UU Laboratory Journal

Visiting Student

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Contents

September Review

1 Research Topic

From September, I began to do some research in Roland's group with *Molcas 8.0* software and multiconfigurational theory.
The first thing I do is to reproduce the result of Figure 1 in the paper *Chemiluminescence of 1, 2-dioxetane. reaction mechanism uncovered.*[1]
Till now, I summerize the steps to find a resonable reaction path including excited states and corresponding input file of *Molcas 8.0*.
1. Build an initial structure of reactant. Optimize it with force field in Avogadro software. Now copy the .xyz file of reactant to $HOME$/Project/TaskName/.

Bibliography

[1] Luca De Vico, Ya-Jun Liu, Jesper Wisborg Krogh, and Roland Lindh. Chemiluminescence of 1, 2-dioxetane. reaction mechanism uncovered. *The Journal of Physical Chemistry A*, 111(32):8013–8019, 2007. 1

Format Style

1 Format Style

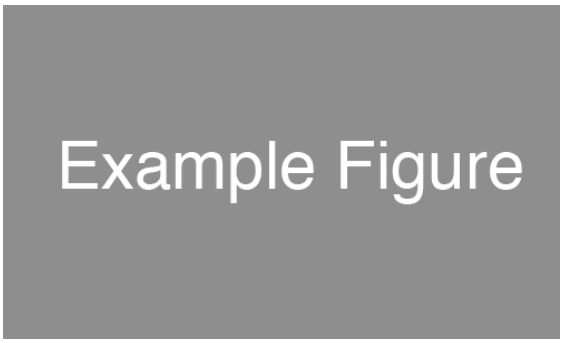

Figure 1: Example figure.

Groups	Treatment X	Treatment Y
1	0.2	0.8
2	0.17	0.7
3	0.24	0.75
4	0.68	0.3

Table 1: The effects of treatments X and Y on the four groups studied.

Table 1 shows that groups 1-3 reacted similarly to the two treatments but group 4 showed a reversed reaction.
This is a bulleted list:

- Item 1
- Item 2
- . . . and so on