

Tutorial

This server runs **AutoMeKin** using the **PM7** semiempirical Hamiltonian. To refine the results install the full package: <https://rxnkin.usc.es/index.php/AutoMeKin>

How to use the server:

1. Click on **Login/Register**
- 2a. If you have already registered, enter your **Email** and **Password**
- 2b. Otherwise, click on **Register** and fill out the form
3. Once you logged in, you will see a screen like this:

Id	Description	Status	Graph	Report	Data	Delete
<div> New Job</div> <div>✓ Completed ⚙ Running ⌚ Waiting ⚫ Error ✖ Deleted</div>						

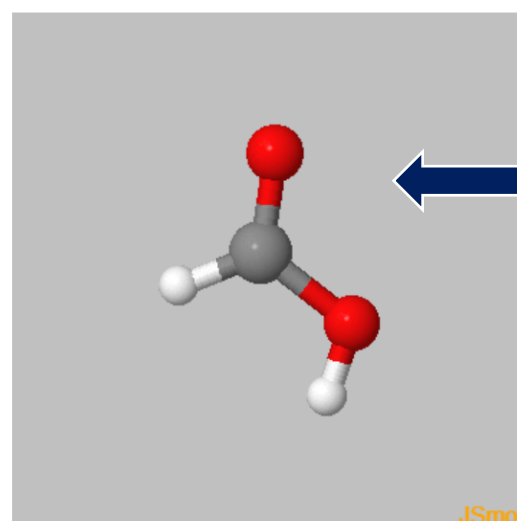
4. Now, to submit a job click on **New Job**

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5. You will be directed to a screen like this where you enter the **details of your job**:

AutoMeKin JOB

Geometry:



1a. The **geometry** file can be loaded by right clicking here. It accepts several formats

NCI(small molecules) Search

1b. Alternatively, you can **search** your molecule **by the name**

XYZ Geometry:

```
5
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.220000
O 1.212436 0.000000 -0.700000
H -0.943102 0.000000 -0.544500
```

1c. **Cartesian coordinates** of the system. If they are changed manually, like adding/removing atoms, update the number of atoms in the first line and hit enter from the end of the last line to update the display above

2. **Charge**

Charge*: 0

3. **Energy or Temperature**

Kinetics: Temperature(K)

Value*: 300

Running Parameters:

Tasks Planned*: 1

Iterations Planned*: 1

cancel

submit your job

6. **submit your job**

Description:

your job description here

5. Short description, e.g.,
name of your system

4. **Tasks and iterations.** The greater these numbers the more MD simulations will be carried out. Be aware of the 5h-limit for your calculations

* Mandatory fields

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6. Now, the screen with the list of jobs will show your job

Id	Description	Status	Graph	Report	Data	Delete
1254	formic acid	⚙️	50%			

🧪 New Job

✓ Completed ⚙️ Running ⌚ Waiting ⚫ Error ✖ Deleted

↑ This is what you have entered in the description

↑ This shows the progress of your job

7. Once your job has finished, you will receive an e-mail and will be able to download the **data** (go to the Wiki and download AutoMeKin's tutorial for details) and **Report**

Id	Description	Status	Graph	Report	Data	Delete
1254	formic acid	✓	📊	📄	📁	🗑️

🧪 New Job

✓ Completed ⚙️ Running ⌚ Waiting ⚫ Error ✖ Deleted

↑ Interactive html with the network, structures and energy profile

↑ Report with a summary of the calculations

↑ Compressed file with all your results