String representation

The feroxide team

April 13, 2018

1 Introduction

Feroxide works by nesting all kinds of elements. This is ideal for calculation purposes, but it can be a pain if you have to type it all out every time again. That is what the string representation was made for. With that, you are able to digitalise complex reactions in only a single line of code, instead of using tens of lines of code to achieve the same thing.

The downside of using string representation is that it is a bit slower at runtime. That is also a reason why you should preferably only initialise a reaction once, instead of having it recreated in a loop.

This paper is made to explain how the string representation of all elements should be created and parsed. It is described from the smallest parts to the biggest parts. Every bigger part depends on the smaller parts.

Note: All whitespace is always ignored. This means that you can place spaces everywhere to increase readability.
However, even though input such as `H 20` is allowed and will succesfully result in H_2O, please do not place (misleading) spaces between MoleculeCompounds.

2 Atom

Atoms are as easy to represent as it can get. Simply enter the atom symbol to refer to the corresponding Atom.

2.1 Examples

- `C` will result in Carbon
- `Co` will result in Cobalt
- `H` will result in Hydrogen

3 MoleculeCompound

MoleculeCompounds are basically atoms with an amount. This is entered by putting a number after the atom symbol. If a number is omitted, one (1) is assumed.

3.1 Examples

- `H2` will result in H_2
- `C3` will result in C_3. This may be used to form butane
- `S` will result in S_1, or simply S

4 Molecule

Molecules are a combination of one or more MoleculeCompounds.

4.1 Examples

- `H2O` will result in H_2O_1, or simply H_2O
- `CH4` will result in C_1H_4, or simply CH_4
- `H3C6H5O7` will result in $H_3C_6S_5$

4.2 Bugs

- Currently you can not add water molecules to the crystal structure of a molecule. For example, the following is **invalid**: `CuSO4.5H2O`
- Molecule structures are not yet implemented. This means isomers such as $CH_3CH_2CH_2OH$ (propan-1-ol) and $CH_3CHOHCH_3$ (propan-2-ol) are the same to feroxide, namely `C3H8O`.

5 Ion

Ions are molecules with charge. This charge is entered after the molecule, seperated with a semi-colon (`;`). Negative charges should have a dash (`-`) **after** the charge. Positive charges can optionally have a plus-sign (`+`).

5.1 Special cases

- If no semi-colon and thus no charge is given, a charge of zero (0) is assumed.
- If only a semi-colon is given, a charge of zero (0) is assumed.
- If only a semi-colon and a plus-sign are given, a charge of positive one (+1) is assumed.
- If only a semi-colon and a dash are given, a charge of negative one (-1) is assumed.
- If the "atom" is an electron (`e`), then a charge of negative one (-1) is assumed. Any given charge will be ignored.

5.2 Examples

- `H2` will result in H_2^0, or simply H_2
- `Na;+` will result in Na_1^{1+}, or simply Na^+
- `Fe;3` will result in Fe^{3+}
- `SO4;2-` will result in $S_1O_4^{2-}$, or simply SO_4^{2-}

- `OH;-` will result in $O_1H_1^{1-}$, or simply OH^-
- `e` will result in e_1^{1-}, or simply e^-
- `e;5` will **also** result in e^-

6 ReactionCompound

ReactionCompounds are Ions (or Molecules - which will be converted to Ions with 0 charge under the hood), but with an amount of moles given. This amount is given at the start. If no amount is given, one (1) is assumed.

6.1 Examples

- `5H2O` will result in $5H_2O_1^0$, or simply $5H_2O$
- `3PO4;3-` will result in $3P_1O_4^{3-}$, or simply $3PO_4^{3-}$
- `Br;-` will result in $1Br_1^{1-}$, or simply Br^-

7 ReactionSide

A ReactionSide contains zero (0) or more ReactionCompounds, seperated by a plus(`+`) sign.

7.1 Examples

- `2H2 + O2` will result in $2H_2^0 + 1O_2^0$, or simply $2H_2 + O_2$
- `H2O + CO2` will result in $1H_2O_1^0 + 1C_1O_2^0$, or simply $H_2O + CO_2$
- `Fe;3 + 3e` will result in $1Fe_1^{3+} + 3e_1^{1-}$, or simply $Fe^{3+} + 3e^-$

8 Reaction

A Reaction contains exactly two (2) ReactionSides, seperated by either `=>` or $\rightarrow$ (`U+2192`) to show a one-side reaction (to the right), or `<=>` or $\rightleftharpoons$ (`U+21CC`) to show an equilibrium.

8.1 Examples

- `2H2 + O2 <=> 2H2O` will result in $2H_2^0 + 1O_2^0 \rightleftharpoons 2H_2O_1^0$, or simply $2H_2 + O_2 \rightleftharpoons 2H_2O$
- `Fe;3 + 3e` $\rightleftharpoons$ `Fe` will result in $1Fe_1^{3+} + 3e_1^- \rightleftharpoons 1Fe_1^0$, or simply $Fe^{3+} + 3e^- \rightleftharpoons Fe$

8.2 Bugs

- It is currently not possible to use `<=` or $\leftarrow$ (`U+2190`) to indicate a one-way reaction to the left.
- Using `<` or `<=` as sign is equal to using `<=>`. This can lead to confusing errors.
- $\rightleftharpoons<>\rightarrow\rightleftharpoons>\rightleftharpoons\rightarrow<\rightleftharpoons=\rightarrow=\rightleftharpoons=<\rightarrow<\rightleftharpoons\rightleftharpoons>==\rightarrow=$ is seen as a valid sign, equal to `<=>`
- While the first (part of a) sign has to be between the two ReactionSides, any other (part of a) sign can be places everywhere to the right of it, and it will be ignored, except when it indicates an equilibrium, in which case the whole reaction will be converted to an equilibrium. *i.e.* `H2 => 2H;1 + 2<=>e` will be equal to `H2 <=> 2H; + 2e`