Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for:

Theoretical study of the pyrolysis of β-1,4-xylan: a detailed investigation on unimolecular concerted reactions.

S1- Rate coefficients involved in the different pathways

Table S1.1

Computed rate coefficients for glycosidic bond fissions of Scheme 2 and for temperatures ranging from 500 to 1200K.

	Glycosidic bond fission			
	A (s^{-1})	n	E (kJ mol^{-1})	K_{750K} (s^{-1})
k_{TS1}	$2.50\ 10^{14}$	0.328	291.58	$1.1\ 10^{-5}$
k_{TS2}	$6.33\ 10^{8}$	1.679	287.36	$4.1\ 10^{-7}$
k_{TS3}	$1.30\ 10^{12}$	0.223	284.18	$9.1\ 10^{-8}$
k_{TS4}	$3.61\ 10^{12}$	0.868	307.61	$4.2\ 10^{-7}$
k_{TS5}	$7.39\ 10^{12}$	0.758	314.01	$1.5\ 10^{-7}$
k_{TS6}	$1.24\ 10^{10}$	0.991	290.50	$5.1\ 10^{-8}$

Table S1.2

Computed rate coefficients for dehydration reactions of Scheme 6 and for temperatures ranging from 500 to 1200K.

	Dehydration reactions			
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS7}	$1.70\ 10^{14}$	0.040	320.75	$1.0\ 10^{-8}$
k_{TS8}	$2.96\ 10^{13}$	0.439	336.81	$1.9\ 10^{-9}$
k_{TS9}	$2.07\ 10^{9}$	1.411	313.76	$3.3\ 10^{-9}$
k_{TS10}	$7.37\ 10^{9}$	1.385	341.16	$1.2\ 10^{-10}$

Table S1.3

Rate coefficients involved radical reactions, for temperatures ranging from 500 to 1200K. *estimated

	Radical reactions			
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
C_4 –O scission	$4.0\ 10^{16*}$	0.0	379.07	$1.6\ 10^{-10}$
Ring opening (C_4-C_5)	$2.11\ 10^{14}$	0.947	377.15	$6.0\ 10^{-10}$

Table S1.4

Computed rate coefficients involved in the thermal decomposition of reducing end-chain (Scheme 8), for temperatures ranging from 500 to 1200K.

Main reactions of fragment 3				
	A (s^{-1})	n	E (kJ mol^{-1})	k_{673K} (s^{-1})
k_{TS1}*	2.50 10^{14}	0.328	291.58	1.1 10^{-5}
k_{TS11}	1.01 10^{10}	1.064	194.43	3.3 10^{-1}
k_{TS12}	6.28 10^{9}	0.851	264.93	6.2 10^{-7}

* Analogy with the computed value from TS1 in scheme 2

Table S1.5

Rate coefficients involved in the thermal decomposition of fragment 5, for temperatures ranging from 500 to 1200K.

Main reactions of fragment 5				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS13}	7.01 10^{10}	0.700	155.52	1.5 10^{2}
k_{TS14}	3.64 10^{12}	-0.362	140.42	5.5 10^{1}
k_{TS15}	5.93 10^{13}	-0.332	241.17	1.1 10^{-4}
k_{TS16}	9.63 10^{12}	0.832	282.09	7.4 10^{-5}

Table S1.6

Rate coefficients involved in the thermal decomposition of fragment 10, for temperatures ranging from 500 to 1200K. Only the lowest energy pathways have been considered.

Main reactions of fragment 10				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS18}	1.08 10^{10}	0.811	157.23	2.6 10^{1}
k_{TS20}	1.54 10^{6}	1.644	234.60	3.8 10^{-6}
k_{TS21}	7.21 10^{7}	1.406	210.12	1.8 10^{-3}
k_{TS23}	1.37 10^{0}	3.706	198.41	9.4 10^{-4}
k_{TS24}	7.06 10^{9}	1.029	194.35	1.9 10^{-1}
k_{TS27}	1.7 10^{11}	0.257	213.59	1.2 10^{-3}

Table S1.7

Rate coefficients involved in the thermal decomposition of fragment 11, for temperatures ranging from 500 to 1200K. Only the two lowest energy pathways have been considered.

Main reactions of fragment 11				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS30}	1.72 10^{4}	1.929	146.52	3.8 10^{-1}
k_{TS31}	5.09 10^{14}	-0.745	182.13	7.6 10^{-1}

Table S1.8

Rate coefficients involved in the thermal decomposition of fragment 18, for temperatures ranging from 500 to 1200K. Only the lowest energy pathways have been considered.

Main reactions of fragment 18				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS33}	$1.89\ 10^{14}$	-0.255	177.86	$1.4\ 10^{1}$
k_{T34}	$3.49\ 10^{10}$	0.438	138.28	$1.5\ 10^{2}$
k_{TS36}	$1.87\ 10^{8}$	0.295	129.75	$1.2\ 10^{0}$
k_{TS37}	$2.24\ 10^{18}$	-1.593	199.41	$7.6\ 10^{-1}$
k_{TS39}	$5.9\ 10^{13}$	-0.140	178.53	$8.6\ 10^{0}$
k_{TS40}	$5.32\ 10^{18}$	-0.915	288.32	$1.0\ 10^{-4}$
k_{TS41}	$1.44\ 10^{13}$	0.556	274.81	$4.1\ 10^{-5}$
k_{TS42}	$1.51\ 10^{9}$	1.409	200.04	$2.0\ 10^{-1}$

Table S1.9

Rate coefficients involved in the thermal decomposition of fragment 15, for temperatures ranging from 500 to 1200K. Only the lowest energy pathways have been considered.

Main reactions of fragment 15				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS46}	$1.27\ 10^{10}$	0.780	205.73	$1.0\ 10^{-2}$
k_{TS50}	$1.10\ 10^{12}$	0.200	187.99	$3.3\ 10^{-1}$
k_{TS51}	$4.17\ 10^{7}$	1.595	172.55	$1.5\ 10^{0}$
k_{TS54}	$2.96\ 10^{6}$	1.961	165.77	$3.7\ 10^{0}$
k_{TS55}	$3.21\ 10^{5}$	1.964	194.10	$4.3\ 10^{-3}$
k_{TS56}	$1.96\ 10^{9}$	0.622	168.41	$2.2\ 10^{-1}$
k_{TS57}	$3.32\ 10^{0}$	2.829	122.93	$1.2\ 10^{0}$
k_{TS58}	$8.38\ 10^{11}$	0.703	156.48	$1.1\ 10^{3}$
k_{TS61}	$6.65\ 10^{12}$	0.270	175.14	$2.5\ 10^{1}$
k_{TS64}	$6.97\ 10^{11}$	0.575	122.63	$9.0\ 10^{4}$
k_{TS25}	$9.48\ 10^{12}$	0.245	194.05	$1.5\ 10^{0}$

Table S1.10

Rate coefficients involved in the thermal decomposition of fragment 34, for temperatures ranging from 500 to 1200K. Only the lowest energy pathways have been considered.

Main reactions of fragment 34				
	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})

k_{TS67}	2.11 10^{12}	0.230	198.78	1.4 10^{-1}
k_{T68}	3.06 10^{13}	0.005	187.28	2.9 10^{0}
k_{TS69}	4.15 10^{13}	-0.547	170.67	1.4 10^{0}
k_{TS70}	1.21 10^{14}	-0.351	152.05	3.1 10^{2}
k_{TS71}	1.08 10^{8}	1.169	168.62	4.5 10^{-1}
k_{TS72}	9.92 10^{8}	1.292	177.78	2.1 10^{0}
k_{TS73}	8.38 10^{5}	2.142	214.76	1.3 10^{-3}
k_{TS74}	2.21 10^{13}	-0.589	163.34	1.9 10^{0}
k_{TS75}	4.58 10^{17}	-1.377	210.04	1.2 10^{-1}

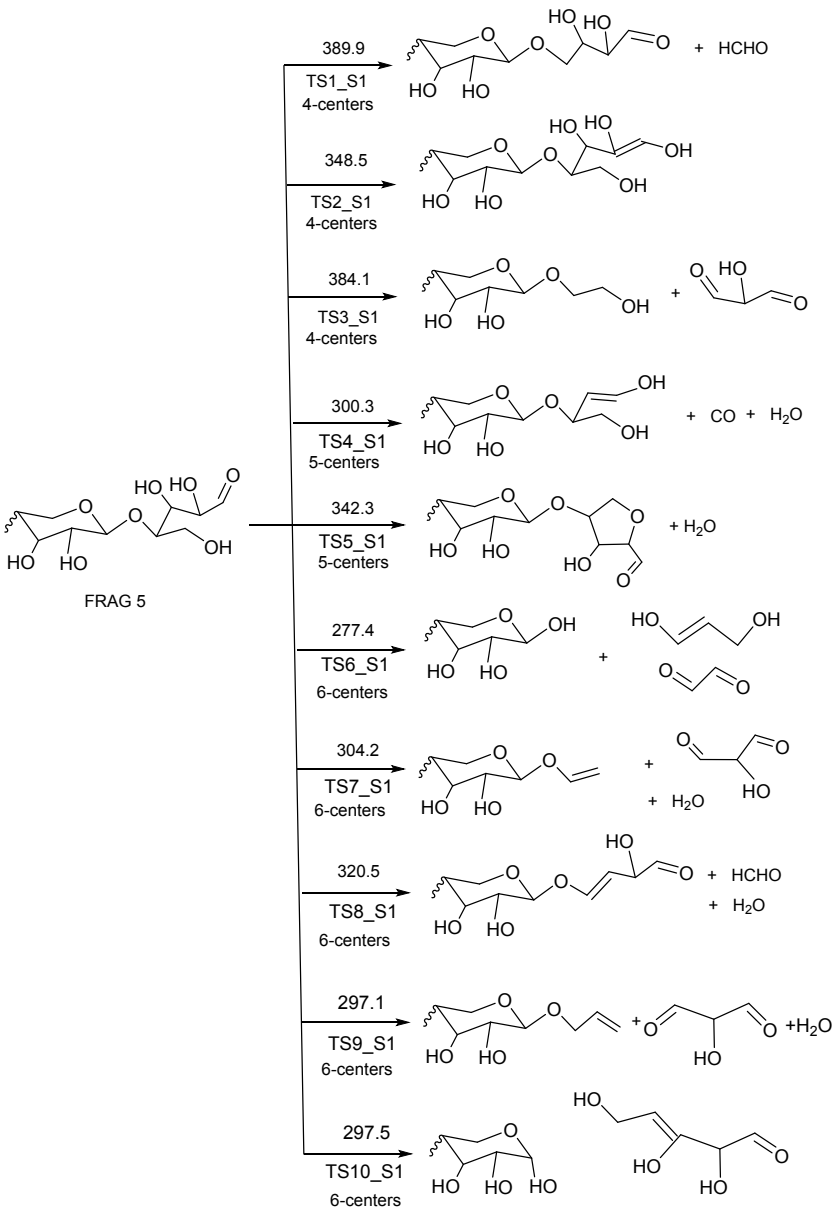
Table S1.11

Rate coefficients involved in the thermal decomposition of fragment 1, for temperatures ranging from 500 to 1200K. Only the lowest energy pathways have been considered.*taken from TS1

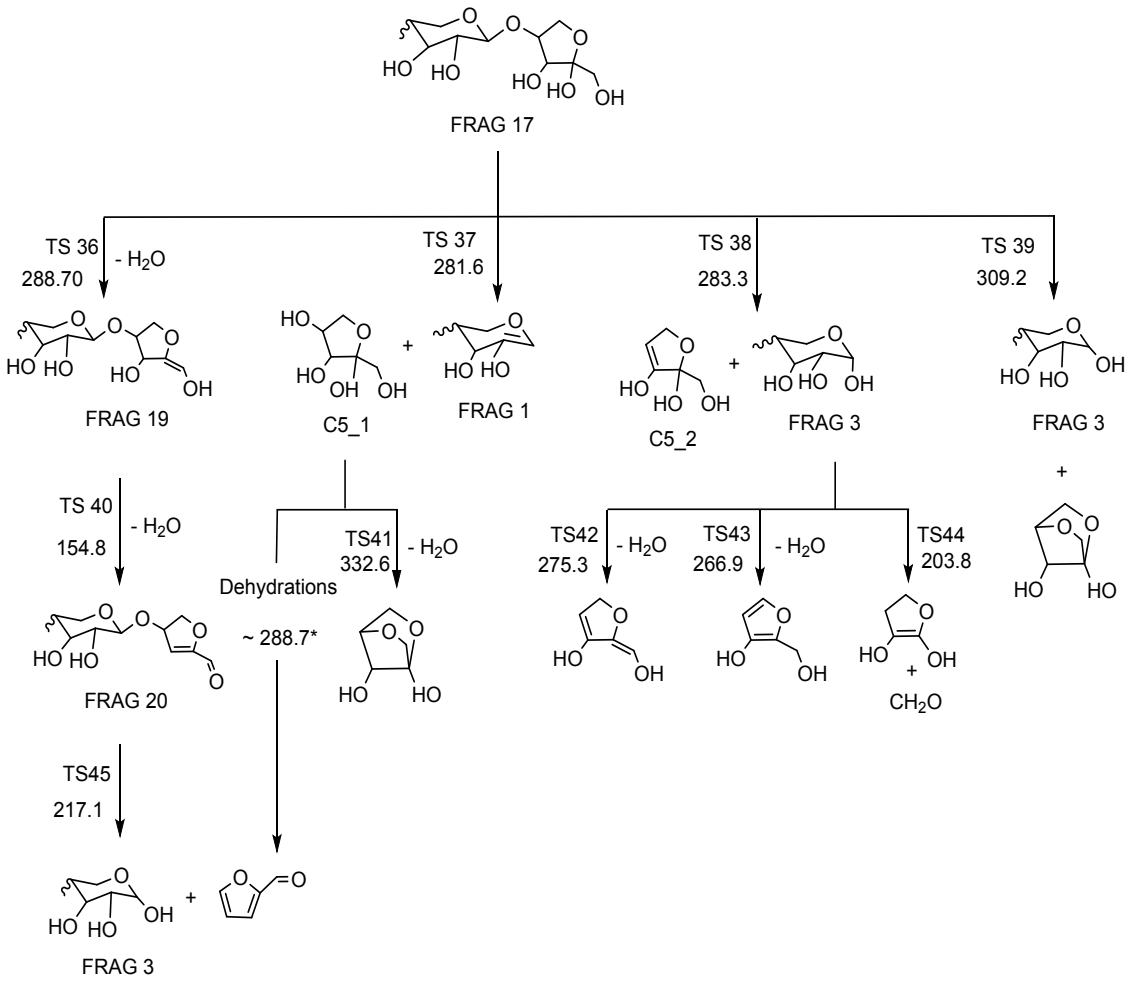
Main reactions of fragment 1

	A (s^{-1})	n	E (kJ mol^{-1})	$k_{\_750K}$ (s^{-1})
k_{TS76}*	2.50 10^{14}	0.328	291.58	1.1 10^{-5}
k_{T77}	1.97 10^{10}	1.204	285.56	7.4 10^{-7}
k_{TS78}	4.11 10^{12}	0.613	201.21	2.3 10^{0}
k_{TS81}	2.81 10^{10}	0.778	200.62	5.2 10^{-2}
k_{TS84}	2.13 10^{3}	2.838	227.53	4.4 10^{-5}
k_{TS85}	5.56 10^{14}	-0.395	169.95	5.9 10^{2}
k_{TS86}	6.89 10^{2}	2.932	226.35	3.2 10^{-5}

S2- Minor pathways involved in the thermal degradation of fragment 5 (Energy in kJ mol^{-1})



S3- Pathways investigated in the thermal degradation of fragment 17 (Energy in kJ mol^{-1})



S3-Cartesian coordinates of reactants and TS for lower energy paths

Scheme 2

Reactant for TS1, TS2 and TS3

Z_{at}	X	Y	Z
6	3.845038	-0.897990	0.132338
6	3.644581	0.581669	-0.190079
6	2.643168	-1.691372	-0.376230
1	3.943405	-1.024790	1.214354
6	2.298607	1.085091	0.335551
1	3.650384	0.727534	-1.279965
1	2.583846	-1.653764	-1.473888
1	2.696924	-2.738313	-0.077189
6	1.158609	0.187552	-0.153053
1	2.306820	1.045073	1.432823
1	1.061072	0.265581	-1.248259
8	1.432935	-1.182152	0.191022
8	-0.010282	0.562472	0.476812
6	-1.260865	0.283130	-0.179553
6	-1.905238	-1.002659	0.352126
6	-2.160783	1.495402	0.092369
1	-1.093450	0.180337	-1.258711
6	-3.343414	-1.105729	-0.156920
1	-1.911634	-0.928569	1.451097
1	-2.210470	1.667847	1.177971
1	-1.739905	2.385708	-0.374987
6	-4.117577	0.179854	0.120335
1	-3.322368	-1.298122	-1.234343
1	-4.241965	0.332935	1.203826
8	-3.459890	1.311812	-0.446074
8	2.040945	2.402098	-0.122431
1	2.809589	2.935671	0.111623
8	-1.212974	-2.174529	-0.051182
1	-0.273382	-2.058861	0.164116
1	-5.109454	0.149198	-0.332818
1	4.763579	-1.271551	-0.334000
1	-3.834297	-1.960171	0.318832
8	4.632674	1.430839	0.406402
1	5.471294	1.317634	-0.051747

TS1

Z_{at}	X	Y	Z
6	2.745834	-1.094933	1.180102
6	3.027888	0.408376	1.290325
6	3.111505	-1.615348	-0.198574
1	1.686938	-1.267932	1.386269
6	2.268924	1.110204	0.177602
1	4.102616	0.612749	1.186337
1	4.189821	-1.604059	-0.375967
1	2.737022	-2.621949	-0.375122
6	2.224589	0.427492	-1.086742
1	1.079271	0.949745	0.340356
1	1.942294	0.965453	-1.982463
8	2.534335	-0.816898	-1.288313
8	-0.054860	0.463020	-0.449507
6	-1.431736	0.262438	-0.526517
6	-1.843078	-1.040632	0.170760
6	-2.229771	1.429110	0.080865
1	-1.733576	0.177049	-1.585569
6	-3.354352	-1.226662	0.119646
1	-1.523466	-0.963028	1.223629
1	-1.923202	1.572449	1.129821
1	-2.028020	2.350921	-0.466794
6	-4.039024	0.020306	0.684382
1	-3.663919	-1.382924	-0.918654
1	-3.817530	0.121256	1.759381
8	-3.635936	1.206072	0.003736
8	2.568859	2.481736	0.018161
1	2.011764	2.976873	0.627705
8	-1.182375	-2.155540	-0.431722
1	-0.322440	-1.808757	-0.705524
1	-5.122839	-0.038005	0.569300
1	3.326500	-1.653487	1.921209
1	-3.652759	-2.111956	0.691787
8	2.553641	0.953357	2.519870
1	3.208076	0.803866	3.208978

TS2

Z_{at}	X	Y	Z
6	-3.909127	0.652272	0.285295

6	-3.803107	-0.836387	0.607604
6	-2.953805	0.991074	-0.858506
1	-3.646727	1.234954	1.173459
6	-2.353868	-1.250728	0.868393
1	-4.168701	-1.428244	-0.243858
1	-3.267740	0.484834	-1.784230
1	-2.936881	2.064682	-1.056102
6	-1.431011	-0.849056	-0.303417
1	-1.989432	-0.727497	1.763543
1	-1.782080	-1.349737	-1.225510
8	-1.619558	0.613162	-0.532363
8	-0.139498	-1.076205	-0.062561
6	1.627697	-0.014429	-1.004975
6	1.536585	0.872419	0.098263
6	2.646947	-1.114639	-0.985605
1	1.000827	0.118199	-1.876862
6	2.760820	1.040948	0.984063
1	0.797230	-0.002004	0.538357
1	2.196733	-2.008012	-0.531315
1	2.936653	-1.365588	-2.008317
6	3.574242	-0.254464	1.012645
1	3.366171	1.864237	0.591369
1	3.045977	-1.029182	1.586432
8	3.833399	-0.729957	-0.308249
8	0.764894	2.028097	-0.029026
1	-0.148330	1.739729	-0.233431
1	4.550608	-0.092743	1.470347
1	-4.936674	0.912890	0.005416
1	2.447501	1.314877	1.994751
8	-2.265643	-2.656681	1.037326
1	-2.938339	-2.897301	1.685541
8	-4.535675	-1.207723	1.786585
1	-5.478864	-1.171884	1.599433

TS3

Z_{at}	X	Y	Z
6	3.805210	-0.720785	-0.348399
6	2.921878	-1.959367	-0.309296
6	1.101954	-0.599145	0.119802
6	1.669595	0.714458	0.394079
6	2.964790	0.497264	-0.689146
1	2.553773	-2.234134	-1.305339
1	3.402403	-2.822045	0.146172
1	4.290852	-0.564811	0.617456
1	0.496881	-0.723279	-0.781700
1	2.198908	0.690195	1.370048
1	2.515417	0.418202	-1.688870
8	1.763398	-1.674609	0.553066
8	-0.571087	-0.705486	1.346956
8	1.047270	1.825590	0.062359
1	-0.352829	0.040495	1.928195
6	-1.897691	-0.408929	0.833167
6	-1.912697	0.915904	0.069317
6	-2.378457	-1.558795	-0.044965
1	-2.559051	-0.320844	1.702174
6	-3.335112	1.144489	-0.438942
1	-1.239877	0.822549	-0.795131
1	-1.696557	-1.692317	-0.900964
1	-2.412813	-2.494332	0.514744
6	-3.793002	-0.073162	-1.246048
1	-4.004042	1.304905	0.412256
1	-3.190862	-0.167596	-2.163546
8	-3.696785	-1.288055	-0.491672
8	-1.450727	1.955652	0.901186
1	-0.496830	2.095275	0.649077
1	-4.840998	0.009036	-1.536078
1	-3.363157	2.044841	-1.058882
8	3.685772	1.681329	-0.563136
1	3.008455	2.382530	-0.515521
1	4.588788	-0.855622	-1.101571

Reactant for TS4

Z_{at}	X	Y	Z
6	-3.427028	-1.043885	-0.192657
6	-3.362413	0.442907	0.153408
6	-2.174413	-1.737537	0.337312
1	-3.487346	-1.163369	-1.278263
6	-2.051137	1.068368	-0.328660
1	-3.409559	0.571751	1.244404
1	-2.143728	-1.707096	1.436299
1	-2.130092	-2.781550	0.026840
6	-0.849858	0.263992	0.174564
1	-2.028737	1.047154	-1.426251
1	-0.782283	0.331037	1.272620
8	-0.998703	-1.118766	-0.195284
8	0.295713	0.749312	-0.423535
6	1.552736	0.548697	0.247039
6	2.286022	-0.683044	-0.292123
6	2.384035	1.811981	-0.007625
1	1.377623	0.429055	1.322941
6	3.721661	-0.716565	0.230037
1	2.318146	-0.603019	-1.388975
1	2.428350	2.001140	-1.090013
1	1.917545	2.672237	0.472056
6	4.419965	0.612519	-0.046928
1	3.686750	-0.877746	1.316600
1	4.527187	0.757933	-1.131526
8	3.689685	1.687261	0.535723
8	-1.918127	2.393831	0.156112
1	-2.718674	2.867683	-0.098578
8	1.684818	-1.915013	0.088104
1	0.742688	-1.880720	-0.146765
1	5.412487	0.623537	0.403443
8	-4.402746	1.213216	-0.459870
1	-5.241093	1.021893	-0.027932
8	4.470671	-1.751537	-0.393627
1	3.946342	-2.558548	-0.326105
1	-4.320796	-1.501964	0.245579

TS4

Z_{at}	X	Y	Z
6	0.986156	-1.066957	0.212642
6	1.464625	1.548988	-0.112509
6	2.853060	1.199829	-0.638946
6	3.334835	-0.131115	-0.057634
6	2.389375	-1.303343	-0.350694

1	1.002699	-0.762456	1.273851
1	2.827173	1.130116	-1.730286
1	3.425887	-0.046210	1.034850
1	1.488427	1.683731	0.978791
8	0.579850	0.486661	-0.464274
8	2.876574	-2.486409	0.267210
1	3.807968	-2.557457	0.024154
8	-1.379590	0.576000	2.175184
1	2.298969	-1.438609	-1.435701
6	-3.223272	0.450195	-1.121792
6	-2.558156	-1.728595	-0.538169
6	-1.736682	-1.179150	0.608826
6	-1.678701	0.206912	0.830511
6	-2.735297	1.079109	0.186691
1	-2.420591	0.480119	-1.871592
1	-1.524723	-1.836509	1.442059
1	-0.527127	0.470169	0.086782
1	-1.907607	-1.884375	-1.405071
8	-3.652319	-0.879888	-0.880106
8	0.040080	-1.826578	-0.174940
1	-1.130145	1.506265	2.164524
8	-2.152796	2.380447	-0.025617
1	-2.859239	3.026320	-0.128702
1	-3.579776	1.176389	0.882470
1	-2.991810	-2.689295	-0.258790
1	1.082769	2.470391	-0.559285
1	-4.086784	0.993441	-1.512393
1	3.559003	1.996032	-0.374191
8	4.601346	-0.530515	-0.605407
1	5.293004	0.042776	-0.260775

Reactant for TS5

Z_{at}	X	Y	Z
6	3.830582	-0.931938	0.075086
6	3.674388	0.580922	-0.131225
6	2.608469	-1.667652	-0.466745
1	3.933686	-1.155497	1.142248
6	2.321690	1.069371	0.410388
1	3.743419	0.810453	-1.202161
1	2.548004	-1.566230	-1.560819
1	2.631519	-2.731468	-0.226836
6	1.181364	0.233013	-0.153668
1	2.285827	0.980212	1.500549
1	1.113612	0.345867	-1.250326
8	1.404480	-1.160404	0.124555
8	-0.009498	0.614576	0.448374
6	-1.247654	0.265593	-0.201529
6	-1.889231	-0.981912	0.420347
6	-2.161904	1.487264	-0.031889
1	-1.064867	0.081054	-1.267518
6	-3.328989	-1.126629	-0.077061
1	-1.894127	-0.827293	1.511247
1	-2.213965	1.745323	1.036742
1	-1.747764	2.342112	-0.568111
6	-4.111202	0.170551	0.099588
1	-3.306860	-1.401439	-1.136412
1	-4.236642	0.409101	1.167315
8	-3.458593	1.257872	-0.555224
8	-1.202118	-2.179963	0.101194
1	-0.251187	-2.029321	0.234275
1	-5.102773	0.099806	-0.349737
1	4.731148	-1.302752	-0.425122
1	4.490064	1.122849	0.354952
1	-3.814405	-1.945262	0.462818
1	2.150666	2.118940	0.156667

TS5

Z_{at}	X	Y	Z
6	3.308466	-1.550363	0.498364
6	3.717271	-0.109925	0.165116
6	2.090228	-1.956295	-0.330464
1	3.055370	-1.629929	1.561660
6	2.509909	0.833023	0.270179
1	4.118664	-0.075504	-0.856007
1	2.362820	-1.998977	-1.398619
1	1.721271	-2.943716	-0.042305
6	1.318668	0.315543	-0.550155
1	2.176113	0.916330	1.310185
1	1.613556	0.256470	-1.618864
8	1.003482	-1.054090	-0.144985
8	0.210218	1.075662	-0.396107
6	-1.996167	0.949289	-0.615452
6	-2.277346	-0.515454	-0.833047
6	-2.016427	1.535466	0.673268
1	-1.870195	1.582750	-1.482355
6	-3.104951	-1.057897	0.333721
1	-1.316055	-1.037756	-0.863877
1	-0.777495	1.485005	0.632294
1	-2.272129	2.590404	0.746592
6	-2.496105	-0.587545	1.652504
1	-4.134490	-0.697207	0.247887
1	-1.458070	-0.930673	1.744897
8	-2.540459	0.838930	1.771669
8	-3.007606	-0.703202	-2.048282
1	-2.385930	-0.753861	-2.781664
1	-3.064118	-0.964007	2.503535
1	4.133109	-2.245622	0.305929
1	4.521529	0.227170	0.826400
1	-3.126780	-2.149163	0.290384
1	2.760949	1.838399	-0.079305

Reactant for TS6

Z_{at}	X	Y	Z
6	3.605040	1.411063	-0.083356
6	3.643320	-0.078180	0.232987
6	2.298377	1.996954	0.459000
1	3.650193	1.548757	-1.169976
6	2.394174	-0.794950	-0.279763
1	3.684918	-0.190762	1.326644
1	2.283356	1.921742	1.554885
1	2.186625	3.047409	0.185181
6	1.128980	-0.093517	0.219593
1	2.383144	-0.761325	-1.377054
1	1.047677	-0.189059	1.313792
8	1.187379	1.309731	-0.117453
8	0.033385	-0.640391	-0.413513

6	-1.246989	-0.553720	0.238401
6	-2.060112	0.636160	-0.279989
6	-1.977935	-1.866667	-0.068132
1	-1.099374	-0.453279	1.320241
6	-3.503396	0.548086	0.215579
1	-2.067747	0.586226	-1.379009
1	-1.989995	-2.025975	-1.156132
1	-1.457157	-2.704178	0.395667
6	-4.095565	-0.819774	-0.113083
1	-3.499116	0.678919	1.306706
1	-4.171837	-0.940385	-1.203322
8	-3.297703	-1.853847	0.453783
8	2.359989	-2.133497	0.184645
1	3.207699	-2.535497	-0.039828
8	-1.557664	1.897252	0.145882
1	-0.614260	1.942003	-0.079816
1	-5.092416	-0.917160	0.316690
8	4.762219	-0.730950	-0.357391
1	5.561157	-0.309288	-0.020392
8	-4.316585	1.542629	-0.393121
1	-3.860279	2.385787	-0.285651
8	4.751449	1.992151	0.544292
1	4.956153	2.834765	0.127442

TS6

Z_{at}	X	Y	Z
6	-3.813491	-0.138399	-1.178242
6	-3.357708	1.118145	-0.419824
6	-3.559491	-1.423235	-0.376023
1	-3.251888	-0.175224	-2.119103
6	-1.918558	0.916387	0.051787
1	-4.007549	1.255881	0.457638
1	-4.231035	-1.452147	0.492363
1	-3.741172	-2.310766	-0.982712
6	-1.871089	-0.403128	0.837937
1	-1.281139	0.821135	-0.834954
1	-2.535660	-0.340633	1.714368
8	-2.193467	-1.511422	0.052635
8	-0.551102	-0.637408	1.358425
6	1.033543	-0.585701	0.087732
6	1.645984	0.706809	0.346023
6	1.802540	-1.810899	0.497109
1	0.406931	-0.684535	-0.792410
6	2.942797	0.493655	-0.703016
1	2.165318	0.685146	1.330340
1	2.168559	-1.730765	1.527634
1	1.213478	-2.719213	0.388167
6	3.745000	-0.752878	-0.365586
1	2.516082	0.425364	-1.710477
1	4.207303	-0.651362	0.624648
8	2.898287	-1.903478	-0.421176
8	-1.435731	1.940036	0.882249
1	-0.494748	2.110299	0.581316
8	1.055403	1.849403	0.035006
1	-0.352431	0.178569	1.852744
1	4.527615	-0.925007	-1.105976
8	3.688355	1.656935	-0.545739
1	3.021566	2.369790	-0.500399
8	-3.418477	2.254701	-1.259515
1	-4.341055	2.380985	-1.508398
8	-5.211401	0.016849	-1.442146
1	-5.445263	-0.463403	-2.241989

Scheme 6

Reactant for TS7 and TS8

Z_{at}	X	Y	Z
6	2.758630	-1.330549	-0.419700
6	4.103911	-0.808232	0.107109
6	4.216539	0.707755	-0.101187
6	2.984974	1.410978	0.461331
6	1.603133	-0.528389	0.161609
1	4.191428	-1.035855	1.177100
1	2.707376	-1.238866	-1.508995
1	2.944314	1.306574	1.555890
1	2.976896	2.475210	0.222392
1	1.549330	-0.648173	1.257964
1	4.296279	0.933871	-1.169826
8	1.783132	0.874072	-0.111536
8	0.416562	-0.941151	-0.429873
6	-0.821013	-0.648344	0.243940
6	-1.482450	0.623103	-0.299599
6	-1.731658	-1.858986	-0.001436
1	-0.634297	-0.532211	1.318735
6	-2.916373	0.739061	0.218628
1	-1.516085	0.539666	-1.396538
1	-1.783523	-2.052507	-1.082913
1	-1.320347	-2.743906	0.485362
6	-3.692829	-0.545163	-0.055613
1	-2.873608	0.900737	1.304854
1	-3.803734	-0.690718	-1.139783
8	-3.028699	-1.658105	0.536255
8	-0.820411	1.821822	0.078116
1	0.129866	1.717116	-0.103359
8	-3.600604	1.815781	-0.408669
1	-3.026690	2.588795	-0.344269
1	-4.685792	-0.495214	0.390987
1	5.114590	1.103027	0.384438
1	4.927643	-1.328510	-0.388830
1	2.618047	-2.384941	-0.167595

TS7

Z_{at}	X	Y	Z
6	2.701981	-1.308166	-0.597045
6	4.078279	-0.842877	-0.101007
6	4.197496	0.682831	-0.201240
6	3.007252	1.346562	0.484262
6	1.579367	-0.551615	0.099327
1	4.215843	-1.149809	0.943539
1	2.599879	-1.131607	-1.672358
1	3.030172	1.147657	1.566759
1	3.008743	2.428636	0.339678
1	1.564283	-0.753781	1.183424
1	4.217747	0.988669	-1.252813
8	1.764783	0.880289	-0.061226

8	0.370612	-0.906481	-0.475525
6	-0.828640	-0.570428	0.250572
6	-1.481603	0.609563	-0.274382
6	-1.681494	-1.828020	0.393120
1	-0.586973	0.606719	1.247025
6	-2.970514	0.755890	-0.040435
1	-1.118220	1.059226	-1.196190
1	-1.603840	-2.422556	-0.532914
1	-1.343507	-2.453528	1.221031
6	-3.615167	-0.618886	-0.252215
1	-3.149897	1.043566	0.999908
1	-3.478579	-0.951709	-1.291287
8	-3.050612	-1.536454	0.665815
8	-0.750635	1.717582	0.910385
1	0.134090	1.887546	0.528651
8	-3.573088	1.685678	-0.932676
1	-3.313402	2.575108	-0.669688
1	-4.683465	-0.563490	-0.041828
1	5.125759	1.035352	0.260370
1	4.869985	-1.331687	-0.675396
1	2.559786	-2.378117	-0.422913

TS8

Z_{at}	X	Y	Z
6	2.842873	-1.350580	-0.276075
6	4.154347	-0.658627	0.128277
6	4.153176	0.810461	-0.317743
6	2.873706	1.502378	0.147692
6	1.648243	-0.531216	0.192666
1	4.270828	-0.706849	1.218493
1	2.773563	-1.441834	-1.364572
1	2.852640	1.573996	1.246351
1	2.785129	2.511627	-0.256341
1	1.613441	-0.484775	1.296641
1	4.209643	0.869066	-1.410038
8	1.713596	0.799747	-0.306783
8	0.475535	-1.122220	-0.291340
6	-0.746713	-0.745738	0.336882
6	-1.334088	0.498883	-0.274790
6	-1.721410	-1.921504	0.131714
1	-0.599444	-0.578859	1.409043
6	-2.737913	0.678332	-0.307166
1	-0.659706	1.157791	-0.804107
1	-1.726798	-2.204973	-0.929683
1	-1.399676	-2.780152	0.720457
6	-3.625645	-0.562615	-0.210584
1	-2.621247	1.242536	0.801722
1	-3.832465	-0.931012	-1.226212
8	-3.017860	-1.572737	0.577773
8	-1.509868	1.919804	1.353415
1	-1.134307	2.447512	2.075290
8	-3.266033	1.612594	-1.227359
1	-3.072340	2.494717	-0.890093
1	-4.574602	-0.319130	0.265779
1	5.023593	1.339927	0.083475
1	5.007632	-1.192491	-0.298670
1	2.778874	-2.356059	0.148687

Reactant for TS9 and TS10

Z_{at}	X	Y	Z
6	1.056141	1.505941	-0.192003
6	1.253245	0.054223	0.240726
6	-0.310443	1.991420	0.290959
1	1.108244	1.570958	-1.282759
6	0.080597	-0.823065	-0.203251
1	1.309683	-0.000573	1.337549
1	-0.343738	2.020881	1.391322
1	-0.533596	2.992320	-0.079292
6	-1.246860	-0.202202	0.237723
1	0.070398	-0.876874	-1.300114
1	-1.314106	-0.221181	1.339320
8	-1.347184	1.149353	-0.206315
8	-2.286369	-0.917300	-0.344685
8	2.423761	-0.551981	-0.322959
1	3.207185	-0.184228	0.097533
8	0.180112	-2.117473	0.367745
1	1.051098	-2.458946	0.133999
1	-3.118365	-0.519753	-0.064559
1	1.848644	2.140590	0.220933

TS9

Z_{at}	X	Y	Z
6	0.761937	1.643476	0.066848
6	1.158492	0.201149	-0.208691
6	-0.623600	1.708849	0.709684
1	0.763170	2.184580	-0.885038
6	0.134099	-0.742381	-0.448209
1	1.358692	-0.461089	0.859623
1	-0.583106	1.372985	1.755356
1	-1.016300	2.725353	0.691079
6	-1.261686	-0.474392	0.071864
1	0.259652	-1.583494	-1.116214
1	-1.332731	-0.790517	1.121690
8	-1.565030	0.912235	-0.015522
8	-2.149314	-1.173233	-0.745651
8	2.336419	0.117640	-0.980966
1	2.760936	-0.726292	-0.786907
8	1.042623	-1.783010	1.160587
1	1.094533	-2.541643	1.764735
1	-3.045651	-0.924714	-0.491518
1	1.501513	2.118991	0.716187

TS10

Z_{at}	X	Y	Z
6	1.042440	1.594768	-0.279831
6	1.324087	0.154425	0.150492
6	-0.267491	2.080951	0.331452
1	0.972860	1.632279	-1.370979
6	0.062803	-0.676868	0.045757
1	1.658941	0.137922	1.189974
1	-0.233023	2.039938	1.428034
1	-0.486196	3.105208	0.030245
6	-1.228262	-0.080001	0.046269
1	0.150558	-1.725937	-0.197559
1	-1.241360	-0.394231	1.273202
8	-1.371760	1.304745	-0.146405
8	-2.221239	-0.766649	-0.634521

8	2.326255	-0.379758	-0.715705
1	2.720686	-1.154088	-0.300057
8	-0.349032	-1.114959	2.085906
1	-0.203662	-1.689408	2.855390
1	-3.071727	-0.524275	-0.251555
1	1.872075	2.236572	0.025461

Scheme 8

FRAG3 for TS11

Z_{at}	X	Y	Z
6	1.761197	0.218398	-0.187935
1	1.675576	0.330076	-1.281018
6	2.971702	1.000371	0.327915
1	2.966160	0.936228	1.424098
6	3.077647	-1.778326	-0.449366
1	3.031085	-1.705417	-1.545682
8	2.833428	2.343362	-0.103070
8	-4.797668	0.609183	-0.322518
8	1.910344	-1.178422	0.123567
6	-3.495878	0.550371	0.183684
1	-3.502355	0.680589	1.280638
6	-2.802068	-0.764243	-0.175616
1	-2.810031	-0.855761	-1.269907
6	-1.357577	-0.756637	0.313800
1	-1.356171	-0.715831	1.413020
6	-0.640586	0.496090	-0.203574
1	-0.487877	0.407275	-1.285718
6	-1.476170	1.746961	0.102873
1	-1.490428	1.914280	1.189096
8	-3.556125	-1.820659	0.411097
8	-0.772584	-1.974703	-0.127640
8	0.626143	0.682942	0.447644
8	-2.795418	1.621545	-0.410390
6	4.273942	0.391435	-0.197903
1	4.305293	0.562742	-1.283578
6	4.338857	-1.107924	0.089298
1	4.414208	-1.269410	1.168467
1	0.176672	-1.948280	0.079831
1	-3.067569	-2.640360	0.270311
1	-5.197432	-0.256965	-0.173336
1	3.638163	2.806876	0.157478
1	-1.034690	2.621612	-0.372676
1	5.225104	-1.550566	-0.378765
1	3.035133	-2.833414	-0.178699
8	5.324945	1.134302	0.430020
1	6.155509	0.963750	-0.025078

TS11

Z_{at}	X	Y	Z
8	0.579563	-0.615038	-0.584673
8	2.646290	-2.348018	0.244794
8	1.924937	1.188794	-0.248120
6	1.683609	-0.175003	0.126320
6	2.891789	-1.039263	-0.241684
6	4.172552	-0.461177	0.364481
6	4.335663	1.014280	0.000980
6	3.068200	1.772773	0.387398
8	-4.376663	-0.833313	1.012992
8	-3.464346	2.085717	-0.189500
8	-0.754629	1.939630	-0.074638
8	-2.871277	-1.680426	-0.300343
6	-3.808499	-0.233746	0.005025
6	-2.816796	0.903005	0.259594
6	-1.454561	0.754227	-0.431171
6	-0.723499	-0.518633	0.013065
6	-1.456819	-1.771102	-0.478647
1	3.448113	-2.861580	0.090526
1	1.499824	-0.226203	1.211108
1	2.982912	-1.036899	-1.335891
1	4.101060	-0.568344	1.456608
1	4.511259	1.107066	-1.074622
1	2.925389	1.773052	1.477567
1	-3.530501	-1.742783	0.695345
1	-2.813169	2.796439	-0.128769
1	0.177744	1.866238	-0.340166
1	-4.362329	-0.123249	-0.934701
1	-2.648611	0.946865	1.343335
1	-1.599285	0.714826	-1.520801
1	-0.621252	-0.516603	1.105114
1	-1.249653	-1.891652	-1.545287
1	-1.095070	-2.659571	0.042298
1	3.099658	2.808658	0.050161
1	5.199433	1.444154	0.519989
8	5.234668	-1.287072	-0.124847
1	6.031898	-1.124708	0.389197

FRAG3 for TS12

Z_{at}	X	Y	Z
6	1.742810	0.253671	-0.161289
1	1.703041	0.422325	-1.250194
6	2.959924	0.962455	0.439773
1	2.919264	0.801308	1.525787
6	2.975366	-1.763344	-0.520449
1	2.920023	-1.633283	-1.610682
8	2.933962	2.350162	0.136626
8	-4.822814	0.782829	-0.335691
8	1.822213	-1.155187	0.087693
6	-3.523466	0.693833	0.169303
1	-3.526486	0.815750	1.267119
6	-2.852308	-0.627464	-0.203732
1	-2.858686	-0.705344	-1.299084
6	-1.407499	-0.655715	0.288239
1	-1.407528	-0.627791	1.388132
6	-0.664041	0.589947	-0.211595
1	-0.499525	0.507866	-1.292416
6	-1.483040	1.851529	0.099270
1	-1.496490	2.011466	1.187203
8	-3.626230	-1.676632	0.368176
8	-0.853009	-1.880092	-0.168421
8	0.601310	0.757644	0.454372
8	-2.801276	1.757416	-0.416204
6	4.246141	0.370218	-0.129765
1	4.307944	0.640503	-1.190459
6	4.259778	-1.155467	0.034034
1	4.350091	-1.421323	1.092367

1	0.100582	-1.874661	0.024791
1	-3.154705	-2.504128	0.214515
1	-5.235430	-0.080787	-0.207824
1	2.128299	2.718192	0.516980
1	2.897228	-2.828172	-0.298863
1	-1.028154	2.723057	-0.371516
1	5.121133	-1.588884	-0.483479
1	5.104092	0.830676	0.365629

TS12

Z_{at}	X	Y	Z
6	-3.621452	-0.617604	-0.311720
6	-2.763936	0.474872	0.222490
6	-1.349916	0.644843	-0.210837
6	-0.565930	-0.583054	0.361831
6	-1.442935	-1.837710	0.273728
8	-4.862400	-0.483884	-0.129365
8	-3.779896	1.857526	-0.604973
8	-0.860628	1.880081	0.270743
8	0.655654	-0.782981	-0.353672
8	-2.712848	-1.534862	0.800106
1	-3.256853	-1.090799	-1.242257
1	-3.024097	0.794021	1.223539
1	-1.287433	0.594715	-1.305450
1	-0.347554	-0.364878	1.413698
1	-1.495040	-2.177727	-0.772520
1	-4.591355	1.285219	-0.468992
1	-3.838493	2.635606	-0.035762
1	0.102714	1.883232	0.128499
8	3.058677	-2.298306	-0.241797
8	1.830663	1.162662	-0.014988
6	1.822595	-0.254748	0.193674
6	3.013512	-0.905414	-0.514460
6	4.318006	-0.278070	-0.030726
6	4.264595	1.250461	-0.155853
6	3.009130	1.796806	0.516028
1	2.239398	-2.689869	-0.565757
1	1.867278	-0.455606	1.277087
1	2.883841	-0.723360	-1.590163
1	4.472053	-0.569744	1.014686
1	4.259711	1.544331	-1.210588
1	3.045967	1.636474	1.602859
1	2.876695	2.863294	0.331396
1	-1.002544	-2.643537	0.868602
1	5.148839	1.703690	0.302561
1	5.150320	-0.694623	-0.602589

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FRAG5

Z_{at}	X	Y	Z
8	0.319832	-0.574435	-0.645012
8	2.236737	-2.583973	-0.115842
8	1.761686	1.071872	-0.033501
6	1.424679	-0.308135	0.144089
6	2.580966	-1.210583	-0.303700
6	3.874110	-0.821418	0.416692
6	4.140534	0.686752	0.298524
6	2.907910	1.478859	0.725033
8	-4.175852	3.067064	0.119259
8	-3.287612	0.778015	1.173577
8	-0.981173	1.979420	-0.295307
8	-0.953614	-2.874516	0.143396
6	-3.648362	2.307642	-0.655099
6	-3.124384	0.951768	-0.212082
6	-1.662517	0.791393	-0.663354
6	-0.996792	-0.452322	-0.061910
6	-1.702296	-1.777698	-0.351605
1	2.387646	-2.825909	0.805304
1	1.198684	-0.483164	1.210184
1	2.690355	-1.081687	-1.383541
1	3.779597	-1.089415	1.479173
1	4.387396	0.943418	-0.736634
1	2.706182	1.340145	1.797489
1	-0.064934	-2.828716	-0.239586
1	-3.644864	1.610710	1.519883
1	-0.022071	1.839965	-0.359095
1	-3.535214	2.552045	-1.727513
1	-3.726232	0.200153	-0.749052
1	-1.660811	0.677613	-1.759105
1	-0.905951	-0.316185	1.019238
1	-2.667438	-1.803692	0.156536
1	-1.872403	-1.875298	-1.433729
1	3.024629	2.546496	0.536988
1	4.996339	0.973626	0.917435
1	4.705767	-1.405196	0.014134

TS13

Z_{at}	X	Y	Z
8	-0.160364	0.341517	0.011487
8	-2.442292	2.024953	0.035336
8	-1.446142	-1.517418	-0.212345
6	-1.429376	-0.174170	0.254041
6	-2.452903	0.693439	-0.492978
6	-3.844195	0.060505	-0.440978
6	-3.794186	-1.416261	-0.856598
6	-2.719607	-2.149072	-0.057637
8	4.394506	-0.973725	-0.476334
8	3.270709	1.467384	-0.927212
8	3.041965	-0.472303	1.411837
8	-0.038105	2.475778	1.866382
6	3.325397	-0.887782	-1.205936
6	2.665716	0.322405	-1.318176
6	1.937349	-0.585191	0.755889
6	0.792052	0.350428	1.080772
6	1.131143	1.802824	1.419214
1	-3.098039	2.088646	0.738919
1	-1.654879	-0.161515	1.334477
1	-2.108730	0.779290	-1.527140
1	-4.223535	0.130859	0.589372
1	-3.563495	-1.498179	-1.923558
1	-2.989944	-2.183283	1.009345
1	-0.666818	2.507176	1.129223
1	4.141855	1.222416	-0.572903
1	3.868789	-0.805529	0.705777

1	2.877657	-1.782051	-1.646469
1	1.751158	0.463048	-1.875437
1	1.611124	-1.571923	0.416585
1	0.319247	-0.087688	1.974380
1	1.854100	1.829135	2.235133
1	1.572040	2.297975	0.551759
1	-2.585118	-3.174097	-0.404912
1	-4.766844	-1.891770	-0.696245
1	-4.530379	0.630498	-1.073028

TS14

Z_{at}	X	Y	Z
8	-0.739282	0.736744	-0.542301
8	-3.359725	1.775201	-0.068007
8	-1.490971	-1.389933	-0.176051
6	-1.715654	-0.005212	0.111881
6	-3.086652	0.425535	-0.414836
6	-4.177162	-0.456464	0.188737
6	-3.858690	-1.942483	-0.026091
6	-2.445382	-2.260400	0.453429
8	4.718398	-0.506529	0.931869
8	3.682856	1.225924	-0.548860
8	1.217093	-1.363585	-0.875525
8	1.993555	2.574481	1.052400
6	3.569320	-0.850860	0.445077
6	3.005611	0.118253	-0.472591
6	1.522707	0.022406	-0.864686
6	0.576200	0.816393	0.059471
6	0.886179	2.315093	0.220789
1	-2.675139	2.325826	-0.465219
1	-1.662383	0.147058	1.202538
1	-3.062654	0.301323	-1.506273
1	-4.245236	-0.232259	1.259780
1	-3.938365	-2.196655	-1.088130
1	-2.369893	-2.149932	1.544680
1	2.788793	2.329980	0.537942
1	4.807982	0.442810	0.588049
1	0.255826	-1.489656	-0.790945
1	3.178201	-1.837070	0.655247
1	3.487625	-0.805027	-1.144712
1	1.426517	0.453404	-1.869316
1	0.558515	0.347386	1.050354
1	1.004191	2.769834	-0.772080
1	0.012078	2.769938	0.693571
1	-2.140281	-3.273488	0.189771
1	-4.576304	-2.569607	0.511915
1	-5.139943	-0.189296	-0.253050

TS15

Z_{at}	X	Y	Z
8	-0.510135	0.610985	-0.645330
8	-2.927867	1.976556	-0.082900
8	-1.412486	-1.388958	-0.052646
6	-1.500770	0.035873	0.130197
6	-2.861171	0.572308	-0.326395
6	-3.997384	-0.200918	0.346562
6	-3.810477	-1.716748	0.186513
6	-2.420391	-2.133269	0.653750
8	4.577214	-0.433682	1.548472
8	4.142766	-0.581288	-1.111587
8	1.166124	-1.610319	-1.001538
8	0.223608	2.978457	0.547551
6	3.407237	-0.390865	1.154122
6	3.062697	-0.570641	-0.222251
6	1.775268	-0.169521	-0.849114
6	0.808782	0.707364	-0.066935
6	1.192178	2.191019	-0.121507
1	-3.238701	2.128465	0.816918
1	-1.347740	0.258941	1.199396
1	-2.908145	0.454712	-1.412188
1	-4.010188	0.050451	1.417146
1	-3.934752	-2.002169	-0.862754
1	-2.302627	-1.968457	1.733993
1	-0.620375	2.866166	0.087570
1	4.929790	-0.568049	-0.541173
1	0.245682	-1.703260	-0.644405
1	2.577706	-0.281450	1.878963
1	2.104519	-1.838322	-0.334997
1	1.898462	0.173105	-1.873963
1	0.754374	0.391533	0.978317
1	2.145315	2.352730	0.383063
1	1.299914	2.497749	-1.169883
1	-2.214947	-3.182993	0.443254
1	-4.567277	-2.257716	0.762389
1	-4.953778	0.125802	-0.068912

TS16

Z_{at}	X	Y	Z
8	-0.296373	0.180944	0.061617
8	-2.949941	1.924230	-0.216561
8	-2.625082	-1.237747	1.488364
6	-2.447465	-0.009957	1.116010
6	-2.769506	0.515810	-0.187691
6	-3.706786	-0.325654	-1.035871
6	-3.302744	-1.795887	-0.854217
6	-3.328761	-2.190304	0.612477
8	5.073504	-1.626355	-0.137084
8	3.538941	0.010660	1.326777
8	1.648517	-1.440087	-0.458086
8	-0.022432	3.074940	0.178298
6	4.369972	-0.863995	-0.755185
6	3.441796	0.119282	-0.070811
6	2.008632	-0.079564	-0.604875
6	0.951446	0.812232	0.114618
6	0.888059	2.217192	-0.496804
1	-3.794356	2.165126	0.181639
1	-2.008572	0.620195	1.880486
1	-1.617411	0.400974	-0.536214
1	-4.754446	-0.174365	-0.743102
1	-2.300355	-1.954448	-1.260641
1	-4.345757	-2.238987	1.008687
1	-0.914547	2.725474	0.054765
1	4.072000	-0.777989	1.508622
1	0.700224	-1.388774	-0.230628

1	4.367155	-0.846822	-1.862102
1	3.770716	1.125606	-0.379772
1	2.023859	0.180720	-1.678434
1	1.252393	0.906424	1.167448
1	1.864840	2.705572	-0.431428
1	0.621137	2.131193	-1.561057
1	-2.829012	-3.138202	0.803050
1	-3.982612	-2.461868	-1.392876
1	-3.616859	-0.026498	-2.081795

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Z_{at}	X	Y	Z
8	-0.473101	0.440819	-0.818443
8	-2.733673	1.927362	0.004676
8	-1.489084	-1.527394	-0.308662
6	-1.454046	-0.137582	-0.020152
6	-2.794023	0.537960	-0.344166
6	-3.949604	-0.184585	0.349148
6	-3.886561	-1.696933	0.092864
6	-2.494586	-2.226873	0.427882
8	3.045683	-0.000838	-0.887137
8	0.109349	2.825296	0.576616
6	1.860489	-0.085868	-1.089476
6	0.821974	0.653420	-0.257718
6	1.077437	2.167824	-0.216781
1	-3.068029	2.040608	0.901522
1	-1.218291	0.006927	1.048992
1	-2.915911	0.505780	-1.430036
1	-3.879747	-0.001212	1.431807
1	-4.105038	-1.909049	-0.958607
1	-2.297298	-2.133747	1.507420
1	-0.764040	2.671873	0.182212
1	1.441227	-0.709563	-1.904653
1	0.865358	0.259485	0.765479
1	2.055911	2.356205	0.226476
1	1.082000	2.556744	-1.243550
1	-2.384338	-3.276651	0.153956
1	-4.638431	-2.218128	0.693619
1	-4.900819	0.237913	0.014407

TS18

Z_{at}	X	Y	Z
8	0.759198	-0.445286	-0.703409
8	3.010272	-2.200636	-0.446085
8	1.990034	1.312440	0.041056
6	1.868613	-0.097782	0.074432
6	3.112462	-0.783716	-0.507555
6	4.373284	-0.266078	0.194997
6	4.413167	1.267221	0.235613
6	3.100226	1.805431	0.795220
8	-2.600550	0.754647	-0.560405
8	-2.817056	-1.508275	0.127113
6	-1.375480	0.583071	-0.938194
6	-0.473732	-0.131493	-0.162750
6	-1.639681	-1.839893	-0.243432
1	3.187928	-2.489758	0.455967
1	1.711558	-0.423884	1.121593
1	3.140722	-0.537593	-1.572166
1	4.383074	-0.654264	1.224373
1	4.560753	1.666555	-0.772891
1	2.985114	1.521415	1.852950
1	-2.924749	-0.231545	-0.145548
1	-1.101498	0.857409	-1.960674
1	-0.535121	-0.088348	0.920276
1	-1.447611	-2.123629	-1.286963
1	-0.971515	-2.324267	0.477635
1	3.041203	2.892163	0.728308
1	5.250850	1.613653	0.849137
1	5.253668	-0.677117	-0.305099

TS20

Z_{at}	X	Y	Z
8	-0.640988	0.424449	-0.697102
8	0.743759	-1.946382	0.168559
8	1.231268	1.632370	-0.381588
6	0.558135	0.451847	0.012164
6	1.429803	-0.769650	-0.326430
6	2.818972	-0.648060	0.303449
6	3.456899	0.701551	-0.050022
6	2.480547	1.827763	0.280090
8	-3.917847	1.359951	0.384581
8	-1.812417	-1.777018	1.168045
6	-2.729798	1.387570	0.089901
6	-1.855175	0.232633	0.025351
6	-2.426843	-1.117496	-0.128257
1	1.285348	-2.723407	-0.005564
1	0.357763	0.477287	1.096907
1	1.493331	-0.824905	-1.418617
1	2.712171	-0.736088	1.391382
1	3.698983	0.739980	-1.116982
1	2.320710	1.890666	1.367663
1	-0.913725	-2.083013	0.898428
1	-2.211503	2.348758	-0.108749
1	-1.619452	-0.641050	1.338783
1	-3.499445	-1.157525	0.034543
1	-2.085370	-1.718165	-0.967812
1	2.847576	2.795114	-0.064671
1	4.391303	0.838789	0.502947
1	3.454190	-1.478766	-0.024883

TS21

Z_{at}	X	Y	Z
8	0.712051	0.263068	-0.885727
8	-1.225408	2.319981	-0.320385
8	-0.785448	-1.363580	-0.493867
6	-0.424364	-0.009145	-0.361052
6	-1.598725	0.991923	-0.626010
6	-2.868871	0.551075	0.107254
6	-3.159618	-0.936365	-0.119395
6	-1.939413	-1.768012	0.257974

8	0.603211	0.230482	1.915274
8	3.468639	-1.117828	-0.706861
6	1.732780	-0.107641	1.399909
6	2.240658	0.684620	0.370617
6	3.388105	0.281544	-0.501932
1	-1.112326	2.400985	0.634107
1	-0.210210	0.160943	0.913869
1	-1.764569	0.979027	-1.707649
1	-2.734654	0.735002	1.182041
1	-3.408381	-1.118294	-1.170474
1	-1.724063	-1.675703	1.331017
1	2.641484	-1.387516	-1.126956
1	2.116775	-1.115654	1.567590
1	1.951573	1.728526	0.352861
1	3.305182	0.823514	-1.452635
1	4.332084	0.586771	-0.036300
1	-2.078332	-2.824563	0.026280
1	-4.020138	-1.255419	0.477123
1	-3.702097	1.177400	-0.222530

FRAG13

Z_{at}	X	Y	Z
8	0.959782	0.326110	-0.633305
8	-1.160354	2.235190	-0.335175
8	-0.454126	-1.385845	-0.123969
6	-0.213146	0.005246	0.050826
6	-1.366303	0.840445	-0.521817
6	-2.698494	0.375705	0.080740
6	-2.869870	-1.145358	-0.022946
6	-1.634491	-1.843985	0.536433
8	4.414104	0.172505	0.513356
6	3.178301	0.580624	0.092116
6	2.120783	-0.205653	-0.100844
1	-1.201507	2.434433	0.606935
1	-0.090876	0.212896	1.131522
1	-1.362415	0.689702	-1.604278
1	-2.723202	0.671265	1.139737
1	-3.000058	-1.438751	-1.069667
1	-1.548317	-1.665546	1.619967
1	4.417895	-0.782406	0.646305
1	3.143460	1.644701	-0.101874
1	2.123089	-1.278511	0.070741
1	-1.665455	-2.921991	0.372307
1	-3.762559	-1.471001	0.520850
1	-3.516001	0.906809	-0.412968

TS23

Z_{at}	X	Y	Z
8	0.859493	0.855685	-0.394061
8	-1.613906	2.254178	0.040576
8	-0.213184	-1.149872	-0.282131
6	-0.258732	0.210554	0.132880
6	-1.530934	0.899072	-0.379885
6	-2.768206	0.094598	0.040594
6	-2.631993	-1.390103	-0.320768
6	-1.305980	-1.930313	0.205677
8	4.171557	-0.094512	-0.203669
6	2.966878	-0.401135	-0.510188
6	2.087205	0.491200	0.157443
1	-1.738982	2.280279	0.995921
1	-0.229191	0.243150	1.240946
1	-1.454047	0.939030	-1.469413
1	-2.893891	0.192082	1.128893
1	-2.661199	-1.516820	-1.407877
1	-1.299843	-1.930247	1.307096
1	3.532962	0.920664	0.279746
1	2.756142	-1.211673	-1.207484
1	2.068693	0.304793	1.237326
1	-1.116507	-2.949737	-0.133352
1	-3.463324	-1.967119	0.097085
1	-3.653966	0.539971	-0.418964

TS24

Z_{at}	X	Y	Z
8	1.215163	0.260534	-0.809717
8	-1.554599	2.160203	0.323446
8	-0.562985	-1.230808	1.188257
6	-0.527748	0.069747	0.898621
6	-1.525702	0.750810	0.157516
6	-2.890938	0.072916	0.053515
6	-2.666604	-1.434686	-0.111194
6	-1.804206	-1.964041	1.022460
8	-0.999441	0.883725	-3.575013
6	-0.329476	1.060979	-2.377788
6	0.624447	0.138064	-1.903615
1	-1.729786	2.366074	1.247315
1	0.333948	0.577630	1.303241
1	-1.116554	0.702071	-1.031004
1	-3.486704	0.277424	0.951252
1	-2.178900	-1.637204	-1.070469
1	-2.336074	-1.904251	1.978202
1	-0.873345	-0.023530	-3.878105
1	-0.284974	2.103310	-2.085970
1	0.690092	-0.820698	-2.469589
1	-1.495562	-2.996574	0.862155
1	-3.616281	-1.977578	-0.113292
1	-3.435871	0.486629	-0.797960

FRAG16

Z_{at}	X	Y	Z
8	0.924017	1.230864	-0.391183
8	-1.608872	2.554477	-0.103289
8	-0.076340	-0.806270	-0.222823
6	-0.183274	0.570541	0.126457
6	-1.463413	1.185221	-0.455717
6	-2.680189	0.352951	-0.030333
6	-2.479541	-1.141427	-0.313386
6	-1.151109	-1.608537	0.273707
8	3.621712	-1.064897	0.081903
6	2.746806	-0.426549	-0.447358
6	2.165864	0.837655	0.172415
1	-1.810565	2.617340	0.837085
1	-0.193461	0.651530	1.232442
1	-1.355174	1.175777	-1.543231
1	-2.841747	0.498347	1.047811

1	-2.473734	-1.322043	-1.393160
1	-1.173347	-1.558503	1.373196
1	2.865763	1.655144	-0.030380
1	2.335085	-0.696350	-1.438613
1	2.101049	0.709547	1.259881
1	-0.912607	-2.633049	-0.013828
1	-3.301436	-1.727362	0.110344
1	-3.568165	0.740096	-0.535959

TS27

Z_{at}	X	Y	Z
8	0.960432	0.504942	-0.467571
8	-1.417151	2.094673	-0.148528
8	-0.203168	-1.412111	-0.310384
6	-0.151216	-0.019528	-0.108810
6	-1.460295	0.734437	-0.527830
6	-2.702629	0.013570	0.002708
6	-2.642703	-1.491476	-0.279459
6	-1.341270	-2.070855	0.262561
8	0.466245	0.313982	2.297810
6	1.700909	0.255957	1.942526
6	2.143520	1.156739	0.979908
1	-1.472406	2.153061	0.812701
1	-0.163141	0.131284	1.183502
1	-1.464350	0.738230	-1.621942
1	-2.765984	0.177271	1.087273
1	-2.697402	-1.677378	-1.357550
1	-1.302306	-1.979751	1.356666
1	3.120459	1.035736	0.529323
1	2.273048	-0.648218	2.168065
1	1.677556	2.127388	0.897198
1	-1.225331	-3.123810	0.003008
1	-3.493216	-2.003787	0.181385
1	-3.591525	0.469793	-0.441333

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FRAG11

Z_{at}	X	Y	Z
8	-0.552992	0.546980	-0.629697
8	-2.856940	1.990449	0.160705
8	-1.590441	-1.441542	-0.293078
6	-1.563689	-0.065509	0.094150
6	-2.895169	0.619152	-0.238910
6	-4.062411	-0.146748	0.386940
6	-3.995224	-1.639379	0.032676
6	-2.615161	-2.201444	0.362329
8	5.016186	-1.066083	0.955897
8	3.813245	0.829924	-0.448772
8	1.285024	-1.601576	-0.660928
8	0.098744	2.951928	0.572390
6	3.711520	-1.333810	0.508487
6	3.136501	-0.161381	-0.259587
6	1.706135	-0.256111	-0.782862
6	0.751271	0.701896	-0.033995
6	1.072168	2.194167	-0.128290
1	-3.088713	2.056769	1.094306
1	-1.366341	-0.001333	1.177995
1	-2.985782	0.632742	-1.328065
1	-4.015602	-0.031446	1.479706
1	-4.191414	-1.779760	-1.034973
1	-2.439444	-2.192138	1.448180
1	-0.767769	2.775517	0.176369
1	5.246784	-0.183805	0.625673
1	0.320110	-1.653875	-0.757580
1	3.045936	-1.560246	1.352057
1	3.686458	-2.216808	-0.142284
1	1.731970	0.055774	-1.836398
1	0.697010	0.406331	1.020589
1	2.037735	2.410700	0.325691
1	1.121666	2.487317	-1.184589
1	-2.496566	-3.225549	0.007733
1	-4.760980	-2.197470	0.580113
1	-5.006330	0.296870	0.060270

TS30

Z_{at}	X	Y	Z
8	-0.704305	0.888590	-0.385422
8	-3.184217	2.257553	-0.000730
8	-1.738834	-1.139686	-0.184029
6	-1.799129	0.251038	0.173300
6	-3.083455	0.890089	-0.375610
6	-4.312701	0.084459	0.060744
6	-4.152932	-1.410555	-0.241632
6	-2.833059	-1.916597	0.326474
8	5.213400	-0.485978	-0.322124
8	3.133719	-0.264065	1.363987
8	1.010106	-1.735424	-0.024210
8	2.778054	1.551536	0.180641
6	3.930842	-0.629350	-0.878853
6	2.838671	-0.195724	0.077417
6	1.395155	-0.431272	-0.385824
6	0.560316	0.694419	0.245889
6	1.407257	1.953449	0.040308
1	-3.459021	2.312135	0.921447
1	-1.774092	0.324192	1.276354
1	-2.994912	0.891542	-1.465050
1	-4.453327	0.220230	1.143198
1	-4.164544	-1.580556	-1.322904
1	-2.834756	-1.868665	1.425265
1	3.019906	0.990030	1.224979
1	5.097652	-0.584730	0.635770
1	0.047282	-1.788331	-0.147367
1	3.708701	-1.683254	-1.116645
1	3.880714	-0.057435	-1.808057
1	1.352824	-0.297296	-1.478423
1	0.418125	0.473259	1.309771
1	1.250608	2.341916	-0.968848
1	1.184740	2.742610	0.760076
1	-2.626839	-2.945956	0.031438
1	-5.198961	0.498068	-0.426553
1	-4.983364	-1.980594	0.186434

TS31

Z_{at}	X	Y	Z
8	-0.038526	0.381483	0.136735
8	2.172251	1.991390	0.745837
8	1.309723	-1.266516	-0.622655
6	1.226068	0.138703	-0.384157
6	2.281811	0.568562	0.637807
6	3.677676	0.128089	0.185210
6	3.696939	-1.371861	-0.141512
6	2.581439	-1.703429	-1.127247
8	-0.807537	-2.599902	0.837157
8	-3.858160	-1.353037	0.234276
8	-3.318610	0.354531	-1.433944
8	-0.322449	3.182679	-0.407319
6	-1.738478	-1.669463	1.351410
6	-2.604292	-0.992500	0.301364
6	-2.296808	-0.014602	-0.740653
6	-1.062433	0.889237	-0.739242
6	-1.422170	2.302544	-0.272846
1	2.740685	2.306164	1.455982
1	1.377558	0.681801	-1.328632
1	2.019111	0.094739	1.592242
1	3.950756	0.711823	-0.701548
1	3.555681	-1.962114	0.769747
1	2.765405	-1.226123	-2.099995
1	0.411030	2.863060	0.139390
1	-0.082146	-2.125836	0.397953
1	-4.203751	-0.713151	-0.485106
1	-1.246397	-0.893222	1.944944
1	-2.421884	-2.227946	1.992451
1	-1.856705	-1.171875	-1.045162
1	-0.680396	0.946477	-1.762463
1	-2.229730	2.684229	-0.896032
1	-1.776612	2.255122	0.766684
1	2.479300	-2.776852	-1.287314
1	4.662965	-1.658610	-0.567855
1	4.411071	0.366032	0.962604

FRAG17

Z_{at}	X	Y	Z
8	-0.731479	1.003060	-0.317811
8	-3.330909	2.151833	-0.049853
8	-1.585992	-1.113626	-0.096699
6	-1.777604	0.280064	0.221040
6	-3.098179	0.788848	-0.377127
6	-4.264153	-0.108646	0.053630
6	-3.968339	-1.590157	-0.208403
6	-2.625530	-1.967012	0.404468
8	4.158923	-1.714762	-0.383297
8	3.061378	0.075390	1.436274
8	1.204912	-1.577158	0.090949
8	2.737375	1.637248	-0.207142
6	3.955512	-0.355954	-0.767890
6	2.823061	0.260120	0.051528
6	1.419384	-0.245834	-0.330681
6	0.543771	0.835384	0.307923
6	1.400755	2.095646	0.096173
1	-3.567784	2.216284	0.882213
1	-1.792806	0.373861	1.323657
1	-2.982248	0.767031	-1.463720
1	-4.442657	0.040550	1.128518
1	-3.935412	-1.783539	-1.285386
1	-2.662955	-1.894135	1.501467
1	3.414909	-0.817631	1.549809
1	3.331314	-2.195386	-0.521364
1	0.251035	-1.741370	0.007951
1	3.733584	-0.263685	-1.836896
1	4.883260	0.175043	-0.551469
1	1.308083	-0.163318	-1.420792
1	0.407163	0.614710	1.371239
1	1.027326	2.668443	-0.754709
1	1.430763	2.735777	0.980258
1	-2.327048	-2.982889	0.141861
1	-5.170192	0.215550	-0.463946
1	-4.757332	-2.221665	0.211926

FRAG18

Z_{at}	X	Y	Z
8	0.106681	0.549197	-0.583092
8	-2.447651	1.843620	-0.403029
8	-0.837075	-1.454800	-0.061258
6	-0.979589	-0.030958	0.060213
6	-2.254263	0.455024	-0.650504
6	-3.494701	-0.346141	-0.230348
6	-3.220875	-1.851154	-0.269485
6	-1.943189	-2.185310	0.491872
8	1.653190	-2.033943	1.144089
8	2.829864	0.970876	-1.538193
8	-0.027817	2.984561	0.885402
6	2.753915	-1.921829	0.263210
6	3.389444	-0.503225	0.230998
6	2.501125	0.521561	-0.459276
6	1.213374	0.994657	0.224974
6	1.173827	2.527104	0.297602
1	-2.992071	1.904782	0.395974
1	-1.007416	0.236610	1.124810
1	-2.090077	0.333987	-1.723881
1	-3.117276	-2.170381	-1.311683
1	-2.049096	-1.949587	1.557455
1	-0.761415	2.772255	0.286114
1	0.825767	-1.915211	0.649224
1	2.494962	-2.219347	-0.759351
1	3.543077	-2.589307	0.615442
1	1.134917	0.562480	1.225277
1	1.996179	2.887600	0.921958
1	1.310810	2.923076	-0.714275
1	-1.681322	-3.238918	0.394717
1	-4.070222	-2.396602	0.155741
1	-4.319916	-0.083669	-0.901965
1	3.541537	-0.185584	1.271981
8	4.632742	-0.588975	-0.426876
1	4.547082	-0.079832	-1.248457
8	-3.804215	0.106458	1.101768
1	-4.704775	-0.144920	1.328199

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TS32

Z_{at}	X	Y	Z
8	-0.099899	0.906900	-0.834471
8	-2.074670	2.287466	0.745692
8	-1.392063	-0.932134	-0.978433
6	-1.111339	0.302947	-0.334679
6	-2.390388	1.149231	-0.031276
6	-3.491085	0.290715	0.595379
6	-3.704008	-1.004933	-0.194386
6	-2.386957	-1.754558	-0.332518
8	0.876168	-2.607874	-0.754134
8	0.273525	-0.233561	1.690475
8	2.056402	2.823871	-1.263256
6	2.103456	-1.924131	-0.634205
6	2.277032	-1.231598	0.735191
6	1.357537	-0.049779	1.013034
6	1.493213	1.219222	0.430792
6	2.523350	1.690717	-0.547043
1	-1.899602	2.009102	1.652328
1	-0.677320	-0.037805	0.855774
1	-2.724287	1.540918	-0.997437
1	-3.201604	0.044520	1.626295
1	-4.099733	-0.781104	-1.190715
1	-2.007988	-2.071108	0.647302
1	1.197725	2.591727	-1.637393
1	0.176663	-1.980495	-0.999423
1	2.246344	-1.202005	-1.444868
1	2.901727	-2.666313	-0.704689
1	0.916822	2.013129	0.889699
1	3.415772	2.011601	-0.000166
1	2.835863	0.888455	-1.220835
1	-2.480589	-2.637512	-0.964946
1	-4.435124	-1.645793	0.307953
1	-4.409937	0.880250	0.652914
1	2.067808	-1.981517	1.505782
8	3.644563	-0.805866	0.784492
1	3.880377	-0.613464	1.697769

TS33

Z_{at}	X	Y	Z
8	0.630501	0.743270	-0.335269
8	3.136200	1.726360	-1.299098
8	1.652207	-1.053967	0.622684
6	1.753548	-0.089045	-0.408386
6	3.008229	0.780879	-0.244118
6	4.250499	-0.109366	-0.117765
6	4.057361	-1.209365	0.933544
6	2.756657	-1.959764	0.664683
8	-4.345514	0.362437	-0.334890
8	-1.524131	0.385046	1.407809
8	-2.084508	2.300178	0.152033
6	-3.942570	-0.733155	0.482651
6	-2.580885	-1.278037	0.026474
6	-1.461793	-0.276164	0.296181
6	-0.566848	0.127965	-0.692966
6	-1.607662	1.901639	-0.977841
1	3.444343	1.271702	-2.091016
1	1.776450	-0.607758	-1.387238
1	2.866643	1.372247	0.663877
1	4.446754	-0.574993	-1.095024
1	4.013339	-0.769306	1.934857
1	2.819135	-2.514426	-0.284818
1	-1.660521	1.440018	1.065895
1	-3.886357	1.162830	-0.030206
1	-4.691254	-1.516311	0.348064
1	-3.901046	-0.457489	1.538720
1	-0.554889	-0.406221	-1.638381
1	-0.659545	2.322897	-1.323370
1	-2.314992	1.610833	-1.762119
1	2.523552	-2.671106	1.457749
1	4.901120	-1.906664	0.919987
1	5.115412	0.517860	0.111833
1	-2.348096	-2.172310	0.618946
8	-2.623884	-1.679470	-1.335027
1	-3.213155	-1.057792	-1.784242

TS34

Z_{at}	X	Y	Z
8	-0.136411	-0.022840	0.101068
8	-1.847334	2.209028	0.151493
8	-1.887014	-1.467822	0.002784
6	-1.482228	-0.174778	0.420242
6	-2.271481	0.918955	-0.312375
6	-3.775626	0.702804	-0.152216
6	-4.157578	-0.740999	-0.509859
6	-3.271030	-1.723965	0.251821
8	4.318501	0.809172	0.064379
8	3.153670	-0.781363	1.354378
8	0.964634	2.250977	1.242627
6	3.306175	1.086689	-0.679401
6	2.294795	-0.939702	-0.794936
6	2.131960	-0.661641	0.552608
6	0.813850	-0.207187	1.153318
6	0.907816	1.068111	2.017140
1	-2.461964	2.524835	0.822711
1	-1.645687	-0.077987	1.508474
1	-1.986678	0.867112	-1.366716
1	-4.050805	0.898990	0.894930
1	-4.031174	-0.906002	-1.584575
1	-3.471382	-1.663632	1.333258
1	0.128892	2.324087	0.754043
1	3.922843	0.086934	0.905194
1	3.424032	0.973028	-1.758741
1	2.530825	1.763018	-0.316182
1	0.496311	-1.035815	1.803321
1	0.052394	1.096361	2.706094
1	1.815344	1.018545	2.620439
1	-3.442476	-2.752780	-0.066244
1	-5.209645	-0.927649	-0.273207
1	-4.321115	1.423065	-0.768174
1	1.488111	-0.849779	-1.505567
8	3.357787	-1.652429	-1.248000
1	3.968297	-1.781776	-0.506102

FRAG21

Z_{at}	X	Y	Z
8	-0.457191	0.227641	0.598263
8	-2.430961	-1.812388	0.778163
8	-1.956876	1.684277	-0.297786
6	-1.643853	0.311651	-0.139636
6	-2.742062	-0.429681	0.633239
6	-4.099754	-0.204943	-0.040376
6	-4.356544	1.285895	-0.300063
6	-3.166156	1.901892	-1.029446
8	5.437699	0.685615	0.080429
8	1.725968	-1.346537	0.885015
6	4.159830	0.458523	0.653745
6	3.143362	0.062045	-0.426953
6	1.777211	-0.208052	0.124148
6	0.706911	0.565601	-0.070937
1	-2.610594	-2.262682	-0.054936
1	-1.500651	-0.146359	-1.135872
1	-2.746879	-0.023630	1.648158
1	-4.108614	-0.745036	-0.998561
1	-4.503476	1.812272	0.648427
1	-3.069817	1.476125	-2.040352
1	5.618618	-0.065647	-0.498798
1	3.852752	1.391316	1.131588
1	4.203778	-0.325031	1.422089
1	0.707863	1.470846	-0.662086
1	-3.261571	2.983938	-1.124852
1	-5.267232	1.420991	-0.892155
1	-4.885724	-0.645142	0.578348
1	3.082984	0.869968	-1.159341
8	3.645926	-1.077822	-1.145580
1	3.409041	-1.866175	-0.640740
1	0.811779	-1.469924	1.181816

FRAG22

Z_{at}	X	Y	Z
8	0.144633	0.585999	-0.239276
8	-2.087340	2.322425	-0.326352
8	-1.189790	-1.253010	-0.119747
6	-1.105160	0.155143	0.154185
6	-2.166817	0.930603	-0.634791
6	-3.559813	0.350104	-0.377845
6	-3.575557	-1.171102	-0.586407
6	-2.458990	-1.827892	0.219382
8	1.537350	-1.921613	0.371861
8	0.928807	2.865731	1.063572
6	3.428081	-0.607197	0.086705
6	2.120174	-0.666654	0.358309
6	1.239153	0.486418	0.720169
6	1.885892	1.871934	0.734611
1	-2.563114	2.491231	0.494992
1	-1.255622	0.307290	1.238203
1	-1.905751	0.849143	-1.692951
1	-3.849171	0.575840	0.659043
1	-3.434473	-1.405509	-1.646277
1	-2.637146	-1.712959	1.298843
1	0.218766	2.816879	0.407241
1	0.791154	0.304362	1.706389
1	2.661660	1.916393	1.500662
1	2.342574	2.074733	-0.241376
1	-2.370983	-2.892604	0.000966
1	-4.541687	-1.588715	-0.286547
1	-4.285955	0.847788	-1.025549
1	4.000952	0.307594	0.096491
8	4.177870	-1.706339	-0.206577
1	3.581690	-2.469014	-0.207863
1	0.603099	-1.856043	0.102536

TS36

Z_{at}	X	Y	Z
8	-0.720833	0.357243	1.114464
8	-1.653643	-2.053913	0.219775
8	-2.672562	1.408606	0.574349
6	-1.843183	0.305329	0.281232
6	-2.577189	-1.004850	0.568935
6	-3.872274	-1.074118	-0.240241
6	-4.706027	0.197822	-0.015493
6	-3.845125	1.439379	-0.246508
8	0.985758	1.852709	-1.853205
8	1.056089	-1.416411	0.036812
6	1.744217	0.786165	-2.095857
6	2.519056	0.310615	-0.667987
6	1.389259	-0.150221	0.112588
6	0.472011	0.869558	0.557762
1	-2.021845	-2.910834	0.458470
1	-1.541283	0.339816	-0.778040
1	-2.781155	-1.034456	1.645535
1	-3.610363	-1.170124	-1.300292
1	-5.093467	0.219157	1.008344
1	-3.551968	1.517349	-1.303829
1	0.396574	1.470029	-0.509255
1	2.638562	1.001562	-2.703620
1	1.232059	-0.106390	-2.499498
1	0.926193	1.614314	1.210827
1	-4.372108	2.353333	0.028332
1	-5.567519	0.212117	-0.690060
1	-4.442964	-1.967849	0.033377
1	3.247126	-0.466903	-0.895278
8	3.132453	1.476527	-0.175932
1	2.666259	2.219302	-0.600330
1	0.129587	-1.577977	0.339128

TS37

Z_{at}	X	Y	Z
8	-0.118677	0.542871	0.786291
8	-2.509862	0.326566	2.391390
8	-1.273499	-0.043580	-1.066791
6	-1.243143	-0.158129	0.365673
6	-2.501800	0.469549	0.977984
6	-3.761352	-0.118676	0.330330
6	-3.696980	-0.064564	-1.201615
6	-2.394984	-0.686611	-1.691420
8	1.424638	0.047932	-1.529805

8	3.474277	0.812840	1.542524
6	3.087942	-1.046693	-0.262089
6	1.765438	-0.489300	-0.360791
6	1.110126	-0.140891	0.857685
6	2.221864	1.136612	1.591626
1	-2.793272	-0.566191	2.618234
1	-1.170550	-1.225465	0.636478
1	-2.441784	1.544966	0.790947
1	-3.862133	-1.166423	0.649746
1	-3.747952	0.973669	-1.544557
1	-2.365888	-1.763600	-1.472205
1	3.551139	-0.195005	0.485837
1	1.135552	-0.908147	1.629954
1	1.886544	2.000822	0.991891
1	1.739481	1.120084	2.580664
1	-2.252105	-0.553559	-2.764096
1	-4.547923	-0.594344	-1.640788
1	-4.637061	0.412794	0.710598
1	3.155583	-1.940969	0.355866
8	3.808522	-1.244581	-1.447333
1	3.639346	-0.504026	-2.040562
1	0.484733	0.325924	-1.502981

FRAG23

Z_{at}	X	Y	Z
8	0.197828	1.128031	-0.094218
8	-2.454518	2.218481	-0.151060
8	-0.633556	-0.999568	0.022641
6	-0.891843	0.392496	0.311086
6	-2.140835	0.864652	-0.448646
6	-3.326505	-0.067268	-0.167647
6	-2.963206	-1.541239	-0.385599
6	-1.699564	-1.883764	0.393509
8	2.114967	-1.240752	0.218961
6	3.624240	0.483518	-0.180875
6	2.405505	0.108377	0.224386
6	1.383306	1.061119	0.739164
1	-2.792314	2.272261	0.750007
1	-1.051440	0.482514	1.403387
1	-1.887994	0.852268	-1.511727
1	-3.643490	0.075847	0.875763
1	-2.788419	-1.733738	-1.448931
1	-1.876690	-1.811885	1.476896
1	1.074151	0.793540	1.758858
1	-1.341607	-2.890353	0.173539
1	-3.783761	-2.191810	-0.066846
1	-4.168571	0.233363	-0.795813
1	3.957447	1.511174	-0.172901
8	4.569801	-0.392673	-0.619909
1	4.170426	-1.274392	-0.613080
1	1.155013	-1.352420	0.083349
1	1.797741	2.069940	0.753128

FRAG24

Z_{at}	X	Y	Z
8	-0.068546	-1.472355	-0.400744
8	-1.018291	0.875584	-1.602928
8	-2.009445	-1.764312	0.758721
6	-1.172884	-0.803862	0.143603
6	-1.896571	-0.091465	-1.006078
6	-3.210842	0.522319	-0.525454
6	-4.042375	-0.519910	0.237043
6	-3.192273	-1.187549	1.316507
8	1.852416	0.364190	-1.193138
6	3.444427	-0.395935	0.395089
6	2.060908	-0.506725	-0.168202
6	1.140313	-1.370623	0.273532
1	-1.123242	1.720020	-1.149796
1	-0.836369	-0.067865	0.894182
1	-2.080709	-0.839937	-1.780877
1	-2.984520	1.364674	0.145131
1	-4.404814	-1.286593	-0.455119
1	-2.918089	-0.458564	2.095178
1	1.309898	-2.053694	1.096259
1	-3.723568	-2.010222	1.796165
1	-4.920065	-0.050117	0.691873
1	-3.763863	0.929736	-1.376119
1	4.169090	-0.684615	-0.379350
8	3.733076	0.916722	0.874822
1	3.551493	1.530976	0.154547
1	0.915890	0.347716	-1.468964
1	3.560632	-1.073193	1.241206

TS39

Z_{at}	X	Y	Z
8	-0.191423	-1.248745	-1.028355
8	1.512598	-1.989731	1.199133
8	0.723141	0.809986	-1.134102
6	0.502884	-0.401275	-0.387360
6	1.806662	-0.937868	0.291721
6	2.629252	0.169996	0.950648
6	2.803874	1.369815	0.016001
6	1.436010	1.847685	-0.456531
8	-2.655250	1.104684	-0.658283
6	-1.577057	0.334955	1.279371
6	-2.301769	0.001765	0.111030
6	-2.255964	-1.264652	-0.383924
1	1.283847	-1.603658	2.051510
1	-0.189190	0.005323	0.603547
1	2.378814	-1.400347	-0.517381
1	2.111560	0.500708	1.863219
1	3.408940	1.089531	-0.852756
1	0.850721	2.208101	0.401961
1	-2.006808	-2.091677	0.263453
1	1.520574	2.664103	-1.176445
1	3.325487	2.184945	0.528121
1	3.593498	-0.240929	1.263811
1	-1.463818	-0.389642	2.077194
8	-1.531616	1.614684	1.711007
1	-1.867141	2.168320	0.985864
1	-2.192467	1.054265	-1.505853
1	-2.664074	-1.502929	-1.355834

TS40

Z_{at}	X	Y	Z
8	-0.722513	-1.171198	0.782474
8	-0.339741	-4.440242	0.271213
8	-2.009896	-2.134368	-1.860622
6	-1.114458	-2.666368	-1.095477
6	-1.373959	-3.491700	0.058961
6	-2.787258	-4.051526	0.148504
6	-3.762674	-2.944123	-0.272756
6	-3.437616	-2.441498	-1.667986
8	1.600625	-0.488247	1.891376
6	0.522458	0.732579	3.572006
6	0.472468	0.141279	2.378054
6	-0.706437	0.068404	1.435940
1	0.070354	-4.258132	1.123154
1	-0.096799	-2.447914	-1.396279
1	-1.249414	-2.571044	0.805226
1	-2.887154	-4.933095	-0.494460
1	-3.711523	-2.114566	0.437253
1	-3.671558	-3.180615	-2.437482
1	-1.635652	0.268712	1.991358
1	-3.940186	-1.506593	-1.909270
1	-4.794162	-3.307981	-0.279385
1	-2.989242	-4.372721	1.172450
1	-0.321557	1.249191	4.005472
8	1.647155	0.768022	4.364746
1	2.338800	0.274114	3.905696
1	1.243953	-1.093420	1.214947
1	-0.612522	0.866082	0.676096

TS41

Z_{at}	X	Y	Z
8	-0.340758	-0.064634	-1.211806
8	-2.498410	2.327901	0.012574
8	-2.059423	-0.946145	1.460503
6	-1.829468	0.264410	1.036906
6	-2.498978	0.910743	-0.073256
6	-3.819819	0.268965	-0.485014
6	-3.645840	-1.254329	-0.438668
6	-3.207688	-1.700780	0.945271
8	0.427437	-2.148530	-2.751930
6	2.200698	-0.927282	-3.809404
6	1.081548	-0.942685	-2.833401
6	0.658259	0.085983	-2.046614
1	-3.134895	2.603192	0.682146
1	-1.001390	0.750582	1.540709
1	-1.689623	0.659216	-0.880289
1	-4.628939	0.582577	0.188029
1	-2.900936	-1.558611	-1.178660
1	-3.999589	-1.566667	1.687257
1	1.171601	1.049459	-2.109112
1	-2.873875	-2.736753	0.970094
1	-4.580422	-1.768051	-0.681066
1	-4.084089	0.602349	-1.490029
1	2.941699	-1.696151	-3.545442
8	1.771695	-1.131460	-5.167174
1	1.216901	-1.919021	-5.174655
1	-0.257651	-2.000355	-2.077511
1	2.693423	0.045457	-3.786954

TS42

Z_{at}	X	Y	Z
8	0.421553	-2.036751	-1.193856
8	-0.186717	-0.403896	2.178930
8	-2.453032	-0.830462	-0.627128
6	-1.565743	-1.054007	0.337032
6	-0.783427	-0.047549	0.944498
6	-1.288346	1.390706	0.844958
6	-1.926407	1.591200	-0.535256
6	-2.968034	0.517946	-0.802245
8	2.279310	-1.075998	0.559827
6	2.453259	1.009454	-0.605366
6	1.730124	-0.285032	-0.420688
6	0.930255	-0.915984	-1.404163
1	-0.867674	-0.404520	2.859948
1	-1.430990	-2.102192	0.565816
1	0.259649	0.005345	0.191712
1	-2.021135	1.585526	1.637977
1	-1.155036	1.555678	-1.310739
1	-3.821043	0.618683	-0.122898
1	0.629305	-0.303542	-2.273008
1	-3.334789	0.538322	-1.827567
1	-2.405291	2.572073	-0.606024
1	-0.448456	2.072906	0.990795
1	2.081202	1.519572	-1.495818
8	2.263474	1.921328	0.485697
1	2.520152	1.462428	1.294050
1	1.818754	-1.930064	0.512963
1	3.525993	0.814168	-0.742080

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FRAG15

Z_{at}	X	Y	Z
8	-0.404502	-0.282604	-0.551683
6	-1.643010	-0.112303	0.108225
6	-2.494592	1.013078	-0.473321
6	-2.363675	-1.450160	-0.086577
1	-1.479449	0.084476	1.177519
6	-3.858557	0.984607	0.209641
1	-2.624455	0.841115	-1.551097
1	-2.305568	-1.731534	-1.140924
1	-1.890075	-2.228166	0.508045
6	-4.537623	-0.382253	0.149619
1	-3.699706	1.187753	1.281750
8	-3.761965	-1.468548	0.299098
8	-1.852934	2.260091	-0.251967
1	-2.451748	2.955593	-0.550409
8	-4.684035	1.982614	-0.350209
1	-5.595278	1.656635	-0.307413
8	-5.735649	-0.475308	0.068818
6	0.681462	0.491515	-0.040466
1	1.562278	0.185043	-0.604282
1	0.506617	1.560826	-0.173183
1	0.844164	0.276993	1.023495

TS46

Z_{at}	X	Y	Z
8	2.263157	-0.454214	-0.391305
6	0.999407	-0.286292	0.219839
6	0.254990	0.966235	-0.253650
6	0.217119	-1.537523	-0.196398
1	1.106618	-0.247116	1.313150
6	-1.230031	0.893704	0.098392
1	0.318780	1.002807	-1.351560
1	0.172997	-1.605024	-1.286316
1	0.688618	-2.432861	0.199228
6	-1.798081	-0.421234	0.293106
1	-1.218005	0.450310	1.373459
8	-1.150375	-1.571589	0.312466
8	0.814612	2.137416	0.308239
1	0.123591	2.815490	0.255557
8	-1.996483	1.892683	-0.060144
1	-3.412692	0.420790	0.228919
8	-3.106576	-0.502172	0.396543
6	3.333652	0.285672	0.200318
1	4.234638	-0.002009	-0.340623
1	3.172112	1.362067	0.113041
1	3.448149	0.021536	1.259015

FRAG26

Z_{at}	X	Y	Z
8	-2.229278	-0.696105	0.490862
6	-1.058758	-0.409836	-0.244436
6	-0.352039	0.878012	0.244768
6	-0.133747	-1.615565	-0.053338
1	-1.294859	-0.285325	-1.310951
6	1.045117	0.940069	-0.349110
1	-0.243315	0.787795	1.335783
1	0.012471	-1.802050	1.014387
1	-0.576219	-2.499962	-0.507877
6	1.881288	-0.336043	-0.229122
8	1.129041	-1.426256	-0.712006
8	-1.084010	2.038281	-0.073954
1	-0.476599	2.633675	-0.540930
8	1.431317	1.918951	-0.947362
8	2.242293	-0.463760	1.126385
6	-3.415298	-0.027022	0.062254
1	-4.228122	-0.437884	0.661037
1	-3.346735	1.051940	0.216590
1	-3.612716	-0.227651	-0.998460
1	2.909196	-1.155779	1.206638
1	2.751017	-0.261826	-0.884770

TS50

Z_{at}	X	Y	Z
8	-2.162907	-0.806986	0.246862
6	-1.020690	-0.477762	-0.507279
6	-0.370066	0.851814	-0.094657
6	-0.031783	-1.634808	-0.304687
1	-1.276368	-0.379129	-1.572886
6	1.076492	0.902355	-0.195290
1	0.102000	0.589481	1.035770
1	0.085191	-1.832644	0.765256
1	-0.405343	-2.535199	-0.788570
6	1.964618	-0.308679	-0.319351
8	1.244774	-1.363238	-0.908397
8	-0.943507	2.005812	-0.159115
8	1.543393	2.108694	-0.208798
8	2.479138	-0.620866	0.954332
6	-3.345473	-0.080469	-0.099952
1	-4.137199	-0.467439	0.541132
1	-3.212457	0.990451	0.064367
1	-3.611503	-0.258733	-1.149981
1	3.165241	-1.291177	0.848995
1	2.767220	-0.074506	-1.025952
1	0.662896	2.637392	-0.245109

TS51

Z_{at}	X	Y	Z
8	-1.706378	-1.031185	0.528661
6	-1.006492	-0.473072	-0.565930
6	-0.364952	0.919352	-0.231922
6	0.026485	-1.509450	-0.990532
1	-1.686993	-0.296137	-1.410239
6	1.157055	0.875291	-0.278211
1	-0.627648	1.151289	0.808647
1	-0.435970	-2.493736	-1.066902
1	0.471659	-1.246434	-1.953094
6	1.846219	-0.239756	0.507586
8	1.106258	-1.629004	-0.035334
8	-0.853243	1.909608	-1.106207
1	-0.092242	2.436923	-1.395922
8	1.789960	1.698524	-0.901590
8	1.469607	-0.444259	1.745656
6	-2.925988	-0.375497	0.851012
1	-3.363110	-0.924346	1.684092
1	-2.766108	0.665494	1.155444
1	-3.616235	-0.392279	-0.001878
1	0.894389	-1.467790	1.119609
1	2.900278	-0.354429	0.225125

FRAG29 for TS54

Z_{at}	X	Y	Z
8	-2.131907	-0.615346	0.548171
6	-1.134374	-0.567848	-0.459927
6	-0.400019	0.777381	-0.411360
6	-0.134213	-1.697635	-0.187834
1	-1.582438	-0.665805	-1.457314
6	0.903667	0.798621	0.372478
1	-0.020798	-1.842438	0.891128
1	-0.465764	-2.635519	-0.630789
6	1.826865	-0.342088	-0.117525
8	1.114323	-1.365386	-0.799563

8	-0.829116	1.786698	-0.927558
8	1.543779	2.044669	0.283707
8	2.499109	-0.843392	1.010877
6	-3.340326	0.077134	0.236794
1	-4.016122	-0.101967	1.072451
1	-3.175685	1.152509	0.122292
1	-3.785709	-0.316722	-0.685056
1	3.175285	-1.462526	0.712719
1	2.524504	0.058752	-0.856415
1	0.943618	2.629173	-0.205823
1	0.646185	0.578519	1.419969

TS54

Z_{at}	X	Y	Z
8	-2.073806	-0.445837	0.561142
6	-1.002618	-0.414550	-0.366528
6	-0.295912	0.946223	-0.290072
6	-0.060329	-1.554733	0.008405
1	-1.368685	-0.535514	-1.394685
6	1.036276	1.035714	0.450864
1	0.072563	-1.575731	1.095661
1	-0.469605	-2.514459	-0.310484
6	2.063544	0.111952	-0.233828
8	1.197348	-1.351985	-0.653323
8	-0.768245	1.941729	-0.796508
8	1.532981	2.347123	0.441390
8	2.926930	-0.573896	0.455664
6	-3.273733	0.200926	0.133613
1	-4.006307	0.025061	0.920393
1	-3.128427	1.275952	-0.001202
1	-3.633434	-0.234910	-0.806313
1	2.185984	-1.517663	0.024135
1	2.347772	0.483028	-1.227333
1	0.906851	2.878501	-0.077746
1	0.904395	0.688475	1.483406

FRAG29 for TS55

Z_{at}	X	Y	Z
8	-2.106417	-1.052963	-0.396077
6	-0.990755	-0.430204	-1.031657
6	-0.538177	0.849189	-0.313935
6	0.160914	-1.454016	-0.976384
1	-1.250836	-0.153846	-2.059172
6	0.351892	0.633401	0.896512
1	-0.011284	-2.134848	-0.137927
1	0.219185	-2.033723	-1.895995
6	1.597283	-0.172355	0.432809
8	1.414269	-0.781815	-0.838671
8	-0.798933	1.961701	-0.712994
8	0.724273	1.850719	1.491456
8	1.881181	-1.122582	1.429884
1	2.728779	-1.533661	1.224458
1	2.427135	0.523475	0.290540
1	0.348838	2.552539	0.936507
1	-0.200388	0.017202	1.616659
6	-3.287577	-0.309616	-0.346686
6	-4.476463	-1.263532	-0.227122
1	-3.397509	0.307730	-1.253646
6	-5.762910	-0.465066	0.032590
1	-4.262423	-1.937387	0.612585
6	-4.343990	1.371985	0.967841
6	-5.595590	0.528038	1.190902
1	-6.588713	-1.157396	0.228156
1	-6.011829	0.074069	-0.889016
1	-4.117532	2.004132	1.827091
1	-4.460967	2.020080	0.086543
1	-6.475002	1.175077	1.270005
1	-5.497761	-0.007005	2.141223
8	-3.203177	0.527537	0.796605
8	-4.548563	-1.991179	-1.451583
1	-5.207736	-2.686272	-1.362116

TS55

Z_{at}	X	Y	Z
8	-0.177454	0.838840	-0.901201
6	1.253006	1.406127	0.494933
6	1.115904	0.155488	1.102950
6	2.433984	1.743258	-0.347921
1	0.594732	2.212859	0.787512
6	2.098269	-0.950667	0.756450
1	2.070661	2.033453	-1.345255
1	2.941331	2.616706	0.074554
6	2.891688	-0.603582	-0.518588
8	3.408260	0.718855	-0.430414
8	0.024003	-0.109680	1.722837
8	3.045831	-1.135420	1.810919
8	2.149414	-0.832041	-1.680384
1	1.267232	-0.429573	-1.608094
1	3.776365	-1.236117	-0.572071
1	2.566356	-1.370452	2.612965
1	1.536856	-1.874087	0.576360
6	-1.190727	0.169808	-0.470375
6	-2.558535	0.926741	-0.376228
1	-0.896670	-0.048870	0.753249
6	-3.651719	0.008357	0.175216
1	-2.798473	1.233944	-1.398463
6	-2.268037	-1.975508	-0.479707
6	-3.657118	-1.349935	-0.534787
1	-4.617734	0.511795	0.082052
1	-3.471884	-0.144594	1.248593
1	-2.212732	-2.897727	-1.058685
1	-1.982732	-2.201041	0.556862
1	-4.382008	-2.023928	-0.067770
1	-3.955404	-1.228858	-1.581519
8	-1.288727	-1.103249	-1.062994
8	-2.430211	2.127098	0.359603
1	-2.373783	1.913005	1.298357

FRAG25

Z_{at}	X	Y	Z
8	-0.418373	0.503801	-0.537188
8	-2.858068	1.905494	-0.291431
8	-1.423110	-1.484627	-0.090636
6	-1.498629	-0.069207	0.110922
6	-2.791023	0.493811	-0.493685
6	-4.009085	-0.244030	0.066441

6	-3.841189	-1.764684	-0.068438
6	-2.503267	-2.205986	0.517938
8	4.404393	-1.343829	-1.219389
8	3.414526	0.602719	1.399736
8	1.436949	-1.594382	0.116196
8	0.083490	3.091798	0.244343
6	4.331775	-0.995175	-0.071640
6	3.180058	-0.129984	0.468436
6	1.828788	-0.270115	-0.228526
6	0.792443	0.771232	0.203169
6	1.145872	2.224936	-0.114410
1	-3.174909	2.084404	0.601536
1	-1.463691	0.138711	1.194423
1	-2.725055	0.356397	-1.576019
1	-4.121975	0.015900	1.129088
1	-3.879651	-2.052615	-1.123812
1	-2.482290	-2.047010	1.606122
1	-0.715566	2.796617	-0.216750
1	0.512729	-1.732513	-0.154116
1	5.127720	-1.187734	0.674387
1	1.988945	-0.188510	-1.312948
1	0.593801	0.669772	1.274976
1	2.015653	2.532370	0.465372
1	1.384389	2.314417	-1.183710
1	-2.301640	-3.259875	0.324600
1	-4.656992	-2.286829	0.440971
1	-4.911278	0.103086	-0.443423

TS56

Z_{at}	X	Y	Z
8	-0.535272	0.863699	-1.144688
8	-3.187180	1.804187	-1.179102
8	-1.089255	-0.919948	0.166570
6	-1.450155	0.411075	-0.205936
6	-2.844236	0.457024	-0.847439
6	-3.880866	-0.204374	0.062013
6	-3.408142	-1.593135	0.512636
6	-2.003161	-1.504814	1.101755
8	1.373380	0.172493	2.180554
8	2.912338	-1.290612	-0.573297
8	2.390571	0.552883	-2.050146
8	-0.511347	3.638665	-1.282078
6	1.653630	-0.689192	1.383089
6	2.130507	-0.428961	-0.003538
6	1.854232	0.709896	-0.890706
6	0.613204	1.583606	-0.678437
6	0.668224	2.877457	-1.486528
1	-3.537953	2.241669	-0.394802
1	-1.433150	1.048540	0.695786
1	-2.776460	-0.072058	-1.801366
1	-4.030333	0.431087	0.947347
1	-3.394594	-2.279712	-0.339854
1	-2.009285	-0.914708	2.030801
1	-1.264486	3.101592	-1.568975
1	2.961523	-0.871050	-1.523477
1	1.570626	-1.766828	1.610749
1	2.672755	1.069602	-0.011046
1	0.495439	1.816076	0.383796
1	1.508372	3.490740	-1.151697
1	0.820316	2.632455	-2.542113
1	-1.600882	-2.492765	1.330671
1	-4.094901	-2.009998	1.255959
1	-4.841226	-0.257708	-0.457085

TS57

Z_{at}	X	Y	Z
8	-0.565551	0.846679	-0.368851
8	-3.029099	2.278900	-0.163412
8	-1.643284	-1.146558	-0.065558
6	-1.691584	0.265249	0.192090
6	-2.941608	0.888426	-0.447616
6	-4.202697	0.134339	-0.011182
6	-4.058883	-1.379502	-0.208827
6	-2.773791	-1.868075	0.447214
8	3.894229	-1.034915	-1.738465
8	3.232841	-0.209139	1.604608
8	1.070221	-1.746815	0.423501
8	2.904799	1.501202	0.261117
6	4.063453	-0.624933	-0.621444
6	2.926250	-0.245053	0.333938
6	1.492739	-0.522304	-0.127172
6	0.668412	0.698102	0.327632
6	1.548553	1.908585	0.008019
1	-3.345206	2.396114	0.739503
1	-1.704595	0.417038	1.287416
1	-2.810347	0.818972	-1.530460
1	-4.384062	0.342981	1.053486
1	-4.028401	-1.620230	-1.276206
1	-2.820608	-1.747206	1.539460
1	3.120600	1.039094	1.360607
1	0.128577	-1.834972	0.201575
1	5.064208	-0.502138	-0.164035
1	1.484464	-0.553917	-1.224465
1	0.482375	0.611499	1.404780
1	1.452634	2.173688	-1.046807
1	1.319807	2.783900	0.617364
1	-2.575809	-2.918126	0.229641
1	-4.917021	-1.906692	0.219478
1	-5.060550	0.529664	-0.560556

FRAG32

Z_{at}	X	Y	Z
8	0.033563	0.477054	-0.396417
8	-2.575659	1.520434	-0.592761
8	-0.755823	-1.376320	0.648922
6	-1.030646	-0.007843	0.365473
6	-2.320982	0.115600	-0.448832
6	-3.479167	-0.595106	0.259711
6	-3.096462	-2.032932	0.635885
6	-1.781736	-2.032039	1.407798
8	1.760265	-2.390561	-1.615696
8	2.068930	-1.334758	0.931167
8	3.155152	1.523621	-0.864474
8	-0.451780	3.187148	0.544110

6	2.435066	-1.403044	-1.498335
6	2.686445	-0.715619	-0.153169
6	2.374680	0.791746	-0.303102
6	1.033084	1.281722	0.253807
6	0.774777	2.760561	-0.023967
1	-3.187134	1.666019	-1.320918
1	-1.124876	0.553993	1.306501
1	-2.124372	-0.336702	-1.427668
1	-3.727067	-0.022855	1.161139
1	-2.979860	-2.645811	-0.263650
1	-1.898800	-1.527836	2.378066
1	-1.182204	2.778216	0.054641
1	2.931656	-0.917811	-2.361791
1	1.016995	1.091699	1.332818
1	1.567322	3.356491	0.432070
1	0.804267	2.936208	-1.105012
1	-1.411657	-3.041433	1.588283
1	-3.882597	-2.491209	1.243706
1	-4.366788	-0.580841	-0.380631
1	1.167174	-1.609628	0.686435
1	3.772553	-0.756071	0.001180

TS58

Z_{at}	X	Y	Z
8	0.414072	0.785757	0.261057
8	2.986702	1.896606	0.547224
8	1.305659	-1.117088	-0.599987
6	1.543985	0.266152	-0.385102
6	2.765455	0.489578	0.506158
6	3.979869	-0.257581	-0.063353
6	3.649638	-1.722267	-0.377944
6	2.395212	-1.791213	-1.241960
8	-2.930190	-2.961870	0.024553
8	-3.078375	-0.709769	1.478617
8	-2.907155	0.542495	-1.052115
8	-2.716169	2.836768	-0.483748
6	-1.982062	-2.222458	-0.063269
6	-1.955702	-0.877224	0.659466
6	-1.838327	0.221827	-0.396988
6	-0.692026	0.997191	-0.545095
6	-1.651511	2.690243	0.203933
1	3.606516	2.097655	1.254874
1	1.694732	0.771239	-1.354036
1	2.508275	0.106882	1.502258
1	4.292520	0.261252	-0.976954
1	3.476802	-2.283369	0.546325
1	2.577111	-1.340284	-2.228788
1	-3.025311	1.654487	-0.910544
1	-1.089244	-2.465835	-0.664141
1	-0.501860	1.482547	-1.498009
1	-1.713991	2.380375	1.255520
1	-0.768755	3.290183	-0.042773
1	2.058200	-2.817255	-1.394078
1	4.485815	-2.200769	-0.897176
1	4.814033	-0.187487	0.641968
1	-3.749247	-1.344386	1.184331
1	-1.047032	-0.855954	1.269954

FRAG33

Z_{at}	X	Y	Z
8	-0.650400	0.924638	-0.239340
8	-3.167585	2.266272	-0.353760
8	-1.680398	-1.092902	0.102116
6	-1.799490	0.332451	0.254517
6	-3.006628	0.865676	-0.532764
6	-4.276975	0.092124	-0.162255
6	-4.064880	-1.424052	-0.249301
6	-2.832595	-1.820059	0.553472
8	4.557595	-1.248959	1.521682
8	3.600180	-0.340122	-0.795068
8	1.049354	-1.714097	0.732697
8	2.786901	1.290850	0.685000
6	3.452887	-0.771641	1.564874
6	2.824120	-0.103083	0.328932
6	1.358401	-0.509602	0.058492
6	0.543058	0.714634	0.507067
6	1.534040	1.850371	0.274357
1	-3.536501	2.431852	0.521104
1	-1.918055	0.549990	1.333452
1	-2.774851	0.732409	-1.592515
1	-4.561945	0.357985	0.866264
1	-3.924695	-1.727300	-1.291717
1	-2.989123	-1.631026	1.626008
1	0.109062	-1.877938	0.562524
1	2.861633	-0.726907	2.493352
1	1.243400	-0.622890	-1.025130
1	0.307381	0.624486	1.575643
1	1.553749	2.130939	-0.785227
1	1.344077	2.736869	0.878444
1	-2.584147	-2.874632	0.427063
1	-4.941282	-1.958501	0.130383
1	-5.093109	0.420145	-0.810461
1	4.492762	-0.565646	-0.488516

TS61

Z_{at}	X	Y	Z
8	-0.775208	1.104242	-0.292398
8	-3.146444	2.023800	1.045029
8	-1.773595	-0.871033	-0.779361
6	-1.768152	0.217682	0.130153
6	-3.123973	0.938011	0.124436
6	-4.249792	-0.067928	0.397943
6	-4.144893	-1.305408	-0.503947
6	-2.731094	-1.876953	-0.443272
8	3.291678	-1.505599	1.242207
8	3.632236	-0.198588	-1.304257
8	1.015849	-1.529577	0.643137
8	2.809487	1.665561	-0.280153
6	3.237171	-0.223144	1.087103
6	3.117680	0.349712	-0.174706
6	1.095920	-0.504909	-0.132557
6	0.541051	0.866914	0.207092
6	1.407403	1.914683	-0.513208
1	-3.255101	1.674708	1.936671
1	-1.545366	-0.157108	1.145736

1	-3.243013	1.389087	-0.864115
1	-4.182328	-0.383349	1.449744
1	-4.373929	-1.034765	-1.539721
1	-2.511908	-2.276819	0.558311
1	2.120781	-1.788776	1.008764
1	3.035286	0.428481	1.942695
1	1.200062	-0.692167	-1.208921
1	0.557806	1.002172	1.295667
1	1.199393	1.867936	-1.586215
1	1.201737	2.920822	-0.153479
1	-2.583907	-2.679635	-1.166656
1	-4.870745	-2.065512	-0.197531
1	-5.213955	0.433292	0.280242
1	4.003101	-1.063154	-1.070148

FRAG35

Z_{at}	X	Y	Z
8	0.740101	1.082560	0.389596
8	3.320897	2.130373	-0.309840
8	1.569794	-1.031001	0.452872
6	1.747490	0.262265	-0.112760
6	3.114976	0.847484	0.265083
6	4.225259	-0.140208	-0.116291
6	3.941353	-1.552439	0.412812
6	2.536821	-1.988381	0.007909
8	-4.714272	2.121091	-3.067654
8	-3.086397	0.310469	-1.715954
8	-2.094082	-1.058423	0.543090
8	-2.811440	1.854141	0.022558
6	-4.084179	2.428336	-1.890252
6	-3.332932	1.562323	-1.210633
6	-1.156183	-0.368132	0.875209
6	-0.578819	0.729978	-0.011182
6	-1.397253	2.037943	0.105411
1	3.483462	2.030708	-1.254649
1	1.659430	0.183202	-1.214121
1	3.104262	1.011085	1.345729
1	4.300271	-0.173457	-1.212989
1	4.018161	-1.567835	1.504755
1	2.465070	-2.104875	-1.083976
1	-4.253463	3.436473	-1.545561
1	-0.678160	-0.479743	1.863864
1	-0.589871	0.376745	-1.047790
1	-1.212037	2.476440	1.086810
1	-1.052462	2.733492	-0.665472
1	2.250480	-2.933557	0.469925
1	4.677749	-2.263352	0.025037
1	5.180486	0.240567	0.253133
1	-2.972317	-0.323377	-0.980158
1	-4.532465	1.193665	-3.268636

TS64

Z_{at}	X	Y	Z
8	0.848776	0.921819	0.619106
8	1.597793	2.837442	-1.296412
8	2.249510	-0.608407	-0.323079
6	1.502990	0.576267	-0.566787
6	2.427922	1.724863	-0.969301
6	3.298702	1.300537	-2.161901
6	3.990364	-0.046857	-1.914992
6	2.958802	-1.080169	-1.473197
8	-1.257206	-1.268205	-2.313230
8	-2.278470	1.174384	-1.802563
8	-0.412580	-2.061048	2.178449
8	-2.812827	0.564305	0.340025
6	-1.764023	-0.978833	-1.071109
6	-2.399117	0.239483	-0.798990
6	0.322238	-1.177190	1.811896
6	-0.173780	0.044543	1.059557
6	-1.261178	0.714259	1.670324
1	2.158724	3.598445	-1.475928
1	0.776952	0.387478	-1.372628
1	3.053986	1.952619	-0.096726
1	2.649695	1.231596	-3.042884
1	4.750887	0.052425	-1.133417
1	2.246921	-1.296079	-2.282932
1	-2.015920	-1.852858	-0.485391
1	1.411390	-1.188499	1.988241
1	-0.701546	-0.491761	0.020313
1	-1.853784	0.186468	2.401759
1	-1.270659	1.794639	1.681196
1	3.423308	-2.018762	-1.168827
1	4.498101	-0.388484	-2.822521
1	4.035428	2.083579	-2.371100
1	-2.571070	2.025242	-1.451098
1	-1.294094	-0.464096	-2.848492

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FRAG34

Z_{at}	X	Y	Z
8	0.172078	-1.009435	-0.160426
8	2.737501	-2.046984	-0.922200
8	1.121599	0.940118	0.526712
6	1.355643	-0.448147	0.320603
6	2.471237	-0.667303	-0.711004
6	3.730067	0.102970	-0.293469
6	3.418799	1.568330	0.038212
6	2.262422	1.641399	1.030182
8	-3.036028	2.223288	-0.546137
8	-3.874997	-0.253924	-0.910384
8	-3.071285	-1.159968	1.422633
6	-2.164400	1.386989	-0.481272
6	-2.488390	-0.090303	-0.690881
6	-2.070609	-0.881633	0.543905
6	-0.812133	-1.251418	0.783902
1	3.197447	-2.401094	-0.152819
1	1.632343	-0.912638	1.285676
1	2.097057	-0.295020	-1.668490
1	4.158702	-0.385010	0.594268
1	3.141514	2.109229	-0.872450
1	2.556803	1.216659	2.002069
1	-1.113551	1.629355	-0.259543
1	-0.521499	-1.805890	1.670027
1	1.929608	2.666632	1.196818
1	4.300806	2.064605	0.455394

1	4.476061	0.021721	-1.087794
1	-4.249445	0.643352	-0.950666
1	-1.912050	-0.440560	-1.555003
1	-3.902018	-1.046955	0.932013

TS67

Z_{at}	X	Y	Z
8	-0.034202	1.497589	1.753019
8	-1.407603	1.691553	-1.483892
8	-2.606388	-0.295190	1.297800
6	-2.112945	0.684001	0.564804
6	-1.460186	0.509595	-0.687819
6	-1.750036	-0.790875	-1.431714
6	-1.816609	-1.932750	-0.409107
6	-2.802583	-1.614071	0.700436
8	4.012250	-1.259472	0.205489
8	1.440352	-1.568887	-0.414629
8	2.040174	1.286666	-1.169060
6	3.261894	-0.451889	0.696531
6	1.759315	-0.484417	0.440862
6	1.303318	0.858017	-0.069646
6	0.728262	1.809150	0.813758
1	-2.299454	1.930960	-1.757891
1	-2.236143	1.660116	1.011884
1	-0.257355	0.465269	-0.410085
1	-2.695069	-0.703346	-1.982167
1	-0.818938	-2.108719	-0.002236
1	-3.835080	-1.622764	0.337482
1	3.620082	0.355375	1.361050
1	0.831059	2.868745	0.504636
1	-2.722552	-2.304927	1.538485
1	-2.134465	-2.862667	-0.890221
1	-0.958007	-0.976614	-2.158643
1	2.284346	-1.966191	-0.682912
1	1.274543	-0.620682	1.417887
1	1.539563	1.962196	-1.639058

TS68

Z_{at}	X	Y	Z
8	-0.038525	-0.405583	-0.637363
8	-1.221852	2.194179	-0.804389
8	-2.016291	-1.314562	0.027696
6	-1.252039	-0.118269	-0.006670
6	-1.967042	0.979624	-0.806114
6	-3.389237	1.181568	-0.270650
6	-4.142043	-0.149115	-0.141572
6	-3.295788	-1.149318	0.640379
8	4.068268	-0.486924	-1.426762
8	3.512233	1.200487	0.972523
8	2.466355	-1.085253	1.882861
6	2.928546	-0.372093	-1.210253
6	2.395321	0.698033	0.296277
6	1.789409	-0.423287	0.916759
6	0.875043	-1.155031	0.122589
1	-1.336872	2.626788	0.049161
1	-1.071139	0.223849	1.029754
1	-1.991663	0.652283	-1.848518
1	-3.323973	1.654610	0.720454
1	-4.351729	-0.560774	-1.134074
1	-3.169700	-0.816398	1.682656
1	1.844739	-1.217410	-0.942175
1	0.517364	-2.119852	0.471029
1	-3.747085	-2.142177	0.654540
1	-5.103790	0.000422	0.359590
1	-3.920364	1.882148	-0.920007
1	4.249924	1.265646	0.350553
1	1.759896	1.433742	-0.186180
1	3.234428	-0.538225	2.116378

TS69

Z_{at}	X	Y	Z
8	-0.141578	0.641846	0.408764
8	1.430361	0.084834	-1.862640
8	1.703091	0.748024	1.751647
6	1.168546	0.180806	0.568880
6	1.976707	0.622834	-0.657483
6	3.452077	0.262364	-0.469147
6	3.976727	0.767750	0.883059
6	3.044852	0.326552	2.009275
8	-2.796708	0.301081	-2.759269
8	-3.911899	-0.711973	-0.796916
8	-3.236868	-0.693244	1.686974
6	-2.024832	0.238371	-1.723137
6	-2.658109	-0.420434	-0.591981
6	-2.246203	-0.286987	0.861718
6	-1.076741	0.170443	1.318454
1	1.739743	-0.821396	-1.972009
1	1.171660	-0.921425	0.661365
1	1.856739	1.706212	-0.741371
1	3.554783	-0.831970	-0.512361
1	4.032893	1.860938	0.876228
1	3.072584	-0.767444	2.129248
1	-0.987089	0.536495	-1.804136
1	-0.842611	0.270453	2.369904
1	3.318361	0.778830	2.962986
1	4.987787	0.390932	1.066531
1	4.034005	0.669931	-1.299714
1	-3.677514	-0.032298	-2.373472
1	-1.866013	-1.240768	-1.081704
1	-3.994506	-0.868336	1.088035

C4H6O4

Z_{at}	X	Y	Z
8	-2.872764	0.400938	-0.633522
8	2.746076	-0.218261	0.330867
8	1.031675	1.069702	-1.231010
8	-1.158329	-0.886875	0.928447
6	1.640005	-0.703353	0.285689
6	0.559127	-0.082248	-0.583311
6	-0.685818	0.265055	0.280687
6	-1.766713	0.886079	-0.588347
1	1.361763	-1.600324	0.861277
1	-1.488499	1.783035	-1.163973
1	1.967142	1.165312	-0.986586
1	0.253042	-0.846007	-1.314915
1	-2.093791	-0.982533	0.684021
1	-0.379745	1.028867	1.012240

TS70

Z_{at}	X	Y	Z

8	-2.233566	-0.178947	-1.551425
8	1.297325	-0.926577	1.078408
8	1.847351	1.433912	-0.184280
8	-0.585260	0.425726	1.497606
6	1.058716	-0.810229	-0.184086
6	1.207398	0.432856	-0.795482
6	-0.890028	0.587968	0.255371
6	-1.755736	-0.395823	-0.460592
1	0.664400	-1.646475	-0.766258
1	-1.938373	-1.340030	0.091193
1	2.099526	1.128550	0.704714
1	0.981052	0.613201	-1.838322
1	0.291473	-0.311298	1.567829
1	-0.862578	1.594917	-0.168569

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Z_{at}	X	Y	Z
8	0.229420	-0.445287	-1.123074
8	-0.725116	2.126813	-0.436818
8	-1.603887	-1.410891	-0.176513
6	-0.759012	-0.260756	-0.167793
6	-1.567765	0.987018	-0.534457
6	-2.776931	1.131370	0.397120
6	-3.594296	-0.156249	0.446694
6	-2.667913	-1.330762	0.767899
8	3.576344	1.304209	0.759743
8	3.407689	-1.388447	0.379389
6	2.485448	0.776919	0.075189
6	2.422245	-0.546581	-0.070725
6	1.301369	-1.299404	-0.730069
1	-1.301052	2.901650	-0.433371
1	-0.322077	-0.140393	0.837454
1	-1.914557	0.851562	-1.570126
1	-2.401592	1.365795	1.398780
1	-4.072230	-0.334237	-0.524313
1	-2.262963	-1.230549	1.786573
1	0.944124	-2.097073	-0.068622
1	-3.195694	-2.282914	0.708055
1	-4.384107	-0.070276	1.198807
1	3.705426	2.220845	0.503329
1	1.710012	1.447681	-0.265552
1	4.112629	-0.843807	0.755081
1	1.665579	-1.779186	-1.642756
8	-3.542531	2.286870	0.033868
1	-4.032432	2.090675	-0.773583

TS71

Z_{at}	X	Y	Z
8	-0.548341	-0.088639	1.589870
8	0.769096	2.041003	0.328738
8	0.878097	-1.615376	0.694319
6	0.316094	-0.299252	0.675119
6	1.423632	0.779820	0.542517
6	2.395074	0.478703	-0.591273
6	2.922270	-0.948396	-0.468109
6	1.739584	-1.917326	-0.398816
8	-1.111869	1.523605	-1.616726
8	-2.835638	-1.463642	-0.524373
6	-1.485755	0.246991	-1.367428
6	-2.392329	-0.164769	-0.366235
6	-2.480941	0.503129	0.820962
1	1.462903	2.695691	0.178243
1	-0.266986	-0.248591	-0.437392
1	1.972141	0.810424	1.491103
1	1.854970	0.591956	-1.541785
1	3.529471	-1.036633	0.437922
1	1.171914	-1.897973	-1.341823
1	-3.057992	0.110465	1.647186
1	2.079781	-2.940639	-0.235706
1	3.559067	-1.197562	-1.324505
1	-0.637291	1.914682	-0.853479
1	-1.402235	-0.399504	-2.237878
1	-2.781099	-1.922919	0.321813
1	-2.164082	1.531643	0.894631
8	3.415832	1.484619	-0.507520
1	3.952906	1.462899	-1.305998

FRAG37

Z_{at}	X	Y	Z
8	-0.040788	-0.134604	0.126770
8	1.957715	-0.801877	-1.806233
8	1.534052	0.670077	1.548162
6	1.316366	-0.232971	0.485371
6	2.169370	0.114142	-0.741578
6	3.644120	0.206074	-0.333611
6	3.835275	1.113014	0.889507
6	2.890578	0.686059	2.007944
8	-3.149211	1.187321	-2.424921
8	-4.188463	-0.061903	-0.353648
8	-3.083868	-1.188736	1.731181
6	-2.237684	0.694036	-1.474041
6	-2.958917	-0.002929	-0.337826
6	-2.260772	-0.615237	0.801196
6	-0.929575	-0.659742	1.006584
1	2.423793	-1.623817	-1.616091
1	1.533445	-1.263402	0.822861
1	1.816841	1.080420	-1.111786
1	4.004764	-0.805191	-0.094817
1	3.624708	2.153424	0.622264
1	3.162690	-0.310903	2.387251
1	-1.533940	-0.006896	-1.938975
1	-0.529852	-1.123175	1.901934
1	2.904986	1.383497	2.845552
1	4.870719	1.070463	1.241319
1	4.228284	0.556422	-1.187856
1	-4.035113	0.958889	-2.103428
1	-3.987500	-1.046057	1.402096
1	-1.631754	1.509752	-1.059318

TS72

Z_{at}	X	Y	Z
8	-0.416778	0.634826	0.454773
8	2.149898	1.584157	-1.736895
8	2.314490	-1.576660	0.016527
6	1.897662	-0.529603	-0.664743
6	2.533697	0.730976	-0.676603
6	3.999975	0.774796	-0.256872
6	4.217104	-0.221572	0.890731
6	3.688756	-1.598467	0.525410
8	2.063412	0.131005	3.988464

8	2.258293	2.611783	3.095877
8	1.329273	3.687692	0.878216
6	1.155748	0.511202	2.973407
6	1.527347	1.878386	2.416807
6	1.045332	2.364880	1.130830
6	-0.104789	1.826907	0.438010
1	2.445260	1.207248	-2.572350
1	0.939160	-0.680358	-1.146569
1	1.945923	1.354858	0.263868
1	4.636973	0.525794	-1.113810
1	3.730717	0.128053	1.804820
1	4.286475	-2.067581	-0.261370
1	1.136440	-0.255620	2.201843
1	-0.630369	2.553066	-0.207620
1	3.645769	-2.266607	1.383445
1	5.282010	-0.316369	1.121648
1	4.258201	1.789284	0.052745
1	2.424733	0.957121	4.345697
1	1.869850	3.987146	1.629124
1	0.126832	0.584668	3.359042

C3H6O2

Z_{at}	X	Y	Z
6	1.482728	-1.317314	0.364501
1	2.562801	-1.145462	0.406830
1	1.155862	-1.723289	1.322891
6	0.763002	-0.049916	0.049824
6	-0.135305	0.542691	0.841949
1	-0.417604	0.158287	1.813256
8	1.118355	0.492612	-1.154951
1	0.618745	1.314402	-1.263691
8	-0.652817	1.777378	0.452012
1	-1.600683	1.800601	0.614552
1	1.298906	-2.062800	-0.415189

TS73

Z_{at}	X	Y	Z
6	1.463499	-1.252586	0.376288
1	2.533006	-1.049666	0.277234
1	1.241254	-1.610575	1.381419
6	0.660054	-0.046824	0.056309
6	-0.310723	0.664523	0.833972
1	-1.306449	0.512656	0.404905
8	0.767326	0.572018	-1.065583
1	0.075614	1.427089	-0.404224
8	-0.349665	0.554230	2.234773
1	0.181604	1.261557	2.609915
1	1.215176	-2.029582	-0.354930

C4H6O4_2

Z_{at}	X	Y	Z
8	2.464399	0.675266	-0.517287
8	-2.976054	0.103307	-0.063612
8	-0.971162	-1.522617	-0.765736
8	0.862993	0.401481	1.597216
6	-1.724290	0.325619	0.529989
6	-0.689924	-0.661177	0.039795
6	0.741776	-0.545701	0.575980
6	1.688048	-0.243984	-0.584684
1	-1.361531	1.340958	0.317058
1	1.615122	-0.907709	-1.461801
1	-2.881597	-0.654585	-0.659894
1	1.595913	0.990563	1.354613
1	-1.784829	0.249235	1.623497
1	1.007415	-1.554428	0.931855

TS74

Z_{at}	X	Y	Z
8	0.150903	1.157655	-1.079086
8	1.978324	1.749887	-1.195169
8	3.577193	-0.521040	0.869855
8	1.576357	-1.840780	-0.507026
6	2.829442	1.600898	-0.077212
6	2.727101	0.131603	0.329284
6	1.387338	-0.500529	-0.128026
6	0.831278	0.325790	-1.273645
1	3.865499	1.841113	-0.328991
1	1.009462	-0.093393	-2.269782
1	0.777873	1.975477	-1.010798
1	2.320942	-2.186890	0.006536
1	2.514946	2.231743	0.763454
1	0.684763	-0.407265	0.714080

TS75

Z_{at}	X	Y	Z
8	1.303666	-1.983544	0.653696
8	-2.837427	-0.518034	0.051741
8	-1.370168	1.369846	0.147242
8	1.374926	1.423953	-0.183012
6	-1.607153	-0.876744	0.141674
6	-0.705780	0.259920	0.267402
6	0.772836	0.361259	0.525288
6	1.529968	-0.916364	0.150786
1	-1.283610	-1.876974	0.433792
1	2.311249	-0.761747	-0.617587
1	-2.347098	0.945196	0.096715
1	0.806722	2.201920	-0.126715
1	-0.919534	-0.699316	-0.937229
1	0.880759	0.494847	1.614712

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FRAG 1

Z_{at}	X	Y	Z
6	3.877385	-1.255446	0.064702
6	3.914657	0.258137	-0.178399
6	2.572129	-1.832154	-0.468513
1	3.950003	-1.468523	1.135984
6	2.651470	0.952218	0.344629
1	3.995240	0.447342	-1.258932
1	2.520625	-1.735520	-1.563178
1	2.455885	-2.886527	-0.214578
6	1.389634	0.244773	-0.173985
1	2.613575	0.904651	1.435924
1	1.308314	0.358184	-1.270951
8	1.450024	-1.162946	0.124465
8	0.283099	0.778167	0.459065

6	-0.999031	0.582328	-0.153305
6	-1.718046	-0.646639	0.407913
6	-1.825925	1.832193	0.142932
1	-0.880669	0.461199	-1.236928
6	-3.185329	-0.555680	0.081565
1	-1.570934	-0.662177	1.498121
1	-1.951884	1.940208	1.228010
1	-1.329256	2.720550	-0.244686
6	-3.763828	0.570683	-0.340419
8	-3.106786	1.771424	-0.482376
8	2.638003	2.337360	0.024837
1	2.848784	2.446956	-0.909253
8	-1.249243	-1.877456	-0.144106
1	-0.293784	-1.922502	0.029048
1	-4.810060	0.632132	-0.605951
1	4.726110	-1.745066	-0.423112
1	4.790106	0.716714	0.287833
8	-3.915775	-1.705952	0.260589
1	-3.308758	-2.444123	0.110877

TS 77

Z_{at}	X	Y	Z
6	-3.991904	0.863079	-0.024499
6	-4.008535	-0.404380	0.837867
6	-3.015589	0.690937	-1.182839
1	-3.681693	1.723904	0.577612
6	-2.594188	-0.822293	1.264084
1	-4.460474	-1.228733	0.268667
1	-3.370601	-0.089512	-1.872506
6	-1.656839	-0.943325	0.037284
1	-2.158058	-0.065221	1.921992
1	-2.067350	-1.707869	-0.654347
8	-1.714050	0.342259	-0.702006
8	-0.380610	-1.197756	0.355983
6	1.377561	-0.754113	-0.909422
6	1.406326	0.502726	-0.252423
6	2.328189	-1.765519	-0.346193
1	0.816625	-0.925533	-1.817531
6	2.668472	0.842815	0.456080
1	0.600512	-0.059804	0.507287
1	2.010464	-2.054186	0.663499
1	2.403727	-2.652212	-0.972453
6	3.714574	0.010528	0.378947
8	3.641705	-1.190446	-0.296323
8	0.753388	1.615618	-0.789920
1	-0.198749	1.382922	-0.833041
1	4.697351	0.228431	0.771766
1	-4.992648	1.082141	-0.411491
1	-4.620868	-0.269191	1.733346
8	2.707456	2.019369	1.145348
1	2.024432	2.591625	0.768032
1	-2.894956	1.613455	-1.754871
8	-2.615693	-2.018146	2.032087
1	-2.823676	-2.760256	1.453437

TS 78

Z_{at}	X	Y	Z
6	-3.810530	-1.319170	-0.336100
6	-3.947254	0.163166	0.031604
6	-2.537926	-1.889550	0.276411
1	-3.766360	-1.435829	-1.423596
6	-2.676824	0.954349	-0.302929
1	-4.140813	0.252061	1.110612
1	-2.599294	-1.894255	1.374463
1	-2.342330	-2.909182	-0.057817
6	-1.437599	0.263039	0.286459
1	-2.528494	0.998675	-1.384903
1	-1.474498	0.281744	1.390499
8	-1.397544	-1.119062	-0.134408
8	-0.300471	0.886565	-0.182846
6	0.878781	0.793022	0.595343
6	1.844944	-0.680402	-0.429585
6	1.685212	1.933239	0.578146
1	0.766498	0.211193	1.505632
6	3.229876	-0.648134	-0.139660
1	1.516240	-0.177835	-1.332905
1	1.367670	2.797631	0.013443
1	2.367708	2.107469	1.395546
6	3.882750	0.565086	-0.285885
8	3.221805	1.592308	-0.673385
8	-2.767597	2.306501	0.121924
1	-3.033889	2.330330	1.047944
8	1.235906	-1.871430	-0.132619
1	0.271401	-1.778029	-0.262309
1	4.913448	0.670885	0.073593
1	-4.677458	-1.886031	0.017437
1	-4.795871	0.624336	-0.479358
8	3.832646	-1.699442	0.498140
1	3.227947	-2.452129	0.456225

TS 81

Z_{at}	X	Y	Z
6	-2.558031	-0.750413	-0.278038
6	-2.214931	0.687261	0.133274
6	-1.482979	-1.704708	0.232469
1	-2.611962	-0.826834	-1.368834
6	-0.781546	1.062608	-0.261733
1	-2.313074	0.784937	1.224380
1	-1.491187	-1.740466	1.333450
1	-1.626253	-2.719592	-0.140285
6	0.194791	-0.016517	0.226987
1	-0.684833	1.108840	-1.349360
1	0.227177	-0.021920	1.334102
8	-0.190620	-1.304911	-0.227305
8	1.461602	0.256309	-0.289603
6	2.506029	-0.440600	0.256796
6	3.760614	-0.243367	-0.132690
1	2.231804	-1.164435	1.018564
1	4.007616	0.471707	-0.907111
1	4.558260	-0.810860	0.325919
8	-0.424100	2.357055	0.204027
1	-0.569613	2.400744	1.155808
1	-3.535871	-1.042352	0.118322
1	-2.906050	1.407968	-0.310595

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Z_{at}	X	Y	Z
6	-0.748495	-0.714171	-0.008893

6	0.096550	0.337621	-0.005621
1	-0.394159	-1.735601	-0.004526
6	1.537114	0.193168	0.003958
8	2.267770	1.172970	0.006630
8	-2.085975	-0.600586	-0.017727
1	-2.322087	0.338988	-0.021474
1	1.936281	-0.835987	0.008671
8	-0.411294	1.605607	-0.011495
1	0.350778	2.208662	-0.007812

TS 84

Z_{at}	X	Y	Z
6	-0.695148	-0.489796	0.022313
6	0.117607	0.675301	0.202064
1	-1.308805	-0.771599	-0.833308
6	1.576044	0.452051	0.199423
8	2.324306	1.393813	0.000329
8	-0.582771	-1.245890	1.032856
1	0.073194	-0.163108	1.465701
1	1.934524	-0.571172	0.392624
8	-0.284538	1.903778	-0.230426
1	0.532386	2.408335	-0.400332

TS 85

Z_{at}	X	Y	Z
6	1.087803	-0.484146	0.578527
6	-0.517458	0.295568	-0.838849
1	0.041083	-0.728562	1.215165
6	-1.097516	-0.874467	-0.368227
8	-1.334885	-0.962155	0.894931
8	2.230426	-0.435297	0.546240
1	-1.147869	-1.752612	-1.019140
8	-0.607924	1.447958	-0.112361
1	-1.134106	1.242016	0.677889
1	-0.191396	0.446339	-1.859060

TS 86

Z_{at}	X	Y	Z
6	0.615239	0.479778	0.306889
1	0.690746	1.473913	0.750255
6	-0.470566	-0.438597	0.265544
1	-0.248682	-1.311252	0.887153
8	1.606591	-0.027400	-0.321338
1	0.671659	-0.870319	-0.638734
8	-1.805802	-0.045880	0.403764
1	-2.130657	0.247522	-0.451922