



### Initial atom features

Feature

Atom type

Degree

Explicit Valence

Hybridization

H count

Electronegativity

Atomic number

Part of an aromatic ring

### atom message

$$\text{atom message} = \mathbf{A}_{\text{bond}(1,2)} \times \text{atom 2} + \mathbf{A}_{\text{bond}(1,3)} \times \text{atom 3}$$

### atom embedding

$$\text{atom embedding} = \text{RNN}(\text{atom message}, \text{atom embedding})$$

Apply update in 2 to all atoms

### graph embedding

$$\text{graph embedding} = f_{\text{down}} \left( \sum_{\text{atoms}} \sigma[f_{\text{gate}}(\text{atom embedding})] f_{\text{up}}(\text{atom embedding}) \right)$$