



RMG-Py Release Updates

Connie Gao

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RMG Study Group

Progress since last summer

- New-style adjacency list completely merged (See RMG Study Group on new-style adjacency list for more details)
 - Uses triple bonded version of CO
 - Families now well defined with distinctions between singlet vs. triplet requirements
- Database Format Improvements
 - Kinetics libraries and training reactions now separate dictionaries from rates
 - Lots of unit tests in place for checking database errors


Adjacency list backwards compatibility

- Old style (RMG-Java) adjacency lists can be used as input in RMG-Py. So can intermediate style adjacency lists.
 - Errors will be raised if electronic state is not specific enough, e.g.

```
1 C 2 {2,S} {3,S}
2 H 0 {1,S}
3 H 0 {1,S}
```

- Default multiplicity used: $2s + 1$

How to fetch old style adjlists from RMG-website



Documentation
Learn more about the RMG software

Database
Browse the RMG database of chemical parameters

Draw Group
Draw a group structure from its adjlist

Molecule Search
Draw a molecule from its adjlist and search its properties

Kinetics Search
Search for the kinetics of a chemical reaction

Solvation Search
Search for the solvation properties of a reaction between a solvent and a solute

Simulation & Tools
Additional tools to supplement RMG

RMG » Molecule Search 8+1 [Log in](#)


Molecule Search

Use this form to find a species from its adjacency list. You can quickly fill in the adjacency list part of the form by entering any species identifier, such as a SMILES, InChI, CAS number, or species name in the 'species identifier' field and pressing tab. This is translated into an adjacency list using the NCI Chemical Identifier Resolver. Do not submit the form until the adjacency list has loaded.

Species Identifier:

```
1 C u0 p0 c0 {2,S} {5,S} {6,S} {7,S}
2 C u0 p0 c0 {1,S} {3,D} {4,S}
3 O u0 p2 c0 {2,D}
4 C u0 p0 c0 {2,S} {8,S} {9,S} {10,S}
5 H u0 p0 c0 {1,S}
6 H u0 p0 c0 {1,S}
7 H u0 p0 c0 {1,S}
8 H u0 p0 c0 {4,S}
9 H u0 p0 c0 {4,S}
10 H u0 p0 c0 {4,S}
```

Adjacency List:

Molecule Structure: 

Molecular Weight: 58.08

InChI: InChI=1S/C3H6O/c 1-3(2)/h1-2H3

SMILES: CC(C)=O

Adjacency List:

```
1 C u0 p0 c0 {3,S} {4,S} {5,S} {6,S}
2 C u0 p0 c0 {3,S} {7,S} {8,S} {9,S}
3 C u0 p0 c0 {1,S} {2,S} {10,D}
4 H u0 p0 c0 {1,S}
5 H u0 p0 c0 {1,S}
6 H u0 p0 c0 {1,S}
7 H u0 p0 c0 {2,S}
8 H u0 p0 c0 {2,S}
9 H u0 p0 c0 {2,S}
10 O u0 p2 c0 {3,D}
```

Old Adjacency List:

```
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {4,S}
3 O 0 {2,D}
4 C 0 {2,S}
```

Names: propan-2-one
ACETONE
67-64-1
NSC135802

Click 'Draw Molecule' Button

Old style adjacency list appears below new style adjlist

How to convert new style adjlists into old style adjlists



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Simulation & Tools

Additional tools to supplement RMG

RMG » Simulation and Tools

Simulation

1. **Create Input File:** generate an input file for an RMG-Py job through a web form, or upload an existing input file for easy editing through the web form.
2. **Submit Job:** Submit a RMG-Py job online by providing your email address. We will email you the result when it's done.

Tools

1. **Visualize Chemkin File:** visualize a model by supplying its chemkin file and RMG-generated species dictionary.
2. **Model Comparison:** compare two RMG-generated models by supplying their individual chemkin files and species dictionaries.
3. **Convert Adjacency Lists:** convert adjacency lists in a text file to old-style adjacency lists which are compatible with RMG-Java.
4. **Merge Models:** merge two RMG-generated models by supplying their individual chemkin files and species dictionaries.
5. **Generate Flux Diagram:** generate a flux diagram video by supplying a RMG input file and completed mechanism, or with a customized set of concentration profiles from a Chemkin job.
6. **PopulateReactions:** generate all possible reactions from a set of initial species.
7. **Plot Kinetics:** plot forward along with a RMG dictionary.
8. **Create RMG-Java Kine**

Go to Simulation & Tools Section



Simulation & Tools

Additional tools to supplement RMG

Convert adjacency lists tool can mass convert .txt file of new adjlists into old adjlists

RMG » Simulation and Tools » Convert Adjacency Lists

Convert Adjacency Lists

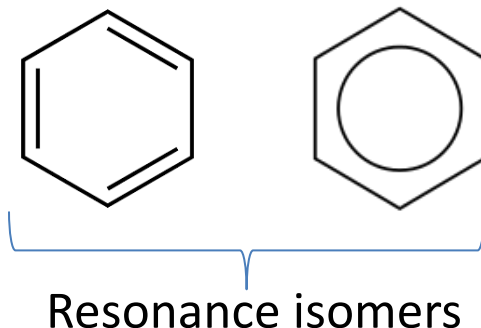
Upload your RMG Dictionary text file and convert them back into old style adjacency lists compatible with RMG-Java. Not that adjacency lists containing heteroatoms such as N, Ar, Ne, and He are not compatible with old style adjacency lists and will result in conversion failure.

RMG Dictionary: No file chosen

Changes to aromaticity detection

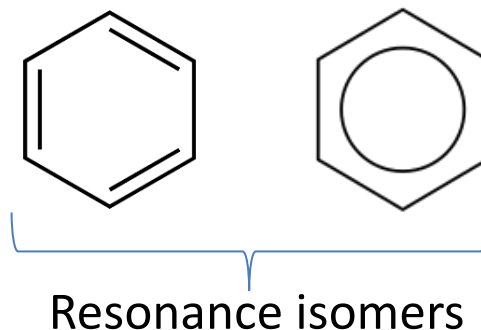
- Use RDKit to detect aromaticity in rings and convert a copy of the molecule to one with Cb bonds. Retain aromatic form as a resonance isomer
 - Convert to Cb bonds only if ring size is 6-membered and all ring members are carbons

Benzene



Thermo for aromatics

Benzene



- Algorithm fetches thermodynamic parameters from all resonance isomers and chooses thermo from isomer with more stable enthalpy
 - Can now obtain aromatic Benson group corrections
- Retains symmetry number correction since aromatic resonance isomer has both more stable enthalpy and higher symmetry number
- Now exhibits identical behavior of RMG-Java

Pull request 1: Handling duplicate reactions in reaction libraries and seed mechanisms

- Allow duplicate Pdep + Non-pdep reactions in reaction libraries and seed mechanisms

```
NNH (38) =N2+H (5)          3.300e+08  0.000      0.000  
DUPLICATE
```

```
NNH (38) +M=N2+H (5) +M      1.300e+14  -0.110     4.980  
CH4 (16) /2.00/  CO2 (17) /2.00/  C2H6 (27) /3.00/  
H2O (28) /6.00/  H2 (4) /2.00/  Ar/0.70/  
DUPLICATE
```

- Previously, RMG was only including one of the reactions, now it includes both as intended

Some issues remaining on handling duplicate PLOG reactions

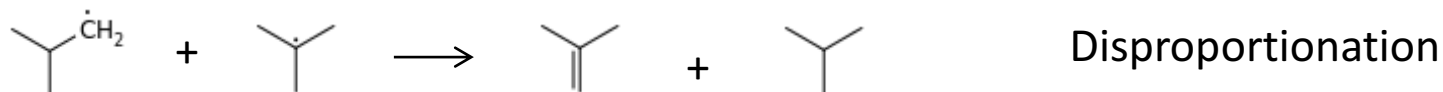
CHEMKIN can read the following format:

```
OH(5)+CO(10)=CO2(11)+H(2)      1.000e+00 0.000      0.000
  PLOG/ 0.001      9.300e+10 0.000      0.000      /
  PLOG/ 0.001      7.100e+05 1.800      1.133      /
  PLOG/ 100.000    1.500e+11 0.000      1.987      /
  PLOG/ 100.000    1.900e+05 1.940      0.000      /
  PLOG/ 2000.000   3.700e+07 1.340      2.186      /
```

Both RMG-Py and RMG-Java require conversion to the following:

```
OH(5)+CO(10)=CO2(11)+H(2)      1.000e+00 0.000      0.000
  PLOG/ 0.001      9.300e+10 0.000      0.000      /
  PLOG/ 100.000    1.500e+11 0.000      1.987      /
  PLOG/ 2000.000   3.700e+07 1.340      2.186      /
DUPLICATE
OH(5)+CO(10)=CO2(11)+H(2)      1.000e+00 0.000      0.000
  PLOG/ 0.001      7.100e+05 1.800      1.133      /
  PLOG/ 100.000    1.900e+05 1.940      0.000      /
  PLOG/ 2000.000   0.000e+00 0.000      0.000      /
DUPLICATE
```

Pull request 2: Handling duplicate reactions in a reaction family with multiple transition states



- Reaction can occur via two transition states, which may have differing kinetics.
- RMG was previously considering them as degenerate reactions
 - Picked up either set of kinetics randomly and increased degeneracy
- Fix: Check template of reaction and increase degeneracy only if templates are identical, otherwise add duplicate kinetics

Task List for Release

- Packaging RMG
 - Package RMG as an executable for Windows (py2exe or NSIS), Linux (Freeze or PyInstaller), and Mac (py2app)
- Comprehensive and working examples
 - May need to compare against RMG-Java
 - Crash checks
- Optional: Easy comparison txt files for kinetic and thermo values in database
- RMG-Py publication