GRRM NEWS No. 002

GRRM NEWS reports recent developments of the SHS algorithm and its applications. An ***updated*** version of ***GRRM*1.20** has been released on 1 Feb. 2008. Performance of the GRRM program has been considerably improved. Applications to large systems containing more than 100 atoms have become possible by the ***LADD*** algorithm and the use of the ***ONIOM*** method.

1) **L**arge **ADD** (LADD) algorithm has been introduced for searching lower energy structures including the global minimum in a very efficient way. This option is recommended to be used for the rapid search of lower lying structures among huge numbers of isomers. Typical applications have been made in J. Phys. Chem. A 2007, 111, 4527.
2) Use of the **ONIOM** method as well as various quantum mechanical techniques incorporated in the Gaussian program is introduced as options. The QM/MM treatments have made it possible to apply the GRRM program to very large systems involving hundreds of atoms. A typical example has been published in J. Phys. Chem. A 2007, 111, 13168.
3) Some modifications have been made to speed up standard procedures in *GRRM*1.00.

For the use of the new version ***GRRM*1.20**, a request or an inquiry should be sent to the following e-mail address.

Request or inquiry to: ohnok@qpcrkk.chem.tohoku.ac.jp

GRRM program has been used by many groups in the world, including Keiji Morokuma and his colleagues in United States, China, and Japan. Frank Jensen has reported Ohno and Maeda's approach as a novel method for searching all possible reaction pathways in his book entitled "Introduction to Computational Chemistry, Second Edition, Wiley, Chichester, 2007".

The world of GRRM is to be extended by parallel computing. The forthcoming version of GRRM will make it possible to use multi-core processors. GRRM holds promise for applications to organo-metallic compounds and catalysts. Moreover, an extension to vibrational spectroscopy also holds promise for various applications, which could not be made by other computer programs.

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GRRM*1.20** is an ***updated version of the first program based on the **SHS** algorithm for an automated exploration of reaction pathways by using energies from solutions of $H\Psi=E\Psi$.

***GRRM* 1.20** copes with various problems in chemistry by automated exploration of reaction pathways.

O ***GRRM* 1.20 automatically explores unknown isomers.**

O ***GRRM* 1.20 automatically explores unknown synthetic routes.**

O ***GRRM* 1.20 automatically explores unknown dissociation channels.**

***GRRM* 1.20** develops an unexplored world of chemistry by elucidating unknown reaction networks.

○ ***GRRM* 1.20 is useful for production of the Atlas for the chemical world.**

○ ***GRRM* 1.20 is useful for design of new chemical compounds and reactions.**

○ ***GRRM* 1.20 is useful for designing new tactics for energy/environment problems.**

○ ***GRRM* 1.20 is useful for elucidation of catalysis and design of new catalysts.**

***GRRM* 1.20** 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 **SIRFO** and **BFGS** methods**.**
- **Optimization of transition structures** Transition structures can be optimized by **SIRFO** 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.

***Program Package & Requirement for GRRM* 1.20**

***GRRM* 1.20** utilizes energies obtained by **Gaussian03**.

***GRRM* 1.20** can be used under a Linux/Unix environment.

***GRRM* 1.20** can be used for research and education, after application to the following address by E-mail. ohnok@qpcrkk.chem.tohoku.ac.jp