Supporting Information: Equivariant Neural Networks Utilizing Molecular Clusters for Accurate Molecular Crystal Lattice Energy Predictions

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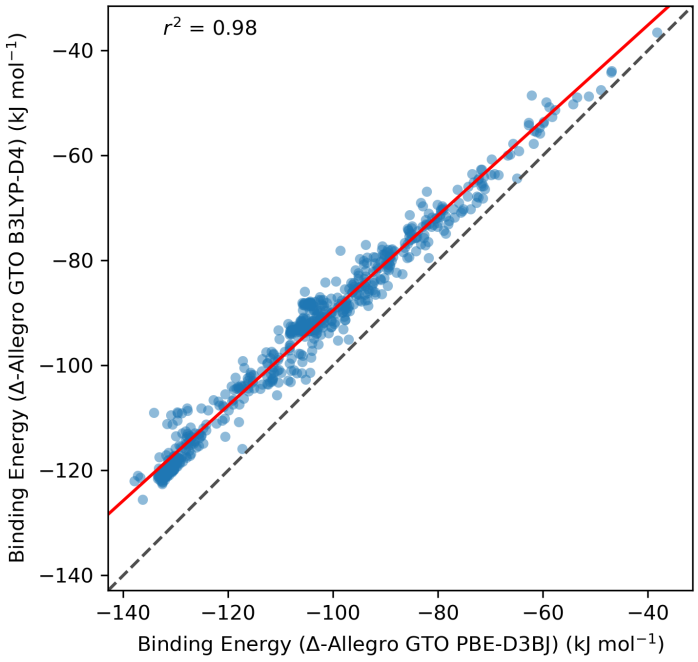

Figure S1: Parity plot for the binding energies predicted by the Δ-Allegro model ($r_{\text{cutoff}} = 6.0$ Å) using PBE-D3BJ and B3LYP-D4 theoretical methods.

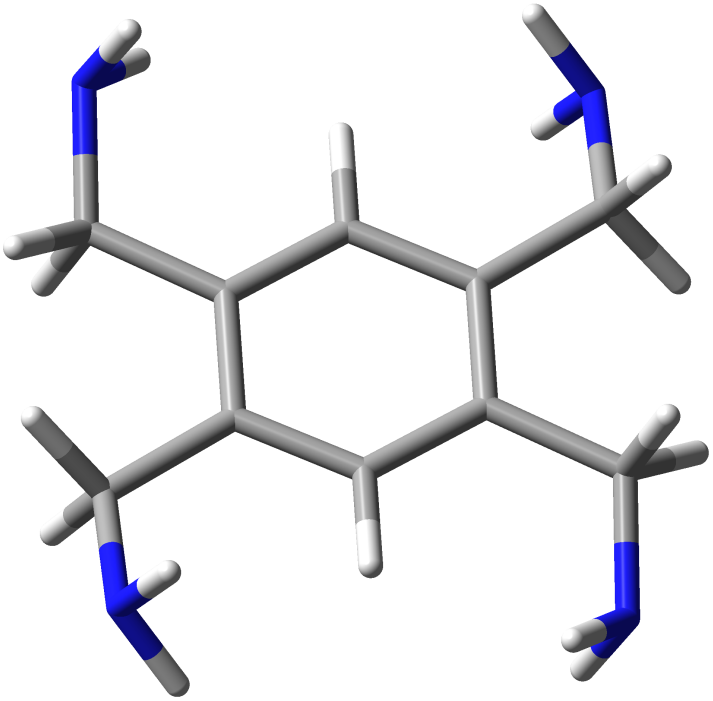

Figure S2: Alternate conformation for Benzene-1,2,4,5-tetrayltetramethanamine.

Table S1: Training and validation errors of the Allegro models on the molecular cluster dataset for Benzene-1,2,4,5-tetrayltetramethanamine.

Model	Training Energy MAE (mHa)	Validation Energy MAE (mHa)
Allegro	0.414	0.545
Δ-Allegro	0.322	0.418

Table S2: Training and validation errors of the Allegro model ($l_{max} = 3$, $multiplicity = 2$) on the molecular cluster dataset for oxabicyclo[3.2.0]hepta-1,4-diene.

Model	Training Energy MAE (mHa)	Validation Energy MAE (mHa)
Allegro	0.09	0.13

Table S3: Training and validation errors of the Allegro model ($l_{max} = 3$, $multiplicity = 2$) on the molecular cluster dataset for Hydantoin.

Model	Training Energy MAE (mHa)	Validation Energy MAE (mHa)
Allegro	0.20	0.41