

Describe molecules by a heterogeneous graph neural network with transformer-like attentions for supervised property predictions

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Table S1. The number of parameters in different setting of HiddenState and LayerNum. The column HiddenState represents the dimension of the hidden states of a given model. The column LayerNum is the number of graph layers. The NumParam is the total number of the MolHGT parameters.

HiddenState	LayerNum	NumParam	HiddenState	LayerNum	NumParam
200	2	3461643	520	2	23137132
200	3	5035293	520	3	33708542
200	4	6608943	520	4	44279952
240	2	4968392	560	2	26821941
240	3	7229962	560	3	39079671
240	4	9491532	560	4	51337401
280	2	6747421	600	2	30778129
280	3	9821711	600	3	44846979
280	4	12896001	600	4	58915829
320	2	8798249	640	2	35007438
320	3	12810059	640	3	51012208
320	4	16821869	640	4	67016978
360	2	11121778	680	2	39508006
360	3	16195908	680	3	57573496
360	4	21270038	680	4	75638986
400	2	13716986	720	2	44281815
400	3	19978236	720	3	64532825
400	4	26239486	720	4	84783835
440	2	16585015	760	2	49326763
440	3	24158185	760	3	71888093
440	4	31731355	760	4	94449423
480	2	19724603	800	2	54645072
480	3	28734493	800	3	79641522
480	4	37744383	800	4	104637972