Automated Exploration of Chemical Reaction Pathways

“GRRM” ~Global Reaction Route Mapping~

GRRM developed by K. Ohno and S. Maeda enables one to follow all reaction pathways from an equilibrium (EQ) point towards structures of transition states (TS) surrounding the EQ point. Subsequent downward followings from already found TSs can easily be made as conventional intrinsic reaction coordinate (IRC) followings to reach some EQ points and dissociation channels (DC).

Feature:

Cooperating with quantum chemistry programs such as Gaussian 03/09 and Molpro, GRRM enables one to perform high speed exploration of chemical reaction pathways in 3N-6 dimensional potential energy surfaces (which was previously limited to 4 atoms) by scaled hypersphere search (SHS) method which is based on anharmonic downward distortion (ADD).

Functions:

- Opt. of EQ EQ structures can be optimized by SIRFO and BFGS methods.
- Opt. of TS TS structures can be optimized by SIRFO and Bofill’s methods.
- IRC search IRC can be traced by Page and McLver methods.
- One step TS search An efficient search of via a TS between a reactant and a product without any initial guess.
- Intermediate search Hypersphere-contraction-mode SHS enables one to explore the multi-step reaction pathways
- Excited-state analysis Minimum energy points on seams of crossings can be searched. With a help of Molpro, excited potential energy surfaces can be searched more effectively.

Free of charge for academic users

HPC SYSTEMS Inc. sells GRRM-ready servers

GRRM innovates compound synthesis method by automated exploration of chemical reaction pathways based on precise quantum chemistry calculation.

GRRM job management by a batch job system

Energy profile chart - Chart of energy differences from EQ0 at a molecular structure change

Microiteration - In connection with QM/MM, the microiteration technique can be used to reduce the computational demands drastically, and it extends the range of application of GRRM considerably

Large ADD following (LADD) A very efficient (1/5~1/10) search of lower lying structures can be made by the LADD algorithm

ONIOM and various QM/MM methods ONIOM as well as various methods available in the Gaussian program can be used as options in combination with the above techniques

GRRM auto-visualization - Geographic view of the structure transitions drawn by circles and lines

3D View of EQ/TS/DDC/UDC - 3D view of molecular structure by HTML5 rotatable by mouse operations

Energy profile chart - Chart of energy differences from EQ0 at a molecular structure change

3D Animation of molecular structure change synchronizing with energy profile chart

Packed together with GRRM in HPC SYSTEMS’ servers (in plan)

Visomin enables you to analyze the output of GRRM (text-based, very huge, ex. over 200 files in 5 atoms system) with a lightweight graphical format. Why not improve your productivity with faster analysis?