

A APPENDIX

A.1 MODEL INITIAL INPUT

Given an input graph $G(V, E, P)$, our objective is to determine the input node feature matrix X and spatial positional encoding S utilizing Equation 3. In this section, we present the methodology for obtaining X . For the atomic-level approach, we initially obtain the node embedding from the pre-trained Uni-Mol model Zhou et al. (2023). Since Uni-Mol solely incorporates atom type information, we manually augment the node features with additional attributes and concatenate them accordingly.

number	feature	range
1	chirality	[0, 3]
2	charge	[0, 10]
3	hyb	[0, 6]
4	numH	[0, 8]
5	valence	[0, 7]
6	degree	[0, 10]
7	aromatic	[0, 1]
8	is_protein	[0, 1]

Table 2: Node feature table