Automated Exploration of Chemical Reaction Pathways
"GRRM" ~Global Reaction Route Mapping~

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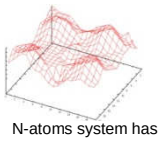
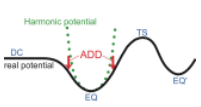
GRRM developed by K. Ohno and S. Maeda enables one to follow all reaction pathways from an equilibrium (EQ) point towards structures of transition states (TS) surrounding the EQ point. Subsequent downward followings from already found TSs can easily be made as conventional intrinsic reaction coordinate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

Feature:

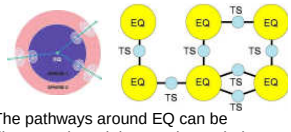
Cooperating with quantum chemistry programs such as Gaussian 03/09 and Molpro, GRRM enables one to perform high speed exploration of chemical reaction pathways in 3N-6 dimensional potential energy surfaces (which was previously limited to 4 atoms) by scaled hypersphere search (SHS) method which is based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



N-atoms system has 3N-6 dimensional potential energy surfaces(PES)



Reaction pathways follows the direction that ADD in PES increases



The pathways around EQ can be discovered at minima on the scaled hypersphere which would have a constant energy when the potentials are harmonic

Functions:

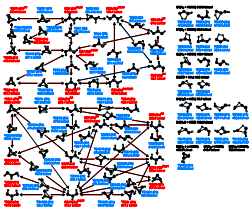
Opt. of EQ EQ structures can be optimized by SIRFO and BFGS methods.
Opt. of TS TS structures can be optimized by SIRFO and Bofill's methods.
IRC search IRC can be traced by Page and McIver methods.
One step TS search An efficient search of via a TS between a reactant and a product without any initial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

Free of charge for academic users

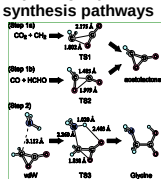
HPC SYSTEMS Inc. sells GRRM-ready servers

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

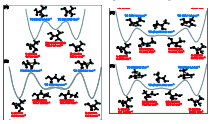
GRRM of CH_3NO system



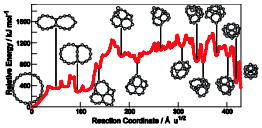
Exploring Glycine synthesis pathways



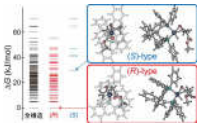
Designing Alanine D-L conversion pathways



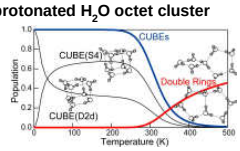
Multistep reaction pathways of C_{20} cluster



Stereoselectivity catalyst on Chiral system

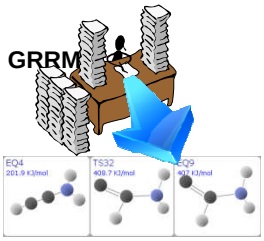


Structural transition of protonated H_2O octet cluster



Assistance tool for searching GRRM
"Visomin" ~Visual Frontend for GRRM~

Developed by HPC SYSTEMS Inc. from full scratch.
Visomin parses lots of GRRM output files, and makes a simple figure on a web-based interface.
It assists you powerfully on the analysis of reaction pathways derived from GRRM.



Features:

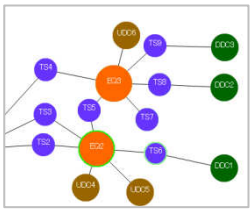
1) 2D geographically view of GRRM of EQ/TS/DDC/UDCs outputted from GRRM
2) Intuitive view of molecular structure change with an energy profile chart and a 3D animation
3) New web standard HTML5-based GUI (Google Chrome or Safari are recommended)

Functions:

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 - 3D animation synchronizing with energy profile chart while highlighting the step
GRRM job management by a batch job system - Interface for managing GRRM computation jobs

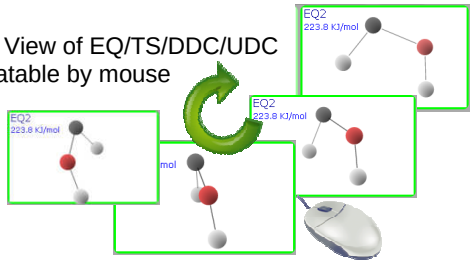
Packed together with GRRM in HPC SYSTEMS' servers (in plan)

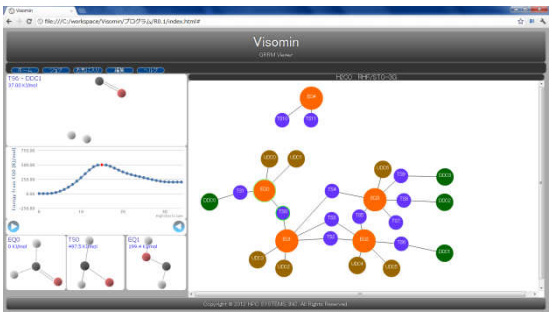
Visomin enables you to analyze the output of GRRM (text-based, very huge, ex. over 200 files in 5 atoms system) with a lightweight graphical format. Why not improve your productivity with faster analysis ?



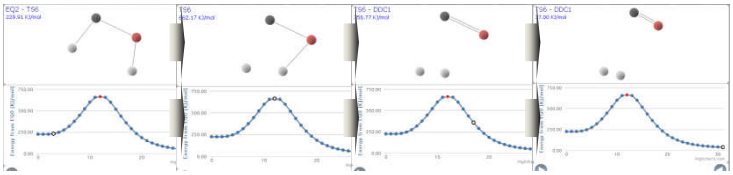
Auto-visualized GRRM

3D View of EQ/TS/DDC/UDC rotatable by mouse





Screenshot



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