Software

Product Name	Reaction plus Pro ver. 1.0
Number of addressable intermediate conformation	Unlimited
Automatic correlation for coordinate axis of initial structure	○
Optimized calculation based on calculation result	○
Quantum chemical calculation technique	All calculation technique of Opt keyword of Gaussian
Basis sets	All basis sets of Gaussian
Input by GUI	Possible by using GaussView *1
Animation display	Possible by using GaussView, VMD *1
Maximum parallel cpu cores	The number of core/nodes *2
Job scheduler	LSF, Lava, Sun Grid Engine, Open Grid Scheduler, PBS Pro, Torque
Bundled item	Software, manual, tutorial
Operating environment *3	OS: RedHat Enterprise Linux 6.x or CentOS 6.x Software: Gaussian09 Rev. C01~ *4
Price	ASK

*1 Checked by GaussView 5.0.8 for Windows, VMD 1.9.1 for Windows.
*2 No parallel computing between nodes support.
*3 Not guaranteed to all operating environment.
*4 To operate this software, Gaussian09 Rev. C01~ (Intel EMT64T Linux ver.) is needed.

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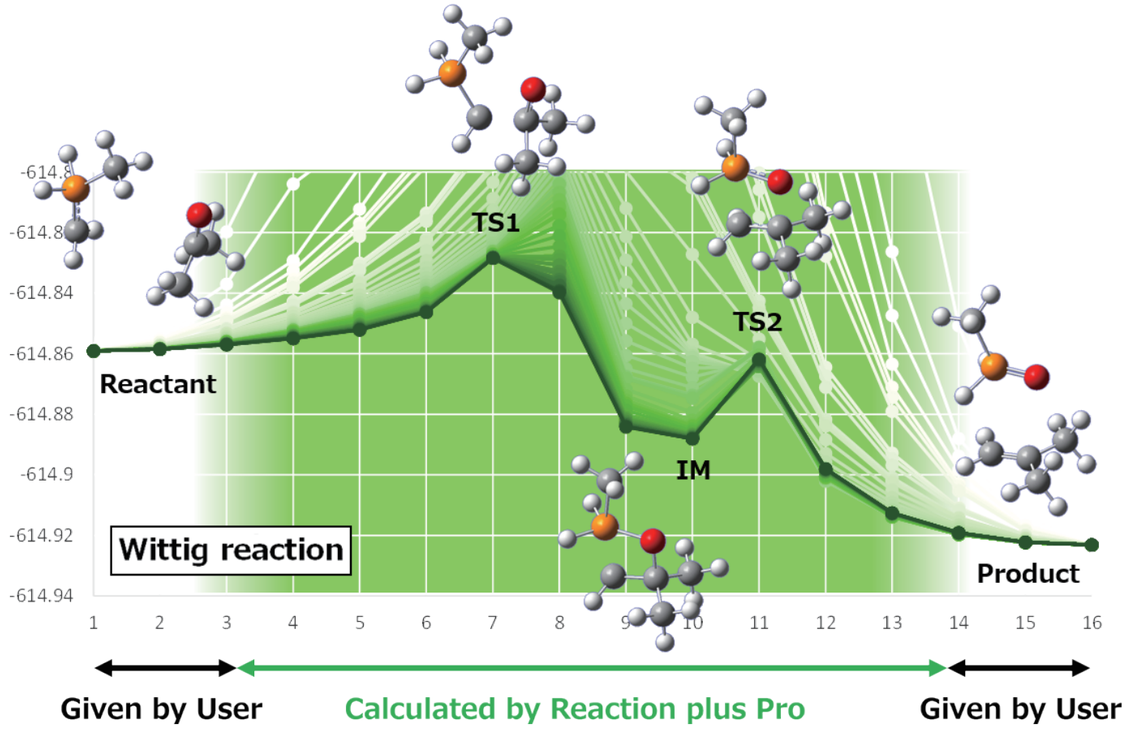
Transition states and reaction paths can be obtained by specifying the reactant and product geometries.

≫ Optimal path can be obtained very quickly if you have some speculation.

Complicated paths can be also available by specifying the multiple intermediate geometries.

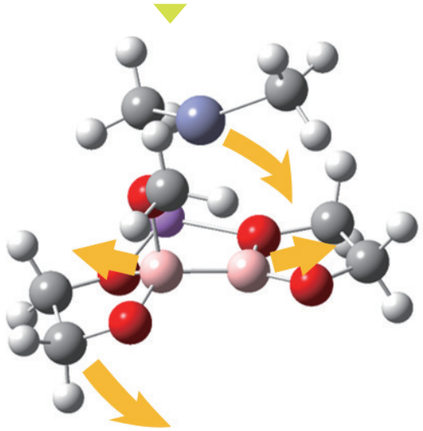
≫ Visualization of the reaction using GaussView, VMD, Avogadro, and so on.



Examples

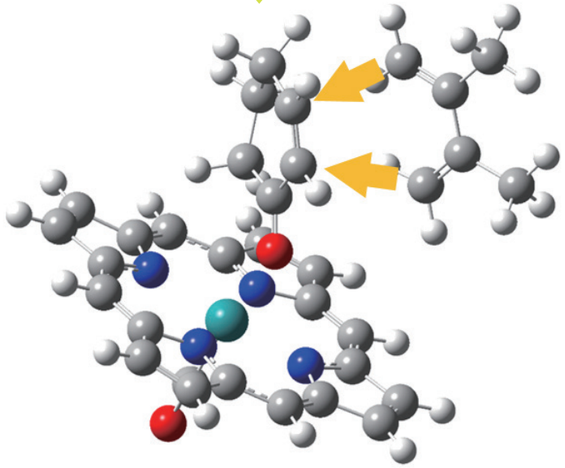
Uchiyama Lab., Univ. of Tokyo

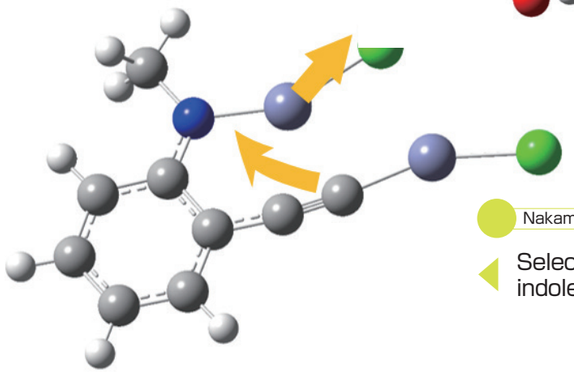
Reaction design based on calculations:
Generation of Borylzincate complexes



Matsubara Lab., Kyoto Univ.

Cycloaddition reactions catalyzed by
Ru-porphyrin complexes



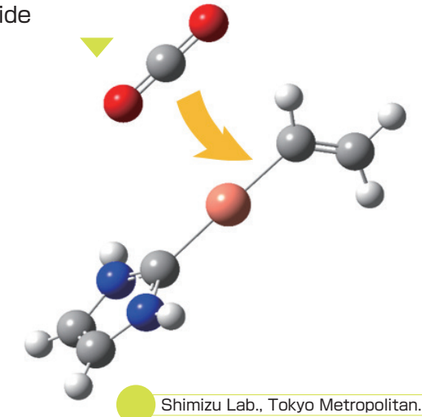


Nakamura Lab., Univ. of Tokyo

Selective syntheses of substituted
indoles via Zn catalysis

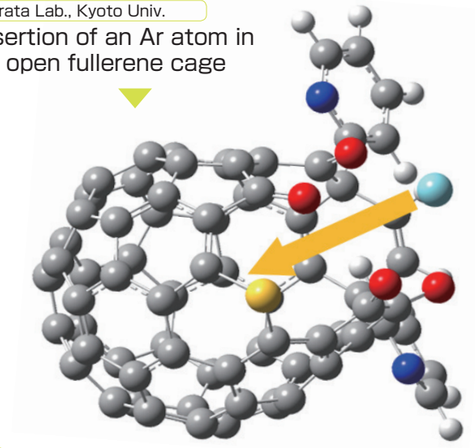
Tsuji Lab., Kyoto Univ.

Fixation reaction of carbon
dioxide



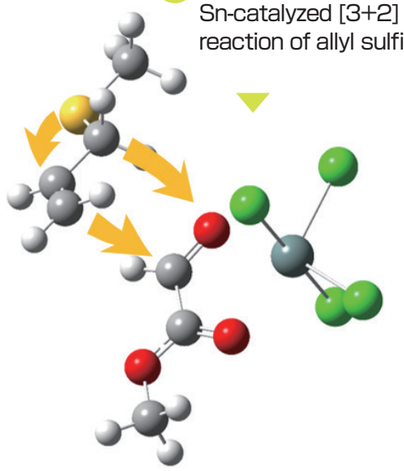
Murata Lab., Kyoto Univ.

Insertion of an Ar atom in
an open fullerene cage

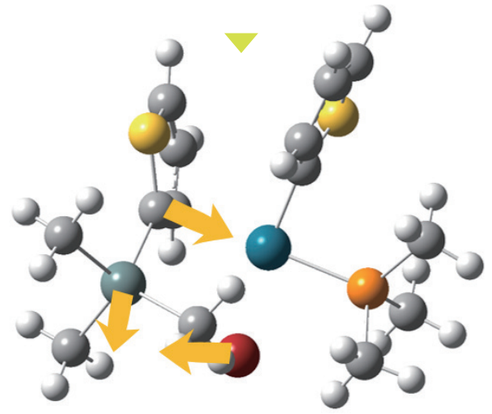


Shimizu Lab., Tokyo Metropolitan. Univ.

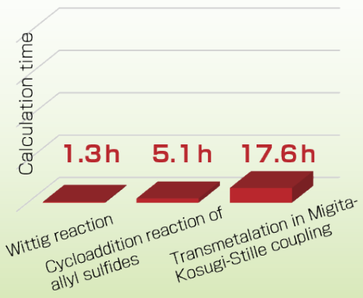
Sn-catalyzed [3+2] cycloaddition
reaction of allyl sulfides

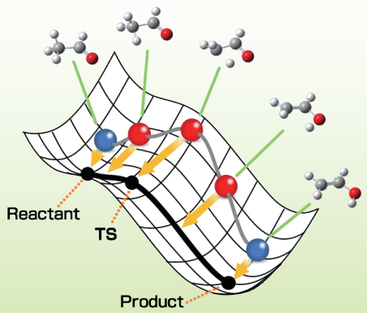


Transmetalation process in Migita-
Kosugi-Stille coupling reaction



Features

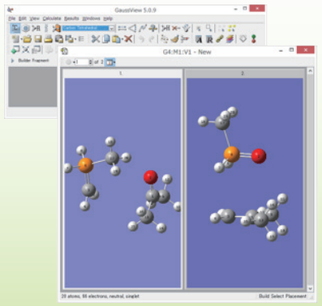




Reaction paths are found very quickly!

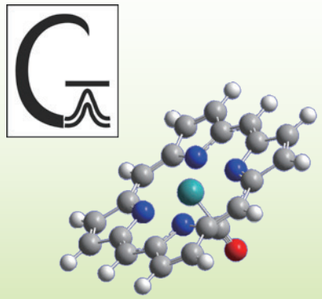
Reaction path s can be calculated very fast. Most reaction paths are found in a half to several days.

Reaction plus Pro is based on Nudged Elastic Band (NEB) method which can optimize whole reaction paths as well as transition states.



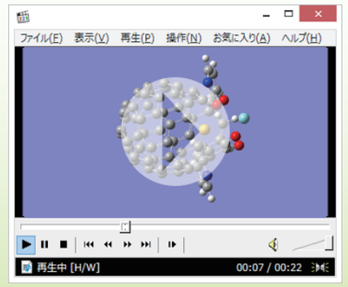
Input creation is very easy!

Input files for Reaction plus Pro can be created with your favorite viewer software such as GaussView.



Many methods on Gaussian are available!

Many calculation method and basis sets on Gaussian are available. PCM solvent effect and reaction paths for excited states can also be calculated.



You can see the reaction process animations!

Output file is compatible with Gaussian log format and XYZ format. You can see animations of reaction processes using GaussView or VMD.