

(a)

Stage 1: fragments-to-moleculeFragments
encoder

Transformer encoder

(Teacher forcing)

SMILES
tokens

Transformer decoder

(Weights transfer)

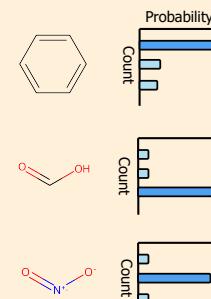
Multi-spectra
encoder

Transformer encoder

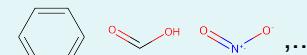
(Teacher forcing)

SMILES
tokens

Transformer decoder

**Stage 2: spectra-to-molecule**

(b)

Fragments encoder

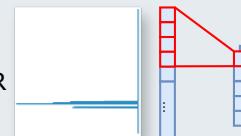
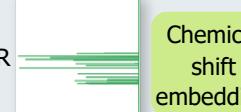
Fragment embedding

2,1,3,...

Count embedding

MLP
(GELU + LN)**Multi-spectra encoder**

IR

Transformer
encoder ^1H NMRTransformer
encoder ^{13}C NMRChemical
shift
embeddingTransformer
encoder