ABSRP Users Guidance

Automatic Bond Separation Reaction Platform

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Software and environment requirements:

RDkit 2019

python 3.7

perl 5.0

Gaussian09

Linux

Note: Your computer must meet the above requirements.

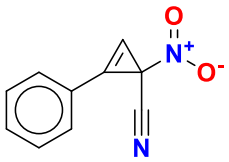
Table 1. Script list of ABSRP (**$Path** represents the path of ABSRP, for example '/d/ABSRP' or '..').

Tool	Code	Command and Description
CBH Generator	CBHGenerator.pyc	**python $Path/CBHGenerator.pyc –m file.mol –r [0/1]** To perform an automatic bond dissociation reaction. The input required after the argument '-m' is a molecular file in '*.mol' format, and the '1' or '0' after the argument '-r' indicates RCBH or CBH scheme, with RCBH as the default. The output is two files named '*.prod' and '*.reac' that record the BSR products and the added reactants, respectively.
QC Engine	BuildGjf.pl	**perl $Path/BuildGjf.pl Nproc Nmem file.mol** To transform a '*.mol' file to a '*.gjf' file for quantum chemistry calculation using Gaussian09, if the ***Energetic Material Studio*** is not available. Nproc and Nmem are integers to allocate the numbers of processor and memory required. **Note**: You should create a file named 'INPUT.txt', before running this command, in which each row contains a Gaussian calculation condition. If 'INPUT.txt' is missing, the default setting '#P OPT Freq M062X/6-31+G(2df,p) INT=UltraFine' will be employed.
	AutoG09.pl	**perl $Path/AutoG09.pl** To run Gaussian09 tasks automatically and continuously, with error checking on each finished '*.log' file, if the ***Energetic Material Studio*** is not available. To repeat the above command *N* times means creating N queue for automatic calculation. Omit this script, if only one molecule is to be calculated. **Note:** A running directory should be created in the location of the '*.gjf' files, and the script must executing in the running directory. The parent directory works as a job-pool, and the script will grab the job

		files from the job-pool into the running directory one by one.
Enthalpy Library	EnthalpyLibrary	An directory under ABSRP, with reusable library of thermal enthalpies for organic fragments.
Error Corrector EOF Calculator	CalcEOF.pl	**perl $Path/CalcEOF.pl $Path/ Name.log** The 2 tools are merged in this script to perform 5 jobs, include (1) reading thermal enthalpy H_{mol}^{low} from a Gaussian '*.log' file, (2) reading organic fragments from the '*.prod' and '*.reac' files, (3) querying their thermal enthalpies from the Enthalpy Library and providingΔCBH_{corr}, (4) correcting H_{mol}^{low} to H_{mol}^{G4}, (5) Calculating $\Delta_f H^{\ominus}$.

Example:

Calculating the $\Delta_f H^{\ominus}$ of



Work flow:

```
cd Example
python ../CBHGenerator.pyc -m TANHAR.mol
perl ../BuildGjf.pl 4 4 TANHAR.mol
g09 M062X6-31xG2dfp.TANHAR.gjf
perl ../CalcEOF.pl ../ M062X6-31xG2dfp.TANHAR.log
```

Output:

M062X6-31xG2dfp.TANHAR.log,111.31(kcal/mol)