Pre-Processing

Network Generation

Kinetics & TD Generation

Post-Processing

A Chemical Knowledge Based Approach

Reaction Family Recipe: an Example

The bond scission of two tertiary carbon atoms

**RECIPE:**

**Reactant Pattern:**

\[ \text{C(C)C(C)(C)} \]

**Transformations:**

1) **Break_Bond** (Atom1 , Atom 2)
2) **Atom 1:** **Gain_Electron**
3) **Atom 2:** **Gain_Electron**

**Constraints:**

- Atom count in molecule > 9
- Subatomic pattern identified: sub-molecular pattern
- Reactive centers that undergo transformations

**Unit Operations**

**Atom Connectivity:**

- Make_Bond
- Break_Bond

**Electronic Configuration:**

- Gain_Electron
- Lose_Electron

**Bond Order:**

- Increase
- Decrease

**Molecular:**

- # atoms in molecule, total # of unpaired electrons, etc...

**Atomic:**

- Presence of charge or aromaticity, etc...

Thermodynamic Properties: Benson GA

**SENSORS GROUP ADDITIVE VALUE:**

- Kin energy corrections and non-nearest neighbor interactions can be represented by SMARTS strings

**GROUP ADDITIVITY:**

- + Add: 1, 4, 2 (ligands)

**From:** M.K. Sabbe, Ph.D thesis

Conclusion

**CHEM-O-INFORMICS IS A HIGHLY ACTIVE FIELD THAT OFFERS A MULTITUDE OF POWERFUL GRAPH-THEORY BASED ALGORITHMS TO ACCOMPLISH NON-TRIVIAL COMPUTATIONAL TASKS.**

**THE PRESENT AUTOMATIC REACTION NETWORK GENERATION TECHNOLOGY IS GREATLY BENEFITING FROM THE ADVANCES MADE IN CHEMO-INFORMATICS, AND HAS ADOPTED FEATURES LIKE SMARTS LANGUAGE, INCHI, SUBSTRUCTURE MATCHING, ETC...**

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