RMG-Py Release Updates

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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

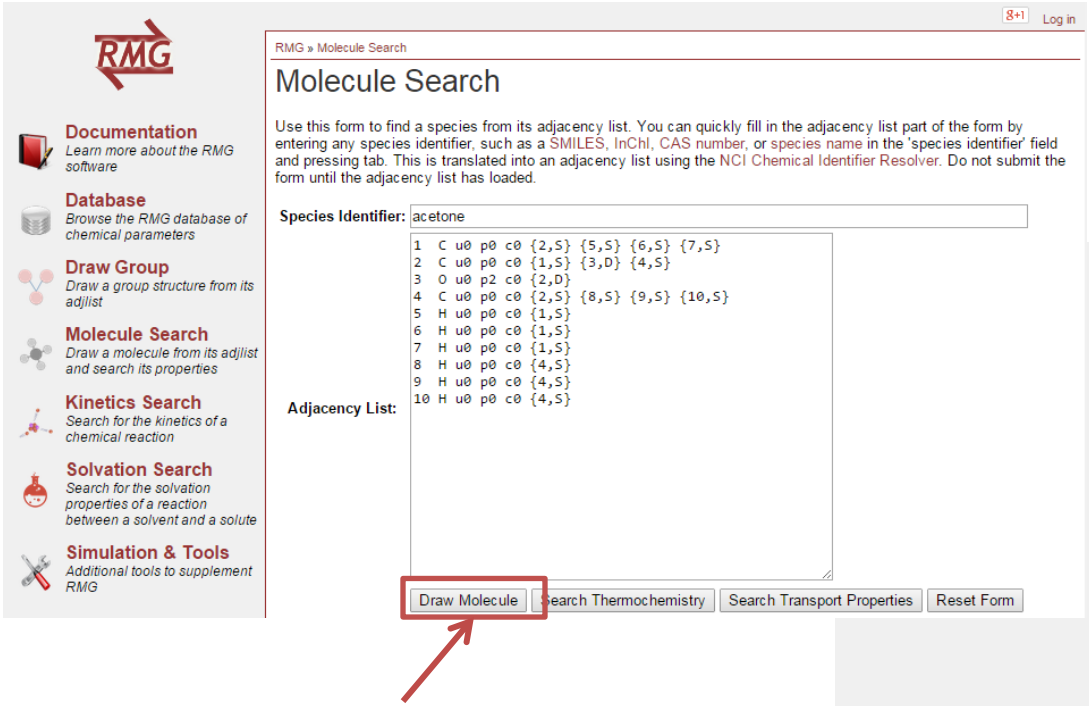
Adjacency list backwards compatibility

- 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}
```

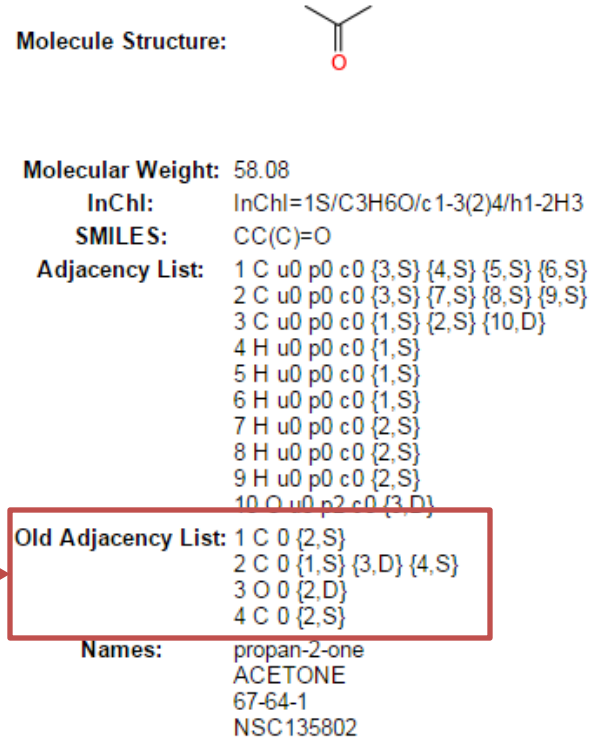
  - Default multiplicity used: 2s + 1

How to fetch old style adjlists from RMG-website

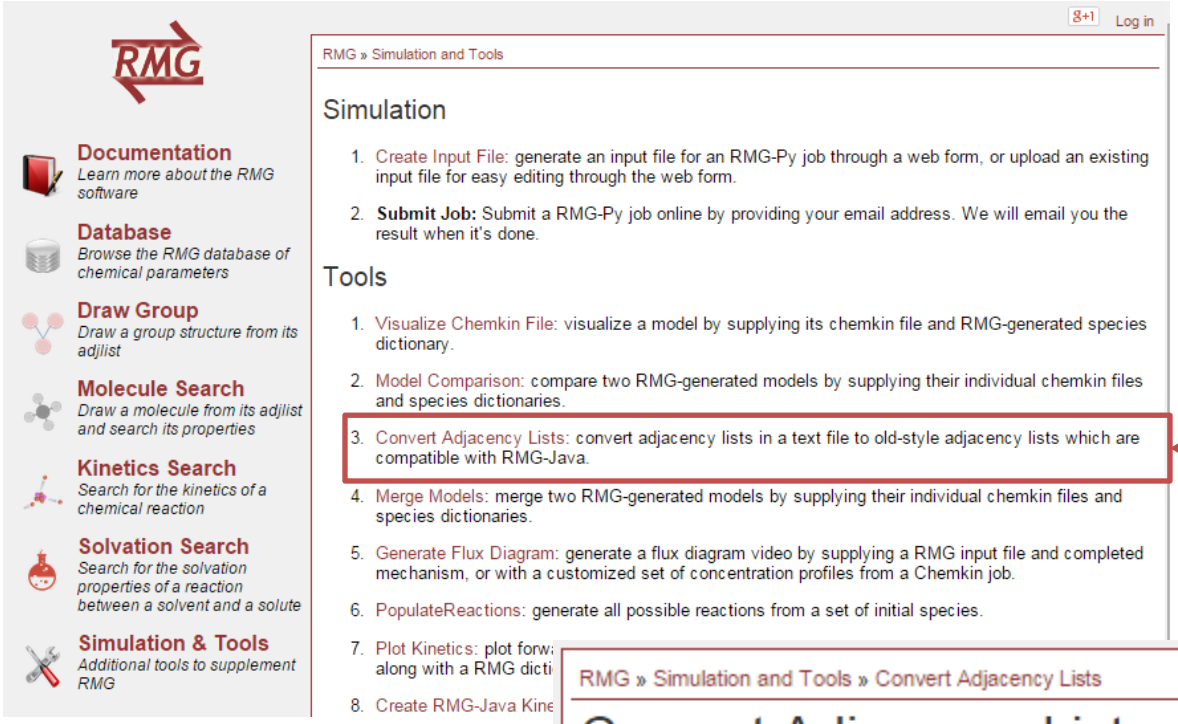


Click ‘Draw Molecule’ Button

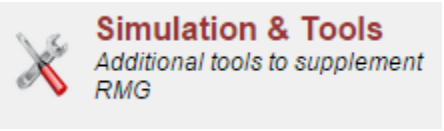
Old style adjacency list appears below new style adjlist



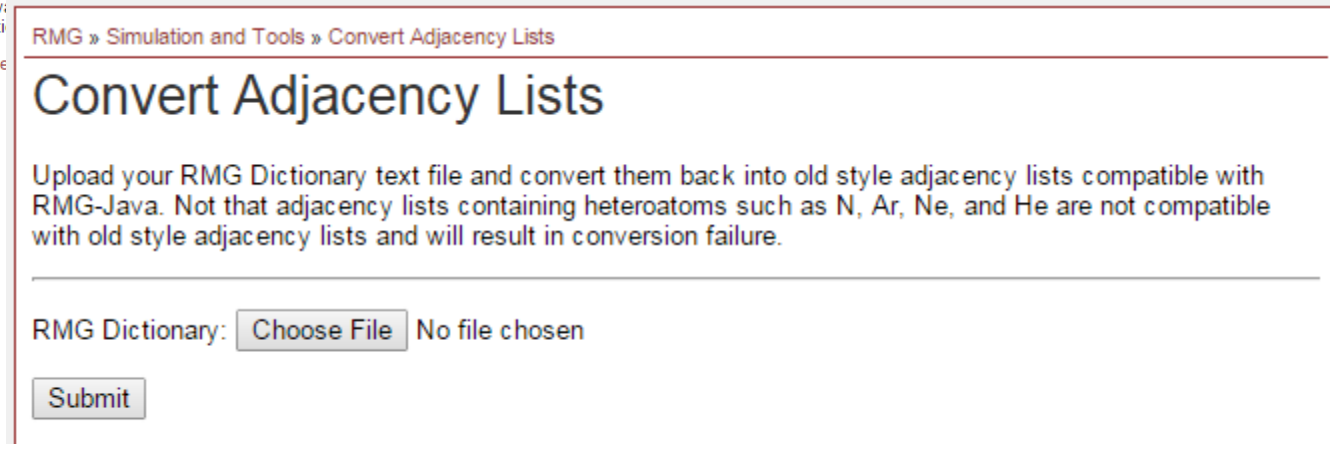
How to convert new style adjlists into old style adjlists



Go to Simulation & Tools Section



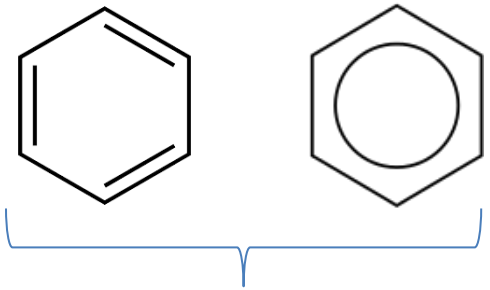
Convert adjacency lists tool can mass convert .txt file of new adjlists into old adjlists



Changes to aromaticity detection

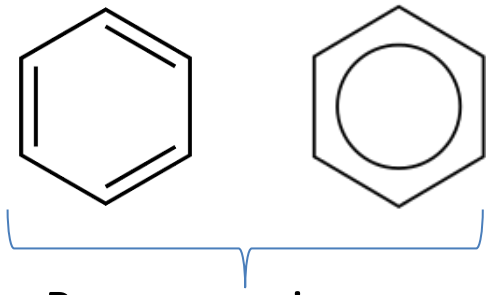
- Use RDKit to detect aromaticity in rings and convert a copy of the molecule to one with Cb bonds. Retain aromatic form as a resonance isomer
  - Convert to Cb bonds only if ring size is 6-membered and all ring members are carbons

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

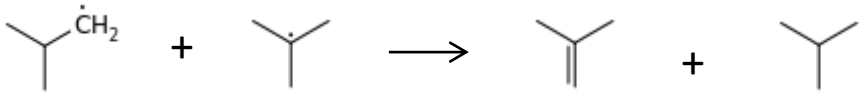
CHEMKIN can read the following format:

```
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



Disproportionation

- 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