Atom 

Your worries Argon

Team: HackWorse

Atom

- Chemistry, simplified
- Algorithmic computational solution for chemical reactions

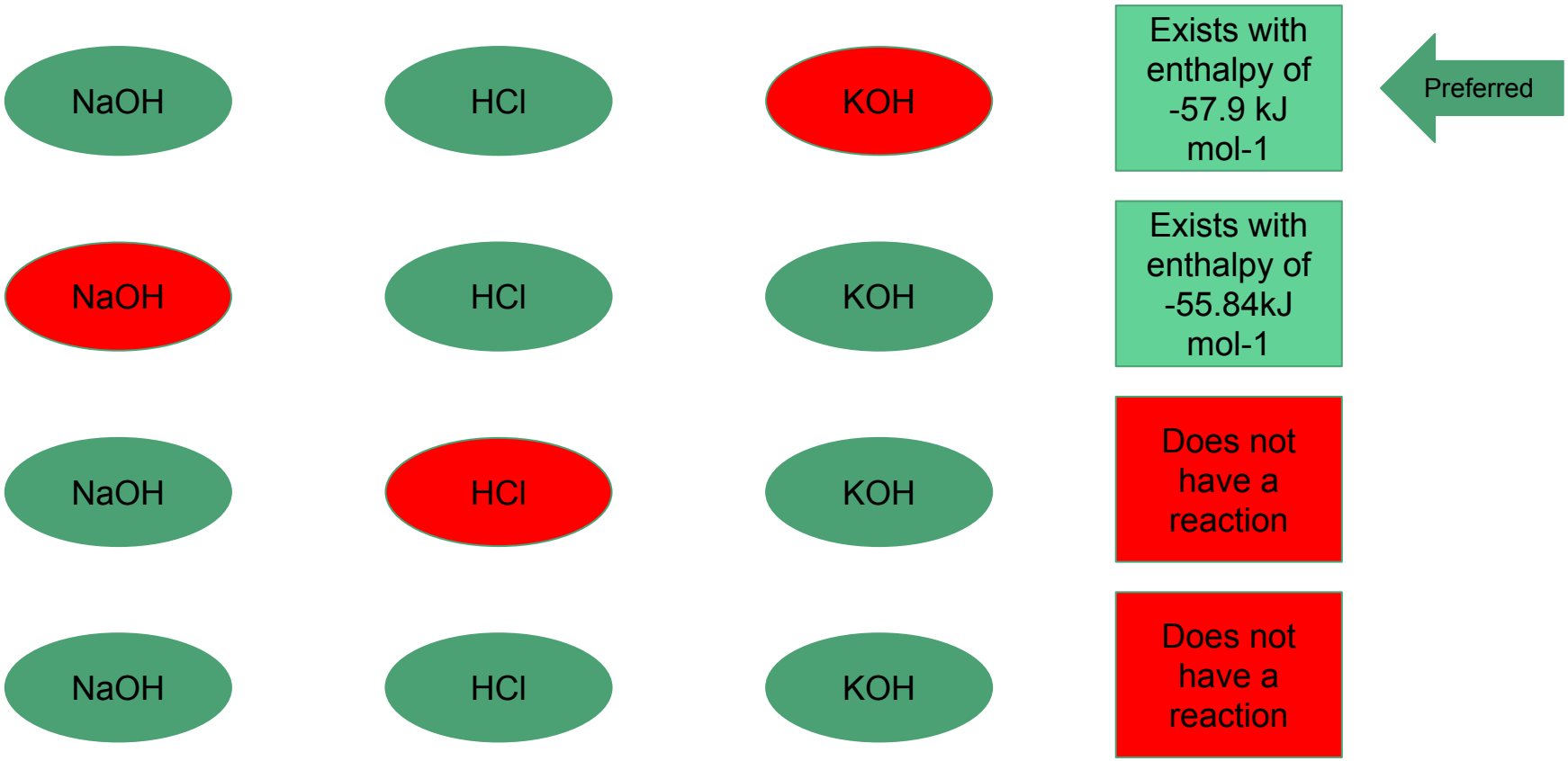
Features

- Solves convoluted reactions
- Balances chemical equations
- Depicts intermediate steps in a chain reaction
- Provides an interface for fetching definitions, product/reactant details, etc

The Algorithm

- A subset of reactants need to be considered to determine the series of reactions that will occur with the given products
- We consider them as masks and iterate through possible reactants and store the reaction with the highest negative enthalpy
- The final product is obtained after all the possible reactions are complete
- The balanced equations are displayed along the way

The Algorithm for NaOH + HCl + KOH



Chain Reactions

products $CaCO_3 + S + H_2O + O_2$

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The following equations were used to arrive at the final product

$2\ H_2O + 3\ O_2 + 2\ S \rightarrow 2\ H_2SO_4$

$1\ CaCO_3 + 1\ H_2SO_4 \rightarrow 1\ CO_2 + 1\ CaSO_4 + 1\ H_2O$

The final product is

$2\ CaCO_3 + 3\ O_2 + 2\ S + 1\ H_2O \rightarrow 2\ CO_2 + 2\ CaSO_4 + 1\ H_2O$

Algorithms/ Technologies

1. Recursive Gaussian elimination: Balancing chemical reactions
2. Iterative bitmasking: To calculate potential products based on Enthalpy
3. Zulip: Chat platform for building the intelligent bot
4. BeautifulSoup/urllib: Web scraping
5. Wikipedia/Google APIs: Populating data
6. Sympy: Computations have been done using Sympy

Majority of development has been done using Python 3.6.9

Demonstration:

https://www.youtube.com/watch?v=xw-rXj-ALys

Devfolio:

https://devfolio.co/submissions/atom

GitHub:

https://github.com/mnaveenkumar2009/HackWorse