Preliminary remarks

SPARQL endpoints:
- rhea.rdf does not contain the cross-references to UniProt protein entries. They are available through the UniProt SPARQL endpoint (https://sparql.uniprot.org/sparql).

In Rhea RDF (rhea.rdf), all data are represented as subclasses of rdfs:Class, i.e. there are no instances.
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Conventions

Namespaces / prefixes:
  rh:  <http://rdf.rhea-db.org/>  
  rdfs: <http://www.w3.org/2000/01/rdf-schema#>  
  ch:   <http://purl.obolibrary.org/obo/>  
  ch2: <http://purl.obolibrary.org/obo/chebi#>  
  ch3: <http://purl.obolibrary.org/obo/chebi/>  
  up:  <http://purl.uniprot.org/core/>  
  ec:  <http://purl.uniprot.org/enzyme/>  

ch:CHEBI** == (rdfs:subClassOf ch:CHEBI_24431) or (rdfs:subClassOf ch:CHEBI_36342)  
ch:CHEBI_24431 chemical entity  
ch:CHEBI_36342 subatomic particle
Reactions, sides and participants

RHEA:10736  (APPROVED)
a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH


- **Reaction Side**: a primary alcohol
  - CHEBI:15794
  - Formula: C2H5OH
  - Charge: 0

- **Reaction Side**: NAD^+ (rh:transformableTo)
  - CHEBI:57540
  - Formula: C2H9N3O14P2
  - Charge: +2

- **Reaction Side**: an aldehyde
  - CHEBI:77478
  - Formula: C2H4O2
  - Charge: +1

- **Reaction Side**: H^+
  - CHEBI:15376
  - Formula: H
  - Charge: +2

**Reaction Participant**:

- rh:Reaction
- rh:ReactionSide
- rh:ReactionSide
- rh:transformableTo
- rh:transformableTo
- rh:contains
- rh:contains
- […]

reaction side

reaction participant
Definition:
A chemical or transport reaction of biological interest with unspecified direction. It is composed of two reaction sides. 

All the reactions published by Rhea are rdfs:subClassOf of rh:Reaction.
Definition:
A chemical or transport reaction (rh:Reaction) is composed of two reaction sides (rh:ReactionSide), sometimes denoted as left and right reaction sides.

In a rh:Reaction, the rh:ReactionSide are arbitrarily defined. They are linked by the predicate rh:side.

In a rh:DirectionalReaction, one rh:ReactionSide represents the substrate(s) (reactant(s), input) of the reaction, whereas the other represents the product(s) (output). In that case, the predicates rh:substrate and rh:product are used to denote the links.

In a rh:BidirectionalReaction, depending on the context, one rh:ReactionSide represents either the substrate(s) or the product(s). In that case, the predicate rh:substrateOrProduct is used to denote the links.

The link between the two reaction sides of a given reaction is denoted by the rh:transformableTo predicate.

A rh:ReactionSide gathers all the reaction participants (rh:ReactionParticipant) that are transformed into another rh:ReactionSide.
Reaction and reaction sides (example)

```
"a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH"
```
Definition: A chemical entity (subclass of rh:Compound) that is transformed in a chemical reaction or translocated in a transport reaction. There are three kinds of participants: small molecules (rh:SmallMolecule), macromolecules (rh:GenericCompound), and polymers (rh:Polymer).

A reaction side (rh:ReactionSide) contains (rh:contains) participants (rh:ReactionParticipant). The stoichiometric coefficient of a participant is defined in a subproperty of rh:contains (rh:contains1, rh:contains2, rh:containsN,...).
"5-oxo-L-proline + ATP + 2 H2O = ADP + H(+) + L-glutamate + phosphate"
A diagram illustrating the relationships between different types of compounds, specifically highlighting the classes `rh:ReactionParticipant`, `rh:SmallMolecule`, `rh:GenericCompound`, and `rh:Polymer`. The diagram also includes a classification of `rdfs:subClassOf rh:Compound`, indicating a hierarchical structure within the Rhea ontology.
Definition:
A chemical compound that is a low molecular weight (MW) molecule involved as participant, in a chemical or transport reaction.
It is a subclass of rh:Compound.
It is a subclass of a given ChEBI chemical entity.
"ethanol + NAD(+) = acetaldehyde + H(+) + NADH"

"a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH"
Definition:
A macromolecule involved as participant, in a chemical or transport reaction. Its chemical structure is not fully described but simplified to the functional group(s) involved in the reaction. These reactive part(s) are chemically defined. rh:GenericCompound represents three kind of macromolecules: proteins (rh:GenericPolypeptide), nucleic acids (rh:GenericPolynucleotide) and heteropolysaccharides (rh:GenericHeteropolysaccharide). rh:GenericCompound is a subclass of rh:Compound and is subclassed in rh:GenericPolypeptide, rh:GenericPolynucleotide, rh:GenericHeteropolysaccharide.
A protein (polypeptide sequence).
It is a subclass of rh:GenericCompound.

A DNA or RNA nucleic acid (polynucleotide sequence).
It is a subclass of rh:GenericCompound.

An heteropolysaccharide.
It is a subclass of rh:GenericCompound.
**Definition:**
The reactive part of a macromolecule (rh:GenericCompound). It has a defined chemical structure.
It is a subclass of a given ChEBI chemical entity.
**Definition:**
A simple polymer (a molecule with defined repeated unit(s) and polymerization index (PI) involved as participant, in a chemical or transport reaction. It is defined by an underlying ChEBI polymer and a PI (n, n+1, n-1, etc). It is a subclass of rh:Compound.
"[(1->4)-alpha-D-galacturonosyl](n) + UDP-alpha-D-galacturonate = [(1->4)-alpha-D-galacturonosyl](n+1) + H(+) + UDP"
**Transport reaction and Location**

<table>
<thead>
<tr>
<th>rh:isTransport</th>
<th>Boolean flag indicating if a reaction is a transport reaction. In transport reaction, the same compound is found in both reaction sides but with a different location.</th>
</tr>
</thead>
<tbody>
<tr>
<td>rh:Location</td>
<td>The location of a reaction participant (rh:ReactionParticipant) in a transport reaction.</td>
</tr>
<tr>
<td>rh:In</td>
<td>It is a subclass of rh:Location.</td>
</tr>
<tr>
<td>rh:Out</td>
<td>It is a subclass of rh:Location.</td>
</tr>
</tbody>
</table>

![Diagram showing the relationship between `rh:Reaction`, `rh:ReactionSide`, `rh:ReactionParticipant`, `rh:isTransport`, `rh:contains`, `rh:location`, `rh:In`, and `rh:Out`.](diag.png)
Transport reaction (example)

"ATP + H2O + sulfate(out) = ADP + H(+) + phosphate + sulfate(in)"

- rdfs:subClassOf rh:Reaction
- rdfs:subClassOf rh:SmallMolecule
- rdfs:subClassOf rh:Reaction
- rdfs:subClassOf rh:Side
- rdfs:subClassOf rh:Location
- rdfs:label "sulfate"
- ch2:smiles "[O-]S([O-])(=O)=O"
## Links to EC numbers and cross-references

<table>
<thead>
<tr>
<th><strong>rh:ec</strong></th>
<th>The nomenclature committee of the IUBMB defines enzyme classes based, among others, on the catalyzed reaction(s). The enzyme classes are identified by an Enzyme Commission number (EC number). rh:ec is used between a rh:Reaction (the catalyzed reaction) and a complete EC number (the enzyme class).</th>
</tr>
</thead>
</table>
| **rdfs:seeAlso** | The cross-references to other metabolic/protein resources. There are two kind of cross-references:  
- Manually curated (KEGG reaction, MetaCyc reaction, EcoCyc reaction)  
- Computed based on ChEBI participants (Reactome (hsa reaction), MACiE reaction)  
The MetaCyc/EcoCyc reactions are linked to either rh:Reaction (no define direction), rh:DirectionalReaction or rh:BidirectionalReaction.  
The KEGG reactions are linked to rh:BidirectionalReaction.  
The cross-references to UniProt protein entries are not part of the rhea.rdf distribution. They are available from the uniprot.rdf distribution. |
EC numbers and cross-references (example)

- **rh:10736**
  - (rdfs:subClassOf rh:Reaction)
  - rh:ec
  - rh:bidirectionalReaction

- **rh:10738**
  - (rdfs:subClassOf rh:DirectionalReaction)
  - rh:bidirectionalReaction
  - rdfs:seeAlso
  - rdfs:seeAlso
    - <http://identifiers.org/kegg.reaction/R00623>

- **rh:10739**
  - (rdfs:subClassOf rh:BidirectionalReaction)
  - rdfs:seeAlso
  - rdfs:seeAlso
  - rdfs:seeAlso
The relation between a rh:Reaction, a rh:DirectionalReaction or rh:BidirectionalReaction and a PubMed URI.
Reaction hierarchical classification

- **rh:12044**
  - (rdfs:subClassOf rh:Reaction)
  - rdfs:label
  - rh:equation
    - "a triacylglycerol + H2O = a diacylglycerol + a fatty acid + H(+)

- **rh:35667**
  - (rdfs:subClassOf rh:Reaction)
  - rdfs:label
  - rh:equation
    - "a triacylglycerol + H2O = a 1,2-diacylglycerol + a fatty acid + H(+)"

- **rh:38379**
  - (rdfs:subClassOf rh:Reaction)
  - rdfs:label
  - rh:equation
    - "(9Z)-octadecenoate + 1,2-di-(9Z-octadecenoyl)-glycerol + H(+) = 1,2,3-tri-(9Z-octadecenoyl)-glycerol + H2O"
### Rhea curation status

<table>
<thead>
<tr>
<th>rh:Status</th>
<th>Curation status of a reaction (rh:Reaction).</th>
</tr>
</thead>
<tbody>
<tr>
<td>rh:Approved</td>
<td>Manually curated reaction. The reaction is evidenced and is chemically balanced at the level of mass and charge. It is a subclass of rh:Status.</td>
</tr>
<tr>
<td>rh:Preliminary</td>
<td>Manually curated reaction. The reaction is indirectly evidenced and/or some knowledge is missing (e.g. it has some undefined participant(s)). The reaction is possibly not balanced at the level of mass and charge. It is a subclass of rh:Status.</td>
</tr>
<tr>
<td>rh:Obsolete</td>
<td>The reaction is no more valid.</td>
</tr>
</tbody>
</table>

(rdfs:subClassOf rh:Status)
Definition:
A chemical or transport reaction of biological interest with a direction specified by substrates and products. All the directional reactions published by Rhea are rdfs:subClassOf rh:DirectionalReaction.
"acetaldehyde + H(+) + NADH => ethanol + NAD(+)"

"ethanol + NAD(+) = acetaldehyde + H(+) + NADH"

"an aldehyde + H(+) + NADH => a primary alcohol + NAD(+)"

"a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH"
Definition:
A chemical or transport reaction of biological interest which can happen in one direction or the other, depending on the physiological conditions.

All the bidirectional reactions published by Rhea are rdfs:subClassOf rh:BidirectionalReaction.
"ethanol + NAD(+) ⇌ acetaldehyde + H(+) + NADH"

rh:contains
..."ethanol + NAD(+) = acetaldehyde + H(+) + NADH"
...
"ethanol + NAD(+) ⇔ acetaldehyde + H(+) + NADH"

"a primary alcohol + NAD(+) = an aldehyde + H(+) + NADH"