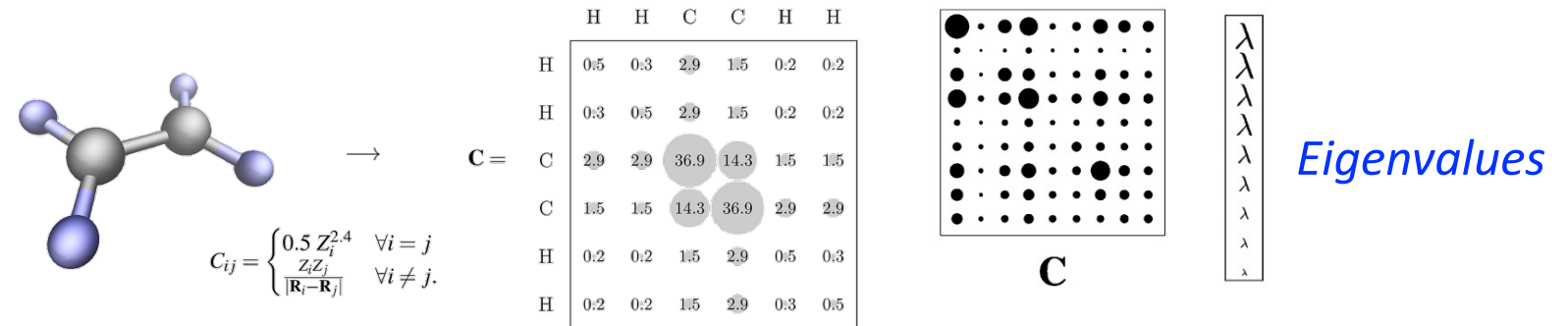


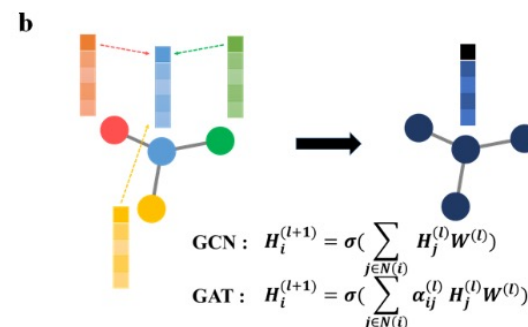
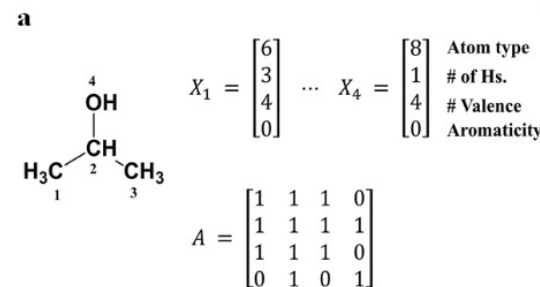
- Input features using 3D coordinates



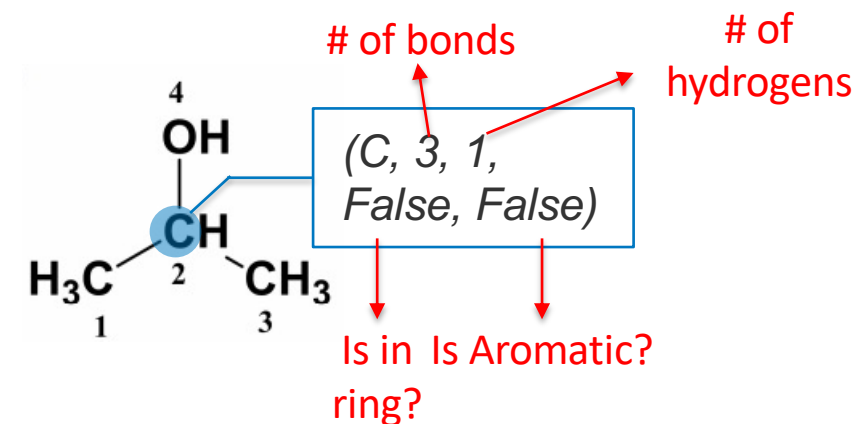
$$C_{ij} = \begin{cases} 0.5 Z_i^{2.4} & \forall i = j \\ \frac{Z_i Z_j}{|R_i - R_j|} & \forall i \neq j. \end{cases}$$

*J. Chem. Theory Comput.*, **2013**, 9, 3404.

- Input features w/o 3D coordinates

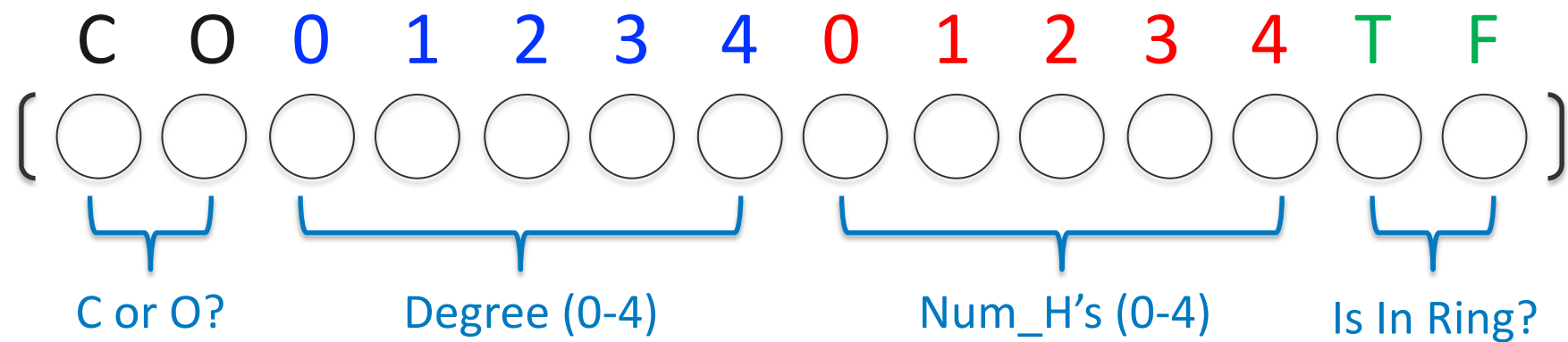


- Atom features



*arXiv: 1805.10988v2*

# One-hot Vector - Example



e.g.) Carbon, Degree 4, 3 hydrogens, not in the ring  
(1,0, 0,0,0,0,1, 0,0,0,1,0, 0, 1)