M winmostar tutorial GAMESS Chemical Reaction Analysis (Heat of Formation and Activation Energy)

V11.5.6

5 February 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 <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual.</u>
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
 - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
 - <u>Winmostar Basic Training Session</u>: 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.
 - <u>Individual Training Session</u>: 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 <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

Calculate the heat of formation and activation energy for the following two chemical reactions at the B3LYP/6-31G* level.

- A. For cases where the transition state structure can be somewhat predicted: Vacuum Diels-Alder reaction of butadiene and ethylene. $(C_4H_6 + C_2H_4 \rightarrow C_6H_{10})$
- B. For cases where the initial structure of the transition state is calculated by another method: $S_N 2$ reaction of bromoethane and Cl- ion in DMSO solution ($CH_3CH_2Br + Cl^- \rightarrow CH_3CH_2Cl + Br^-$)

Note:

• The initial structure for the transition state calculation of the S_N2 reaction will use the results from MOPAC transition state calculations. Please complete the content of MOPAC (Transition State and IRC) tutorial beforehand.



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.



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. Diels-Alder Reaction between Butadiene and Ethylene

A. Calculation Procedure

Perform structure optimization calculations for the reactants (C_4H_6 , C_2H_4), the product (C_6H_{10}), and the transition state, and determine their respective energies. From the summation and subtraction of these energies, calculate the heat of formation and the activation energy for this reaction.



A. Calculation Procedure

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

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.
- B. Enter 'Diels_Alder' for **Project name** and click **Save**.

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	Element H 1 ~	+ 🔍 🔍 🖓 💠	+H % % Fragment -CH3 V
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			Create new project (Import File)
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C) UserData folder	C:¥winmos11¥UserData	¥
Description (Or	ational)		
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			Save

From Label/Charge menu at the top right of Main Window, select Number & Element to display the names of each atom in Viewport.





- A. Select –**C2H3** from **Fragment** at the top of Main Window and click **Replace** once.
- B. Click on **4H** atom (yellow) so it is marked with a thick red circle, then click **Replace** again to create cis-butadiene.



- A. Select **GAMESS** from **Solver** and click **Workflow Setup**.
- B. In GAMESS Workflow Setup window, click OK.
- By default, the structure optimization is carried out at the B3LYP/6-31G* level.
- If you want to reduce computational accuracy to finish calculations more quickly, change Basis set to STO-3G.

If you switch to STO-3G, it is necessary to run not only butadiene but all molecules in this Diels-Alder reaction at the STO-3G level.



A. Change Prefix for working folder name to 'butadiene'.

C. Click **Run**.

- B. Set # of MPI Procs according to the number of cores on your computer. When running on a remote machine, also configure settings such as the profile.
 - M Job Setting X Run local job Program GAMESS (1) C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe Path O Run remote job Remote Server Profile pbs_example gamess (Default) New -I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23:50:00 Control... Do not run job after saving files Parallelization # of Threads / MPI Proc 1 # of MPI Procs 1 Prefix for working folder budadiene Descriptions for jobs (Optional) Run

- A. After the calculation is complete and the status of the working folder changes to **END** or **END(-)**, click **Log (Extracted)** in Action.
- B. In **Extracted Log** window, copy the number after E= at the end of the last NSERCH line into Excel or a similar program. This value (-155.98651 Hartree) represents the energy of butadiene in its stable structure.
- C. Close **Extracted Log** window.

♦ Project			
Working Folders (Diels_Alder)	Options ▼		
		FINAL R-B3LYPV1R ENERGY IS -155.9865123817 AFTER 8 ITERATIONS NSERCH: 15 E= -155.9865123817 GRAD. MAX= 0.0004731 R.M.S.=	0.0001593
⊙ budadiene1_6₩S_OPT	END	FINAL R-B3LYPV1R ENERGY IS -155.9865133141 AFTER 8 ITERATIONS NSERCH: 16 E= -155.9865133141 GRAD. MAX= 0.0002712 R.M.S.=	0.0000903
		FINAL R-B3LYPV1R ENERGY IS -155.9865136514 AFTER 8 ITERATIONS NSERCH: 17 E= -155.9865136514 GRAD. MAX= 0.0001316 R.M.S.= FINAL R-B3LYPV1R ENERGY IS -155.9865137283 AFTER 8 ITERATIONS NSERCH: 18 E= -155.9865137283 GRAD. MAX= 0.0000941 R.M.S.=	0.0000403
		**** FOULLIBRIUM GEOMETRY LOCATED *****	0.0000272
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Action (ethylene2_GMS_OPT)		<	
Coordinate (Initial)		Export	Close
🔁 Coordinate (Final), Charge &	Dipole		
Log			
Log (Extracted)			
Animation			
•			

C. Structure Optimization Calculation (Ethylene)

- A. Click Edit | Reset Structure to revert to the initial C-H state.
- B. Select **-C2H3** from **Fragment** at the top of Main Window, then click **Replace** once to create Ethylene.



C. Structure Optimization Calculation (Ethylene)

- A. Click **Morkflow Setup**).
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In **GAMESS Workflow Setup** window, click **OK**.
- D. In **Job Setting** window, change **Prefix for working folder name** to 'ethylene' and click **Run**.
- If you want to reduce the calculation accuracy to finish the calculation faster, change Basis set to STO-3G.

		Run local job	
GAMESS Workflow Setup	- 🗆 X	Program GAMESS (1) V	
		Path C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.e	xe
eset Optimize V	# of Jobs: + 1 -	O Run remote job	
En	able parameter/structure scan Config	Remote Server Profile pbs_example \lor Config	
(st job		Solver gamess V	
		Template Script (Default) V New	Edit.
ask Optimize V Method B3LTP(same as Gaus: V	basis set 6-31G*	Option I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23	:50:00
Charge 0 V Multiplicity 1 V	Solvent [None] V	Test Connection	
	Detaile	Information	
	Details		
		Do not run job after saving files	
Reset Import 🔽 Export	ок	Parallelization	
		# of MPI Procs 1 v # of Threads / MPI c 1 v	
		Prefix for working folder ethylene	
		Descriptions for jobs (Optional)	
		Run Run	$\boldsymbol{\boldsymbol{X}}$
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WINMOSTAT Copyright 2	008-2023 X-Ability Co., Ltd	I. Powered by ChatGPT-4	

C. Structure Optimization Calculation (Ethylene)

- A. After the calculation is complete and the status of the working folder changes to END or END(-), click Log (Extracted) in Action.
- B. In **Extracted Log** window, copy the number after E= at the end of the last NSERCH line into Excel or a similar program. This value (-78.58746 Hartree) represents the energy of Ethylene in its stable structure.
- C. Close Extracted Log window.

♥ Project			
Working Folders (Diels_Alder)	Options ▼	FINAL R-B3LYPV1R ENERGY IS -78.5870120987 AFTER 16 ITERATIONS NSERCH: 0 E= -78.5870120987 GRAD. MAX= 0.0124467 R.M.S.= FINAL R-B3LYPV1R ENERGY IS -78.5874254653 AFTER 10 ITERATIONS	0.0061245
budadiene1_GMS_OPT • ethylene2_GMS_OPT	END END	NSERCH: 1 E= -78.5874254653 GRAD. MAX= 0.0023467 R.M.S.= FINAL R-B3LYPV1R ENERGY IS -78.5874614846 AFTER 8 ITERATIONS NSERCH: 2 E= -78.5874614846 GRAD. MAX= 0.0005779 R.M.S.= FINAL R-B3LYPV1R ENERGY IS -78.5874675865 AFTER 8 ITERATIONS NSERCH: 3 E= -78.5874675865 GRAD. MAX= 0.0000325 R.M.S.=	0.0003426
		***** EQUILIBRIUM GEOMETRY LOCATED ***** EXECUTION OF GAMESS TERMINATED NORMALLY 07:56:59 29-JAN-2024	
Action (ethylene2_GMS_OPT)		< Export	Close
Coordinate (Final), Charge & I Cog Log Log Animation	Dipole		

D. Structure Optimization Calculation (Cyclohexene)

- A. Click Edit | Reset Structure.
- B. Select -CYCLOHEXYL(EQ) from Fragment at the top of Main Window, then click Replace once.
- C. Click sequentially on the atoms **13H** and **15H** (yellow), and then click **Delete Atom** twice.
- D. Click **Quick Optimization** to create Cyclohexene.



D. Structure Optimization Calculation (Cyclohexene)

- A. Click 🗹 (Workflow Setup) .
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In **GAMESS Workflow Setup** window, click **OK**.
- D. In **Job Setting** window, change **Prefix for working folder name** to 'cyclohexene' and click **Run**.

Job Setting
 Run local job

• If you want to reduce the calculation accuracy to finish the calculation

faster, change Basis set to STO-3G.

		Program	GAMESS (1) V
M GAMESS Workflow Setup	- 🗆 X	Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe
Preset Optimize V	# of Jobs: + 1 -	O Run remote job	
En	nable parameter/structure scan Config	Remote Server Profile	pbs_example V Config
		Solver	gamess 🗸
1st job	+ -	Template Script	(Default) V New Edit
Task Optimize V Method B3LYP(same as Gaus: V	Basis set 6-31G*	Option	+ nodes=1:ppn=%WM_NUM_PROC% + walltime=23:50:00
Charge 0 V Multiplicity 1 V	Solvent [None] ~		Test Connection ਰਿੱਊ Control
	Details	Information	
		Do not run job after saving	g files
Reset Import 🚩 Export	ОК	Parallelization # of MPI Procs 1 ~	# of Threads / MPI D
		Prefix for working folder Descriptions for jobs (Optiona	cydohexene
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D. Structure Optimization Calculation (Cyclohexene)

- A. After the calculation is complete and the status of the working folder changes to **END** or **END(-)**, click **Log (Extracted)** in Action.
- B. In **Extracted Log** window, copy the number after E= at the end of the last NSERCH line into Excel or a similar program. This value (-234.64826 Hartree) represents the energy of Ethylene in its stable structure.
- C. Close Extracted Log window.

➢ Project		
orking Folders (Diels_Alder)	Options 🔻	
		NSERCH: 17 E= -234.6482643680 GRAD. MAX= 0.0001959 R.M.S.=
budadiene1_GMS_OPT	END	NSERCH: 18 E= -234.6482648038 GRAD. MAX= 0.0001802 R.M.S.=
ethylene2_GMS_OPT	END	FINAL R-B3LYPV1R ENERGY IS -234.6482650020 AFTER 8 ITERATIONS
⊙ cyclohexene3_6MS	END	FINAL R-B3LYPV1R ENERGY IS -234.6482650797 AFTER 8 ITERATIONS
		NSERCH: 20 E= -234.6482650797 GRAD. MAX= 0.0000707 R.M.S.=
		***** EQUILIBRIUM GEOMETRY LOCATED *****
		EXECUTION OF GAMESS TERMINATED NORMALLY THU APP 21 16:40:10 2022
		<
Action (cyclohexene3_GMS_OPT)		
ᅼ Coordinate (Initial)		Export
ᅼ Coordinate (Final), Charge &	Dipole	
🚾 Log		
Log (Extracted)		

- A. Click Edit | Reset Structure.
- B. Select -

C6H5 from **Fragment** at the top of Main Window, then click **Replace** once to create Benzene.

- C. Rotate the molecule by clicking and dragging near the molecule (light blue) until it aligns as shown in the bottom-right figure.
- D. Click on the atoms **7C**, **5C**, **4C** in the order.



- A. Press and hold **Ctrl** and click on the atoms **1C**, **2H**, **4C**, and **8H** to select them as a group, indicated by blue circles.
- B. Rotate the molecule by clicking and dragging near the molecule to align it as shown in the central figure.
- C. Click Modify Selected Group and select Translate (Mouse).



- A. Consider the overlap of π orbitals between two molecules in the Diels-Alder reaction and position the carbon skeletons of butadiene and ethylene accordingly. Drag the screen to move the C₂H₂ part until the Length is approximately 2.0 Å and the Angle is about 100°, as shown in the lower-left figure. Since the goal is to create an initial structure for the transition state, the values do not need to be matched precisely.
- B. Click near the molecule once to deselect the group selection (blue circles), then click and drag near the molecule again to rotate it as shown in the central lower figure.
- C. While holding **Ctrl**, click on atoms **1C**, **3C**, **4C**, and **5C** to select them as a group (blue circles), and then click **Add Hydrogen to Marked Atom** once. This completes the initial structure for the transition state calculation. In GAMESS, only atomic coordinates are used, and bond information is not utilized so it's rolt a problem if a bond remains between C_4H_6 and C_2H_4 .



- A. Click 🗹 (Workflow Setup) .
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In GAMESS Workflow Setup window, change Preset to IR + Optimize(TS) + IR.
- D. In **Job Setting** window, change **Prefix for working folder name** to 'ts' and click **Run**.

Iob Setting

If you want to reduce the calculation accuracy to finish the

calculation faster, change Basis set to STO-3G.

GAMESS Workflow Setup	- 🗆 ×	Run local job	
		Program	GAMESS (1) V
reset IR + Optimize(TS)+IR V	# of Jobs: + 2 -	Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe
Optimize Energy Enal IR	ble parameter/structure scan Config	O Run remote job	
TDDFT Optimize(TS)	+ -	Remote Server Profile	pbs_example V Config
Task Optimize(TDDFT) Optimize+IR eas Gaus: ~	Basis set 6-31G* \checkmark	Solver	gamess 🗸
Optimize + IR + Raman Charge Optimize + TDDFT	Solvent [None] ~	Template Script	(Default) V New Edit
Optimize +IR + TDDFT Optimize +IR + Raman + TDDFT		Option	-I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23:50:00
IR + Optimize(TS)+IR IR + Optimize(TS)+IR + IRC RESP Charge Optimize +RESP Charge	Details		Test Connection
Add preset Edit preset list	+ -	Information	
barge 0 V Multiplicity 1 V	Solvent [None]	Do not run job after saving	files
	fi recircit	Parallelization	
Same conditions as previous job	Details	# of MPI Procs 1 V	# of Threads / MPP Proc 1
		Prefix for working folder	ts
Reset Import 🔽 Export	ок	Descriptions for jobs (Optional)	
			Run Run
	1		

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- A. After the calculation is completed and the status of the work folder changes to **END** or **END(-)**, click on the folder 'ts5_GMS_OPTTS-IR' in Working folders, and then click **IR/Raman** in Action.
- B. In **IR Spectrum** window, if there is only one negative value (appearing as negative but actually an imaginary value) in the list of vibration frequencies at the top left, it signifies that the transition state structure has been obtained.
- C. After clicking on the first peak, click **Animation**. If the vibration between the carbons of butadiene and ethylene is displayed, it indicates that the desired transition state has been achieved.



- A. Click Log (Extracted) in Action.
- B. In Extracted Log window, copy the number after E= at the end of the last NSERCH line into Excel or a similar program. This value (-234.54391 Hartree) represents the energy of Ethylene in its stable structure.
- C. Close Extracted Log window.

➢ Project	
Working Folders (Diels_Alder)	Options 🔻
Name	Status
budadiene1_GMS_OPT	END
ethylene2_GMS_OPT	END
cyclohexene3_GMS_OPT	END
ts4_GMS_FR	END
	R END
<	>
Action (tes GMS_OPTTS-IP)	
Coordinate (Initial)	
Coordinate (Final), Charge	& Dipole
🚾 Log	
Log (Extracted)	

F. Reaction Energy Calculation

The calculation is performed as follows. (Heat of Reaction) = (Energy of Products) - (Energy of Reactants) (Activation Energy) = (Energy of Transition State) – (Energy of Reactants) This reaction is exothermic by 46.6 kcal/mol, and the activation energy required to overcome the transition state is 18.9 kcal/mol.



B. SN2 Reaction of Bromoethane with Cl- Ion

A. Calculation Procedure

Perform structure optimization calculations for the reactants (CH_3CH_2Br , Cl^-), products (CH_3CH_2Cl , Br^-), and the transition state in DMSO solution, a non-protic polar solvent, using the PCM method. The energies obtained from these calculations are used to compute the heat of reaction and activation energy for the reaction. Note:

 The initial structure for the transition state calculation should utilize results from MOPAC calculations. Therefore, it's necessary to complete MOPAC (Transition State & IRC Calculation) tutorial in advance.



A. Calculation Procedure

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.
- B. Enter 'SN2' for **Project name** and click **Save**.

		🞯 Winmostar (PF	REMIUM) V11.5.	5										
		<u>File E</u> dit Select	<u>V</u> iew <u>Q</u> M	<u>M</u> D <u>S</u> olid	<u>A</u> dd-On	Tools	<u>W</u> indow	<u>H</u> elp						
		🕞 🚘 🕶 [B <mark></mark> () B R	e 🖻 🝷	1	0	f y	Sol	ve				
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					ß	Crea	te New Pi	roject (3D)	🗸					
					Q	Cre	ate new pr	oject (2D)						
		N. Destant			3	Creat	e new proje	ect (SMILES)						
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Project nam	e		SN2											
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		ened folder	C:¥winmos	11¥UserDa	ta									
	OUserDat	a folder	C:¥winmos	11¥UserDa	ta¥									
Description	(Optional)												1	
											Save			

B. Structural Optimization Calculation (Bromethane)

- A. Select **-CH3** from **Fragment** at the top of Main Window and click **Replace** twice to create ethane.
- B. With the **H** atom (yellow) marked with a thick red circle, select **Br 35** from **Element for editing operations** at the top of Main Window.
- C. Click **Change Element** to create bromoethane.



B. Structural Optimization Calculation (Bromethane)

- A. Click \mathbf{M} (Workflow Setup).
- B. In **GAMESS Workflow Setup** window, change **Solvent** to **DMSO (PCM)** and click **OK**.
- C. In **Job Setting** window, **Prefix for working folder name** to "bromoethane" and click **Run**.

 \cdot If you want to finish the calculation faster by reducing the calculation accuracy, change Basis set to STO-3G.

If you change to STO-3G, it's necessary to perform all the molecules involved in this SN2 reaction at STO-3G as well.

			Run local job	
GAMESS Workflow Setup		- 🗆 ×	Program	GAMESS (1) V
	(16 B		Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe
Preset Optimize	 (modified) 	# of Jobs: + 1 -	○ Run remote job	
	Enable param	eter/structure scan Config	Remote Server Profile	pbs_example v Config
			Solver	gamess 🗸
1st job		+ -	Template Script	(Default) V New Edit
Task Optimize ~ Method	B3LYP(same as Gaus: V Basis se	t 6-31G* ~	Option	-I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23:50:00
Charge 0 V Multiplie	ity 1 V Solvent	DMSO (PCM)		Test Connection
		C6H5Cl (PCM) CH5Cl (SMD) CH3NO2 (PCM) CH3NO2 (PCM) CH3NO2 (PCM)	Information	-
		C6H12 (PCM)	Do not run job after savi	ng hies
		C6H12 (SMD)	Parallelization	
Reset Import 🔻 Export		ANILINE (SMD)	# of MPI Procs 1	# of Threads / MPI Proc
±	<u> </u>	ACETONE (PCM) ACETONE (SMD)	Prefix for working folder	bromoethane
	BBr	THF (rCM) THF (SMD) DMSO (PCM) DMSO (SMD)	Descriptions for jobs (Option	
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B. Structural Optimization Calculation (Bromethane)

- A. After the calculation has finished and the status of the working folder changes to END or END(-), click Log in Action.
- B. Copy the value from the line "TOTAL FREE ENERGY IN SOLVENT" found near the end of the displayed log into Excel or similar.

➢ Project	
Working Folders (SN2)	Options 🔻
Name	Status
● bromoethane1_6MS	. END
Action (bromoethane1_GMS_OP	די)
🖰 Coordinate (Initial)	
🔁 Coordinate (Final), 🗲 roe	<u>& Dipo</u> le
🚾 Log	
Log (Extracted)	
Animation	
🗲 MO & Charge	
Show in Explorer	

C. Structural Optimization Calculation (Chloroethane)

- A. Click **Br** atom of bromoethane to mark it with a thick red circle.
- B. From Element for editing operations at the top of Main Window, select Cl 17.
- C. Click **Change Element** to create chloroethane.



C. Structural Optimization Calculation (Chloroethane)

- A. Click **(Workflow Setup**).
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In GAMESS Workflow Setup window, with Solvent set to DMSO(PCM), click OK.
- D. In **Job setting** window, change **Prefix for working folder name** to "chloroethane" and click Run.
- \cdot If you want to speed up the calculation by reducing the calculation accuracy, change Basis set to STO-3G.

		🚳 Job Setting	- 🗆
GAMESS Workflow Setup	– 🗆 ×	● Run local job	
		Program GAMESS (1) V	
eset Optimize v (modified)	# of Jobs: + 1 -	Path C:¥Users¥Public¥gamess-64¥games	s.2023.R1.intel.exe
Enable p	arameter/structure scan	◯ Run remote job	
= P		Remote Server Profile pbs_example	 ✓ Config
t job	+ -	Solver gamess	\sim
k Ontimize V Method B3LYP/same as Gauss V Ba	sis set 6-316*	Template Script (Default)	V New Edit
		Option -I nodes=1:ppn=%WM_NUM_PROC	% -l walltime=23:50:00
arge 0 V Multiplicity 1 V So	lvent DMSO (PCM) 🗸	Test Connection	Control
	Details	Information	
		Do not run job after saving files	
Land Toront - Toront		Parallelization	
eset Import	OK	# of MPI Procs 1	×
		Prefix for working folder chloroethane	
		Descriptions for jobs (Optional)	
			Rin Run
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C. Structural Optimization Calculation (Chloroethane)

- A. After the calculation has finished and the status of the working folder changes to END or END(-), click Log in Action.
- B. Copy the value from the line "TOTAL FREE ENERGY IN SOLVENT" found near the end of the displayed log into Excel or similar.

अ Project	
Working Folders (SN2)	Options V
Name	Status
bromoethane1 GMS OPT	END
⊙ chloroethane2_6≝	END
Action (chloroothano? CMS_ODT)	
Coordinate (Initial)	
Coordinate (Final), Charles	Dipole
🔤 Log	
Log (Extracted)	
Animation	
📑 MO & Charge	
Show in Explorer	

D. Energy Calculation (Cl Ion)

- A. Click Edit | Reset Structure.
- B. Click on the right **H** atom (yellow) to mark it with a thick red circle, then click **Delete Atom** to leave only the **C** atom.
- C. From Element for editing operations at the top of Main Window, select Cl 17.
- D. Click **Change Element** to change it to a **Cl** atom.



D. Energy Calculation (Cl Ion)

- A. Click **(Workflow Setup**).
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In **GAMESS Workflow Setup** window, with **Solvent** set to **DMSO(PCM)** and **Charge** set to **-1**, and then click **OK**.
- D. In **Job setting** window, change **Prefix for working folder name** to "cl" and click **Run**.
- \cdot If you want to speed up the calculation by reducing the calculation accuracy, change Basis set to STO-3G.

	 Run local job 	
	Program	GAMESS (1) V
	Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe
Config	○ Run remote job	
	Remote Server Profile	pbs_example \checkmark Config
-	Solver	gamess 🗸
	Template Script	(Default) V New Edit
~	Option	-I nodes=1:ppn=%WM_NUM_PROC% -I walltime=23:50:00
\sim		Test Connection
	Information	
	Do not run job after saving	fles
	Parallelization	4
	# of MPI Procs 1 ~	# of Thread PI Proc 1 V
	Prefix for working folder	
	Descriptions for jobs (Optional	
		Path Config Confi

D. Energy Calculation (Cl Ion)

- A. After the calculation has finished and the status of the working folder changes to END or END(-), click Log in Action.
- B. Copy the value from the line "TOTAL FREE ENERGY IN SOLVENT" found near the end of the displayed log into Excel or similar.

➢ Project	
Working Folders (SN2)	Options ▼
Name	Status
bromoethane1_GMS_OPT	END
chloroethane2_GMS_OPT	END
⊙ c13_6₩S_0PT	END
Antine (-12 CMC ODT)	
Action (CI3_GMS_OPT)	
Coordinate (Initial)	
Coordinate (Final), Chrige &	Dipole
🚾 Log	
Log (Extracted)	
Animation	
HO & Charge	
Show in Explorer	

E. Energy Calculation (Br Ion)

- A. With **CI** atom displayed, select **Br 35** from **Element for editing operations** at the top of Main Window.
- B. Click Change Element to change it to a Br atom.





E. Energy Calculation (Br Ion)

- A. Click **(Workflow Setup**).
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In **GAMESS Workflow Setup** window, with **Solvent** set to **DMSO(PCM)** and **Charge** set to **-1**, and then click **OK**.
- D. In **Job setting** window, change **Prefix for working folder name** to "br" and click **Run**.

M Job Setting

• If you want to speed up the calculation by reducing the calculation accuracy, change Basis set to STO-3G.

		•	
GAMESS Workflow Setup	- 🗆 X	● Run local job	
		Program GAMESS (1) V	
optimize v (modified)	# of Jobs: + 1 -	Path C:¥Users¥Public¥gamess-64¥gamess.2023.R	intel.exe
Enable	parameter/structure scan Config	O Run remote job	
		Remote Server Profile pbs_example V Co	onfig
job	+ -	Solver gamess V	
Optimize V Method B3LYP(same as Gaus: V	asis set 6-31G* V	Template Script (Default) V	lew Edit
		Option I nodes=1:ppn=%WM_NUM_PROC% -I wallt	me=23:50:00
rge -1 V Multiplicity 1 V	olvent DMSO (PCM) V	Test Connection	Control
		Information	
	Details		
		Do not run job after saving files	
asat Import 🗶 Evport		Parallelization	
		# of MPI Procs 1 v # of Threads PI Proc 1 v	
	•	Prefix for working folder br	
		Descriptions for jobs (Optional)	
			tun
• -			
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		- /	

- 🗆 X

E. Energy Calculation (Br Ion)

- A. After the calculation has finished and the status of the working folder changes to END or END(-), click Log in Action.
- B. Copy the value from the line "TOTAL FREE ENERGY IN SOLVENT" found near the end of the displayed log into Excel or similar.

ders (SN2) Options ▼ Status thane1_GMS_OPT END	ns ▼
Status thane1_GMS_OPT END	
thane1_GMS_OPT END	
ethane2_GMS_OPT END #S_OPT END	
MS_OPT END	
GMS_OPT) late (Initial) late (Final) late (F	

Assuming MOPAC (Transition State & IRC) tutorial has already been completed.

- A. Select File | Import File.
- B. Enter "ts.arc" (the file name of the transition state calculation result from MOPAC (Transition State & IRC) tutorial) and click **Open**.
- C. If prompted with "Do you want to dixcard the current content ana load a new structure?", click **Discard and Import**.

<u>F</u> ile	<u>E</u> dit Select <u>V</u> iew <u>Q</u> M <u>M</u> D <u>S</u> olic	
D	New Project Ctrl+Alt+N	
	New Project with Current Model	
6	Open Project Ctrl+Alt+O	
	Open Recent Project	Import File X
	Project	•
	New File Ctrl+N	Do you want to discard the current content and load a new structure?
	Open File Ctrl+O	
	Open Recent File	Discard and import
S	Reload	
B	Save File Ctrl+S	
₽	Save File As Shift+Ctrl+S	
	Close Ctrl+W	
ц,	Import File	
	Import Recent File	•
	Import	

- A. Click \mathbf{M} (Workflow Setup).
- B. If 'Do you want to continue from previous run?' appears, click No.
- C. In **GAMESS Workflow Setup** window, change **Preset** to **IR + Optimize(TS)+IR**. Change **Charge** to **-1** and **Solvent** to **DMSO(PCM)** in **1st job**, then click **OK**.
- D. In **Job Setup** window, change **Prefix for working folder name** to "ts" and click **Run**.
- If you wish to reduce the calculation accuracy for a quicker completion, change Basis set to STO-3G.

		Run local job			
GAMESS Workflow Setup	- 🗆 X	Program	GAMESS (1) V		
Preset IR + Optimize(TS)+IR ied)	# of Jobs: + 2 -	Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe		
Enable	e parameter/structure scan Config	O Run remote job			
		Remote Server Profile	pbs_example V Config		
Tark ID Method D21/20/ama as Cause of L	+ -	Solver	gamess 🗸		
BSLTP(same as Gause V	basis set 6-316- V	Template Script	(Default) V New Edit		
Charge -1 dtiplicity 1 v	Solvent DMSO (PCM)	Option	-l nodes=1:ppn=%WM_NUM_PROC% -l walltime=23:50:00 V		
	C6H50 (PCM) C6H5Cl (SMD) CH3N02 (PCM) CH3N02 (SMD)		Test Connection		
2nd tob	NEPTANE (PCM) C6H12 (PCM) C6H12 (SMD) ANIL INF (PCM)	Information			
Task Optimize(TS)+IR V Method B3LYP(same as Gause V	ANILINE (SMD) ACETONE (PCM) ACETONE (SMD)	Do not run job after savin	g files		
Charge -1 V Multiplicity 1 V	Solvent THF (PCM) THF (SMD)	Parallelization			
Same conditions as previous job Continue from previous job	DMSO (PCM) DMSO (SMD)	# of MPI Procs 1 ~	# of Thread PI Proc 1		
	Details	Prefix for working folder	ts		
		Descriptions for jobs (Optiona			
Reset Import	ок		Refit Run		
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- A. After the calculation ends and the status of the working folder changes to **END** or **END(-)**, click on the "ts6_GMS_OPTTS-IR" folder in Working Folders, then click **IR/Raman** in Action.
- B. If there is only one negative value (shown as a negative value, but technically an imaginary value) in the list of vibrational frequencies at the top left of **IR Spectrum** window, it means that the transition state structure has been obtained.
- C. Click on the first peak and then click **Animation**. If the vibration between Cl⁻, Br⁻, and carbon is displayed, it means the desired transition state has been achieved.



A. Copy the value from the line "TOTAL FREE ENERGY IN SOLVENT" written towards the end of the displayed log into Excel or similar software.

×	Project	
Wo	rking Folders (SN2)	Options V
	Name	Status
	bromoethane1_GMS_OPT	END
	chloroethane2_GMS_OPT	END
_	c13_GMS_OPT	END
_	br 4_GMS_OPT	END
C	ts5_GMS_IR ts6_GMS_OPTTS-IR	END
Act	tion (ts6_GMS_OPTTS-IR)	
e	Coordinate (Initial)	
	Coordinate (Einal) Char	Dipolo
		Dipole
L	og (Extracted)	
F	Animation	
4	MO & Charge	
	IR/Raman	
2	Show in Evalurar	

G. Reaction Energy Calculation

The heat of reaction is calculated as follows: Heat of Reaction = Energy of Products - Energy of Reactants Activation Energy = Energy of Transition State - Energy of Reactants This reaction is exothermic by 6.5 kcal/mol, and the activation energy required to surpass the transition state is 14.3 kcal/mol.

	エネルギー	1	-3113.4621	tate L1	
Reactants	-2653.11658 + (-460.36842) = -3113.48500 Hartree		Hartree	1	
Transition State	-3113.46211 Hartree	rgy			Heat of Reaction
Products	-539.43004 + (-2574.06531) = -3113.49535 Hartree	Ene	\bigvee		
Heat of Reaction	-3113.49535 – (-3113.48500) = -0.01035 Hartree = -6.5 kcal/mol		Reactants -3113.48500 Hartree	Products	Heat of Reaction -6.5 kcal/mol
Activation Energy	-3113.46211- (-3113.48500) = 0.02286 Hartree			-3113.4953 Hartree	5
	=14.3 kcal/mol		Reaction	Coordinate	

G. Reaction Energy Calculation

For reference, we summarize the comparison of the heat of reaction and activation energy in DMSO solution and in vacuum. The energy values in vacuum were calculated by setting **Solvent** to **[None]** in **GAMESS Workflow Setup** window. The heat of reaction differs by about 6 kcal/mol between DMSO solution and vacuum, but the trend is the same. On the other hand, the sign of the activation energy is reversed, with the transition state being more stable than the reactants in vacuum. Comparing the energy of each molecule, the atoms with a charge of -1, Cl- and Br-, are significantly stabilized in solution, but the stabilization in solution for the transition state, which has an overall charge of -1, is smaller compared to Cl- and Br-. For reactions involving molecules with a significant charge imbalance, solvent effects can be important.

	溶液中	真空中
Reactants	-2653.11658 + (-460.36842) = -3113.48500 Hartree	-2653.1127 + (-460.2522) = -3113.3649 Hartree
Transition State	-3113.46211 Hartree	-3113.3782 Hartree
Products	-539.43004 + (-2574.06531) = -3113.49535 Hartree	-539.4263 +(-2573.9586) = -3113.3849 Hartree
Heat of Reaction	-3113.49535 – (-3113.48500) = -0.01035 Hartree = -6.5 kcal/mol	-3113.3849 - (-3113.3649) = -0.0200 Hartree = -12.6 kcal/mol
Activation Energy	-3113.46211- (-3113.48500) = 0.02286 Hartree = 14.3 kcal/mol	-3113.3782 - (-3113.3649) = -0.0133 Hartree = -8.3 kcal/mol

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