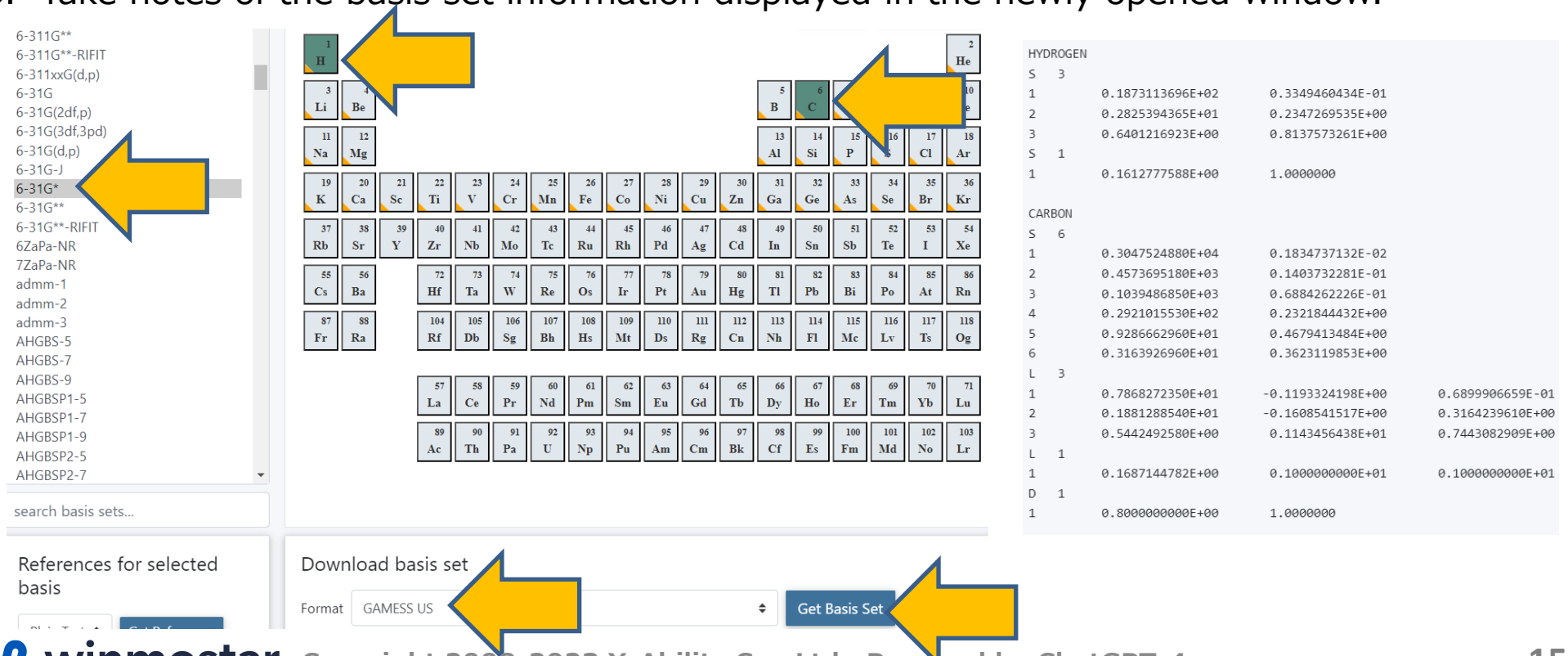
C. Execution of Calculate (Basis Set and ECP Configuration)

Retrieve the basis set and ECP values from Basis Set Exchange website.

(https://www.basissetexchange.org/)

A. Select 6-31G* for the basis set, choose C and H for the elements, select GAMESS US as Format, and click Get Basis Set.

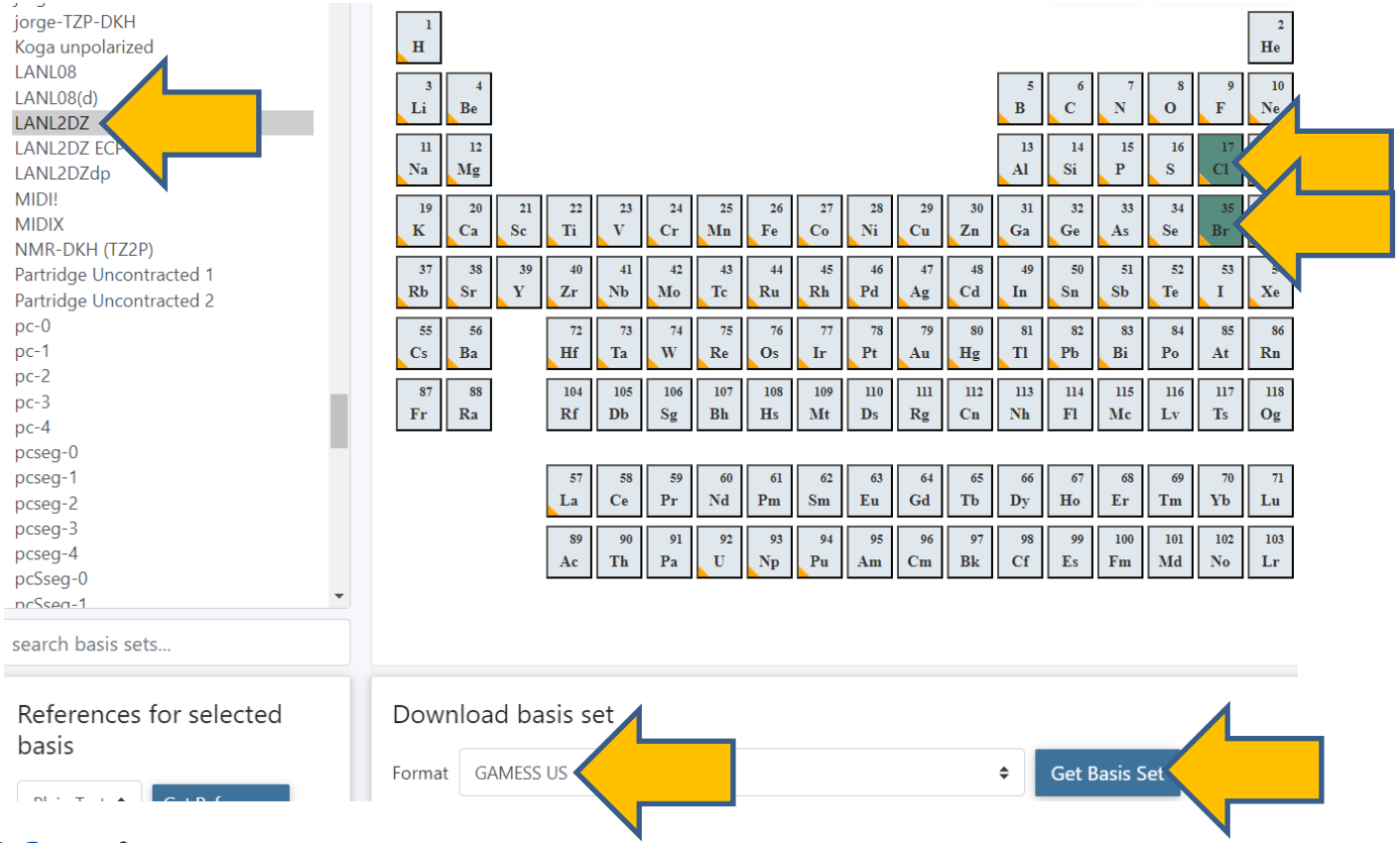
B. Take notes of the basis set information displayed in the newly opened window.



C. Execution of Calculate (Basis Set and ECP Configuration)

A. Select LANL2DZ for the basis set/ECP, choose Cl and Br for the elements, select GAMESS US as Format, and click Get Basis Set.

B. Take notes of the basis set and ECP information displayed in the newly opened window.




```
CHLORINE
S   2
1         2.2310000              -0.4900589
2         0.4720000               1.2542684
S   1
1         0.1631000               1.0000000
P   2
1         6.2960000              -0.0635641
2         0.6333000               1.0141355
P   1
1         0.1819000               1.0000000

BROMINE
S   2
1         1.1590000              -3.0378769
2         0.7107000               3.3703735
S   1
1         0.1905000               1.0000000
P   2
1         2.6910000              -0.1189800
2         0.4446000               1.0424471
P   1
1         0.1377000               1.0000000

$END

$ECP
CL-ECP GEN    10    2
5     ----- d-ul potential -----
    -10.0000000       1      94.8130000
     66.2729170       2     165.6440000
    -28.9685950       2      30.8317000
    -12.8663370       2      10.5841000
     -1.7102170       2       3.7704000
```

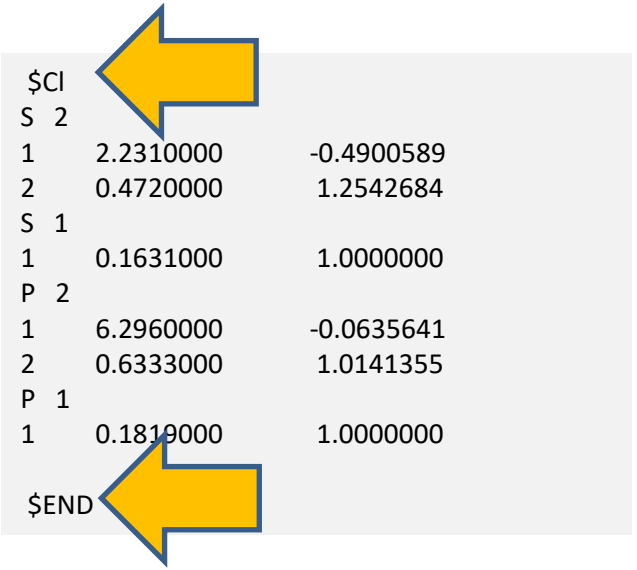
C. Execution of Calculate (Basis Set and ECP Configuration)

Modify the basis set data for all elements to fit the input format using the data obtained from Basis Set Exchange website. Here, we use the data for chlorine (from 'CHLORINE' to the blank line) as an example.

Change the element name 'CHLORINE' to ' $Cl' and be sure to include one space at the beginning. The character following the $ is the keyword for the basis set of each element, and the keyword name can be arbitrary. In this tutorial, to keep it short, we have used the element symbols as keywords.

After the last blank line (leave the blank line), add ' $END'. Similarly, ensure to include one space at the beginning. Note that case distinction does not matter in GAMESS inputs.

```
CHLORINE
S  2
1      2.2310000          -0.4900589
2      0.4720000           1.2542684
S  1
1      0.1631000           1.0000000
P  2
1      6.2960000          -0.0635641
2      0.6333000           1.0141355
P  1
1      0.1819000           1.0000000
```

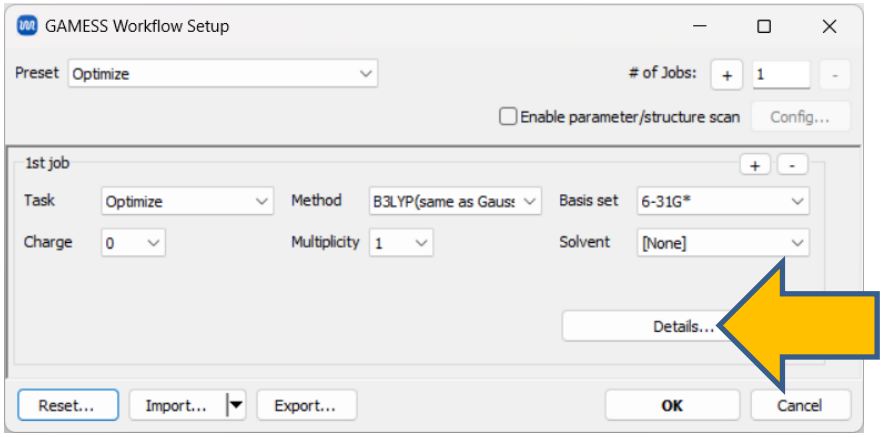


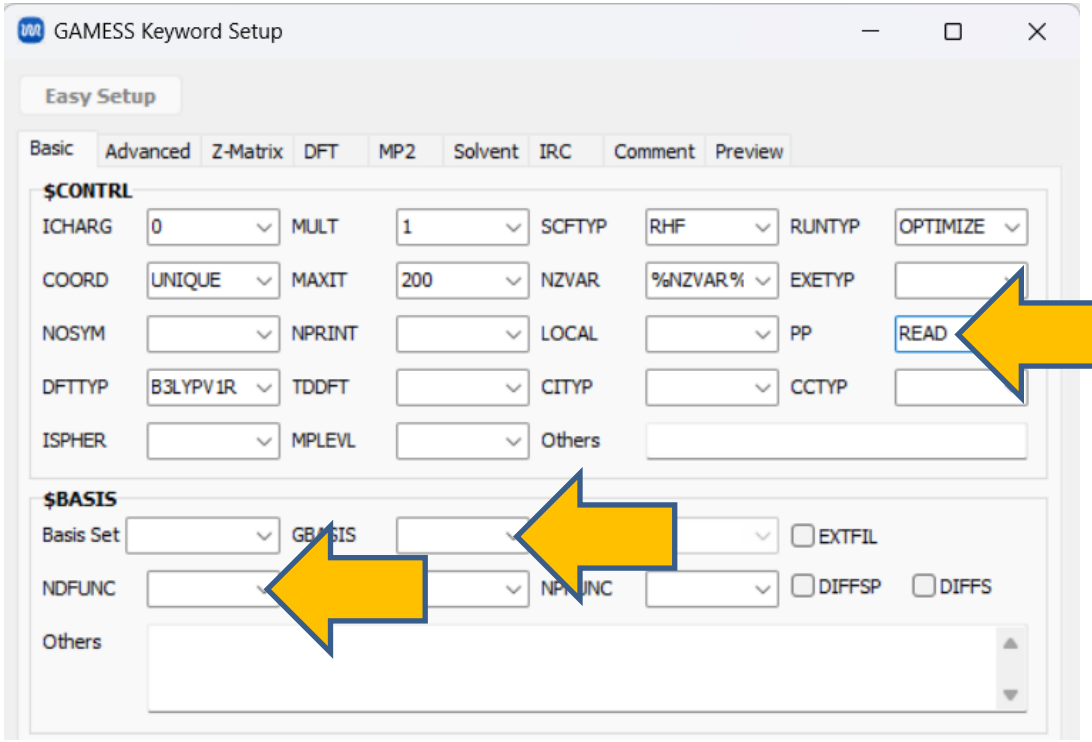
C. Execution of Calculate (Basis Set and ECP Configuration)

A. Select **GAMESS** from **Solver** and click **Workflow Setup**.

B. In **GAMESS Workflow Setup** window, click **Details**.

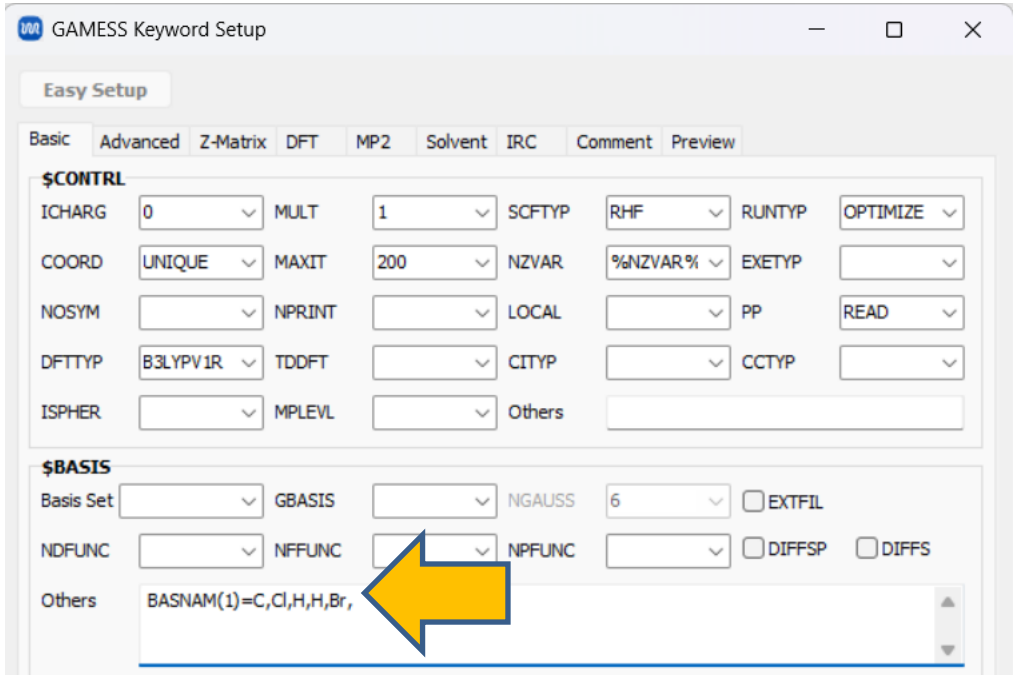
C. In **GAMESS Keyword Setup** window, change **PP** under **$CONTRL** to **READ** and leave **GBASIS** and **NDFUNC** under **$BASIS** blank.

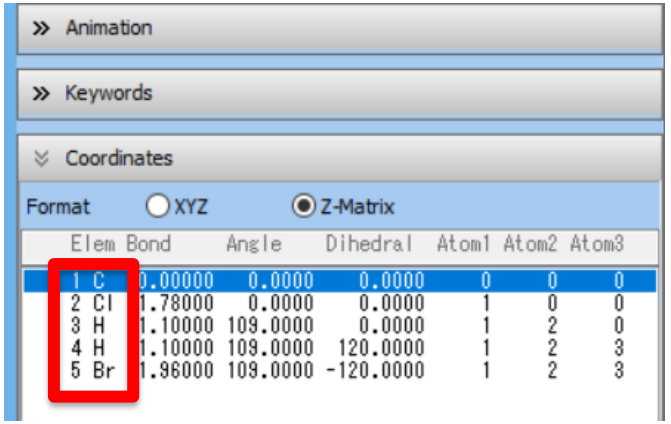




C. Execution of Calculate (Basis Set and ECP Configuration)

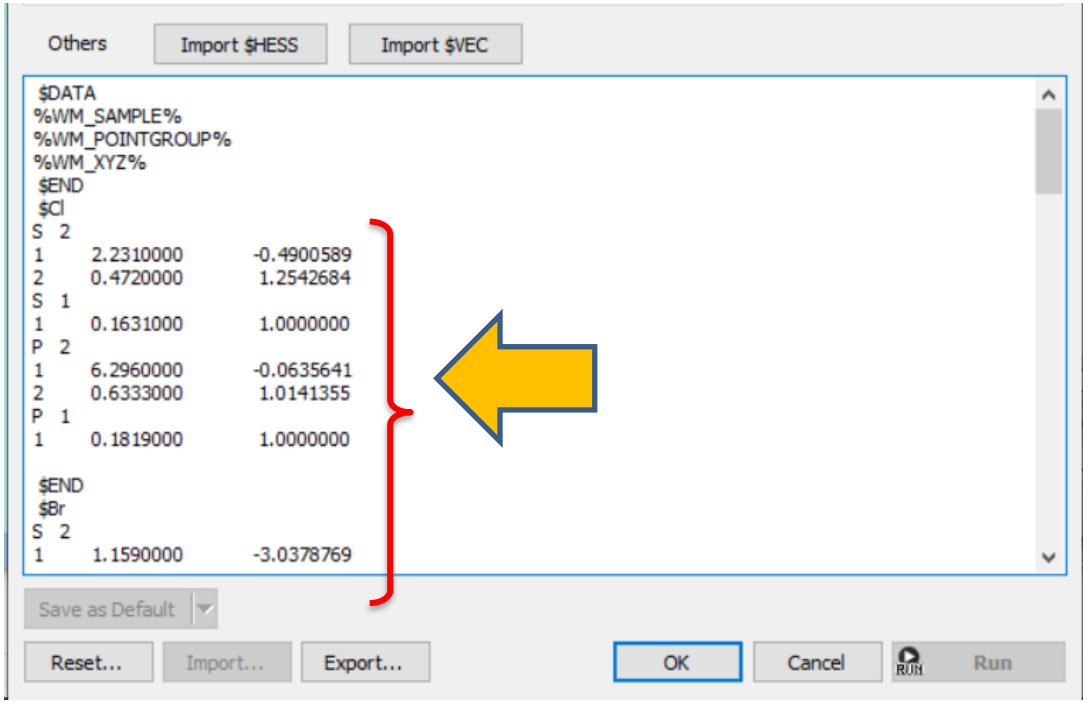
A. In **$BASIS** section's **Others**, enter '`BASNAM(1)=C,Cl,H,H,Br,`'. After BASNAM(1)=, list the basis set keywords for each atom starting from the first, as determined on p.17. Due to GAMESS specifications, a line of computational conditions can only read up to 80 characters, so in this tutorial, we use element symbols as keywords because they are shorter. If the molecular size is large and exceeds 80 characters, please divide the information into multiple lines. Verify the arrangement of atoms in Coordinate Viewer on the right of Main Window.





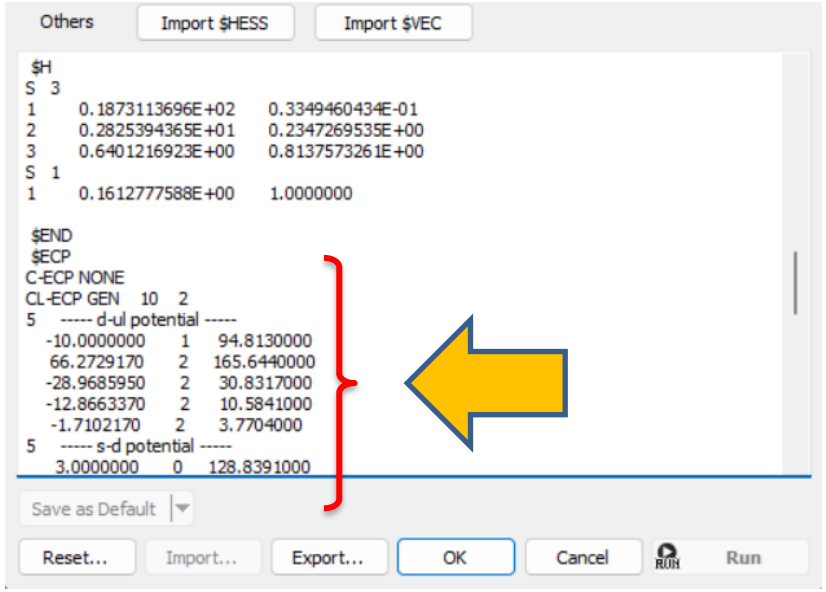
C. Execution of Calculate (Basis Set and ECP Configuration)

A. In **GAMESS Keyword Setup** window, add the basis set information for each element, as modified on page 17, below $END on the fifth line in **Others** section.



C. Execution of Calculate (Basis Set and ECP Configuration)

A. Next, append the ECP information for all atoms after the basis set data in **Others** section. The first line should start with ' $ECP' (with one space at the beginning), and from the second line onwards, enter the data for each atom line by line. For atoms not using ECP, write only one line 'Element name-ECP NONE' (for example, for carbon, write 'C-ECP NONE'). For atoms using ECP, enter the data obtained from p.16. Do not insert blank lines between the data for each atom, and finally, write ' $END' (with one space at the beginning).




```
 $ECP
C-ECP NONE
CL-ECP GEN   10   2
5    ----- d-ul potential -----
   -10.0000000     1    94.8130000
    66.2729170     2   165.6440000
   -28.9685950     2    30.8317000
   -12.8663370     2    10.5841000
    -1.7102170     2     3.7704000
5    ----- s-d potential -----
     3.0000000     0   128.8391000
    12.8528510     1   120.3786000
   275.6723980     2    63.5622000
   115.6777120     2    18.0695000
    35.0606090     2     3.8142000
6    ----- p-d potential -----
     5.0000000     0   216.5263000
     7.4794860     1    46.5723000
   613.0320000     2   147.4685000
   280.8006850     2    48.9869000
   107.8788240     2    13.2096000
    15.3439560     2     3.1831000
H-ECP NONE
H-ECP NONE
```

```
BR-ECP GEN   28   3
4    ----- f-ul potential -----
   -28.0000000     1   213.6143969
  -134.9268852     2    41.0585380
   -41.9271913     2     8.7086530
    -5.9336420     2     2.6074661
4    ----- s-f potential -----
     3.0000000     0    54.1980682
    27.3430642     1    32.9053558
   118.8028847     2    13.6744890
    43.4354876     2     3.0341152
5    ----- p-f potential -----
     5.0000000     0    54.2563340
    25.0504252     1    26.0095593
    92.6157463     2    28.2012995
    95.8249016     2     9.4341061
    26.2684983     2     2.5321764
5    ----- d-f potential -----
     3.0000000     0    87.6328721
    22.5533557     1    61.7373377
   178.1241988     2    32.4385104
    76.9924162     2     8.7537199
     9.4818270     2     1.6633189
$END
```

C. Execution of Calculate (Basis Set and ECP Configuration)

A. In **GAMESS Keyword Setup** window, click **OK**.
B. In **GAMESS Workflow Setup** window, click **OK**.
C. In **Job Setting** window, click **Run** to start the calculation.

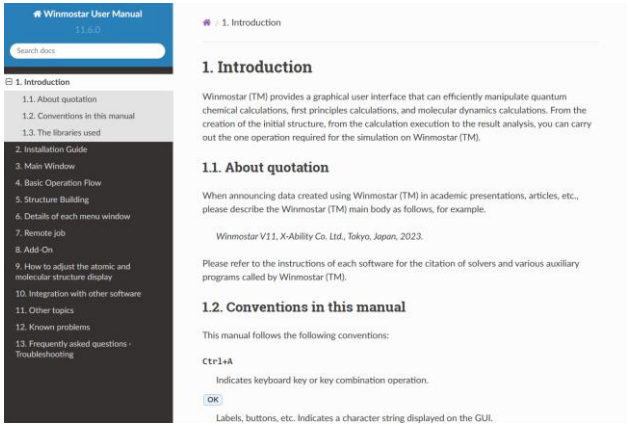
Supplementary

A. If there are multiple atoms of the same element using ECP, write the ECP data only for the first atom; for the second and subsequent atoms, only enter 'Element name--ECP'. For example, for CH_2Cl_2 (where the 2nd and 5th atoms are Cl using LANL2DZ), it would be as follows:

```
 $ECP
C-ECP NONE
CL-ECP GEN    10    2
5     ----- d-ul potential -----
   -10.0000000      1     94.8130000
    66.2729170      2    165.6440000
   -28.9685950      2     30.8317000
   -12.8663370      2     10.5841000
    -1.7102170      2      3.7704000
5     ----- s-d potential -----
     3.0000000      0    128.8391000
    12.8528510      1    120.3786000
   275.6723980      2     63.5622000
   115.6777120      2     18.0695000
    35.0606090      2      3.8142000
6     ----- p-d potential -----
     5.0000000      0    216.5263000
     7.4794860      1     46.5723000
   613.0320000      2    147.4685000
   280.8006850      2     48.9869000
   107.8788240      2     13.2096000
    15.3439560      2      3.1831000
H-ECP NONE
H-ECP NONE
CL-ECP
 $END
```

Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult Frequently asked questions.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through Contact page, detailing the steps to reproduce the issue and attaching any generated files at that time.