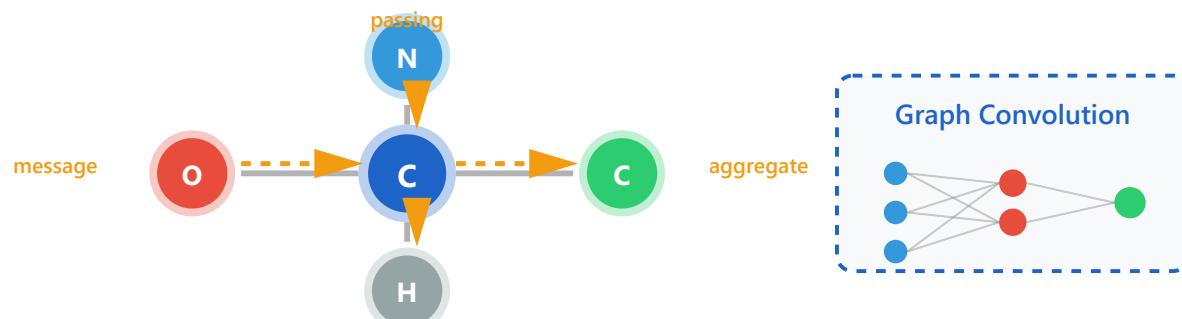


# Graph Neural Networks



● Atoms (Nodes)

— Bonds (Edges)

— Message Flow

## Molecular graphs

Atoms as nodes, bonds as edges

## Message passing

Information flow between atoms

## Graph convolutions

Feature aggregation operations

## Attention mechanisms

Weighted information aggregation

## Pooling strategies

Graph-level representations