

Supplementary Information

Listed below are the Cartesian coordinates of all fully hydrated silicate structures (minima and saddle points) discussed in this work. All minima have been fully optimized at the HF/6-31G(d) level of theory. Transition states have been located as the maxima of constrained internal coordinate scans, also performed at the HF/6-31G(d) level of theory, where the constrained coordinates were pertinent Si-O bonds between hydrogen-bonded oligomers (during Si-O bond formation processes) or Si-OH bonds during dehydration reactions.

Only trimerisation and tetramerization reactions are considered here; dimerization reactions were considered in our previous works.¹

- (1) McIntosh, G. J. *Phys. Chem. Chem. Phys.* **2012**, *14*, 996.

3R-1

3TS-2

Atom	x	y	z	Atom	x	y	z
Si	-0.246612	1.525078	-0.746028	Si	-0.75204	0.114339	-1.33409
Si	2.38387	-1.967041	-1.250381	Si	2.782971	-0.14637	-0.6268
O	2.643921	-0.855525	-0.089823	O	2.630989	1.460717	-0.96085
H	1.88922	-0.294559	0.140489	H	1.84625	1.58801	-1.48212
O	1.827207	-1.287048	-2.619161	O	3.094229	-1.20554	-1.85131
H	1.200935	-0.567885	-2.569889	H	2.313875	-1.28529	-2.39096
O	1.370065	-3.162482	-0.734638	O	1.881059	-0.84551	0.599689
H	0.547755	-2.897255	-0.32236	H	1.012178	-1.06998	0.281932
O	3.805873	-2.708403	-1.561202	O	4.246557	-0.04405	0.157621
H	3.780836	-3.658475	-1.620497	H	4.626632	-0.87944	0.394632
O	-1.803438	1.950088	-0.594974	O	-1.15204	-0.79177	0.013795
O	0.305465	0.504039	0.307105	O	0.762262	-0.12739	-1.65412
O	-0.041249	0.908344	-2.2767	O	-1.77209	-0.24268	-2.55269
H	-0.541552	1.316543	-2.969486	H	-2.70264	-0.05385	-2.46858
O	0.512905	3.014614	-0.709402	O	-1.1065	1.684049	-0.88474
H	1.459709	2.987615	-0.732621	H	-0.5765	2.052945	-0.17684
O	2.710549	-5.48975	-1.628094	O	3.991645	-3.2071	0.153894
H	2.355358	-5.65119	-2.491583	H	3.855826	-2.88763	-0.73391
H	2.066356	-4.940853	-1.182089	H	3.216611	-2.91965	0.621922
O	5.615058	-1.009476	0.307226	O	3.025917	3.4325	0.990458
H	4.720711	-0.722089	0.46215	H	3.015863	2.815931	0.254358
H	5.507368	-1.671373	-0.366063	H	3.694958	3.104787	1.575991
O	-0.888297	-1.944216	0.596744	O	-4.63262	0.275937	-1.88888
H	-0.841876	-2.106343	1.530518	H	-4.61216	1.147503	-1.50873
H	-0.521205	-1.054036	0.476179	H	-4.61407	-0.30643	-1.1355
Si	-3.295377	2.040737	0.038946	O	0.182936	2.80079	1.46555
O	-3.693037	3.613373	0.12629	H	1.058573	3.164443	1.344884
H	-2.998138	4.236679	-0.072922	H	0.302374	2.063104	2.056772
O	-4.394031	1.281087	-0.886653	O	0.814076	0.271064	2.898893
H	-4.41848	0.333025	-0.787934	H	1.319523	0.126839	3.687024
O	-3.311975	1.288404	1.495632	H	1.327786	-0.08577	2.165777
H	-2.523713	1.29965	2.036369	Si	-2.2958	-1.29545	1.034443
O	-1.272919	5.245513	-0.227016	O	-3.68293	-0.45405	0.840743
H	-0.653894	4.556194	-0.468344	H	-3.64813	0.499234	0.834624
H	-1.019055	5.527249	0.641025	O	-2.75618	-2.84243	0.770018
O	-3.845445	-1.378246	0.347146	H	-2.21491	-3.51086	1.163292
H	-3.795338	-0.734596	1.047841	O	-1.6915	-1.21166	2.549124
H	-2.95179	-1.696278	0.245924	H	-0.90245	-0.69641	2.696631
O	-0.756648	0.934121	2.783901	O	-3.62174	2.342616	0.04731
H	-0.19819	1.453779	3.344437	H	-3.57471	3.123948	0.581324
H	-0.271239	0.790047	1.957597	H	-2.74937	2.229329	-0.3482

3R-2

Atom	x	y	z
Si	0.579176	-0.49443	1.017135
Si	-2.47751	0.64152	0.181448
O	-1.88395	1.786428	1.255091
H	-1.06934	1.578738	1.68816
O	-3.35582	-0.63907	0.795949
H	-2.86994	-1.30244	1.273141
O	-2.02321	0.690527	-1.43571
H	-1.15519	0.349769	-1.59069
O	-3.8621	1.554399	-0.20941
H	-4.47825	1.602706	0.505977
O	1.618547	-1.01004	-0.15254
O	-0.89411	-0.43061	0.45275
O	0.670758	-1.54352	2.275472
H	1.434614	-1.45915	2.837633
O	1.148118	0.944865	1.583658
H	1.249156	1.628619	0.914642
O	3.091344	-0.17673	3.380909
H	2.557527	0.488317	2.949168
H	3.834212	-0.31522	2.808757
O	1.162735	2.6252	-0.70616
H	0.326545	3.089379	-0.77712
H	1.164312	1.9729	-1.39928
Si	1.755486	-1.24078	-1.73599
O	3.318653	-1.34656	-2.20663
H	3.643205	-2.22515	-2.34459
O	1.045079	-2.59661	-2.26874
H	0.168302	-2.81727	-1.9417
O	1.104519	0.113178	-2.42263
H	1.02994	0.121551	-3.36717
O	-1.46686	-2.81887	-1.02348
H	-2.29034	-2.67881	-1.49046
H	-1.35401	-2.01747	-0.50886
O	-1.49858	3.820687	-0.76154
H	-1.73824	3.437474	0.080961
H	-2.02556	3.315182	-1.37156
O	-3.97549	-1.62355	-1.9486
H	-4.19757	-1.46028	-1.03481
H	-3.58607	-0.79671	-2.21927
O	-1.90801	-3.12848	2.071679
H	-1.78785	-3.46533	1.191004
H	-1.08252	-2.7121	2.302668

3TS-3

Atom	x	y	z
Si	-1.14945	-1.10872	0.554819
Si	1.82689	-1.62214	0.504453
O	2.491576	-2.90875	1.270121
H	1.905493	-3.31284	1.894912
O	2.513922	-0.18504	0.922596
H	3.412066	-0.25961	0.571041
O	1.521492	-1.82501	-1.09168
H	2.373752	-1.80286	-1.5346
O	4.047107	-1.35433	-0.72245
H	4.708272	-2.01921	-0.59315
O	-1.26249	0.512111	0.469267
O	0.30275	-1.51073	1.136898
O	-2.30307	-1.68982	1.530164
H	-3.18958	-1.37362	1.353464
O	-1.3281	-1.75322	-0.95038
H	-0.50331	-1.83917	-1.42556
O	-3.927	-2.67306	-1.72435
H	-3.02337	-2.3695	-1.63073
H	-3.95522	-3.51044	-1.28166
O	-4.68539	-0.65804	0.284204
H	-4.66136	-1.26246	-0.45425
H	-4.36826	0.176699	-0.05147
Si	-1.64294	1.84344	-0.37277
O	-3.2302	1.6835	-0.78736
H	-3.6075	2.401536	-1.27599
O	-1.51779	3.16282	0.560314
H	-0.65747	3.573138	0.667983
O	-0.7734	1.959143	-1.73732
H	0.182584	1.954706	-1.68513
O	1.196105	3.944726	0.904641
H	1.630839	3.538394	0.159152
H	1.351844	3.349506	1.636723
O	4.334948	0.760904	-2.34406
H	4.301679	-0.06569	-1.8177
H	5.163858	1.166993	-2.13356
O	2.038179	1.934851	-1.07953
H	2.082256	1.260856	-0.40402
H	2.751105	1.703341	-1.67886
O	1.268209	1.684905	2.749225
H	1.763616	1.020021	2.27325
H	0.36087	1.414431	2.676601

3R-3

Atom	x	y	z
Si	-0.01054	0.012159	0.003783
Si	-0.00198	0.005193	3.068554
O	1.552953	0.003986	3.294177
H	2.191828	-0.15862	4.924667
O	-0.75097	-1.18558	3.963788
H	-1.5668	-1.49261	3.593545
O	-0.72221	1.442022	3.49127
H	-0.73463	1.576627	4.434677
O	2.475899	-0.16001	5.852548
H	2.751365	-1.04674	6.038628
O	0.69671	1.469081	-0.09114
O	-0.47763	-0.26298	1.519522
O	-1.29662	-0.06466	-0.97925
H	-1.16778	0.273052	-1.86322
O	1.082757	-1.11957	-0.49146
H	1.821746	-1.25037	0.112048
O	-0.19672	0.999973	-3.50723
H	0.498912	0.372694	-3.67593
H	0.262208	1.772508	-3.1922
O	3.224429	-0.9668	1.300912
H	2.711638	-0.7307	2.08519
H	3.547249	-0.1378	0.962771
Si	1.916581	2.45738	-0.50209
O	2.20459	2.332963	-2.10806
H	2.576582	1.51026	-2.41054
O	1.489625	3.98788	-0.20405
H	1.046809	4.137482	0.633215
O	3.275814	1.99245	0.287752
H	3.333648	2.221944	1.215098
O	2.300807	-0.54024	-2.95567
H	1.902585	-0.86263	-2.14092
H	2.952437	-1.17723	-3.21421
O	0.57953	3.927762	2.509445
H	1.402363	3.615451	2.876356
H	-0.04149	3.227625	2.700931
O	2.95875	2.300006	3.129332
H	3.549174	2.313039	3.870795
H	2.43232	1.483446	3.218808
O	-0.35927	0.505172	6.405112
H	0.588121	0.393932	6.450276
H	-0.66892	-0.26362	5.937187

3TS-4

Atom	x	y	z
Si	1.540922	1.01307	-0.19472
Si	-1.37597	0.623101	-0.25467
O	-1.05114	-0.88923	-0.48668
H	-4.99079	-0.85537	-0.18194
O	-2.28963	1.255781	-1.47591
H	-2.40651	2.200684	-1.44312
O	-2.13331	0.960542	1.178193
H	-2.44209	0.178931	1.641688
O	-4.76036	-1.7747	-0.20411
H	-4.1905	-1.86986	-0.97071
O	1.583643	-0.59574	-0.16251
O	0.020396	1.551912	-0.21657
O	2.395711	1.592824	1.05998
H	3.026967	0.965853	1.412212
O	2.323253	1.538295	-1.55738
H	1.849219	1.428865	-2.37113
O	5.163144	1.014209	-1.07693
H	4.278243	1.172476	-1.40101
H	5.386364	1.79174	-0.58288
O	4.313943	-0.64066	1.312097
H	4.730729	-0.36211	0.501423
H	3.732986	-1.36156	1.076091
Si	0.823008	-2.00916	0.107727
O	2.266819	-2.80767	0.591037
H	2.195693	-3.72342	0.818681
O	-0.03312	-2.18992	1.515601
H	0.505132	-2.48039	2.238222
O	0.396727	-2.94494	-1.17389
H	1.100144	-3.50143	-1.47427
O	-2.03891	3.614252	2.124445
H	-2.17187	2.686904	1.913508
H	-1.18354	3.655187	2.530644
O	-1.63646	4.095927	-0.74337
H	-1.89479	4.154953	0.174523
H	-0.79472	3.654579	-0.72201
O	-2.86103	-1.64418	2.093418
H	-3.47479	-1.86161	1.395015
H	-2.00201	-1.92541	1.783402
O	-2.90744	-1.67222	-2.4121
H	-2.13386	-1.69182	-1.83838
H	-2.9694	-0.75138	-2.63928

3R-4

Atom	x	y	z
Si	0.198523	-0.21068	-0.36627
Si	-0.05391	-0.24606	2.53777
O	1.526127	-0.29369	2.47283
H	1.170509	-0.38581	6.417942
O	-0.59831	-1.60401	3.281583
H	-1.54328	-1.72818	3.252922
O	-0.62211	1.081005	3.318828
H	0.061655	1.597061	3.759758
O	2.058387	-0.22137	6.13045
H	2.273244	-0.95395	5.549166
O	1.746644	-0.3626	0.00803
O	-0.68425	-0.22077	1.005672
O	-0.05002	1.127576	-1.25599
H	0.764054	1.482476	-1.61502
O	-0.28859	-1.47228	-1.31915
H	-0.25589	-2.33002	-0.91742
O	0.872228	-0.68724	-3.94426
H	0.526313	-1.14395	-3.18154
H	0.293979	0.056091	-4.05511
O	2.670075	1.326926	-2.36593
H	2.479093	0.589001	-2.93561
H	3.155043	0.965534	-1.62096
Si	2.776896	-0.00165	1.282726
O	4.030039	0.312621	0.05767
H	4.873624	0.584547	0.390135
O	2.873924	1.589266	1.850429
H	3.400275	2.146098	1.297045
O	3.670522	-1.23824	1.990381
H	4.423217	-1.48531	1.475117
O	-3.37524	1.657054	3.024662
H	-2.44342	1.580428	3.240116
H	-3.41106	2.213248	2.258303
O	-3.35342	-1.17364	2.28208
H	-3.58292	-0.29989	2.593918
H	-2.87972	-1.02323	1.471891
O	1.69854	2.206488	4.437554
H	1.952069	1.488392	5.01456
H	2.180355	2.061701	3.622912
O	2.332043	-2.49147	4.325568
H	2.808933	-2.1004	3.593049
H	1.425623	-2.48057	4.036652

3TS-5

Atom	x	y	z
Si	1.947829	-0.16745	-0.25191
Si	-0.59151	1.376031	-0.38933
O	-1.24905	-0.07195	-0.71394
H	-5.71991	0.45427	0.251074
O	-0.68965	2.314112	-1.71109
H	-0.23894	3.154524	-1.65312
O	-1.34273	2.096167	0.867893
H	-1.91913	1.544267	1.410603
O	-5.21626	-0.30769	0.50207
H	-4.799	-0.62192	-0.30281
O	0.955772	-1.38674	-0.63463
O	0.990335	1.13581	-0.01279
O	2.85938	-0.52636	1.033908
H	2.790477	-1.44673	1.320092
O	2.989598	0.161519	-1.48063
H	2.603807	0.415879	-2.30772
O	5.649091	0.227678	0.058489
H	5.127059	0.271797	-0.73412
H	5.010049	-0.01481	0.720016
O	2.558248	-3.28655	1.439113
H	3.18095	-3.71766	0.870274
H	1.673559	-3.5211	1.077636
Si	-0.63821	-1.58135	-0.32061
O	0.144374	-3.81435	0.415714
H	-0.273	-4.60474	0.732714
O	-1.00286	-1.65079	1.276029
H	-0.66244	-2.49527	1.576655
O	-1.41007	-2.57579	-1.35471
H	-1.06219	-3.44808	-1.16631
O	-0.2359	4.552904	1.77032
H	-0.74186	3.76643	1.558128
H	0.292485	4.321714	2.522212
O	1.062956	4.456921	-0.81661
H	0.684537	4.684675	0.032155
H	1.786507	3.874136	-0.62227
O	-2.91787	0.271778	2.270343
H	-3.71639	0.082235	1.781062
H	-2.34122	-0.47617	2.12192
O	-3.8061	-0.95659	-1.91285
H	-3.34804	-1.79234	-1.89862
H	-3.09504	-0.33306	-1.79683

3R-5

Atom	x	y	z
Si	1.47536	-0.90723	-0.22901
Si	-0.6782	0.960314	-1.05428
O	-1.6253	-0.21668	-0.47633
O	-1.05918	1.292843	-2.59845
H	-0.47344	1.92628	-3.00429
O	-0.81862	2.296136	-0.11596
H	-1.47552	2.274187	0.582141
O	0.29893	-1.42512	0.75676
O	0.867066	0.417747	-0.98339
O	2.842176	-0.51019	0.554674
H	2.787746	0.245397	1.138447
O	1.913977	-2.06054	-1.29063
H	1.190174	-2.56935	-1.65514
O	4.90554	-2.34117	-0.72954
H	4.110496	-2.57033	-1.19795
H	4.602689	-1.68127	-0.11561
O	2.35168	1.737922	2.294829
H	2.951893	1.843616	3.020532
H	1.496898	1.525422	2.688586
Si	-1.33925	-1.21777	0.822769
O	-0.09841	1.115609	3.520211
H	-0.72622	1.824825	3.445418
O	-1.8525	-0.63942	2.185383
H	-0.57189	0.357898	3.154699
O	-2.01462	-2.6707	0.41451
H	-2.61334	-3.01461	1.071258
O	1.59549	3.843232	0.114601
H	0.702747	3.504279	0.123302
H	2.059378	3.289268	0.734703
O	1.548796	2.819718	-2.68512
H	1.677293	3.340282	-1.89407
H	1.905895	1.967915	-2.46255
O	-2.64906	1.935524	2.065442
H	-3.57599	2.066669	1.922883
H	-2.50482	0.973812	2.122717
O	-0.66893	-3.15508	-2.09692
H	-1.15912	-3.25125	-1.28103
H	-1.12637	-2.47816	-2.57961
O	-3.44447	-2.69907	3.07706
H	-2.97726	-3.14002	3.772805
H	-2.96561	-1.87313	2.9229

3R-6

Atom	x	y	z
Si	1.10327	-0.25275	-0.10816
Si	-2.99709	0.465674	-0.37777
O	-1.89232	1.542679	-0.61737
H	-0.33013	1.232379	-0.97884
O	-2.71464	-1.00888	-1.09899
H	-1.82867	-1.33685	-0.96535
O	-4.50111	0.877336	-0.97942
H	-4.49407	1.708351	-1.43282
O	-3.22729	0.16619	1.241022
H	-4.01221	-0.33043	1.452891
O	2.624404	-0.64004	-0.5288
O	0.623353	0.976094	-1.03849
O	0.106756	-1.53198	-0.34141
H	0.330812	-2.29028	0.191371
O	1.228978	0.102495	1.487748
H	0.467615	0.468804	1.958655
O	-5.97817	-1.01028	0.732821
H	-5.78059	-1.74897	0.162128
H	-5.89565	-0.24716	0.169098
O	-1.1982	3.566138	1.080281
H	-0.35828	3.843667	0.742318
H	-1.52789	2.912294	0.442699
O	1.78555	-2.93365	1.709619
H	1.710208	-2.11984	2.196489
H	2.664907	-2.93819	1.349115
O	-0.97702	1.197369	2.764892
H	-1.76446	0.769734	2.428643
H	-1.02481	2.086581	2.415926
O	-4.92297	-2.73922	-1.44104
H	-4.10095	-2.25082	-1.35001
H	-5.31394	-2.41672	-2.24133
Si	4.163728	-0.35086	-0.10176
O	4.940188	-1.77127	0.166002
H	5.425178	-2.11785	-0.56945
O	4.949353	0.392218	-1.31184
H	4.42967	1.031637	-1.79901
O	4.154298	0.491081	1.291755
H	3.301214	0.58923	1.704052
O	2.900539	2.166336	-2.36102
H	2.875268	3.055519	-2.03542
H	2.079226	1.762444	-2.07391

3TS-7

Atom	x	y	z
Si	-0.8645	-0.03135	-0.28422
Si	2.733771	-0.2167	-0.21736
O	1.346939	-0.93041	-0.3983
H	0.04295	-1.1923	-1.85138
O	2.72741	1.386746	-0.627
H	1.831147	1.718771	-0.59063
O	3.958814	-0.83668	-1.17218
H	3.841407	-1.74814	-1.40115
O	3.265335	-0.36001	1.347348
H	4.163276	-0.07858	1.496157
O	-2.44652	0.482618	-0.34978
O	-0.84486	-0.88626	-1.69435
O	-0.06633	1.408057	-0.26561
H	-0.64787	2.146303	-0.08878
O	-0.92722	-0.86289	1.125114
H	-0.1222	-1.15924	1.548539
O	6.083977	0.381442	0.529409
H	5.991412	1.268108	0.188943
H	5.736697	-0.17746	-0.15893
O	1.05795	-3.62013	0.190933
H	0.121443	-3.76452	0.172378
H	1.176933	-2.69867	-0.07512
O	-1.90083	3.499535	0.771207
H	-1.65117	3.530099	1.685039
H	-2.74338	3.050004	0.746063
O	1.267605	-1.99054	2.706849
H	1.993603	-1.42325	2.454676
H	1.349799	-2.75569	2.146043
O	5.155172	2.796225	-0.91223
H	4.268359	2.448204	-0.79266
H	5.340953	2.691242	-1.83515
Si	-3.88907	0.365499	0.342004
O	-4.39182	1.87608	0.80296
H	-5.12763	2.206492	0.306293
O	-5.01455	-0.14012	-0.72119
H	-4.67882	-0.66936	-1.44413
O	-3.77626	-0.57282	1.667166
H	-2.88585	-0.87245	1.837542
O	-3.46127	-1.66383	-2.64916
H	-3.39949	-2.59167	-2.46847
H	-2.5928	-1.30844	-2.45081

3R-7

Atom	x	y	z
Si	0.219457	0.741758	0.311059
Si	2.440156	-1.5218	0.323421
O	1.513638	-2.55069	-0.56006
H	0.675286	-2.13747	-0.76117
O	2.892547	-2.15871	1.757831
H	2.516235	-1.74421	2.533271
O	1.066363	1.997601	-0.4336
H	0.535945	2.781101	-0.46403
O	3.860423	-1.36089	-0.52233
H	4.631735	-1.47077	0.016631
O	-1.26857	1.737254	0.132759
O	1.682678	-0.13667	0.499885
O	-0.06722	0.690488	1.978793
H	-0.71031	1.32686	2.279496
O	-0.43343	-0.51692	-0.60882
H	-1.35083	-0.44183	-0.83377
O	-2.55492	1.995827	3.209857
H	-2.9204	1.118818	3.204121
H	-2.95332	2.441817	2.46803
Si	-2.73147	1.806837	-0.47111
O	-3.66663	2.736044	0.529849
H	-4.38992	3.192427	0.123794
O	-2.83047	2.464646	-1.9587
H	-2.07923	2.310451	-2.52904
O	-3.36411	0.283875	-0.55458
H	-3.37354	-0.18733	0.274223
O	-2.56595	-0.87801	2.14953
H	-2.54005	-1.8112	2.313337
H	-1.65449	-0.58827	2.101116
O	-0.25401	1.690852	-3.19958
H	0.375589	1.78891	-2.48906
H	-0.22808	0.769007	-3.42186
O	3.234436	-3.38417	-2.84308
H	2.517666	-3.37466	-2.2155
H	3.801764	-2.69477	-2.51987
O	3.925708	1.66666	-1.22448
H	3.050381	1.864751	-0.90054
H	4.001149	0.724605	-1.1244
O	1.724978	-0.49309	3.806518
H	2.389319	0.160597	3.977104
H	1.104473	-0.07173	3.204771

3TS-8

Atom	x	y	z
Si	-0.07787	0.100146	-0.21431
Si	-2.74148	-1.18486	-0.62843
O	-3.21092	-0.25632	0.648224
H	-2.523	0.024218	1.243765
O	-3.00988	-2.7685	-0.40012
H	-2.53581	-3.1893	0.320138
O	-0.59323	1.596944	-0.77743
H	0.099528	2.154671	-1.10634
O	-3.7093	-0.75493	-1.8762
H	-4.12724	-1.47541	-2.32575
O	1.460205	0.087457	-0.75358
O	-1.18187	-0.8688	-0.92301
O	0.596825	-1.98926	0.737262
H	0.668133	-2.4782	-0.07309
O	-0.32645	0.339108	1.406297
H	-0.04088	-0.43504	1.878604
O	4.654515	-2.35891	-1.17202
H	4.217221	-2.41071	-0.32658
H	4.358491	-1.54125	-1.55592
Si	2.769935	0.997877	-0.46407
O	3.790948	0.66067	-1.70469
H	4.625694	1.107524	-1.69147
O	2.400087	2.585401	-0.49179
H	2.007754	2.954334	0.301204
O	3.43782	0.672656	0.977857
H	3.453112	-0.24084	1.265278
O	3.13178	-2.08567	1.426118
H	3.227073	-2.57025	2.233794
H	2.167641	-2.07512	1.203691
O	0.653562	3.213058	1.803262
H	-0.15456	3.656723	1.558888
H	0.383626	2.311937	1.957691
O	-4.68101	2.193805	0.014911
H	-4.33059	1.353987	0.306392
H	-4.6702	2.137883	-0.93181
O	-2.06281	3.633982	0.579736
H	-1.68534	2.913513	0.07653
H	-2.99875	3.458775	0.586732
O	-1.33545	-3.53445	1.755184
H	-0.98019	-4.39645	1.918887
H	-0.58858	-2.97526	1.454576

3TS-8

Atom	x	y	z
Si	-0.2446	0.588695	-0.49296
Si	-2.81928	-0.65706	-1.21639
O	-3.13532	-0.47665	0.386288
H	-2.33702	-0.47992	0.918677
O	-2.75425	-2.21013	-1.6843
H	-2.07907	-2.72805	-1.23968
O	-0.40886	2.23114	-0.27349
H	-0.5039	2.734151	-1.07053
O	-4.07294	0.014128	-2.03179
H	-4.54029	-0.57991	-2.60167
O	1.163121	0.397833	-1.31738
O	-1.44374	0.14698	-1.53121
O	-0.32385	-0.20444	0.855945
O	3.816128	-2.50101	1.330252
H	3.202873	-2.00055	1.864543
H	4.244221	-1.84202	0.796471
Si	2.735748	0.23956	-1.5234
O	3.018964	-1.18756	-2.29163
H	3.659666	-1.16408	-2.98815
O	3.387867	1.372029	-2.51748
H	3.712657	2.15583	-2.09764
O	3.535556	0.318993	-0.1068
H	3.043188	0.257733	0.714946
O	2.040951	-0.34532	2.194398
H	1.836762	0.223632	2.930275
H	1.192318	-0.42453	1.730188
O	-0.26875	1.195853	3.39973
H	-0.75337	2.0101	3.302096
H	-0.43831	0.721636	2.585627
O	-4.43964	2.014498	1.08585
H	-4.10474	1.12631	0.964523
H	-4.73056	2.282591	0.224313
O	-1.90107	3.353795	2.028975
H	-1.37441	3.078524	1.283007
H	-2.77567	3.015082	1.855004
O	-0.62187	-3.0249	0.030274
H	0.227527	-3.33823	-0.277
H	-0.45159	-2.18845	0.464149
O	2.117613	-3.65101	-0.81448
H	2.667799	-3.46991	-0.05505
H	2.337933	-2.97351	-1.44593

4R-1

Atom	x	y	z
14	0.491844	1.041583	-0.10614
14	4.19733	-0.87166	0.348466
8	3.018564	-0.89576	1.47417
1	2.102275	-0.86449	1.155683
8	4.209711	0.539769	-0.49289
1	3.391604	0.895936	-0.83185
8	4.082058	-2.11673	-0.70945
1	3.253075	-2.23074	-1.17221
8	5.612197	-0.9902	1.139436
1	6.380083	-0.9707	0.579538
8	-1.01289	1.507447	-0.53513
8	0.536486	-0.43271	0.463539
8	1.455668	1.224009	-1.4581
1	1.33454	0.557926	-2.12527
8	1.082821	2.208838	0.890196
1	1.443222	1.939633	1.730946
8	0.891872	4.304847	-1.1273
1	1.009238	3.959399	-0.24559
1	1.177904	3.587781	-1.6827
8	6.678612	-0.78563	-1.69961
1	6.12854	-0.00953	-1.71674
1	6.079044	-1.50804	-1.8528
8	-0.7738	0.070574	2.933641
1	-0.29389	-0.31256	2.196656
1	-0.10842	0.49387	3.463877
8	2.198136	1.067902	3.344334
1	2.635713	0.352585	2.877495
1	2.873797	1.538238	3.813265
8	1.393886	-1.91262	-1.75584
1	0.738359	-2.54333	-2.0267
1	1.037789	-1.51295	-0.95552
14	-2.58099	1.295025	-0.20682
8	-3.47108	2.424018	-0.9436
1	-3.04702	3.267776	-1.10112
8	-3.06575	-0.15782	-0.74639
8	-2.84686	1.350643	1.412877
1	-2.16892	1.021744	2.006907
8	-1.9449	4.816292	-1.48826
1	-1.99863	5.13344	-2.37902
1	-1.01638	4.636393	-1.3276
14	-2.99581	-1.76538	-0.61867
8	-1.46763	-2.27218	-0.32857
1	-0.84291	-1.67022	0.085463
8	-3.48264	-2.42763	-2.027
1	-3.55592	-3.37479	-2.00157
8	-3.96958	-2.28491	0.589375
1	-4.46648	-1.64098	1.093077
8	-5.28257	-0.09396	1.943138
1	-4.51859	0.483201	1.94443
1	-5.91801	0.324042	1.377431
8	-3.02923	-4.9323	-0.25274
1	-3.57632	-4.44406	0.354728
1	-2.15162	-4.59875	-0.10306

4TS-2

Atom	x	y	z
14	0.612546	0.891041	-0.50254
14	3.489232	-0.96689	0.20984
8	3.853061	0.450663	-0.55568
1	3.186948	0.833101	-1.10951
8	3.251231	-2.3061	-0.71068
1	2.369803	-2.45894	-1.02433
8	2.793968	-0.97534	1.720534
1	1.849016	-0.98965	1.644894
8	5.071682	-1.22915	0.728407
1	5.122647	-1.85704	1.435306
8	-0.94941	0.728697	-0.94631
8	1.378247	-0.47293	-0.33514
8	1.336499	1.838967	-1.6797
1	1.217852	1.530429	-2.5685
8	0.555208	1.859998	0.830325
1	1.309223	1.888992	1.427249
8	0.449932	4.481859	-0.77758
1	0.437938	4.1409	0.109946
1	0.87075	3.782362	-1.27224
8	6.121586	-3.14966	-1.32721
1	6.165719	-2.39906	-0.74395
1	5.183855	-3.27127	-1.42674
8	2.772357	1.810085	2.604104
1	2.887661	0.862677	2.600328
1	3.600634	2.147906	2.26802
8	5.392264	2.032837	1.255046
1	4.986328	1.627682	0.489037
1	5.924547	1.336702	1.618729
8	0.039869	-2.80165	-1.00323
1	-0.32541	-3.13927	-0.19285
1	0.385363	-1.92986	-0.78402
14	-2.4699	0.971114	-0.43733
8	-3.28339	2.003671	-1.37511
1	-2.99706	2.915045	-1.42652
8	-3.29314	-0.41361	-0.44749
8	-2.37268	1.524859	1.114357
1	-1.4909	1.757917	1.394875
8	-2.26962	4.682517	-1.60004
1	-2.29446	5.051487	-2.47197
1	-1.3497	4.690272	-1.32615
14	-3.30588	-2.02614	-0.5574
8	-2.50275	-2.6836	0.705487
1	-2.949	-2.58738	1.545987
8	-2.64684	-2.59306	-1.92431
1	-1.69585	-2.70856	-1.9065
8	-4.89417	-2.44813	-0.53526
1	-5.11392	-3.23959	-1.00622
8	-4.3683	0.796709	3.033064
1	-3.65886	1.05804	2.44461
1	-5.08251	1.39412	2.858632
8	-4.59933	-2.0559	2.573253
1	-5.22197	-2.12902	1.859397
1	-4.57276	-1.12968	2.811862

4R-2

Atom	x	y	z
14	0.676735	0.876439	-0.55954
14	3.211591	-0.98266	0.145854
8	3.775815	0.426914	-0.55869
1	3.234533	0.822901	-1.22462
8	3.141752	-2.37054	-0.76179
1	2.313038	-2.56394	-1.17583
8	2.529719	-1.05431	1.690067
1	1.585531	-1.09774	1.664538
8	4.779791	-1.26775	0.791496
1	4.760063	-1.95713	1.440316
8	-0.89765	0.685365	-0.92115
8	1.436004	-0.51372	-0.46518
8	1.329153	1.833934	-1.75963
1	1.140002	1.559791	-2.64749
8	0.698718	1.799649	0.794169
1	1.458289	1.79953	1.388227
8	0.7071	4.526262	-0.79128
1	0.762932	4.259647	0.118948
1	1.036456	3.768221	-1.2693
8	6.061045	-3.01218	-1.23832
1	6.023643	-2.28846	-0.61992
1	5.137538	-3.18351	-1.38649
8	2.82082	1.648343	2.635691
1	2.815906	0.69285	2.634887
1	3.704752	1.873487	2.34764
8	5.498837	1.558213	1.407347
1	5.084589	1.508036	0.549359
1	5.650777	0.634551	1.585002
8	-0.0864	-2.79163	-1.21192
1	-0.44512	-3.13317	-0.39985
1	0.313145	-1.95191	-0.97961
14	-2.39607	1.024608	-0.39052
8	-3.14287	2.124228	-1.30528
1	-2.82663	3.027235	-1.3149
8	-3.30098	-0.30679	-0.41715
8	-2.24415	1.540162	1.168719
1	-1.35286	1.757258	1.430751
8	-2.05984	4.77653	-1.41406
1	-2.15108	5.238934	-2.2356
1	-1.12293	4.767703	-1.2064
14	-3.3713	-1.91359	-0.59291
8	-2.52113	-2.64586	0.59579
1	-2.9248	-2.58386	1.461136
8	-2.8011	-2.43672	-2.01628
1	-1.85678	-2.59168	-2.05094
8	-4.96771	-2.28873	-0.50362
1	-5.24067	-3.04545	-1.00304
8	-4.13467	0.755326	3.176228
1	-3.46784	1.0338	2.547602
1	-4.82946	1.396852	3.12147
8	-4.48692	-2.05955	2.600852
1	-5.16057	-2.08012	1.931357
1	-4.41857	-1.14821	2.884164

4TS-3

Atom	x	y	z
14	0.598603	1.199301	-0.600898
14	2.768362	-1.038724	-0.344227
8	3.885136	0.000586	-0.983952
1	3.526459	0.607586	-1.61743
8	2.467084	-2.369018	-1.249001
1	3.266467	-2.892289	-1.21509
8	2.862087	-1.171103	1.28204
1	3.653972	-1.69182	1.43607
8	4.763305	-2.430846	0.081955
1	4.801262	-3.330807	0.381058
8	-0.977315	1.02048	-0.907802
8	1.344904	-0.206157	-0.543227
8	1.226066	2.128291	-1.822036
1	0.921607	1.909993	-2.693105
8	0.728045	2.068087	0.773197
1	1.492263	1.929099	1.350671
8	0.407068	4.730671	-0.562918
1	0.526641	4.244719	0.247147
1	0.810836	4.165816	-1.214934
8	6.954537	-1.121543	0.916688
1	6.170178	-1.629831	0.619445
1	7.508917	-1.055293	0.152008
8	2.902134	1.473247	2.369102
1	2.857579	0.521871	2.285365
1	3.789534	1.68342	2.077464
8	5.494803	1.398656	1.018812
1	5.043086	1.028897	0.264346
1	6.105778	0.702419	1.256946
8	-0.171807	-3.604027	-1.326766
1	-0.445989	-3.547117	-0.417624
1	0.6893	-3.190135	-1.374417
14	-2.458554	1.06044	-0.239043
8	-3.407609	2.151037	-0.958025
1	-3.141848	3.069862	-0.946723
8	-3.185212	-0.362862	-0.370906
8	-2.247744	1.415489	1.358407
1	-1.370444	1.686805	1.610006
8	-2.420487	4.85387	-0.959957
1	-2.614718	5.432451	-1.684054
1	-1.470484	4.884194	-0.828982
14	-3.216999	-1.965242	-0.587351
8	-2.359965	-2.717722	0.580646
1	-2.755996	-2.683581	1.450215
8	-2.635709	-2.434747	-2.020669
1	-1.756154	-2.82024	-2.022868
8	-4.812636	-2.359899	-0.499149
1	-5.070781	-3.115252	-1.008564
8	-4.221278	0.561804	3.264875
1	-3.506199	0.862229	2.703932
1	-4.946215	1.147589	3.094895
8	-4.391269	-2.257823	2.575418
1	-5.018522	-2.274856	1.861746
1	-4.379394	-1.358317	2.899875

4R-3

Atom	x	y	z
14	-0.84569	1.105501	-0.73074
14	-2.98061	-1.11419	-0.56741
8	-3.73598	-1.46029	-1.99193
1	-3.34685	-2.14467	-2.51739
8	-2.62338	0.362224	2.683354
1	-3.15466	0.84275	3.303172
8	-2.4704	-2.58583	-0.00695
1	-2.04331	-2.56838	0.85082
8	-3.84613	-0.23335	0.395958
1	-3.1959	0.141701	1.923235
8	0.665153	1.029378	-1.30741
8	-1.55748	-0.32585	-0.96304
8	-0.71889	1.476881	0.860513
1	-1.3313	1.125724	1.506106
8	-1.58668	2.314391	-1.52701
1	-2.5351	2.38858	-1.40227
8	-0.19893	4.297941	0.891423
1	-0.55904	4.486562	0.03342
1	-0.46842	3.396883	1.065637
8	-6.25612	-0.90151	1.70285
1	-6.14062	-1.83259	1.831304
1	-5.48678	-0.62702	1.194206
8	-0.39349	-2.88589	-1.99944
1	-0.5028	-1.93907	-1.99371
1	-0.9938	-3.1671	-1.31098
8	-4.36805	2.159129	-0.87482
1	-4.95856	1.931985	-1.58035
1	-4.29539	1.357377	-0.33719
8	-1.05776	-2.09359	2.472751
1	-0.16612	-1.82525	2.26752
1	-1.51398	-1.31132	2.773171
14	2.267685	0.961834	-1.39359
8	2.933631	2.394287	-1.73464
1	2.949559	3.005061	-0.99542
8	2.883924	0.326619	-0.04606
8	2.682363	-0.10157	-2.58467
1	2.603544	0.196808	-3.48011
8	2.60578	3.580189	0.847293
1	2.630429	2.849911	1.457767
1	1.721877	3.942679	0.904341
14	2.888004	-0.36884	1.407475
8	2.604213	0.801833	2.513218
1	2.974336	0.672174	3.375016
8	4.334174	-1.01057	1.769496
1	4.579083	-1.83309	1.347872
8	1.703188	-1.49901	1.444663
1	1.679143	-2.05217	0.667244
8	2.327066	-2.74699	-1.24893
1	1.453882	-3.01812	-1.54085
1	2.540858	-1.98401	-1.78168
8	4.769048	-3.35462	0.117245
1	3.941352	-3.36384	-0.36336
1	5.445187	-3.20231	-0.52883

4TS-4

Atom	x	y	z
14	-1.45455	1.339429	-1.25624
14	-1.87652	0.013129	1.281182
8	-0.98889	0.272426	2.663943
1	-0.36624	-0.42828	2.834265
8	1.101139	4.746361	1.113594
1	1.190025	3.996189	1.699392
8	-3.46209	0.043051	1.77839
1	-3.59828	-0.082	2.706354
8	-1.44062	-1.22384	0.448855
1	1.500665	4.479059	0.287256
8	-0.24569	0.341958	-1.67011
8	-1.72246	1.37936	0.339064
8	-1.04216	2.835456	-1.74934
1	-1.24837	3.546086	-1.13542
8	-2.77817	0.805963	-2.07421
1	-3.47734	1.432799	-2.19925
8	1.942964	3.586185	-1.46682
1	1.097898	3.222057	-1.71283
1	2.539513	2.854276	-1.32727
8	1.156365	2.277943	2.700692
1	1.71921	1.621711	2.304656
1	0.309441	1.842067	2.770227
8	-4.64757	-1.36688	-0.69885
1	-4.01069	-0.91667	-1.24421
1	-4.45043	-1.06683	0.183457
8	-1.64589	4.522535	0.417141
1	-1.8907	3.758733	0.927393
1	-0.76178	4.753836	0.713346
8	-0.99565	-3.55321	1.70398
1	-1.26227	-2.75466	1.21642
1	-1.36968	-4.27298	1.211636
14	0.50006	-1.07344	-1.49924
8	1.626841	-1.02114	-2.74802
1	1.60173	-0.20719	-3.23375
8	1.406267	-1.17998	-0.17781
8	-0.33041	-2.43558	-1.83323
1	-0.14643	-2.8072	-2.68457
8	3.806774	1.396739	-0.72089
1	3.474281	1.078612	0.112922
1	4.144435	0.622071	-1.15773
14	2.149035	-1.51527	1.201846
8	2.794136	-0.06603	1.697044
1	3.380714	-0.12142	2.440869
8	3.35791	-2.57375	0.930346
1	3.833106	-2.43016	0.11661
8	1.196541	-2.02552	2.399411
1	0.56724	-2.73478	2.231113
8	-2.80488	-3.84925	-0.94224
1	-3.52549	-3.25173	-0.76481
1	-2.05472	-3.27349	-1.0606
8	4.236145	-1.45618	-1.72497
1	4.818663	-1.81912	-2.37825
1	3.368253	-1.38779	-2.13079

4R-4

Atom	x	y	z
14	-1.94192	1.130286	0.800658
14	-1.79215	-1.79912	0.719362
8	-1.3168	-2.40285	2.18285
1	-1.85748	-3.0959	2.535372
8	-2.83638	-2.89699	0.132955
1	-3.04209	-2.82573	-0.80225
8	-0.50647	-1.50506	-0.17135
8	-0.5243	0.98858	0.044393
8	-2.56432	-0.3653	0.961989
8	-1.87245	1.960197	2.180598
1	-1.1358	1.85201	2.791364
8	-2.98605	2.009331	-0.14654
1	-3.3812	2.74163	0.309413
8	1.660481	2.692844	1.161367
1	1.066694	2.122415	0.676837
1	2.53928	2.345208	1.000332
8	1.132592	-1.16536	3.335175
1	1.775475	-1.28196	2.641417
1	0.350165	-1.6308	3.050123
8	-4.91979	-0.01484	-1.1939
1	-4.37159	0.752385	-1.05628
1	-4.80355	-0.52146	-0.39878
8	0.468319	1.649912	3.646238
1	0.72626	0.727943	3.650203
1	1.025757	2.07822	3.000494
14	0.164495	-0.10722	-1.05707
8	0.917839	1.197621	-1.94301
1	0.373924	1.96883	-2.07014
8	1.697885	-0.68856	-0.7659
8	-0.76844	-0.55807	-2.38545
1	-0.55309	-0.01895	-3.13352
8	4.1456	1.341872	0.630698
1	3.939345	0.478241	0.974262
1	4.120665	1.246431	-0.31964
14	2.610761	-1.93115	-0.36972
8	3.171241	-1.59288	1.165266
1	3.807863	-2.2031	1.513664
8	3.900661	-2.03276	-1.36373
1	4.062719	-1.23035	-1.85293
8	1.825438	-3.35498	-0.36653
1	0.88166	-3.23832	-0.30237
8	-3.2137	-2.06626	-2.53823
1	-3.84067	-1.36566	-2.37838
1	-2.3594	-1.63827	-2.60412
8	3.677196	0.877869	-2.23404
1	3.929974	1.457335	-2.93912
1	2.71596	0.958995	-2.14657
8	0.765631	5.036423	-0.23451
1	1.512994	5.349545	-0.72514
1	1.099199	4.335285	0.328794
8	-0.9771	3.552376	-2.09491
1	-0.51026	4.109494	-1.47488
1	-1.66621	3.122221	-1.60083

4TS-5

Atom	x	y	z
14	-1.77226	1.423059	-1.34015
14	-2.11032	0.263663	1.353638
8	-1.4734	1.342999	2.431192
1	-1.76051	1.242312	3.328986
8	1.725567	4.14142	1.013889
1	1.841668	3.45262	1.664426
8	-3.35695	-0.48444	2.06046
1	-3.32468	-1.44544	2.088925
8	-0.99268	-0.78286	0.850611
1	1.963139	3.743747	0.175256
8	-0.37155	0.603865	-1.21329
8	-2.57178	1.133908	0.054985
8	-1.5681	2.988229	-1.64098
1	-1.37956	3.564099	-0.89297
8	-2.69134	0.815899	-2.56018
1	-2.77022	1.360322	-3.33168
8	2.254334	2.657428	-1.41405
1	1.582885	1.995445	-1.53713
1	3.084476	2.184482	-1.36479
8	1.606675	1.792019	2.784174
1	2.16345	1.124476	2.394328
1	0.707687	1.531909	2.611938
8	-4.67133	-1.05758	-1.3931
1	-4.12158	-0.47225	-1.90769
1	-4.75469	-0.63909	-0.54487
8	-1.08047	4.217713	0.821355
1	-1.33108	3.551221	1.451006
1	-0.12873	4.322791	0.913953
8	-2.79191	-3.24003	1.943727
1	-1.85197	-3.10778	1.973874
1	-2.97416	-3.45197	1.023908
14	0.013623	-0.81458	-0.48222
8	1.356207	-1.14705	-2.65743
1	1.06101	-0.5358	-3.31829
8	1.48993	-0.78993	0.180649
8	-0.43697	-2.18876	-1.22166
1	0.115937	-2.21306	-2.02078
8	4.639229	1.053727	-1.01705
1	4.462072	0.758617	-0.13152
1	4.48499	0.296499	-1.58296
14	2.657921	-1.55934	0.964951
8	3.484392	-0.31998	1.681575
1	4.123858	-0.56448	2.337037
8	3.589211	-2.48237	0.024434
1	3.756354	-2.19813	-0.88169
8	2.125752	-2.53139	2.169915
1	2.108579	-3.45713	1.970508
8	-3.04112	-3.47236	-0.86744
1	-3.65109	-2.78935	-1.13764
1	-2.17171	-3.1451	-1.0931
8	3.858459	-1.31525	-2.44807
1	4.208654	-1.74924	-3.21314
1	2.852446	-1.22071	-2.59277

4R-5

Atom	x	y	z
14	1.821771	0.536505	1.728451
14	2.466819	0.58445	-1.19115
8	2.838608	2.105335	-1.67372
1	3.147236	2.208898	-2.56318
8	-0.88864	4.253722	-0.14802
1	-1.02347	3.771478	-0.96121
8	3.346711	-0.4596	-2.05247
1	2.923218	-1.28963	-2.30138
8	0.871147	0.306181	-1.33386
1	-1.32439	3.756019	0.542803
8	0.338712	0.130094	1.20289
8	2.785038	0.501459	0.407709
8	1.882254	1.942653	2.508271
1	1.866156	2.748154	1.980335
8	2.36494	-0.59618	2.790973
1	2.656723	-0.24957	3.623691
8	-1.78537	2.512285	2.019719
1	-1.19654	1.781674	1.868304
1	-2.64965	2.127207	2.148012
8	-0.94747	2.55591	-2.59016
1	-1.75145	2.052238	-2.67224
1	-0.30033	1.927799	-2.28667
8	4.087545	-2.43315	1.221519
1	3.603298	-1.90208	1.847377
1	4.283535	-1.84599	0.501393
8	1.845272	3.958958	0.570001
1	2.264508	3.617108	-0.21268
1	0.941505	4.170684	0.3212
8	1.831975	-2.77641	-2.47283
1	1.049559	-2.50185	-1.99198
1	2.156989	-3.49875	-1.94176
14	-0.13579	-0.47677	-0.26598
8	-1.39841	-2.9717	1.88329
1	-0.7824	-2.71579	2.557346
8	-1.63545	0.12312	-0.54707
8	-0.09345	-2.03621	-0.39236
1	-0.95737	-2.76463	1.047936
8	-4.35255	1.068303	2.20204
1	-4.47395	0.920395	1.269142
1	-4.22905	0.19433	2.556289
14	-2.94154	-0.47859	-1.28932
8	-3.24193	0.526616	-2.55216
1	-4.11195	0.513216	-2.92473
8	-4.28488	-0.42733	-0.35968
1	-4.34633	-1.11146	0.306045
8	-2.64437	-2.00929	-1.74548
1	-1.7934	-2.34717	-1.45902
8	1.96102	-4.17604	0.067571
1	2.685116	-3.74557	0.514143
1	1.23555	-3.5542	0.086497
8	-4.02625	-2.03033	2.015606
1	-4.55399	-2.7904	2.220004
1	-3.11236	-2.33766	2.002011

4TS-6

Atom	x	y	z
14	-2.03986	-1.63424	-0.55796
14	0.959033	-1.48142	-1.11921
8	1.918645	-2.82294	-1.15372
1	1.793648	-3.42843	-1.87114
8	4.338038	-1.77614	0.337511
1	3.865171	-1.2919	1.014402
8	1.327045	-0.50122	-2.36641
1	2.213029	-0.13419	-2.32638
8	1.31577	-0.83128	0.308444
1	3.680109	-2.31742	-0.09144
8	-2.57355	-0.14927	-0.92232
8	-0.58735	-1.90923	-1.24042
8	-1.89726	-1.75285	1.085106
1	-1.22948	-1.19817	1.477663
8	-3.05301	-2.77644	-1.08077
1	-3.98358	-2.67581	-0.88515
8	-4.53605	-0.67785	1.919902
1	-4.32688	0.173081	1.535729
1	-3.70389	-1.14374	1.908066
8	6.659148	-3.27318	1.322359
1	5.980877	-2.7323	0.92163
1	6.224152	-3.74368	2.0194
8	0.009986	1.900855	-3.52126
1	-0.83294	1.957086	-3.08154
1	0.371496	1.055787	-3.26767
8	-5.73238	-2.37716	-0.03549
1	-6.02653	-3.13798	0.44614
1	-5.48435	-1.72571	0.624305
8	3.872046	0.51228	-1.5872
1	3.594983	1.221626	-1.01725
1	4.250694	-0.15662	-1.02124
14	-2.04139	1.270683	-0.26216
8	-3.21742	1.69801	0.825331
1	-2.86604	2.016656	1.655752
8	-0.60722	1.127087	0.323708
8	-2.11595	2.407669	-1.48229
1	-2.985	2.73813	-1.6653
8	-1.87574	1.964486	3.344699
1	-1.10133	1.533285	2.982633
1	-2.31102	1.31073	3.874966
14	1.42855	0.441845	1.304444
8	0.408892	0.309129	2.606525
1	0.896971	0.046343	3.376467
8	2.889974	0.06671	2.073479
1	3.458654	0.8119	2.209897
8	1.864525	1.88122	0.674968
1	1.173546	2.296103	0.158378
8	0.630563	3.773022	-1.36
1	0.731046	3.270439	-2.16655
1	-0.29318	3.673303	-1.1553
8	2.90717	4.775442	0.288352
1	2.205131	4.755055	-0.35521
1	2.848874	3.92348	0.703183

4R-6

Atom	x	y	z
14	-2.01845	-1.59208	-0.87069
14	0.932538	-1.49917	-1.2635
8	1.841414	-2.87318	-1.29573
1	1.820609	-3.38168	-2.09459
8	4.214153	-2.0162	0.314428
1	3.687251	-1.4852	0.923551
8	1.449274	-0.45174	-2.40185
1	2.334936	-0.10406	-2.25532
8	1.023829	-0.93842	0.229564
1	3.582028	-2.53758	-0.17095
8	-2.26276	0.008717	-0.74093
8	-0.60936	-1.86777	-1.62724
8	-1.95551	-2.23089	0.652185
1	-1.146	-2.08384	1.128719
8	-3.20329	-2.29847	-1.70129
1	-4.1103	-2.14289	-1.43952
8	-4.4362	-1.13884	1.862195
1	-4.10255	-0.24674	1.777885
1	-3.66661	-1.6849	1.726334
8	6.316269	-3.57722	1.574794
1	5.70285	-3.03461	1.079585
1	5.867642	-3.78096	2.383333
8	0.009248	1.937437	-3.30253
1	-0.87161	1.840954	-2.96179
1	0.450287	1.109291	-3.12274
8	-5.7966	-1.87862	-0.51571
1	-6.25966	-2.686	-0.33941
1	-5.47715	-1.5611	0.332456
8	3.894311	0.480956	-1.37822
1	3.477857	1.02617	-0.71152
1	4.259566	-0.26592	-0.91019
14	-1.80545	1.246434	0.221948
8	-2.89106	1.299153	1.452592
1	-2.53977	1.536711	2.313647
8	-0.30588	1.129579	0.679782
8	-1.98191	2.630476	-0.66991
1	-2.85339	3.001279	-0.68586
8	-1.58722	1.605608	3.927093
1	-0.79134	1.203854	3.56309
1	-1.93619	0.979522	4.546439
14	1.219145	0.419748	1.2019
8	0.549842	0.246499	2.749172
1	1.207442	-0.13104	3.3169
8	2.757672	-0.20573	1.829267
1	3.371904	0.499808	1.976812
8	2.066065	1.723279	0.580941
1	1.539506	2.386167	0.143742
8	0.68339	3.776923	-1.14708
1	0.700172	3.295478	-1.97331
1	-0.20928	3.654681	-0.8366
8	2.100507	6.27623	-0.66247
1	1.56538	5.523121	-0.9075
1	2.797928	5.918237	-0.13098

4TS-7

Atom	x	y	z
14	-2.21429	-1.09908	-1.07894
14	0.768228	-1.28366	-1.65049
8	1.356713	-2.78357	-1.94366
1	1.296018	-3.10801	-2.83124
8	4.226747	-2.38896	-0.71085
1	3.962992	-1.94876	0.121472
8	1.400227	-0.17407	-2.65574
1	2.335348	0.030339	-2.51271
8	1.051946	-0.99171	-0.09602
1	3.44522	-2.83161	-1.01811
8	-2.30647	0.397789	-0.44691
8	-0.83899	-1.26643	-1.9147
8	-2.22688	-2.18197	0.167105
1	-1.39063	-2.49678	0.486564
8	-3.46404	-1.35949	-2.05943
1	-4.3457	-1.18726	-1.7286
8	-4.5254	-1.23849	1.787168
1	-4.06677	-0.43167	2.012979
1	-3.83585	-1.81606	1.472498
8	4.460024	-3.44491	2.602275
1	4.806414	-3.81218	1.800144
1	4.092147	-2.59499	2.328142
8	0.023559	2.359195	-2.97651
1	-0.89848	2.15142	-2.89779
1	0.48182	1.519945	-2.99793
8	-5.94577	-0.97648	-0.65933
1	-6.57336	-1.68373	-0.71667
1	-5.59172	-1.00051	0.232934
8	3.96714	0.268107	-1.76891
1	3.710011	0.676391	-0.945
1	4.260267	-0.61235	-1.52664
14	-1.71691	1.284388	0.780934
8	-2.60284	0.965037	2.115249
1	-2.10212	0.79374	2.918603
8	-0.1698	0.993619	1.000162
8	-1.85666	2.873163	0.38461
1	-2.67927	3.303187	0.570993
8	-0.87453	0.260333	4.225352
1	-0.06047	0.08144	3.746166
1	-1.04829	-0.51185	4.745756
14	1.28253	0.190139	1.015844
8	1.318421	-0.34806	2.55011
1	2.18049	-0.79421	2.616344
8	3.487511	-1.04981	1.498553
1	4.16497	-0.40556	1.660006
8	2.3291	1.33767	0.511016
1	1.912333	2.15913	0.250664
8	0.881267	3.68894	-0.55772
1	0.694824	3.36683	-1.44052
1	0.043659	3.642423	-0.10562
8	2.372507	6.182037	-0.17188
1	1.823831	5.421465	-0.35392
1	3.198091	5.828773	0.129098

4R-7

Atom	x	y	z
14	-2.04017	-1.18991	-1.19883
14	0.846711	-0.72092	-1.86521
8	1.682115	-2.06949	-2.29487
1	1.67568	-2.3219	-3.20747
8	4.293226	-1.78396	-0.6935
1	4.08641	-1.69079	0.236796
8	1.312942	0.558859	-2.75972
1	2.223124	0.827697	-2.59418
8	1.096366	-0.56631	-0.29366
1	3.498506	-2.10411	-1.1085
8	-2.40071	0.152169	-0.35414
8	-0.74535	-0.91754	-2.1408
8	-1.69853	-2.40004	-0.13131
1	-0.82111	-2.43532	0.231335
8	-3.28082	-1.61644	-2.13122
1	-4.14958	-1.68302	-1.73473
8	-4.03709	-2.22738	1.711826
1	-3.74767	-1.37695	2.037202
1	-3.26583	-2.58559	1.281793
8	5.330517	-4.11168	1.222181
1	5.334753	-3.68983	0.371036
1	4.784026	-3.54418	1.757494
8	-0.48031	2.850029	-2.67926
1	-1.34652	2.46741	-2.62452
1	0.119371	2.121087	-2.83181
8	-5.67842	-1.97187	-0.58644
1	-6.12876	-2.79477	-0.71839
1	-5.25389	-2.0313	0.27306
8	3.846584	1.001335	-1.63492
1	3.473269	1.358331	-0.83047
1	4.202479	0.147578	-1.3937
14	-1.96838	0.998425	0.966808
8	-2.63109	0.292307	2.280135
1	-2.01272	0.074038	2.988435
8	-0.38155	1.097914	1.073667
8	-2.51036	2.536506	0.796368
1	-3.39672	2.732685	1.063297
8	-0.58721	-0.44858	4.049977
1	0.21897	-0.39129	3.505533
1	-0.57162	-1.30685	4.449606
14	1.134382	0.441464	1.034072
8	1.515273	-0.34492	2.316913
1	2.958613	-1.27062	2.28871
8	3.835644	-1.68875	2.180836
1	4.441269	-1.10724	2.620658
8	2.096971	1.714605	0.603352
1	1.623345	2.522742	0.415787
8	0.256664	3.98477	-0.1264
1	0.048616	3.734924	-1.0276
1	-0.5009	3.713358	0.3822
8	1.383964	6.598546	0.570734
1	0.935437	5.807044	0.279275
1	2.205235	6.299404	0.935342

4R-8

Atom	x	y	z
14	-0.30309	-1.48979	-0.31538
14	-4.31757	0.670775	0.460093
8	-3.19381	-0.20426	1.114824
1	-1.67341	-0.1076	0.821528
8	-5.2139	-0.21843	-0.64722
1	-4.95567	-1.12755	-0.69426
8	-3.78609	1.985084	-0.40659
1	-3.02192	1.857734	-0.95903
8	-5.40433	1.302815	1.523941
1	-6.1001	1.809966	1.126188
8	1.274894	-1.78412	-0.07529
8	-0.69668	-0.23143	0.639644
8	-0.52652	-1.14042	-1.90012
1	-0.83014	-0.26042	-2.11511
8	-1.13622	-2.85249	-0.01046
1	-1.60986	-2.91066	0.818581
8	0.190804	-3.82929	-2.7188
1	-0.25429	-4.14574	-1.94021
1	-0.11457	-2.93021	-2.81261
8	-6.57139	2.327154	-1.39881
1	-6.50261	1.381149	-1.47701
1	-5.66659	2.606833	-1.29686
8	0.2031	-1.26135	3.245264
1	-0.13274	-0.62833	2.617115
1	-0.51884	-1.87533	3.341175
8	-2.50605	-2.39318	2.478877
1	-2.86947	-1.57679	2.082259
1	-3.22979	-2.83272	2.902691
8	-1.25352	1.67839	-2.1242
1	-1.23228	2.191089	-2.92096
1	-0.54215	2.001915	-1.5685
14	2.69826	-1.17508	0.381575
8	3.905938	-2.07773	-0.19352
1	3.710614	-2.63587	-0.947
8	2.828487	0.353547	-0.15466
8	2.785229	-1.11318	2.018261
1	2.002469	-1.36679	2.510996
8	3.088127	-3.60728	-2.48958
1	3.289187	-3.18231	-3.31206
1	2.138123	-3.73676	-2.48929
14	2.409619	1.902419	-0.32014
8	0.786356	2.033773	-0.17147
1	0.307663	1.365991	0.321197
8	2.769404	2.5123	-1.78208
1	3.495383	3.126774	-1.82577
8	3.234206	2.796782	0.77859
1	3.527201	2.355489	1.578694
8	4.130238	1.215808	2.974935
1	3.673638	0.390531	2.80215
1	5.055107	1.011925	2.944467
8	4.671237	4.616506	-0.87787
1	4.350759	4.165445	-0.09805
1	4.247131	5.463669	-0.88574

4TS-9

Atom	x	y	z
14	-1.30605	-0.10979	-0.5725
14	1.242882	0.090472	1.025213
8	1.066967	-1.29198	1.898692
1	0.156248	-1.56649	1.956129
8	0.850683	1.352878	1.960023
1	0.716449	2.18476	1.500164
8	-1.26913	-0.86042	-2.02824
1	-2.1696	-0.90671	-2.33944
8	2.794286	0.142702	0.57696
8	-3.58037	-0.35608	-1.08433
8	0.343257	0.032281	-0.32095
8	-1.74007	1.4798	-0.51117
1	-2.60881	1.666405	-0.86806
8	-1.65987	-1.00817	0.774816
1	-2.54961	-0.91555	1.114118
8	-4.37842	2.908793	-0.72867
1	-4.32908	3.073202	0.205324
1	-5.04751	2.238169	-0.83695
14	-4.83407	-0.6233	-0.18632
8	-6.05266	0.471946	-0.47743
1	-6.92062	0.197426	-0.21783
8	-5.54606	-2.10066	-0.309
1	-4.9373	-2.83142	-0.27227
8	-4.41	-0.48238	1.427943
1	-4.21159	0.398767	1.731667
8	-3.07462	2.178373	1.974699
1	-2.56754	2.296169	2.767108
1	-2.4396	2.032674	1.27444
8	-2.85864	-3.62795	-0.38506
1	-2.72257	-3.3791	-1.29028
1	-2.36375	-2.97938	0.106577
8	3.522441	-2.82904	2.131057
1	2.685757	-2.37162	2.212839
1	3.408462	-3.43712	1.412482
8	1.804914	-0.82782	-2.67561
1	1.195008	-1.28382	-3.24043
1	1.254899	-0.47427	-1.97762
8	0.385618	3.461158	0.169496
1	1.180093	3.514974	-0.35743
1	-0.26885	2.986333	-0.33671
14	4.24696	-0.18197	-0.01986
8	4.180459	-1.29199	-1.21393
1	3.446451	-1.24207	-1.82908
8	4.847935	1.244977	-0.56593
1	5.704731	1.169351	-0.97445
8	5.271235	-0.7623	1.108787
1	4.913593	-1.48637	1.621996
8	7.171132	-0.53941	-1.24472
1	7.122726	-0.78586	-0.32709
1	6.539261	-1.1026	-1.6786
8	3.174712	3.656297	-0.7356
1	3.675984	2.844043	-0.78494
1	3.490147	4.096509	0.042137

4R-9

Atom	x	y	z
14	-1.98063	1.153252	-0.32166
14	0.853271	0.983892	1.22425
8	0.839321	0.078571	2.611377
1	0.220277	0.420807	3.255936
8	1.054252	2.539294	1.669168
1	1.057152	3.168409	0.94438
8	-2.48835	1.650765	1.228279
1	-1.63703	1.902505	2.940155
8	2.189764	0.474735	0.430499
8	-2.34502	-0.45817	-0.70706
8	-0.44454	0.697526	0.363421
8	-1.12914	1.989083	-1.53691
1	-1.75867	2.458662	-2.06795
8	-1.06058	1.961415	3.702903
1	-0.4179	2.617949	3.457264
8	-4.77797	-0.26804	-2.95403
1	-3.95143	-0.46889	-3.37238
1	-4.82282	-0.85506	-2.20287
14	-2.99632	-1.67891	0.11452
8	-4.45767	-1.98459	-0.59414
1	-4.81791	-2.84767	-0.44492
8	-2.18716	-3.08266	-0.01329
1	-1.37396	-3.16537	0.482977
8	-3.14726	-1.28206	1.691388
1	-3.01304	-0.36477	1.907621
8	-3.48725	1.777755	-0.93939
1	-3.34174	2.055602	1.136594
1	-3.94309	1.250034	-1.58323
8	0.366511	-2.75556	1.287931
1	0.852976	-2.54405	0.492557
1	0.177891	-1.91785	1.701449
8	2.857733	-2.02655	2.901634
1	2.339632	-1.2348	3.036058
1	2.217832	-2.68119	2.641878
8	-0.11696	-0.70486	-2.62071
1	-0.86649	-0.94004	-2.07976
1	-0.092	0.244751	-2.5423
8	0.963931	3.844815	-0.83394
1	1.766854	3.628996	-1.30305
1	0.28136	3.265355	-1.17098
14	2.974431	-0.62031	-0.438
8	1.951166	-1.75788	-1.01959
1	1.275453	-1.45121	-1.63356
8	3.733433	0.17345	-1.65671
1	4.339842	-0.36824	-2.15484
8	4.111636	-1.40621	0.428324
1	3.870695	-1.66128	1.321809
8	5.244617	-2.3302	-2.09003
1	5.247105	-2.28799	-1.13722
1	4.541072	-2.92781	-2.31028
8	3.600708	3.062485	-1.89411
1	3.622343	2.106669	-1.89998
1	4.145693	3.320684	-1.16298

4TS-10

Atom	x	y	z
14	1.675451	0.9812	0.156153
14	-1.14726	1.402869	-1.15709
8	-1.32462	1.259572	-2.78042
1	-0.69336	1.795313	-3.25608
8	-1.33503	2.962538	-0.7614
1	-1.33884	3.202905	0.169794
8	2.485757	2.169703	-0.62807
1	1.525249	2.975361	-2.27514
8	-2.2867	0.476385	-0.46639
8	2.302096	-0.50881	-0.0413
8	0.299509	0.808483	-0.75071
8	1.029411	1.378493	1.619262
1	1.775547	1.582986	2.190798
8	0.840005	3.300014	-2.85647
1	0.272949	3.814395	-2.2928
8	2.846305	-0.91689	3.349585
1	3.099051	-0.08362	2.931486
1	3.189689	-1.57012	2.750779
14	3.495027	-1.52331	-0.38402
8	3.859909	-2.35794	0.981328
1	4.672501	-2.84385	0.969575
8	3.015371	-2.5037	-1.5944
1	2.07309	-2.5962	-1.72248
8	4.89742	-0.83144	-0.86691
1	4.947801	-0.56867	-1.77501
8	3.511027	1.36286	1.723985
1	3.219513	2.412138	-0.06504
1	4.445099	1.229563	1.64175
8	0.151588	-2.09338	-1.68484
1	-0.33738	-2.37669	-0.91494
1	0.38154	-1.19008	-1.4777
8	-2.20104	-1.49422	-3.38607
1	-2.04892	-0.55416	-3.44909
1	-1.37342	-1.85007	-3.07053
8	-0.09723	-0.98318	2.796567
1	0.752918	-1.28056	3.117198
1	0.103337	-0.10112	2.493615
8	-1.19892	3.270014	2.003974
1	-1.95864	2.837286	2.389707
1	-0.45457	2.682124	2.103492
14	-2.85141	-0.91506	0.121563
8	-1.64788	-1.89628	0.621218
1	-1.12837	-1.6669	1.399458
8	-3.86849	-0.53006	1.346944
1	-4.46616	-1.22843	1.602963
8	-3.70502	-1.73593	-1.00135
1	-3.35187	-1.73402	-1.89527
8	-5.28735	-3.07857	0.993899
1	-5.02568	-2.86329	0.101164
1	-4.73391	-3.80243	1.256083
8	-3.76689	2.047269	2.673881
1	-3.78273	1.153463	2.334745
1	-4.32364	2.545252	2.090501

4R-10

Atom	x	y	z
14	-1.71337	0.630287	-0.16146
14	1.069522	1.37305	1.149125
8	1.015549	0.751897	2.659538
1	0.205828	0.955745	3.135425
8	1.058469	2.994441	1.194586
1	0.682007	3.428532	0.426467
8	-2.72452	0.797402	1.023445
1	-2.07337	1.234724	2.625239
8	2.461828	0.833515	0.502302
8	-1.80344	-0.92291	-0.77578
8	-0.14309	0.819325	0.247076
8	-1.88088	1.618901	-1.47362
1	-2.72661	1.522865	-1.91243
8	-1.59907	1.490361	3.43196
1	-1.67538	2.433034	3.489433
8	-4.56577	0.764749	-2.19023
1	-4.98402	1.083379	-1.3907
1	-4.51163	-0.18119	-2.09441
14	-2.72343	-2.17179	-0.2934
8	-4.04211	-2.1645	-1.27828
1	-4.64263	-2.89273	-1.20512
8	-1.97741	-3.60238	-0.49788
1	-1.2048	-3.74119	0.042807
8	-3.0998	-1.98396	1.278066
1	-3.17245	-1.05724	1.523549
8	-5.23974	1.728715	0.4599
1	-4.37749	1.394501	0.750803
1	-5.19471	2.670166	0.55171
8	0.413952	-2.80201	1.224864
1	0.918875	-2.39878	0.518801
1	-0.16321	-2.12462	1.557218
8	2.677116	-1.68582	2.936518
1	2.208115	-0.86435	3.073067
1	2.020197	-2.29828	2.618258
8	0.268944	-0.87657	-2.80167
1	-0.51745	-1.01665	-2.2767
1	0.228231	0.03467	-3.06332
8	0.095024	3.801957	-1.36841
1	0.868481	3.535306	-1.85778
1	-0.58847	3.15849	-1.54779
14	3.20235	-0.37133	-0.27132
8	2.129162	-1.49818	-0.76909
1	1.558575	-1.28256	-1.51233
8	3.995705	0.305187	-1.53293
1	4.742752	-0.18717	-1.86402
8	4.296667	-1.11942	0.679906
1	3.963589	-1.39009	1.539275
8	6.077979	-1.76557	-1.48259
1	5.796715	-1.72455	-0.57074
1	5.777483	-2.6035	-1.80832
8	2.933381	3.061432	-1.92459
1	3.315945	2.190615	-1.99705
1	3.070635	3.305241	-1.0173

4TS-11

Atom	x	y	z
14	-1.32768	0.503472	0.799739
14	0.632239	2.43974	-0.15266
8	1.097479	3.330301	1.137181
1	1.211422	2.837512	1.948653
8	0.706581	3.387811	-1.48027
1	0.255882	4.222546	-1.39824
8	0.006545	-0.33459	1.062722
1	0.678578	0.591959	2.544525
8	1.590962	1.173906	-0.39498
8	-2.40843	-0.23705	-0.16731
8	-0.8975	1.912007	0.053097
8	-2.0949	0.918933	2.185158
1	-2.73892	0.285844	2.500328
8	0.973642	1.23617	3.197351
1	0.209764	1.392583	3.739294
8	-3.66908	-1.47741	2.775886
1	-2.89126	-2.03262	2.803895
1	-4.10802	-1.70065	1.961217
14	-2.90994	-1.5715	-0.92387
8	-4.30057	-2.11903	-0.23517
1	-5.08609	-1.98339	-0.74604
8	-3.24567	-1.23256	-2.47538
1	-2.72056	-0.54765	-2.89211
8	-1.82055	-2.76572	-0.70068
1	-0.92569	-2.46093	-0.85647
8	-1.09858	-2.78835	2.205247
1	-0.64687	-1.98833	1.934407
1	-1.35336	-3.19499	1.383028
8	4.23474	-3.4239	0.765947
1	3.655096	-2.66722	0.867297
1	3.795098	-4.15206	1.183337
8	3.779999	0.163254	3.407267
1	3.769501	-0.15871	2.514202
1	2.941896	0.599976	3.523217
8	-1.52719	0.959724	-3.23549
1	-1.53331	1.409605	-2.39823
1	-0.6079	0.92828	-3.49514
8	-0.93307	5.255684	0.186021
1	-0.27647	5.026034	0.836694
1	-1.64805	4.647814	0.332723
14	1.643188	-0.45883	-0.42938
8	0.459712	-1.26446	-1.28581
1	0.748852	-1.4145	-2.17689
8	2.868364	-0.55485	-1.56801
1	3.320121	-1.37966	-1.72014
8	2.354323	-1.26526	0.83494
1	1.73366	-1.37438	1.544523
8	4.507654	-2.96729	-2.01914
1	5.363695	-2.59106	-2.17208
1	4.514547	-3.29137	-1.11858
8	1.453825	1.264634	-3.56915
1	2.088595	0.742101	-3.08366
1	1.414116	2.097138	-3.10882

4R-11

Atom	x	y	z
14	-1.08571	-0.00679	1.147683
14	1.418113	1.421122	0.711051
8	2.473519	1.256466	1.97362
1	2.232756	0.531989	2.54696
8	1.689641	2.896501	0.068618
1	2.041528	3.564308	0.651041
8	-0.29162	-1.12538	0.302182
1	1.087894	-1.59997	1.92256
8	1.62697	0.305956	-0.41111
8	-2.47289	0.471042	0.472979
8	-0.09564	1.292263	1.29249
8	-1.40005	-0.55379	2.65795
1	-2.28042	-0.90707	2.793985
8	1.424291	-1.39024	2.791165
1	0.63311	-1.29408	3.314042
8	-4.00151	-1.78796	2.441976
1	-3.66405	-2.43126	1.819995
1	-4.53954	-1.1982	1.923294
14	-3.63497	0.368714	-0.64768
8	-5.06752	0.071281	0.104685
1	-5.71364	0.759598	0.033002
8	-3.80031	1.778474	-1.42871
1	-3.00423	2.259712	-1.66393
8	-3.33869	-0.92278	-1.59466
1	-2.4212	-0.95583	-1.88268
8	-2.6177	-3.14274	0.24455
1	-1.77232	-2.70202	0.264105
1	-3.06868	-2.7403	-0.49206
8	4.215666	-3.01637	-0.55456
1	3.27387	-2.96827	-0.71319
1	4.350881	-2.62024	0.302428
8	4.301365	-1.49093	2.011138
1	4.186347	-0.59457	1.718137
1	3.497893	-1.69918	2.477379
8	-1.27226	3.0718	-1.87676
1	-0.86363	3.240413	-1.03663
1	-0.56628	2.725828	-2.42404
8	2.880798	4.074279	2.479256
1	2.984185	3.133752	2.606393
1	2.263434	4.364451	3.137126
14	0.783072	-0.93344	-1.19036
8	-0.64064	-0.62335	-2.0451
1	-0.42043	-0.503	-2.95998
8	1.649143	-0.71776	-2.65626
1	2.574864	-0.935	-2.68216
8	1.375935	-2.47663	-0.90464
1	0.892535	-2.93698	-0.23479
8	4.658231	-1.14266	-2.66314
1	4.923065	-0.33901	-2.23774
1	4.678832	-1.82157	-1.98722
8	1.297507	2.17686	-2.99015
1	1.485956	1.236636	-3.00379
1	1.726261	2.500728	-2.20603

4TS-12

Atom	x	y	z
14	1.55178	-0.04055	-1.45993
14	-1.01115	1.357196	-1.08406
8	-2.26313	1.417406	-2.13246
1	-2.68049	0.587202	-2.35822
8	-0.93285	2.807626	-0.35176
1	-1.47422	3.506188	-0.71194
8	0.781515	-1.30252	-0.75333
1	-2.84122	-1.65533	-1.46287
8	-1.20778	0.174481	0.007195
8	2.542405	0.622041	-0.36437
8	0.390472	1.033266	-1.84785
8	2.360015	-0.48901	-2.77867
1	3.279755	-0.73352	-2.66136
8	-3.29506	-1.26117	-2.20445
1	-3.89868	-1.93253	-2.49773
8	4.948347	-1.34	-1.88127
1	4.625535	-2.08045	-1.37048
1	5.226514	-0.69694	-1.23603
14	3.421847	0.565084	0.99512
8	5.009338	0.464613	0.573664
1	5.57725	1.105489	0.97818
8	3.259997	1.911144	1.869819
1	2.375481	2.229169	2.077155
8	3.07306	-0.8185	1.78918
1	2.146841	-1.00869	1.950808
8	3.401991	-3.06963	-0.09173
1	2.523671	-2.90993	-0.418
1	3.459018	-2.53309	0.695447
8	-4.37689	-3.42444	-0.21553
1	-3.55161	-3.22494	0.212708
1	-4.93667	-2.66564	-0.06133
8	-5.64487	-0.76699	-0.15495
1	-5.32186	-0.35219	0.647854
1	-5.052	-0.47783	-0.83788
8	0.576922	2.644603	2.238616
1	0.12627	2.858831	1.427272
1	-0.0627	2.16304	2.766103
8	-2.68955	4.253318	-2.18489
1	-2.87603	3.34134	-2.39706
1	-2.20288	4.600491	-2.92018
14	-0.47703	-1.24419	0.334483
8	0.297512	-1.35971	1.75744
1	-0.40889	-1.31981	2.421086
8	-2.14867	-1.16911	2.345603
1	-2.45194	-1.99781	2.693395
8	-1.4279	-2.50402	-0.14617
1	-0.97927	-3.09285	-0.7399
8	-4.37921	0.294865	2.140469
1	-3.56332	-0.2506	2.148463
1	-4.78685	0.156078	2.984119
8	-1.63903	1.297032	3.542526
1	-1.75565	0.385789	3.243924
1	-2.38556	1.750362	3.171255

4R-12

Atom	x	y	z
14	-1.18105	-1.49665	-0.40393
14	1.458726	-1.24587	0.926056
8	2.716845	-2.26582	0.747373
1	2.882428	-2.60812	-0.13621
8	1.47395	-0.78739	2.498064
1	2.011936	-1.31471	3.08574
8	-0.53857	-0.4138	-1.44341
1	2.163285	-3.29452	-2.32672
8	1.582418	0.06981	-0.01137
8	-2.2938	-0.76029	0.511182
8	0.052524	-1.97496	0.552257
8	-1.80419	-2.7744	-1.16699
1	-2.69455	-2.66129	-1.50444
8	2.984835	-3.0208	-1.93995
1	3.251938	-2.22356	-2.40779
8	-4.36707	-1.78858	-2.0469
1	-4.06489	-1.04823	-2.57163
1	-4.75027	-1.38984	-1.27119
14	-3.30528	0.487992	0.758953
8	-4.83129	0.020913	0.340731
1	-5.44422	-0.00726	1.062087
8	-3.37626	0.849127	2.335085
1	-2.57201	0.84219	2.85997
8	-2.91113	1.706836	-0.23551
1	-1.96655	1.93963	-0.28893
8	-3.04312	0.628661	-3.01741
1	-2.13441	0.353233	-2.96322
1	-3.16486	1.181969	-2.24892
8	3.621768	-0.5244	-3.11281
1	2.794533	-0.04634	-3.09103
1	4.158655	-0.06002	-2.47388
8	4.399572	1.160469	-0.82138
1	4.072487	2.025272	-1.05231
1	3.680045	0.748259	-0.35418
8	-0.91456	0.739668	3.729388
1	-0.39235	-0.0013	3.439934
1	-0.32353	1.483924	3.626159
8	3.304553	-2.83333	3.477242
1	3.432325	-2.86074	2.530638
1	2.891063	-3.65319	3.711234
14	0.495054	0.817148	-1.04686
8	-0.22357	2.040348	-0.3998
1	0.516494	3.322725	0.278231
8	1.079803	4.038553	0.654184
1	0.506518	4.773136	0.825493
8	1.340429	1.145624	-2.42524
1	1.680547	2.034667	-2.45583
8	2.849141	3.639225	-1.53811
1	2.311848	3.899986	-0.78494
1	3.170772	4.436779	-1.93511
8	1.436679	2.333557	3.076319
1	1.384041	2.920032	2.325066
1	1.742695	1.498547	2.739079

4R-13

Atom	x	y	z
14	1.277302	0.22682	0.619497
14	0.605342	3.04059	-0.16194
8	-0.68182	2.346721	-0.90897
1	-0.60491	1.381188	-0.83931
8	1.636787	3.805312	-1.15749
1	2.413075	3.307756	-1.41505
8	1.205653	-0.35556	2.147842
1	0.375976	-0.2075	2.606896
8	-0.02332	4.194338	0.828089
1	0.484979	4.989715	0.905011
8	2.755602	-0.27196	0.078285
8	1.370757	1.876463	0.652951
8	-0.20405	-1.21487	-2.75917
1	0.258522	-0.78015	-3.46261
8	0.089563	-0.19244	-0.3289
1	0.055537	-0.7797	-1.92617
8	3.794011	1.908079	-1.63238
1	4.703227	2.055621	-1.40943
1	3.520713	1.164105	-1.09689
14	3.700641	-1.58589	0.283635
8	5.251298	-1.11999	0.020915
1	5.719134	-1.65845	-0.6017
8	3.488944	-2.12207	1.80438
1	2.796646	-1.69001	2.297699
8	3.439109	-2.73442	-0.83332
1	2.574865	-3.13208	-0.94394
8	0.762831	-3.64874	-1.40376
1	0.088823	-3.65466	-0.73338
1	0.474734	-2.9814	-2.02211
8	-1.42433	0.30984	3.059013
1	-1.61187	1.246759	3.081131
1	-2.07087	-0.06454	2.467894
8	-3.39104	2.455081	0.059871
1	-2.47435	2.539054	-0.20351
1	-3.86905	2.525449	-0.76098
8	-2.13931	3.159804	2.686095
1	-1.42654	3.602336	2.234487
1	-2.83748	3.089147	2.043173
8	-3.10209	-4.71768	1.620345
1	-2.26861	-4.26776	1.556359
1	-3.70489	-4.14414	1.160387
14	-3.02578	-1.47925	-0.30639
8	-1.63447	-2.20487	0.119856
1	-0.89999	-1.56808	0.118455
8	-2.9154	-0.86977	-1.82983
1	-2.08724	-1.03332	-2.28333
8	-3.43096	-0.32377	0.758558
1	-3.49132	0.595599	0.498778
8	-4.21233	-2.61661	-0.27337
1	-4.3422	-3.10564	-1.07365
8	-3.35844	1.906829	-2.82624
1	-3.33873	0.978189	-2.60658
1	-2.45939	2.20287	-2.7411

4TS-14

Atom	x	y	z
14	0.875298	0.012802	-0.75859
14	-0.26469	-2.55165	0.580497
8	-1.68994	-1.85625	1.001317
1	-1.86647	-1.02726	0.549916
8	0.625488	-2.98321	1.869823
1	1.313888	-2.38363	2.151397
8	0.962319	0.104282	-2.39451
1	0.16303	-0.14078	-2.86204
8	-0.67193	-3.95132	-0.18435
1	-0.05195	-4.66265	-0.10518
8	2.438435	0.241488	-0.29007
8	0.53463	-1.56051	-0.38971
8	1.418951	1.709412	2.289951
1	1.78279	0.868846	2.550605
8	-0.06649	1.011832	0.005648
1	1.012684	1.541875	1.432878
8	2.771315	-1.11238	2.533045
1	3.350282	-1.36288	3.240355
1	3.320742	-1.02758	1.754128
14	3.953055	0.215781	-0.81987
8	4.725922	-0.80145	0.238586
1	5.66331	-0.69176	0.313594
8	4.045238	-0.37627	-2.33185
1	3.229561	-0.33357	-2.82197
8	4.673428	1.669125	-0.74937
1	4.41923	2.244854	-0.02706
8	3.680241	3.23346	1.459155
1	3.351808	4.085901	1.207454
1	2.922174	2.749192	1.798981
8	-1.71737	-0.61959	-3.12417
1	-1.97779	-1.5332	-3.01973
1	-2.09573	-0.16764	-2.376
8	-4.33759	-2.51895	0.066903
1	-3.50326	-2.4572	0.528168
1	-5.01397	-2.44525	0.72645
8	-2.67951	-3.31079	-2.32313
1	-2.01676	-3.68073	-1.74743
1	-3.43328	-3.14519	-1.76539
8	-3.94837	4.788897	-1.50361
1	-3.02579	4.573903	-1.58137
1	-4.2769	4.082391	-0.95831
14	-2.32839	1.845183	0.235339
8	-1.63566	2.935107	-0.75918
1	-0.73807	2.672438	-0.93764
8	-1.89203	1.796232	1.816202
1	-0.97164	1.62606	1.978192
8	-2.65976	0.364735	-0.44836
1	-3.59186	0.176978	-0.4496
8	-3.88499	2.43494	0.394217
1	-4.08021	2.791604	1.249293
8	-3.15671	-0.54929	3.319912
1	-2.85818	0.305551	3.025701
1	-2.60654	-1.16583	2.849732

4R-14

Atom	x	y	z
14	0.679506	-0.00452	-0.80746
14	-0.67659	-2.39073	0.732306
8	-2.07122	-1.61821	1.094767
1	-2.20686	-0.80148	0.598894
8	0.181418	-2.81294	2.044851
1	0.923781	-2.26501	2.290128
8	0.638575	-0.03516	-2.43521
1	-0.19707	-0.27666	-2.84319
8	-1.10014	-3.7976	-0.00492
1	-0.55833	-4.54796	0.195058
8	2.272866	0.135221	-0.44727
8	0.188668	-1.45676	-0.24803
8	1.918371	1.731706	2.142253
1	2.063369	0.829186	2.413793
8	-0.05434	1.192279	-0.0654
1	1.502715	1.659448	1.28613
8	2.563107	-1.19914	2.543196
1	3.08103	-1.45314	3.295467
1	3.119148	-1.32094	1.772208
14	3.732871	-0.29439	-0.97041
8	4.255071	-1.39333	0.158285
1	5.166666	-1.64679	0.115435
8	3.655286	-0.99576	-2.43436
1	2.845543	-0.85583	-2.91459
8	4.773246	0.946242	-1.01767
1	4.779445	1.545535	-0.27059
8	4.495548	2.620531	1.310289
1	4.471227	3.557541	1.171252
1	3.638512	2.380389	1.671801
8	-2.04414	-0.63258	-3.04821
1	-2.38059	-1.51438	-2.89316
1	-2.32982	-0.11338	-2.30109
8	-4.64811	-2.74775	0.321093
1	-3.82801	-2.46918	0.725144
1	-5.32041	-2.1737	0.661945
8	-3.08777	-3.24037	-2.16357
1	-2.40166	-3.61209	-1.61791
1	-3.81853	-3.09999	-1.5675
8	-3.60511	4.905811	-1.57269
1	-2.68589	4.807352	-1.78908
1	-3.71311	4.229098	-0.90721
14	-1.62775	2.077391	0.17677
8	-1.13699	3.247036	-0.90704
1	-0.29139	3.057668	-1.28399
8	-1.30231	2.202836	1.819462
1	-0.41841	1.992363	2.085559
8	-2.43214	0.685752	-0.41634
1	-3.36138	0.881146	-0.38397
8	-3.178	2.826138	0.414219
1	-3.23375	3.27544	1.244645
8	-2.71758	0.198734	3.572031
1	-2.36523	0.953119	3.106714
1	-2.50816	-0.54763	3.023147

4TS-15

Atom	x	y	z
14	0.633524	-0.0462	-1.00146
14	-0.56098	-2.30868	0.914414
8	-2.00362	-1.64621	1.294422
1	-2.22318	-0.84308	0.807146
8	0.343206	-2.66927	2.21062
1	1.006925	-2.03878	2.484321
8	0.660544	-0.50377	-2.5641
1	-0.20627	-0.72816	-2.91183
8	-0.87164	-3.74752	0.180707
1	-0.28269	-4.45396	0.40662
8	2.197412	0.324855	-0.65087
8	0.221984	-1.30212	-0.06525
8	1.961662	1.957111	1.772114
1	1.94269	1.217218	2.373701
8	-0.23783	1.240311	-0.68175
1	1.951238	1.55597	0.907627
8	2.597086	-0.88649	2.611425
1	3.140886	-1.03521	3.373259
1	3.138676	-1.0603	1.841533
14	3.681023	-0.16544	-1.08269
8	4.133533	-1.19805	0.133606
1	4.979285	-1.61565	0.044636
8	3.647392	-0.94201	-2.50628
1	2.798228	-0.98427	-2.93701
8	4.73079	1.061645	-1.16702
1	4.812775	1.643497	-0.41142
8	4.629142	2.790657	1.157817
1	4.655367	3.717277	0.960403
1	3.762012	2.619738	1.529506
8	-2.12248	-0.95801	-2.75628
1	-2.46717	-1.83417	-2.58454
1	-2.48256	-0.39609	-2.07434
8	-4.55136	-2.94767	0.612063
1	-3.73713	-2.61847	0.988617
1	-5.17409	-2.23553	0.671532
8	-3.0338	-3.57674	-1.84847
1	-2.27878	-3.82852	-1.32546
1	-3.73289	-3.4496	-1.21172
8	-4.62519	4.526108	-1.09856
1	-3.80789	4.542752	-1.57854
1	-4.426	3.893295	-0.39605
14	-1.65899	1.972897	-0.05717
8	-1.77084	3.159072	-1.19265
1	-1.0834	3.086629	-1.83956
8	-1.07798	2.347241	1.44316
1	-0.12855	2.359063	1.510858
8	-2.61316	0.605854	-0.21013
1	-3.46358	0.920922	0.109928
8	-3.64008	2.666758	0.718724
1	-3.51096	3.051536	1.58516
8	-1.0459	0.380907	3.666181
1	-1.23642	1.091446	3.05863
1	-1.50172	-0.37518	3.317768

4R-15

Atom	x	y	z
14	0.687417	0.008614	0.911214
14	-0.00725	2.55333	-0.91439
8	-1.31447	2.105571	-1.77588
1	-2.18026	2.222413	-1.38636
8	1.192139	3.022133	-1.88591
1	1.988174	2.495874	-1.99486
8	0.944095	0.345548	2.483362
1	0.19656	0.686441	2.983441
8	-0.45548	3.859638	-0.00418
1	0.204111	4.534231	0.079309
8	2.07746	-0.68207	0.413155
8	0.4601	1.361664	0.060136
8	0.879491	-2.18917	-2.38774
1	0.114509	-1.68476	-2.68007
8	-0.5223	-1.00282	0.661545
1	0.720562	-2.36674	-1.46826
8	3.586384	1.56198	-2.10154
1	3.527279	0.672248	-2.44061
1	3.892654	1.454859	-1.20469
14	3.602733	-0.77929	0.934066
8	4.283501	0.694805	0.602067
1	5.069353	0.910195	1.084627
8	3.695666	-1.06583	2.533279
1	2.95162	-0.74045	3.030918
8	4.403374	-1.95387	0.155519
1	4.292216	-1.94596	-0.79294
8	3.513821	-1.36815	-2.60011
1	3.823314	-1.77069	-3.40026
1	2.579236	-1.60329	-2.52967
8	-1.53378	1.143604	3.520875
1	-1.90179	1.918542	3.098459
1	-2.00352	0.400879	3.144647
8	-3.93611	2.30574	-0.59325
1	-4.52684	2.93123	-0.99061
1	-4.28904	1.429437	-0.79634
8	-2.64161	3.316597	1.90084
1	-1.90404	3.642212	1.392453
1	-3.21525	2.909042	1.258035
8	-3.30016	-4.41729	-1.12188
1	-3.16462	-3.46081	-1.11314
1	-4.21493	-4.54762	-0.91543
14	-1.95316	-1.79627	0.75543
8	-1.65485	-3.34254	1.244347
1	-1.96494	-4.00348	0.634664
8	-2.77655	-1.75723	-0.58125
1	-4.13296	-0.79599	-0.99125
8	-2.68923	-1.04661	2.056
1	-3.43	-1.5175	2.410905
8	-4.82349	-0.21373	-1.36075
1	-4.73391	-0.31053	-2.29991
8	-1.50712	-0.72347	-2.84397
1	-1.96183	-1.10497	-2.08291
1	-1.39919	0.199696	-2.63599

4TS-16

Atom	x	y	z
14	0.794379	-0.72521	-0.92492
14	-0.64275	-0.43466	1.582752
8	-1.82124	-0.0832	0.580609
1	-3.46725	-0.34487	1.324663
8	-0.10273	0.756534	2.577082
1	0.828152	0.740305	2.811555
8	0.561079	-2.14565	-1.70736
1	-0.29113	-2.55953	-1.57203
8	-1.07218	-1.67396	2.604432
1	-0.85989	-1.51115	3.513056
8	2.326307	-0.30975	-1.21198
8	0.646777	-0.95684	0.692136
8	0.190898	3.464623	1.613525
1	0.002177	2.730464	2.192679
8	-4.33284	-0.62793	1.649149
1	-0.42146	3.305477	0.898067
8	2.71501	0.971495	3.14979
1	2.910436	1.816014	2.752547
1	3.209224	0.343046	2.629206
14	3.794507	-0.26953	-0.49987
8	3.567975	-0.87436	1.023705
1	2.699368	-1.23584	1.167176
8	4.842337	-1.14912	-1.36437
1	4.471442	-1.92002	-1.78916
8	4.395651	1.2288	-0.40035
1	3.901668	1.887384	0.082382
8	2.93707	3.200848	1.247088
1	3.327942	4.064148	1.255415
1	1.980761	3.333819	1.243177
8	3.160966	-3.37352	-2.30442
1	3.133341	-4.11906	-1.7205
1	2.283139	-2.9944	-2.2822
8	-3.19992	-3.47322	1.977324
1	-3.88961	-2.81984	2.024005
1	-2.4365	-3.02081	2.329313
8	-2.14366	-2.76572	-0.68962
1	-2.13893	-1.87359	-0.34516
1	-2.3733	-3.30733	0.062238
8	-3.10649	4.447911	-2.01533
1	-2.54229	3.797052	-2.43789
1	-3.98451	4.097974	-2.08355
14	-1.69756	1.151572	-1.15647
8	-1.52748	2.224185	-2.48495
1	-1.29149	1.789225	-3.29132
8	-1.88353	2.3813	-0.05675
1	-2.17125	3.181267	-0.48694
8	-0.23121	0.413135	-1.37954
1	-4.79713	0.163077	1.88701
8	-3.00749	0.377996	-1.74709
1	-3.5491	-0.24313	-1.28036
8	-5.00275	-1.7232	-0.97217
1	-4.32837	-2.37929	-1.10868
1	-4.98589	-1.51364	-0.0431

4R-16

Atom	x	y	z
14	1.23153	0.12747	0.73248
14	3.83522	-0.1808	-0.8138
8	3.25225	0.86641	-1.9272
1	2.31011	1.00743	-1.8917
8	4.13949	-1.6776	-1.3512
1	3.4963	-2.3648	-1.1676
8	1.2146	1.22448	1.93393
1	0.37456	1.31862	2.38525
8	5.26244	0.46964	-0.342
1	5.9497	-0.1493	-0.1407
8	0.42815	-1.1946	1.19365
8	2.77022	-0.2512	0.40887
8	-0.5691	-0.7774	-2.9519
1	-0.0041	-0.3031	-2.3486
8	0.6145	0.70598	-0.6649
1	-1.4242	-0.3529	-2.8581
8	2.08911	-3.588	-0.6456
1	1.25544	-3.5374	-1.1079
1	1.86115	-3.5635	0.27736
14	-0.7305	-2.1539	1.76357
8	0.03708	-3.5693	2.0841
1	-0.4535	-4.2459	2.52813
8	-1.4232	-1.5894	3.11089
1	-1.617	-0.6544	3.16679
8	-1.895	-2.3887	0.63786
1	-1.599	-2.7419	-0.2001
8	-0.6172	-3.2733	-1.8181
1	-0.9599	-3.9205	-2.4197
1	-0.6116	-2.4285	-2.2904
8	-1.5319	1.26937	2.67894
1	-1.7594	2.13066	3.00788
1	-1.7513	1.29989	1.73095
8	4.16276	3.443	-0.6492
1	3.87492	2.83329	-1.3218
1	4.8147	2.95328	-0.1623
8	1.73999	4.0556	1.10074
1	1.68537	3.1736	1.45641
1	2.48509	4.04234	0.50598
8	-6.1027	0.09528	-1.9903
1	-5.7628	-0.3973	-1.2492
1	-6.0493	1.00039	-1.702
14	-3.2237	0.93509	-0.6616
8	-4.0045	-0.3312	0.06281
1	-3.4468	-1.062	0.31593
8	-3.0092	0.49395	-2.2578
1	-3.8277	0.28073	-2.6931
8	-1.8645	1.36504	-0.0039
1	-0.3022	1.03818	-0.5557
8	-4.3871	2.12089	-0.6615
1	-4.0812	2.97468	-0.3876
8	-1.3299	4.03396	0.97729
1	-0.403	4.24945	0.91833
1	-1.4391	3.2062	0.51038

4TS-17

Atom	x	y	z
14	0.62968	-0.3275	-0.5116
14	3.58786	0.25272	0.31751
8	3.45169	-0.7582	1.609
1	2.54041	-0.9873	1.77088
8	4.02549	1.76994	0.7082
1	3.34485	2.44052	0.77214
8	0.85231	-1.4177	-1.7319
1	0.05262	-1.7939	-2.068
8	4.85573	-0.3608	-0.5399
1	5.396	0.28809	-0.9674
8	-0.111	1.07575	-0.8742
8	2.20622	0.23963	-0.4857
8	-0.4526	0.90512	3.22735
1	0.29862	0.55108	2.76148
8	0.65055	-0.8174	1.08579
1	-1.1726	0.3579	2.91705
8	1.92132	3.77304	0.7778
1	1.19925	3.73104	1.39706
1	1.49423	3.77889	-0.0746
14	-0.9613	2.32941	-1.3715
8	0.0058	3.66012	-1.4953
1	0.19697	3.93164	-2.3826
8	-1.6242	2.10606	-2.8319
1	-1.8869	1.21927	-3.0815
8	-2.1294	2.64243	-0.2626
1	-1.8217	2.99733	0.5701
8	-0.7551	3.44832	2.18351
1	-1.0549	4.06561	2.83701
1	-0.6671	2.59407	2.62235
8	-2.3949	-0.6167	-3.1166
1	-3.3357	-0.6991	-3.0259
1	-2.0368	-0.8833	-2.2677
8	4.52814	-3.2399	0.35822
1	4.24902	-2.6437	1.04757
1	4.90825	-2.653	-0.2864
8	1.92169	-4.0669	-0.875
1	1.76839	-3.2044	-1.2512
1	2.76761	-4.0008	-0.4377
8	-5.3295	-1.1927	2.22857
1	-5.3251	-0.4553	1.62784
1	-5.1916	-1.9479	1.66558
14	-2.6726	-1.0931	0.35123
8	-3.7092	0.11823	-0.0485
1	-3.3483	1.00197	-0.0792
8	-2.2986	-0.9454	1.96913
1	-3.0614	-1.0777	2.52481
8	-1.3334	-1.1656	-0.4908
1	-0.1059	-1.3234	1.34822
8	-3.6135	-2.436	0.16913
1	-3.1327	-3.2501	0.0532
8	-1.0577	-4.0648	-0.3323
1	-0.1745	-4.4228	-0.3723
1	-0.9517	-3.1283	-0.4742

4R-17

Atom	x	y	z
14	-0.506	0.48951	-1.3439
14	-1.6865	1.71247	1.19001
8	-0.466	2.79742	1.15413
1	1.64121	3.18819	1.63063
8	-1.5461	0.93689	2.61829
1	-2.0466	0.13827	2.80725
8	-0.9383	0.46658	-2.9742
1	-0.7583	1.28048	-3.4197
8	-3.1544	2.47886	1.14345
1	-3.5156	2.74411	1.9776
8	-0.7978	-1.2023	-1.3417
8	-1.6436	0.75982	-0.1041
8	1.08317	-0.1591	3.3653
1	0.30944	0.37602	3.20074
8	2.5619	3.11831	1.40012
1	1.67435	-0.0108	2.62963
8	-2.7091	-1.5868	3.17799
1	-1.9469	-2.0458	3.51915
1	-2.8223	-1.9453	2.29889
14	-1.2701	-2.5152	-0.5867
8	-2.5703	-2.1078	0.36541
1	-2.7931	-1.1984	0.19257
8	-1.6469	-3.6741	-1.6628
1	-1.7693	-3.3423	-2.5508
8	-0.1029	-3.1322	0.39339
1	-0.1662	-3.0017	1.33608
8	0.00134	-2.7082	3.30297
1	0.55359	-3.3525	3.72426
1	0.45811	-1.8605	3.36623
8	-1.9664	-2.0332	-4.0811
1	-2.8502	-1.7187	-4.2106
1	-1.4935	-1.2934	-3.6936
8	-2.6993	4.09255	-1.331
1	-2.2249	4.7767	-0.8776
1	-3.1081	3.57508	-0.6425
8	-0.1716	2.25174	-1.4839
1	-0.1103	2.82132	0.2588
1	-0.9222	2.76834	-1.7581
8	5.31676	-1.4764	0.3684
1	4.68578	-2.1546	0.14964
1	5.35566	-0.9321	-0.4113
14	2.44529	-0.3317	-0.4482
8	2.49315	-1.9617	-0.4871
1	1.69574	-2.439	-0.2609
8	2.87724	0.16371	1.0879
1	3.7369	-0.1731	1.32809
8	1.03019	0.32801	-0.7227
1	2.74911	2.18377	1.41739
8	3.59977	0.1728	-1.4865
1	3.50983	1.09914	-1.7179
8	2.68342	2.92489	-1.6077
1	1.7496	2.73498	-1.7037
1	2.77624	3.2113	-0.7026

4TS-18

Atom	x	y	z
14	0.07023	-0.4854	-1.31
14	-2.0988	-1.7996	0.32509
8	-3.1084	-0.5526	0.09211
1	-3.5294	1.37541	0.89865
8	-1.5642	-1.8136	1.87257
1	-0.7655	-2.3142	2.06021
8	0.35205	-0.3355	-2.9238
1	-0.3832	0.12431	-3.3141
8	-2.9034	-3.213	0.05429
1	-2.8106	-3.8769	0.72247
8	1.57539	-1.0764	-0.92
8	-0.8604	-1.6845	-0.7092
8	-0.5374	0.49293	3.36038
1	-1.0593	-0.189	2.94083
8	-3.4384	2.31773	1.00632
1	-0.5582	1.24092	2.76674
8	0.88499	-3.101	2.51415
1	1.30749	-2.443	3.05942
1	1.48057	-3.2095	1.77677
14	2.97975	-1.2354	-0.1979
8	3.03285	-2.7026	0.57108
1	3.82725	-3.2002	0.43695
8	4.20567	-1.1749	-1.2609
1	3.95289	-1.0638	-2.1781
8	3.20085	-0.0734	0.94111
1	2.89304	-0.2628	1.82653
8	2.00142	-0.5682	3.55288
1	2.41993	-0.2824	4.35359
1	1.13544	-0.1393	3.52305
8	2.99097	-0.9742	-3.8721
1	2.84966	-1.8328	-4.2467
1	2.12302	-0.6731	-3.5958
8	-5.6728	-2.2445	-0.7
1	-5.3335	-1.3843	-0.4826
1	-4.918	-2.8106	-0.5805
8	-1.9718	0.35741	-2.0821
1	-2.8076	-0.066	-0.7133
1	-2.4484	-0.1779	-2.7053
8	1.1318	5.217	1.2114
1	1.89241	4.65366	1.11193
1	0.77904	5.29294	0.33091
14	0.41725	2.35536	0.01863
8	2.01215	2.50548	0.32931
1	2.50988	1.71346	0.52757
8	-0.4396	2.64715	1.41422
1	-0.2437	3.51045	1.76995
8	0.00752	0.86599	-0.4007
1	-2.5309	2.45117	1.25975
8	0.07474	3.50424	-1.0715
1	-0.8226	3.48755	-1.4263
8	-2.5549	3.01916	-1.8251
1	-2.4042	2.08541	-2.0379
1	-3.067	3.00134	-1.0217

4R-19

Atom	x	y	z
14	3.098852	-0.9264	-0.70539
14	1.463608	1.553613	-0.25145
8	0.418048	0.840546	-1.2746
1	-4.2909	3.982351	-0.0983
8	1.924064	2.968371	-0.88811
1	2.471595	3.530146	-0.34101
8	0.818394	1.733023	1.232335
1	-0.13542	1.64674	1.343081
8	-3.89098	3.135528	0.041831
1	-3.39704	2.918221	-0.75564
8	1.834906	-1.31158	-1.65779
8	2.750322	0.550573	-0.10192
8	3.369986	-2.02982	0.438346
1	2.588495	-2.45387	0.813785
8	4.494729	-0.84908	-1.5575
1	4.55609	-0.17731	-2.22195
8	6.362205	-2.59275	0.161683
1	6.146673	-2.05697	-0.59239
1	5.518664	-2.72116	0.581328
8	0.898715	-2.98991	1.256863
1	0.52463	-2.80861	2.118892
1	0.256391	-2.69693	0.614385
14	0.322948	-0.71732	-1.78834
8	-2.61481	-0.77748	3.339094
1	-2.36072	0.038006	2.913526
8	-0.66475	-1.58273	-0.85187
1	-3.23501	-1.17835	2.732016
8	-0.13257	-0.72607	-3.3507
1	-1.00692	-1.03949	-3.53665
8	3.103682	2.071854	2.915853
1	2.205783	1.96057	2.605693
1	3.546838	1.272336	2.659595
8	3.762086	4.152794	1.024681
1	3.61204	3.561156	1.763705
1	4.656066	4.005103	0.747803
8	-1.93194	1.386448	1.46329
1	-2.48083	2.15604	1.346044
1	-2.21847	0.778294	0.76304
8	-2.48298	1.976314	-2.06814
1	-2.64454	1.132673	-1.62297
1	-1.53745	2.051484	-2.11858
14	-4.39688	-0.73843	-0.22743
8	-5.4684	0.518389	-0.15273
1	-5.09008	1.378019	0.000887
8	-4.43484	-1.60348	1.195521
1	-5.19818	-2.152	1.30814
8	-5.09177	-1.77132	-1.32065
1	-5.62928	-1.34504	-1.97236
8	-2.92689	-0.24939	-0.50656
1	-1.54852	-1.19892	-0.66931
8	-0.26185	-2.28337	3.81617
1	-1.09763	-1.83272	3.66554
1	0.265351	-1.68509	4.327447

4TS-20

Atom	x	y	z
14	2.673752	-1.13628	-0.61222
14	1.170657	1.350428	-0.17472
8	-0.09994	0.449367	-0.57793
1	-4.50573	3.771214	-0.81403
8	1.238873	2.563079	-1.25342
1	1.972989	3.173684	-1.19301
8	0.983685	1.923674	1.360341
1	0.097612	2.243822	1.525759
8	-3.9372	3.070141	-0.52737
1	-3.33365	2.868314	-1.25199
8	1.20629	-1.67595	-0.94665
8	2.519055	0.442717	-0.15548
8	3.459999	-1.95701	0.54351
1	2.911516	-2.24259	1.281548
8	3.63236	-1.20846	-1.94668
1	3.174326	-1.42991	-2.7461
8	6.191533	-2.36064	-0.7304
1	5.661558	-1.99264	-1.42793
1	5.566395	-2.46314	-0.0207
8	1.421634	-2.56663	2.367542
1	1.207954	-1.83945	2.950976
1	0.687529	-2.61377	1.758066
14	-0.39999	-1.16031	-0.84764
8	-2.36853	0.04241	3.400298
1	-2.32665	0.808042	2.832624
8	-0.79415	-2.04561	0.48018
1	-2.80952	-0.61787	2.874566
8	-0.84048	-1.60948	-2.35714
1	-1.75561	-1.441	-2.52846
8	3.864022	2.553933	1.717584
1	2.952023	2.544492	1.992937
1	4.024357	1.665889	1.417351
8	3.69172	4.003184	-0.76838
1	3.859638	3.649067	0.106228
1	4.355806	3.629803	-1.33237
8	-1.90389	1.942633	1.243944
1	-2.5725	2.536468	0.915758
1	-1.82836	1.254455	0.581004
8	-2.11466	2.005052	-2.30131
1	-2.1678	1.138541	-1.88672
1	-1.19746	2.249306	-2.24206
14	-3.8798	-0.88687	-0.31584
8	-5.00776	0.302593	-0.23975
1	-4.71377	1.208536	-0.24913
8	-3.67354	-1.62066	1.173567
1	-4.30355	-2.29751	1.380233
8	-4.60114	-2.06417	-1.22508
1	-5.31171	-1.76507	-1.77388
8	-2.45791	-0.39017	-0.7762
1	-1.68075	-1.96727	0.809284
8	0.557503	-0.14314	3.713931
1	-0.39857	-0.17234	3.723955
1	0.789317	0.508327	3.061079

4R-21

Atom	x	y	z
14	1.999197	-0.72872	-1.6418
14	1.925817	1.435122	0.41959
8	0.747475	2.028139	-0.53153
1	-1.38516	4.471486	2.80974
8	3.124873	2.514707	0.558775
1	3.863477	2.20803	1.078948
8	1.31001	1.068447	1.887749
1	0.354081	1.124753	1.983077
8	-1.90559	4.022724	2.157522
1	-1.54945	4.289998	1.308818
8	0.63086	-0.01558	-2.12901
8	2.47502	0.066357	-0.29532
8	1.891479	-2.31324	-1.3322
1	1.606772	-2.59111	-0.46116
8	3.10789	-0.62023	-2.84526
1	2.983862	0.091094	-3.45817
8	3.880756	-3.55458	-3.30961
1	3.963389	-2.61732	-3.4405
1	3.194989	-3.61731	-2.65434
8	1.085934	-2.88056	1.34422
1	1.103865	-3.68069	1.855951
1	0.266468	-2.44667	1.594429
14	-0.31096	1.20349	-1.52728
8	-1.35228	-1.74119	2.310103
1	-1.40955	-0.79271	2.413549
8	-1.59808	0.705499	-0.79425
1	-2.00402	-1.94379	1.639452
8	-0.60117	2.283679	-2.74176
1	-1.44651	2.182805	-3.15662
8	2.600389	-1.11307	3.198023
1	2.107485	-0.32224	2.986675
1	2.351084	-1.7235	2.508697
8	4.780728	0.418962	1.849107
1	4.26716	-0.10295	2.462873
1	4.762881	-0.07312	1.037456
8	-1.48846	1.142879	1.926279
1	-1.75725	2.035473	2.139173
1	-1.62046	1.042975	0.972433
8	-0.55336	4.646933	-0.31316
1	-1.00228	4.619265	-1.14865
1	0.069596	3.92451	-0.35729
14	-4.40824	-1.14198	-0.49946
8	-5.3984	-1.17158	0.800849
1	-5.43218	-0.37402	1.309627
8	-2.87846	-1.61459	-0.14403
1	-2.22685	-0.9467	-0.40028
8	-5.06734	-2.23067	-1.52587
1	-4.45547	-2.69264	-2.08061
8	-4.33382	0.371327	-1.09442
1	-3.44247	0.735184	-1.09953
8	0.434677	-3.07011	4.43276
1	-0.31865	-2.68411	3.997373
1	1.128661	-2.42163	4.372323

4TS-22

Atom	x	y	z
14	1.80195	-1.1249	-1.1017
14	1.64813	1.81574	-0.7149
8	0.19929	1.62861	-1.4206
1	-2.289	4.78546	0.56807
8	2.53768	2.93303	-1.4729
1	3.44153	2.98042	-1.168
8	1.4443	2.21629	0.85846
1	0.56008	2.16427	1.22622
8	-2.8201	4.16212	1.04527
1	-3.3153	3.67597	0.38301
8	0.18327	-0.9519	-1.0939
8	2.4058	0.35932	-0.8034
8	2.34779	-2.1976	-0.0221
1	2.37519	-1.9425	0.90123
8	2.28829	-1.7049	-2.554
1	1.72586	-1.5132	-3.2927
8	3.92363	-4.1862	-1.7795
1	3.58016	-3.5391	-2.3843
1	3.56541	-3.9094	-0.9439
8	2.15152	-1.2008	2.64257
1	2.20381	-1.734	3.43043
1	1.24053	-0.9058	2.63958
14	-0.8058	0.32918	-1.5045
8	-0.7061	-0.7336	2.98548
1	-0.9435	0.17848	2.82561
8	-2.0119	0.39487	-0.483
1	-1.2086	-1.2441	2.3485
8	-1.2522	0.15713	-3.0657
1	-2.0737	-0.3201	-3.1279
8	3.69648	1.43323	2.50031
1	2.92178	1.86144	2.14395
1	3.42568	0.52633	2.61208
8	4.96653	2.00681	-0.0773
1	4.74883	1.86693	0.84417
1	4.83452	1.15957	-0.4848
8	-1.2335	1.83466	1.752
1	-1.708	2.6653	1.74043
1	-1.5119	1.3657	0.95503
8	-3.9508	2.40387	-0.8825
1	-3.2796	1.71437	-0.9086
1	-4.7771	1.94618	-0.7984
14	-3.3126	-1.3632	-0.0238
8	-4.107	-0.24	0.88727
1	-3.6311	0.56262	1.03508
8	-1.9523	-1.996	0.67164
1	-1.1468	-1.8319	0.19338
8	-4.4247	-2.6054	0.18923
1	-4.8747	-2.6033	1.02052
8	-3.3667	-1.3944	-1.6872
1	-3.9519	-2.089	-1.9628
8	0.75086	-2.0508	5.13081
1	0.07274	-1.672	4.57388
1	0.81092	-1.4912	5.89253

4R-22

Atom	x	y	z
14	1.85193	-0.9844	-1.2185
14	1.51893	1.89635	-0.5319
8	0.05903	1.6915	-1.2155
1	-2.391	4.61824	0.74851
8	2.3166	3.12811	-1.209
1	3.22157	3.21068	-0.9145
8	1.33317	2.13949	1.0746
1	0.45378	2.04133	1.44353
8	-2.9046	3.97749	1.22193
1	-3.4276	3.51576	0.56371
8	0.22608	-0.9055	-1.2722
8	2.35015	0.50091	-0.7714
8	2.41758	-2.1103	-0.2072
1	2.43361	-1.9198	0.73238
8	2.42714	-1.4098	-2.6907
1	1.87449	-1.2131	-3.435
8	4.22094	-3.8211	-2.0473
1	3.85064	-3.1507	-2.6093
1	3.80435	-3.6536	-1.2098
8	2.20851	-1.3378	2.52315
1	2.28219	-1.9493	3.25029
1	1.28967	-1.0703	2.55724
14	-0.8401	0.34645	-1.4889
8	-0.6635	-1.0245	2.92048
1	-0.9587	-0.1181	2.87347
8	-2.0262	0.21516	-0.4279
1	-1.1514	-1.4906	2.23617
8	-1.3471	0.3797	-3.0333
1	-2.1454	-0.1337	-3.1296
8	3.66518	1.35192	2.59442
1	2.8573	1.7657	2.30081
1	3.44457	0.42563	2.63404
8	4.82493	2.25947	0.06491
1	4.63874	2.00975	0.97007
1	4.78133	1.44591	-0.4221
8	-1.3453	1.64278	1.8939
1	-1.8166	2.47599	1.88015
1	-1.5697	1.20535	1.06753
8	-4.1501	2.25397	-0.6747
1	-3.4489	1.61657	-0.8062
1	-4.8876	1.7301	-0.386
14	-3.1647	-1.3194	-0.1254
8	-4.0064	-0.3659	0.96361
1	-3.5447	0.39199	1.28565
8	-1.8632	-2.133	0.55177
1	-1.0451	-2.0067	0.08753
8	-4.316	-2.5749	-0.0227
1	-4.6835	-2.6951	0.83937
8	-3.3029	-1.3165	-1.8046
1	-3.9023	-2.0057	-2.0607
8	0.86188	-2.5354	4.87991
1	0.16128	-2.1176	4.38166
1	0.86764	-2.1203	5.73114

4TS-23

Atom	x	y	z
14	2.28451	1.44378	-0.8876
14	3.16856	-1.1839	0.24616
8	1.66088	-1.1997	0.85896
8	4.26285	-1.3599	1.42522
1	4.86837	-2.0946	1.36002
8	3.33633	-2.4149	-0.8179
1	2.52301	-2.7581	-1.1926
8	0.82215	0.87154	-0.4528
8	3.34112	0.26394	-0.4816
8	2.39885	1.67581	-2.5032
1	2.6576	0.929	-3.025
8	2.55117	2.86563	-0.1803
1	1.86387	3.18184	0.41781
8	3.70751	4.48877	-2.5667
1	3.54448	4.41461	-1.6334
1	3.2819	3.71902	-2.9249
14	0.3435	-0.2855	0.59322
8	-0.8283	-1.1462	-0.1087
8	-0.1465	0.34525	2.00923
1	-1.0879	0.27822	2.16983
8	5.71027	-3.6136	0.27943
1	4.97671	-3.5241	-0.3248
1	6.49176	-3.3932	-0.2088
8	0.66948	-3.0518	-1.7369
1	0.216	-3.7758	-2.1469
1	0.01518	-2.5837	-1.2194
14	-2.4467	-0.7487	-0.2552
8	-3.0646	-2.0696	-0.9332
1	-4.0013	-2.2018	-1.0852
8	-2.4124	0.58436	-1.2339
1	-1.6593	0.63492	-1.808
8	-4.9878	0.31498	-0.0109
1	-4.8989	0.7509	-0.8483
8	-2.8299	-0.3661	1.27879
1	-3.7206	3.2E-05	1.2502
8	-2.2834	3.19172	0.32578
1	-2.3524	2.4288	-0.2407
1	-3.1064	3.20096	0.81298
8	-7.1872	-1.1192	0.07912
1	-6.4	-0.5217	0.06559
1	-7.3289	-1.3503	0.9863
8	2.53744	-0.453	4.04107
1	1.70306	-0.3331	3.60372
1	3.13108	-0.7823	3.37615
8	0.3663	3.43057	1.52307
1	0.2835	2.6492	2.05818
1	-0.4819	3.50256	1.08164
8	-5.742	-2.8083	-1.6226
1	-5.9384	-2.4468	-2.4758
1	-6.3162	-2.3414	-1.0081
8	-4.9315	2.61648	1.4449
1	-5.0323	1.78333	0.94647
1	-5.7368	3.09951	1.32646

4R-23

Atom	x	y	z
14	2.83357	-0.9557	0.23549
14	1.24121	0.52987	-1.8126
8	0.23499	-0.7394	-1.6722
1	-4.9992	2.72815	0.31712
8	1.67761	0.72931	-3.3558
1	2.3463	1.39905	-3.4872
8	0.55098	1.86242	-1.1762
1	-0.4031	1.90245	-1.0685
8	-4.8021	3.10838	-0.5358
1	-5.1301	2.46385	-1.1585
8	1.44267	-1.7951	0.37138
8	2.56127	0.17709	-0.9005
8	3.33093	-0.2693	1.61155
1	2.96954	0.59206	1.83193
8	4.03217	-1.9887	-0.1807
1	3.77453	-2.7785	-0.6359
8	6.05117	-1.578	2.13092
1	5.78914	-1.9486	1.29672
1	5.31759	-1.0168	2.35575
8	1.98249	2.16863	2.11751
1	1.83083	2.30544	3.04915
1	1.12206	1.912	1.79004
14	0.06585	-1.8655	-0.4997
8	-0.7892	1.11957	1.98543
1	-1.2877	1.57654	1.30608
8	-1.1952	-1.4872	0.43986
1	-0.8508	0.19833	1.74673
8	-0.0901	-3.3506	-1.1302
1	-0.9923	-3.6208	-1.2743
8	2.49046	3.87001	-0.4015
1	1.69531	3.42047	-0.6775
1	2.63803	3.55042	0.48303
8	3.86147	2.54038	-2.6031
1	3.54026	3.13716	-1.9269
1	4.28324	1.83785	-2.1244
8	-2.1495	1.91732	-0.3953
1	-2.8292	2.57753	-0.5264
1	-2.6317	1.07938	-0.3727
8	-5.5876	0.5014	-1.7464
1	-6.397	0.26261	-1.3158
1	-4.8842	0.12749	-1.2013
14	-2.8351	-1.7054	0.30013
8	-3.6341	-0.3926	0.00402
1	-4.5022	0.62827	1.21816
8	-3.2363	-2.4436	1.71693
1	-4.1131	-2.2679	2.02644
8	-4.9677	1.25207	1.79046
1	-4.3614	1.46917	2.48553
8	-2.9582	-2.8265	-0.9307
1	-3.4941	-2.54	-1.6575
8	0.33008	1.89868	4.54479
1	-0.2474	1.63287	3.83099
1	0.45017	1.13215	5.08852

4R-24

Atom	x	y	z
14	2.4683	-0.9922	-0.5139
14	-1.7292	0.22264	-0.3814
8	-1.0788	-0.7684	0.74594
1	-0.1099	-0.743	0.8227
8	-1.1307	-0.0603	-1.8617
1	-0.1956	-0.2256	-1.9699
8	-1.5577	1.79466	0.05908
1	-0.6752	2.10241	0.26725
8	-3.3202	-0.0502	-0.4381
8	3.97942	-0.4241	-0.6297
8	1.60658	-0.4574	0.68284
8	1.69393	-0.6493	-1.9465
1	2.22381	-0.6814	-2.7311
8	2.72825	-2.6429	-0.4748
1	1.95481	-3.1751	-0.3487
8	-5.2166	2.75281	-1.8425
1	-5.6012	1.90121	-1.6445
1	-4.4527	2.56768	-2.3734
8	-2.9231	-2.1084	2.4777
1	-2.1914	-1.76	1.96556
1	-3.2086	-1.3915	3.03061
8	1.18002	2.25241	0.85616
1	1.21369	2.44847	1.78394
1	1.39317	1.30958	0.78429
14	5.32915	0.40467	-0.2677
8	6.56718	-0.6457	-0.3017
1	6.34305	-1.5619	-0.4484
8	5.61446	1.58657	-1.3451
1	5.09691	2.37812	-1.2227
8	5.14149	1.13194	1.18893
1	4.61989	0.69624	1.86119
8	5.53325	-3.3924	-0.446
1	4.59884	-3.2037	-0.5318
1	5.64381	-3.7659	0.41742
8	3.81473	3.50728	0.04096
1	4.26092	3.01927	0.72675
1	2.90146	3.24093	0.10783
8	3.13448	-0.021	2.91161
1	3.12062	-0.7447	3.5217
1	2.52519	-0.2452	2.19327
14	-4.7609	-0.3343	0.23393
8	-4.8969	0.48666	1.62752
1	-4.6859	1.42216	1.58517
8	-5.8918	0.09058	-0.8743
1	-6.5897	-0.5392	-1.0378
8	-4.9964	-1.9239	0.54654
1	-4.4021	-2.2757	1.21136
8	-4.0401	3.08995	0.87763
1	-4.4806	3.229	0.04259
1	-3.1459	2.8397	0.65294
8	-7.2952	-2.4837	-1.035
1	-6.6008	-2.6298	-0.3946
1	-7.0297	-2.9441	-1.8195

4TS-25

Atom	x	y	z
14	1.88454	-0.4787	-0.8926
14	-1.2491	0.05215	-0.1603
8	-1.1076	-1.0759	1.05595
1	-0.2033	-1.2001	1.30457
8	-0.9665	-0.4784	-1.7131
1	-0.4674	0.10724	-2.2673
8	-1.1839	1.7009	0.10281
1	-0.2941	2.02345	0.11366
8	-2.9176	0.00411	-0.193
8	3.35316	-0.5707	-0.2478
8	0.80162	0.17795	0.06459
8	1.9695	0.47165	-2.2543
1	2.59526	0.20467	-2.9144
8	1.52032	-2.0309	-1.3359
1	0.61945	-2.1236	-1.6299
8	-3.7834	3.22657	-1.0197
1	-4.4148	2.52717	-1.1666
1	-2.9357	2.79467	-1.0147
8	-3.3365	-2.4453	2.30403
1	-2.5255	-2.0949	1.93632
1	-3.7388	-1.7095	2.7522
8	3.01072	3.05333	-0.7762
1	2.71942	2.82255	0.10121
1	2.63024	2.40303	-1.3583
14	4.82223	-0.5937	0.44744
8	5.06153	-2.0642	1.08577
1	4.57482	-2.7915	0.70275
8	5.98326	-0.2661	-0.6409
1	6.13195	0.66029	-0.8182
8	4.85661	0.57717	1.59206
1	4.01248	0.91733	1.87709
8	3.27663	-4.0163	-0.1527
1	2.68435	-3.4379	-0.6324
1	2.7389	-4.4852	0.47055
8	5.90527	2.63946	-0.4294
1	5.83819	2.39642	0.48759
1	5.02004	2.90253	-0.676
8	2.16255	1.76391	1.85442
1	1.66935	2.04421	2.6138
1	1.60881	1.14645	1.35913
14	-4.4456	-0.1755	0.20199
8	-4.6955	0.27282	1.75671
1	-4.3173	1.11661	2.00469
8	-5.3437	0.71018	-0.8514
1	-6.1692	0.33012	-1.1363
8	-4.9982	-1.7191	0.06778
1	-4.601	-2.3129	0.70296
8	-3.2881	2.80216	1.87864
1	-3.7014	3.26499	1.15483
1	-2.4843	2.46578	1.49018
8	-7.2329	-1.4468	-1.6749
1	-6.6128	-1.8354	-1.0595
1	-6.9243	-1.6876	-2.5378

4TS-26

Atom	x	y	z
14	0.992855	-1.886186	0.067277
14	-1.782907	-1.376872	-0.794087
8	-2.999572	-2.307112	-0.256181
1	-2.899416	-2.65678	0.629861
8	-2.206194	-0.924585	-2.286595
1	-1.75562	-0.16757	-2.672447
8	0.491354	-1.081757	1.402309
1	-1.459877	-2.766676	2.604056
8	-1.548914	-0.066932	0.173648
8	1.90844	-0.846167	-0.789317
8	-0.365427	-2.203545	-0.765494
8	1.818453	-3.22975	0.392346
1	2.768437	-3.135167	0.46081
8	-2.399789	-2.84622	2.494471
1	-2.779283	-2.06901	2.904387
8	4.606273	-2.377976	0.287691
1	4.96914	-1.82859	0.978997
1	4.497139	-1.777928	-0.44128
8	2.570796	0.634847	-0.883862
1	3.987792	0.256289	-1.718604
1	3.865851	-0.376482	-2.412558
8	1.847503	1.672014	-1.955144
1	2.410862	1.844651	-2.697772
1	3.292085	1.277519	0.445459
14	2.610462	1.596299	1.029065
8	5.584088	0.035685	1.64149
1	4.826249	0.51474	1.303827
8	6.317251	0.319221	1.112506
1	-3.350252	-0.253316	3.396715
8	-2.532391	0.203746	3.203725
1	-3.97503	0.069944	2.759504
8	-3.458107	2.220897	0.582843
1	-2.92999	2.692306	1.218984
1	-2.985408	1.412877	0.400315
8	-0.867912	1.402955	-3.138196
1	-0.036497	1.47828	-2.676916
1	-1.408631	2.124298	-2.817648
8	-4.776756	-2.541571	-2.729146
1	-4.527663	-2.725341	-1.830172
1	-4.097485	-1.9422	-3.017696
14	-0.250235	0.365989	1.115514
8	0.743077	1.355515	0.397336
1	0.416902	2.976587	-0.033854
8	0.177127	3.916998	-0.141302
1	0.871682	4.307122	-0.654264
8	-0.876118	0.926178	2.5307
1	-0.845229	1.871479	2.649968
8	-1.351803	3.786038	2.216931
1	-0.796069	4.055056	1.482745
1	-1.496849	4.550019	2.758054
8	-2.26486	3.589738	-1.790639
1	-1.502446	3.819112	-1.265729
1	-2.877136	3.193971	-1.174834

4R-26

Atom	x	y	z
14	-0.9167	-2.0024	-0.2156
14	1.77361	-1.3976	0.78787
8	3.11793	-2.1544	0.28911
1	3.11875	-2.4672	-0.6161
8	2.03972	-0.9908	2.32671
1	1.54068	-0.2603	2.70476
8	-0.4001	-1.1452	-1.5323
1	1.8778	-2.6508	-2.7162
8	1.47782	-0.045	-0.1204
8	-1.7837	-0.9422	0.64374
8	0.45818	-2.3517	0.58619
8	-1.7509	-3.325	-0.5905
1	-2.7035	-3.2232	-0.578
8	2.80451	-2.5988	-2.5172
1	3.10617	-1.76	-2.8656
8	-4.473	-2.3792	-0.2125
1	-5.1151	-2.0021	-0.8045
1	-4.2272	-1.6425	0.3425
14	-2.3793	0.61759	0.55038
8	-3.8299	0.1593	1.41185
1	-3.6391	-0.407	2.14684
8	-1.9014	1.70979	1.7444
1	-2.5829	1.79441	2.3967
8	-3.3375	1.10623	-0.7315
1	-2.825	1.47865	-1.4331
8	-6.0531	0.14897	-0.8312
1	-5.1876	0.54041	-0.9444
1	-6.1696	0.16691	0.11022
8	3.47187	0.13683	-3.2522
1	2.59943	0.49868	-3.112
1	4.01276	0.52067	-2.5721
8	3.40898	2.23523	-0.4814
1	2.87395	2.75512	-1.072
1	2.91215	1.44014	-0.3069
8	0.65148	1.29289	3.19409
1	-0.1675	1.41742	2.71924
1	1.21852	2.01645	2.93243
8	4.75649	-2.3387	2.86526
1	4.58462	-2.4883	1.94229
1	3.99444	-1.8446	3.14586
14	0.22054	0.31285	-1.127
8	-0.8994	1.19024	-0.3919
1	-0.5779	2.93245	0.18271
8	-0.3124	3.85469	0.27824
1	-0.9483	4.23121	0.87231
8	0.82737	1.05667	-2.4506
1	0.7968	2.01002	-2.4781
8	1.26682	3.86285	-2.0257
1	0.69365	4.11835	-1.3006
1	1.34367	4.6069	-2.6075
8	2.14615	3.50668	1.95023
1	1.40786	3.73613	1.39373
1	2.80012	3.14256	1.35946

4TS-27

Atom	x	y	z
14	1.35824	-1.5853	-0.4362
14	-1.5394	-1.3355	-0.985
8	-2.3923	-2.6318	-0.5059
1	-2.0398	-3.1607	0.2108
8	-2.3451	-0.723	-2.2289
1	-2.1936	0.19069	-2.5098
8	0.77225	-1.3289	1.10525
1	-0.341	-3.4798	1.87995
8	-1.4187	-0.2359	0.25354
8	2.15541	-0.215	-0.7883
8	0.00908	-1.7593	-1.3211
8	2.30916	-2.8748	-0.5259
1	3.255	-2.7333	-0.5998
8	-1.242	-3.7788	1.85139
1	-1.7024	-3.2953	2.53587
8	5.07362	-2.281	-0.9405
1	5.30766	-1.3845	-0.6912
1	5.23496	-2.3436	-1.872
14	2.18235	1.17571	0.09462
8	2.93192	2.47002	-0.5278
1	2.34051	2.8054	-1.2031
8	0.68807	2.11115	-1.66
1	0.95901	1.88089	-2.5398
8	3.30187	0.84789	1.30599
1	3.03533	0.20417	1.9475
8	5.69311	0.44993	-0.184
1	5.02487	0.6024	0.48545
1	5.52189	1.12121	-0.8328
8	-2.63	-1.9066	3.6041
1	-2.0522	-1.1549	3.49175
1	-3.4317	-1.6863	3.14724
8	-3.6406	1.80043	1.03874
1	-2.9605	2.1706	1.59321
1	-3.2306	1.05213	0.6181
8	-1.8417	1.88284	-2.8321
1	-0.9967	2.01217	-2.3817
1	-2.4478	2.51291	-2.4499
8	-4.5951	-2.8045	-2.6084
1	-4.0965	-3.0794	-1.847
1	-4.1437	-2.0143	-2.8829
14	-0.1805	-0.0036	1.28651
8	0.76104	1.2639	0.93178
1	-0.0712	3.35196	-0.7555
8	-0.4625	4.03632	-0.1764
1	0.08668	4.80097	-0.2831
8	-0.7433	0.16028	2.80734
1	-0.8197	1.07356	3.07791
8	-1.2749	3.01589	2.41002
1	-0.8265	3.27516	1.59928
1	-1.5298	3.82214	2.83832
8	-3.2773	3.83166	-1.1049
1	-2.4114	4.07371	-0.7875
1	-3.6175	3.21724	-0.459

4R-27

Atom	x	y	z
14	2.17858	0.93618	-0.8273
14	-0.0294	1.59193	1.07737
8	-0.3881	3.1746	1.04283
1	-0.3975	3.6144	0.19139
8	-0.3346	1.1109	2.57967
1	-0.6176	0.21515	2.79318
8	0.88713	1.10333	-1.8589
1	0.05629	3.50567	-2.1369
8	-0.9422	0.77099	-0.0385
8	2.57405	-0.6243	-0.8973
8	1.52021	1.31982	0.6236
8	3.37958	1.92384	-1.2578
1	4.13363	1.83896	-0.6801
8	-0.5513	4.06133	-1.6629
1	-1.4281	3.78667	-1.9288
8	4.45059	0.7756	1.22224
1	4.34595	-0.1703	1.3452
1	3.84707	1.16473	1.84273
14	1.6249	-1.9919	-0.9142
8	1.65058	-2.7933	0.4151
1	0.32612	-3.3298	1.14732
8	-0.4818	-3.6609	1.61731
1	-0.1878	-4.3837	2.1547
8	2.10125	-2.8563	-2.2361
1	2.29741	-2.3446	-3.0077
8	3.92233	-2.0375	1.84603
1	4.55117	-2.6636	1.51534
1	3.08277	-2.2864	1.43272
8	-3.0944	2.76005	-2.3522
1	-2.6854	1.93499	-2.6003
1	-3.6063	2.55248	-1.5784
8	-3.912	0.52755	-0.0584
1	-3.9161	-0.1182	-0.758
1	-2.9899	0.70601	0.10966
8	-1.3754	-1.3765	3.20968
1	-0.9931	-2.1172	2.74303
1	-2.3059	-1.3876	2.99345
8	-0.8708	3.82206	3.97949
1	-0.7863	4.00498	3.05014
1	-0.7663	2.87835	4.02056
14	-0.3956	0.16214	-1.4652
8	0.11225	-1.3523	-1.2851
1	-1.9876	-3.6153	0.57212
8	-2.85	-3.6218	0.13696
1	-3.1296	-4.5274	0.13541
8	-1.5719	0.26792	-2.5861
1	-2.1365	-0.5003	-2.6516
8	-3.4724	-1.7895	-1.9804
1	-3.1596	-2.4378	-1.3445
1	-4.129	-2.2218	-2.5098
8	-4.088	-1.602	2.04264
1	-3.8417	-2.2894	1.43206
1	-4.1949	-0.8144	1.51454

4TS-28

Atom	x	y	z
14	-0.76212	-2.409632	-0.440308
14	-1.873538	1.020537	-0.223167
8	-3.332161	0.960536	0.536984
1	-3.934889	0.284287	0.227782
8	-1.845292	2.474384	-0.964443
1	-1.087576	2.7484	-1.483927
8	-0.445601	-1.60445	0.955563
1	-4.010916	-1.847509	-0.380318
8	-0.720726	1.075346	1.016408
8	0.337368	-2.096156	-1.605682
8	-1.476348	-0.2579	-1.062946
8	-2.318307	-2.778859	-0.811518
1	-2.477274	-3.704593	-0.680015
8	-4.737387	-1.490766	0.126087
1	-4.507955	-1.670646	1.033029
8	2.235583	-3.02386	1.737993
1	1.926677	-2.282577	2.251419
1	1.44881	-3.394472	1.342668
8	1.194414	-0.722867	-1.796018
1	-0.220363	-3.947778	0.027059
1	0.274334	-4.388876	-0.649351
8	0.508161	0.250732	-2.898068
1	-0.436002	0.254795	-2.726184
1	2.705535	-1.017673	-2.307691
14	3.313241	-1.350978	-1.653661
8	4.249025	-1.894581	0.059708
1	4.929105	-2.549917	-0.019005
8	3.568504	-2.28177	0.619914
1	-3.148973	-1.173604	2.697632
8	-2.299561	-1.519139	2.448422
1	-3.159568	-0.286332	2.348986
8	0.882292	3.672236	1.572995
1	1.39624	3.241728	2.247083
1	0.153792	3.089491	1.377222
8	0.454141	3.158578	-2.550785
1	0.690181	2.292126	-2.867846
1	1.203716	3.472632	-2.048277
8	-4.398239	3.789409	0.012112
1	-4.398788	2.930059	0.418346
1	-3.598756	3.771007	-0.503298
14	0.316143	-0.16154	1.016727
8	1.328035	-0.064521	-0.281088
1	3.014005	0.825395	0.098191
8	3.859659	1.129704	0.426941
1	4.404619	0.350011	0.38384
8	1.202974	-0.239067	2.380185
1	1.661603	0.522519	2.723827
8	2.921565	1.989845	2.948178
1	3.426157	1.783442	2.156991
1	3.534873	2.110531	3.660039
8	2.633349	3.878485	-0.719761
1	3.257853	3.184977	-0.543185
1	2.064688	3.924114	0.049141

4R-28

Atom	x	y	z
14	-0.967894	-2.037028	-0.569327
14	-1.798467	1.014801	-0.260586
8	-3.241496	1.018242	0.501107
1	-3.866238	0.315953	0.308133
8	-1.775444	2.333606	-1.204309
1	-0.961105	2.675446	-1.580842
8	-0.480409	-1.487754	0.961899
1	-4.153108	-1.77021	-0.224382
8	-0.608823	1.155696	0.905774
8	0.318468	-1.950843	-1.657764
8	-1.452394	-0.360793	-1.016004
8	-2.529908	-2.534679	-0.900461
1	-2.589305	-3.469807	-0.759617
8	-4.788764	-1.328768	0.338236
1	-4.517468	-1.54583	1.225385
8	1.643121	-3.552905	1.70738
1	1.481377	-2.825049	2.295331
1	0.843063	-3.620113	1.175976
14	1.404922	-0.763553	-1.699069
8	-0.525142	-3.691617	-0.148725
1	-0.034535	-4.100343	-0.847364
8	0.991674	0.356821	-2.818761
1	0.056396	0.349947	-2.99427
8	2.916541	-1.228282	-2.052598
1	3.303508	-1.870951	-1.457086
8	3.808469	-3.093551	-0.057724
1	4.09236	-3.960866	-0.31149
1	3.099133	-3.223472	0.580067
8	-3.017449	-1.154582	2.789229
1	-2.200471	-1.504287	2.448374
1	-3.018388	-0.241504	2.522091
8	0.854577	3.655509	1.916621
1	1.448656	3.201355	2.503252
1	0.197829	3.017656	1.649947
8	0.629537	3.232596	-2.405125
1	1.028003	2.404841	-2.65474
1	1.249347	3.659288	-1.814251
8	-4.378316	3.739755	-0.470641
1	-4.385544	2.966943	0.082028
1	-3.56952	3.638785	-0.96086
14	0.388379	-0.125615	1.068533
8	1.46342	-0.088641	-0.183524
1	3.096933	0.890845	0.012926
8	3.861411	1.439242	0.19821
1	4.574394	1.060959	-0.300828
8	1.172919	-0.14142	2.483483
1	1.803733	0.534209	2.715945
8	3.141895	1.914049	2.908539
1	3.613657	1.825688	2.079212
1	3.775203	1.820204	3.607275
8	2.523567	4.142533	-0.40958
1	3.085348	3.384056	-0.292068
1	1.949938	4.152076	0.356036

4TS-29

Atom	x	y	z
14	-1.595259	0.983393	-0.899849
14	1.140462	2.032821	-0.157391
8	0.905892	3.39872	0.681731
1	0.002501	3.628175	0.912851
8	2.549957	2.198719	-0.928922
1	2.916033	1.42965	-1.374011
8	-1.365601	0.43433	0.641751
1	-2.182545	3.771969	0.10547
8	1.229638	0.712642	0.857614
8	-1.533816	-0.34497	-1.868585
8	-0.109336	1.700699	-1.147168
8	-2.649024	2.14409	-1.268901
1	-3.506322	1.782471	-1.008396
8	-1.907424	3.890913	1.008898
1	-2.525488	3.35093	1.502034
8	-3.427006	-1.744541	1.527592
1	-2.670923	-1.488607	2.039581
1	-3.609392	-0.991314	0.92544
14	-0.482853	-1.569192	-1.729045
8	-3.950296	0.278795	-0.171943
1	-4.626437	-0.088172	-0.725983
8	0.715616	-1.365776	-2.83283
1	0.531069	-0.727995	-3.510035
8	-1.09533	-3.041694	-1.947924
1	-1.773052	-3.368589	-1.349715
8	-3.030637	-3.931914	-0.117923
1	-3.881326	-4.102543	-0.498411
1	-3.163952	-3.208443	0.509098
8	-4.02289	2.030671	1.967925
1	-4.127301	1.419956	1.221794
1	-3.771252	1.482387	2.698097
8	3.752864	-0.524788	2.14647
1	3.284745	-1.133987	2.706347
1	3.105111	0.094193	1.821818
8	3.384476	-0.218676	-2.150502
1	2.595227	-0.696573	-2.385821
1	3.874674	-0.800783	-1.570465
8	3.396738	5.027945	-0.083563
1	2.576163	4.893081	0.377228
1	3.506215	4.216059	-0.565767
14	0.00608	-0.356339	0.970491
8	0.196246	-1.486697	-0.223669
1	1.300323	-3.029618	0.112609
8	1.899743	-3.726296	0.383442
1	1.598999	-4.513784	-0.052286
8	-0.106687	-1.06434	2.414424
1	0.57415	-1.645773	2.743519
8	2.044225	-2.844737	3.085439
1	2.080236	-3.354921	2.274961
1	1.973118	-3.457039	3.805471
8	4.468472	-2.078798	-0.196031
1	3.793348	-2.742343	-0.106137
1	4.401488	-1.542321	0.593225

4R-29

Atom	x	y	z
14	-1.699113	0.287444	-0.919679
14	0.673479	2.08956	-0.427487
8	0.120453	3.467205	0.219372
1	-0.834778	3.584371	0.206977
8	1.998513	2.453369	-1.276305
1	2.485756	1.740764	-1.699537
8	-1.330633	-0.081959	0.697896
1	-2.965838	2.728346	-0.487374
8	1.081436	0.983876	0.750143
8	-1.230433	-1.128957	-1.665882
8	-0.482499	1.342953	-1.289702
8	-3.146619	0.766061	-1.134822
1	-4.485797	0.458833	-0.182435
8	-2.725813	3.435807	0.112859
1	-3.076967	3.160263	0.956123
8	-3.661307	-2.005752	1.441617
1	-2.867086	-1.482413	1.476372
1	-4.350038	-1.386036	1.207309
14	0.02819	-2.082764	-1.339688
8	-5.183556	0.269035	0.479948
1	-6.014372	0.470346	0.072809
8	1.242699	-1.981823	-2.441267
1	1.153228	-2.521489	-3.214885
8	-0.412673	-3.638924	-1.268835
1	-1.340453	-3.812182	-1.088458
8	-3.213699	-3.608851	-0.882817
1	-3.374483	-2.916536	-1.513192
1	-3.416606	-3.21151	-0.033405
8	-3.683061	1.859533	2.431051
1	-4.322089	1.372223	1.914609
1	-2.903201	1.318013	2.434312
8	3.985757	0.772202	1.862725
1	3.733927	0.177987	2.561014
1	3.174201	1.132174	1.517816
8	3.289651	0.196335	-2.375518
1	2.643804	-0.492321	-2.49927
1	3.934921	-0.157742	-1.76418
8	2.219881	5.479989	-0.79351
1	1.442553	5.230744	-0.306167
1	2.496064	4.660173	-1.187698
14	0.219767	-0.358263	1.082823
8	0.721687	-1.565565	0.063034
1	2.26568	-2.597058	0.551238
8	3.040548	-3.03725	0.905004
1	2.962224	-3.949697	0.658087
8	0.348843	-0.819294	2.62026
1	1.194753	-1.034618	3.003525
8	3.013743	-1.63074	3.387834
1	3.163627	-2.261078	2.682088
1	3.203744	-2.066488	4.207747
8	4.964967	-0.932524	-0.273977
1	4.517253	-1.719405	0.016311
1	4.804368	-0.28714	0.413826

4TS-30

Atom	x	y	z
14	-1.683917	1.030243	-1.330197
14	1.081586	1.932235	-0.160982
8	0.890055	3.261379	0.752328
1	0.030792	3.389052	1.158959
8	2.401043	2.188813	-1.071845
1	2.639929	1.462931	-1.651265
8	-1.313521	0.28083	0.917627
1	-2.24373	2.824108	1.048002
8	1.30268	0.57523	0.731927
8	-1.618229	-0.573324	-1.621892
8	-0.221398	1.697246	-1.110213
8	-2.119662	1.667673	-2.81267
1	-1.395737	1.920309	-3.366937
8	-1.855852	3.357158	1.737302
1	-1.988259	2.835215	2.522558
8	-4.563098	-0.202118	1.221912
1	-4.2071	-0.040401	2.09133
1	-4.017537	0.337971	0.652052
14	-0.772808	-1.909793	-1.304913
8	-2.996811	1.601352	-0.495556
1	-3.541739	2.117034	-1.077699
8	0.304741	-2.222531	-2.513336
1	-0.045	-2.633667	-3.291461
8	-1.745999	-3.199392	-1.205498
1	-2.574403	-3.1085	-0.728761
8	-4.215883	-2.806409	0.157837
1	-4.960244	-2.829751	-0.427659
1	-4.271217	-1.955241	0.603811
8	-2.60434	0.79767	3.228556
1	-2.126905	0.590715	2.407473
1	-2.140121	0.324848	3.906735
8	4.087211	-0.330047	1.537445
1	3.821222	-0.94278	2.214045
1	3.300374	0.15583	1.303426
8	2.782777	-0.265429	-2.583954
1	2.002313	-0.804391	-2.664183
1	3.409534	-0.800884	-2.096819
8	3.179254	5.029789	-0.269751
1	2.426337	4.84179	0.279662
1	3.291203	4.221739	-0.758406
14	0.055266	-0.447891	1.110046
8	0.175019	-1.702784	0.004102
1	1.512246	-3.009672	0.178774
8	2.206658	-3.64946	0.358786
1	1.913991	-4.468159	-0.019396
8	0.306771	-1.068467	2.599382
1	1.126833	-1.507231	2.799722
8	2.786328	-2.636822	2.956927
1	2.682142	-3.169745	2.167825
1	2.774772	-3.224929	3.699614
8	4.424667	-1.92947	-0.85365
1	3.819829	-2.610004	-0.577662
1	4.499411	-1.350407	-0.095239

4R-30

Atom	x	y	z
14	-1.63116	1.0522	-1.065902
14	1.252563	1.890253	-0.310786
8	1.263778	3.259759	0.568103
1	0.428057	3.512874	0.961749
8	2.583678	1.935205	-1.236733
1	2.751817	1.15001	-1.761661
8	-1.276168	0.437234	0.625734
1	-2.005036	3.188746	0.974156
8	1.346913	0.555309	0.670567
8	-1.604609	-0.538595	-1.634305
8	-0.108355	1.736295	-1.163536
8	-2.189715	1.697424	-2.54958
1	-1.594333	1.566679	-3.272189
8	-1.465912	3.622973	1.63159
1	-1.639877	3.136109	2.429839
8	-4.66786	0.086337	1.228871
1	-4.307678	0.216748	2.100251
1	-4.157585	0.680882	0.677579
14	-0.855487	-1.912489	-1.307412
8	-2.941193	1.824134	-0.310961
1	-3.419328	2.309961	-0.971457
8	0.223484	-2.345886	-2.47554
1	-0.130147	-2.804702	-3.224648
8	-1.87965	-3.159057	-1.142216
1	-2.734291	-2.978173	-0.744914
8	-4.432438	-2.449076	-0.064206
1	-5.005108	-2.273557	-0.798618
1	-4.458526	-1.648942	0.467827
8	-2.492304	1.051887	3.085342
1	-2.157946	0.889645	2.199861
1	-1.941154	0.509803	3.636237
8	3.979809	-0.587346	1.672175
1	3.573154	-1.114762	2.350765
1	3.296239	-0.002514	1.356296
8	2.827628	-0.639063	-2.537531
1	2.010115	-1.115365	-2.642125
1	3.378192	-1.195801	-1.987388
8	3.774829	4.653379	-0.489402
1	3.001513	4.580218	0.059034
1	3.761836	3.839895	-0.981574
14	0.043181	-0.376074	0.996785
8	0.097929	-1.713248	0.021269
1	1.259602	-3.15106	0.345206
8	1.875326	-3.828151	0.637042
1	1.516308	-4.655339	0.34373
8	0.031857	-0.837563	2.557071
1	0.747978	-1.370136	2.891311
8	2.292719	-2.597021	3.167862
1	2.224223	-3.199004	2.425177
1	2.381427	-3.12063	3.952538
8	4.252712	-2.34038	-0.628238
1	3.603666	-2.970644	-0.335254
1	4.349852	-1.731804	0.103652

4TS-31

Atom	x	y	z
14	-1.595259	0.983393	-0.899849
14	1.140462	2.032821	-0.157391
8	0.905892	3.39872	0.681731
1	0.002501	3.628175	0.912851
8	2.549957	2.198719	-0.928922
1	2.916033	1.42965	-1.374011
8	-1.365601	0.43433	0.641751
1	-2.182545	3.771969	0.10547
8	1.229638	0.712642	0.857614
8	-1.533816	-0.34497	-1.868585
8	-0.109336	1.700699	-1.147168
8	-2.649024	2.14409	-1.268901
1	-3.506322	1.782471	-1.008396
8	-1.907424	3.890913	1.008898
1	-2.525488	3.35093	1.502034
8	-3.427006	-1.744541	1.527592
1	-2.670923	-1.488607	2.039581
1	-3.609392	-0.991314	0.92544
14	-0.482853	-1.569192	-1.729045
8	-3.950296	0.278795	-0.171943
1	-4.626437	-0.088172	-0.725983
8	0.715616	-1.365776	-2.83283
1	0.531069	-0.727995	-3.510035
8	-1.09533	-3.041694	-1.947924
1	-1.773052	-3.368589	-1.349715
8	-3.030637	-3.931914	-0.117923
1	-3.881326	-4.102543	-0.498411
1	-3.163952	-3.208443	0.509098
8	-4.02289	2.030671	1.967925
1	-4.127301	1.419956	1.221794
1	-3.771252	1.482387	2.698097
8	3.752864	-0.524788	2.14647
1	3.284745	-1.133987	2.706347
1	3.105111	0.094193	1.821818
8	3.384476	-0.218676	-2.150502
1	2.595227	-0.696573	-2.385821
1	3.874674	-0.800783	-1.570465
8	3.396738	5.027945	-0.083563
1	2.576163	4.893081	0.377228
1	3.506215	4.216059	-0.565767
14	0.00608	-0.356339	0.970491
8	0.196246	-1.486697	-0.223669
1	1.300323	-3.029618	0.112609
8	1.899743	-3.726296	0.383442
1	1.598999	-4.513784	-0.052286
8	-0.106687	-1.06434	2.414424
1	0.57415	-1.645773	2.743519
8	2.044225	-2.844737	3.085439
1	2.080236	-3.354921	2.274961
1	1.973118	-3.457039	3.805471
8	4.468472	-2.078798	-0.196031
1	3.793348	-2.742343	-0.106137
1	4.401488	-1.542321	0.593225

4R-31

Atom	x	y	z
14	-1.699113	0.287444	-0.919679
14	0.673479	2.08956	-0.427487
8	0.120453	3.467205	0.219372
1	-0.834778	3.584371	0.206977
8	1.998513	2.453369	-1.276305
1	2.485756	1.740764	-1.699537
8	-1.330633	-0.081959	0.697896
1	-2.965838	2.728346	-0.487374
8	1.081436	0.983876	0.750143
8	-1.230433	-1.128957	-1.665882
8	-0.482499	1.342953	-1.289702
8	-3.146619	0.766061	-1.134822
1	-4.485797	0.458833	-0.182435
8	-2.725813	3.435807	0.112859
1	-3.076967	3.160263	0.956123
8	-3.661307	-2.005752	1.441617
1	-2.867086	-1.482413	1.476372
1	-4.350038	-1.386036	1.207309
14	0.02819	-2.082764	-1.339688
8	-5.183556	0.269035	0.479948
1	-6.014372	0.470346	0.072809
8	1.242699	-1.981823	-2.441267
1	1.153228	-2.521489	-3.214885
8	-0.412673	-3.638924	-1.268835
1	-1.340453	-3.812182	-1.088458
8	-3.213699	-3.608851	-0.882817
1	-3.374483	-2.916536	-1.513192
1	-3.416606	-3.211151	-0.033405
8	-3.683061	1.859533	2.431051
1	-4.322089	1.372223	1.914609
1	-2.903201	1.318013	2.434312
8	3.985757	0.772202	1.862725
1	3.733927	0.177987	2.561014
1	3.174201	1.132174	1.517816
8	3.289651	0.196335	-2.375518
1	2.643804	-0.492321	-2.49927
1	3.934921	-0.157742	-1.76418
8	2.219881	5.479989	-0.79351
1	1.442553	5.230744	-0.306167
1	2.496064	4.660173	-1.187698
14	0.219767	-0.358263	1.082823
8	0.721687	-1.565565	0.063034
1	2.26568	-2.597058	0.551238
8	3.040548	-3.03725	0.905004
1	2.962224	-3.949697	0.658087
8	0.348843	-0.819294	2.62026
1	1.194753	-1.034618	3.003525
8	3.013743	-1.63074	3.387834
1	3.163627	-2.261078	2.682088
1	3.203744	-2.066488	4.207747
8	4.964967	-0.932524	-0.273977
1	4.517253	-1.719405	0.016311
1	4.804368	-0.28714	0.413826

4TS-32

Atom	x	y	z
14	2.304819	-0.156841	-0.697326
14	-0.249903	-0.341485	1.364662
8	0.255069	-1.348565	2.562629
1	1.135157	-1.669625	2.417228
8	-1.798071	-0.08583	2.01965
1	-2.095889	-0.781038	2.60168
8	2.089722	1.500391	-0.569622
8	0.16974	1.25131	1.214552
8	1.224632	-0.606501	-1.877635
8	1.770602	-0.771785	0.673172
8	3.806442	-0.488288	-1.183233
1	4.503149	-0.014992	-0.73314
14	-0.343405	-0.293103	-1.578238
8	-0.725123	-0.944023	-0.120337
8	-1.342709	-0.772958	-2.7351
1	-2.08076	-1.338891	-2.509388
14	0.592914	1.996153	-0.17897
8	-0.422333	1.343648	-1.314551
8	0.430531	3.5898	-0.048675
1	-0.160736	4.084809	-0.616508
8	-2.236796	-2.750195	3.263151
1	-1.304684	-2.63522	3.4136
1	-2.290525	-3.198688	2.422908
8	-4.079878	-0.155065	0.081563
1	-3.374587	-0.180926	0.728018
1	-4.05028	0.721779	-0.29041
8	-1.651738	4.962299	-1.449042
1	-1.968367	5.728177	-0.989894
1	-2.326451	4.288862	-1.355741
8	-3.092343	2.573711	-0.762552
1	-2.332219	2.097791	-1.088538
1	-2.936743	2.691346	0.177398
8	3.432034	0.355362	2.684736
1	2.873751	-0.089712	2.039971
1	2.850023	0.920634	3.174735
8	-1.846028	-3.545174	0.402587
1	-1.577763	-2.663005	0.154954
1	-2.496657	-3.780682	-0.248603
8	5.065744	1.480774	0.559875
1	4.712373	1.172658	1.393446
1	4.419316	2.093881	0.230144
8	1.533318	-3.795932	-2.838037
1	1.580414	-2.853957	-2.944815
1	1.550012	-3.935166	-1.894572
8	-3.60481	-2.22097	-1.744773
1	-3.870663	-1.54566	-1.111126
1	-4.337448	-2.353041	-2.330767
8	1.31705	-3.771901	0.149823
1	1.49767	-2.848938	0.313307
1	0.380019	-3.886506	0.266783
8	-2.392765	2.728363	2.010233
1	-1.513961	3.087457	2.024161
1	-2.264418	1.79476	2.186057

4R-32

Atom	x	y	z
14	2.188472	-0.589199	-0.694014
14	-0.155638	-0.297634	1.333196
8	0.048036	-1.347903	2.61475
1	0.828708	-1.877609	2.53809
8	-1.637368	0.277372	2.022875
1	-2.021618	-0.305356	2.668972
8	2.340041	1.065902	-0.651346
8	0.442535	1.26485	1.145258
8	1.063187	-0.881034	-1.866659
8	1.48676	-0.981855	0.707581
8	3.587517	-1.303031	-1.036142
1	4.366534	-0.916237	-0.639079
14	-0.421157	-0.248333	-1.586831
8	-0.892378	-0.780723	-0.117599
8	-1.488408	-0.557298	-2.741116
1	-2.327555	-0.950418	-2.500888
14	0.967343	1.869595	-0.271817
8	-0.16008	1.378495	-1.384343
8	1.153192	3.464121	-0.230233
1	0.598705	4.056226	-0.739339
8	-2.603925	-2.324684	3.39266
1	-1.65359	-2.292774	3.427952
1	-2.80067	-2.714858	2.545898
8	-3.959555	0.577671	0.20678
1	-3.230428	0.418921	0.809105
1	-3.807239	1.446995	-0.151053
8	-0.760423	5.198235	-1.4554
1	-0.90653	5.990983	-0.957546
1	-1.532205	4.646001	-1.32236
8	-2.547308	3.101042	-0.693123
1	-1.91455	2.48259	-1.049263
1	-2.338779	3.175432	0.241849
8	3.448375	-0.12347	2.686208
1	2.785158	-0.469697	2.088233
1	3.009755	0.552968	3.185041
8	-2.519676	-3.074252	0.451054
1	-2.084331	-2.249603	0.24202
1	-3.212651	-3.139224	-0.196258
8	5.247309	0.508685	0.485296
1	4.856909	0.3489	1.34309
1	4.748767	1.228821	0.116973
8	0.70937	-4.073996	-2.892052
1	0.931347	-3.153861	-2.962631
1	0.621259	-4.234158	-1.956254
8	-3.987892	-1.47568	-1.677831
1	-4.07756	-0.773994	-1.022432
1	-4.763004	-1.446471	-2.221711
8	0.334983	-4.069521	0.088581
1	0.719871	-3.222938	0.285643
1	-0.603648	-3.963595	0.215101
8	-1.764557	3.107743	2.050061
1	-0.839468	3.319294	2.054301
1	-1.777341	2.156323	2.187017

4TS-33

Atom	x	y	z
14	1.528507	-1.89152	0.946688
14	0.55781	0.286709	-0.651723
8	1.220754	1.412844	-1.594639
1	2.164538	1.498907	-1.479011
8	-1.67478	2.232894	-1.320269
1	-1.69303	2.859916	-2.032974
8	0.524694	-2.832193	0.041286
8	-0.350432	-0.853455	-1.40549
8	0.578189	-1.3192	2.155777
8	1.842293	-0.592233	-0.018823
8	2.845929	-2.620083	1.483973
1	3.619907	-2.66938	0.919483
14	-0.767169	-0.472954	1.73698
8	-0.247532	0.693132	0.712078
8	-1.60383	0.08016	2.979235
1	-1.885223	0.999529	2.979669
14	-0.85534	-2.164317	-0.540812
8	-1.621702	-1.518548	0.773561
8	-1.732175	-3.193966	-1.38737
1	-2.690089	-3.242908	-1.347821
8	0.921033	4.404272	-2.058773
1	0.77945	3.462257	-2.110243
1	0.293011	4.692191	-1.404927
8	-3.778803	2.435635	0.338826
1	-3.043443	2.415893	-0.31233
1	-4.252538	1.620018	0.221564
8	-4.555373	-3.179502	-1.397394
1	-4.858402	-3.063113	-2.287987
1	-4.708702	-2.340673	-0.955397
8	-4.373054	-0.594778	-0.28805
1	-3.658644	-0.790192	0.309732
1	-3.943956	-0.282003	-1.093079
8	6.148134	-0.001923	-0.816583
1	5.472026	0.645009	-0.60504
1	6.565107	0.294831	-1.613413
8	-0.402211	3.797932	0.565767
1	-0.821922	3.175307	-0.055877
1	-0.859693	3.666352	1.388163
8	4.955242	-2.606398	-0.423485
1	5.415837	-1.771011	-0.511417
1	4.569267	-2.780381	-1.271583
8	3.841968	1.51446	-0.228867
1	3.366036	0.814781	0.209508
1	3.526787	2.342718	0.145422
8	-2.455093	2.737928	2.695699
1	-2.98871	2.660498	1.888934
1	-2.981674	3.205566	3.328955
8	2.500247	3.913397	0.421426
1	2.382438	4.284051	-0.448689
1	1.595401	3.774884	0.7066
8	-2.96973	0.248304	-2.543466
1	-2.27891	-0.350626	-2.794733
1	-2.488323	0.997282	-2.124732

4R-33

Atom	x	y	z
14	0.947064	-2.216895	0.758854
14	0.186403	0.183146	-0.614877
8	0.614432	1.386834	-1.498841
1	-0.637772	2.563909	-1.898449
8	-1.393361	3.154705	-2.055782
1	-1.030951	3.984784	-2.334225
8	-0.355886	-2.938671	0.042093
8	-1.087948	-0.749211	-1.20333
8	0.312921	-1.543483	2.123055
8	1.319477	-0.964839	-0.231115
8	2.170365	-3.198261	1.060606
1	2.893207	-3.239191	0.427376
14	-0.912782	-0.468348	1.947755
8	-0.389328	0.645496	0.878199
8	-1.438917	0.207967	3.30555
1	-1.327047	1.159133	3.348461
14	-1.653006	-2.009824	-0.302332
8	-2.0911	-1.298133	1.129876
8	-2.827587	-2.841085	-1.002899
1	-3.609983	-2.408178	-1.347758
8	3.170574	1.600019	-2.414294
1	2.252141	1.487013	-2.119175
1	3.131493	1.825383	-3.333292
8	-2.762337	3.443787	0.63067
1	-2.279441	3.421846	-0.193333
1	-3.365339	2.704756	0.592867
8	-5.013973	-1.258558	-1.951034
1	-4.585304	-0.599782	-2.490831
1	-5.321479	-0.781398	-1.187998
8	-4.178767	0.872423	0.140744
1	-3.664367	0.250991	0.646659
1	-3.774007	0.902192	-0.724454
8	5.004949	-0.525438	-1.411989
1	5.248954	-0.124934	-0.578591
1	4.36922	0.074176	-1.796921
8	1.217636	3.458371	0.531243
1	0.99653	2.802175	-0.129731
1	0.717249	3.211861	1.302501
8	4.117689	-3.165757	-0.957147
1	4.421538	-2.265151	-1.113288
1	3.763124	-3.466955	-1.782399
8	5.285585	0.917277	1.122247
1	4.614626	0.534394	1.671914
1	4.931704	1.757397	0.821811
8	-1.04562	3.027171	2.83108
1	-1.617919	3.174592	2.070764
1	-1.173253	3.7696	3.405832
8	4.05988	3.205819	-0.073239
1	3.87924	2.814596	-0.924611
1	3.200379	3.42033	0.286354
8	-3.060064	0.837552	-2.572879
1	-2.30736	0.287117	-2.360993
1	-2.701663	1.714349	-2.692599