**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 ‘..’).

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| --- | --- | --- |
| **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 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 providing, (4) correcting to , (5) Calculating . |

**Example：**

Calculating the of

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**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)**