## A Machine Learning Based Approach to Reaction Rate Estimation Supporting Information

Matthew S. Johnson and William H. Green\*

Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, United States

E-mail: whgreen@mit.edu

## 1 Histograms of Errors for Additional Families

We present histograms of errors for three additional reaction families: radical recombination, disproportionation, and ketoenol. These families were excluded from the original manuscript primarily because they are smaller, have lower variances in their rate coefficients and/or less homogeneous training sets than the included families. The training sets for Radical recombination and disproportionation are best described as a combination of experimentally informed estimates with some careful calculations. Ketoenol's training set is mostly calculations.



Figure 1: Histogram for radical recombination errors. Dark green is overlap. Trained on 145 reactions.



Figure 2: Histogram for disproportionation errors. Dark green is overlap. Trained on 137 reactions.



Figure 3: Histogram for ketoenol errors. Dark green is overlap. Trained on 8 reactions.