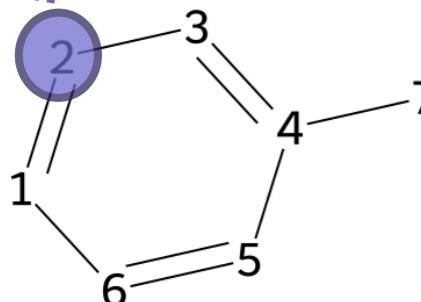
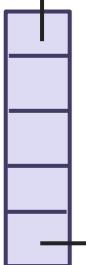


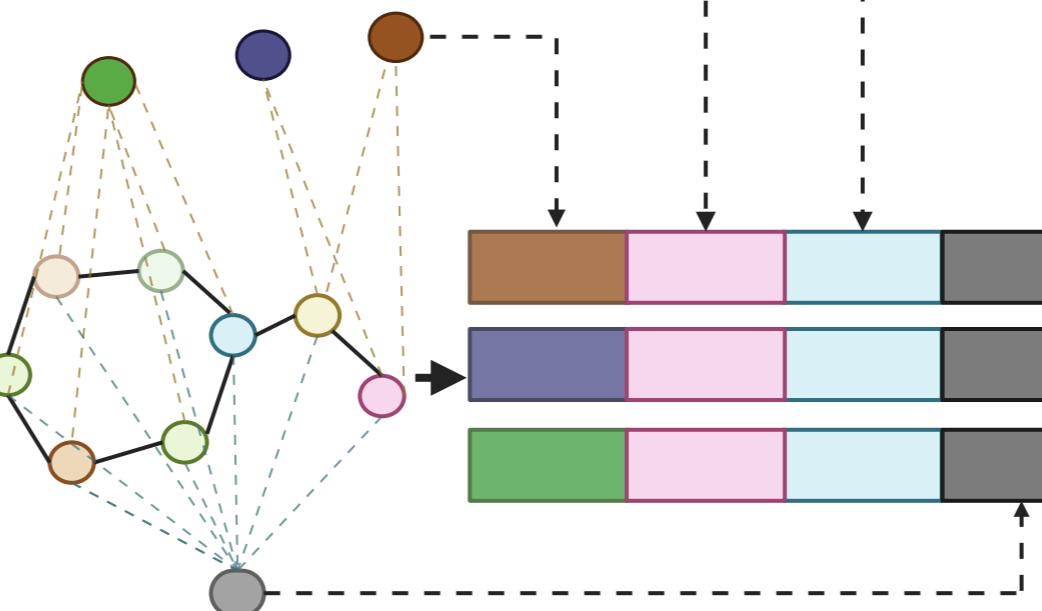
- Atom type
- Connection degree
- Hybridization number
- Formal Charge
- Is aromatic ?


 $N_{\text{atom}} \times d_0$

	3	4	201
1	0	0	1
2	0	0	1
3	0	0	1
4	0	0	1
5	0	0	1
6	0	0	1
7	1	1	0
8	1	1	0

 $N_{\text{atom}} \times F$

Graph
Convolution
Network

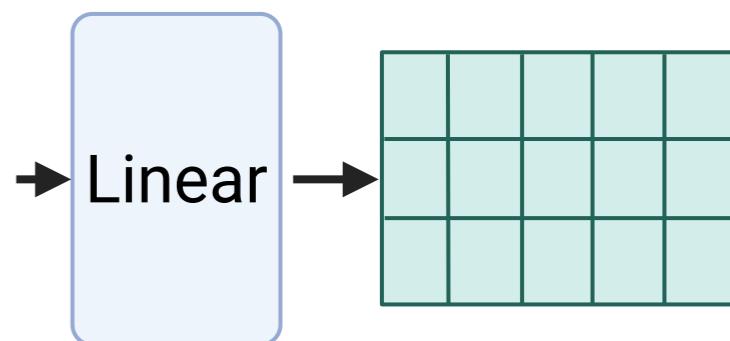

 $N_{\text{atom}} \times D_{\text{graph}}$

0	
1	
2	
3	
4	
.	
.	
.	
160	

Positional
embedding

0	
1	
2	
3	
4	
.	
201	
.	
204	

Functional groups
embedding


 $F \times D_{\text{concat}}$
 $F \times D$