rxnSMILES4AtomEco:

rxnSMILES4AtomEco is a package that provides functions to calculate the atom economy of chemical reactions using reaction SMILES.

Features:

- Calculation of atom economy for reactions
- Handling of multiple reactions in a single calculation
- Support for different types of reaction SMILES
- Programmatic output of atom economy numerical value: verbose- and numberic output.

Usage:

To use the package, simply import the relevant functions and provide reaction SMILES as input.

Example verbose output:

```
from rxnSMILES4AtomEco import atom_economy
reactions_smiles = "C.O>catalyst>{3}[HH]"
atom_economy(reactions_smiles)

::: {.cell}
``` {.python .cell-code}
from rxnSMILES4AtomEco import atom_economy
reactions_smiles = "C.O>catalyst>{3}[HH]"
atom_economy(reactions_smiles)
```

:::
```

Example numeric output:

```
from rxnSMILES4AtomEco import get_atom_economy
reactions_smiles = "C.O>catalyst>{3}[HH]"
value = get_atom_economy(reactions_smiles)
print(value)

::: {.cell}
``` {.python .cell-code}
from rxnSMILES4AtomEco import get_atom_economy
reactions_smiles = "C.O>catalyst>{3}[HH]"
value = get_atom_economy(reactions_smiles)
print(value)
```

:::
```