M winmostar tutorial GAMESS Bimolecular Calculations (Dispersion Force Corrections)

V11.6.5

14 March 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

 Traditional methods like HF or conventional DFT (B3LYP, PBE, etc.) cannot handle dispersion forces (also known as weak interactions) such as van der Waals forces or π-π interactions. To accurately calculate dispersion forces, methods that correct for dispersion based on interatomic distances (like B3LYP-D3), improved DFT functionals (such as cam-B3LYP, M06 series), or high-precision second-order perturbation (MP2) methods are needed. This tutorial describes the calculation of a benzene dimer using the B3LYP-D3 method.



Preference of Operating Environment

• For GAMESS

FollowtheGAMESSInstallationManualathttps://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en_win.pdfto install GAMESS.

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 prior to V10, it is necessary to display the final structure of the original job each time. However, in project mode, the final structure is automatically carried over.

For basic operation instructions, please refer to GAMESS Fundamentals tutorial.

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

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			+fi 5 % Fragment -CH3 V Repla
	 Recent projects 		
	Project	Status	Project mode
			🕞 Create New Project (3D)
			Create new project (2D)
			S Create new project (SMILES)
	ℽ Project		Create new project (Import File)
	Working Folders	Options V	
New p	roject		
Project na	me	Benzene_dimer	
location	 Arbitrary folder 	C:¥winmos11¥UserData	Brow
	O Last opened folder	C:¥winmos11¥UserData	
	O UserData folder	C:¥winmos11¥UserData	¥
	O Users¥Public folder	C:¥Users¥Public¥	
Description	(Optional)		

- A. Select **-C6H5** from **Fragment** at the top of Main Window, and click **Replace** once to create benzene.
- B. Click **File | Export File**, enter 'benzene' as the file name, and click **Save**. When 'Successfully exported benzene.wmm' is displayed, click **OK**. This completes the saving of this benzene structure file.





- A. Hold **Ctrl** and drag over the entire benzene to select all atoms as a group.
- B. Click **(Modify Selected Group)** and select **Translate(Numerical)**.
- C. In **Translate Group** window, enter **4.0** in **Z** field and click **OK**.



- A. Click File | Import File, select 'benzene.wmm' file saved in p.7, and click Open.
- B. When prompted with 'Do you want to discard the current content and load a new structure?', click **Append file**.
- C. Click **(Align View to X-Axis)** to confirm that the benzene dimer has been successfully created.



B. Execution of Calculate

- A. Select **GAMESS** from **Solver** and click **Workflow Setup**.
- B. In GAMESS Workflow Setup window, change Method to B3LYP-D3 (same as Gaussian).
- C. Click **OK**.
- To speed up the calculation by reducing accuracy, change **Basis set** to **STO-3G**.

	W GAMESS Workflow Setup	- 🗆 X
Solver GAMESS	Preset Optimize	# of Jobs: + 1 - er/structure scan Config
Repla GAMESS Gaussian Tempo LAMMPS Gromacs Quantum ESPRESSO Towhee	1st job Task Optimize Method B3LYP-D3(same as Gz Basis set Charge 0 Multiplicity B3LYP(same as Gaussian) B3LYP-D3(same as Gaussian) B3LYP-D3(same as Gaussian) B3LYP-D3(same as Gaussian) B3LYP-D3(same as Gaussian) B3LYP-D3(original) B3LYP-D3(original) B3PW91 PBE PBE PBE0 wB97X wB97X-D	+ - 6-31G* ~ Details
	Reset Import V Export M06 M06-2X	ок

B. Execution of Calculate

- A. Set the # of MPI Procs according to the number of cores in your computer. When running on a remote machine, also set up profiles and other settings.
- B. Click Run.

🞯 Job Setting			_		×
Run local job					
Program	GAMESS (1) \vee				
Path	C:¥Users¥Public¥gamess-64¥gamess.2023.R1.intel.exe				
○ Run remote job					
Remote Server Profile	pbs_example	\sim	Config		
Solver	gamess	\sim			
Template Script	(Default)	\sim	New	Edit	
Option	-I nodes=1:ppn=%WM_NUM_PR(DC% -	walltime=23:50:	:00	\sim
	Test Connection		Ê₽ Control		
Information					
Do not run job after savin	g files				
Parallelization					
# of MPI Procs 1 ~	# of Threads / MPI Proc 1	~			
Prefix for working folder	work				
Descriptions for jobs (Optiona	al)				
			Run		

C. Computational Analysis

- A. After the calculation has finished and the status of the work folder changes to **END** or **END(-)**, click **Animation** in **Action** at the bottom right of Main Window to display the results of the structure optimization calculation in Animation area.
- B. Click **I**ay) button to play the animation and display the final optimized structure.

℅ Project	
Working Folders (Benzene_dimer)	Options ▼
• work1_6MS_0PT	END
Action (work1_GMS_OPT)	
Action (work1_GMS_OPT)	
Action (work1_GMS_OPT) Coordinate (Initial)	Dipole
Action (work1_GMS_OPT) Coordinate (Initial) Coordinate (Final), Charge & D Log	Dipole
Action (work1_GMS_OPT) Coordinate (Initial) Coordinate (Final), Charge & D Log Log Log Log	Dipole
Action (work1_GMS_OPT) Coordinate (Initial) Coordinate (Final), Charge & D Log Log Log Log Animation	Dipole
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➢ Animation				
 			Reload	Options ▼
Speed				Open Viewer
NSERCH= NSERCH= NSERCH= NSERCH=	44 Eel= -458.83 45 Eel= -458.83 46 Eel= -458.83 47 Eel= -458.83	353856 Grad= 0 353862 Grad= 0 353861 Grad= 0 353867 Grad= 0	.0002387 .0001227 .0001530 .0000920	~
Frame			48	/ 48
Result	***** EQUILIBR	UM GEOMETRY	LOCATED *	****
Plot C	Column 4	 Custom 	Plot	
$\mathcal{M}_{\mathbf{n}}$				
-458.83	5386700	****	• • • • • • • •	

C. Computational Analysis

A. Click (Align View to X-Axis), then click on two carbon atoms in overlapping positions when viewed from above the benzene rings. Verify that the distance between the planes of the benzene dimer, indicated by the Length value, is approximately 3.7 Å.

• (Comparison) When the structure optimization calculation is performed using **B3LYP** instead of **B3LYP-D3**, as **Method** on p.10, the two benzene molecules become more stable as they move apart, and the energy change becomes negligible at around 6^{A} , at which point the calculation ends.



Supplement: Specifying -D3 with Other Functionals

- A. Click **Details** in **GAMESS Workflow Setup** window.
- B. In **GAMESS Keyword Setup** window, change **DFTTYP** in **\$CONTRL** section to the desired functional.
- C. Click **DFT** tab and change **IDCVER** in **\$DFT** section to **3**.

	🛛 🚧 GAMESS Keyword Setup - 🗆 🗙
GAMESS Workflow Setup	
reset Optimize V (modified) # of Jobs: + 1	Easy Setup
Enable parameter/structure scan Config	Basic Advanced Z-Matrix DFT MP2 Solvent IRC Comment Preview
1st job + - Task Optimize v Method B3LYP-D3(same as G: v Basis set STO-3G v	SCONTRL ICHARG 0 V MULT 1 V SCFTYP RHF V RUNTYP OPTIMIZE V
Charge 0 V Multiplicity 1 V Solvent [None] V	COORD UNIQUE V MAXIT 200 V NZVAR %NZVAR% V EXETYP V
Details	
Reset Import 🔽 Export OK Cancel	ISPHER NONE V Others
	GAMESS Keyword Setup — ×
	Easy Setup
	Basic Advanced Z-Matrix DFT RC Comment Preview
	Others 1
	\$TDDFT NSTATE V NRAD V NLEB V
M winmostar Copyright 2008-2023 X-,	Ability Co., Ltd. Powered by ChatGPT-4

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.)
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