

RMG Study Group Agenda for 2014-02-21

TOPICS

Adjacency List Syntax

Extensibility
Including charges for ions
Multiplicity as a species property or not?
Wildcards
Back-portability to Java
Rings
Cis-Trans

Database Format

Rates rule storage in CSV format
Adjlists and dictionaries in separate txt file
How to link long form comments and indexing
How to store original reaction (how do training reactions fit into our new scheme? and how can we provide mechanism for suggesting new groups?)

Database Testing

Ensuring children are actually children of groups
Testing if groups are incorporated into tree
Testing that adjlists are valid and identical going between rules and groups (this will no longer be a problem in the future when we store only one copy of the dictionary)
Adjlist validity checks (Implemented in Py. Known not to be implemented in Java.)
Mass balance checks (Just implemented in Py. What about Java?)
Duplicate checks for both thermo and reaction libraries (Just implemented in Py. What is the status in Java?)

Database Development (low priority)

Connie would like thermo and kinetics depositories of trusted values
Visualization of tree and sparsity in rate rules (Something for the web. Not a priority)
Constant evaluation of accuracy of rate rule algorithm given the current group and tree structure (ie. Josh Allen's training rate tests)
Better visualization of groups and GUI for editing rules. (Summer urops? Richard's students?)

New and Pressing Issues

Resonance isomer identification for dienes (along with recent bugfix in Java. Need to check Py)
Species constraints and forbidden species in Py
Seed mechanism handling and pdep in Py

Require Python > 2.7? (would allow ordered dictionaries)
Use the "real" cclib not our fork?

TASK LIST

Someone to decide and convert to new adjlist format
Someone to convert old database to new format and port over all existing comments
Someone to write database parser (or converter) for Java
Someone to write new database parser for Py
Someone to write database testing code
Someone to include aromaticity perception in Py
One person to handle each pressing issue listed above.
Everyone to write more documentation (specific assignments and times?)