GRRM17

GRRM: introduction

GRRM program can search/predict the complete reaction paths, intermediates, and transition states automatically. Development of GRRM program was started on 2002 by Prof. Koichi Ohno and master course student Satoshi Maeda (currently professor at Hokkaido University). In 2009, Dr. Keiji Morokuma, one of the world's leading theoretical chemists, joined the development team. GRRM program has been opening a new world of quantum chemistry. GRRM program is an advanced technology developed in Japan and its functionality is still developong.

Newly installed GRRM17 is a successor version to GRRM11 and GRRM14.
Further details can be found at web page of Institute for Quantum Chemical Exploration,
https://iqce.jp/GRRM/index_e.shtml.

Manual

GRRM17 user manual is available at the following site. (PDF version of mannual is not available.)
https://afir.sci.hokudai.ac.jp/documents/manual/54
Detailed information, input file, utilization of MPI, and interface to other programs (Molpro, GAMESS, Trubomole, SIESTA) can be found at this site. Althoug the manual is available to anyone, tutorial on that site is available only for registered users.

RCCS prepared samples using Gaussian (g09 or g16). Gaussian 09 (g09) may be well-tested than g16 in case of GRRM17.

There are some changes from GRRM14. Please be careful upon migration.
(e.g. You may need to use "ADDF" keyword instead of "GRRM" in GRRM17.)

Sample job scripts

There are some samples under /local/apl/lx/GRRM17/samples directory. "ADDF" samples may need several hours to finish. Please be careful when running them.

RCCS specific problem of SC-AFIR calculation with Gaussian

This problem was solved by the update on Feb 7, 2022.

Citation

You should respect the following official guideline upon publishing your results.
https://afir.sci.hokudai.ac.jp/documents/manual/52