

**The Mechanism of Selective Catalytic Reduction of NO_x on Cu-SSZ-13 –
A Computational Study**

Supporting Information

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Table S1. Computed energy components for optimized structures for Cu-SSZ-13 structures.

Structure	E(SCF)/(kcal/mol)	ZPE/(kcal/mol)	TS(gas)/(kcal/mol) 298.15 K	G(gas)/(kcal/mol)
	cc-pVTZ(-f)/(LACVP3P)	6-31G**/LACVP	6-31G**/LACVP	6-31G**/LACVP
1	-3664238.17	168.67	80.82	-3664150.32
2	-3745704.88	172.67	87.00	-3745619.21
2A	-3745697.41	171.30	87.75	-3745613.86
3	-3745702.53	173.68	87.11	-3745615.96
4	-3781186.07	196.24	89.87	-3781079.65
5	-3664643.30	173.47	81.55	-3664551.37
6	-3746119.14	177.51	86.04	-3746027.68
7	-3700126.35	200.31	92.03	-3781081.85
7A	-3781594.24	204.19	85.43	-3700011.46
8	-3758928.12	178.72	88.16	-3758837.56
8A	-3840402.52	184.04	89.85	-3840308.33
8B	-3794406.42	203.04	92.48	-3794295.86
8A-TS	-3840386.72	183.17	88.33	-3840291.88
9	-3840398.55	184.49	88.64	-3840302.70
9-TS	-3840366.82	183.08	88.13	-3840271.86
10	-3840376.83	183.04	94.03	-3840287.82
11	-3793258.31	181.30	90.43	-3793167.43
12	-3840433.76	185.25	90.93	-3840339.44
NH₃	-35457.89	21.11	14.38	-35451.15
N₂	-68676.83	3.37	13.66	-68687.12
NO	-81453.73	2.73	14.64	-81465.64
NO⁺	-81235.58	3.38	14.14	-81246.34
HNO₃	-176163.15	16.02	19.06	-176166.19
NO₃⁻	-175822.94	8.66	18.62	-175832.90
HNO₂	-129006.12	12.23	17.67	-129011.56
NO₂⁻	-128648.35	4.75	17.34	-128660.94
N₂O	-115808.43	6.87	15.69	-115817.25
H₂O	-47924.00	13.08	13.88	-47924.80
H₃N⁺-NO	-116745.89	26.97	20.32	-116739.23
NH₄⁺ - -H₂N-NO	-152229.26	48.11	21.96	-152203.11
NH₄⁺ + H₂N-NO	-116534.91	20.82	17.56	-116531.65
13/A'	-3781193.24	195.50	92.10	-3781089.84
TS8	-3781125.32	193.09	90.07	-3781022.31
TS9	-3781159.73	192.34	89.33	-3781056.72
TS10	-3781182.33	195.46	90.72	-3781077.59
TS11	-3781149.46	192.65	85.26	-3781042.05
TS12	-3781146.47	193.81	88.10	-3781040.76
TS13	-3781176.22	193.99	92.05	-3781074.28
TS14	-3781157.52	191.82	90.59	-3781056.28
13-TS	-3781186.85	194.27	89.39	-3781081.97
14	-3781188.72	196.13	92.05	-3781084.64
14-TS	-3781186.57	194.35	89.59	-3781081.81
15	-3781186.13	194.68	92.60	-3781084.05
15-TS	-3781178.06	192.78	90.71	-3781076.00
16	-3741316.72	177.67	84.55	-3741223.60
17	-3776798.06	202.96	86.78	-3776681.88

17-TS	-3776780.56	198.72	85.82	-3776667.66
18	-3776789.66	200.58	87.50	-3776676.59
19	-3858272.73	206.77	90.31	-3858156.27
20	-3810310.91	189.67	87.59	-3810208.83
21	-3810342.02	190.99	89.43	-3810240.45
22	-3693772.77	169.57	81.35	-3693684.55

Table S2. Electronic energy component for small molecules computed with DFT and CCSD(T) for NO_s reduction.

Molecule	E(SCF)/(kcal/mol)	E (kcal/mol)
	cc-pVTZ(-f)/(LACV3P)	(CCSD(T)/cc-pVQZ)
NH ₃	-35457.89	-35449.66
N ₂	-68676.83	-68651.81
NO	-81453.73	-81421.68
NO ⁺	-81235.58	-81210.41
HNO ₃	-176163.15	-176083.28
NO ₃ ⁻	-175822.94	-175747.56
HNO ₂	-129006.12	-128950.84
NO ₂ ⁻	-128648.35	-128596.90
N ₂ O	-115808.43	-115750.63
H ₂ O	-47924.00	-47916.23
H ₃ N ⁺ -NO	-116745.89	-116665.36
NH ₄ ⁺ ---H ₂ N-NO	-152229.258	-4142318.89
NH ₄ ⁺ + H ₂ N-NO	-116534.905	-116458.99

Table S3. Coupled-cluster electronic energies with zero-point energy and entropy corrections for unassisted decomposition of nitrosamide.

Structure	E(SCF)/(kcal/mol)	ZPE/(kcal/mol)	TS(gas) (kcal/mol)	G(gas)/(kcal/mol)
	(CCSD(T)/cc-pVQZ)	6-31G**/LACVP	6-31G**/LACVP	6-31G**/LACVP
A	-116492.92	19.60	18.52	-116491.84
B	-116485.31	21.15	17.58	-116481.73
C	-116459.98	17.14	17.60	-116460.44
D	-116493.13	20.36	17.79	-116490.56
E	-116487.20	19.48	17.81	-116485.53
F	-116493.44	19.86	17.89	-116491.48
TS1	-116429.87	16.28	17.81	-116431.40
TS2	-116459.98	17.14	17.60	-116460.44
TS3	-116484.08	19.16	17.68	-116482.60
TS4	-116452.03	17.42	18.69	-116453.30
TS5	-116454.54	17.55	18.79	-116455.78
TS6	-116483.67	18.76	17.77	-116482.68
TS7	-116465.95	16.04	23.74	-116473.65

Table S4: Cartesian coordinates of optimized structures**1**

Al	8.481919520	1.223572488	6.354284266
Cu	6.783507369	3.589544587	6.128531420
O	5.117822306	4.834039310	9.017505785
O	6.818995161	1.974403226	9.219045043
O	8.580147130	4.943053987	9.130282542
O	8.615757940	3.046222770	6.479814808
O	4.858695602	2.980776442	6.246511775
O	6.785662860	5.643982369	6.197482175
O	6.899272647	6.984304374	9.897774741
O	4.187422334	2.388587752	9.744040685
O	9.443772577	2.451892877	9.666356521
O	9.476815411	5.463888580	5.851932353
O	6.745384611	1.384643253	5.845238334
O	4.068473242	5.421915920	5.941582595
O	5.167545691	7.321559608	7.608453955
O	4.905629295	0.715671827	7.782475169
O	10.716115627	3.987223471	7.811234045
O	8.701429070	0.498750262	7.932988888
O	8.528186516	7.187454932	7.733365305
O	2.877633457	3.861347205	7.924531490
Al	5.292583551	6.589638474	9.245816668
Si	5.313011266	1.273631029	9.320508277
Si	9.923686384	3.981521584	9.288556268
Si	10.016735115	3.962939112	6.315502385
Si	5.148270914	1.290766021	6.275110855
Si	5.258171529	6.544494609	6.199931886
Si	8.270040712	6.491295658	6.275531769
Si	3.489513532	3.968407595	6.417188431
Si	3.791395899	3.954173043	9.361496715
Si	8.337175521	6.574700835	9.293733098
Si	8.327711973	1.286067630	9.323447537
O	9.661315588	0.819829288	5.128291831
H	10.117279485	-0.035102138	5.160435504
O	10.982875297	3.323620469	5.163471636
H	10.718676399	2.383219348	4.977005056
O	8.082645907	7.684019855	5.130003301
H	8.675265029	8.447273153	5.243558275
O	5.273036347	7.475161339	4.847254190
H	6.156923545	7.872272890	4.694908916
O	2.412301379	3.324012198	5.332987482
H	1.481104230	3.384697725	5.616648951
O	2.833753471	4.574800059	10.542781853
H	3.047889223	5.545424625	10.647737247
O	3.942539642	7.027385156	10.308291613
H	3.639631209	7.945237983	10.378558567
O	9.603726348	7.127035459	10.234618250
H	9.349081745	7.819975573	10.867039697
O	10.932345595	4.535582638	10.460344774
H	10.772614770	5.490530790	10.626134576
O	8.201363862	0.208617197	10.593768586
H	8.930524485	-0.428451826	10.677172086
O	5.314955204	0.005998667	10.361088099
H	6.218721951	-0.170153006	10.703942226
O	4.212022636	0.551951116	5.148637027
H	3.445092569	1.193578329	4.818620732

2

Al	8.071018140	5.915881046	7.535669472
Cu	6.895758510	5.708280794	4.935264000
O	3.926020247	9.517304986	5.710678602
O	5.785312940	8.872212460	8.351051863
O	7.336685645	10.319386226	5.759257923
O	8.492195452	6.446650091	5.812571030
O	4.189149982	5.725669943	5.740592972
O	6.012866330	7.933130695	3.529409953
O	5.378762934	11.691811528	4.388195561
O	3.082195128	8.767474336	8.190814121
O	8.280509178	9.901591788	8.253320275
O	8.668633022	7.970831495	3.682168651
O	6.465880613	5.317617387	6.841803844
O	3.463723532	7.064178248	3.638932691
O	4.009023559	9.673477115	2.868396724
O	4.498268464	6.495115388	8.369940975
O	9.589490993	8.910411328	6.129115005
O	7.940475920	7.252514287	8.638843455
O	7.386128315	10.323341552	3.126441501
O	2.135140131	7.539885659	6.030582907
Al	3.910795274	10.677606103	4.371372647
Si	4.415144833	8.093676910	8.865043150
Si	8.700681174	10.214266339	6.690792273
Si	9.440649297	7.637249336	5.107489826
Si	4.836441950	5.376391532	7.234685913
Si	4.448045455	8.124015560	2.842353654
Si	7.386787937	8.694087129	2.946140035
Si	2.852152525	6.447326142	5.052312387
Si	2.648466385	9.049972647	6.607301715
Si	6.927348570	11.258006124	4.453871272
Si	7.324045362	8.729702133	8.933419234
O	9.080316418	4.606606064	8.063167494
H	9.364586651	4.611449613	8.990906192
O	10.931580955	7.070921881	4.690897911
H	11.617915509	7.164783847	5.395492925
O	7.383643836	8.341883611	1.314645421
H	7.908169529	8.955998315	0.771281461
O	4.587184998	7.452533448	1.321995734
H	5.407535755	7.770472392	0.885862494
O	1.775597499	5.250270166	4.683833191
H	0.849431378	5.534718803	4.772141965
O	1.381472261	10.095384589	6.576820855
H	1.526388221	10.763601231	5.848115562
O	2.389036251	11.562431860	4.516030625
H	1.988803801	11.981081292	3.737560389
O	7.943069401	12.590695779	4.499895903
H	7.468395310	13.431608522	4.384531935
O	9.596415691	11.587776196	6.607827335
H	9.224664378	12.205903340	5.937782032
O	7.168323528	9.013108872	10.572261188
H	7.968217815	8.859997418	11.102472328
O	4.316526326	8.118661443	10.508830615
H	5.134908146	8.487694177	10.902935788
O	4.371361661	3.885122371	7.768843728
H	3.816900866	3.914187766	8.568343780
N	5.974362909	5.247945524	3.453950712
O	5.060175692	5.172699305	2.770015868

2A

Al	8.407721865	1.367104870	6.222553368
Cu	6.776222833	3.863969714	6.228013495
O	5.085529296	4.845737021	9.104533435
O	6.785654591	1.959280530	9.111924712
O	8.543277667	4.968590248	9.107071576
O	8.571434070	3.172296445	6.478015391
O	4.821196763	3.152453912	6.297464546
O	6.703288057	5.869614306	6.339231289
O	6.884746611	6.948526644	10.067761161
O	4.179430673	2.370090277	9.778368803
O	9.405198996	2.443198683	9.560230020
O	9.377331778	5.633542480	5.937577146
O	6.666253953	1.507437651	5.771130878
O	3.986858823	5.596568981	6.130373427
O	5.075699563	7.428378292	7.864391568
O	4.789895298	0.812379543	7.697242300
O	10.693883793	4.069541021	7.784790498
O	8.676528911	0.553391489	7.752781299
O	8.481520292	7.319300698	7.889879883
O	2.834506314	3.895236035	8.025742669
Al	5.259072825	6.583220055	9.441119950
Si	5.274483904	1.272774989	9.244965622
Si	9.881835975	3.989465325	9.252921842
Si	9.949246020	4.113152322	6.310985872
Si	5.087922230	1.463238249	6.225362915
Si	5.153636925	6.730583295	6.413606321
Si	8.202631587	6.680707077	6.408074392
Si	3.433785199	4.102550678	6.517370904
Si	3.768853897	3.945298525	9.446491725
Si	8.308565780	6.586304393	9.401166539
Si	8.300465936	1.277374984	9.175835184
O	9.549780370	1.037190411	4.937820561
H	9.999562198	0.179379084	4.891204126
O	10.876132584	3.543607264	5.091390104
H	10.601300848	2.615627466	4.860677295
O	8.008339718	7.899772408	5.293837430
H	8.608086719	8.657998042	5.399916956
O	5.140239995	7.735936892	5.116047373
H	6.028016253	8.110673590	4.937574278
O	2.326926826	3.534204419	5.427754548
H	1.404408261	3.638826061	5.716961276
O	2.833078950	4.511526321	10.672718778
H	3.051655511	5.474609553	10.830512198
O	3.943618745	6.947592220	10.574850027
H	3.664811890	7.859750408	10.745610868
O	9.587385390	7.073245772	10.363140546
H	9.321535937	7.683978808	11.071475902
O	10.868186741	4.494033765	10.463406716
H	10.714882766	5.446585263	10.653206017
O	8.197461407	0.138750359	10.396018192
H	8.888700581	-0.544624290	10.376105214
O	5.311708521	-0.052860118	10.210577124
H	6.227202736	-0.242830193	10.514293833
O	4.191658126	0.772602428	5.037675898
H	3.228003949	0.846236920	5.142075245
N	6.630059143	3.558132591	3.609440302
O	7.240773170	2.761020408	3.016255091

3

O	11.262191179	3.748185205	2.431805881
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O	5.047684449	4.943715152	6.337661884
O	6.817151707	1.979578432	6.595323936
O	8.606274316	5.021278404	6.644284263
O	8.969895279	2.782981643	3.393693294
O	6.809197407	6.331359021	3.296035761
O	4.563451808	2.687981692	3.112754898
O	4.798727016	7.738999746	2.128400028
O	4.399637942	0.118713702	2.483858783
O	9.329481960	0.060875203	2.329303097
O	8.764392055	7.993836968	2.502574309
O	2.322374259	3.837794924	2.310427151
O	6.839190691	6.997319948	6.929675763
O	4.211476256	2.500106542	6.886159985
O	9.391461812	2.510968446	6.834202034
O	9.235956872	5.398386197	3.036159351
O	4.391421450	5.343294886	3.081554877
O	6.774526353	1.334239137	3.093170148
O	4.883529938	7.386446677	4.816212003
O	5.004858903	0.780425425	5.004054188
O	10.570881197	4.143101544	5.011093651
O	8.626531983	0.535322565	5.152678727
O	8.752818521	7.126999037	5.019192492
O	3.040836335	3.898918770	4.918690314
Al	5.160033199	6.747500081	6.431181630
Si	5.261586614	1.314188444	6.529235101
Si	9.919203687	4.019615174	6.505037122
Si	10.012636320	4.022386811	3.456569326
Si	5.197557932	6.743605241	3.374861381
Si	5.168720339	1.207529716	3.427441983
Al	8.518643143	1.043507353	3.476987656
Si	8.371779548	6.730801506	3.474389368
Si	3.562188050	3.969784308	3.368071381
Si	3.692147449	4.005112677	6.427935930
Si	8.339698939	1.271840554	6.541570893
Si	8.366538827	6.716299155	6.568943475
O	2.634138380	4.611287913	7.499888088
O	3.884474633	7.122368025	7.564455924
O	9.448017201	7.392315438	7.593073134
O	11.001512023	4.572021331	7.610250667
O	8.308935735	0.208582463	7.804780740
O	5.197328529	0.084182992	7.595135637
H	3.478759829	7.993240490	7.581424808
H	2.856412950	5.547133653	7.710588146
H	6.053023288	-0.144768625	7.987671778
H	4.417303096	-0.803234564	2.761375122
H	1.872925192	4.657069718	2.076457269
H	10.049774363	0.416810501	1.803661773
H	11.770617982	4.512850449	2.141479078
H	9.375774546	8.631940395	2.886354596
H	5.030978848	8.666132907	2.247081333
H	10.154719588	6.803642225	7.890515983
H	11.914084103	4.272518737	7.531744214
H	8.907475862	-0.543605829	7.728257352
Cu	6.786013677	4.067699406	6.722976208
N	7.305407688	3.007922513	2.034941709
O	6.674477769	3.887434832	2.261985023

4

O	11.253520078	3.639105237	2.582493083
O	5.077928739	4.940031697	6.406816621

O	6.852003045	2.056737237	6.719849176
O	8.628365593	5.057771124	6.816067121
O	8.735854812	3.176447660	3.402609891
O	7.031070777	6.000485400	3.639355168
O	4.506711553	2.612623518	3.180333106
O	5.433737436	7.553752960	2.111568692
O	4.314872902	0.052418485	2.630675105
O	9.457335017	0.584562416	2.198572061
O	8.419686473	8.091396647	2.742906816
O	2.351190113	3.898424282	2.361142004
O	6.819671413	7.028378058	7.109347147
O	4.187903327	2.485069651	6.955360223
O	9.431998785	2.533177113	7.051818284
O	9.654140091	5.715524265	3.213893188
O	4.559238791	5.254270582	3.069004560
O	6.734662343	1.218830223	2.956655003
O	4.984561745	7.347496377	4.819137653
O	5.126740494	0.762718817	5.105354712
O	10.604980955	4.112297143	5.160653657
O	8.679074576	0.800741674	5.063390736
O	8.847526513	7.254092992	5.276909743
O	3.031201447	3.966163811	4.985832038
Al	5.178480540	6.749311642	6.477808760
Si	5.313058409	1.341144858	6.634756708
Si	9.949313521	4.046834962	6.665084743
Si	10.030939264	4.138329170	3.584620101
Si	5.464020306	6.596923638	3.463607965
Si	5.190938146	1.152928244	3.506123360
Al	8.478085657	1.387689562	3.389378087
Si	8.485697853	6.760225147	3.741693705
Si	3.597696844	3.957234808	3.440565555
Si	3.702606130	4.015556101	6.508950962
Si	8.378927954	1.346162449	6.544329042
Si	8.375089083	6.761651277	6.798733061
O	2.644530956	4.623229075	7.596264381
O	3.818481604	7.123090811	7.530379301
O	9.393652324	7.413819636	7.917739609
O	11.030995260	4.638320342	7.772563122
O	8.331815852	0.115403790	7.669719556
O	5.262709929	0.123311792	7.734122967
H	3.387085552	7.988561041	7.477175023
H	2.867412709	5.587753946	7.738672189
H	6.168168111	-0.146416285	7.995762575
H	4.674629560	-0.850298276	2.665346152
H	1.803799080	4.700737730	2.337481055
H	10.313840681	1.009647352	2.029214748
H	12.032792758	4.219247974	2.563983147
H	8.974759692	8.836463827	3.028882207
H	6.228177534	8.122447283	2.075005068
H	10.131118353	6.815584090	8.144562314
H	11.939522883	4.300601588	7.706299225
H	8.886073640	-0.646663195	7.428528752
Cu	6.812580030	4.115031708	6.834074929
N	6.324307501	1.910227728	0.823505829
O	5.200829273	1.780251539	0.651686302
N	6.754423197	3.768973187	1.401006423
H	7.072132407	4.294333600	0.581701731
H	7.512431440	3.655061343	2.106046464
H	5.930601441	4.208604616	1.837336996

Al	8.419410443	1.158948811	6.310931738
Cu	6.777899855	3.811110144	6.037123308
O	5.321144196	4.765338280	9.387773937
O	6.778224260	2.006061373	9.276480088
O	8.385750413	4.948554156	9.241003178
O	8.530998912	2.971738278	6.424699831
O	4.971521427	2.853054791	6.131814137
O	6.786016266	5.893570427	6.090264534
O	6.924045158	7.094274108	9.907006002
O	4.224152486	2.315776978	9.868245840
O	9.359361343	2.481992330	9.746532702
O	9.420997035	5.419023651	5.772065356
O	6.747599547	0.888101620	5.781896595
O	4.188935840	5.364330539	5.821979038
O	4.991792597	7.155343306	7.692342192
O	4.865784059	0.745907952	7.790936192
O	10.525010013	4.081132291	7.843573495
O	8.678041694	0.519230529	7.949031414
O	8.593549737	7.146383537	7.716262556
O	3.220058515	3.944417999	7.926468813
Al	5.313711119	6.682404601	9.347489555
Si	5.320148821	1.186879214	9.314960492
Si	9.791207809	4.010916428	9.327986275
Si	9.904054028	3.904642113	6.311425381
Si	5.220453092	1.145236012	6.219312322
Si	5.235438106	6.602553967	6.188175260
Si	8.328389919	6.559493168	6.198289615
Si	3.686407927	3.890533566	6.344300384
Si	3.827688989	3.840854354	9.461434640
Si	8.346721941	6.622104152	9.274046141
Si	8.299495637	1.287595675	9.325784560
O	9.726972448	0.815071390	5.185618948
H	10.095524623	-0.076184672	5.101588710
O	10.975420204	3.259743190	5.262663650
H	10.719309912	2.308931412	5.080706231
O	8.246837573	7.802022453	5.106100416
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O	5.116223402	7.740798315	5.009620632
H	5.989230005	8.091293593	4.743850525
O	2.470131563	3.266027872	5.419280084
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H	3.411781718	7.746661265	10.287855319
O	9.613212513	7.242465646	10.178026012
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O	10.793552930	4.593518360	10.491362175
H	10.722581943	5.573874704	10.552036373
O	8.173820584	0.182922413	10.583231142
H	8.801773821	-0.556196613	10.511377787
O	5.358564184	-0.091627526	10.333691079
H	6.272802495	-0.233086834	10.674965353
O	4.141948495	0.436670293	5.198512670
H	3.326903691	0.955434295	5.068171328
H	6.177714815	4.274429012	9.465967070

Cu	6.440669263	6.162210118	4.765537350
O	4.125564733	9.804529806	5.924188402
O	5.828904025	8.561151313	8.301128737
O	7.125718164	10.444302035	5.789011028
O	7.843706519	6.944196864	5.969619196
O	4.601884000	6.130472495	5.955740517
O	5.964993849	7.983989992	3.487717717
O	5.359425747	11.650815084	4.134495717
O	3.198768435	8.761406278	8.285716965
O	8.209932036	9.726799042	8.154505241
O	8.658019380	7.844581927	3.589250837
O	6.467689518	5.030989790	7.501838662
O	3.572884334	6.805183118	3.606410182
O	3.731762498	9.448532812	3.016126788
O	4.295083037	6.331700187	8.617439881
O	9.471032344	9.108985676	5.825915316
O	8.070257278	7.085625835	8.875139403
O	7.417929843	10.243298799	3.095718721
O	2.408606976	7.765946998	5.873725151
Al	3.898101422	10.696627472	4.239421664
Si	4.452909853	7.931057570	9.003315032
Si	8.570037126	10.240374828	6.637270021
Si	9.154173103	7.618384648	5.177150491
Si	4.878975695	5.307919075	7.447286011
Si	4.407558528	7.991980614	2.784189035
Si	7.395874549	8.611821264	2.875084054
Si	3.179137865	6.488277243	5.169425685
Si	2.745901572	9.118870889	6.764774051
Si	6.914268014	11.241466985	4.347115199
Si	7.374134346	8.550008270	8.952608182
O	9.468491861	5.067776299	7.218851825
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O	10.448726054	6.624162242	5.211913312
H	10.312061616	5.934597643	5.927928383
O	7.354580001	8.244781498	1.254745198
H	8.236281293	8.169933176	0.798876984
O	4.526139069	7.516322921	1.216264485
H	5.426084689	7.651695214	0.851087454
O	2.242827055	5.129692279	5.317911632
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O	1.550470807	10.208250502	6.713616411
H	1.675303728	10.837715159	5.936921836
O	2.368364681	11.511226576	4.550338460
H	1.745358001	11.551219085	3.806709707
O	7.936155439	12.546925065	4.492712503
H	7.946371828	13.230881312	3.378248615
O	9.389187758	11.655556993	6.750854122
H	9.141567258	12.295673510	6.049702143
O	7.155446362	9.000034003	10.553451476
H	7.828547924	8.626820054	11.148500997
O	4.418798574	8.169094731	10.622256748
H	5.273159415	8.552935958	10.928833948
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Al	8.338478964	1.296607934	6.329671409
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Cu	7.133998407	3.965226105	4.965284714
O	5.310382903	4.713368934	9.584318991
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O	8.435072064	3.104377941	6.428433286
O	5.084810277	2.949608693	6.275035428
O	6.818339150	5.802575652	6.117197233
O	6.878292175	7.090753367	10.069043598
O	4.140310720	2.263735825	9.894675352
O	9.322562548	2.447141170	9.844875236
O	9.466453209	5.501168249	5.871223106
O	6.713401208	0.915091822	5.704377543
O	4.165030402	5.388137094	5.825174192
O	5.053067960	7.030348366	7.781490361
O	4.911962366	0.756164623	7.804459301
O	10.431523504	4.104330254	7.971552770
O	8.569464927	0.617708139	7.952587689
O	8.504477094	7.097475484	7.875827493
O	3.258102254	4.025751658	8.002841474
Al	5.297673681	6.622488844	9.465630832
Si	5.277700739	1.170350972	9.358289250
Si	9.748184272	3.989585350	9.475501322
Si	9.858565587	3.957298569	6.419697631
Si	5.226400670	1.260837823	6.251984140
Si	5.280738228	6.542091090	6.252948408
Si	8.302171056	6.560023830	6.333158507
Si	3.761749596	3.911799554	6.430591870
Si	3.803421635	3.820239019	9.548404736
Si	8.297043385	6.593905943	9.451599124
Si	8.238563788	1.289735961	9.389581002
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O	10.966418758	3.304204941	5.407360645
H	10.692248634	2.363034565	5.204473778
O	8.212063212	7.868554667	5.309726636
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O	5.194671209	7.743686455	5.130056157
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O	2.544782557	3.209806028	5.538642107
H	1.644686125	3.490539155	5.777262719
O	2.814154173	4.491672078	10.643522595
H	3.040101931	5.465668993	10.755678515
O	3.893458482	6.915055720	10.487523587
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O	9.591948716	7.159810016	10.340368234
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O	10.793413085	4.517380027	10.627765477
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O	8.148586619	0.106209258	10.575081077
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O	4.093581359	0.656762473	5.210886973
H	3.261785979	1.170883461	5.238916173
H	6.158192321	4.203688701	9.631153502
N	6.566881618	2.928124081	3.351652558
H	5.622025785	3.152810966	3.016185706
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7A

Al	7.849717207	6.029926582	7.508164349
Cu	6.576722617	5.880936609	4.578797610
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O	7.092310082	10.478389386	5.817897147
O	7.762014543	6.988945658	5.970003935
O	4.521534230	6.186997382	6.004585298
O	5.983388838	7.822225764	3.518763462
O	5.365755600	11.730466234	4.181810717
O	3.202253680	8.888796518	8.322886195
O	8.209484008	9.803437977	8.181796667
O	8.667245347	7.825047944	3.604701173
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O	8.082737508	7.149879758	8.855830248
O	7.361297820	10.174026079	3.150610467
O	2.348785364	7.847654328	5.944402710
Al	3.931844211	10.720329790	4.241004821
Si	4.435881595	8.033761292	9.042774092
Si	8.547747773	10.276513879	6.644138241
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Si	4.779868677	5.396608719	7.490081327
Si	4.419688386	7.945717143	2.829591341
Si	7.367014570	8.544700190	2.908234440
Si	3.106766257	6.556290537	5.235137851
Si	2.730962148	9.209619769	6.796956297
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Si	7.381950236	8.613499749	8.972719714
O	9.265644842	4.993080531	7.167353142
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O	1.557179245	10.325079434	6.741861476
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O	7.974338118	12.524944013	4.316323268
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H	7.874152896	8.651425774	11.162265936
O	4.410266460	8.282615200	10.661699055
H	5.277962180	8.630997382	10.969420218
O	3.897618262	4.002952352	7.500874595
H	3.077984845	4.081715309	6.971325239
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Al	8.431864846	1.155189717	6.423065698
Cu	6.906231651	3.748240752	5.381602845
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O	8.484414349	2.981741187	6.422188141
O	5.128548649	2.867522587	6.265869606
O	6.829502067	5.770422239	6.218309859
O	6.914907728	7.119172594	9.944439456
O	4.198105523	2.303739099	9.939337798
O	9.348773118	2.492341544	9.902418666
O	9.470239675	5.392128075	5.846149888
O	6.785938356	0.830562561	5.848339761
O	4.228347658	5.320735525	5.826870391
O	4.987905865	7.077739180	7.731533211
O	4.926165817	0.736633323	7.887591518
O	10.471351043	4.023805682	7.941784685
O	8.668871462	0.567135224	8.079011159
O	8.620277964	7.114321837	7.787592566
O	3.290710075	3.954115397	7.974891190
Al	5.310147661	6.666873327	9.402622878
Si	5.320987100	1.184889977	9.425583344
Si	9.781184078	4.009431146	9.446746680
Si	9.900683321	3.864959022	6.393331908
Si	5.276330322	1.147977743	6.318477698
Si	5.293714990	6.529541967	6.238609702
Si	8.345511781	6.496304901	6.286520888
Si	3.791808401	3.848958923	6.406974510
Si	3.837287926	3.837750995	9.530432072
Si	8.346098856	6.624899695	9.355460058
Si	8.291853177	1.298422333	9.475487264
O	9.766078788	0.779453323	5.338553789
H	10.144962765	-0.111685867	5.315726675
O	11.003341948	3.209337950	5.383838785
H	10.758086795	2.252538013	5.215310034
O	8.224271358	7.722465237	5.174247829
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O	5.260935125	7.670226298	5.058266960
H	6.158549099	7.982032635	4.819911497
O	2.615001087	3.124674986	5.495799357
H	1.708100947	3.453610215	5.615538506
O	2.843904623	4.553576153	10.589143213
H	3.087801318	5.524625049	10.700334379
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H	3.381042624	7.734803826	10.263053433
O	9.611273818	7.237849322	10.259496828
H	9.206212886	7.601511624	11.212742347
O	10.820584985	4.606376063	10.568471452
H	10.748263779	5.585441549	10.628926322
O	8.177642680	0.171917651	10.711458560
H	8.798807552	-0.570585125	10.616219440
O	5.331937104	-0.095810555	10.445157613
H	6.237040751	-0.241390555	10.804484645
O	4.158692766	0.502807264	5.299218875
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O 5.491770537 4.433672576 3.068060170
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8A

Al 8.416655311 1.189615910 6.436847329
Cu 6.929870078 3.694053330 5.225356150
O 5.319795568 4.733542145 9.540142579
O 6.771067285 2.032017544 9.467811311
O 8.399759199 4.970454417 9.385008051
O 8.441923994 3.020793491 6.450945237
O 5.173617537 2.903754365 6.295488668
O 6.793249902 5.773214518 6.156500194
O 6.893030662 7.104055865 10.008675053
O 4.188861359 2.285997817 9.959213860
O 9.352770807 2.512172153 9.930646962
O 9.433439754 5.435638051 5.882387174
O 6.782227831 0.838576229 5.850607463
O 4.175957338 5.340707508 5.861555049
O 5.017215147 7.065553863 7.763501400
O 4.944708724 0.745022746 7.899779875
O 10.469421523 4.021203819 7.947794580
O 8.673181467 0.602884346 8.089436634
O 8.514379926 7.148013102 7.808145823
O 3.279679552 3.933435575 7.991476158
Al 5.299098446 6.645597365 9.437728548
Si 5.327387116 1.186143463 9.442901205
Si 9.790892121 4.024772267 9.460902488
Si 9.861874497 3.902309186 6.411222123
Si 5.278526641 1.177593430 6.332517555
Si 5.263280300 6.533005907 6.253289942
Si 8.284124771 6.527828775 6.301122660
Si 3.804886679 3.849499577 6.427664836
Si 3.823125476 3.818278983 9.548766695
Si 8.316480013 6.633630137 9.383826171
Si 8.294356501 1.322984023 9.492538795
O 9.742165827 0.832892735 5.332168655
H 10.137418738 -0.051363713 5.313168484
O 10.935973032 3.263231844 5.359666120
H 10.700768096 2.300491220 5.202407879
O 8.192787311 7.765953597 5.196997245
H 8.952069074 8.371462962 5.158587327
O 5.186494869 7.698850589 5.098133428
H 6.074346713 8.017494699 4.837434859
O 2.649183172 3.090246710 5.511576150
H 1.729201010 3.364081970 5.666452021
O 2.824391946 4.527001880 10.607370408
H 3.060676989 5.500447696 10.716553520
O 3.909149534 6.937292699 10.477660204
H 3.341819102 7.692166659 10.253524482
O 9.604357962 7.211705761 10.273583496
H 9.349965947 7.856677771 10.954914560
O 10.845007374 4.623355830 10.566294506
H 10.743639631 5.593885879 10.668811191
O 8.186406780 0.181486693 10.716019783
H 8.799249622 -0.564653796 10.597463239
O 5.350177681 -0.099584141 10.455562292
H 6.258288248 -0.241017751 10.809789151
O 4.137299841 0.564563469 5.322213100
H 3.371640919 1.163507872 5.204688473
H 6.169246794 4.230610372 9.611099503

O 5.554113372 3.987147004 3.641489675
O 5.768561423 4.901552719 2.798238858
N 8.132999438 3.844451364 3.635447723
O 7.999782196 4.711140276 2.870197106

8B

Al 8.367634279 1.281315188 6.397900375
Cu 6.872739876 3.871855033 5.076018384
O 5.354291633 4.788025622 9.512628437
O 6.829559820 1.931955592 9.348291607
O 8.341578714 4.943130677 9.489760837
O 8.385298478 3.087954528 6.534125773
O 5.177995726 2.986559204 6.227042200
O 6.752246726 6.006380364 6.303072300
O 6.862393550 7.123083696 10.039839065
O 4.299091591 2.289132708 9.970168949
O 9.363440961 2.457654004 9.892717408
O 9.357412682 5.501731084 5.922938692
O 6.754270804 0.859689915 5.819025406
O 4.179211087 5.425289768 5.944145952
O 4.887122442 7.223517266 7.838717515
O 4.872858192 0.814622651 7.810034604
O 10.429417814 4.112730056 7.999533884
O 8.784609579 0.584618211 7.972992346
O 8.607521248 7.154743756 7.946044327
O 3.311264802 3.919065184 8.027283015
Al 5.258098855 6.706072835 9.470800786
Si 5.354324027 1.159353003 9.349473463
Si 9.749950182 4.007077207 9.509937747
Si 9.781661754 3.981189146 6.478071078
Si 5.253781023 1.262842155 6.255686372
Si 5.199376282 6.673654314 6.342064196
Si 8.285360393 6.642866750 6.412702468
Si 3.807243917 3.912816718 6.449098213
Si 3.897029510 3.814864034 9.569451313
Si 8.303243881 6.615532988 9.491709881
Si 8.355503510 1.247942813 9.394521645
O 9.600938966 0.997963522 5.141113617
H 9.940732052 0.098651331 5.010817767
O 10.860996169 3.377135062 5.395227501
H 10.669536694 2.408884555 5.241526236
O 8.275623648 7.922972749 5.360049330
H 9.099052157 8.436005745 5.303314158
O 5.089240900 7.813340295 5.158517838
H 5.963962109 8.175243380 4.918451363
O 2.591775481 3.200043074 5.568593070
H 1.710267967 3.275097819 5.973349608
O 2.911528414 4.491444742 10.660822555
H 3.121109072 5.471717858 10.771202047
O 3.883697635 6.951309105 10.545620453
H 3.257519036 7.637403313 10.261418304
O 9.557502969 7.139947962 10.459648659
H 9.291771965 7.792272932 11.129074106
O 10.788604690 4.559968003 10.653134305
H 10.681466217 5.523821274 10.802375712
O 8.250935737 0.066606618 10.577984723
H 8.864145077 -0.675471967 10.438793401
O 5.366073641 -0.178609448 10.295700972
H 6.268483241 -0.340904514 10.652365608
O 4.126406835 0.677819947 5.210429622

H	3.374725892	1.294135914	5.091358977
H	6.241836255	4.354082804	9.583871082
O	5.631460533	4.327258964	3.422648269
O	4.482328294	3.802102461	3.389393248
N	8.213350416	3.217209798	3.585045292
H	9.027344137	3.837970290	3.503121888
H	7.760684878	3.156874063	2.667505280
H	8.595940122	2.286256731	3.825699973

8A-TS

Al	8.524537137	1.222585183	6.437094194
Cu	7.014413300	3.534851690	5.447094212
O	5.293480354	4.799826415	9.443004201
O	6.817960847	1.974374961	9.292934299
O	8.353632630	5.011525405	9.444502423
O	8.534818686	3.059392669	6.580737058
O	5.164180025	2.940760352	6.434609544
O	6.791918177	5.838296641	6.344907577
O	6.818112948	7.143745719	10.026773182
O	4.248994701	2.303368179	9.829970469
O	9.345307389	2.542440035	9.891769058
O	9.426112920	5.518385192	5.952965888
O	6.848081730	0.986088018	5.882580743
O	4.195897000	5.420659875	5.893341896
O	4.932266456	7.212017804	7.771224872
O	4.938106797	0.645962758	7.830345653
O	10.501577355	4.169600278	8.035997264
O	8.829185832	0.577020518	8.048405933
O	8.547818912	7.217469312	7.908938776
O	3.206481063	4.002729159	7.963196851
Al	5.226733497	6.720053130	9.423547265
Si	5.359029940	1.164945141	9.346892434
Si	9.761038492	4.088358115	9.520126830
Si	9.918736506	4.018046780	6.495290755
Si	5.300708653	1.223287500	6.322388413
Si	5.277390149	6.618131980	6.297002697
Si	8.276301670	6.600935134	6.404234978
Si	3.811276462	3.927189167	6.422940109
Si	3.826248413	3.838415943	9.489242482
Si	8.267542028	6.680410946	9.461648813
Si	8.353323368	1.313945734	9.419316185
O	9.787111537	0.963317497	5.245667742
H	10.200327377	0.096200467	5.123489363
O	11.013046321	3.396621411	5.457947697
H	10.760185905	2.460967945	5.213106380
O	8.183295299	7.844397292	5.305621886
H	9.018019561	8.109925266	4.877547549
O	5.261520455	7.746020108	5.103003296
H	6.158226905	8.076086719	4.888037146
O	2.755198758	3.153282375	5.409255682
H	1.712199815	3.565181834	5.431155299
O	2.858002077	4.478278532	10.618075830
H	3.058241846	5.459254818	10.732654197
O	3.839743107	6.936799437	10.485906915
H	3.240583327	7.673919192	10.287239372
O	9.514452697	7.221416833	10.428982969
H	9.266059806	7.930508158	11.045561299
O	10.764670815	4.654006549	10.686690671
H	10.638171699	5.616692232	10.831360161
O	8.228460461	0.173579601	10.640916449

H	8.835148722	-0.576443774	10.512926976
O	5.388494258	-0.081604874	10.406173838
H	6.305232773	-0.227573105	10.736397846
O	4.234088027	0.679621013	5.202475574
H	3.488242389	1.295881352	5.044878762
H	6.168621008	4.348077732	9.525747755
O	5.869500761	4.085780169	3.992725769
O	6.271689478	3.623725460	2.744044686
N	7.661538802	3.515149234	2.562239875
O	8.308423597	3.572270343	3.589426653

9

Al	8.464420484	1.179551531	6.436388128
Cu	6.915584816	3.625529005	5.391262321
O	5.311084051	4.798232641	9.425782091
O	6.814815056	1.995583980	9.388316488
O	8.398680611	4.988609648	9.396856968
O	8.437107181	3.019878565	6.536841933
O	5.187996261	2.917631939	6.356343367
O	6.799286557	5.871529076	6.395781113
O	6.875695353	7.126171147	9.980895297
O	4.258427692	2.319738676	9.927450017
O	9.361972182	2.512674231	9.917100967
O	9.394524063	5.456408244	5.943180200
O	6.813178870	0.875794299	5.862715092
O	4.215430553	5.393853544	5.939346128
O	4.910445234	7.237825263	7.772313740
O	4.933994746	0.719454886	7.874078267
O	10.484042798	4.037137696	7.973966854
O	8.754909262	0.568204428	8.069543884
O	8.657373892	7.212323215	7.898653405
O	3.236564684	3.890446134	7.965808990
Al	5.268780774	6.723627864	9.408658475
Si	5.357422923	1.183776052	9.404664362
Si	9.789379076	4.038255982	9.479750620
Si	9.855634652	3.935331286	6.445879431
Si	5.295937054	1.183281207	6.327158403
Si	5.275703606	6.622932981	6.310223960
Si	8.305798808	6.587975800	6.410647986
Si	3.820060967	3.888359073	6.422015046
Si	3.841885197	3.837146825	9.504799168
Si	8.331869861	6.657179158	9.438669838
Si	8.339708702	1.301572519	9.458874935
O	9.768489292	0.874124804	5.298711509
H	10.203863910	0.009549886	5.266108651
O	10.926516175	3.314477159	5.386024497
H	10.698962244	2.360517378	5.185239661
O	8.197451098	7.816892129	5.298886265
H	8.962643185	8.412245578	5.229432441
O	5.262117716	7.726840583	5.095400956
H	6.165470950	8.016329492	4.851213357
O	2.729931782	3.145918216	5.419985629
H	1.824386081	3.498719740	5.412818488
O	2.866127337	4.550535223	10.578065945
H	3.115227017	5.521204571	10.703983685
O	3.914226892	6.973173696	10.506093138
H	3.321761724	7.713660589	10.298245185
O	9.563276543	7.195644193	10.429062629
H	9.259233797	7.766824113	11.154533597
O	10.833227752	4.632039534	10.596185780

H	10.695597640	5.592744076	10.745956991
O	8.223570382	0.162283221	10.682131945
H	8.840883811	-0.581060693	10.567786791
O	5.378143434	-0.096087999	10.424010545
H	6.288267266	-0.243652569	10.770647039
O	4.182381114	0.619097670	5.263071944
H	3.438867653	1.239560907	5.115337541
H	6.181096090	4.333312346	9.497538896
O	5.838213361	4.307503584	3.944629127
O	6.520131122	4.195799197	2.666964641
N	7.759238253	3.774249440	2.674300345
O	8.219980625	3.434653176	3.778521119

9-TS

Al	8.491671162	1.343587249	6.361243019
Cu	6.779739612	3.914828294	5.310630947
O	5.340714238	4.773107065	9.436210527
O	6.846118187	2.008879804	9.351682943
O	8.403084763	4.966051394	9.528759532
O	8.402228593	3.191406465	6.387311924
O	5.203030650	2.960691182	6.409698377
O	6.865803580	5.938705350	6.395666679
O	6.887202101	7.105936497	10.098460435
O	4.259255606	2.287002694	9.797445845
O	9.398810916	2.495366199	9.968784981
O	9.490892675	5.596211678	5.970815839
O	6.867530920	0.961074729	5.765970829
O	4.277906302	5.497419134	5.935454940
O	4.997393952	7.251926033	7.849912744
O	5.042625998	0.671559167	7.796370154
O	10.420850811	4.059387326	7.997812560
O	8.821231323	0.710246295	7.982394080
O	8.681405406	7.188209331	8.031159860
O	3.261662252	4.001038396	7.917677121
Al	5.298820061	6.690029314	9.483027714
Si	5.399034512	1.170348099	9.332737240
Si	9.803810814	4.028731637	9.534254686
Si	9.861188675	4.036629651	6.439201763
Si	5.357760869	1.240656608	6.274013936
Si	5.341544371	6.709215523	6.361913965
Si	8.375633520	6.668892279	6.498579469
Si	3.866717457	3.969354626	6.379424886
Si	3.854991406	3.825472581	9.448625842
Si	8.345927816	6.633408450	9.569636960
Si	8.374791577	1.322370419	9.417767274
O	9.862257005	0.998063850	5.297299503
H	10.385908780	0.209230545	5.511723362
O	10.972770305	3.436439061	5.407538786
H	10.764667329	2.472271198	5.218537506
O	8.257659190	7.955922574	5.458942084
H	9.024926110	8.550784910	5.409569303
O	5.344492448	7.863065691	5.195893626
H	6.255466820	8.133739978	4.954445332
O	2.791032823	3.266007495	5.344794674
H	2.234791427	4.003261652	4.685022705
O	2.878321047	4.474776887	10.563910144
H	3.097479152	5.448152391	10.703545296
O	3.900652706	6.917863012	10.525101942
H	3.307244771	7.647706749	10.284456237
O	9.578009940	7.171828001	10.557960803

H	9.268851015	7.695500884	11.316439751
O	10.891073848	4.601692128	10.620988687
H	10.763987765	5.558250335	10.798939402
O	8.245951053	0.111520507	10.568562854
H	8.871313579	-0.621704878	10.436834081
O	5.407550721	-0.093207823	10.372381192
H	6.320464830	-0.264705203	10.699453408
O	4.239723047	0.710774969	5.194821024
H	3.534917438	1.360737057	4.998571851
H	6.200556242	4.294118296	9.538274879
O	5.572457313	4.417941070	4.059985531
O	6.049020994	2.562844368	2.630636353
N	7.238642432	2.502909716	2.802609069
O	7.908685275	2.969056884	3.718453044

10

Al	8.250380169	1.148153946	6.396510419
Cu	6.719282166	3.659654724	5.250647597
O	5.277944535	4.749262615	9.539477168
O	6.777484614	2.015389782	9.501479431
O	8.360198294	4.970460478	9.330173945
O	8.237841381	2.993424337	6.376002668
O	4.993564771	2.816605163	6.446573819
O	6.619761438	5.692699481	6.229302091
O	6.850807172	7.107819389	9.951218796
O	4.227079191	2.296485157	10.109434403
O	9.366668067	2.523245505	9.852688401
O	9.233000759	5.399963486	5.772601908
O	6.594572925	0.761997547	5.919747519
O	3.999439145	5.239387064	5.980773649
O	4.880348096	7.082893357	7.766708193
O	4.877187043	0.676570288	8.068324604
O	10.341249343	3.984992608	7.785940034
O	8.632982289	0.610486940	8.038577117
O	8.428533069	7.129941271	7.727016771
O	3.147129904	3.874402288	8.165652138
Al	5.235739255	6.662691948	9.429764366
Si	5.334024207	1.173566865	9.572663116
Si	9.758821505	4.032417037	9.337813163
Si	9.672013208	3.865794795	6.280634978
Si	5.116849102	1.095806435	6.479930356
Si	5.084341042	6.458085575	6.283569177
Si	8.100497722	6.485833423	6.249076149
Si	3.632390975	3.764216356	6.590232023
Si	3.801263591	3.808512607	9.683367677
Si	8.265242617	6.633744322	9.312065268
Si	8.304489239	1.320390729	9.459983678
O	9.517178497	0.801816200	5.223909572
H	9.921117059	-0.077558918	5.181557775
O	10.695392393	3.216495275	5.188866091
H	10.459292400	2.250296485	5.047330314
O	7.917915548	7.721279092	5.154678350
H	8.586478060	8.426038728	5.185792216
O	4.976601696	7.545674587	5.059807230
H	5.854440778	7.884021353	4.787616809
O	2.457286415	2.994314904	5.711011933
H	1.545986946	3.314739487	5.818740637
O	2.866171734	4.530835528	10.789947235
H	3.088773811	5.511043070	10.855338071
O	3.888170549	6.962709525	10.519165448

H	3.288775849	7.689703049	10.286311870
O	9.572390222	7.223453084	10.163594830
H	9.347034184	7.900885110	10.822937720
O	10.877056864	4.666245706	10.356134228
H	10.752726139	5.631919590	10.478652710
O	8.267759476	0.177964931	10.684804960
H	8.884163186	-0.560494871	10.539579446
O	5.407931892	-0.076681457	10.626761889
H	6.336437672	-0.224995080	10.918874834
O	3.928257242	0.462001190	5.540906072
H	3.164727280	1.063270185	5.425364560
H	6.139619719	4.268353963	9.610525473
O	6.100988689	3.924762702	3.609598776
O	8.291396127	5.480901400	2.816114486
N	9.354503787	4.892174815	2.861304138
O	10.490429294	5.187291856	2.570465534

11

Al	8.607963230	1.507634661	6.316107865
Cu	7.427678946	3.669279446	4.902008655
O	5.060278360	4.996300984	9.027322184
O	6.847651074	2.338537136	9.407017845
O	9.203540846	5.375426321	9.751608629
O	8.768208609	3.334648476	6.311455251
O	4.937804801	3.143166073	5.909203610
O	6.997244409	5.932849445	6.062770262
O	6.905960063	6.545575890	9.897053969
O	4.140114861	2.541176650	9.602202096
O	9.463030060	2.730590727	9.738105925
O	9.728326986	5.749810474	5.822593165
O	6.986558818	1.623889951	5.529412563
O	4.282658959	5.674830016	5.877670685
O	5.403724503	7.536819083	7.514818742
O	5.260158261	1.079471358	7.624483265
O	10.750265264	4.284553021	7.851095204
O	8.637701071	0.859147004	7.939999242
O	8.603350735	7.201786435	7.807200404
O	3.000276832	3.999864241	7.632931859
Al	5.155666642	6.747461600	9.050833788
Si	5.385929880	1.541750208	9.216266729
Si	10.253267519	4.128535583	9.411781474
Si	10.185313797	4.221934153	6.299593652
Si	5.410130524	1.560168199	6.059280203
Si	5.496755159	6.758633521	6.076848776
Si	8.453637652	6.712230864	6.228770393
Si	3.659695186	4.170577937	6.129449328
Si	3.705332558	4.077114901	9.150315868
Si	8.528887206	6.813808808	9.391038765
Si	8.322770624	1.586546965	9.367071385
O	9.941624754	1.075076874	5.268770456
H	10.230691110	0.159300117	5.146023896
O	11.267877924	3.571039446	5.261883686
H	11.025258494	2.620411438	5.092106142
O	8.461044510	8.068789671	5.274202402
H	9.143389117	8.053774252	4.581062053
O	5.458138980	7.775949030	4.781317096
H	6.311294886	8.235162888	4.654559254
O	2.478051922	3.818834870	5.031110150
H	1.586850411	4.039390264	5.351988273
O	2.630231451	4.685488974	10.238308598

H	2.819860907	5.635526947	10.414522616
O	3.950294563	7.363180565	10.142694717
H	3.632268228	8.275203331	10.069739978
O	9.051914876	8.081488139	10.290671949
H	9.613858203	8.710889400	9.807906257
O	11.612769078	4.230206526	10.332101648
H	11.538193057	3.815536736	11.207247692
O	8.277306015	0.429403507	10.576401281
H	8.833313186	-0.344053955	10.377845689
O	5.348981113	0.206416870	10.176863379
H	6.223963326	0.042711440	10.588297625
O	4.603712874	0.513621938	5.075399510
H	3.677997450	0.349903819	5.323069428
N	6.931118337	4.879871221	2.754285919
O	8.008096741	5.055439574	3.421104194
O	6.212876296	3.992175902	3.344749485
H	6.785478844	5.588591333	10.120067811

12

Al	8.642533767	1.337625782	6.230519710
Cu	7.411036678	3.581210148	4.949415521
O	5.380263481	4.955246213	9.236208507
O	6.795016425	2.345562275	9.297449854
O	8.589593441	5.189097561	9.109616230
O	9.011792548	3.119908472	5.993795843
O	4.808761062	3.050705081	6.024165859
O	7.025567689	6.001188474	6.142706597
O	7.010053158	7.252609844	9.839147298
O	4.160482409	2.535928539	9.497355405
O	9.411259467	2.734160797	9.789277860
O	9.707959828	5.703769232	5.901044507
O	6.949246814	1.640699084	5.605691856
O	4.397989676	5.654240279	5.626429746
O	5.173048173	7.386667994	7.551595215
O	5.191480995	0.911320922	7.614379814
O	10.708924407	4.078940616	7.836481692
O	8.649846522	0.881683663	7.926482014
O	8.736116846	7.461101447	7.710796492
O	3.243743765	4.410102007	7.733965460
Al	5.415952610	6.873027188	9.204665323
Si	5.372896258	1.461006115	9.165690778
Si	9.939937068	4.217811753	9.301259777
Si	10.268730725	4.189934947	6.249775591
Si	5.367099683	1.492326081	6.075973165
Si	5.514536775	6.789050468	6.077562838
Si	8.498674200	6.768070994	6.225237300
Si	3.701799274	4.261383342	6.141430590
Si	3.837785825	4.116129971	9.236172857
Si	8.461246336	6.849595757	9.233450060
Si	8.303952752	1.601833228	9.337694033
O	9.705198742	0.429210983	5.198164243
H	9.831210989	-0.519216656	5.368709155
O	11.541740596	3.876612271	5.251564802
H	11.601547010	2.942921385	4.970898986
O	8.428732521	7.980997752	5.090896280
H	9.171013512	8.608744098	5.081954163
O	5.548197974	7.904238005	4.868724145
H	6.450849641	8.249058151	4.705002859
O	2.396228897	3.874334348	5.213166992
H	1.830486412	4.623549319	4.956690798

O	2.924113713	4.740484995	10.421042069
H	3.150927488	5.713636077	10.530544879
O	4.007959344	7.166507441	10.223359199
H	3.419612645	7.880809636	9.929234128
O	9.694040625	7.371427942	10.235421593
H	9.384820157	7.937421243	10.963013205
O	10.956543659	4.830187734	10.431201586
H	10.790808195	5.788973747	10.575839535
O	8.143757514	0.453329361	10.546808731
H	8.803543239	-0.260129761	10.501987173
O	5.333271719	0.212698671	10.222860429
H	6.230624590	0.041246510	10.590496400
O	4.625980009	0.476218150	5.008804957
H	3.705261256	0.241079266	5.218407437
N	6.765302613	4.948828260	2.990525083
O	7.945403964	5.021153965	3.527305589
O	6.011764840	4.052702087	3.560171316
O	6.397444519	5.644203717	2.067037501
H	6.189914299	4.401287296	9.364112067

NH₃

N	4.598089354	21.807577361	7.944458995
H	4.598085140	22.747555075	8.354729676
H	5.412114788	21.337613134	8.354723804
H	3.784059777	21.337615607	8.354724841

N₂

O	6.726320310	20.775069144	-0.393075440
H	6.344462515	21.456880752	0.213018243
H	6.736635137	19.876917906	0.020745217
H	6.277702587	20.771356289	-1.274500449

H₂O

O	6.752495832	20.787407559	-0.397663229
H	6.752495832	21.549669549	0.205418442
H	6.752495832	20.025145565	0.205418444

NO

N	6.948690690	2.313223376	5.606694231
O	6.948690690	3.349536735	6.150412961

NO⁺

N	6.948690690	2.353286625	5.627710918
O	6.948690690	3.314462547	6.132013474

HNO₃

N	-0.436691126	-0.122800216	5.997595824
O	-0.180396329	-1.302639047	6.081693297
O	-0.289777542	0.669902510	5.074306261
O	-1.011164906	0.425080900	7.197941874
H	-1.134960279	1.364894871	6.935262654

NO₃⁻

N	-0.608687073	-0.157340334	6.128947217
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O	-0.221935466	-0.982233030	5.236704328
O	0.101021608	0.865656952	6.399702130
O	-1.706352682	-0.354704961	6.744753333

HNO₂

N	-0.541431192	-0.183617518	6.007043301
O	-0.253712843	0.595362457	5.139811420
O	-1.050302503	0.437641675	7.166226010
H	-1.041326418	1.407341463	6.951236008

NO₂⁻

N	-0.527352707	-0.131251420	5.805678775
O	-0.055668899	-1.323728133	5.900417205
O	0.050901556	0.753891855	6.537532690

N₂O

N	6.948690832	2.210862484	5.552995896
O	6.948690630	3.271603549	6.109434683
N	6.948690617	1.192097639	5.018580063

H₃N⁺-NO

O	4.952479664	4.967295938	8.544132717
N	6.020534884	5.083657645	8.875073795
N	7.200367019	5.802296548	7.404854902
H	7.897198687	6.392231190	7.876545974
H	6.659768896	6.345428257	6.718812800
H	7.659383253	4.998698339	6.956128084

NH₄⁺-H₂N-NO

O	5.703460587	5.956777179	9.196186358
N	5.619574390	5.304325745	8.206633770
N	6.961255839	4.696479069	7.811796083
H	7.549187294	4.575776375	8.652614546
H	7.655780990	5.694489848	6.723399011
H	6.753608745	3.789910772	7.370813183
N	8.117763967	6.392579908	5.981853925
H	7.892842886	6.094860653	5.021429912
H	9.142081335	6.409293851	6.089920799
H	7.757149718	7.347861545	6.120923669

NH₄⁺+H₂N-NO

O	5.381920191	4.914994738	8.300413416
N	6.474347369	5.486898155	8.443729557
N	7.227123342	5.918228631	7.497367232
H	6.787155584	5.622201898	9.441133464
H	8.050899123	6.331850572	7.969056985

A

O	5.387398146	4.950157061	8.235600423
N	6.422654791	5.459092089	8.663100741
N	7.219867286	5.949056131	7.692143464
H	8.093331504	6.383112259	7.978237515
H	6.930637276	5.872863052	6.709019472

B

O	6.798396110	5.639454707	9.788326006
N	6.556938440	5.551449710	8.564271888
N	7.231878946	5.935369440	7.545887164
H	5.661316955	5.092139366	8.288017088
H	8.088775061	6.361930694	7.953376171

C

O	5.378581858	4.967585438	7.882954142
N	6.497124766	5.511382517	8.457305750
N	7.268499542	5.982091360	7.589471234
H	8.072148781	6.363411989	8.121463815
H	5.501397623	5.106030351	6.904723032

D

O	5.371756978	4.966271169	7.872511572
N	6.516282759	5.518499037	8.476776657
N	7.253593496	5.974668134	7.581320026
H	8.061240775	6.359565638	8.106721030
H	4.880935967	4.652298088	8.658171475

E

O	6.794942375	5.681374083	9.820189615
N	6.500012042	5.496592006	8.471135890
N	7.278922651	5.944744223	7.618774318
H	8.113585144	6.436844803	8.040461952
H	7.651922967	6.183465317	9.879840333

F

O	6.850611513	5.634857000	9.810132450
N	6.444143508	5.510159042	8.439320943
N	7.254044379	6.013716808	7.656761726
H	8.068353779	6.427000824	8.173317805
H	6.116402789	5.194060216	10.285075178

TS1

O	5.508623352	4.789826666	8.489749791
N	6.438010195	5.593871528	8.546762583
N	7.091910710	6.082224788	7.483977163
H	7.660578236	5.800107610	8.643268048
H	6.801535163	5.595094582	6.598489192

TS2

O	5.438048054	4.993642578	8.011007731
N	6.415174151	5.452872732	8.728123328
N	7.217334145	5.933988120	7.843887516
H	8.088789511	6.365796839	8.184410165
H	6.270463455	5.495805929	7.055464225

TS3

O	6.434925306	5.069123064	9.512821106
N	6.626253146	6.174481156	8.584143941
N	7.645957781	5.955977646	7.916345952

H	7.683078749	6.758854526	7.250309629
H	6.953190325	5.347831590	10.295274182

TS4

O	6.746566012	5.891473075	9.851019236
N	6.441484272	5.545120620	8.418079899
N	7.377849776	5.643264886	7.664079887
H	8.154607663	5.495254194	7.048838314
H	7.711899191	6.101963936	9.842060444

TS5

O	6.767195313	5.906197470	9.872189164
N	6.412695251	5.568075838	8.375703331
N	7.385538427	5.594468593	7.688186023
H	8.129494869	5.573820903	7.020569445
H	5.867580113	5.836147813	10.254489395

TS6

O	6.817107452	5.594317285	9.843247640
N	6.439713877	5.544181134	8.402884562
N	7.284746767	6.025487584	7.655746207
H	8.118346813	6.367945074	8.197204072
H	7.488321157	4.883303309	9.918092642

TS7

O	6.822506970	5.728591510	9.932970515
N	6.326317792	5.553962909	8.168515194
N	7.375188553	5.905730530	7.759908652
H	7.830545220	6.002915801	8.837022369
H	6.824146724	4.850554937	10.374134804

13/A'

O	11.297990058	3.474416873	2.704135060
O	5.028315491	5.030722881	6.344163180
O	6.795727549	2.099414841	6.842488014
O	8.545111737	5.111735877	6.846480034
O	8.766579583	2.853081559	3.204949503
O	6.917291117	5.842846545	3.813987023
O	4.884401845	2.675566607	3.313551811
O	5.569351179	7.265375775	1.952766665
O	4.259614745	0.137166716	2.727504493
O	9.648901699	0.084304231	2.662570299
O	8.281436435	7.798665007	2.584770499
O	2.480189714	3.484262862	2.376907235
O	6.788195094	7.149176317	6.939422551
O	4.178656991	2.591231216	7.064852575
O	9.325968253	2.599032125	7.371971151
O	9.516707794	5.459250429	3.172200769
O	4.384884518	5.242047084	3.048233153
O	6.837530234	0.819285144	3.190617626
O	4.917032928	7.414192652	4.667498536
O	5.053797006	0.790547786	5.222861080
O	10.317817968	3.866523127	5.197467067
O	8.787333833	0.869199470	5.354411106
O	8.886849951	7.166059795	5.151692113
O	3.033264768	3.840337992	4.973437537

Al	5.133673456	6.845924853	6.347287017
Si	5.243826324	1.387858325	6.730280243
Si	9.816847730	4.041297822	6.757332094
Si	9.981887811	3.934174307	3.583940777
Si	5.395460604	6.479885866	3.430149098
Si	5.294663702	1.092114839	3.595463748
Al	8.524526882	1.002250232	3.607753031
Si	8.389338826	6.556868919	3.697119920
Si	3.691891598	3.797079252	3.457384207
Si	3.674528856	4.070278455	6.491700303
Si	8.321345887	1.388671707	6.797839855
Si	8.339148385	6.814608109	6.695961308
O	2.592256055	4.750716566	7.512816349
O	3.798585175	7.260649930	7.414254869
O	9.341400687	7.532436491	7.788991097
O	10.999022987	4.727087128	7.688493244
O	8.214958885	0.167554461	7.926442294
O	5.157850476	0.214815270	7.878691577
H	3.368012682	8.125047351	7.339458563
H	2.831350549	5.713826529	7.628041195
H	6.051157368	-0.068751558	8.163736522
H	4.658028219	-0.713251782	2.478664406
H	1.595243386	3.626598877	2.752383527
H	10.415744740	0.561118247	2.310351297
H	12.094374458	4.020539852	2.810531837
H	8.854284172	8.561436786	2.773190841
H	6.396564738	7.797246870	1.949882536
H	10.120379914	6.987040710	8.007097182
H	11.774052276	4.176042861	7.887487243
H	8.780470813	-0.597594779	7.723810697
Cu	6.698688966	4.165150416	6.974401539
N	7.061978111	4.509652046	1.248017075
O	7.272974791	3.259856827	1.306001885
N	6.016600337	4.836183242	0.556844408
H	5.715891825	5.819393246	0.724655462
H	8.131671889	3.081898856	2.300972724
H	5.377218716	4.094360175	0.235422239

TS8

O	10.565990452	2.925101291	2.988185731
O	4.035884974	4.021656219	6.127442335
O	5.792864502	1.036682739	6.447966272
O	7.460161654	4.033443587	7.064778613
O	7.990572892	2.365509521	3.189729191
O	6.202775091	5.254610789	3.964137878
O	4.626207431	2.196690911	3.221343702
O	5.038054489	6.938869855	2.206935717
O	3.680733533	0.103275975	1.871970809
O	9.253744587	-0.153443696	2.364540094
O	7.710199076	7.364747763	3.260473752
O	2.499375092	2.739814048	1.603637812
O	5.668775266	6.044979709	7.203995377
O	3.158866129	1.497245077	6.342076472
O	8.245874825	1.471975959	7.298267535
O	8.817240928	4.923656062	3.549619875
O	3.825269024	4.720707445	2.794929865
O	6.297395650	0.144039825	2.599576438
O	4.060693856	6.624913572	4.798730339
O	4.352889505	-0.148163784	4.487578249
O	9.382907224	3.045403859	5.421239568

O	7.947629206	0.090582151	4.991281651
O	7.995419136	6.296041763	5.739904174
O	2.300781158	3.045951975	4.301972537
Al	4.091787130	5.817348532	6.392931876
Si	4.279523124	0.339007665	6.058479994
Si	8.752530062	2.993246561	6.946791207
Si	9.204783142	3.347975818	3.817476319
Si	4.713535767	5.912936333	3.495239351
Si	4.791295531	0.554839632	3.037441266
Al	7.898194566	0.435920166	3.259454943
Si	7.661638487	5.959960914	4.160475588
Si	3.291271785	3.168973487	2.977818911
Si	2.698791545	3.045031198	5.914029850
Si	7.330861646	0.355090649	6.448394444
Si	7.240113596	5.739038421	7.133360122
O	1.464381539	3.559769984	6.857204113
O	2.637700355	6.074261808	7.345487080
O	8.073422138	6.297372661	8.439442032
O	9.845493667	3.541917368	8.057229616
O	7.154189480	-1.031832949	7.348651818
O	4.036974115	-0.937344851	7.064597997
H	2.175717621	6.924161650	7.290674418
H	1.663202819	4.488064592	7.162626600
H	4.884149012	-1.317332854	7.372517279
H	4.020421178	-0.552177237	1.240164694
H	2.640800965	1.786428656	1.413324740
H	9.978597560	0.475586290	2.221964672
H	11.388377943	3.372636284	3.248126186
H	8.225192769	8.082465106	3.667638737
H	5.781439420	7.539062397	2.424220418
H	8.860999169	5.762913582	8.651472944
H	10.548329619	2.924987147	8.320253060
H	7.762143432	-1.746591728	7.092539558
Cu	5.633493031	3.073963324	6.804821741
H	7.493598916	2.745273311	2.328485277
O	6.843010805	3.153292824	1.086059858
N	6.447180673	4.337688102	1.205212772
N	5.742757764	4.857829719	0.157948392
H	6.926767243	5.322748249	0.690029811
H	5.364594788	5.736168926	0.608953738

TS9

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O	5.014504907	5.018279985	6.334142713
O	6.788690090	2.101835423	6.863051743
O	8.559167044	5.088137170	6.877105645
O	8.704398684	2.882589773	3.245599293
O	6.912823177	5.860681255	3.681477174
O	4.984511698	2.778891016	3.287863428
O	5.475200335	7.379577448	1.973306572
O	4.218042227	0.285032080	2.691910458
O	9.699890140	0.153930127	2.699785230
O	8.337543290	7.876322065	2.624281269
O	2.524378601	3.502568313	2.350060808
O	6.782801744	7.097772783	7.013664978
O	4.170100175	2.598851986	7.107668947
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O	6.831162360	0.825974085	3.178719663

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Si 5.298494002 1.170672342 3.577310254
Al 8.509796259 0.997678990 3.628321979
Si 8.377747697 6.593140802 3.683807917
Si 3.718053599 3.835076712 3.441080641
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O 3.784827475 7.241281414 7.421291380
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O 8.189259291 0.160527305 7.948661075
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H 11.821193196 4.145731537 7.820270473
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Cu 6.695001376 4.170825817 6.969165998
H 8.113726203 3.117354729 2.413491358
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TS10

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O 6.997902913 5.683315576 3.781192992
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O 5.543939128 6.872352820 1.933580583
O 4.382621698 -0.341296432 3.040186650
O 9.240663488 0.342922756 2.292152383
O 8.041450887 7.889999965 2.653143258
O 2.099414147 3.888179751 2.703643348
O 6.749294564 7.119586128 6.985350503
O 4.289113418 2.512819099 7.274358625
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O 5.173070211 0.801216415 5.349587870
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O 8.790718702 7.247569681 5.162230397
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Si 5.415744600 6.199095227 3.496400321
Si 5.133258199 0.973331287 3.701540981
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Si 8.358813254 6.623594585 3.698105817
Si 3.439998872 3.672714494 3.634927285
Si 3.726215007 3.969867805 6.695250159
Si 8.439878303 1.450781925 6.646693458
Si 8.310426579 6.845975585 6.714628429
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TS11

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O	6.822013072	7.029617801	7.211609335
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O	5.157470708	1.087902046	4.867008489
O	10.502117234	4.196852700	5.019751371
O	8.610164587	0.956972079	4.898312481
O	8.704619912	7.250721228	5.218327569
O	2.900927259	4.014746483	5.108975737
Al	5.177993862	6.836119521	6.542246007
Si	5.308505078	1.440918478	6.471552438
Si	9.938220572	4.100555740	6.549507502
Si	10.158027012	4.316960759	3.390067325
Si	5.317694234	6.761831718	3.523344392
Si	5.065852690	1.569058533	3.297455762
Al	8.416284668	1.550899334	3.260521712
Si	8.283228393	6.782279062	3.686315420
Si	3.330591006	4.232020467	3.522310541
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Si	8.374194181	1.415883932	6.431691721
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O	2.708890357	4.663160137	7.755200970
O	3.823850872	7.177860928	7.616985092
O	9.443916338	7.449352462	7.813059779
O	11.069828443	4.663684333	7.619200128
O	8.350535481	0.127249377	7.481163791
O	5.233665606	0.067897935	7.368963231
H	3.381954562	8.038554675	7.567195344
H	2.922526826	5.633511875	7.881871763
H	6.114798260	-0.197323450	7.701425666
H	4.543471807	-0.526451073	2.728416376
H	1.147170704	4.295276627	3.195980932
H	9.694190464	0.084984537	1.871554933
H	12.009159783	5.102497646	2.428053307
H	8.627105726	8.926860822	3.136256104
H	6.163750395	8.197206653	2.094768223
H	10.196858502	6.858267965	8.003017885
H	11.977812586	4.341602075	7.492631890
H	8.989147253	-0.579823500	7.289835180
Cu	6.766378350	4.175637836	6.843383303
H	6.829697545	2.366738031	1.824084881
N	7.683671049	2.594112881	-0.383678375
H	8.190979179	0.990366263	0.595058372
O	8.097604752	1.333204165	-0.328978237
N	7.276454143	3.132056312	0.739443998
H	8.119725448	3.553623403	1.154263763

TS12

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O	8.565277668	5.184020345	6.668348498
O	9.822329082	2.676949676	3.037630807
O	6.822612625	5.770412556	3.505823142
O	4.294049152	2.721201240	2.862766322
O	5.468686940	7.238119442	1.735204578
O	5.506982936	0.399603675	2.274416242

O	8.247288069	0.174979142	2.374662817
O	8.203420795	7.721713888	2.329521013
O	1.970978211	3.952990600	2.399612152
O	6.754601253	7.163565999	6.840835753
O	4.224324698	2.629669441	6.900028690
O	9.477492843	2.734542866	7.097822084
O	9.421975453	5.394304495	3.021289128
O	4.166241036	5.381318751	3.004918404
O	6.991598677	2.496915851	3.100399916
O	4.999157613	7.502404877	4.496040302
O	5.401371092	1.273710318	4.862219440
O	10.608950195	4.224071619	5.113016851
O	8.635220075	1.043032718	5.136448017
O	8.709928500	7.204483143	4.911963137
O	2.912832667	3.881118386	4.903248385
Al	5.127064138	6.889707289	6.167793097
Si	5.376617463	1.542330375	6.481071629
Si	9.941065520	4.235062604	6.598758132
Si	10.406999383	4.123493923	3.450786155
Si	5.326506024	6.512181808	3.253356496
Si	5.486578449	1.693129189	3.273457219
Al	8.562245257	1.538073149	3.446572062
Si	8.301487944	6.499096206	3.473933085
Si	3.343079626	3.995228659	3.311140534
Si	3.671923802	4.112697453	6.363959391
Si	8.412136999	1.541843988	6.652250537
Si	8.303137677	6.874859903	6.497606897
O	2.660695131	4.767265335	7.469143243
O	3.748974670	7.280229221	7.187586817
O	9.359914469	7.636170882	7.505014577
O	10.973984721	4.948480981	7.684549987
O	8.437462346	0.286651966	7.740534545
O	5.198507200	0.145826079	7.325817421
H	3.333228077	8.153625498	7.144383727
H	2.854911664	5.745781342	7.533561409
H	6.031851317	-0.144683945	7.744038343
H	6.441306971	0.061986217	2.193453678
H	1.163755913	3.949174817	2.940458117
H	8.792013271	-0.623235609	2.447336055
H	12.039433171	5.272983359	2.468697785
H	8.683301564	8.528800650	2.583733129
H	6.318795083	7.735690102	1.696402163
H	10.084066688	7.046292304	7.794642680
H	11.913518767	4.724783690	7.573642253
H	9.080822592	-0.411173387	7.529837245
Cu	6.718598720	4.284888144	6.817110815
H	7.148724440	2.970488440	2.120073691
N	7.218585076	4.625194239	0.474791872
H	5.716775943	5.723645115	0.808606979
O	5.927114013	4.756718182	0.838773483
N	7.706874286	3.490908641	0.873288154
H	7.523247027	2.835343909	0.100361222

TS13

O	11.493439024	3.943745030	2.765741638
O	5.040725210	4.919571220	6.441015733
O	6.904561350	2.038587541	6.765711192
O	8.584740872	5.064433878	6.990548934
O	9.010224501	2.978043027	3.080258030
O	6.873508952	5.937136588	3.743355846

O	4.785195933	2.774602760	2.950561993
O	5.348802772	7.629502652	2.247667721
O	4.413541752	0.207296627	2.529543423
O	9.550137824	0.116603934	2.475786975
O	8.279973748	8.052135618	2.846789895
O	2.395732965	3.711302311	2.377488665
O	6.743548804	7.001655373	7.231560478
O	4.277045192	2.457780916	7.131936747
O	9.440038486	2.554549641	7.330173225
O	9.474768416	5.653509129	3.235371586
O	4.289430167	5.401999130	3.227703755
O	6.920537437	1.152508555	3.017618214
O	4.949759138	7.402586708	4.947551360
O	5.113620296	1.014882933	5.014381306
O	10.308984160	3.957013844	5.198805768
O	8.915669083	0.941461791	5.221621919
O	8.753010186	7.164387011	5.343680802
O	3.179340977	3.620132580	4.977625998
Al	5.105839493	6.729981893	6.572243864
Si	5.353355317	1.341190694	6.597477159
Si	9.879595484	4.044657470	6.783790716
Si	10.084443751	4.172490386	3.584897459
Si	5.334559114	6.635160569	3.565106355
Si	5.342812396	1.263961961	3.394934150
Al	8.609929438	1.147921049	3.496075460
Si	8.316961491	6.701862534	3.817618675
Si	3.653844944	3.907360770	3.426976227
Si	3.720238412	3.912639977	6.520090297
Si	8.446084943	1.370959408	6.700286145
Si	8.294184568	6.760689800	6.897224418
O	2.567790614	4.552680586	7.484953518
O	3.739405354	7.048177474	7.636541617
O	9.305539509	7.498095403	7.968465226
O	11.082659677	4.704835448	7.702106671
O	8.344338903	0.085774153	7.752840303
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H	3.284714055	7.902312024	7.588151333
H	2.804749515	5.504922321	7.684994769
H	6.213447265	-0.237473615	7.868905433
H	4.674045327	-0.724122468	2.621248677
H	1.846414640	4.505690382	2.266509681
H	10.478425650	-0.045671113	2.697040562
H	11.987325191	4.757904198	2.572845455
H	8.699910176	8.833155917	3.246040140
H	6.209232835	8.084387693	2.156453116
H	10.124827157	6.997708656	8.137319989
H	11.922276029	4.217982986	7.745910219
H	8.962882838	-0.641030142	7.567058821
Cu	6.762052370	4.100685826	6.952424870
H	8.430211576	3.204068109	2.188033503
H	4.889482721	3.173848572	1.076074145
O	5.413003856	3.509683756	0.296609945
N	6.565049381	4.033383762	0.934682402
N	7.423132618	3.155355998	1.113186211
H	7.115697461	2.207636190	0.796595215

TS14

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O	8.584159473	5.131985189	6.867052611
O	8.642078501	3.007395969	3.269662360
O	7.021195110	5.906533499	3.607575571
O	5.133904236	2.675898046	3.600208135
O	5.487526418	7.404705866	1.949898187
O	4.291630381	0.190686960	2.839891672
O	9.773274187	0.406247918	2.538057815
O	8.451817317	7.974350388	2.636825528
O	2.927295142	3.257410857	2.243232036
O	6.779914276	7.109340420	6.982640333
O	4.222120434	2.562264168	7.024781831
O	9.401741986	2.632777764	7.371132137
O	9.599673093	5.568252196	3.138401940
O	4.499503943	5.229503067	3.059072206
O	6.912719734	0.709347322	3.229415403
O	5.021890815	7.392500931	4.665155990
O	5.165494651	0.636962145	5.331135144
O	10.319786521	3.916618004	5.171698189
O	8.902948330	0.961080907	5.320596237
O	8.877217563	7.187079729	5.182935311
O	3.054657104	3.817839747	4.916277856
Al	5.145775910	6.808218631	6.332861148
Si	5.320616398	1.368957871	6.790694105
Si	9.866251927	4.080856241	6.751743614
Si	9.960043021	4.030505237	3.573029930
Si	5.466313920	6.536778234	3.358020136
Si	5.401195695	1.031695530	3.727439063
Al	8.579041093	1.077496662	3.588186982
Si	8.463923894	6.674551708	3.669034805
Si	3.904357722	3.762555827	3.500883047
Si	3.693361392	4.032182227	6.447712279
Si	8.408099032	1.422057160	6.777470461
Si	8.337679592	6.828253534	6.725616824
O	2.604695604	4.705947797	7.462743087
O	3.774812389	7.204715788	7.361454230
O	9.314145011	7.577042940	7.820124872
O	11.069450524	4.771169892	7.647120100
O	8.317220273	0.180187630	7.879779364
O	5.244958866	0.298356874	8.033305315
H	3.340159035	8.066546724	7.280597025
H	2.830762318	5.674276886	7.573478579
H	6.132185044	-0.043451695	8.265626299
H	4.708122182	-0.372052458	2.166181343
H	2.123889883	3.791437266	2.117182092
H	10.538435833	0.969719814	2.339815443
H	12.009191734	3.930758934	2.637175050
H	8.923399875	8.755658407	2.972389375
H	6.288033286	7.960598579	1.884745482
H	10.136143439	7.088053617	8.008172953
H	11.802369025	4.194827356	7.919547084
H	8.917526897	-0.562683866	7.697566493
Cu	6.748955982	4.167301704	6.866228171
H	8.020715911	3.268146768	2.492838828
O	4.984821223	3.521733019	0.204778103
N	6.265101409	2.572904704	0.858718782
N	6.879840935	3.501171116	1.297812553
H	5.966721432	4.241241383	0.895714367
H	4.176359886	3.324138479	0.756898247

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O	11.350952981	3.507225554	2.724564848
O	5.032558701	5.020794529	6.340253311
O	6.812477943	2.096577683	6.854039734
O	8.557780050	5.105847939	6.848552881
O	8.835352225	2.805944118	3.245298894
O	6.917427777	5.847033577	3.786896585
O	4.940429829	2.713124456	3.374913709
O	5.556659594	7.300085517	1.968454580
O	4.261896401	0.205003687	2.732207057
O	9.641142809	0.021859090	2.681121438
O	8.306854722	7.785826869	2.576756586
O	2.512866128	3.517441555	2.375939594
O	6.797833950	7.139030044	6.948292938
O	4.189055716	2.584233840	7.073379623
O	9.343087280	2.598733289	7.377116935
O	9.511555917	5.433848204	3.170976897
O	4.386124955	5.255409530	3.053878640
O	6.858379138	0.816147907	3.203041610
O	4.924857315	7.412895318	4.687863797
O	5.074833000	0.780123083	5.240030606
O	10.355932775	3.875649044	5.213019636
O	8.797344660	0.836218924	5.380615622
O	8.885329995	7.154020406	5.148873760
O	3.025510603	3.826309402	4.982213462
Al	5.141852584	6.835364253	6.363541572
Si	5.262119869	1.384850185	6.746016674
Si	9.837296472	4.041634318	6.764905129
Si	10.012430771	3.919850321	3.596335619
Si	5.395284959	6.491986307	3.440919987
Si	5.324436248	1.114676082	3.619572303
Al	8.550861396	0.983167627	3.628157327
Si	8.399020213	6.544410954	3.691841249
Si	3.711917374	3.807262873	3.477057673
Si	3.679386913	4.059916302	6.498623823
Si	8.339438756	1.381999865	6.816318483
Si	8.348698552	6.805747533	6.697653677
O	2.598104651	4.742679372	7.519693286
O	3.810582159	7.248936612	7.435181692
O	9.353212182	7.529558301	7.784367993
O	11.006885265	4.730280397	7.710446128
O	8.225865254	0.175950328	7.961405064
O	5.171648204	0.217274248	7.899624278
H	3.374431603	8.110088977	7.353621638
H	2.838233391	5.705190441	7.638655537
H	6.064890494	-0.067452273	8.184324302
H	4.628750646	-0.661171873	2.487354783
H	1.631614429	3.211594456	2.866843346
H	10.428114580	0.475609171	2.342365180
H	12.115557217	4.098723451	2.821680378
H	8.862898293	8.555442776	2.786621630
H	6.388843087	7.824135339	1.963322032
H	10.139334229	6.990201495	7.992578623
H	11.784486368	4.182736014	7.909043375
H	8.790244225	-0.592828031	7.769312473
Cu	6.713168598	4.160582729	6.964836904
N	6.956709950	4.527413039	1.209292749
O	7.112163589	3.260604627	1.225755932
N	5.922263182	4.914983951	0.546431836
H	5.671148990	5.912206901	0.744269426
H	8.047822751	3.065162346	2.178667264
H	5.245946145	4.215556576	0.204817685

O	11.261391816	3.544046878	2.642285054
O	5.101141265	4.973109705	6.486290319
O	6.854943659	2.068223013	6.743340132
O	8.608875703	5.141048588	6.839183330
O	8.701441126	3.084476061	3.280428635
O	7.006854795	5.920555494	3.663363934
O	4.625035350	2.549792553	3.208796582
O	5.440844007	7.459206708	2.086329014
O	4.315191241	-0.021690234	2.725499753
O	9.580154997	0.411857495	2.403071230
O	8.356309021	7.979479813	2.637209979
O	2.352188684	3.717685393	2.459608018
O	6.823944583	7.147683670	7.028356133
O	4.223848009	2.522133652	7.075796630
O	9.385049789	2.625483456	7.248808794
O	9.602468140	5.620361931	3.164612683
O	4.582308239	5.145366023	3.034006876
O	6.801649945	1.009804593	3.166700769
O	4.919811505	7.274806684	4.783129757
O	5.029002402	0.764018245	5.202599478
O	10.448111502	4.018629145	5.166374499
O	8.853326083	0.899987712	5.209960031
O	8.863050797	7.248615654	5.192073133
O	3.111650964	3.921981768	5.031241178
Al	5.174403433	6.781287723	6.469803366
Si	5.309498460	1.347368628	6.704521481
Si	9.900312363	4.092558480	6.712052665
Si	9.989235490	4.057083318	3.566999111
Si	5.437527905	6.521123376	3.448790935
Si	5.242801553	1.053761967	3.577369596
Al	8.516563842	1.249529405	3.491299620
Si	8.460487210	6.693940297	3.691152915
Si	3.644853464	3.833678763	3.478159930
Si	3.736778292	4.029002117	6.571651753
Si	8.405628417	1.400802872	6.664804280
Si	8.373342020	6.840772147	6.737995150
O	2.644160826	4.671475479	7.606095073
O	3.841667524	7.182530659	7.544670700
O	9.391963666	7.546169746	7.823585424
O	11.049534663	4.742599928	7.709770547
O	8.328240529	0.174805930	7.794114016
O	5.295519454	0.157129017	7.838013171
H	3.415565578	8.050728206	7.493994743
H	2.878971132	5.632678287	7.747896375
H	6.207652784	-0.076527046	8.111265468
H	4.562759594	-0.948504816	2.880744470
H	1.606042687	4.290202829	2.703991907
H	10.381547289	0.903788164	2.162673236
H	12.090995335	4.034665007	2.764099274
H	8.905690268	8.745703074	2.873834352
H	6.267028450	7.981188237	2.027835895
H	10.170654263	6.995156890	8.028318767
H	11.879176975	4.246126615	7.803724326
H	8.921723068	-0.571337678	7.602110722
Cu	6.821399437	4.127102533	6.903139716
N	6.619232848	2.901643348	0.769205075
O	5.387942985	2.995257555	0.224421181
N	6.740964046	3.692225141	1.730131349

H	5.921070008	4.263331332	2.061110191
H	7.654807842	3.552456296	2.356476851
H	5.390051542	2.296169961	-0.465028622

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O	11.657015751	3.948141963	2.731351395
O	5.022894335	4.922795022	6.318985090
O	6.910829239	2.070310775	6.994384774
O	8.562687479	5.067320937	6.824650341
O	9.303138175	2.717223856	3.036831739
O	6.851257650	5.662273298	3.681997249
O	4.450429006	2.544144133	3.232802151
O	5.467613122	7.115330170	1.918908848
O	4.583661357	-0.063492341	2.765632032
O	9.091790685	-0.230873353	2.595067548
O	8.125241626	7.732637031	2.557658782
O	2.067301852	3.765368763	2.595439690
O	6.748226103	7.045683590	6.987940746
O	4.262743373	2.476432255	7.127396252
O	9.484427164	2.606489110	7.263097578
O	9.460482594	5.430070345	3.086138689
O	4.218149297	5.168483638	3.165566721
O	6.849105660	1.447858616	3.023410025
O	4.973004145	7.331280910	4.660586237
O	5.315895789	0.880150344	5.189644679
O	10.449387256	4.012776612	5.145516034
O	8.719961336	0.922807412	5.265218493
O	8.734809324	7.100518071	5.089354153
O	2.934477083	3.700707348	5.126772822
Al	5.116399768	6.744398759	6.341827067
Si	5.392938644	1.347178027	6.762420745
Si	9.910914677	4.090024560	6.682550555
Si	10.188445594	3.983200068	3.492920416
Si	5.324698826	6.342447898	3.423460650
Si	5.290288959	1.190001441	3.571051802
Al	8.603579460	1.157724077	3.515383332
Si	8.298734015	6.455462568	3.631125076
Si	3.416117240	3.792835132	3.546516105
Si	3.695485224	3.950738850	6.584399082
Si	8.445970616	1.401905734	6.769649505
Si	8.298654725	6.757227068	6.664638259
O	2.688528953	4.607975546	7.692392015
O	3.743496961	7.140791111	7.365504799
O	9.334068522	7.518762599	7.694573161
O	11.026656539	4.823760223	7.665899362
O	8.448088455	0.146377548	7.863522168
O	5.287196532	0.057711907	7.774397781
H	3.299422626	7.998158157	7.282716675
H	2.869979382	5.589850197	7.739075091
H	6.167362335	-0.200519171	8.114774006
H	5.148892408	-0.848189119	2.667116377
H	1.304136905	3.170590560	3.083494936
H	10.007016155	-0.536154460	2.678200114
H	12.131476980	4.795377502	2.751564208
H	8.610785324	8.528677411	2.835529156
H	6.223496792	7.746564961	1.975876389
H	10.109855501	6.967957953	7.916330390
H	11.920845517	4.443787810	7.659943221
H	9.029941974	-0.592011381	7.615543971
Cu	6.734654328	4.123465582	6.959500849

N	6.344434688	4.218815927	1.222374765
O	6.766202506	5.279420068	0.520652347
N	7.127871924	3.242417821	1.174362840
H	6.913884128	2.301136060	2.045991191
H	8.033546060	3.375013026	0.686425362
H	6.143565931	6.020507063	0.862838341

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O	11.124314243	3.422906022	2.584079207
O	5.098819843	4.981654484	6.448412959
O	6.879630059	2.070028497	6.889471736
O	8.644512775	5.071934340	6.894366877
O	8.563222220	3.022439983	3.187913502
O	6.910790146	5.874056982	3.626003962
O	4.844744452	2.720546645	3.170718306
O	5.358054453	7.495184924	2.101891854
O	4.115004595	0.178442455	2.820280172
O	9.547958763	0.365207121	2.409176855
O	8.323784416	7.929464797	2.636888598
O	2.402092418	3.537441240	2.508852585
O	6.861259405	7.071037630	7.087053301
O	4.271485950	2.564440442	7.243921031
O	9.450267117	2.528190641	7.255075009
O	9.492570954	5.526182113	3.074497042
O	4.331681272	5.311255472	3.172519005
O	6.734531086	0.883794570	3.064129300
O	5.016195177	7.385646234	4.826857605
O	5.064950072	0.961418372	5.222617126
O	10.324233963	3.920882741	5.106884029
O	8.728691125	0.913953736	5.189584681
O	8.836579999	7.106766065	5.162181008
O	3.156055841	3.718693262	5.082989884
Al	5.205101964	6.794063145	6.483943234
Si	5.320049298	1.391418629	6.778175342
Si	9.907217271	4.005457053	6.697932562
Si	9.877373373	3.980475134	3.520131364
Si	5.366495761	6.564636999	3.468595872
Si	5.225501025	1.129541246	3.585921107
Al	8.425376060	1.166988499	3.457796636
Si	8.371354594	6.616141576	3.657226251
Si	3.659893812	3.857548919	3.521625843
Si	3.753250063	4.018114146	6.606533179
Si	8.394230791	1.358162210	6.692771668
Si	8.398638202	6.769643396	6.738549958
O	2.646952776	4.722399089	7.580588829
O	3.871649798	7.199151468	7.560013100
O	9.452832371	7.523940006	7.755095645
O	11.137474223	4.638811328	7.599859720
O	8.347570255	0.083284271	7.763523691
O	5.267841647	0.106638092	7.799616129
H	3.425227372	8.054016688	7.467003510
H	2.904872652	5.679455403	7.721886317
H	6.167139935	-0.167200810	8.074896199
H	4.376067243	-0.755014341	2.751080939
H	1.601475801	4.066796828	2.675741494
H	10.367196795	0.849970144	2.217785261
H	11.986712343	3.845861348	2.736070060
H	8.851863322	8.689380789	2.936190154
H	6.177169184	8.023901601	2.032529587
H	10.250722320	6.998605323	7.948600817

H	11.874396272	4.041757493	7.815641937
H	8.907397871	-0.669042993	7.505550179
Cu	6.811682876	4.136891804	6.960511017
N	6.637812477	3.785929774	0.295163710
O	5.568090700	3.151775806	0.715033167
N	7.588169497	3.922501089	1.127154023
H	8.345561304	4.455383566	0.672443651
H	7.905990559	3.449759473	2.200894266
H	5.528627700	2.970943148	1.728989833

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O	11.093630657	3.257430280	2.728498123
O	5.048882942	4.979041171	6.337308113
O	6.815728255	2.087395011	6.981032685
O	8.579992982	5.078269880	6.948156669
O	8.552159015	2.987060694	3.450231123
O	7.030218427	5.838950242	3.574423560
O	4.845050798	2.559183894	3.376280547
O	5.495629214	7.302257224	1.917017606
O	4.184657922	0.008356686	2.934219416
O	9.598116473	0.405764690	2.583926061
O	8.497466384	7.896840276	2.656850255
O	2.541914940	3.402023543	2.357556624
O	6.783879205	7.074958350	7.007537579
O	4.178521340	2.568427895	7.090426472
O	9.372221711	2.566769796	7.418119402
O	9.612622266	5.477605254	3.187963003
O	4.472784728	5.176778300	3.084411803
O	6.789295708	0.755811556	3.177598147
O	5.069843190	7.353050745	4.645705640
O	5.171813213	0.711961494	5.346123727
O	10.348322794	3.867192817	5.258874332
O	8.736072819	0.860327161	5.406732646
O	8.871652743	7.092703680	5.210094784
O	3.045899182	3.817763906	4.966473551
Al	5.158449970	6.791871366	6.324663299
Si	5.268372914	1.373973221	6.844385677
Si	9.858722835	4.022296025	6.827641228
Si	9.918463071	3.937412857	3.669371223
Si	5.463080435	6.459367102	3.343717085
Si	5.247948509	1.005288242	3.709601381
Al	8.452311164	1.093662581	3.682486214
Si	8.475019825	6.597533972	3.687944396
Si	3.723879405	3.758500409	3.453055074
Si	3.677807671	4.042573332	6.483350720
Si	8.335541957	1.372330927	6.878236257
Si	8.339097200	6.773155702	6.760223718
O	2.595706336	4.734878587	7.496618292
O	3.779122044	7.234112849	7.324358483
O	9.323336625	7.541272150	7.834558714
O	11.053031625	4.694184083	7.749476604
O	8.253209473	0.140034573	7.992107486
O	5.143937627	0.227706980	8.015699711
H	3.340259504	8.086008486	7.185913838
H	2.823783679	5.703944291	7.586276561
H	6.026102188	-0.084915370	8.303098203
H	4.302660443	-0.936564789	3.130102474
H	1.682735949	4.111120654	2.475561649
H	10.388341854	0.944661523	2.415477767
H	11.938915075	3.733384500	2.678614091

H	9.034741698	8.646130083	2.965044633
H	6.218800669	7.958353350	1.904638864
H	10.133494936	7.041851744	8.044715201
H	11.883655305	4.196587104	7.827844674
H	8.846758397	-0.607267084	7.805647200
Cu	6.720776547	4.155298562	6.999715774
N	7.295959756	2.732886614	0.198245457
O	7.044682945	3.618551534	1.611088898
N	7.144340299	1.571581409	0.385333659
H	7.868956503	3.321938261	2.635557803
H	6.904705916	1.178139207	1.359435997
H	7.140227221	4.545145114	1.311024461

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Al	8.379887840	1.141960594	6.371038193
Cu	6.865553165	3.466428787	5.220055900
O	5.134318516	4.956532668	9.493901206
O	6.840634848	1.982931557	9.342507781
O	8.500825260	4.991237488	9.359820792
O	8.390177866	2.986685050	6.413991417
O	5.097993998	2.946809179	6.216708348
O	6.708095331	5.856314223	6.233725793
O	6.787960721	7.050221437	9.828337174
O	4.281201997	2.442763229	10.011431767
O	9.419604552	2.489726121	9.789787080
O	9.319890549	5.447153769	5.800960231
O	6.692922359	0.869079903	5.876368954
O	4.109231634	5.408372509	5.950366352
O	4.947648443	7.135520988	7.860682256
O	4.822670576	0.864052637	7.918949837
O	10.458216170	4.014407831	7.791791007
O	8.742866725	0.551593706	7.991741052
O	8.511918701	7.183959547	7.770130648
O	3.198290988	3.860722104	7.996590365
Si	5.261210237	6.588183155	9.393890711
Si	5.336885779	1.294865984	9.440771492
Si	9.853072546	4.004929018	9.339183064
Si	9.787324471	3.908476857	6.284395509
Si	5.183146715	1.209781849	6.348840669
Si	5.204072922	6.585383002	6.319252539
Si	8.214542434	6.560871382	6.269105797
Si	3.726410063	3.887168868	6.447266290
Si	3.813839304	3.940718704	9.548715361
Si	8.301082344	6.610942208	9.321649098
Si	8.349620070	1.290205652	9.389395441
O	9.625353175	0.833658005	5.169461328
H	10.055793605	-0.031922122	5.112020040
O	10.807438785	3.298760837	5.168047782
H	10.557054152	2.345468082	4.987604543
O	8.106825022	7.799329597	5.165981102
H	8.914801629	8.316076468	5.002660939
O	5.074336703	7.822806303	5.250635273
H	5.946118889	8.127978986	4.927877561
O	2.564920763	3.202243534	5.480504416
H	1.649280814	3.370880543	5.762751467
O	2.669111543	4.528849385	10.569183444
H	2.841135415	5.460384222	10.813743569
O	4.126689628	7.211069154	10.435180857
H	3.862482207	8.133518429	10.279607120
O	9.453875794	7.225355414	10.339362779

H	9.439990056	8.345228379	10.426308348
O	10.983389114	4.572640824	10.390225267
H	10.831526214	5.503142669	10.644505323
O	8.268426521	0.163612179	10.626330064
H	8.874644688	-0.585994893	10.497250114
O	5.339682702	-0.004187657	10.443694700
H	6.252669456	-0.188857997	10.758474675
O	4.049746491	0.588866647	5.332725928
H	3.289061054	1.190807019	5.201219044
O	7.529486221	3.933994529	3.583292426
H	8.144167608	4.694628429	3.614201506

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Al	8.256200996	1.234876683	6.353429181
Cu	7.155103634	3.832519367	4.848814555
O	5.134783776	4.973883368	9.593861083
O	6.797534941	1.917431211	9.328824957
O	8.480964821	4.893290204	9.452111090
O	8.348914191	3.067872706	6.289370115
O	5.068085454	2.979982988	6.289458494
O	6.852188641	5.845433432	6.481607424
O	6.834845176	7.007970986	9.936943114
O	4.253513370	2.457709925	10.010410858
O	9.356391232	2.384509475	9.936886448
O	9.471137549	5.453888357	5.944415050
O	6.603317405	0.831202555	5.885716092
O	4.218598070	5.462133809	6.000402935
O	5.007666261	7.157944975	7.944239436
O	4.746069428	0.855387986	7.919702280
O	10.409701725	3.824329455	7.906898476
O	8.763247718	0.644104614	7.931738781
O	8.682525040	7.136943993	7.967648875
O	3.184341095	3.981793420	8.045784287
Si	5.298040439	6.600855876	9.477778966
Si	5.269880074	1.279797444	9.436405756
Si	9.814101388	3.887339743	9.456802311
Si	9.815459608	3.870342238	6.371166543
Si	5.119874736	1.281562609	6.364910056
Si	5.349726478	6.589229172	6.420528894
Si	8.360741225	6.551708116	6.456193856
Si	3.754074552	3.956038699	6.503778722
Si	3.802766596	3.975257820	9.595865585
Si	8.345607556	6.524029313	9.478131929
Si	8.302981329	1.228890984	9.384828834
O	9.427680985	0.879839299	5.046641498
H	9.795866521	-0.016228235	4.988520831
O	10.868713382	3.245979138	5.280616889
H	10.590325523	2.310998800	5.078355705
O	8.282351315	7.816909270	5.384742332
H	9.102393562	7.866425872	4.726982093
O	5.328943280	7.818884481	5.337777869
H	6.224202567	8.019891452	4.992447018
O	2.551614940	3.358684245	5.519508637
H	1.649974873	3.587924157	5.804120729
O	2.662635581	4.530898736	10.642798185
H	2.828083499	5.459411474	10.899543417
O	4.177552111	7.269828485	10.505945646
H	3.906149359	8.178292896	10.291775550
O	9.467560827	7.058543681	10.575195142
H	9.389156119	8.072858843	10.845514596

O	10.962442265	4.466453564	10.480062039
H	10.763287498	5.368132724	10.801475326
O	8.173116706	0.003826857	10.517715937
H	8.820061906	-0.713325613	10.408523919
O	5.241920571	-0.010526183	10.452224037
H	6.153397781	-0.255849474	10.724123444
O	3.995738289	0.691099341	5.306840118
H	3.211967445	1.273490721	5.245029624
O	6.282956199	4.919337397	3.626868401
H	5.333715489	4.966169012	3.861472151
N	7.443592874	2.336290496	3.460699724
H	7.463248280	2.776438386	2.536553012
H	6.645432812	1.694966404	3.530833027
H	8.298800218	1.788078729	3.663034742

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Al	8.292443439	1.217291752	6.309149631
Cu	7.090469109	3.888592923	5.206432853
O	5.126443666	4.955557271	9.551442610
O	6.773363730	1.908260297	9.239047351
O	8.527517474	4.886131328	9.448933282
O	8.411291176	3.052777752	6.428225268
O	5.008854859	2.985001557	6.298365070
O	6.877515870	5.797721770	6.406539059
O	6.850984740	6.964721834	9.952718728
O	4.219422448	2.440656632	9.899125573
O	9.336945110	2.346184122	9.853295217
O	9.513941618	5.442606295	5.960531499
O	6.621342215	0.904604847	5.824027977
O	4.226493408	5.472373547	5.968502163
O	5.086309769	7.142652305	7.914523055
O	4.738110804	0.801626541	7.838657364
O	10.509999283	3.873803785	7.931943277
O	8.727782310	0.555963929	7.889681718
O	8.637793779	7.137288292	7.950612589
O	3.125606861	4.051123192	8.016115795
Si	5.321525668	6.579025615	9.456802819
Si	5.249014116	1.260259365	9.351358671
Si	9.843348894	3.853745542	9.457445112
Si	9.880218189	3.859686788	6.406836696
Si	5.118427545	1.281178844	6.299781059
Si	5.372922454	6.580432539	6.384071045
Si	8.391852495	6.536692019	6.436767902
Si	3.707863487	3.982110443	6.482644959
Si	3.780471501	3.974712709	9.552745292
Si	8.365754670	6.511878616	9.472099078
Si	8.269905864	1.194791326	9.317493060
O	9.524824391	0.893419543	5.073752836
H	9.946912186	0.020041951	5.071819280
O	10.888571645	3.222579815	5.290254035
H	10.579050710	2.287860236	5.084817374
O	8.313076432	7.795312522	5.358387690
H	9.159224995	7.779812173	4.625473440
O	5.370115414	7.820773743	5.315244778
H	6.262373426	8.023199034	4.963733868
O	2.515140256	3.413656504	5.474945226
H	1.610821032	3.656107567	5.739066017
O	2.667752155	4.509756920	10.637876749
H	2.817938155	5.443281413	10.884409186
O	4.183964290	7.257164619	10.456549720

H	3.955768578	8.183672107	10.271587288
O	9.501680791	7.082646015	10.534061015
H	9.506939797	8.042817241	10.709182053
O	10.957148890	4.359327926	10.556743387
H	10.823464667	5.290035147	10.821648364
O	8.121907089	-0.007471001	10.475989178
H	8.697793424	-0.772554925	10.306583531
O	5.217190321	-0.010481283	10.390038276
H	6.131689937	-0.252745066	10.658641760
O	4.015310941	0.699463462	5.217431090
H	3.218231321	1.261323369	5.157662982
O	6.129976019	4.842482673	3.667525966
H	5.158237520	4.800597832	3.767869939
N	7.324805658	2.772631611	3.488679698
H	6.938135945	1.842997053	3.697012079
H	8.323317231	2.661451967	3.277699581
H	6.553535992	3.857821266	3.211553276

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Al	8.256904069	1.228712093	6.317435953
Cu	7.203108490	3.939535034	4.941758822
O	5.145637840	4.942850673	9.678961888
O	6.745260905	1.924465747	9.353666900
O	8.503362061	4.879821012	9.464562607
O	8.365437354	3.077377109	6.327698596
O	5.064699157	2.976603517	6.270198245
O	6.890655818	5.849525264	6.342562736
O	6.857743498	6.983244602	9.958748138
O	4.183348276	2.435519819	9.970304987
O	9.315421493	2.349374166	9.928021763
O	9.522505339	5.440335475	5.970869275
O	6.604574359	0.841025865	5.844544413
O	4.262602907	5.452909309	5.918621771
O	5.069609620	7.060426992	7.943961645
O	4.742629542	0.845762521	7.888773189
O	10.445759082	3.812001454	7.937211342
O	8.679807244	0.623031487	7.926500569
O	8.652325315	7.126575659	7.959192683
O	3.228013412	4.076432185	8.031828349
Si	5.324949154	6.560216218	9.505315716
Si	5.225567087	1.265406953	9.418490905
Si	9.816065849	3.843070594	9.476043703
Si	9.857622703	3.842524413	6.394957479
Si	5.120712147	1.271605296	6.330507770
Si	5.370350951	6.579069880	6.394784944
Si	8.410243156	6.551194140	6.433305807
Si	3.767431745	3.963965813	6.485687950
Si	3.789995339	3.975853276	9.601197620
Si	8.364776618	6.504650864	9.481762137
Si	8.240585717	1.208995667	9.378897952
O	9.525945561	0.855862676	5.134925799
H	9.943859959	-0.017868075	5.190190778
O	10.903047996	3.190021879	5.323262010
H	10.591589529	2.256342526	5.119453653
O	8.325975336	7.812800260	5.361828137
H	9.161281772	8.260909706	5.132477027
O	5.325232468	7.852017696	5.362373463
H	6.215044247	8.103663043	5.040115001
O	2.529309725	3.386523103	5.537896926
H	1.639471253	3.601075850	5.867539605

O	2.624653942	4.518299045	10.626911297
H	2.770202231	5.446447838	10.892927099
O	4.191391606	7.275611451	10.482594357
H	3.963451667	8.194550149	10.263222682
O	9.507344273	7.036948578	10.556116944
H	9.493043814	8.141655674	10.729443970
O	10.949471056	4.378228572	10.541065436
H	10.780283849	5.289330573	10.850901538
O	8.105841085	-0.020552825	10.510019572
H	8.707367901	-0.767209612	10.349564440
O	5.176312496	-0.020758114	10.438905257
H	6.085881301	-0.273995561	10.711841113
O	3.984290691	0.670775014	5.293907718
H	3.190051927	1.236973364	5.242822912
O	6.026289609	4.909836106	3.479408833
H	5.082179344	4.881288628	3.738571101
N	7.271843938	2.647236789	3.414479337
H	6.883455593	1.759592248	3.773943159
H	8.253714373	2.422776801	3.195238337
H	6.253008682	4.047042761	2.993664518

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Al	8.438186349	1.303650578	6.374878225
Cu	7.173394298	3.918625600	4.969948899
O	5.006596698	4.748653147	9.481747938
O	6.949970276	1.830639437	9.316817203
O	8.396420262	4.908669953	9.651339258
O	8.449865118	3.115089702	6.477257077
O	5.056322758	2.811955846	6.265775887
O	6.670873072	5.635193510	6.325936243
O	6.573249155	6.856444328	10.093407450
O	4.381832379	2.184012350	10.035480954
O	9.482758067	2.457017611	9.901442905
O	9.323444198	5.578626530	5.972539545
O	6.811274021	0.814587537	5.893685685
O	3.970447680	5.213454404	6.146964784
O	4.960649981	6.988829412	7.950462408
O	4.942083654	0.671588587	7.902225343
O	10.416566575	4.192888754	8.013303703
O	8.983668097	0.647223955	7.921618514
O	8.247663557	7.082481729	8.020854409
O	3.087281889	3.522844675	8.072430804
Si	5.110174695	6.379587854	9.493477319
Si	5.468656568	1.089404891	9.419131116
Si	9.815139237	4.023802609	9.551837529
Si	9.820327224	4.041225578	6.479781802
Si	5.290212439	1.127204505	6.348048741
Si	5.126173352	6.325365746	6.448595403
Si	8.103655849	6.541797327	6.480221565
Si	3.651748828	3.629087304	6.528487616
Si	3.770107028	3.633373765	9.591325565
Si	8.109461830	6.514350121	9.577034316
Si	8.497658331	1.234067050	9.363912567
O	9.589000773	1.088440144	5.019894472
H	10.004164486	0.219965219	4.898410994
O	10.931816080	3.485130934	5.409999420
H	10.667111521	2.560185451	5.142958102
O	7.943263439	7.908276957	5.547310631
H	8.237048508	7.762614214	4.627416444
O	4.997476685	7.493939896	5.275253235

H	5.839427165	7.999343813	5.208504109
O	2.489097627	2.999939599	5.522638639
H	1.584119723	3.080019506	5.870891585
O	2.640984153	4.127728037	10.677849926
H	2.718288436	5.080061822	10.884025380
O	3.866047525	6.926608274	10.443599237
H	3.625873512	7.864140008	10.359291649
O	9.234663451	7.263250106	10.534953603
H	9.334575550	8.221711879	10.409936306
O	10.910318222	4.594213775	10.639999330
H	10.737747716	5.523808197	10.883380374
O	8.455884739	0.013965581	10.511607546
H	9.106090484	-0.690618396	10.350228085
O	5.539713130	-0.222567514	10.404972857
H	6.467664914	-0.391669750	10.681645104
O	4.235603824	0.432570932	5.278483273
H	3.404513938	0.940628011	5.197095520
N	6.594292316	5.313448723	3.229594504
O	7.163738815	6.393369448	3.321387740
N	7.393993574	2.481924140	3.530459291
H	7.364165928	2.888648203	2.590769706
H	6.647623520	1.782534338	3.619423826
H	8.282507745	1.969009661	3.671759123
O	5.183127631	5.405959745	3.358225625
H	5.003453127	6.339563879	3.676648188

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Al	8.266807541	1.214299516	6.371861024
Cu	7.150782799	3.981770175	4.931468938
O	5.159884747	4.958065861	9.569508159
O	6.801200998	1.927068574	9.374089366
O	8.521965425	4.901025395	9.463133205
O	8.361573157	3.053365791	6.320271504
O	5.090225307	2.955584696	6.253076993
O	6.883749615	5.761299555	6.367682089
O	6.852464285	7.009158742	9.922855516
O	4.250000307	2.461987879	10.028401575
O	9.360599220	2.384313906	9.971634704
O	9.520826298	5.420632224	5.963540990
O	6.625303178	0.772261334	5.935061131
O	4.247943863	5.422540576	5.959550878
O	5.080785774	7.114995339	7.903545252
O	4.752653928	0.881066611	7.933294289
O	10.442572505	3.810939715	7.930752628
O	8.766944871	0.643000585	7.968315200
O	8.648331361	7.127471413	7.941771846
O	3.214077140	3.967937113	8.019987548
Si	5.326533170	6.579205704	9.456781544
Si	5.272517347	1.283145879	9.450524927
Si	9.843468193	3.870808506	9.478540575
Si	9.845552775	3.816275894	6.392771206
Si	5.141271177	1.246041109	6.359348705
Si	5.368856598	6.540234127	6.380788982
Si	8.394232228	6.503833700	6.440454968
Si	3.768573754	3.913284125	6.472261967
Si	3.814463755	3.969556505	5.977206352
Si	8.364976946	6.522909521	9.477181303
Si	8.303292529	1.226743567	9.415575956
O	9.461897448	0.887678739	5.092496057
H	9.803088075	-0.015579383	4.994885126

O	10.895744916	3.186900154	5.309142914
H	10.574788145	2.259905573	5.089781070
O	8.275715461	7.744294044	5.334318659
H	9.116582710	8.081930868	4.969615974
O	5.372010666	7.774366480	5.299148563
H	6.277712302	8.072357085	5.070159102
O	2.546323320	3.337424447	5.507305279
H	1.651909611	3.561202357	5.817464747
O	2.671137318	4.563012996	10.598963386
H	2.843944520	5.492545969	10.845807746
O	4.183373812	7.265788605	10.444547431
H	3.913315777	8.170484506	10.213640892
O	9.497111501	7.081646634	10.546606222
H	9.488992742	8.186640662	10.690038863
O	10.993901027	4.446159352	10.503512183
H	10.809750070	5.351679670	10.819593220
O	8.174683297	0.006275383	10.554151434
H	8.811965061	-0.717408261	10.431597099
O	5.230514361	-0.008492321	10.466109408
H	6.139356916	-0.254510854	10.745752775
O	3.992252205	0.623075024	5.353926735
H	3.228869068	1.220165498	5.233757756
N	6.234540079	5.180245222	3.650073965
O	6.155358437	5.020186337	2.488587627
N	7.439614939	2.858020449	3.411795791
H	8.004778045	2.048915325	3.742148112
H	8.111642389	3.395256547	2.819406696

21

Al	8.415426431	1.256060205	6.298750034
Cu	6.955624474	3.748642920	5.361268505
O	5.102271903	4.930019920	9.401411702
O	6.842634594	1.958688803	9.236984510
O	8.521222534	4.953300460	9.443456571
O	8.521412278	3.069942572	6.472436082
O	5.042551441	3.006839338	6.230860422
O	6.792311492	5.820117329	6.235785672
O	6.770175805	6.976253812	9.907994422
O	4.255091018	2.398447075	9.809914278
O	9.425811814	2.426964397	9.732285096
O	9.452064844	5.512252990	5.888504091
O	6.745884422	1.021487285	5.718109332
O	4.144330593	5.469019289	5.931931159
O	5.067007248	7.165820497	7.836054969
O	4.891880251	0.793786639	7.753981237
O	10.564254962	4.105924667	7.907346011
O	8.746730702	0.535630019	7.878979431
O	8.514482061	7.157283652	7.870795749
O	3.089919107	3.956003240	7.929394083
Si	5.264630354	6.558936288	9.367224127
Si	5.339561670	1.257134751	9.285673731
Si	9.875101694	3.969123243	9.413993424
Si	9.914600999	3.970259928	6.389123024
Si	5.223398705	1.299154366	6.216065514
Si	5.284120383	6.592790382	6.297589337
Si	8.293826873	6.567974304	6.346801395
Si	3.684571437	3.949710294	6.397193094
Si	3.776815517	3.918590595	9.452738908
Si	8.297334353	6.570165105	9.416370567
Si	8.344968161	1.251671573	9.288052801

O	9.673919846	0.956911913	5.089426003
H	10.097560913	0.085636723	5.060820277
O	10.965009651	3.361883943	5.291732626
H	10.694417962	2.418047352	5.089058592
O	8.167473236	7.839839803	5.281144685
H	8.959289951	8.390745203	5.163334005
O	5.232292265	7.821957368	5.215391029
H	6.128117728	8.137506092	4.972983451
O	2.535647896	3.319930333	5.383280342
H	1.615516208	3.484925412	5.651195121
O	2.682980949	4.445750520	10.559461426
H	2.810633379	5.391063861	10.774708577
O	4.084037718	7.172655572	10.360546985
H	3.843995869	8.103334726	10.217221450
O	9.414030841	7.239623304	10.438751584
H	9.316847990	8.184294913	10.641488480
O	10.950787531	4.455057591	10.561865736
H	10.837514757	5.392592403	10.807173677
O	8.239243842	0.100513201	10.501534994
H	8.838875428	-0.652386604	10.362628407
O	5.315567679	-0.028888225	10.307249358
H	6.225193047	-0.226882664	10.623451526
O	4.127886414	0.693732491	5.143554813
H	3.389419354	1.312280078	4.972174297
N	6.796650864	3.282515482	3.410817946
H	7.641138066	3.596545352	2.916111359
H	6.617431318	2.266596867	3.317980919
N	5.649255987	4.116136855	3.033295128
O	4.603108278	3.503712102	3.055152161

22

Al	8.437966898	1.154875191	6.303202466
Cu	6.807891848	3.768676182	6.149759735
O	5.121220779	4.932968576	9.321799237
O	6.844456726	1.946508723	9.195898112
O	8.520918578	4.964314614	9.274302016
O	8.576196193	2.967766224	6.448833716
O	4.972206583	2.886718872	6.164379449
O	6.760472539	5.871389098	6.153973866
O	6.781951322	7.001055667	9.750104544
O	4.278196711	2.419705453	9.829757705
O	9.423364996	2.446791514	9.687859059
O	9.420602096	5.429220073	5.804601773

O	6.749046114	0.910454123	5.812527499
O	4.145078207	5.382641656	5.878737310
O	4.977885098	7.157856803	7.748063380
O	4.840809203	0.759240927	7.804943921
O	10.602209186	4.086465010	7.831658471
O	8.761417478	0.475874040	7.910162167
O	8.524223478	7.184272739	7.718989138
O	3.091383486	3.912710654	7.905757409
Si	5.262817419	6.565585919	9.273997767
Si	5.341169100	1.252883868	9.311540250
Si	9.878310141	3.977773867	9.325574181
Si	9.937358925	3.906860749	6.321034006
Si	5.218728211	1.168765764	6.246077557
Si	5.224908226	6.575916479	6.219348376
Si	8.305344961	6.546998479	6.211869212
Si	3.648840887	3.876791202	6.361955567
Si	3.793115231	3.923683471	9.425297025
Si	8.307321032	6.581529059	9.260792932
Si	8.353176486	1.246099212	9.283924354
O	9.700813609	0.847893995	5.112778339
H	10.101998642	-0.031034244	5.043477367
O	10.978380147	3.279613714	5.230570406
H	10.692095676	2.339481416	5.028108758
O	8.199542154	7.764008802	5.090084010
H	9.040547225	8.123244307	4.751632793
O	5.124811380	7.782128157	5.114434105
H	6.005835350	8.068082791	4.797599963
O	2.482865881	3.261421012	5.364162649
H	1.569483349	3.510206449	5.586069201
O	2.711887683	4.496968786	10.519526859
H	2.871314567	5.438849414	10.731279368
O	4.115224437	7.176597991	10.307799575
H	3.833043381	8.091197125	10.138293845
O	9.433251421	7.198896549	10.304370362
H	9.370209889	8.310782834	10.437199740
O	10.911815891	4.504087438	10.492124487
H	10.781753873	5.445017233	10.718895619
O	8.237526238	0.149694874	10.548403994
H	8.828424397	-0.615504216	10.441610533
O	5.337066087	0.000295242	10.371624970
H	6.252622139	-0.180542885	10.684458218
O	4.155059753	0.483481071	5.191240678
H	3.333981116	0.998691635	5.081923151

Table S5. Vibrational frequencies of the optimized structures

1

42.97	50.24	57.54	65.47	71.79	77.23
80.38	84.31	88.90	93.55	99.15	103.05
109.72	110.89	118.35	122.67	125.30	130.91
134.61	136.58	144.53	152.97	154.67	160.86
167.64	169.86	176.16	176.33	185.56	188.13
190.98	196.40	200.01	202.52	208.03	214.20
216.56	221.96	224.34	229.23	231.86	240.42
241.01	246.44	256.99	261.63	266.80	274.34
282.12	285.63	287.01	290.39	292.89	300.54
306.24	311.64	314.49	315.14	324.19	329.22
331.88	336.70	345.25	349.28	354.04	354.43
356.83	363.54	369.98	374.13	380.66	390.30
402.23	408.83	426.55	431.34	442.21	444.31
448.00	455.94	463.28	480.25	485.07	501.00
507.42	535.20	553.30	562.57	590.66	594.24
598.15	613.76	621.69	630.17	653.57	662.21
667.57	679.96	703.74	710.03	722.28	724.79
744.29	754.15	763.76	767.23	786.18	792.35
800.34	844.14	857.66	858.63	867.46	876.21
886.93	892.27	899.14	905.48	907.72	909.52
914.85	920.30	927.78	933.69	943.51	950.13
967.74	974.83	976.11	982.44	994.50	1001.01
1005.15	1008.73	1022.96	1029.55	1040.22	1049.20
1055.81	1063.62	1076.93	1079.97	1090.42	1097.99
1105.77	1141.65	1196.69	2801.04	3229.85	3373.08
3592.67	3601.26	3624.77	3744.80	3775.00	3785.30
3786.65	3818.38	3819.74			

2

28.66	34.67	40.99	47.46	57.23	60.72
66.23	69.20	72.11	80.82	86.23	89.90
95.30	98.08	101.94	106.43	111.73	113.32
119.93	124.13	130.42	139.28	140.20	144.08
152.00	153.15	155.83	164.85	168.27	171.74
176.27	181.52	185.56	193.33	193.78	198.31
199.34	201.96	208.20	210.54	217.67	221.49
223.59	229.11	235.03	239.39	242.43	247.86
254.36	259.29	265.36	268.34	277.49	283.77
286.48	290.90	295.10	296.43	298.45	305.78
306.16	310.25	313.69	317.95	322.40	328.20
334.30	338.18	348.19	352.15	355.26	356.10
362.82	374.83	378.21	386.84	399.54	406.13
410.63	417.64	428.01	428.20	434.14	443.33
446.28	454.29	463.96	466.81	489.32	492.52
506.04	525.27	526.52	539.16	554.87	568.51
577.22	590.32	601.63	612.10	625.18	653.14
670.31	679.06	686.73	700.04	711.41	737.36
742.41	746.03	762.96	768.44	780.81	805.69
831.10	837.94	851.60	857.50	861.41	869.55
872.35	884.10	895.43	903.14	907.61	911.76
923.52	924.98	933.24	945.77	949.42	955.40
967.39	984.13	990.42	997.81	998.24	1006.74
1007.71	1017.39	1020.05	1033.16	1041.82	1051.84
1062.03	1082.33	1083.32	1096.59	1098.50	1112.21

1120.71	1155.47	1949.23	3267.90	3556.52	3580.54
3613.49	3635.85	3767.12	3769.79	3775.67	3780.38
3785.17	3803.28	3807.84			

2A

16.56	29.96	38.91	45.45	47.47	55.12
64.28	66.24	70.80	78.15	81.52	86.93
87.54	88.38	91.06	103.34	109.67	111.94
115.61	118.58	119.64	123.71	129.01	133.00
140.81	143.13	151.55	156.47	160.76	162.00
166.62	171.17	175.77	180.24	181.50	185.68
189.84	192.44	197.59	198.30	205.70	215.57
216.53	218.98	220.14	228.74	231.59	238.20
241.82	248.28	253.36	257.91	260.60	267.19
273.46	280.74	285.27	286.67	288.33	300.67
304.56	309.04	312.58	315.76	320.23	327.01
328.68	335.82	338.69	343.56	351.92	354.33
355.16	362.01	367.49	372.87	381.37	388.26
401.87	408.90	425.98	430.18	442.53	445.35
448.76	455.88	462.03	483.85	496.00	502.26
504.84	533.19	552.30	562.00	590.09	596.39
596.91	613.10	624.48	629.13	651.73	662.13
666.75	675.91	701.45	709.94	720.61	722.50
743.61	753.50	759.49	765.54	786.87	789.57
807.36	836.76	843.59	854.42	856.99	870.92
876.47	887.27	892.12	901.68	903.69	907.33
910.21	918.33	925.60	931.63	944.55	948.05
967.79	969.89	972.76	975.46	988.26	998.76
1008.62	1011.70	1021.85	1026.61	1034.75	1045.92
1051.58	1059.67	1071.72	1076.01	1092.68	1097.97
1104.92	1144.13	1906.30	3209.19	3365.61	3580.34
3581.29	3638.91	3780.51	3781.24	3782.21	3782.86
3786.20	3815.79	3820.10			

3

15.83	32.57	46.06	51.33	56.16	63.92
64.62	70.53	75.83	79.87	83.63	86.83
92.18	97.97	103.29	105.24	114.06	116.82
120.16	124.79	135.53	136.15	151.21	152.53
159.29	162.67	168.91	174.66	178.91	179.96
183.86	185.74	189.79	190.24	195.76	199.01
204.47	206.47	207.32	212.41	221.78	222.14
226.98	228.46	234.72	238.58	247.04	249.91
253.15	257.84	261.55	267.04	274.29	277.07
286.51	290.57	293.35	293.93	297.81	303.45
304.39	308.87	317.83	319.97	326.04	332.14
333.48	337.50	345.83	348.83	349.54	351.41
356.84	359.31	361.31	365.47	372.00	375.71
385.24	397.54	399.44	413.24	422.57	425.80
438.08	442.08	449.26	458.43	460.90	466.66
476.60	506.27	521.72	531.34	577.78	587.96
599.62	605.94	612.18	631.19	651.84	657.61
692.66	694.89	706.24	722.87	734.45	756.65
765.59	772.09	791.89	796.51	819.28	837.58
841.92	852.59	854.44	856.93	861.14	864.63
871.13	874.40	884.51	901.64	913.39	917.62
921.42	930.42	934.08	936.38	945.41	958.61
966.53	975.28	981.41	987.95	989.88	997.60
1004.50	1008.55	1023.36	1033.49	1050.20	1072.01

1080.00 1091.17 1098.80 1103.30 1116.06 1122.20
1129.02 1146.57 2189.53 3214.00 3680.46 3710.57
3721.11 3736.37 3778.06 3779.33 3780.26 3782.00
3783.75 3787.64 3831.94

4

19.69 34.44 39.56 42.43 47.39 51.97
60.75 64.67 69.06 71.45 75.99 78.90
84.61 85.93 93.88 95.09 97.57 104.84
108.06 112.75 116.70 127.93 136.18 138.40
143.09 147.73 149.25 156.83 160.30 161.61
166.20 167.40 172.72 177.38 179.13 183.63
188.86 190.39 193.48 197.59 203.27 207.67
210.07 213.98 219.82 221.07 226.39 236.74
238.81 243.52 245.22 252.33 254.15 258.17
267.34 270.16 275.25 279.27 282.27 283.13
294.11 298.02 299.14 309.21 311.47 313.92
318.69 322.34 325.95 328.74 331.14 333.23
338.81 343.18 346.58 353.04 355.25 363.10
364.79 367.42 367.80 376.41 390.13 395.52
410.59 415.01 429.29 437.94 445.41 449.17
451.11 460.12 465.26 473.11 486.23 500.16
510.36 516.59 555.18 577.61 586.98 601.74
602.61 626.20 629.74 643.72 667.30 669.49
676.46 698.98 709.02 724.94 733.59 745.34
754.74 768.85 773.54 775.65 780.75 818.14
842.74 848.94 856.72 858.69 862.80 864.84
881.14 884.32 894.72 895.52 903.28 908.64
915.64 916.42 924.73 929.97 939.99 942.87
952.79 967.42 971.59 975.62 990.77 1005.36
1009.98 1011.06 1021.75 1033.81 1052.36 1065.37
1069.72 1074.29 1080.36 1096.56 1108.09 1113.92
1137.94 1148.25 1178.06 1566.97 1622.80 1912.71
3162.37 3279.34 3380.75 3531.68 3642.02 3689.67
3711.77 3777.09 3779.81 3783.85 3785.89 3792.00
3792.28 3793.23 3828.95

5

32.16 35.82 48.31 53.50 63.52 68.50
69.92 79.69 82.36 87.00 89.59 96.45
99.63 102.14 106.80 118.23 118.65 129.48
138.49 143.16 143.75 155.26 156.21 161.77
164.02 166.50 177.51 181.63 184.77 188.85
195.56 199.87 204.77 206.03 212.48 212.96
217.33 221.31 225.91 229.31 233.77 240.86
245.86 251.13 257.37 262.51 269.35 274.49
286.46 287.85 290.02 297.73 305.07 307.80
313.19 315.95 317.88 322.68 325.09 334.39
335.59 338.07 342.84 345.52 348.58 355.52
358.20 362.39 365.89 369.87 383.45 390.29
405.71 412.21 429.77 435.22 441.92 444.78
454.00 462.21 468.02 484.82 506.46 517.29
530.03 536.09 543.26 557.65 559.88 583.47
595.48 599.91 605.55 617.62 626.27 635.13
658.20 669.05 681.31 700.61 707.01 722.72
725.06 744.87 755.73 762.55 767.27 779.82
787.49 793.72 828.54 844.18 852.26 855.53
875.39 885.22 891.94 903.39 908.25 914.06
917.61 923.77 926.36 932.23 941.97 956.60
961.00 965.95 976.81 990.19 998.54 1002.32
1014.25 1019.29 1030.09 1041.03 1046.27 1050.13
1060.60 1063.65 1076.44 1088.74 1098.64 1107.26
1110.51 1126.65 1145.14 1158.31 1172.22 1306.16

3116.45 3253.06 3476.20 3482.87 3530.25 3559.92
3693.74 3735.63 3779.37 3789.82 3813.74 3834.41

6

28.57 37.06 40.44 50.47 54.41 62.81
68.70 71.04 78.29 84.34 86.53 89.64
93.78 97.54 104.64 105.47 108.80 117.09
121.78 126.85 133.46 140.03 143.63 147.66
149.15 154.75 164.13 168.50 170.79 171.58
183.41 186.19 189.32 199.68 201.73 204.67
207.54 210.27 214.23 220.67 221.57 225.24
230.61 235.01 237.99 243.03 247.38 258.37
261.81 266.56 277.49 281.94 290.40 292.63
298.34 305.58 307.70 313.73 317.41 319.38
320.94 331.21 332.04 336.29 337.09 346.43
347.35 352.33 354.86 358.77 361.82 365.12
376.62 388.06 391.49 396.05 401.67 408.52
423.39 429.22 433.26 439.83 445.68 448.5
459.97 461.65 468.02 478.42 507.18 515.62
521.27 534.81 540.28 554.84 570.56 586.36
603.05 604.15 616.33 623.34 635.92 663.51
675.94 692.71 707.05 712.64 729.08 730.26
749.35 759.50 769.61 776.38 777.54 787.28
795.40 843.84 848.91 857.52 862.20 876.67
887.73 892.49 898.89 912.04 917.03 923.81
925.39 933.55 942.15 946.44 961.63 966.27
971.96 977.19 987.27 989.95 1003.68 1010.63
1016.30 1026.71 1037.14 1047.31 1050.62 1057.99
1060.24 1076.10 1078.59 1095.60 1102.78 1107.66
1126.94 1128.73 1166.50 1168.13 1315.70 1790.47
3125.79 3213.82 3486.97 3509.44 3542.55 3621.42
3633.08 3696.52 3775.89 3785.25 3802.41 3826.78

7

27.57 38.03 45.90 53.37 58.75 63.71
71.71 72.85 80.56 83.67 84.81 87.91
88.91 91.97 96.35 99.39 106.44 111.74
119.91 122.63 125.82 127.79 142.61 143.80
148.21 149.54 160.16 165.03 167.65 172.76
175.03 182.99 186.84 196.57 199.01 203.47
207.07 208.32 216.11 218.78 221.34 227.66
228.24 229.89 238.50 242.74 245.71 260.24
265.89 270.94 275.61 282.89 287.25 292.87
296.62 300.06 302.04 306.99 310.81 316.56
318.50 321.54 324.64 331.89 334.51 339.54
342.76 347.94 353.02 356.74 358.80 361.68
364.84 373.65 392.34 393.66 398.86 400.80
419.12 431.11 435.26 441.43 443.43 449.36
454.97 462.65 467.49 471.21 501.44 513.33
520.55 528.81 542.95 553.02 580.91 597.67
600.55 612.31 619.78 626.73 636.31 658.19
669.31 681.92 694.37 705.02 718.28 727.28
735.62 749.79 759.02 766.40 769.13 782.12
783.36 787.81 835.72 845.33 853.38 862.46
865.41 881.45 887.68 896.46 898.47 907.62
910.61 919.79 923.86 929.71 936.36 943.04
954.57 959.64 968.59 978.27 986.73 990.01
998.48 1007.07 1013.08 1027.76 1039.64 1040.98
1044.77 1049.70 1059.44 1072.59 1076.09 1090.37
1098.53 1113.95 1126.38 1159.10 1162.96 1192.65
1612.80 1638.88 3159.48 3250.47 3325.43 3455.18
3484.21 3509.55 3556.38 3631.59 3666.17 3674.38
3776.84 3777.25 3786.11 3786.79 3807.96 3815.60

7A

25.34	34.64	38.50	43.26	51.69	58.39
59.59	64.95	67.20	74.49	80.43	86.86
88.54	90.13	93.82	97.21	100.84	101.23
110.15	116.28	120.96	122.17	127.17	129.86
136.73	142.56	147.06	149.86	154.81	162.34
169.22	171.31	174.33	183.03	185.02	193.37
198.00	202.54	207.32	210.17	211.09	219.30
224.22	225.53	226.71	230.27	234.72	239.10
240.63	242.62	251.02	256.35	261.95	270.06
278.40	284.47	288.98	297.49	298.85	304.97
307.90	312.75	314.43	319.89	322.69	327.28
329.20	334.04	334.90	338.35	345.40	347.79
353.83	355.48	358.35	360.86	364.90	367.33
376.54	383.62	394.42	398.48	400.98	420.08
426.99	435.17	440.23	444.75	452.12	458.55
460.14	465.96	474.55	504.63	514.91	516.59
527.88	532.98	553.82	586.91	598.44	606.08
616.27	624.13	634.28	650.30	668.78	683.07
694.60	706.20	712.22	724.43	731.44	737.46
748.61	758.55	762.84	769.32	780.65	781.72
791.50	845.82	849.75	854.68	862.28	864.62
875.99	888.67	893.02	897.90	907.39	911.14
921.41	925.51	928.95	938.94	940.21	955.09
963.74	964.95	979.76	985.49	993.12	996.12
1003.28	1014.38	1029.77	1040.81	1042.61	1045.09
1049.97	1062.03	1070.97	1075.63	1097.65	1100.76
1105.70	1124.82	1137.01	1164.22	1236.85	1592.63
1635.74	1715.03	3137.33	3251.77	3325.53	3444.51
3501.54	3517.22	3561.55	3620.19	3655.95	3663.30
3778.17	3786.23	3788.62	3791.15	3805.50	3808.12

8

30.95	36.14	45.77	49.55	54.30	56.90
65.37	71.48	75.16	83.68	85.27	87.95
91.38	92.76	101.06	103.31	105.65	110.63
120.81	121.87	128.63	138.44	142.76	144.56
149.52	150.28	158.27	165.11	167.95	168.71
172.02	183.39	184.95	193.91	198.10	202.56
205.14	207.92	216.51	217.97	222.28	223.03
228.59	230.08	238.87	243.21	247.96	258.99
261.58	266.07	275.66	280.98	290.55	292.08
297.51	305.11	308.60	311.29	312.90	319.03
320.87	326.93	330.03	333.25	336.62	339.39
347.77	347.93	352.63	355.54	356.22	362.40
365.52	374.15	388.20	392.09	394.12	407.69
409.85	421.54	428.45	436.02	445.60	447.75
457.37	461.05	465.83	506.32	509.75	515.26
522.02	533.31	546.51	556.49	583.06	600.77
605.23	618.33	624.36	634.90	660.68	674.18
686.86	705.04	710.74	725.26	730.01	746.73
758.76	767.43	773.40	778.29	788.12	795.84
833.00	847.39	858.29	861.33	877.21	885.72
890.27	897.40	910.23	914.16	922.05	925.94
930.03	934.72	938.38	939.98	959.02	967.27
974.71	988.02	995.11	997.34	1010.95	1015.45
1027.65	1040.32	1042.09	1049.66	1054.86	1059.43
1069.26	1076.76	1085.13	1098.63	1105.93	1114.49
1127.65	1159.99	1169.07	1282.28	1378.96	2380.97
3134.44	3240.19	3491.36	3556.92	3580.22	3651.57
3677.42	3695.17	3776.56	3785.43	3808.83	3828.27

8A

32.12	37.05	45.09	51.14	54.13	67.47
69.41	73.17	78.19	83.64	86.07	89.71
90.53	91.61	98.30	100.53	106.40	111.19

120.45	123.23	126.34	126.87	134.40	138.44
140.15	146.32	147.95	152.66	158.27	163.71
167.73	171.75	176.54	179.13	184.06	185.95
195.67	201.55	204.06	206.90	209.04	213.97
219.46	223.54	226.20	231.64	233.18	238.25
242.08	246.63	255.67	261.12	265.05	273.63
275.31	286.37	287.07	290.11	296.48	301.35
304.43	305.65	310.46	312.43	318.48	320.81
322.65	330.60	331.75	336.50	340.35	348.90
351.82	354.56	358.25	360.01	363.42	365.53
375.67	390.71	395.18	399.39	402.35	413.31
424.19	431.64	435.79	444.40	449.75	457.11
459.89	467.08	480.13	503.56	509.55	518.46
524.40	530.86	541.56	556.27	582.36	598.25
605.77	616.34	623.90	633.82	661.70	674.92
694.19	706.77	709.49	725.74	731.28	748.08
758.31	768.72	775.67	780.44	784.07	791.00
839.06	845.39	855.29	862.70	864.99	869.33
887.48	892.80	898.01	907.81	911.92	918.37
922.65	927.95	931.60	937.86	945.86	958.31
969.46	981.13	985.11	988.91	1001.87	1010.03
1015.76	1032.05	1039.20	1042.06	1050.22	1053.29
1064.20	1073.79	1081.14	1099.72	1103.74	1113.99
1127.39	1167.19	1168.50	1346.54	1828.49	3130.02
3212.43	3494.34	3551.02	3618.20	3656.23	3670.89
3775.63	3783.43	3787.38	3788.01	3807.17	3826.93

8B

23.64	30.56	36.28	44.38	44.81	52.46
54.22	62.81	67.02	67.85	77.87	80.17
84.78	87.46	90.39	95.29	99.48	103.12
105.37	110.17	114.88	122.42	127.12	130.25
137.55	139.71	142.92	148.08	154.01	165.19
167.21	171.26	173.06	174.20	179.12	183.53
191.06	192.58	197.62	202.29	205.02	207.02
213.34	218.05	224.48	227.09	230.17	234.16
235.37	241.85	243.99	253.89	259.54	268.60
269.98	278.32	286.40	288.86	295.37	298.05
303.47	307.49	311.95	313.80	320.48	321.23
323.99	333.60	336.76	337.98	340.05	342.84
347.05	349.20	352.45	354.99	356.15	360.11
366.08	371.61	380.69	395.32	399.48	406.25
423.83	436.37	439.07	441.89	454.88	457.20
459.30	464.32	478.96	499.00	509.75	518.68
522.92	540.75	552.43	587.00	596.03	599.17
609.23	614.97	628.51	636.26	670.71	676.43
684.76	702.96	709.84	715.64	726.05	728.94
744.27	753.77	762.94	768.74	781.79	788.88
795.63	846.23	854.74	858.19	865.76	867.64
881.06	890.92	894.74	898.48	905.16	910.13
917.58	924.18	930.90	931.89	937.60	956.80
961.41	965.79	978.82	980.70	989.06	996.04
1003.06	1014.76	1028.74	1037.45	1044.68	1048.21
1056.16	1063.70	1072.87	1082.86	1098.56	1103.23
1107.70	1127.34	1148.70	1169.13	1230.99	1361.74
1610.88	1630.96	3107.85	3272.39	3306.75	3450.02
3478.64	3521.53	3572.69	3614.43	3653.61	3708.73
3773.96	3777.12	3787.24	3791.56	3794.87	3805.88

8A-TS

-269.89	20.46	32.78	38.44	49.11	54.26
54.63	60.65	66.98	71.79	77.71	84.67
86.10	89.21	93.90	95.00	105.03	108.21
118.49	120.48	123.95	127.42	134.01	142.85
146.80	148.89	152.13	153.27	162.95	169.57
171.74	179.60	184.84	187.18	191.37	193.45
198.29	203.84	208.27	210.23	219.36	222.83
225.26	228.91	230.42	233.17	239.70	244.18

250.74	254.82	258.97	268.61	271.50	279.16
288.26	291.11	294.09	300.96	305.32	307.18
311.45	317.90	319.78	321.09	322.40	330.19
332.15	336.17	339.68	348.55	350.28	357.61
359.78	362.47	365.56	368.33	383.98	392.18
400.23	403.10	417.13	423.23	428.71	437.04
441.47	448.96	457.14	460.40	464.21	473.62
479.91	504.18	507.32	513.91	520.22	538.55
541.41	557.97	581.35	599.97	601.59	614.66
623.00	638.40	655.53	663.74	679.55	707.34
709.99	724.08	733.37	748.69	756.28	762.29
772.80	780.48	787.00	795.08	831.57	840.57
844.64	857.57	862.22	871.49	882.61	888.85
897.21	911.63	915.63	917.77	924.10	926.36
928.05	933.30	939.82	945.21	963.86	971.21
975.17	985.44	991.53	998.51	1003.31	1013.77
1028.97	1030.04	1040.65	1044.49	1054.38	1060.90
1073.05	1074.86	1079.72	1094.43	1099.09	1105.23
1128.92	1147.89	1165.97	1306.80	1498.55	2150.05
3129.38	3274.56	3517.45	3544.03	3608.93	3635.64
3653.72	3749.38	3771.92	3788.78	3808.07	3834.59

9

34.03	40.12	41.29	50.17	54.06	63.46
65.99	77.25	80.11	83.50	86.06	88.58
92.80	95.50	97.94	103.80	111.45	117.08
117.73	122.72	124.27	130.91	137.39	140.23
143.53	148.35	154.02	154.10	157.10	163.05
169.43	173.19	177.55	181.96	187.29	193.12
199.94	203.55	207.43	209.27	218.26	223.52
225.73	231.13	234.31	234.88	239.01	243.57
247.58	253.46	254.54	261.23	269.41	278.89
286.38	291.29	295.04	300.17	306.89	309.96
312.11	316.87	319.31	321.98	324.54	332.08
334.30	337.69	338.61	346.87	351.27	355.24
358.63	359.92	365.30	367.20	381.26	390.20
400.62	401.25	413.97	419.30	425.15	429.46
436.70	443.63	446.82	457.22	463.91	466.88
491.58	500.48	505.47	517.66	526.96	531.50
539.55	556.85	586.16	599.35	601.92	613.64
621.00	634.15	660.01	663.91	676.84	684.12
704.37	709.49	727.31	727.95	750.19	758.84
762.68	772.42	779.25	784.34	792.99	830.31
846.59	854.74	857.74	858.31	867.03	882.98
894.27	898.87	908.22	913.82	914.17	918.79
925.36	930.29	933.77	941.84	947.80	957.34
964.77	973.56	985.24	988.57	993.48	999.23
1003.78	1015.63	1027.81	1034.36	1041.70	1051.18
1059.86	1064.05	1075.23	1083.36	1097.29	1103.16
1106.86	1128.06	1153.11	1178.00	1404.74	3081.18
3245.16	3507.10	3550.52	3599.97	3648.21	3652.65
3773.43	3786.14	3787.44	3790.54	3802.92	3829.97

18-TS

-108.93	35.18	38.77	39.66	50.36	57.69
60.59	69.85	72.32	79.45	83.68	85.77
89.61	95.70	96.91	98.77	104.70	113.44
115.66	120.50	126.30	127.90	133.70	135.86
144.06	145.23	148.81	153.71	154.84	164.92
166.80	170.00	174.37	176.76	184.84	186.14
193.13	199.41	206.15	207.84	212.11	214.67
217.98	222.47	224.40	225.13	232.56	237.09
243.83	246.51	249.56	258.10	270.37	275.76
283.37	290.15	294.24	300.94	306.02	309.76
310.92	311.34	317.02	318.90	326.61	332.38
335.15	337.64	339.18	344.51	349.09	350.67
353.16	358.54	360.85	364.59	369.01	374.97
388.22	395.28	401.81	407.38	413.90	424.94

436.13	442.17	448.72	456.61	458.29	466.74
481.37	504.97	513.51	519.28	520.24	529.29
539.95	554.20	584.01	596.48	599.80	613.99
619.12	632.51	652.77	673.65	693.71	703.96
707.19	716.81	724.77	733.02	747.06	759.71
766.65	771.87	783.47	790.14	816.08	831.60
848.07	854.62	859.32	865.96	885.31	889.15
894.64	906.43	907.53	918.85	923.27	926.78
930.03	937.52	941.84	961.25	972.28	973.63
988.13	995.65	1000.73	1009.12	1015.96	1029.15
1031.37	1040.43	1050.11	1052.37	1061.85	1073.44
1075.68	1082.85	1088.84	1101.74	1106.25	1126.93
1158.40	1163.64	1273.46	1304.09	1668.91	2036.46
3128.76	3187.24	3499.08	3555.27	3613.84	3639.35
3660.36	3778.10	3785.38	3786.48	3800.77	3802.01

10

12.16	21.38	34.14	40.87	50.17	54.98
59.67	60.84	63.08	68.95	72.33	74.70
84.09	85.31	88.16	88.61	93.01	95.20
102.00	104.42	109.50	112.54	118.97	121.64
123.04	125.54	129.88	133.82	142.68	143.45
150.01	151.24	158.29	164.20	169.56	171.71
172.32	181.11	185.77	194.29	200.89	203.48
207.91	209.51	218.94	222.50	224.03	231.02
232.22	235.71	240.66	245.95	249.55	256.88
261.70	270.60	281.10	285.55	288.45	295.70
299.93	304.99	309.02	311.49	317.17	320.44
320.87	329.44	331.11	335.21	338.76	348.25
349.44	354.72	357.39	358.36	363.60	365.09
377.62	392.80	398.40	402.27	414.38	421.95
427.80	435.22	444.90	446.58	457.10	459.39
466.18	474.52	504.15	513.21	520.21	528.35
538.37	554.09	581.89	587.38	601.49	604.88
619.98	621.89	633.22	660.15	673.18	688.90
694.55	704.69	710.50	726.42	728.98	748.77
758.38	767.18	777.33	780.41	785.22	792.04
838.76	841.91	855.23	858.79	859.54	864.73
886.41	892.24	898.34	906.01	911.50	917.67
920.49	930.13	934.83	937.93	945.25	960.15
970.13	981.62	986.44	989.83	1002.93	1011.36
1016.25	1031.81	1039.33	1043.93	1050.77	1055.07
1065.74	1074.54	1081.23	1099.61	1104.41	1109.51
1127.33	1163.89	1169.01	1299.64	1689.85	3136.41
3186.53	3501.96	3558.06	3613.42	3657.57	3662.69
3775.54	3787.96	3788.86	3790.78	3806.90	3828.89

11

8.44	21.62	26.54	38.58	47.53	53.00
64.12	65.94	67.46	72.78	75.23	77.21
82.34	86.22	86.42	90.68	94.80	100.20
102.59	107.76	111.60	116.74	118.48	121.78
128.49	132.98	133.41	144.04	149.48	152.45
154.42	165.77	171.07	172.75	173.61	186.42
188.09	193.88	196.13	197.62	199.36	209.48
212.23	214.33	221.91	223.69	229.66	232.57
240.20	248.52	253.92	258.34	266.12	268.45
274.81	276.71	283.06	287.28	293.14	294.33
296.87	302.52	308.31	313.04	316.01	321.40
323.99	335.79	338.45	341.84	346.29	347.83
355.47	357.71	359.67	370.57	372.99	381.43
387.75	393.68	402.29	408.31	410.53	421.72
429.51	434.38	437.42	446.12	457.16	466.63
470.45	484.20	495.37	514.28	524.49	530.41
564.73	573.24	590.42	594.47	611.26	625.32

635.82	640.16	653.33	674.68	697.27	706.57
729.23	740.23	743.16	758.95	764.16	775.79
788.97	792.36	821.36	827.18	842.26	846.90
847.73	855.62	869.24	871.85	881.43	896.95
900.51	912.13	915.25	921.93	930.23	933.48
938.28	946.85	949.36	960.08	967.80	974.72
982.19	987.05	994.48	1008.33	1009.91	1012.50
1020.98	1043.94	1062.94	1070.16	1082.93	1087.78
1111.54	1114.23	1118.72	1122.93	1132.69	1142.58
1158.65	1299.06	3363.91	3514.86	3556.43	3624.19
3695.28	3771.47	3780.03	3780.61	3783.97	3789.88
3797.19	3829.97	3835.54			

12

12.78	26.75	38.04	40.46	47.56	51.28
58.71	64.77	72.50	76.68	78.07	85.35
88.92	93.29	95.00	96.62	100.08	108.73
116.88	125.27	126.85	128.56	134.18	136.31
140.15	146.57	152.48	156.36	158.30	165.08
167.08	170.03	177.63	182.26	184.45	191.84
196.49	199.87	203.30	207.35	212.16	217.50
224.28	224.95	227.35	233.35	236.07	238.90
243.06	249.49	253.39	255.49	267.49	278.67
280.61	283.02	286.94	291.57	301.62	302.40
303.53	306.01	311.31	316.22	319.04	321.34
324.32	331.09	333.19	338.28	339.82	342.15
353.07	356.70	357.95	363.16	366.62	376.71
384.82	399.42	403.99	407.64	418.09	430.90
438.70	444.75	448.54	452.18	460.00	470.96
482.47	501.74	510.67	512.13	524.39	531.87
549.08	551.89	587.63	598.52	612.42	617.03
626.12	640.71	644.41	670.27	697.30	698.33
702.05	709.21	733.46	738.91	754.73	757.32
761.65	771.73	778.98	793.51	817.99	845.76
849.80	853.45	856.96	859.79	861.91	871.10
887.45	892.47	902.65	908.98	916.87	918.61
921.63	935.39	945.56	947.04	948.98	957.86
965.04	980.14	985.95	996.79	999.59	1004.71
1008.70	1019.47	1030.04	1038.00	1047.71	1055.87
1070.13	1071.14	1084.14	1100.04	1104.43	1108.45
1120.28	1132.63	1153.85	1197.37	1590.05	3177.40
3493.40	3553.51	3568.50	3639.39	3722.20	3771.09
3772.11	3775.24	3784.29	3784.83	3786.52	3800.37

NH₃

1071.77	1650.03	1650.06	3377.73	3514.50	3515.22
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N₂

841.59	1641.96	1642.34	3503.34	3616.03	3616.71
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H₂O

1627.84	3709.64	3832.15
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NO

1909.34

NO⁺

2363.65

HNO₃

482.25	547.91	604.25	738.47	853.94	1273.70
1326.55	1765.98	3615.90			

NO₃⁻

683.08	684.01	804.97	1041.84	1418.17	1422.32
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HNO₂

583.13	730.76	843.73	1284.84	1669.07	3445.28
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NO₂⁻

756.31	1253.58	1311.68
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N₂O

585.21	585.46	1320.09	2312.09
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H₃N⁺-NO

36.75	280.82	463.19	599.12	719.99	1146.79
1576.29	1589.34	2064.44	3360.13	3510.71	3518.03

NH₄⁺--H₂N-NO

94.20	168.10	277.40	419.99	547.99	656.29
665.96	743.02	791.86	965.90	1146.32	1445.05
1525.12	1560.22	1568.94	1709.13	1715.18	1720.85
2122.15	2828.01	2921.64	2930.42	3330.86	3476.28

NH₄⁺+H₂N-NO

701.42	797.89	964.91	1232.40	1393.55	1474.39
1670.34	3000.25	3325.47			

A

134.92	583.87	717.83	1030.08	1176.27	1525.27
1564.73	3355.78	3619.25			

B

657.23	871.59	1052.66	1225.41	1398.90	1499.39
1603.45	3191.96	3295.63			

C

643.97	697.42	908.04	941.24	1321.23	1401.99
1575.88	3313.25	3387.37			

D

511.82	640.35	882.82	926.92	1282.93	1401.25
1615.08	3300.57	3676.91			

E

562.52	629.33	861.94	928.80	1249.88	1376.29
1620.37	3017.37	3381.72			

F

482.89	582.48	800.51	982.04	1244.21	1340.43
1663.02	3132.24	3662.28			

TS1

-1818.76 450.48 628.07 913.85 1238.83 1297.77
1567.83 2162.90 3124.53

TS2

-1649.82 549.04 929.18 1153.47 1184.51 1347.70
1422.81 2010.89 3388.61

TS3

-652.21 636.53 774.90 908.22 1234.33 1361.91
1601.08 3222.15 3666.51

TS4

-1272.38 168.70 439.03 595.52 695.27 1208.36
1764.84 3510.63 3801.20

TS5

-1220.72 161.73 448.21 509.16 663.62 1155.71
1845.93 3655.99 3834.47

TS6

-537.21 577.10 698.31 937.22 1203.28 1308.02
1655.90 3096.86 3643.94

TS7

-1453.40 350.50 525.53 747.13 870.26 1174.48
1821.92 2089.97 3641.79

20/A'

17.64 29.60 36.65 43.33 50.74 58.61
59.55 62.00 66.58 70.11 75.19 79.22
82.02 83.20 90.65 95.37 97.49 98.49
104.83 111.76 119.12 120.56 123.50 127.78
130.01 137.12 145.72 148.95 153.49 153.97
157.45 161.86 165.18 169.58 179.12 180.34
182.36 185.47 190.56 194.14 200.18 204.89
209.40 211.39 213.32 214.30 219.17 221.51
227.31 237.59 239.57 248.59 253.92 255.43
259.28 265.95 266.89 273.87 279.36 286.12
291.41 299.62 302.96 307.37 308.86 314.02
319.13 325.44 326.66 330.73 334.49 337.01
341.16 350.03 352.25 353.96 359.20 361.17
367.47 374.22 387.36 397.83 404.15 420.00
427.87 437.26 442.74 448.27 452.95 461.10
465.00 496.31 513.31 525.38 561.33 574.06
581.82 601.29 604.83 609.97 615.91 631.41
652.80 666.43 672.55 681.75 686.65 702.71
712.41 720.62 736.38 749.75 759.32 765.61
767.74 780.48 823.43 829.89 832.58 846.71
853.95 859.88 862.97 867.28 873.65 885.81
890.53 894.85 901.99 906.89 910.51 916.96
926.15 927.66 939.11 946.26 947.24 955.49
963.02 986.72 991.24 999.65 1006.33 1025.43
1033.16 1043.95 1058.90 1064.24 1071.99 1085.39
1092.85 1107.96 1116.38 1122.58 1129.88 1149.53
1153.27 1206.62 1317.98 1350.10 1528.48 1575.86
1663.19 3168.78 3297.71 3413.60 3585.18 3652.01
3724.64 3775.55 3781.03 3790.27 3790.67 3790.78
3791.69 3818.29 3828.08

TS8

-1635.39 33.87 38.01 46.12 49.59 56.08
59.56 66.89 68.69 72.04 74.60 77.82
83.07 89.46 93.81 94.73 99.14 102.08
109.48 110.81 114.01 116.43 122.30 122.50
126.57 133.02 139.33 144.58 148.58 153.62
157.99 162.69 164.39 172.25 178.75 183.04
186.39 188.27 194.12 195.71 197.62 200.89
208.18 208.95 212.12 219.86 223.71 226.65
230.79 235.64 237.70 244.33 251.45 255.90
258.93 265.42 271.25 277.15 279.04 284.36
292.16 297.17 302.00 304.78 308.17 311.86
317.36 322.65 324.61 326.95 336.78 339.73
343.42 349.58 350.36 354.08 359.29 361.14
367.64 373.13 387.84 399.25 404.94 417.81
426.66 431.90 446.36 448.82 452.68 459.35
463.80 496.23 507.39 508.81 530.20 547.65
565.03 565.78 586.07 606.83 613.90 625.63
630.40 656.53 666.10 680.78 682.59 704.42
709.93 712.77 724.29 731.37 747.80 764.13
765.32 782.15 791.41 822.81 827.32 836.25
845.22 853.57 865.28 872.69 876.17 881.82
891.35 895.85 903.93 908.59 913.57 917.88
924.34 927.63 937.77 943.25 956.32 959.65
966.03 982.74 990.81 1003.33 1009.80 1015.20
1024.59 1026.48 1037.85 1050.07 1056.58 1059.95
1073.96 1085.30 1099.51 1108.34 1113.82 1125.94
1134.73 1138.61 1253.90 1349.01 1420.94 1517.59
2204.92 2239.29 3060.21 3329.58 3600.92 3649.43
3680.41 3733.23 3776.77 3777.00 3789.75 3790.87
3792.89 3803.90 3824.61

TS9

-1693.65 26.45 30.52 35.38 39.83 47.57
55.35 59.99 60.41 64.33 68.72 74.18
76.93 79.27 82.53 86.14 93.30 94.31
95.34 98.39 105.46 108.94 114.49 117.06
121.51 125.39 126.58 133.55 143.91 149.17
150.15 153.70 160.40 162.41 164.39 171.80
176.56 181.24 183.35 185.77 191.41 196.42
197.84 202.11 206.91 210.50 212.46 216.43
219.97 222.98 230.22 238.57 241.48 243.81
252.61 256.72 260.04 265.73 270.87 277.32
280.90 290.14 297.25 301.48 302.01 307.58
314.79 316.37 324.32 326.51 329.57 332.80
337.56 340.24 347.57 349.78 355.78 358.85
360.18 365.92 372.70 384.97 397.78 403.25
421.28 428.44 436.30 443.11 446.28 450.00
460.90 463.53 497.83 504.34 518.58 541.32
556.19 565.99 582.02 602.50 609.01 615.93
627.04 653.47 667.86 681.96 684.58 704.62
712.27 719.78 741.65 757.60 763.47 764.58
771.05 781.51 816.91 826.56 842.24 850.05
856.16 859.15 866.29 871.51 873.98 888.16
891.21 903.09 906.21 910.21 914.45 920.11
924.68 927.75 937.42 938.97 947.18 951.12
959.08 964.85 987.25 990.88 996.03 998.85
1009.26 1033.01 1038.65 1052.04 1064.28 1068.21
1078.04 1090.15 1097.46 1104.58 1111.09 1118.13
1138.96 1140.76 1151.32 1334.55 1383.39 1510.23
1996.35 2478.60 3285.50 3296.75 3653.17 3653.54
3732.63 3776.83 3780.08 3789.37 3790.50 3791.61
3794.04 3817.52 3827.99

TS10

-175.87 12.25 25.85 34.89 43.73 50.85
57.73 64.71 68.53 73.08 74.95 75.93
79.50 85.80 94.65 96.44 100.72 104.45
109.92 111.66 116.88 121.76 129.40 131.23

131.94	142.56	147.05	147.74	153.66	159.75
162.75	166.50	168.67	170.33	176.07	179.62
181.95	185.60	190.80	192.93	199.03	204.33
206.82	208.18	212.37	217.77	222.79	228.33
235.71	237.35	241.29	245.49	250.51	257.62
264.23	269.29	270.08	278.23	284.33	286.85
294.21	296.83	305.84	309.90	310.17	315.90
320.72	325.31	329.04	330.87	335.33	341.94
346.72	351.36	356.35	361.54	365.58	370.59
372.23	380.37	389.31	393.05	402.90	413.33
425.33	435.80	440.44	442.53	450.17	458.79
464.75	490.90	499.92	521.55	549.77	557.72
568.44	579.73	604.58	609.43	615.86	625.96
645.45	653.63	659.07	674.91	694.86	699.74
714.74	719.60	742.92	759.25	762.45	763.14
773.58	795.02	818.47	838.84	849.52	850.31
853.98	857.77	863.19	867.32	888.44	890.13
899.54	906.17	907.91	917.91	920.97	925.57
929.97	940.74	945.61	950.54	955.09	963.30
981.06	985.82	998.24	1006.91	1012.60	1019.44
1034.53	1038.78	1052.32	1056.42	1079.28	1083.97
1088.36	1099.25	1101.76	1120.16	1133.78	1143.73
1159.89	1181.14	1456.46	1491.39	1569.68	1640.76
2352.49	2449.67	2951.35	3330.14	3519.80	3672.02
3729.76	3779.79	3780.47	3790.14	3791.51	3792.46
3793.62	3819.61	3833.72			

TS11

-1144.82	8.49	36.12	37.96	41.46	45.62
47.83	49.33	51.87	57.03	66.71	69.98
72.13	75.88	78.93	82.73	86.94	90.08
93.04	98.74	105.01	110.34	112.57	122.07
126.30	129.56	133.32	141.36	146.71	151.98
156.65	162.57	163.25	167.75	170.90	175.83
182.51	188.00	189.29	194.97	199.77	201.40
202.32	210.35	213.06	215.96	217.49	223.74
229.98	235.03	242.25	246.94	249.99	254.38
257.40	261.44	267.18	271.32	274.83	284.39
287.59	294.61	295.92	300.70	307.07	308.94
320.26	322.06	322.62	331.81	332.49	337.45
338.74	344.71	352.39	357.63	359.51	360.91
366.30	380.44	382.64	388.75	394.97	405.11
410.90	420.35	429.94	432.22	434.67	445.01
457.83	462.19	480.95	486.88	511.39	521.46
565.15	573.36	592.36	604.33	605.28	614.34
618.76	624.29	649.68	664.33	681.14	698.88
713.19	715.46	729.52	734.15	740.39	751.62
761.66	775.07	789.68	815.93	836.90	843.67
852.51	857.71	861.00	864.39	867.57	886.20
889.28	893.99	903.71	906.41	907.24	911.72
917.92	927.81	930.17	933.93	945.54	955.30
960.12	968.98	973.18	985.96	993.64	1004.26
1017.86	1026.71	1038.26	1045.52	1059.89	1076.87
1080.29	1096.41	1104.55	1105.73	1123.18	1128.94
1152.87	1173.37	1181.57	1230.32	1353.40	1407.03
1777.48	3254.56	3267.27	3393.06	3668.62	3675.77
3716.33	3781.62	3787.67	3788.89	3790.90	3793.24
3794.13	3796.12	3825.62			

TS12

-1280.63	20.80	30.52	35.50	44.16	47.44
51.29	52.81	56.54	60.64	66.45	68.35
71.83	78.75	81.96	87.70	94.51	99.23
103.94	108.14	115.66	117.67	126.76	133.90
138.57	142.08	147.08	151.73	156.43	160.47
161.95	168.62	171.61	172.96	176.88	180.45
190.11	191.16	196.69	197.75	201.17	204.91
210.18	212.49	213.95	214.94	225.38	226.82

234.83	240.11	241.99	248.38	255.61	258.87
262.59	269.66	275.59	279.21	284.66	287.05
292.29	293.73	302.08	304.61	306.58	309.25
316.29	322.82	327.09	333.94	336.61	341.09
346.48	348.73	358.43	359.64	362.03	365.82
369.13	377.92	391.08	394.20	400.78	407.67
411.22	429.62	432.05	436.96	449.18	459.05
467.02	496.52	511.08	520.86	564.88	575.27
589.51	600.77	609.92	623.84	626.78	647.98
651.95	664.58	671.65	683.39	692.59	706.36
715.89	723.20	729.01	739.51	750.78	764.34
770.20	772.22	773.47	782.08	789.67	812.93
830.93	850.46	853.88	855.13	867.19	870.91
883.66	893.64	899.25	904.35	913.51	916.48
923.22	928.96	931.96	945.87	956.74	958.86
963.77	982.56	985.20	994.32	1000.21	1008.65
1030.16	1037.45	1050.54	1059.76	1081.47	1085.72
1090.86	1106.41	1111.37	1118.22	1130.04	1141.70
1145.61	1160.76	1197.99	1260.40	1354.06	1431.54
1759.27	3285.41	3326.69	3373.90	3443.02	3551.30
3682.45	3708.67	3775.14	3781.73	3783.50	3794.15
3803.62	3821.24	3832.42			

TS13

-397.08	23.50	28.27	35.24	38.50	54.90
56.64	59.40	66.48	67.17	73.55	75.00
78.96	84.95	87.48	94.85	96.02	99.73
101.77	105.27	111.29	115.14	119.20	119.61
128.96	135.73	140.92	145.36	150.46	155.55
156.56	160.28	162.92	165.16	170.62	174.88
176.48	181.10	182.29	186.00	190.30	192.14
198.26	202.03	206.98	214.78	216.26	220.82
224.89	228.72	237.40	237.91	242.64	249.41
260.44	261.15	263.39	270.30	276.90	281.67
287.79	293.28	295.87	300.56	305.71	312.24
313.28	315.33	324.30	325.96	330.85	336.48
339.65	342.77	350.15	353.81	356.57	360.22
363.05	377.30	378.35	385.39	389.28	403.79
413.57	423.04	425.53	433.69	440.33	447.64
455.34	458.68	468.30	492.54	504.56	519.81
550.13	563.29	575.99	603.47	607.48	615.57
625.22	646.23	659.66	672.19	675.96	679.46
705.80	713.42	721.72	745.25	753.57	774.75
775.75	779.53	827.89	829.41	843.02	851.26
854.64	856.86	865.11	865.76	873.64	884.21
885.76	896.59	903.71	908.65	914.05	919.89
922.12	927.12	928.36	940.12	944.97	952.06
961.58	969.16	971.82	985.19	997.21	1000.59
1008.23	1035.86	1040.47	1060.34	1063.81	1075.98
1083.83	1088.94	1097.18	1105.73	1118.01	1129.43
1145.57	1159.99	1277.64	1365.23	1442.80	1607.87
1934.90	3195.07	3249.78	3364.99	3648.78	3685.37
3738.65	3780.39	3781.85	3783.80	3790.19	3790.97
3793.47	3825.40	3835.79			

TS14

-1781.87	30.37	33.69	38.55	48.61	53.02
55.56	60.43	63.90	65.75	68.72	74.48
74.75	76.56	81.37	87.57	89.77	92.96
103.78	108.28	110.77	114.47	117.98	124.32
127.79	132.20	136.69	140.80	144.25	150.39
152.98	160.45	162.96	165.02	166.71	170.46
174.80	179.92	183.08	188.82	190.88	194.45
198.85	206.59	210.29	211.21	218.49	221.85
225.67	230.12	232.62	235.41	248.09	248.21
252.55	262.00	265.24	266.19	272.39	282.30
284.25	290.80	295.42	296.31	303.37	308.21
312.03	316.16	319.44	324.90	328.36	331.39

335.66	341.02	345.10	346.21	352.49	358.87
360.68	365.22	373.03	384.20	394.99	405.01
419.00	427.44	434.14	439.02	442.54	450.54
452.83	463.27	468.22	497.82	508.19	519.11
548.33	554.92	565.47	583.44	599.16	611.23
619.07	629.09	654.19	673.43	679.79	697.94
708.93	717.82	731.99	741.15	748.64	762.88
774.05	780.66	783.57	802.92	809.34	827.90
842.35	847.92	852.71	862.69	866.05	871.79
877.26	883.19	885.86	891.14	896.45	903.97
911.31	913.30	919.70	923.34	934.68	943.71
947.10	957.58	959.07	965.50	983.07	988.31
1000.46	1007.65	1031.75	1036.97	1056.02	1062.52
1066.18	1082.77	1085.75	1093.63	1103.29	1111.23
1114.74	1132.06	1152.05	1271.80	1276.04	1734.28
1939.18	2752.86	3269.31	3368.98	3670.27	3703.27
3738.98	3772.87	3781.44	3782.57	3789.20	3792.79
3794.63	3796.59	3828.13			

13/A'

17.64	29.60	36.65	43.33	50.74	58.61
59.55	62.00	66.58	70.11	75.19	79.22
82.02	83.20	90.65	95.37	97.49	98.49
104.83	111.76	119.12	120.56	123.50	127.78
130.01	137.12	145.72	148.95	153.49	153.97
157.45	161.86	165.18	169.58	179.12	180.34
182.36	185.47	190.56	194.14	200.18	204.89
209.40	211.39	213.32	214.30	219.17	221.51
227.31	237.59	239.57	248.59	253.92	255.43
259.28	265.95	266.89	273.87	279.36	286.12
291.41	299.62	302.96	307.37	308.86	314.02
319.13	325.44	326.66	330.73	334.49	337.01
341.16	350.03	352.25	353.96	359.20	361.17
367.47	374.22	387.36	397.83	404.15	420.00
427.87	437.26	442.74	448.27	452.95	461.10
465.00	496.31	513.31	525.38	561.33	574.06
581.82	601.29	604.83	609.97	615.91	631.41
652.80	666.43	672.55	681.75	686.65	702.71
712.41	720.62	736.38	749.75	759.32	765.61
767.74	780.48	823.43	829.89	832.58	846.71
853.95	859.88	862.97	867.28	873.65	885.81
890.53	894.85	901.99	906.89	910.51	916.96
926.15	927.66	939.11	946.26	947.24	955.49
963.02	986.72	991.24	999.65	1006.33	1025.43
1033.16	1043.95	1058.90	1064.24	1071.99	1085.39
1092.85	1107.96	1116.38	1122.58	1129.88	1149.53
1153.27	1206.62	1317.98	1350.10	1528.48	1575.86
1663.19	3168.78	3297.71	3413.60	3585.18	3652.01
3724.64	3775.55	3781.03	3790.27	3790.67	3790.78
3791.69	3818.29	3828.08			

13-TS

-1255.89	29.94	37.63	40.53	49.17	54.04
59.53	65.58	68.97	72.79	76.02	78.74
81.63	86.36	92.40	96.30	102.74	104.69
111.33	117.72	119.88	124.82	126.06	132.51
138.63	142.85	150.09	152.77	157.28	158.67
164.71	167.41	169.37	172.77	182.08	183.45
184.46	186.88	191.20	194.55	202.09	205.35
208.47	212.96	213.40	217.88	221.31	225.05
229.63	239.69	245.91	248.97	253.02	255.47
264.99	266.10	270.12	276.38	281.18	286.85
293.45	301.33	302.74	307.02	310.72	320.88
321.73	327.12	327.93	331.34	335.10	340.16
341.68	349.42	353.27	358.64	361.70	364.78
374.91	376.39	391.08	402.47	413.71	421.94
438.65	442.90	444.35	449.32	454.70	462.34
466.28	498.30	508.75	523.47	561.08	575.99

582.09	602.60	606.27	611.38	619.23	632.75
652.56	662.46	671.07	683.32	697.77	704.77
713.23	725.02	748.27	756.79	761.56	768.88
778.47	781.59	820.16	825.46	838.16	848.20
858.14	867.22	871.27	879.31	884.52	892.08
895.94	899.90	906.09	911.43	912.86	915.60
920.41	928.72	939.40	941.84	955.59	962.60
969.42	989.63	990.57	995.02	1009.73	1027.59
1035.27	1048.46	1060.96	1065.98	1075.44	1085.72
1098.06	1105.83	1112.40	1120.55	1139.17	1148.35
1199.16	1211.80	1262.93	1341.06	1472.26	1559.31
1600.33	2817.91	3094.54	3295.88	3402.30	3586.65
3648.90	3721.42	3774.62	3780.53	3784.16	3789.48
3791.14	3814.39	3826.39			

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25.42	32.65	35.24	45.36	47.42	55.16
62.20	64.83	68.58	69.13	71.12	73.73
76.91	83.19	84.84	89.78	92.85	95.97
104.36	108.33	111.01	120.25	124.53	133.17
136.33	142.30	145.87	149.65	158.58	162.49
164.79	166.29	168.59	176.44	178.24	181.36
186.64	187.54	194.67	198.97	201.84	203.25
204.82	208.38	209.81	218.60	221.26	224.96
230.59	233.65	238.88	244.79	250.27	251.80
256.98	263.10	266.96	273.77	275.83	283.77
292.28	295.17	301.50	304.26	309.56	318.63
321.88	324.27	328.99	333.21	334.71	339.93
340.72	348.10	353.48	356.71	361.94	369.50
373.20	374.72	390.57	395.65	409.78	417.39
430.88	441.13	446.70	450.91	452.56	463.77
464.49	480.62	493.81	501.59	517.70	554.98
574.14	574.70	585.47	598.59	609.58	625.45
631.54	642.30	649.58	666.03	678.86	696.64
707.49	716.63	723.28	739.97	754.85	764.59
765.95	781.17	822.70	840.45	849.20	854.58
856.18	863.54	868.13	881.54	887.19	888.79
892.80	904.38	908.59	913.33	915.60	924.79
927.64	929.15	941.61	943.79	954.29	967.63
973.11	978.38	986.83	1001.90	1014.10	1015.84
1029.01	1036.82	1042.71	1053.15	1062.98	1069.80
1077.16	1096.16	1110.40	1112.09	1125.90	1132.07
1149.75	1176.52	1301.31	1382.09	1549.87	1668.55
2143.60	3041.54	3290.75	3637.80	3643.98	3663.75
3723.26	3778.70	3784.80	3785.78	3789.11	3789.36
3792.82	3798.11	3829.40			

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-825.90	15.40	29.17	38.00	42.72	53.80
57.61	66.79	68.31	71.04	77.24	80.44
83.03	90.12	94.69	98.54	102.03	109.94
113.16	123.15	126.79	129.84	134.62	139.96
141.67	149.56	149.90	153.50	158.51	160.78
163.62	168.40	170.84	175.55	178.15	180.66
185.08	189.24	190.88	197.13	198.78	205.18
207.92	213.41	216.26	218.63	222.41	230.33
236.52	240.65	246.99	248.30	253.95	261.79
263.75	266.75	275.62	279.28	284.70	285.25
293.38	301.02	304.27	309.07	313.42	319.27
321.30	326.09	331.61	334.39	338.36	342.61
346.05	352.07	359.54	360.25	363.03	369.27
379.78	389.26	395.60	399.43	404.97	415.23
427.81	429.97	436.23	447.71	453.33	458.89
466.61	497.29	511.98	521.19	562.63	573.49
588.99	605.74	613.60	625.14	626.51	642.52
652.34	672.69	673.51	689.69	698.52	704.44
721.86	731.65	747.13	758.49	770.20	777.70
779.43	801.95	820.78	842.09	847.75	854.20

865.89	869.95	875.45	880.55	894.37	900.07
903.88	910.82	913.81	915.63	919.37	928.92
937.49	944.54	952.87	958.55	965.66	971.49
983.03	987.95	995.82	1006.59	1010.32	1029.07
1035.07	1062.09	1065.46	1085.53	1094.02	1096.85
1102.75	1109.40	1114.53	1126.78	1144.43	1157.60
1172.85	1266.90	1278.48	1361.87	1491.98	1606.82
1679.61	2516.15	2852.93	3288.82	3304.01	3544.86
3678.04	3701.14	3773.00	3781.74	3784.05	3789.50
3790.93	3821.77	3829.30			

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10.87	24.95	30.47	36.47	44.78	55.26
56.95	60.43	64.66	66.84	72.37	72.77
76.49	82.98	84.23	88.83	94.30	102.00
102.23	104.80	109.20	115.23	122.55	134.89
144.33	145.72	153.46	156.84	161.46	162.75
166.12	172.02	173.13	179.48	183.11	185.41
188.62	189.21	193.55	195.00	200.15	203.69
207.46	214.93	216.89	225.48	229.34	233.96
241.83	248.02	251.19	254.67	257.38	261.12
266.28	269.19	272.90	281.97	286.96	289.81
293.81	297.82	301.32	304.51	308.83	316.78
322.90	326.14	326.38	331.18	334.48	339.55
340.82	351.42	354.32	357.03	360.17	362.20
370.26	382.58	388.95	398.03	405.60	413.42
429.90	437.17	441.66	443.64	453.07	455.32
464.32	471.27	492.76	514.69	533.23	559.75
565.17	574.01	596.91	614.95	624.75	625.29
647.47	669.89	677.20	686.35	696.82	705.67
713.65	721.28	743.39	758.88	765.85	776.54
779.15	799.97	822.49	832.04	843.39	848.65
853.96	854.75	863.42	868.48	877.33	883.44
886.70	892.08	905.79	909.78	912.82	916.75
921.84	927.08	928.01	941.03	950.44	956.19
968.07	969.08	986.54	994.47	998.10	1001.38
1010.84	1036.23	1040.04	1057.71	1069.26	1076.41
1079.99	1097.49	1108.51	1115.28	1118.50	1141.10
1154.95	1158.36	1205.08	1419.00	1502.63	1569.12
1675.51	2809.33	3254.51	3396.84	3655.06	3691.57
3739.97	3757.30	3776.44	3777.17	3777.99	3778.61
3789.29	3792.84	3824.73			

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-229.59	25.89	34.98	38.70	44.92	47.73
54.41	57.03	62.59	64.76	71.67	72.13
74.94	77.14	85.18	92.10	93.14	96.64
99.77	109.14	111.68	115.10	125.07	128.16
128.54	140.33	143.76	150.80	157.88	159.27
166.65	167.45	169.54	173.94	182.64	183.07
187.40	191.80	193.51	197.29	204.99	208.34
210.78	214.23	216.42	226.96	227.88	231.90
235.08	240.34	243.39	249.66	257.31	259.88
265.25	270.06	271.06	279.67	286.94	288.83
291.64	293.79	305.94	307.90	314.17	318.03
321.33	326.40	329.57	335.40	339.31	342.74
345.81	351.30	354.68	360.74	361.48	363.79
373.28	382.46	388.18	399.39	403.45	418.42
427.41	432.36	439.13	442.70	444.26	451.80
463.51	467.55	485.51	503.33	514.76	532.21
565.33	570.61	583.29	592.23	607.05	614.78
624.61	630.35	652.63	670.38	680.32	706.83
712.04	723.40	734.11	740.50	763.53	771.90
772.17	780.41	824.97	830.94	843.45	852.28
854.84	868.07	870.17	876.12	881.93	885.23
901.59	905.32	912.82	917.32	920.00	924.59
935.01	940.83	942.72	955.27	960.49	960.97
976.05	980.79	987.05	999.80	1002.52	1020.94

1040.45	1043.40	1058.64	1068.34	1073.34	1077.57
1084.07	1095.06	1103.94	1113.91	1119.57	1127.79
1140.64	1151.22	1207.89	1295.20	1509.17	1588.90
1876.38	2164.87	2725.01	3287.16	3667.09	3700.60
3712.28	3740.42	3780.39	3781.06	3783.95	3788.25
3792.40	3794.08	3833.01			

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42.57	48.17	51.98	55.82	63.64	66.75
71.25	75.89	78.81	84.67	87.48	88.35
91.38	100.35	104.72	105.47	107.72	110.50
116.68	121.00	125.64	134.61	144.92	151.71
154.56	161.49	167.00	172.17	174.12	182.97
184.97	190.87	195.42	199.79	203.63	206.64
208.63	212.50	217.10	217.98	225.54	227.87
235.89	242.92	249.78	251.10	258.55	262.21
270.06	274.51	281.24	284.72	292.59	297.87
298.06	300.89	307.75	315.38	317.57	323.33
327.28	332.23	334.52	338.78	344.10	349.80
353.32	355.67	360.09	361.54	366.53	370.71
375.48	381.47	391.09	402.63	406.29	419.22
423.24	425.48	434.57	444.12	452.61	456.97
462.87	464.84	471.26	508.19	520.69	522.95
537.86	547.64	584.31	593.55	609.31	616.46
625.86	639.93	660.30	676.09	683.94	718.58
727.12	733.68	749.14	760.18	764.89	770.36
778.59	784.57	793.18	840.93	857.35	860.88
866.29	870.58	883.32	895.94	896.94	904.23
908.35	913.61	915.23	920.19	920.38	934.63
945.80	958.22	961.31	971.49	973.14	980.45
984.72	987.42	990.83	998.05	999.21	1013.78
1032.35	1037.69	1051.49	1073.66	1075.10	1081.64
1086.64	1088.89	1103.26	1107.33	1109.46	1114.76
1158.61	1302.33	2128.50	3240.08	3582.69	3662.70
3674.36	3675.91	3695.94	3703.69	3773.68	3777.05
3777.42	3785.65	3831.54			

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28.02	45.01	46.38	50.57	56.84	59.85
61.31	67.64	72.15	84.37	85.05	89.63
93.29	94.93	101.23	104.40	105.70	113.09
117.75	119.44	130.18	135.46	139.84	140.24
152.31	155.19	163.22	167.56	172.10	176.28
184.70	186.11	193.89	198.04	201.05	203.06
206.01	210.27	211.07	217.99	220.65	223.13
227.01	228.24	233.79	239.38	243.19	254.76
260.39	273.01	276.37	285.69	292.70	295.53
299.48	302.92	305.46	311.89	313.13	321.83
322.97	329.28	334.52	336.92	339.20	347.28
350.28	351.85	357.47	361.20	364.51	368.10
371.99	373.89	379.62	386.66	387.27	396.07
397.31	408.86	422.14	423.50	427.61	438.66
451.97	456.82	457.76	466.59	469.31	473.91
487.85	514.14	522.56	531.32	546.43	596.96
600.80	611.09	620.18	625.57	645.13	652.20
669.14	692.76	695.88	714.09	726.76	737.12
747.03	757.46	766.14	768.75	781.70	788.36
792.35	807.12	846.41	860.44	866.83	870.64
885.50	891.91	899.51	904.55	905.23	907.41
910.63	918.14	919.62	927.99	937.56	941.15
950.79	956.83	959.40	973.89	974.63	978.07
984.86	990.22	990.86	992.66	995.39	1013.06
1028.78	1039.85	1040.86	1067.85	1071.07	1079.96
1082.71	1094.61	1099.06	1103.78	1113.36	1125.77
1164.73	1207.54	1211.67	1577.08	1621.29	2824.21
2833.64	3266.45	3342.57	3462.65	3543.89	3600.30
3640.97	3672.20	3679.74	3682.50	3690.96	3774.36
3785.21	3785.49	3801.87			

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-884.30	43.46	46.72	53.20	58.24	62.10
64.53	68.08	72.57	78.10	86.97	90.01
90.88	92.98	94.67	100.26	105.02	108.20
112.82	117.83	121.65	126.96	130.03	140.05
143.41	149.15	157.71	165.77	169.08	176.21
178.39	185.91	190.10	195.93	198.51	201.44
204.64	207.87	209.01	217.27	219.95	224.22
227.89	230.69	233.45	237.77	252.86	258.37
271.29	277.44	280.75	288.51	291.34	295.44
297.92	306.81	309.58	310.32	314.45	318.97
319.95	321.73	327.99	330.74	335.57	338.21
341.17	346.93	348.80	351.77	354.66	359.63
363.89	366.08	370.44	373.83	379.76	383.53
394.00	395.76	407.59	417.23	421.11	425.10
430.38	444.96	451.69	455.61	461.33	471.98
477.00	513.15	513.37	526.76	542.06	588.87
596.95	604.46	611.69	618.31	622.20	646.34
659.01	664.19	680.76	685.62	695.48	712.12
726.52	731.52	750.31	754.38	759.56	768.86
774.63	776.03	790.74	818.12	844.17	855.11
863.99	866.07	880.66	889.53	896.58	900.55
904.36	909.36	911.02	916.78	918.43	924.54
936.57	942.21	950.17	958.45	970.44	974.54
977.78	984.36	987.05	990.28	992.12	994.04
1011.41	1029.45	1039.01	1043.80	1070.17	1072.32
1077.65	1080.67	1089.06	1095.24	1101.01	1107.93
1120.53	1173.38	1295.42	1504.11	1540.35	1682.75
2176.94	3168.41	3406.43	3516.57	3577.21	3643.52
3696.72	3697.74	3699.53	3701.78	3731.73	3775.66
3779.50	3786.09	3809.15			

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41.48	45.65	49.08	51.58	59.79	61.56
65.54	66.92	74.22	80.81	86.68	88.74
89.24	92.18	97.00	101.19	103.44	108.08
113.08	115.96	121.08	124.61	130.10	137.13
148.59	152.63	161.43	168.56	170.68	176.94
182.45	189.11	193.25	196.28	197.43	202.39
204.40	206.47	208.38	210.42	218.51	220.33
224.78	229.15	230.99	236.27	252.66	256.84
265.28	266.71	278.52	283.21	287.94	291.18
292.35	297.51	300.46	305.48	308.39	310.03
317.38	320.44	325.08	326.73	330.77	332.21
337.36	347.02	347.82	349.81	357.30	360.48
362.22	364.52	368.49	372.79	378.99	388.94
391.30	404.26	411.57	420.05	421.06	423.36
430.18	443.97	453.47	455.95	457.96	464.38
471.91	498.74	510.30	521.75	533.05	540.93
589.53	596.34	604.11	612.36	619.31	634.34
641.43	664.47	682.37	686.45	710.28	721.40
734.26	748.38	754.44	755.26	762.89	771.93
781.29	785.63	811.22	841.19	856.15	860.77
864.91	874.33	889.90	892.66	901.21	905.31
907.44	911.66	917.35	922.00	925.78	935.25
938.12	941.66	951.27	960.51	970.18	973.85
975.44	984.83	989.64	991.84	996.05	1001.57
1012.74	1030.95	1041.10	1047.14	1072.14	1075.07
1076.65	1083.70	1089.75	1092.43	1103.87	1106.08
1119.91	1168.93	1300.21	1524.43	1577.34	2173.85
2969.36	3180.58	3354.72	3453.11	3591.10	3661.67
3680.28	3693.28	3700.62	3709.76	3743.64	3774.75
3783.32	3786.94	3807.50			

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24.79	39.52	46.10	49.64	54.75	57.98
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62.56	68.09	71.76	75.00	78.42	82.25
87.12	92.82	93.50	101.64	104.24	107.59
112.78	115.42	116.28	121.03	122.93	128.00
132.98	137.23	145.11	147.46	150.47	158.16
160.81	164.25	171.71	173.26	182.47	189.69
194.03	197.82	199.58	205.09	208.41	210.57
212.34	216.72	218.34	225.31	230.17	233.41
238.12	240.72	245.18	256.08	259.40	267.98
272.27	281.73	286.60	290.82	297.11	300.27
302.48	308.02	313.57	314.07	320.77	323.13
329.55	331.85	335.55	340.15	343.27	349.88
352.85	354.02	357.42	358.65	367.23	370.44
373.15	377.40	379.68	394.10	395.71	400.24
410.34	416.84	425.19	437.31	448.40	450.02
457.89	461.57	466.45	470.28	505.97	512.93
526.33	533.20	573.33	581.85	594.59	597.58
610.86	617.68	625.38	642.81	646.05	671.34
691.12	695.47	709.87	716.25	734.98	741.50
746.92	764.29	765.06	767.63	773.27	782.05
789.25	835.50	842.95	850.47	865.76	869.34
870.85	878.66	888.98	894.65	896.77	907.55
909.60	913.79	920.05	922.31	935.44	943.22
949.56	955.56	958.69	970.15	975.41	980.70
984.92	986.11	990.42	993.46	1009.93	1018.30
1035.75	1040.64	1048.42	1069.58	1072.69	1086.49
1092.91	1095.23	1109.10	1115.72	1117.23	1144.35
1214.66	1309.94	1543.32	1594.49	1631.56	3277.47
3289.30	3307.66	3451.91	3527.58	3578.55	3585.73
3686.73	3689.76	3711.94	3723.62	3774.44	3782.39
3789.96	3793.63	3804.56			

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30.35	33.31	43.94	49.74	57.12	60.82
65.91	69.59	72.73	81.98	82.33	88.74
90.13	92.60	99.22	101.42	105.74	112.60
116.64	120.01	123.28	127.75	134.32	142.99
148.33	152.21	162.04	166.60	171.50	174.10
181.81	186.12	191.15	196.42	202.47	204.46
205.59	208.01	210.87	212.86	216.25	219.72
225.21	228.65	232.71	234.41	237.13	251.86
256.94	264.71	266.74	276.14	287.20	289.52
291.03	297.06	297.98	306.41	308.31	314.34
318.56	322.15	324.21	328.93	329.67	334.68
337.14	347.11	347.94	349.22	352.95	358.37
361.84	364.07	370.09	371.00	375.37	379.10
390.46	396.95	411.21	416.60	419.64	423.42
440.46	443.80	454.84	456.98	457.35	463.42
468.40	475.16	487.15	511.72	514.97	526.21
533.43	592.22	599.15	611.11	619.08	622.72
639.68	665.82	687.25	706.97	720.40	739.30
742.65	753.03	757.57	766.39	779.45	785.78
797.28	822.04	843.12	858.33	863.95	866.60
870.57	890.36	892.24	898.05	902.78	907.24
908.09	915.77	921.29	923.43	925.76	935.06
942.26	950.49	958.07	970.63	973.98	976.37
985.27	990.21	993.44	996.92	999.87	1013.42
1031.23	1039.17	1047.07	1069.62	1073.94	1077.57
1082.19	1094.03	1100.97	1103.03	1108.96	1112.12
1179.37	1296.46	1532.02	1754.29	2212.05	3186.81
3226.27	3325.15	3601.70	3630.18	3693.76	3699.80
3700.86	3725.46	3776.40	3784.18	3786.16	3801.83

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28.27	40.93	45.25	50.59	52.13	56.16
61.81	64.36	66.08	71.03	74.07	79.90
83.17	88.19	91.27	95.87	97.62	99.52
106.52	109.21	112.17	116.26	124.42	129.96
132.21	138.12	140.10	150.75	157.74	161.61

165.40	169.18	181.61	186.46	190.99	195.79
199.30	204.47	204.92	208.82	213.64	215.85
219.62	221.40	224.62	231.43	233.98	238.01
240.67	256.56	260.79	266.67	269.36	280.11
282.02	288.47	294.60	298.92	304.37	307.50
309.90	319.70	321.03	327.11	329.35	332.57
337.51	342.13	348.40	350.46	355.47	357.42
359.23	364.07	366.11	367.86	371.37	380.02
395.89	398.71	411.48	417.16	420.38	426.80
433.95	441.30	451.11	453.94	462.77	467.17
469.71	502.58	507.46	516.17	526.54	536.13
592.57	595.10	607.36	614.99	623.32	641.19
645.58	666.70	678.62	694.66	719.81	730.93
749.73	755.03	759.49	764.53	766.78	774.49
787.58	793.03	843.03	849.33	860.50	865.28
871.98	882.40	889.48	896.92	899.35	901.19
910.00	911.89	913.26	919.19	925.60	929.58
938.16	943.83	945.74	955.90	971.51	972.30
979.57	982.11	986.85	989.24	991.12	994.76
1012.74	1031.87	1035.77	1042.79	1067.92	1072.94
1080.08	1089.39	1094.60	1108.05	1109.09	1120.78
1140.63	1163.60	1523.54	1592.57	3226.48	3301.58
3480.45	3583.53	3641.81	3673.06	3683.48	3721.65
3779.26	3782.47	3788.72	3789.05	3797.87	3819.39

38.12	46.37	52.85	55.41	61.51	67.25
69.96	75.42	82.64	83.23	88.23	92.27
97.29	103.96	107.00	111.03	111.37	118.87
125.19	139.78	143.82	151.95	157.06	160.58
166.28	169.78	179.57	182.69	185.53	192.76
196.84	200.63	203.19	204.67	206.93	209.65
216.34	221.36	223.62	231.67	233.13	237.80
251.67	254.91	258.95	260.93	267.76	273.06
282.67	285.57	292.22	298.74	302.10	304.94
311.59	320.85	321.45	327.13	329.95	332.31
335.22	338.05	344.22	346.32	352.83	355.53
358.58	362.01	363.33	369.33	378.70	380.25
395.13	399.07	412.32	422.63	426.00	433.57
443.70	450.24	455.06	462.71	466.22	467.97
518.21	524.36	530.49	546.58	590.26	602.59
606.71	614.43	621.56	645.76	667.32	668.96
690.93	707.69	729.01	747.10	754.34	763.80
772.76	777.38	779.49	789.52	845.77	857.08
861.05	869.84	881.72	887.83	897.74	899.27
908.70	910.94	912.56	915.95	924.50	928.40
931.79	937.89	944.29	954.24	963.56	971.93
979.13	982.52	984.44	987.18	989.54	995.58
1011.20	1030.30	1035.63	1054.14	1068.22	1074.88
1079.82	1081.73	1088.09	1097.21	1105.87	1111.47
1119.54	1168.12	1299.87	2144.02	3219.74	3564.08
3670.43	3671.02	3704.82	3724.75	3745.75	3776.74
3782.47	3785.54	3827.42			