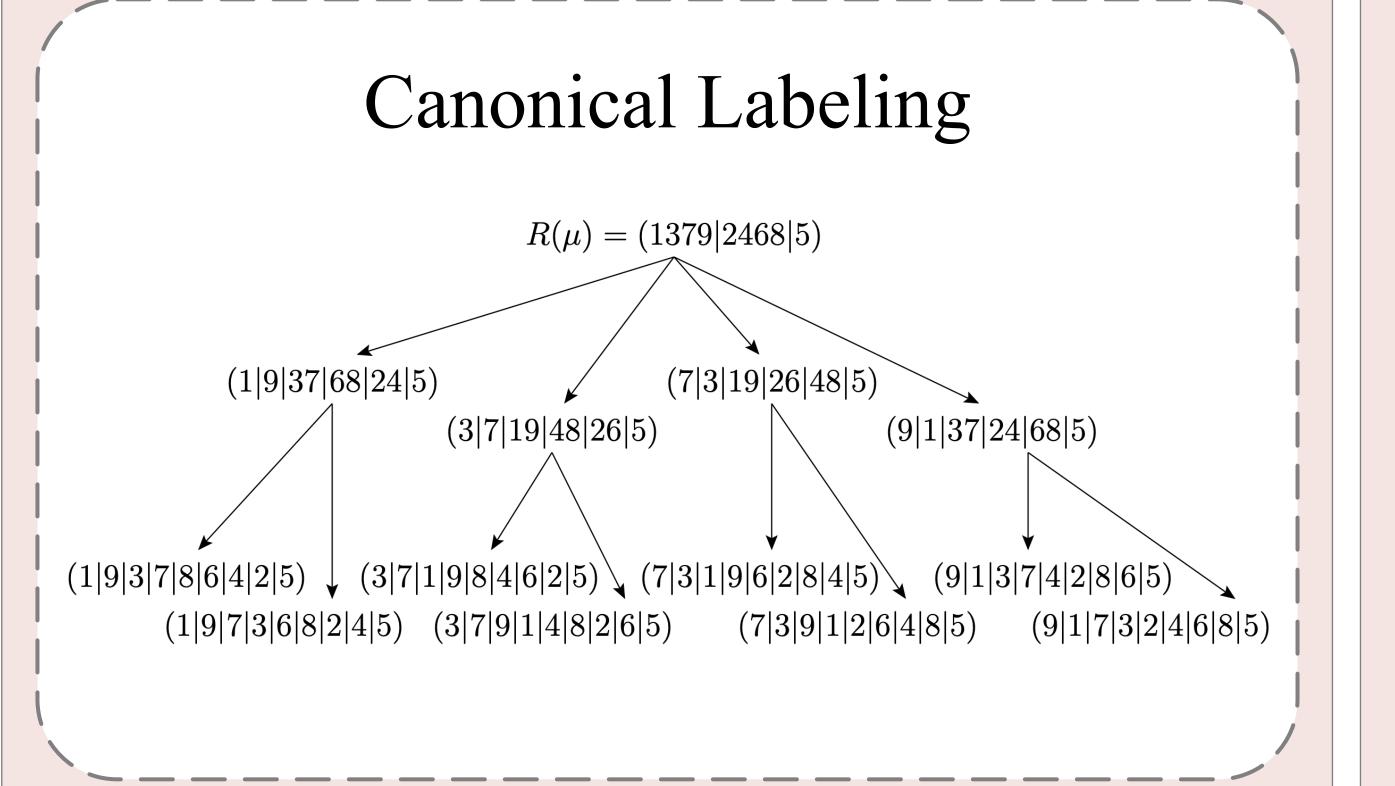
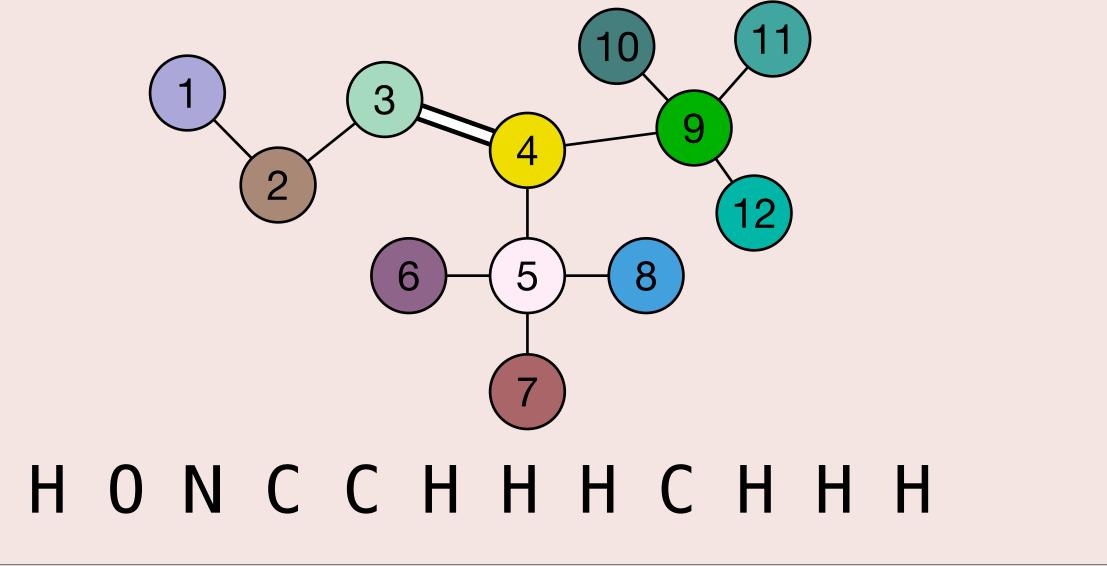
(0.08, -0.69, -1.10) (0.01, 0.00, -0.03) (-0.10, 1.50, 0.00) (0.07, 0.13, -2.24)

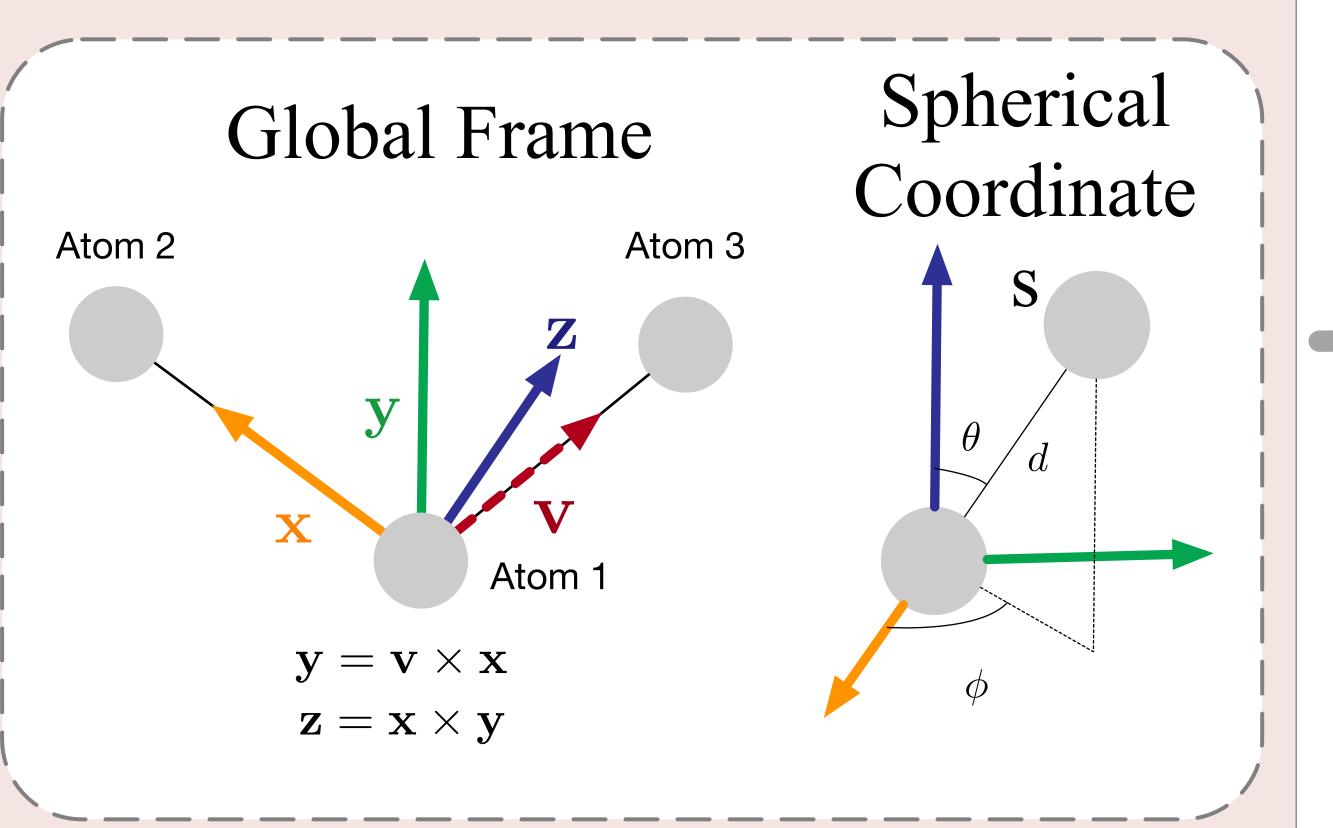
Input Molecule

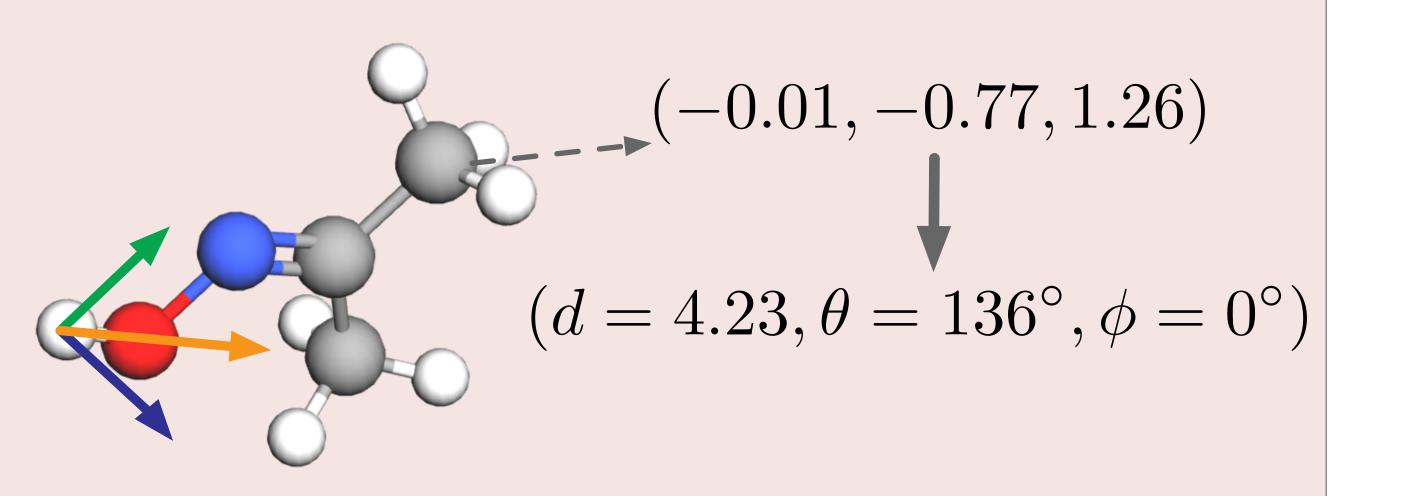
Serialization



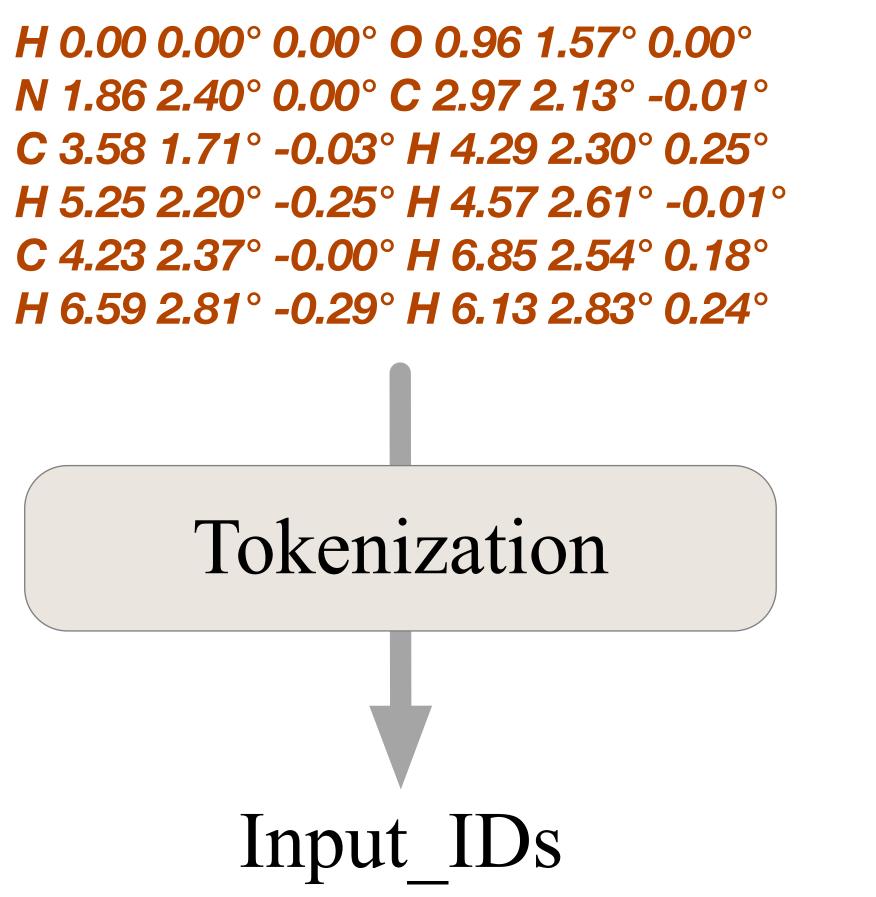


Spherical Representation

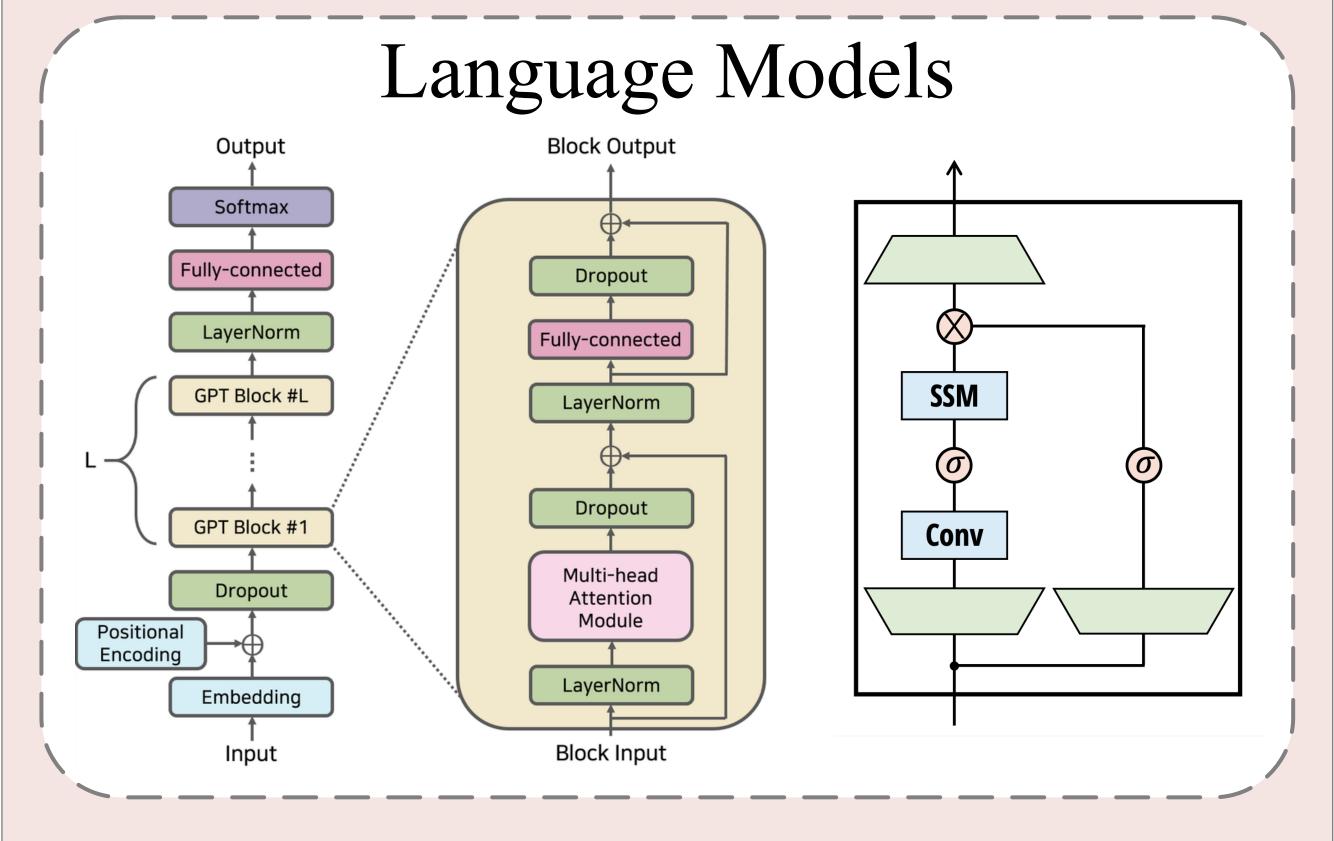




3D Sequence



Training & Generation





Unconditional generation Input: *H 0.00 0.00*° 0.00° O 0.96 1.57° ...





Condition: ε_{homo} property *-5.9484*

Input: *H 0.00 0.00*° 0.00° O 0.96 1. 57