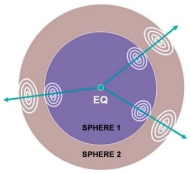

GRRM NEWS No. 005

GRRM NEWS reports recent developments of the ADD/SHS algorithm and its applications. A major revision has been made for the GRRM program. The newest version is ***GRRM***11, which will be released within the earlier half of 2011.

(1) One of the major improvements in *GRRM*11 is parallel treatments of the GRRM procedure around equilibrium (EQ) points. Although the standard GRRM treatments are processed in series from one EQ point to other unprocessed EQ points. Now in GRRM11, the SHS search of reaction channels leading to TS or DC around EQ can be made for several EQ points simultaneously in a parallel mode. This is especially suitable for high performance servers with multi-cores, although this new function is limited to only one-node. This parallel version of GRRM considerably reduces computation time for the global mapping of the entire reaction channels.

(2) Microiteration technique is introduced in *GRRM*11 to drastically reduce computational demands for large systems. A giant system with more than 300 atoms could be handled by using QM/MM methods [Ref.32].

(3) Excited-state potential surfaces can be studied by *GRRM*11. Minimum points on seems of crossings as well as conical intersections can be searched very effectively, which helps to consider unknown chemistry in photochemical processes [Refs. 30, 35, 36].

(4) *GRRM*11 has been strengthened its ability for studying important problems. Surface processes can be treated with fixing geometries of some atoms in the substrate [Ref. 37]. Imposition of special conditions on some bonds limits chemical structures to be searched, and such treatments considerably reduce computation time to obtain interesting reaction channels leading to aimed chemical compounds.

In addition to the new version of *GRRM*11, a graphical display (GDSP) system for GRRM calculations has been developed. GRRM-GDSP is a data handling system, which automatically creates a system of Web pages for viewing lists of obtained geometries and three-dimensional structures based on output data from the GRRM program. Animations around transition structures along IRC pathways can also be produced automatically. Dissociated products are listed for all dissociation channels, and synthetic reaction routes without byproducts can easily be found on the Web representation.

A new GRRM interface has been created. Everything, from input-data preparation and submission of a GRRM-JOB to confirmation of the searched results as well as creation of visualized Web Pages of the GRRM output data, can be handled on a Web Page in the WebGRRM system.

GRRM*11** is an ***updated version of the GRRM program based on the **SHS** algorithm for an automated exploration of reaction pathways by using energies from solutions of $H\Psi = E\Psi$.

***GRRM* 11** copes with various problems in chemistry by automated exploration of reaction pathways.

O ***GRRM* 11 automatically explores unknown isomers.**

O ***GRRM* 11 automatically explores unknown synthetic routes.**

O ***GRRM* 11 automatically explores unknown dissociation channels.**

***GRRM* 11** develops an unexplored world of chemistry by elucidating unknown reaction networks.

○ ***GRRM* 11 is useful for production of the Atlas for the chemical world.**

○ ***GRRM* 11 is useful for design of new chemical compounds and reactions.**

○ ***GRRM* 11 is useful for designing new tactics for energy/environment problems.**

○ ***GRRM* 11 is useful for elucidation of catalysis and design of new catalysts.**

***GRRM* 11** is an epoch-making program of potential analyses for the following problems.

- **Normal coordinate analysis** Normal coordinate calculations can be made at arbitrary structures. Optionally, enthalpy and Gibbs energies can also be obtained.
- **Optimization of equilibrium structures** Equilibrium structures can be optimized by **RFO** and **BFGS** methods**.**
- **Optimization of transition structures** Transition structures can be optimized by **RFO** and **Bofill's** methods**.**
- **IRC search** **IRC** can be traced by **Page** and **McIver** methods**.**
- **GRRM search** Global reaction route mapping (**GRRM**) can be made for the potential surface of a given chemical formula. Starting from an equilibrium structure, automated search of dissociation and isomerization can be performed to explore **GRRM** corresponding to the Atlas of chemical reaction routes. Optionally, exploration of reaction routes can be made for the limited region around a particular structure.
- **One step TS search** An efficient search of the reaction pathway via a transition structure (**TS**) between a reactant and a product can be made automatically without initial guess, and this technique is much more rapid and applicable than any other methods.
- **Intermediate search** Intermediates between a pair of isomers can be found, even if they are far apart. The **SHS** method in the hypersphere-contraction-mode enables us to explore multi-step reaction pathways, even if they amount to several tens of steps.
- **Large ADD following (LADD)** A very efficient search of lower lying structures can be made by the LADD algorithm, which is especially suitable for systems with huge numbers of isomers.
- **ONIOM and various QM&MM methods** ONIOM as well as various methods available in the Gaussian program can been used as options in combination with the above techniques.
- **Microiteration** In connection with QM&MM, the microiteration technique can be used for drastically reducing computational demands, and it extends the range of GRRM considerably.
- **Limited Search** Limited searches fixing geometries of some atoms as well as imposing special conditions on some bonds extend abilities of the GRRM method to many important problems.
- **Excited-State analyses** Minimum energy points on seems of crossings can be searched. With a help of Molpro, excited potential energy surfaces can be searched more effectively.

***Program Package & Requirement for GRRM* 11**

***GRRM* 11** utilizes energies obtained by **Gaussian09** (Gaussian03 can also be used directly).
Conventional packages other than Gaussian09/03 can also be used with additional data handling.

***GRRM* 11** can be used under a Linux/Unix environment.

***GRRM* 11** can be used for research and education, after application to the following address by E-mail.

ohnok@m. tohoku.ac.jp

SHS-GRRM Publication List

1) A Scaled Hypersphere Search Method for the Topography of Reaction Pathways on the Potential Energy Surface.
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S. Maeda and K. Ohno, *J. Phys. Chem. A* 109(25), 5742-5753 (2005).
6) Global Investigation on Potential Energy Surface of CH_3CN: Application of the Scaled Hypersphere Search Method.
Xia Yang, Satoshi Maeda, and Koichi Ohno, *J. Phys. Chem. A* 109(32), 7319-7328 (2005).
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S. Maeda, Y. Watanabe, and K. Ohno, *Chem. Phys. Lett.* 414(4-6), 265-270 (2005).
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K. Ohno and S. Maeda, *Chemistry Letters* 35(5), 492-493 (2006).
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13) Global Mapping of Small Carbon Clusters Using the Scaled Hypersphere Search Method.
B. Hajgato, S. Maeda , and K. Ohno, *AIP Conference Proceedings* 855, 296-304 (2006).
14) Structures of Water Octamers $(H_2O)_8$: Exploration on Ab Initio Potential Energy Surfaces by

the Scaled Hypersphere Search Method.
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