

Sample: ← is the single input / output for experiments

- ID
- name
- user

- chemical compounds: ← compound is useful to describe the reaction

- chemical substance(s)
 - INCHI
 - name
 - molecular mass
 - concentration / amount
 - electron distribution, potentials, etc...

use a different name, e.g.
chemical species

- geometry
- physical state (solid, liquid, ...)
- amount
- role in the experiment (catalyst, carrier, etc.)

- property 1

- property 2

- ...