Supporting information for:

Constant Size Molecular Descriptors For Use With Machine Learning

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1 Bond lengths for connectivity counts

The connectivity count features in Section 5.3 of the main manuscript rely on identifying either the presence of a bond or the bond order. The values in Table S1 were summed to give the atom separation corresponding to the upper limit of a given bond type. The bond order is assigned based on this upper limit and the maximum allowed bond order between the respective elements. For features that rely on only the presence of a bond, a bond is assumes to be present if the atoms are closer than the cutoff for a single bond.

Table S1: All distances listed are in Å.

Element	Single	Aromatic	Double	Triple
С	0.850	0.720	0.690	0.620
Cl	1.045			
\mathbf{F}	1.230			
H	0.600			
N	0.740	0.655	0.630	0.565
O	0.695	0.620	0.590	0.530
P	1.110	0.985	0.945	
\mathbf{S}	1.070	0.945	0.905	

2 Implementation of encoded distance features

For the encoding distance features of Section 5.4 of the main manuscript, there are a few parameters that must be adjusted. These include the β for the encoding functions of Table 2, the start and end points of the grids, and the number of grid points. These parameters were chosen based on model performance for QM7 atomization energies, along with the time and memory involved in the computations. The chosen values are $\beta = 20$, and a grid with $N_{grid} = 100$ points between 0.2Å and 6Å. The following shows how model performance varies with each parameter in turn, holding the remaining parameters at their chosen value.

Figure S1 shows that there is a broad range of values for β that give roughly equal performance on QM7 atomization energies. We chose 20 for β because it is in the center of this range. For large β , the encoding function approaches that of the spike encoding function, leading to poor performance. The dependence on β for $\mathbf{2}^{LP}$ is similar to that seen for $\mathbf{2}^{NP}$ in Figure S1, so $\beta = 20$ was used for both normal and logistic encoding functions.

Figures S2 and S3 show model performance and computation time as a function of the number of grid points, N_{grid} . The computation time increases nearly linearly with N_{grid} . The model performance improves substantially up to about $N_{grid} = 50$ and then levels off. A value of 100 was chosen as a reasonable compromise between performance and computation time.

The dependence of model performance on the start and end points of the grid are shown

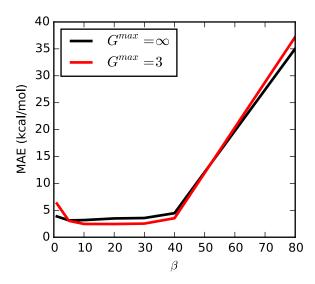


Figure S1: Dependence of MAE on β for KRR models of the QM7 atomization energy. The models use $\mathbf{2}^{NP}$ as a feature vector.

in Figures S5 and S6, respectively. The results are consistent with the distribution of atomic separations in Figure S4. For G^{max} of 3, the distributions lie between 0.8 and 4 Å. For $G^{max} = \infty$, the distributions lie between 0.8 and about 6 Å. The model performance is independent of starting point for values below about 1.0 Å (Figure S5). As the end point is increased in Figure S6, performance initially improves, until about 6 Å and then degrades for larger values. This degradation can be attributed to the loss of grid resolution in the main range of values. We chose a start value of 0.2Å and an end value of 6.0 Å to span the distribution of atomic separations in the QM7 data set, while retaining good model performance.

To reduce computation, we elected to remove all encoded ranges where there were no examples (in the case of the QM7 data set, this means 14 encoded ranges).

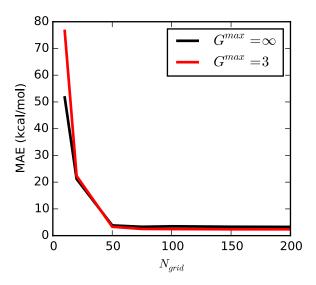


Figure S2: Dependence of MAE on number of grid points for KRR models of the QM7 atomization energy. The models use $\mathbf{2}^{NP}$ as a feature vector.

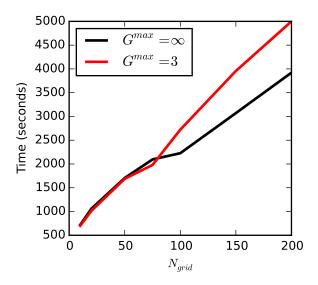


Figure S3: The relation between the time required for training/testing and the number of grid points.

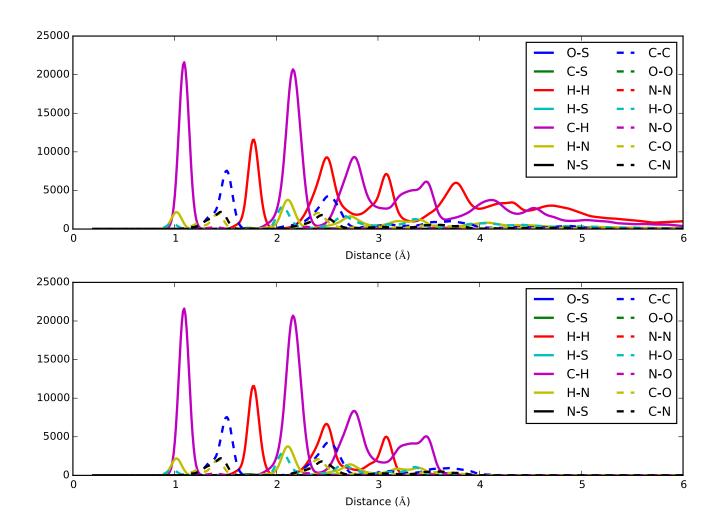


Figure S4: Distribution of bond distances in the QM7 data set, using the normal probability distribution as the encoding function. The upper panel has no restriction on atomic separations. The lower panel is for $G^{max}=3$.

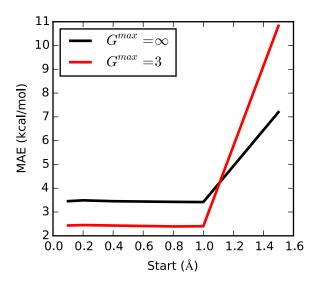


Figure S5: Dependence of MAE on the starting point for grid for KRR models of the QM7 atomization energy. The models use $\mathbf{2}^{NP}$ as a feature vector.

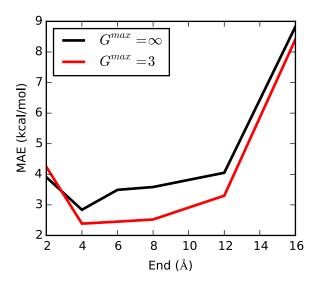


Figure S6: Dependence of MAE on the ending point for grid for KRR models of the QM7 atomization energy. The models use $\mathbf{2}^{NP}$ as a feature vector.

3 Results

Table S2: For the results dealing with learning rates (Table 5, Figure 4, and Figure 5), the following sets of hyperparameters were used.

Feature	α	γ	Kernel
$12^{NP}3^B4^B$	1e-7	1e-5	gauss
BoB	1e-9	1e-5	laplace
2^{LC}	1e-9	1e-5	gauss
2^B	1e-7	0.001	gauss

Tables S3 and S4 list MAEs from LRR and KRR models, respectively, of QM7 atomization energies. Fold lists the standard deviation across the 5 folds. Unless otherwise specified, all encoded distance features use the default values of the previous section. The notation for feature vectors is as in the main manuscript, with the addition of subscripts to encoded distance features to indicate parameters that differ from their default values. Integer subscripts refer to the value of G^{max} , with no subscript indicating $G^{max} = \infty$. Other changes from default values are listed as {key: value}, pairs.

Name	LRR	Fold	α
1	15.7007	0.2515	0.001
$1 \ 2^B$	8.5378	0.1485	0.1
$1\ 2^{B}\ 3$	6.2088	0.1291	0.1
$1\ 2^{B}\ 3\ 4$	5.2756	0.1588	0.1
$1\ 2^{B}\ 3\ 4\ 5$	4.2939	0.1087	1.0
$1\ 2^{B}\ 3\ 4^{B}$	4.5085	0.0763	1.0
$1\ 2^{B}\ 3\ 4^{B}\ 5$	3.7927	0.1324	1.0
$1 \ 2^B \ 3^B$	5.6513	0.1438	0.01
$1 \ 2^B \ 3^B \ 4$	4.9384	0.1694	0.1
$1\ 2^{B}\ 3^{B}\ 4\ 5$	4.0619	0.1123	1.0
$1 \ 2^B \ 3^B \ 4^B$	4.4827	0.0792	1.0
$1 \ 2^B \ 3^B \ 4^B \ 5$	3.7473	0.1413	1.0

$1~2^{LC}$	2.8034	0.1242	0.01
$1\ 2^{LC}\ 3$	2.5502	0.0735	0.01
$1\ 2^{LC}\ 3\ 4$	2.4542	0.0660	0.01
$1 \ 2^{LC} \ 3 \ 4^B$	2.0353	0.0332	0.1
$1 \ 2^{LC} \ 3^B$	2.2607	0.0374	0.01
$1 \ 2^{LC} \ 3^B \ 4$	2.2352	0.0436	0.01
$1 \ 2^{LC} \ 3^B \ 4^B$	2.0144	0.0394	0.1
$1 \ 2_1^{LC}$	6.3336	0.1485	0.01
$1\ 2_1^{LC}\ 3$	5.1905	0.1364	0.01
$1 \ 2_1^{LC} \ 3 \ 4$	4.3768	0.4273	0.001
$1 \ 2_1^{LC} \ 3 \ 4^B$	3.6673	0.1029	1.0
$1 \ 2_1^{LC} \ 3^B$	4.5679	0.2295	0.001
$1 \ 2_1^{LC} \ 3^B \ 4$	3.9977	0.1484	0.01
$1 \ 2_1^{LC} \ 3^B \ 4^B$	3.6471	0.1256	1.0
$1~2_2^{LC}$	2.8404	0.0561	0.001
$1 \ 2_2^{LC} \ 3$	2.7304	0.1345	0.001
$1\ 2_2^{LC}\ 3\ 4$	2.5988	0.0486	0.01
$1 \ 2_2^{LC} \ 3 \ 4^B$	2.0242	0.0405	0.1
$1 \ 2_2^{LC} \ 3^B$	2.4390	0.0456	0.01
$1 \ 2_2^{LC} \ 3^B \ 4$	2.3134	0.0534	0.01
$1 \ 2_2^{LC} \ 3^B \ 4^B$	2.0186	0.0464	0.1
$1~2^{LC}_3$	2.5950	0.0745	0.01
$1 \ 2_3^{LC} \ 3$	2.4634	0.0660	0.01
$1 \ 2_3^{LC} \ 3 \ 4$	2.3820	0.0663	0.01
$1 \ 2_3^{LC} \ 3 \ 4 \ 5$	2.3616	0.0714	0.1
$1 \ 2_3^{LC} \ 3 \ 4^B$	1.8184	0.0555	0.1
$1 \ 2_3^{LC} \ 3 \ 4^B \ 5$	1.8551	0.0652	0.1

$1 \ 2_3^{LC} \ 3^B$	2.1421	0.0584	0.01
$1 \ 2_3^{LC} \ 3^B \ 4$	2.1157	0.0730	0.01
$1\ 2_3^{LC}\ 3^B\ 4\ 5$	2.1545	0.0914	0.1
$1 \ 2_3^{LC} \ 3^B \ 4^B$	1.8220	0.0763	0.1
$1 \ 2_3^{LC} \ 3^B \ 4^B \ 5$	1.8467	0.0761	0.1
$1 \ 2_3^{LC} \ \{'\beta': \ 30.0\}$	2.4833	0.0662	0.01
$1 \ 2_3^{LC} \ \{'\beta': \ 30.0\} \ 3^B$	2.0831	0.0481	0.01
$1 \ 2_3^{LC} \ \{'\beta': \ 30.0\} \ 3^B \ 4^B$	1.7737	0.0677	0.1
$1\ 2_3^{NC}$	2.4833	0.0574	0.01
$1 2_3^{NC} 3^B$	2.0900	0.0476	0.01
$1 \ 2_3^{NC} \ 3^B \ 4^B$	1.7791	0.0677	0.1
$1 \ 2_3^{NC} \ \{'\beta': \ 30.0\}$	2.4728	0.0823	0.1
$1 \ 2_3^{NC} \ \{'\beta': \ 30.0\} \ 3^B$	2.0745	0.0614	0.1
$1 \ 2_3^{NC} \ \{'\beta': \ 30.0\} \ 3^B \ 4^B$	1.7480	0.0625	0.1
$1 \ 2_3^{NP}$	2.4711	0.0775	0.01
$1 \ 2_3^{NP} \ 3^B$	2.0992	0.0402	0.01
$1 \ 2_3^{NP} \ 3^B \ 4^B$	1.7641	0.0353	0.1
$1~2^{SC}_3$	2.8994	0.0542	0.1
$1 \ 2_3^{SC} \ 3^B$	2.4362	0.0608	0.1
$1 \ 2_3^{SC} \ 3^B \ 4^B$	2.0145	0.0427	1.0
$1 \ 2_3^{SC} \ \{'\beta': \ 30.0\}$	2.8994	0.0542	0.1
$1 \ 2_3^{SC} \ \{'\beta': \ 30.0\} \ 3^B$	2.4362	0.0608	0.1
$1 \ 2_3^{SC} \ \{'\beta': \ 30.0\} \ 3^B \ 4^B$	2.0145	0.0427	1.0
$1~2_4^{LC}$	2.9074	0.1089	0.01
$1\ 2_4^{LC}\ 3$	2.5179	0.1151	0.001
$1\ 2_4^{LC}\ 3\ 4$	2.4741	0.1138	0.001
$1\ 2_4^{LC}\ 3\ 4^B$	2.0616	0.0287	0.1

$1 \ 2_4^{LC} \ 3^B$	2.2613	0.0317	0.01
$1 \ 2_4^{LC} \ 3^B \ 4$	2.2239	0.0428	0.01
$1 \ 2_4^{LC} \ 3^B \ 4^B$	2.0277	0.0417	0.1
$1~2_5^{LC}$	2.8299	0.1217	0.01
$1 \ 2_5^{LC} \ 3$	2.5707	0.0637	0.01
$1 \ 2_5^{LC} \ 3 \ 4$	2.4725	0.0653	0.01
$1 \ 2_5^{LC} \ 3 \ 4^B$	2.0565	0.0341	0.1
$1 \ 2_5^{LC} \ 3^B$	2.2785	0.0364	0.01
$1 \ 2_5^{LC} \ 3^B \ 4$	2.2473	0.0509	0.01
$1 \ 2_5^{LC} \ 3^B \ 4^B$	2.0376	0.0422	0.1
$1~2_6^{LC}$	2.8041	0.1241	0.01
$1 \ 2_6^{LC} \ 3$	2.5481	0.0700	0.01
$1\ 2_6^{LC}\ 3\ 4$	2.4512	0.0637	0.01
$1 \ 2_6^{LC} \ 3 \ 4^B$	2.0369	0.0359	0.1
$1 \ 2_6^{LC} \ 3^B$	2.2585	0.0379	0.01
$1 \ 2_6^{LC} \ 3^B \ 4$	2.2323	0.0444	0.01
$1 \ 2_6^{LC} \ 3^B \ 4^B$	2.0161	0.0419	0.1
$1~2_7^{LC}$	2.8045	0.1230	0.01
$1\ 2_7^{LC}\ 3$	2.5507	0.0724	0.01
$1\ 2_7^{LC}\ 3\ 4$	2.4539	0.0650	0.01
$1 \ 2_7^{LC} \ 3 \ 4^B$	2.0343	0.0342	0.1
$1 \ 2_7^{LC} \ 3^B$	2.2605	0.0363	0.01
$1\ 2_7^{LC}\ 3^B\ 4$	2.2346	0.0434	0.01
$1 \ 2_7^{LC} \ 3^B \ 4^B$	2.0136	0.0404	0.1
1 Bag of Bonds	9.7804	0.1511	1.0
1 Bag of Bonds 3	6.2550	0.1560	0.1
1 Bag of Bonds 3 4	5.9116	0.1627	1.0

1 Bag of Bonds 3 4^B	4.1550	0.1231	1.0
1 Bag of Bonds 3^B	4.6733	0.1413	1.0
1 Bag of Bonds 3^B 4	4.5066	0.1433	1.0
1 Bag of Bonds $3^B 4^B$	4.0767	0.1245	1.0
1^C	11.2675	0.2300	0.001
$1^C 2^B$	8.5248	0.1427	0.01
$1^C \ 2^B \ 3$	6.2042	0.1376	0.1
$1^C \ 2^B \ 3 \ 4$	5.2733	0.1665	0.1
$1^C \ 2^B \ 3 \ 4 \ 5$	4.3145	0.1368	1.0
$1^C \ 2^B \ 3 \ 4^B$	4.4981	0.0840	1.0
$1^C \ 2^B \ 3 \ 4^B \ 5$	3.8035	0.1505	1.0
$1^C \ 2^B \ 3^B$	5.6428	0.1452	0.1
$1^C \ 2^B \ 3^B \ 4$	4.9329	0.1640	0.1
$1^C \ 2^B \ 3^B \ 4 \ 5$	4.0597	0.1125	0.1
$1^C \ 2^B \ 3^B \ 4^B$	4.5067	0.0847	1.0
$1^C \ 2^B \ 3^B \ 4^B \ 5$	3.8092	0.1528	1.0
$1^C \ 2^{LC}$	2.7767	0.1252	0.01
$1^C \ 2^{LC} \ 3$	2.5489	0.0551	0.01
$1^C \ 2^{LC} \ 3 \ 4$	2.4661	0.0452	0.01
$1^C \ 2^{LC} \ 3 \ 4^B$	2.0435	0.0318	0.1
$1^C \ 2^{LC} \ 3^B$	2.2727	0.0429	0.01
$1^C \ 2^{LC} \ 3^B \ 4$	2.2458	0.0423	0.01
$1^C \ 2^{LC} \ 3^B \ 4^B$	2.0221	0.0351	0.1
$1^C \ 2_1^{LC}$	6.2415	0.1723	0.01
$1^C \ 2_1^{LC} \ 3$	5.1853	0.1395	0.01
$1^C \ 2_1^{LC} \ 3 \ 4$	4.3757	0.4312	0.001
$1^C \ 2_1^{LC} \ 3 \ 4^B$	3.6495	0.0919	1.0

$1^C \ 2_1^{LC} \ 3^B$	4.5926	0.2839	0.001
$1^C \ 2_1^{LC} \ 3^B \ 4$	3.9817	0.1503	0.01
$1^C \ 2_1^{LC} \ 3^B \ 4^B$	3.6316	0.1142	1.0
$1^C \ 2_2^{LC}$	2.8002	0.1120	0.001
$1^C \ 2_2^{LC} \ 3$	2.7532	0.1308	0.001
$1^C \ 2_2^{LC} \ 3 \ 4$	2.6000	0.0489	0.01
$1^C \ 2_2^{LC} \ 3 \ 4^B$	2.0303	0.0342	0.1
$1^C \ 2_2^{LC} \ 3^B$	2.4398	0.0451	0.01
$1^C \ 2_2^{LC} \ 3^B \ 4$	2.3183	0.0530	0.01
$1^C \ 2_2^{LC} \ 3^B \ 4^B$	2.0154	0.0384	0.1
$1^C \ 2_3^{LC}$	2.5549	0.0811	0.01
$1^C \ 2_3^{LC} \ 3$	2.4589	0.0631	0.01
$1^C \ 2_3^{LC} \ 3 \ 4$	2.3737	0.0684	0.01
$1^C \ 2_3^{LC} \ 3 \ 4^B$	1.8185	0.0554	0.1
$1^C \ 2_3^{LC} \ 3^B$	2.1548	0.0589	0.01
$1^C \ 2_3^{LC} \ 3^B \ 4$	2.1209	0.0784	0.01
$1^C \ 2_3^{LC} \ 3^B \ 4^B$	1.8163	0.0693	0.1
$1^C \ 2_3^{LC} \ 3 \ 4 \ 5$	2.3945	0.0598	0.1
$1^C \ 2_3^{LC} \ 3 \ 4^B \ 5$	1.8658	0.0673	0.1
$1^C \ 2_3^{LC} \ 3^B \ 4 \ 5$	2.1644	0.0843	0.1
$1^C \ 2_3^{LC} \ 3^B \ 4^B \ 5$	1.8469	0.0785	0.1
$1^C \ 2_4^{LC}$	2.8441	0.2314	0.001
$1^C \ 2_4^{LC} \ 3$	2.5473	0.1145	0.001
$1^C \ 2_4^{LC} \ 3 \ 4$	2.4922	0.0605	0.01
$1^C \ 2_4^{LC} \ 3 \ 4^B$	2.0597	0.0330	0.1
$1^C \ 2_4^{LC} \ 3^B$	2.2617	0.0366	0.01
$1^C \ 2_4^{LC} \ 3^B \ 4$	2.2218	0.0388	0.01

$1^C \ 2_4^{LC} \ 3^B \ 4^B$	2.0374	0.0430	0.1
$1^C \ 2_5^{LC}$	2.8058	0.1242	0.01
$1^C \ 2_5^{LC} \ 3$	2.5593	0.1398	0.001
$1^C \ 2_5^{LC} \ 3 \ 4$	2.4842	0.0536	0.01
$1^C \ 2^{LC}_5 \ 3 \ 4^B$	2.0639	0.0341	0.1
$1^C \ 2^{LC}_5 \ 3^B$	2.2910	0.0404	0.01
$1^C \ 2^{LC}_5 \ 3^B \ 4$	2.2564	0.0473	0.01
$1^C \ 2^{LC}_5 \ 3^B \ 4^B$	2.0444	0.0399	0.1
$1^C \ 2_6^{LC}$	2.7776	0.1262	0.01
$1^C \ 2_6^{LC} \ 3$	2.5467	0.0530	0.01
$1^C \ 2_6^{LC} \ 3 \ 4$	2.4624	0.0444	0.01
$1^C \ 2^{LC}_6 \ 3 \ 4^B$	2.0454	0.0340	0.1
$1^C \ 2_6^{LC} \ 3^B$	2.2706	0.0433	0.01
$1^C \ 2_6^{LC} \ 3^B \ 4$	2.2429	0.0429	0.01
$1^C \ 2^{LC}_6 \ 3^B \ 4^B$	2.0239	0.0376	0.1
$1^{C} \ 2^{LC}_{7}$	2.7775	0.1240	0.01
$1^C \ 2^{LC}_7 \ 3$	2.5489	0.0541	0.01
$1^C \ 2^{LC}_7 \ 3 \ 4$	2.4657	0.0441	0.01
$1^C \ 2^{LC}_7 \ 3 \ 4^B$	2.0429	0.0327	0.1
$1^C \ 2^{LC}_7 \ 3^B$	2.2727	0.0415	0.01
$1^C \ 2^{LC}_7 \ 3^B \ 4$	2.2453	0.0416	0.01
$1^C \ 2^{LC}_7 \ 3^B \ 4^B$	2.0214	0.0361	0.1
1^C Bag of Bonds	7.8937	0.1697	0.1
1^C Bag of Bonds 3	5.4190	0.1682	1.0
1^C Bag of Bonds 3 4	5.1525	0.1559	1.0
1^C Bag of Bonds $3 \ 4^B$	4.1234	0.1261	1.0
1^C Bag of Bonds 3^B	4.5804	0.1591	1.0

1^C Bag of Bonds 3^B 4	4.4246	0.1461	1.0
1^C Bag of Bonds 3^B 4^B	4.0642	0.1229	1.0
2	42.5581	0.3532	1.0
2^B	12.916	0.2919	0.001
2^{LP}	4.9019	0.0818	0.01
2^{NC}	4.9497	0.0720	0.1
2^{NP}	4.9553	0.0972	0.1
2^{NP} {'end': 12.0}	5.8791	0.1431	0.1
2^{NP} {'end': 16.0}	12.6072	0.2010	0.01
2^{NP} {'end': 2.0}	6.7371	0.1762	0.001
2^{NP} {'end': 4.0}	4.9788	0.0994	0.01
2^{NP} {'end': 6.0}	4.9553	0.0972	0.1
2^{NP} {'end': 8.0}	4.8223	0.0962	0.1
2^{NP} {'segments': 10}	60.0313	0.9907	0.001
2^{NP} {'segments': 150}	4.9064	0.0941	0.1
2^{NP} {'segments': 200}	4.9032	0.0943	0.1
2^{NP} {'segments': 25}	28.8464	0.4007	0.001
2^{NP} {'segments': 50}	5.9702	0.0741	0.01
2^{NP} {'segments': 75}	5.0141	0.1073	0.01
$2^{NP} \ \{'\beta': \ 1.0\}$	6.6683	0.0815	0.001
$2^{NP} \ \{'\beta': \ 10.0\}$	5.0004	0.0623	0.01
$2^{NP} \ \{'\beta': \ 2.5\}$	5.8535	0.1770	0.001
$2^{NP} \ \{'\beta': \ 30.0\}$	5.0820	0.1035	0.01
$2^{NP} \ \{'\beta': \ 40.0\}$	6.1273	0.0896	0.01
$2^{NP} \ \{'\beta': 5.0\}$	5.4152	0.2241	0.001
$2^{NP} \ \{'\beta':\ 80.0\}$	39.5902	1.0179	1.0
2^{NP} {'start': 0.1}	4.9468	0.0996	0.1

2^{NP} {'start': 0.2}	4.9553	0.0972	0.1
2^{NP} {'start': 0.4}	4.9298	0.1011	0.1
2^{NP} {'start': 0.8}	4.9413	0.1028	0.1
2^{NP} {'start': 1.0}	4.9672	0.0872	0.1
2^{NP} {'start': 1.5}	11.1556	0.2164	0.1
2^{SC}	6.0140	0.1786	1.0
2^{SP}	132.1945	3.0651	1.0
2_1	9.0548	0.2739	0.01
2_1^{LP}	8.6599	0.4742	0.001
2_1^{NC}	8.6347	0.6150	0.01
2_1^{NP}	8.0929	0.2361	0.0001
2_1^{SC}	11.2133	0.1713	1e-05
2_1^{SP}	168.3545	1.3873	0.01
2_2	5.2149	0.1719	0.001
2_2^{LP}	5.0587	0.2155	0.0001
2_2^{NC}	5.0651	0.0696	0.01
2_2^{NP}	5.0130	0.0427	0.001
2_2^{SC}	6.8146	0.1797	0.1
2_2^{SP}	162.2208	1.4962	1.0
2_3	4.5538	0.0915	0.01
2_3^{LC}	4.5538	0.0915	0.01
$2_3^{LC} \ \{'\beta':\ 30.0\}$	4.4312	0.0792	0.01
2_3^{LP}	4.5203	0.0905	0.001
2_3^{NC}	4.4493	0.0769	0.01
$2_3^{NC} \ 2_3^{NP}$	4.4139	0.0935	0.01
$2_3^{NC} \ \{'\beta':\ 30.0\}$	4.3749	0.1100	0.01
2_3^{NP}	2.4711	0.0775	0.01

2_3^{NP} {'end': 12.0}	5.6734	0.1611	0.001
2_3^{NP} {'end': 16.0}	14.2262	0.3014	0.001
2_3^{NP} {'end': 4.0}	4.3218	0.1182	0.001
2_3^{NP} {'end': 6.0}	4.5121	0.1077	0.01
2_3^{NP} {'end': 8.0}	4.5460	0.1004	0.01
2_3^{NP} {'segments': 10}	84.1753	1.0094	0.001
2_3^{NP} {'segments': 150}	4.3073	0.1170	0.001
2_3^{NP} {'segments': 200}	4.3546	0.1049	0.01
2_3^{NP} {'segments': 25}	33.4157	0.8663	0.001
2_3^{NP} {'segments': 50}	5.6196	0.1571	0.001
2_3^{NP} {'segments': 75}	4.5435	0.1103	0.01
$2_3^{NP} \ \{'\beta': \ 1.0\}$	10.9222	0.3285	0.001
$2_3^{NP} \ \{'\beta': \ 10.0\}$	4.6449	0.1176	0.001
$2_3^{NP} \ \{'\beta': \ 2.5\}$	6.6183	0.1584	0.001
$2_3^{NP} \ \{'\beta':\ 30.0\}$	4.5288	0.1102	0.01
$2_3^{NP} \ \{'\beta': \ 40.0\}$	5.9969	0.0569	0.01
$2_3^{NP} \ \{'\beta': 5.0\}$	5.5599	0.2342	0.001
$2_3^{NP} \ \{'\beta':\ 80.0\}$	46.6440	0.8325	0.001
2_3^{NP} {'start': 0.1}	4.4750	0.1120	0.01
2_3^{NP} {'start': 0.2}	4.5121	0.1077	0.01
2_3^{NP} {'start': 0.4}	4.4493	0.1035	0.01
2_3^{NP} {'start': 0.8}	4.3680	0.1384	0.001
2_3^{NP} {'start': 1.0}	4.3581	0.1290	0.001
2_3^{NP} {'start': 1.5}	20.8561	0.3221	0.01
2_3^{SC}	5.7663	0.1090	1.0
$2_3^{SC} \ \{'\beta':\ 30.0\}$	5.7663	0.1090	1.0
2_3^{SP}	147.6294	2.7820	1.0

2	5.1088	0.0731	0.01
2	$\frac{LP}{4}$ 5.0595	0.1353	0.001
2	$^{NC}_{4}$ 4.9912	0.0933	0.01
2	$^{NP}_{4}$ 5.0452	0.1022	0.01
2	$\begin{array}{c} SC \\ 4 \end{array} \tag{6.5754}$	0.1611	1.0
2	SP 141.6751	3.1076	1.0
2	5.2917	0.1083	0.01
2	$\frac{LP}{5}$ 5.2350	0.1373	0.01
2	$\frac{NC}{5}$ 5.2325	0.1401	0.01
2	5.2367	0.1354	0.01
2	$\frac{SC}{5}$ 6.8206	0.2061	1.0
2	$^{SP}_{5}$ 136.9339	3.3614	1.0
2	5.2651	0.1060	0.01
2	$^{LP}_{6}$ 5.2299	0.1349	0.01
2	5.2170	0.1565	0.01
2	5.2317	0.1632	0.01
2	$\frac{SC}{6}$ 6.8510	0.1936	1.0
2	$^{SP}_{6}$ 134.5053	2.7396	1.0
2	5.2689	0.1012	0.01
2	$\frac{LP}{7}$ 5.2327	0.1306	0.01
2	$\frac{NC}{7}$ 5.2210	0.1516	0.01
2	$^{NP}_{7}$ 5.2346	0.1578	0.01
2	$\frac{SC}{7}$ 6.8454	0.1966	1.0
2	SP 134.0674	2.7591	1.0
3	58.6948	0.7411	1.0
3	9.0619	0.3880	0.01
4	94.2483	1.1164	1.0

4^B	81.5092	0.6791	1.0
5	102.1410	1.6964	10.0
5^B	102.4255	1.5005	1.0
Bag of Bonds	9.7960	0.1587	0.01
Bag of Bonds {'strip atoms': True}	17.3518	0.2901	0.01
$Bag of Bonds_1$	12.0466	0.2862	0.01
Bag of Bonds ₁ {'strip atoms': True}	33.0308	0.2570	1.0
Bag of $Bonds_2$	9.1210	0.2327	0.01
Bag of Bonds ₂ {'strip atoms': True}	38.0673	0.7031	0.1
Bag of $Bonds_3$	10.1130	0.2195	0.01
Bag of Bonds ₃ {'strip atoms': True}	34.5855	0.6927	1.0
$Bag of Bonds_4$	10.0033	0.1903	0.01
Bag of Bonds ₄ {'strip atoms': True}	27.7330	0.5014	1.0
Bag of $Bonds_5$	9.8274	0.2079	0.01
Bag of Bonds ₅ {'strip atoms': True}	23.7519	0.2201	0.1
$Bag of Bonds_6$	9.7265	0.1909	0.01
Bag of Bonds ₆ {'strip atoms': True}	21.4671	0.2877	0.01
Bag of Bonds ₇	9.7240	0.1696	0.01
Bag of Bonds ₇ {'strip atoms': True}	20.8799	0.2830	0.01
Coulomb Matrix	27.0624	0.4680	0.01
Coulomb $Matrix_1$	29.4228	0.5601	0.001
Coulomb $Matrix_2$	29.2594	0.3798	0.01
Coulomb $Matrix_3$	30.8664	0.2111	0.1
Coulomb $Matrix_4$	29.5230	0.2349	0.1
Coulomb $Matrix_5$	29.0555	0.4645	0.01
Coulomb $Matrix_6$	29.0772	0.5091	0.01
Coulomb Matrix ₇	29.1617	0.5299	0.01

Table S3: LRR Results

In the following table, the kernel options are for the Gaussian Kernel (gauss) and the Laplacian Kernel (laplace). The hyperparameters α and γ correspond to the regularization term, and the parameter of the kernel respectively.

Name	KRR	Fold	α	γ	Kernel
1	14.5830	0.2586	1e-07	1e-03	gauss
$1~2^B$	6.8788	0.0190	1e-05	1e-03	gauss
$1\ 2^{B}\ 3$	5.2761	0.1257	1e-11	1e-07	gauss
$1\ 2^{B}\ 3\ 4$	3.6420	0.1186	1e-11	1e-07	laplace
$1\ 2^{B}\ 3\ 4\ 5$	3.9640	0.1660	1e-07	1e-07	gauss
$1 \ 2^B \ 3 \ 4^B$	4.1313	0.1067	1e-09	1e-07	gauss
$1\ 2^{B}\ 3\ 4^{B}\ 5$	3.3964	0.1324	1e-07	1e-07	gauss
$1 \ 2^B \ 3^B$	4.5148	0.1139	1e-11	1e-07	laplace
$1 \ 2^B \ 3^B \ 4$	3.4005	0.0678	1e-11	1e-07	laplace
$1\ 2^{B}\ 3^{B}\ 4\ 5$	3.4207	0.2662	1e-09	1e-07	gauss
$1 \ 2^B \ 3^B \ 4^B$	3.8680	0.1343	1e-11	1e-07	laplace
$1 \ 2^B \ 3^B \ 4^B \ 5$	3.3731	0.1299	1e-07	1e-07	gauss
$1~2^{LC}$	2.1640	0.0583	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3$	2.0375	0.0674	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3 \ 4$	1.9351	0.0283	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3 \ 4^B$	1.7372	0.0394	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3^B$	1.8000	0.0338	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3^B \ 4$	1.7596	0.0264	1e-09	1e-07	gauss
$1 \ 2^{LC} \ 3^B \ 4^B$	1.7155	0.0340	1e-09	1e-07	gauss
$1 2_1^{LC}$	5.1025	0.0572	1e-07	1e-07	laplace

$1\ 2_1^{LC}\ 3$	4.4376	0.0748	1e-07	1e-07	laplace
$1\ 2_1^{LC}\ 3\ 4$	3.6197	0.0916	1e-09	1e-07	gauss
$1\ 2_1^{LC}\ 3\ 4^B$	3.2523	0.1262	1e-07	1e-07	laplace
$1 \ 2_1^{LC} \ 3^B$	3.9978	0.0997	1e-09	1e-07	gauss
$1 \ 2_1^{LC} \ 3^B \ 4$	3.3872	0.1052	1e-09	1e-07	gauss
$1 \ 2_1^{LC} \ 3^B \ 4^B$	3.2175	0.0902	1e-07	1e-07	laplace
$1 \ 2_2^{LC}$	1.8764	0.0790	1e-11	1e-07	gauss
$1\ 2_2^{LC}\ 3$	1.8268	0.0397	1e-11	1e-07	gauss
$1\ 2_2^{LC}\ 3\ 4$	1.7407	0.0265	1e-11	1e-07	gauss
$1\ 2_2^{LC}\ 3\ 4^B$	1.6869	0.0118	1e-09	1e-07	gauss
$1 \ 2_2^{LC} \ 3^B$	1.7257	0.0711	1e-11	1e-07	gauss
$1 \ 2_2^{LC} \ 3^B \ 4$	1.7600	0.0405	1e-09	1e-07	gauss
$1 \ 2_2^{LC} \ 3^B \ 4^B$	1.6689	0.0184	1e-09	1e-07	gauss
$1 \ 2_3^{LC}$	1.6752	0.0399	1e-11	1e-07	gauss
$1\ 2_3^{LC}\ 3$	1.6106	0.1316	1e-11	1e-07	gauss
$1\ 2_3^{LC}\ 3\ 4$	1.7256	0.0412	1e-09	1e-07	gauss
$1\ 2_3^{LC}\ 3\ 4\ 5$	1.8862	0.0808	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3 \ 4^B$	1.4622	0.0437	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3 \ 4^B \ 5$	1.6017	0.0713	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3^B$	1.4303	0.0317	1e-11	1e-07	gauss
$1 \ 2_3^{LC} \ 3^B \ 4$	1.5562	0.0576	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3^B \ 4 \ 5$	1.7777	0.0792	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3^B \ 4^B$	1.4481	0.0611	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ 3^B \ 4^B \ 5$	1.5975	0.0710	1e-09	1e-07	gauss
$1 \ 2_3^{LC} \ \{'\beta': \ 30.0\}$	1.8162	0.0409	1e-07	1e-05	gauss
$1 \ 2_3^{LC} \ \{'\beta': \ 30.0\} \ 3^B$	1.6015	0.0446	1e-07	1e-05	gauss
$1 \ 2_3^{LC} \ \{ `\beta `: \ 30.0 \} \ 3^B \ 4^B$	1.4172	0.0658	1e-09	1e-07	gauss

$1 \ 2_3^{NC}$	1.8124	0.0431	1e-07	1e-05	gauss
$1 2_3^{NC} 3^B$	1.6005	0.0445	1e-07	1e-05	gauss
$1 \ 2_3^{NC} \ 3^B \ 4^B$	1.4136	0.0648	1e-09	1e-07	gauss
$1 \ 2_3^{NC} \ \{'\beta': \ 30.0\}$	1.7988	0.0466	1e-07	1e-05	gauss
1 2_3^{NC} {' β ': 30.0} 3^B	1.5968	0.0430	1e-07	1e-05	gauss
1 2_3^{NC} {' β ': 30.0} 3^B 4^B	1.4084	0.0595	1e-09	1e-07	gauss
$1 2_3^{NP}$	1.4487	0.0568	1e-09	1e-05	gauss
$1 \ 2_3^{NP} \ 3^B$	1.1907	0.0413	1e-09	1e-05	gauss
$1 \ 2_3^{NP} \ 3^B \ 4^B$	1.2534	0.0148	1e-07	1e-05	gauss
$1\ 2_3^{SC}$	2.5309	0.0563	1e-07	1e-07	gauss
$1 \ 2_3^{SC} \ 3^B$	2.1568	0.0277	1e-07	1e-07	gauss
$1 \ 2_3^{SC} \ 3^B \ 4^B$	1.7724	0.0485	1e-07	1e-07	gauss
$1 \ 2_3^{SC} \ \{'\beta': \ 30.0\}$	2.5309	0.0563	1e-07	1e-07	gauss
$1\ 2_3^{SC}\ \{'\beta':\ 30.0\}\ 3^B$	2.1568	0.0277	1e-07	1e-07	gauss
1 2_3^{SC} {' β ': 30.0} 3^B 4^B	1.7724	0.0485	1e-07	1e-07	gauss
$1~2_4^{LC}$	2.1115	0.0429	1e-09	1e-07	gauss
$1 \ 2_4^{LC} \ 3$	1.9871	0.0280	1e-09	1e-07	gauss
$1 \ 2_4^{LC} \ 3 \ 4$	1.8957	0.0265	1e-09	1e-07	gauss
$1\ 2_4^{LC}\ 3\ 4^B$	1.6755	0.0287	1e-09	1e-07	gauss
$1 \ 2_4^{LC} \ 3^B$	1.7272	0.0316	1e-09	1e-07	gauss
$1 \ 2_4^{LC} \ 3^B \ 4$	1.6882	0.0395	1e-09	1e-07	gauss
$1 \ 2_4^{LC} \ 3^B \ 4^B$	1.6408	0.0267	1e-09	1e-07	gauss
$1 \ 2_5^{LC}$	2.1486	0.0434	1e-09	1e-07	gauss
$1 \ 2_5^{LC} \ 3$	2.0172	0.0360	1e-09	1e-07	gauss
$1 \ 2_5^{LC} \ 3 \ 4$	1.9350	0.0256	1e-09	1e-07	gauss
$1\ 2_5^{LC}\ 3\ 4^B$	1.7286	0.0320	1e-09	1e-07	gauss
$1 \ 2_5^{LC} \ 3^B$	1.7978	0.0364	1e-09	1e-07	gauss

$1 \ 2_5^{LC} \ 3^B \ 4$	1.7653	0.0317	1e-09	1e-07	gauss
$1 \ 2_5^{LC} \ 3^B \ 4^B$	1.7103	0.0262	1e-09	1e-07	gauss
$1 \ 2_6^{LC}$	2.1624	0.0563	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3$	2.0330	0.0640	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3 \ 4$	1.9336	0.0263	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3 \ 4^B$	1.7354	0.0365	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3^B$	1.8019	0.0335	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3^B \ 4$	1.7596	0.0307	1e-09	1e-07	gauss
$1 \ 2_6^{LC} \ 3^B \ 4^B$	1.7146	0.0290	1e-09	1e-07	gauss
$1 2_7^{LC}$	2.1618	0.0593	1e-09	1e-07	gauss
$1\ 2_7^{LC}\ 3$	2.0361	0.0683	1e-09	1e-07	gauss
$1\ 2_7^{LC}\ 3\ 4$	1.9334	0.0288	1e-09	1e-07	gauss
$1 \ 2_7^{LC} \ 3 \ 4^B$	1.7394	0.0387	1e-09	1e-07	gauss
$1 \ 2_7^{LC} \ 3^B$	1.7999	0.0342	1e-09	1e-07	gauss
$1 \ 2_7^{LC} \ 3^B \ 4$	1.7602	0.0261	1e-09	1e-07	gauss
$1 \ 2_7^{LC} \ 3^B \ 4^B$	1.7178	0.0330	1e-09	1e-07	gauss
1 Bag of Bonds	2.6897	0.0420	1e-07	1e-07	laplace
1 Bag of Bonds 3	2.5241	0.0374	1e-07	1e-07	laplace
1 Bag of Bonds 3 4	2.4971	0.0219	1e-07	1e-07	laplace
1 Bag of Bonds 3 4^B	2.3190	0.0496	1e-07	1e-07	laplace
1 Bag of Bonds 3^B	2.4431	0.0550	1e-07	1e-07	laplace
1 Bag of Bonds 3^B 4	2.4396	0.0386	1e-07	1e-07	laplace
1 Bag of Bonds 3^B 4^B	2.3262	0.0461	1e-07	1e-07	laplace
1^C	9.3266	0.1211	1e-07	1e-03	gauss
$1^C 2^B$	6.6876	0.0054	1e-05	1e-03	gauss
$1^C \ 2^B \ 3$	5.0100	0.1493	1e-11	1e-07	laplace
$1^C \ 2^B \ 3 \ 4$	3.4528	0.0977	1e-11	1e-07	laplace

$1^C \ 2^B \ 3 \ 4 \ 5$	3.7071	0.2631	1e-09	1e-07	gauss
$1^C \ 2^B \ 3 \ 4^B$	4.1354	0.1190	1e-09	1e-07	gauss
$1^C \ 2^B \ 3 \ 4^B \ 5$	3.4048	0.1603	1e-07	1e-07	gauss
$1^C \ 2^B \ 3^B$	4.4394	0.1219	1e-11	1e-07	laplace
$1^C \ 2^B \ 3^B \ 4$	3.3516	0.1076	1e-11	1e-07	laplace
$1^C \ 2^B \ 3^B \ 4 \ 5$	3.3742	0.2473	1e-09	1e-07	gauss
$1^C \ 2^B \ 3^B \ 4^B$	3.8367	0.1346	1e-11	1e-07	laplace
$1^C \ 2^B \ 3^B \ 4^B \ 5$	3.0883	0.1180	1e-09	1e-07	gauss
$1^{C\ LC}2$	2.1566	0.0604	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3$	2.0392	0.0682	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3 \ 4$	1.9410	0.0438	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3 \ 4^B$	1.7412	0.0440	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3^B$	1.8011	0.0456	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3^B \ 4$	1.7589	0.0342	1e-09	1e-07	gauss
$1^C \ 2^{LC} \ 3^B \ 4^B$	1.7131	0.0323	1e-09	1e-07	gauss
$1^C \ 2_1^{LC}$	4.8068	0.0654	1e-07	1e-07	laplace
$1^C \ 2_1^{LC} \ 3$	4.2667	0.1048	1e-07	1e-07	laplace
$1^C \ 2_1^{LC} \ 3 \ 4$	3.5751	0.0890	1e-09	1e-07	gauss
$1^C \ 2_1^{LC} \ 3 \ 4^B$	3.1975	0.1186	1e-07	1e-07	laplace
$1^C \ 2_1^{LC} \ 3^B$	3.8663	0.0792	1e-07	1e-07	laplace
$1^C \ 2_1^{LC} \ 3^B \ 4$	3.3696	0.1026	1e-09	1e-07	gauss
$1^C \ 2_1^{LC} \ 3^B \ 4^B$	3.1662	0.0896	1e-07	1e-07	laplace
$1^C \ 2_2^{LC}$	1.8295	0.0759	1e-11	1e-07	gauss
$1^C \ 2_2^{LC} \ 3$	1.8050	0.0523	1e-11	1e-07	gauss
$1^C \ 2_2^{LC} \ 3 \ 4$	1.7256	0.0217	1e-11	1e-07	gauss
$1^C \ 2_2^{LC} \ 3 \ 4^B$	1.6913	0.0144	1e-09	1e-07	gauss
$1^C \ 2_2^{LC} \ 3^B$	1.7024	0.0744	1e-11	1e-07	gauss

$1^C \ 2_2^{LC} \ 3^B \ 4$	1.7541	0.0452	1e-09	1e-07	gauss
$1^C \ 2_2^{LC} \ 3^B \ 4^B$	1.6689	0.0180	1e-09	1e-07	gauss
$1^C \ 2_3^{LC}$	1.6415	0.0531	1e-11	1e-07	gauss
$1^C \ 2_3^{LC} \ 3$	1.5761	0.1235	1e-11	1e-07	gauss
$1^C \ 2_3^{LC} \ 3 \ 4$	1.5667	0.0710	1e-11	1e-07	gauss
$1^C \ 2_3^{LC} \ 3 \ 4^B$	1.4574	0.0500	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3^B$	1.4337	0.0448	1e-11	1e-07	gauss
$1^C \ 2_3^{LC} \ 3^B \ 4$	1.5515	0.0631	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3^B \ 4^B$	1.4419	0.0565	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3 \ 4 \ 5$	1.8888	0.0783	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3 \ 4^B \ 5$	1.6110	0.0648	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3^B \ 4 \ 5$	1.7805	0.0736	1e-09	1e-07	gauss
$1^C \ 2_3^{LC} \ 3^B \ 4^B \ 5$	1.5937	0.0615	1e-09	1e-07	gauss
$1^C \ 2_4^{LC}$	2.0737	0.0453	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3$	1.9700	0.0327	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3 \ 4$	1.8883	0.0328	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3 \ 4^B$	1.6749	0.0275	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3^B$	1.7232	0.0256	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3^B \ 4$	1.6836	0.0331	1e-09	1e-07	gauss
$1^C \ 2_4^{LC} \ 3^B \ 4^B$	1.6460	0.0305	1e-09	1e-07	gauss
$1^C \ 2_5^{LC}$	2.1359	0.0449	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3$	2.0150	0.0563	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3 \ 4$	1.9425	0.0515	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3 \ 4^B$	1.7331	0.0420	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3^B$	1.7996	0.0420	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3^B \ 4$	1.7614	0.0382	1e-09	1e-07	gauss
$1^C \ 2_5^{LC} \ 3^B \ 4^B$	1.7067	0.0304	1e-09	1e-07	gauss

1^C Bag of Bonds 3 2.5023 0.0458 $1e-07$ <t< th=""><th></th><th></th><th></th><th></th><th></th><th></th><th></th></t<>							
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$1^C 2_6^{LC}$	2.1544	0.0569	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$1^{C} 2_{6}^{LC} 3$	2.0354	0.0666	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$1^{C} 2_{6}^{LC} 3 4$	1.9393	0.0469	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$(^C \ 2^{LC}_6 \ 3 \ 4^B)$	1.7394	0.0425	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$(^{C}\ 2_{6}^{LC}\ 3^{B})$	1.8042	0.0441	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$(^C \ 2_6^{LC} \ 3^B \ 4)$	1.7588	0.0383	1e-09	1e-07	gauss
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	$1^{C} 2_{6}^{LC} 3^{B} 4^{B}$	1.7121	0.0284	1e-09	1e-07	gauss
1^C 2_7^{LC} 3 4^B 1.9396 0.0432 1e-09 1e-07 gauss 1^C 2_7^{LC} 3 4^B 1.7434 0.0431 1e-09 1e-07 gauss 1^C 2_7^{LC} 3^B 4 1.8012 0.0454 1e-09 1e-07 gauss 1^C 2_7^{LC} 3^B 4^B 1.7154 0.0312 1e-09 1e-07 gauss 1^C Bag of Bonds 2.6704 0.0481 1e-07 1e-07 laplace 1^C Bag of Bonds 3 2.5023 0.0458 1e-07 1e-07 laplace 1^C Bag of Bonds 3 2.3144 0.0553 1e-07 1e-07 laplace 1^C Bag of Bonds 3^B 2.4218 0.0532 1e-07 1e-07 laplace 1^C Bag of Bonds 3^B 2.4218 0.0532 1e-07 1e-07 laplace 1^C Bag of Bonds 3^B 2.4156 0.0376 1e-07 1e-07 laplace 1^C Bag of Bonds 3^B 2.3197 0.0511 1e-07 1e-07 laplace 2^D 7.6924 0.1527 1e-07 1e-03 gauss 2^{D} 3.18	1	$1^C 2_7^{LC}$	2.1543	0.0618	1e-09	1e-07	gauss
$1^C \ 2_7^{LC} \ 3 \ 4^B$ 1.7434 0.0431 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B$ 1.8012 0.0454 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B \ 4$ 1.7592 0.0334 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B \ 4^B$ 1.7154 0.0312 1e-09 1e-07 gauss $1^C \ Bag \ of \ Bonds$ 2.6704 0.0481 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.5023 0.0458 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.4678 0.0267 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.3144 0.0553 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.4218 0.0532 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.4 2.4156 0.0376 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.8 2.3197 0.0511 1e-07 1e-07 laplace $2^D \ Bag \ of \ Bonds$ 3.8 2.3197 0.0511 1e-07 1e-07<	1	$1^{C} 2_{7}^{LC} 3$	2.0381	0.0691	1e-09	1e-07	gauss
$1^C \ 2_7^{LC} \ 3^B$ 1.8012 0.0454 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B \ 4$ 1.7592 0.0334 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B \ 4^B$ 1.7154 0.0312 1e-09 1e-07 gauss $1^C \ Bag \ of \ Bonds$ 2.6704 0.0481 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.5023 0.0458 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.4678 0.0267 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.3144 0.0553 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.4218 0.0532 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.4218 0.0376 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.3197 0.0511 1e-07 1e-07 laplace $2^C \ Bag \ of \ Bonds$ 3.1836 0.1023 1e-07 1e-07 laplace $2^B \ Bag \ of \ Bonds$ 3.1836 0.1023 1e-07 1e-07 laplace	1	$1^{C} 2_{7}^{LC} 3 4$	1.9396	0.0432	1e-09	1e-07	gauss
$1^C \ 2_7^{LC} \ 3^B \ 4$ 1.7592 0.0334 1e-09 1e-07 gauss $1^C \ 2_7^{LC} \ 3^B \ 4^B$ 1.7154 0.0312 1e-09 1e-07 gauss $1^C \ Bag \ of \ Bonds$ 2.6704 0.0481 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.5023 0.0458 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 2.4678 0.0267 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 2.3144 0.0553 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 2.4218 0.0532 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 4 2.4156 0.0376 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 4 2.4156 0.0376 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3 4 2.4156 0.0376 1e-07 1e-07 laplace $2^C \ Bag \ of \ Bonds$ 3 4 2.4156 0.0511 1e-07 1e-07 laplace </td <td>1</td> <td>$1^{C} 2_{7}^{LC} 3 4^{B}$</td> <td>1.7434</td> <td>0.0431</td> <td>1e-09</td> <td>1e-07</td> <td>gauss</td>	1	$1^{C} 2_{7}^{LC} 3 4^{B}$	1.7434	0.0431	1e-09	1e-07	gauss
$1^C \ 2_7^{LC} \ 3^B \ 4^B$ 1.7154 0.0312 1e-09 1e-07 gauss $1^C \ Bag \ of \ Bonds$ 2.6704 0.0481 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 2.5023 0.0458 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.4 2.4678 0.0267 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.4 2.3144 0.0553 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.4 2.4218 0.0532 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.4 2.4156 0.0376 1e-07 1e-07 laplace $1^C \ Bag \ of \ Bonds$ 3.8 2.3197 0.0511 1e-07 1e-07 laplace $2^C \ Bag \ of \ Bonds$ 3.8 2.3197 0.0511 1e-07 1e-07 laplace $2^C \ Bag \ of \ Bonds$ 3.8 2.3197 0.0511 1e-07 1e-07 laplace $2^C \ Bag \ of \ Bonds$ 3.1836 0.1023 1e-07 1e-03 gauss $2^{NC} \ Bag \ of \ Bonds$	1	$(^{C}\ 2^{LC}_{7}\ 3^{B})$	1.8012	0.0454	1e-09	1e-07	gauss
1^C Bag of Bonds 2.6704 0.0481 $1e-07$	1	$1^{C} 2_{7}^{LC} 3^{B} 4$	1.7592	0.0334	1e-09	1e-07	gauss
1^C Bag of Bonds 3 2.5023 0.0458 $1e-07$ $1e-07$ $1aplace$ 1^C Bag of Bonds 3 4 2.4678 0.0267 $1e-07$ $1e-07$ $1aplace$ 1^C Bag of Bonds 3 4^B 2.3144 0.0553 $1e-07$ $1e-07$ $1aplace$ 1^C Bag of Bonds 3^B 2.4218 0.0532 $1e-07$ $1e-07$ $1aplace$ 1^C Bag of Bonds 3^B 4 2.4156 0.0376 $1e-07$ $1e-07$ $1aplace$ 1^C Bag of Bonds 3^B 4 2.3197 0.0511 $1e-07$ $1e-07$ $1aplace$ 2^C Bag of Bonds 3^B 4 2.3197 0.0511 $1e-07$ $1e-07$ $1aplace$ 2^C Bag of Bonds 3^B 4 2.3197 0.0511 $1e-07$ $1e-07$ $1aplace$ 2^C Bag of Bonds 3^B 4 2.3197 0.0511 $1e-07$ $1e-07$ $1aplace$ 2^C Bag of Bonds 3^B 4 2.3197 0.0511 $1e-07$	1	$1^{C} 2_{7}^{LC} 3^{B} 4^{B}$	1.7154	0.0312	1e-09	1e-07	gauss
1^C Bag of Bonds 3.4 2.4678 0.0267 $1e-07$	1	C Bag of Bonds	2.6704	0.0481	1e-07	1e-07	laplace
1^C Bag of Bonds 34^B 2.3144 0.0553 $1e-07$	1	C Bag of Bonds 3	2.5023	0.0458	1e-07	1e-07	laplace
1^C Bag of Bonds 3^B 2.4218 0.0532 $1e-07$	1	C Bag of Bonds 3 4	2.4678	0.0267	1e-07	1e-07	laplace
1^C Bag of Bonds 3^B 4 2.4156 0.0376 $1e-07$	1	C Bag of Bonds 3 4^{B}	2.3144	0.0553	1e-07	1e-07	laplace
1^C Bag of Bonds 3^B 4^B 2.3197 0.0511 $1e-07$ $1e-07$ $1aplace$ 2 27.0143 1.2266 $1e-11$ $1e-05$ $gauss$ 2^B 7.6924 0.1527 $1e-07$ $1e-03$ $gauss$ 2^{LP} 3.1836 0.1023 $1e-09$ $1e-05$ $gauss$ 2^{NC} 2.9543 0.0646 $1e-09$ $1e-07$ $gauss$ 2^{NP} 3.4914 0.1005 $1e-07$ $1e-05$ $gauss$	1	C Bag of Bonds 3^{B}	2.4218	0.0532	1e-07	1e-07	laplace
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	C Bag of Bonds 3^{B} 4	2.4156	0.0376	1e-07	1e-07	laplace
2^{B} 7.6924 0.1527 $1e-07$ $1e-03$ gauss 2^{LP} 3.1836 0.1023 $1e-09$ $1e-05$ gauss 2^{NC} 2.9543 0.0646 $1e-09$ $1e-07$ gauss 2^{NP} 3.4914 0.1005 $1e-07$ $1e-05$ gauss	1	C Bag of Bonds 3^{B} 4^{B}	2.3197	0.0511	1e-07	1e-07	laplace
2^{LP} 3.1836 0.1023 1e-09 1e-05 gauss 2^{NC} 2.9543 0.0646 1e-09 1e-07 gauss 2^{NP} 3.4914 0.1005 1e-07 1e-05 gauss	2	2	27.0143	1.2266	1e-11	1e-05	gauss
2^{NC} 2.9543 0.0646 1e-09 1e-07 gauss 2^{NP} 3.4914 0.1005 1e-07 1e-05 gauss	2	Q^B	7.6924	0.1527	1e-07	1e-03	gauss
2^{NP} 3.4914 0.1005 1e-07 1e-05 gauss	2	2^{LP}	3.1836	0.1023	1e-09	1e-05	gauss
9.1011 0.1000 10 01 10 00 gatab	2	2NC	2.9543	0.0646	1e-09	1e-07	gauss
2^{NP} {'end': 12.0} 4.0497 0.0908 1e-09 1e-05 gauss	2	2^{NP}	3.4914	0.1005	1e-07	1e-05	gauss
	2	2^{NP} {'end': 12.0}	4.0497	0.0908	1e-09	1e-05	gauss

2^{NP} {'end': 16.0}	8.8295	0.1648	1e-09	1e-05	gauss
2^{NP} {'end': 2.0}	3.9053	0.5433	1e-09	1e-05	gauss
2^{NP} {'end': 4.0}	2.8394	0.1226	1e-09	1e-05	gauss
2^{NP} {'end': 6.0}	3.4914	0.1005	1e-07	1e-05	gauss
2^{NP} {'end': 8.0}	3.5837	0.0939	1e-07	1e-05	gauss
2^{NP} {'segments': 10}	51.6721	0.8192	1e-09	1e-05	gauss
2^{NP} {'segments': 150}	3.3189	0.0993	1e-07	1e-05	gauss
2^{NP} {'segments': 200}	3.2660	0.1039	1e-07	1e-05	gauss
2^{NP} {'segments': 25}	21.2022	0.3948	1e-09	1e-05	gauss
2^{NP} {'segments': 50}	3.8189	0.1564	1e-09	1e-05	gauss
2^{NP} {'segments': 75}	3.3082	0.0701	1e-09	1e-05	gauss
$2^{NP} \{ \beta' : 1.0 \}$	3.8716	0.1001	1e-07	1e-05	gauss
$2^{NP} \{ '\beta' : 10.0 \}$	3.1849	0.0777	1e-07	1e-05	gauss
$2^{NP} \{ '\beta' : 2.5 \}$	3.0443	0.1656	1e-09	1e-05	gauss
$2^{NP} \{ \beta' : 30.0 \}$	3.5714	0.1258	1e-09	1e-05	gauss
$2^{NP} \{ '\beta' : 40.0 \}$	4.4723	0.1251	1e-09	1e-05	gauss
$2^{NP} \{ \beta' : 5.0 \}$	3.1355	0.0516	1e-07	1e-05	gauss
$2^{NP} \{ \beta' : 80.0 \}$	35.0504	0.8029	1e-07	1e-05	gauss
2^{NP} {'start': 0.1}	3.4565	0.0847	1e-07	1e-05	gauss
2^{NP} {'start': 0.2}	3.4914	0.1005	1e-07	1e-05	gauss
2^{NP} {'start': 0.4}	3.4549	0.1007	1e-07	1e-05	gauss
2^{NP} {'start': 0.8}	3.4270	0.0983	1e-07	1e-05	gauss
2^{NP} {'start': 1.0}	3.4181	0.0877	1e-07	1e-05	gauss
2^{NP} {'start': 1.5}	7.2008	0.0602	1e-07	1e-05	gauss
2^{SC}	4.0910	0.0993	1e-07	1e-07	gauss
2^{SP}	132.0560	3.0004	1e-09	1e-11	gauss
2_1	6.3495	0.1191	1e-07	1e-07	laplace

2_1^{LP}	7.5691	1.6200	1e-09	1e-05	gauss
2_1^{NC}	6.4204	0.6765	1e-07	1e-05	gauss
2_1^{NP}	6.2499	2.0349	1e-11	1e-05	gauss
2_1^{SC}	6.2928	0.1868	1e-09	1e-05	gauss
2_1^{SP}	167.2493	1.5730	1e-09	1e-05	gauss
2_2	3.3990	0.5837	1e-11	1e-07	gauss
2_2^{LP}	2.5101	0.1446	1e-11	1e-05	gauss
2_2^{NC}	2.7340	0.0770	1e-07	1e-05	gauss
2_2^{NP}	2.4360	0.3073	1e-11	1e-05	gauss
2_2^{SC}	3.1870	0.0630	1e-07	1e-05	gauss
2_2^{SP}	160.7898	1.6727	1e-07	1e-05	gauss
2_3	2.7405	0.0779	1e-11	1e-07	gauss
2^{LC}_3	2.7402	0.0769	1e-11	1e-07	gauss
$2_3^{LC} \ \{'\beta':\ 30.0\}$	2.7213	0.0613	1e-11	1e-07	gauss
2_3^{LP}	2.6063	0.0714	1e-09	1e-05	gauss
2_3^{NC}	2.7179	0.0776	1e-11	1e-07	gauss
$2_3^{NC} \ 2_3^{NP}$	2.8589	0.0621	1e-09	1e-07	gauss
$2_3^{NC} \ \{'\beta':\ 30.0\}$	2.8776	0.0932	1e-09	1e-07	gauss
2_3^{NP}	2.4520	0.0817	1e-09	1e-05	gauss
2_3^{NP} {'end': 12.0}	3.3002	0.0953	1e-09	1e-05	gauss
2_3^{NP} {'end': 16.0}	8.4140	0.2894	1e-09	1e-05	gauss
2_3^{NP} {'end': 4.0}	2.3865	0.0690	1e-09	1e-05	gauss
2_3^{NP} {'end': 6.0}	2.4520	0.0817	1e-09	1e-05	gauss
2_3^{NP} {'end': 8.0}	2.5219	0.0522	1e-09	1e-05	gauss
2_3^{NP} {'segments': 10}	76.5502	1.1925	1e-09	1e-05	gauss
2_3^{NP} {'segments': 150}	2.3723	0.0879	1e-09	1e-05	gauss
2_3^{NP} {'segments': 200}	2.3724	0.0866	1e-09	1e-05	gauss

2_3^{NP} {'segments': 25}	22.3027	0.3675	1e-09	1e-05	gauss
2_3^{NP} {'segments': 50}	3.3063	0.1420	1e-09	1e-05	gauss
2_3^{NP} {'segments': 75}	2.5052	0.0509	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta': 1.0\}$	6.2651	0.0677	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta': 10.0\}$	2.4681	0.0623	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta': \ 2.5\}$	3.8039	0.0425	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta':\ 30.0\}$	2.5371	0.1042	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta': \ 40.0\}$	3.5383	0.1359	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta': 5.0\}$	3.0443	0.1656	1e-09	1e-05	gauss
$2_3^{NP} \ \{'\beta':\ 80.0\}$	37.2210	1.4209	1e-09	1e-05	gauss
2_3^{NP} {'start': 0.1}	2.4346	0.0895	1e-09	1e-05	gauss
2_3^{NP} {'start': 0.2}	2.4520	0.0817	1e-09	1e-05	gauss
2_3^{NP} {'start': 0.4}	2.4326	0.0919	1e-09	1e-05	gauss
2_3^{NP} {'start': 0.8}	2.3938	0.0946	1e-09	1e-05	gauss
2_3^{NP} {'start': 1.0}	2.4019	0.0934	1e-09	1e-05	gauss
2_3^{NP} {'start': 1.5}	10.8269	0.2624	1e-09	1e-05	gauss
2_3^{SC}	3.6489	0.1096	1e-09	1e-07	gauss
$2_3^{SC} \ \{'\beta':\ 30.0\}$	3.6489	0.1096	1e-09	1e-07	gauss
2_3^{SP}	146.4782	2.6895	1e-07	1e-05	gauss
2_4	3.3554	0.0558	1e-09	1e-07	gauss
2_4^{LP}	2.9515	0.1458	1e-09	1e-05	gauss
2_4^{NC}	3.1824	0.0796	1e-09	1e-07	gauss
2_4^{NP}	3.0073	0.1094	1e-09	1e-05	gauss
2_4^{SC}	4.1667	0.0960	1e-09	1e-07	gauss
2_4^{SP}	141.7759	3.3160	1e-05	1e-07	gauss
2_5	3.5451	0.0708	1e-09	1e-07	gauss
2_5^{LP}	3.3860	0.1120	1e-09	1e-05	gauss

2_5^{NC}	3.4412	0.0751	1e-09	1e-07	gauss
2_5^{NP}	3.4864	0.0987	1e-09	1e-05	gauss
2^{SC}_5	4.5364	0.0881	1e-09	1e-07	gauss
2_5^{SP}	136.2433	3.4077	1e-09	1e-11	gauss
2_6	3.5102	0.0700	1e-09	1e-07	gauss
2_6^{LP}	3.4702	0.1062	1e-09	1e-05	gauss
2_6^{NC}	3.3962	0.0546	1e-09	1e-07	gauss
2_6^{NP}	3.7576	0.0970	1e-07	1e-05	gauss
2_6^{SC}	4.5080	0.0667	1e-09	1e-07	gauss
2_6^{SP}	133.9029	2.8934	1e-09	1e-11	gauss
27	3.5038	0.0731	1e-09	1e-07	gauss
2_7^{LP}	3.4846	0.1020	1e-09	1e-05	gauss
2_7^{NC}	3.3877	0.0630	1e-09	1e-07	gauss
2_7^{NP}	3.7627	0.0946	1e-07	1e-05	gauss
2_7^{SC}	4.4929	0.0669	1e-09	1e-07	gauss
2_7^{SP}	133.4427	2.8907	1e-09	1e-11	gauss
3	45.2756	1.5846	1e-05	1e-03	gauss
3^B	6.3598	0.2685	1e-11	1e-07	gauss
4	64.2473	1.0873	1e-11	1e-07	laplace
4^B	51.4362	1.2445	1e-11	1e-07	laplace
5	56.4299	3.4445	1e-03	1e-03	laplace
5^B	67.4268	2.0270	1e-05	1e-05	gauss
Bag of Bonds	2.4137	0.0302	1e-09	1e-03	laplace
Bag of Bonds {'strip atoms': True}	2.3973	0.0353	1e-09	1e-03	laplace
$Bag of Bonds_1$	3.3332	0.0958	1e-05	1e-03	laplace
Bag of Bonds ₁ {'strip atoms': True}	3.7842	0.1366	1e-05	1e-03	laplace
$Bag of Bonds_2$	2.1441	0.0892	1e-07	1e-05	laplace

Bag of Bonds ₂ {'strip atoms': True}	3.1378	0.0975	1e-09	1e-03	laplace
Bag of $Bonds_3$	2.3332	0.0880	1e-07	1e-05	laplace
Bag of Bonds ₃ {'strip atoms': True}	3.7245	0.1495	1e-09	1e-05	laplace
$Bag of Bonds_4$	2.5566	0.0916	1e-07	1e-05	laplace
Bag of Bonds ₄ {'strip atoms': True}	3.8601	0.0667	1e-09	1e-03	laplace
Bag of $Bonds_5$	2.6012	0.1162	1e-07	1e-05	laplace
Bag of Bonds ₅ {'strip atoms': True}	3.8341	0.0725	1e-09	1e-03	laplace
Bag of $Bonds_6$	2.5947	0.0917	1e-07	1e-05	laplace
Bag of Bonds ₆ {'strip atoms': True}	3.8087	0.0873	1e-09	1e-03	laplace
Bag of $Bonds_7$	2.5660	0.0843	1e-07	1e-05	laplace
Bag of Bonds ₇ {'strip atoms': True}	3.7550	0.0936	1e-09	1e-03	laplace
Coulomb Matrix	3.3714	0.1643	1e-07	1e-03	laplace
Coulomb Matrix ₁	2.8048	0.1232	1e-07	1e-03	laplace
Coulomb $Matrix_2$	2.9136	0.1867	1e-07	1e-03	laplace
Coulomb Matrix ₃	3.2354	0.1384	1e-07	1e-03	laplace
Coulomb Matrix ₄	3.4033	0.1562	1e-07	1e-03	laplace
Coulomb Matrix ₅	3.3810	0.1651	1e-07	1e-03	laplace
Coulomb Matrix ₆	3.3332	0.1533	1e-07	1e-03	laplace
Coulomb Matrix ₇	3.3273	0.1582	1e-07	1e-03	laplace
Null	179.0135	0.0754	1e-09	1e-11	gauss

Table S4: KRR Results