

1 **Supporting Information**

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3 **How to Complete the Tautomerization and Substrate-**
4 **assisted Activation prior to C-C Bond Fission by**
5 **Meta-Cleavage Product Hydrolase LigY?**

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36 **Part I. Key Bond Distances for the hydrolysis in QM/MM Calculations.**

37 Table S1. Key bond distances (Å) in the QM region (SnB3).

species	H ² -C ⁵	H ³ -O ³	H ⁴ -O ⁷	H ⁵ -O ²	H ² -O ⁵	H ⁵ -C ⁵	C ⁵ -C ⁶	O ¹ -C ⁶
R	2.15	1.85	1.98	1.91	3.52	3.84	1.44	3.95
TS1	1.22	1.87	2.01	1.61	3.72	3.57	1.49	3.92
IM1	1.15	1.88	1.98	1.58	3.77	3.68	1.51	4.03
IM1'	2.77	1.86	1.97	2.12	1.84	1.11	1.52	3.90
TS2	1.10	1.89	1.88	1.18	3.56	2.81	1.53	2.01
IM2	1.11	1.87	1.59	0.99	5.86	2.90	1.55	1.50
TS3	1.09	1.94	1.76	0.97	5.39	3.02	1.98	1.40
P	1.09	2.05	1.76	0.97	5.83	3.25	3.36	1.31

38

39

40 Table S2. Key bond distances (Å) in the QM region (SnA3).

species	H ¹ -C ⁵	H ³ -O ³	H ² -O ¹	H ² -O ²	H ^β -O ⁵	H ^α -O ⁶	C ⁵ -C ⁶	O ¹ -C ⁶
R	2.62	3.66	3.66	0.97	2.89	1.67	1.42	2.95
TS1	1.28	3.60	1.53	1.03	2.91	1.78	1.47	2.73
IM1	1.10	3.68	1.05	1.48	2.93	1.85	1.52	2.78
TS2	1.10	3.62	1.57	1.04	2.89	1.87	1.54	2.14
IM2	1.10	3.61	2.03	0.98	2.80	1.80	1.56	1.52
TS3	1.09	3.54	2.00	0.97	2.93	1.70	2.14	1.40
P	1.09	3.58	3.04	0.97	2.96	1.57	3.60	1.32

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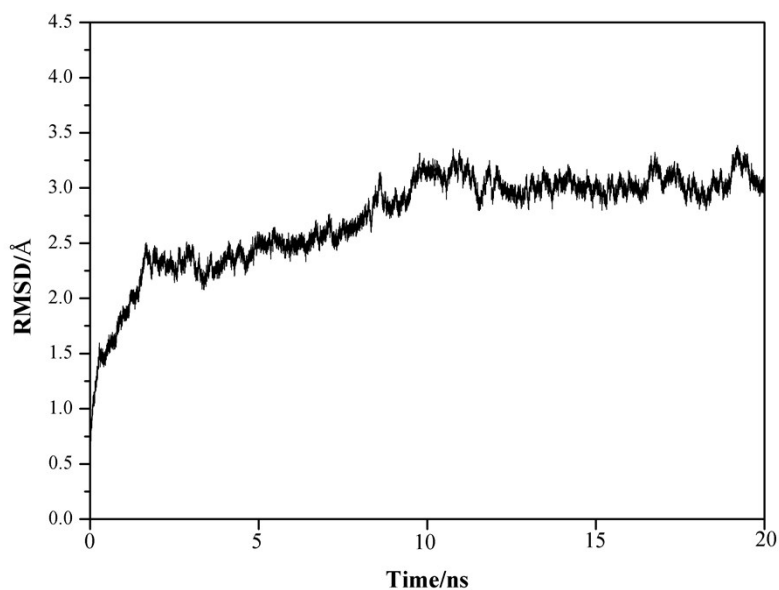
43 Table S3. Key bond distances (Å) in the QM region (SnA4).

species	H ¹ -C ⁵	H ³ -O ³	H ⁷ -O ¹	H ⁷ -N ¹	H ^β -O ⁴	H ^α -O ⁶	C ⁵ -C ⁶	O ¹ -C ⁶
R	3.07	1.88	2.30	1.01	1.81	2.01	1.40	3.19
TS1	1.24	1.98	1.75	1.05	1.85	2.05	1.47	3.22
IM1	1.11	2.12	1.02	1.62	1.86	2.03	1.51	3.72
TS2	1.10	2.11	1.03	1.61	1.87	1.99	1.51	3.19
IM2	1.10	2.20	1.01	1.69	1.85	2.05	1.52	3.05
TS3	1.10	2.17	1.77	1.06	1.86	2.02	1.53	2.33
IM3	1.10	1.98	2.33	1.02	1.86	2.06	1.60	1.48
TS4	1.09	1.85	3.32	1.01	1.78	2.01	2.24	1.38
P	1.09	1.78	3.47	1.01	1.72	1.94	2.85	1.33

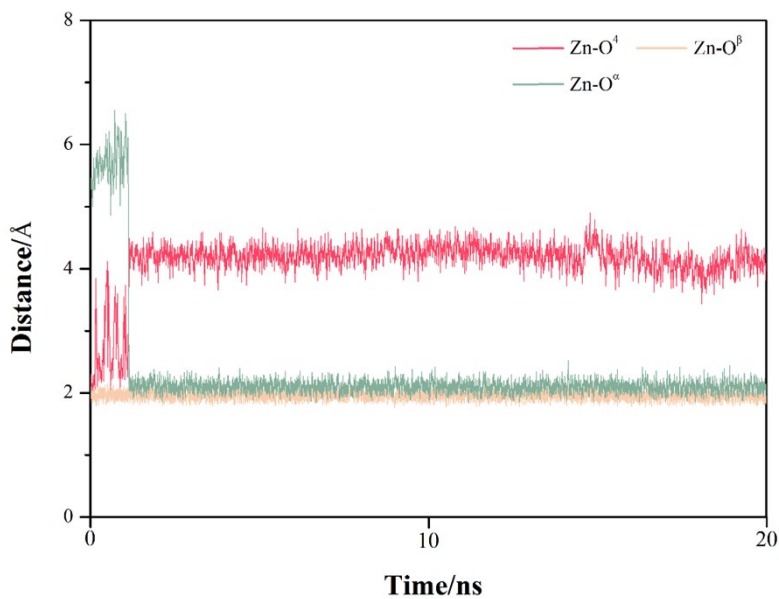
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46 Part II. Variations of Key Distances in Two MD Systems



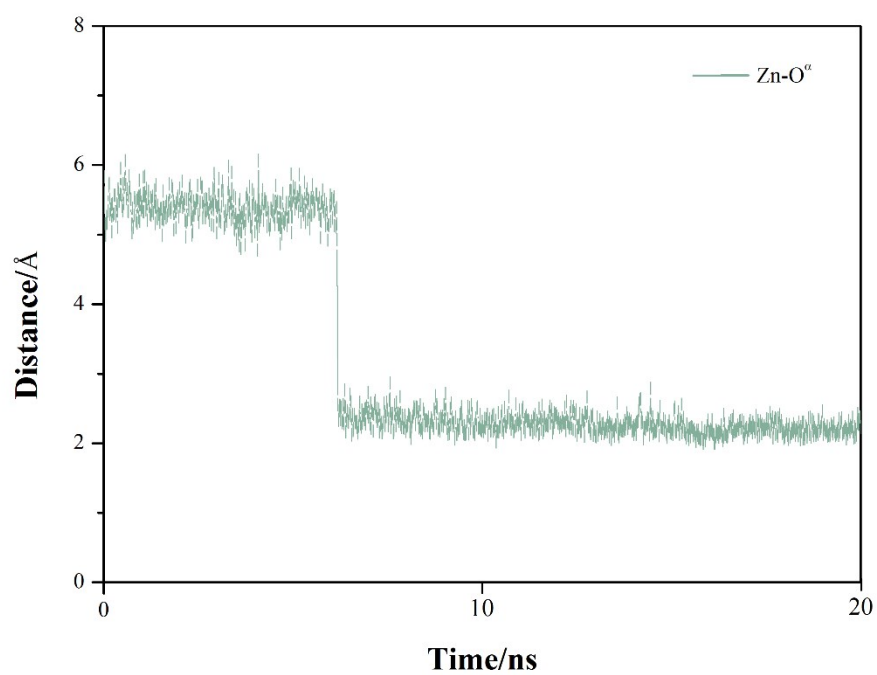
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49 Figure S1 Root-mean-square deviations (RMSD) of the backbone for molecular
50 dynamic simulation of System-A model. And variations of key internuclear distances
51 (Zn-O^δ , Zn-O^β and Zn-O^α) during the molecular dynamics simulation in System-A.

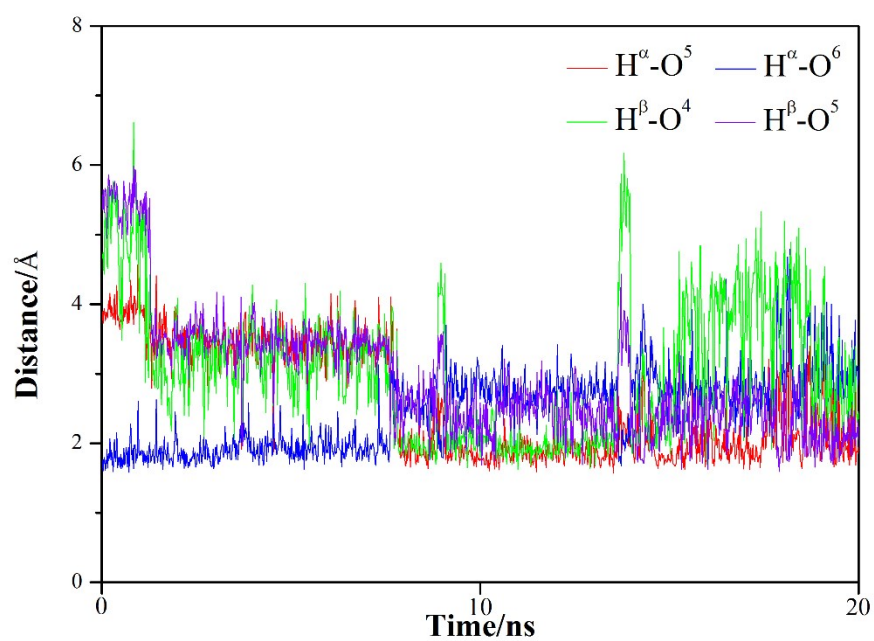
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54 Figure S2 Variation of key internuclear distance (Zn-O^α) during the molecular
55 dynamics simulation in System-B.

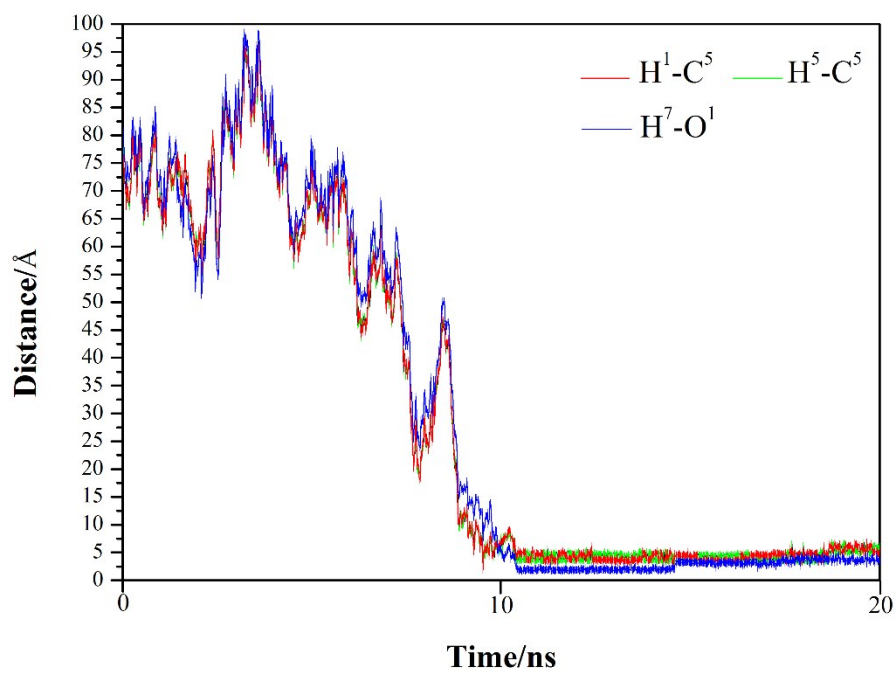
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58 Figure S3 Variations of key internuclear distances between Arg72 and 4-carboxyl of
59 the substrate (H^α-O⁵, H^α-O⁶, H^β-O⁴ and H^β-O⁵) during the molecular dynamics
60 simulation in System-A.

61

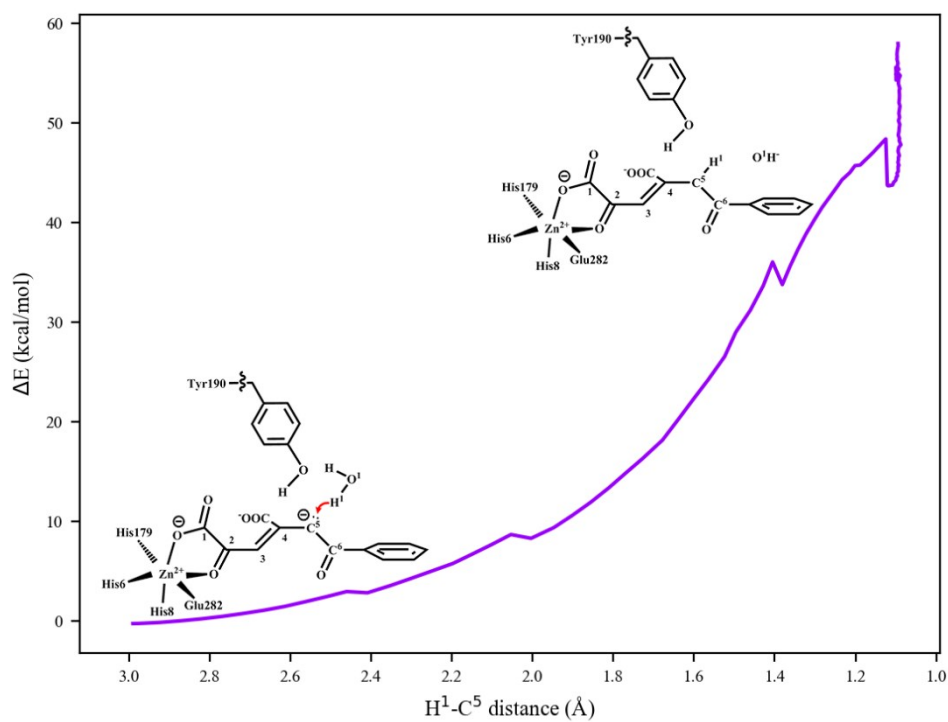


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63 Figure S4 Variations key internuclear distances (H¹-C⁵, H⁵-C⁵ and H⁷-O¹) during the
64 molecular dynamics simulation in System-A. The atoms (H¹, H⁵ and O¹) refer to the
65 catalytic water in SnA4.

66

67 Part III. Proton Transfer Energy Scan

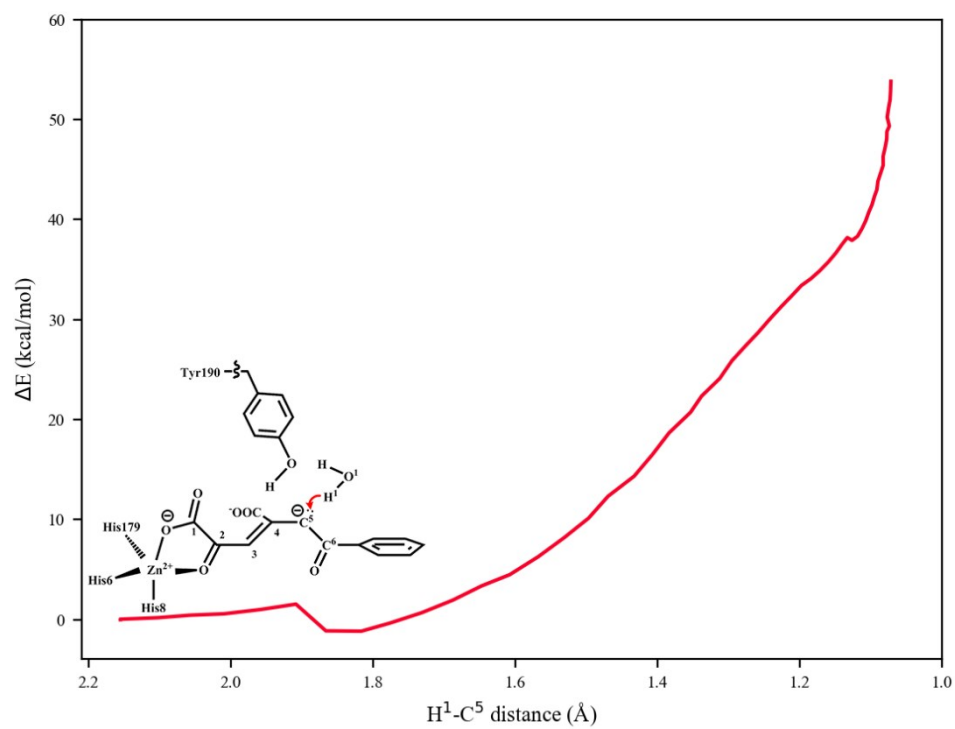


68

69 Figure S5 The M06-2X(B1)/MM energy profile along the forming H¹-C⁵ bond

70 starting from the reactant in SnB1.

71

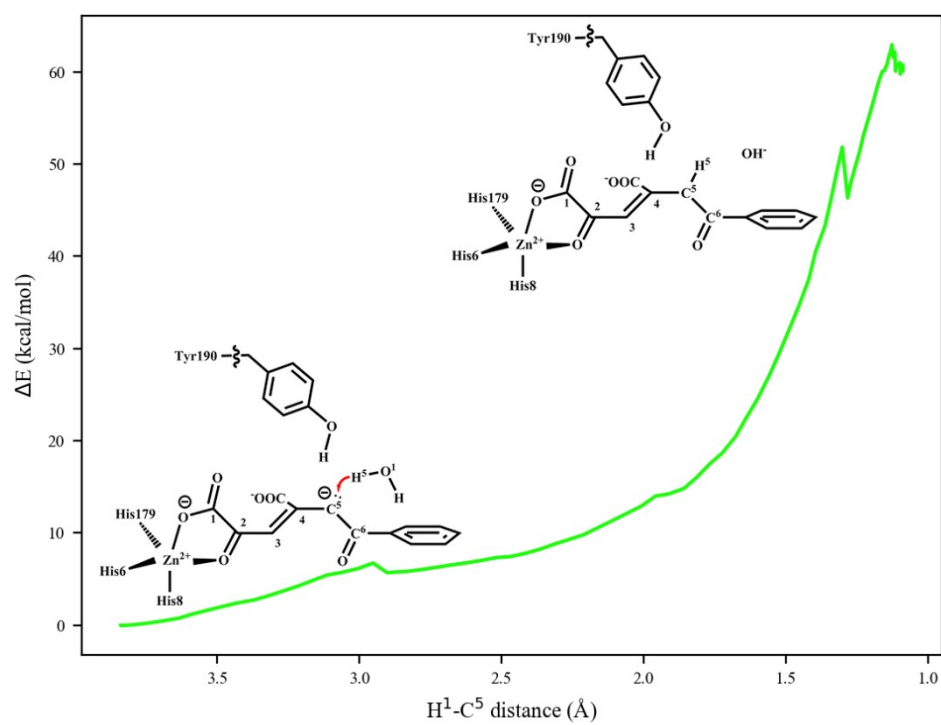


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73 Figure S6 The M06-2X(B1)/MM energy profile along the forming H¹-C⁵ bond

74 starting from the reactant in SnB2.

75

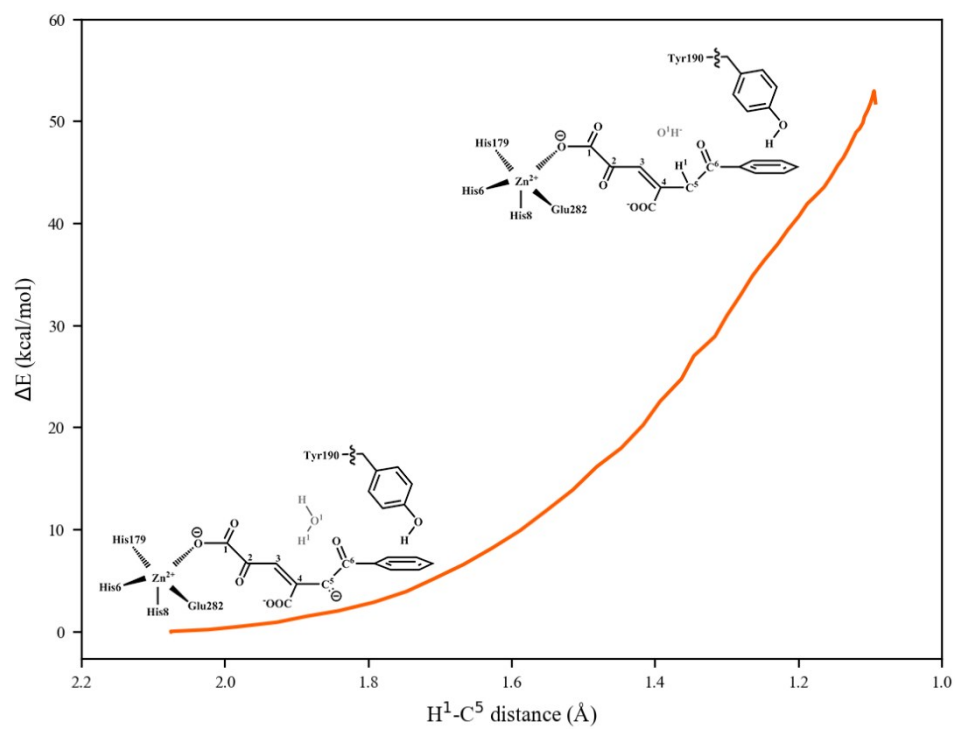


76

77 Figure S7 The M06-2X(B1)/MM energy profile along the forming H¹-C⁵ bond

78 starting from the reactant in SnB3.

79

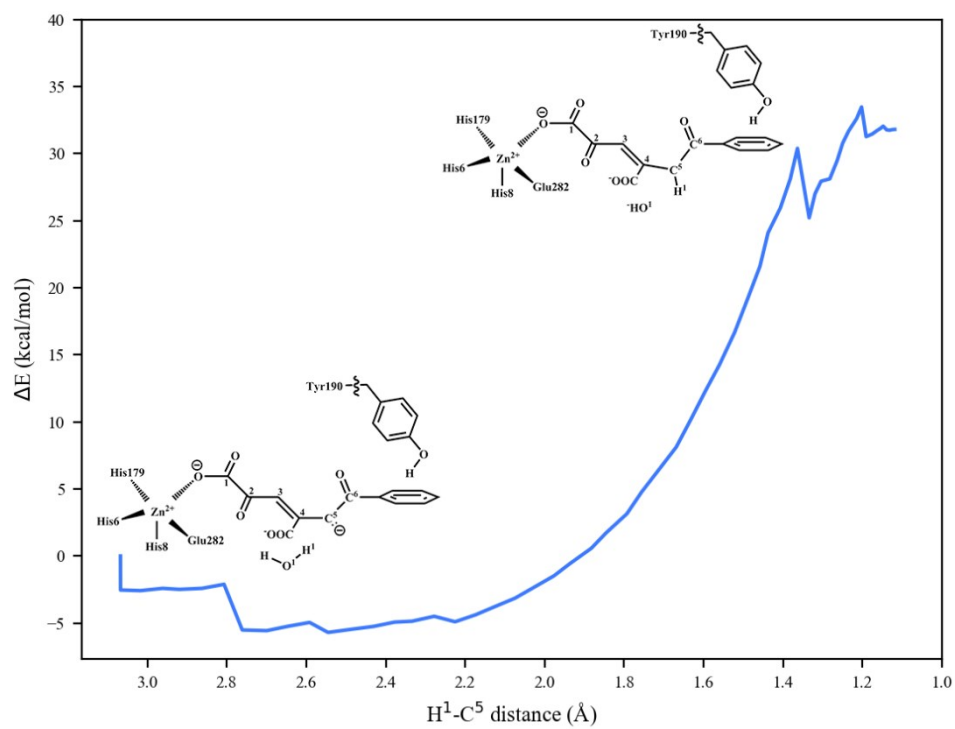


80

81 Figure S8 The M06-2X(B1)/MM energy profile along the forming H¹-C⁵ bond

82 starting from the reactant in SnA1.

83



84

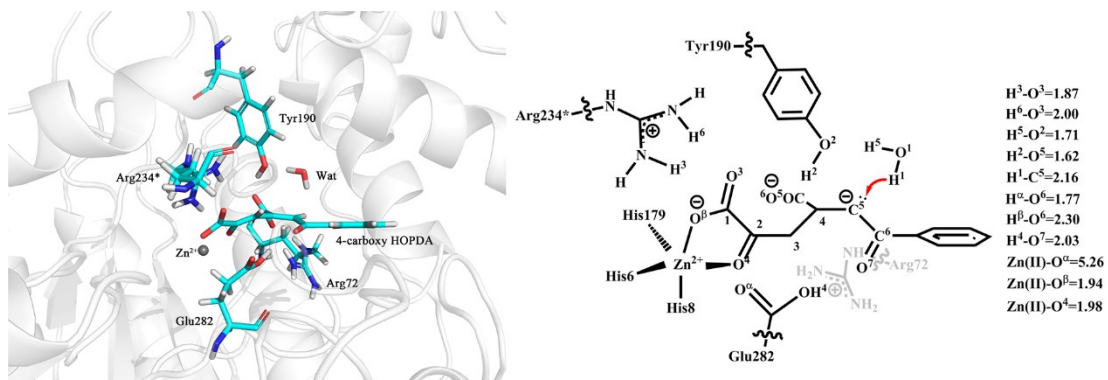
85 Figure S9 The M06-2X(B1)/MM energy profile along the forming H^1-C^5 bond

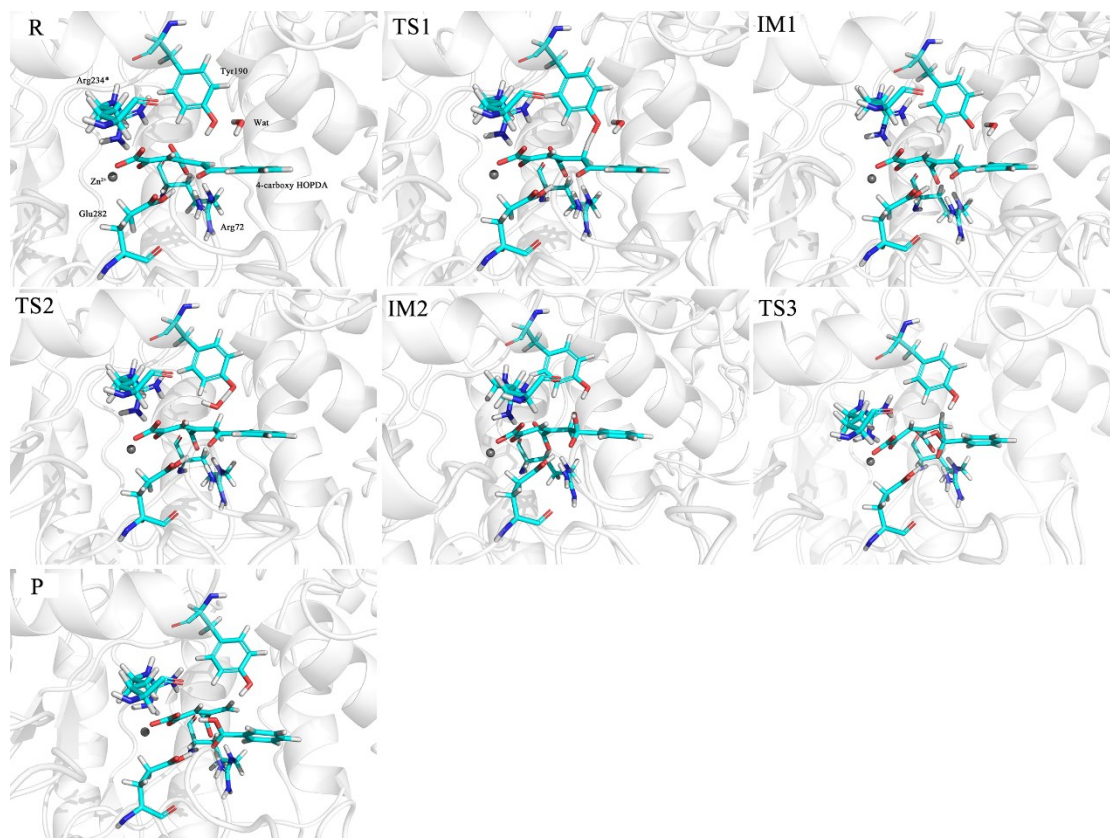
86 starting from the reactant in SnA2.

87

88 Part IV. The Three Dimensional structures among the whole reaction

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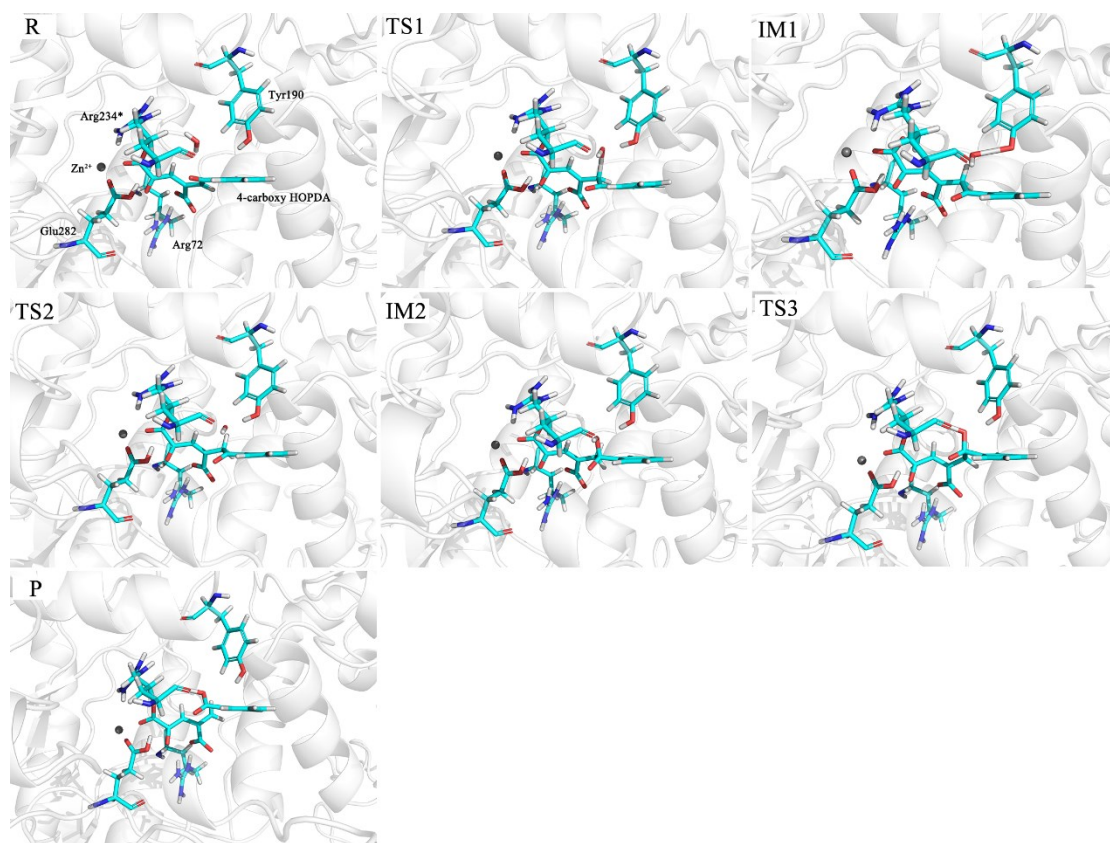


95

96 Figure S11 Optimized structures for the reactant, transition states, intermediates and

97 product among the whole catalytic reaction in SnB3 (calculated at B1 level).

98

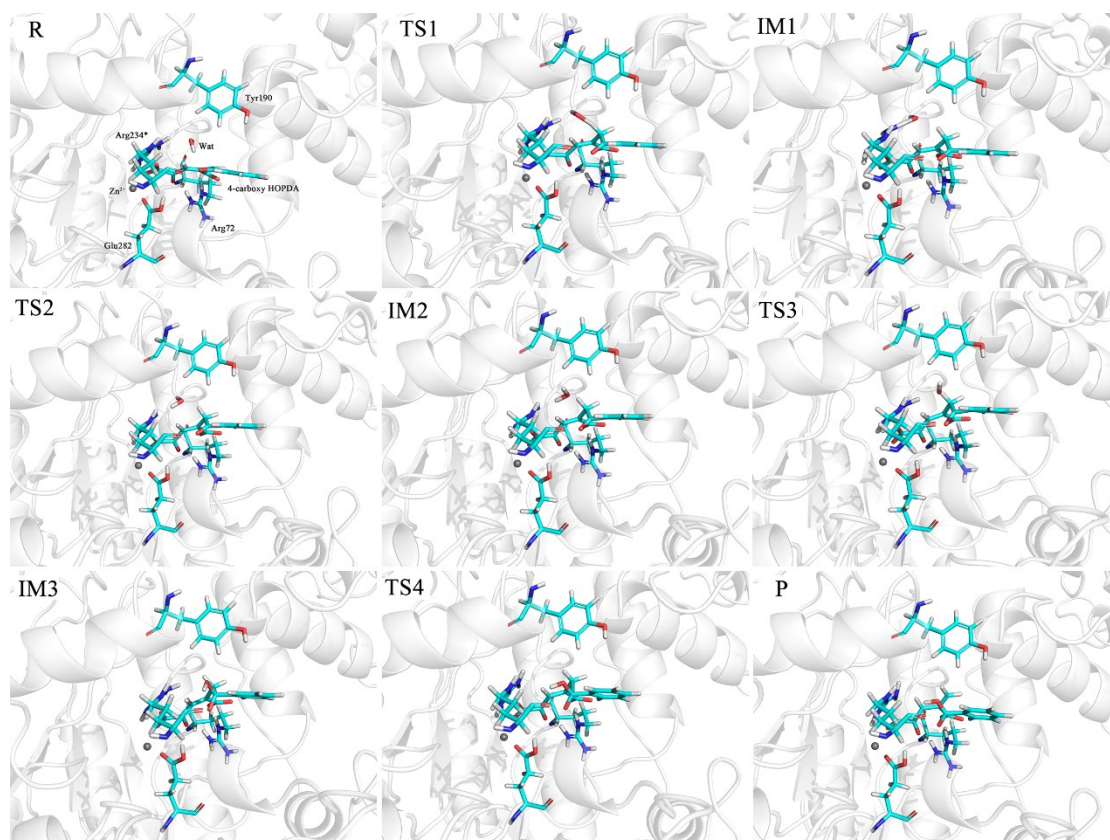


99

100 Figure S12 Optimized structures for the reactant, transition states, intermediates and

101 product among the whole catalytic reaction in SnA3 (calculated at B1 level).

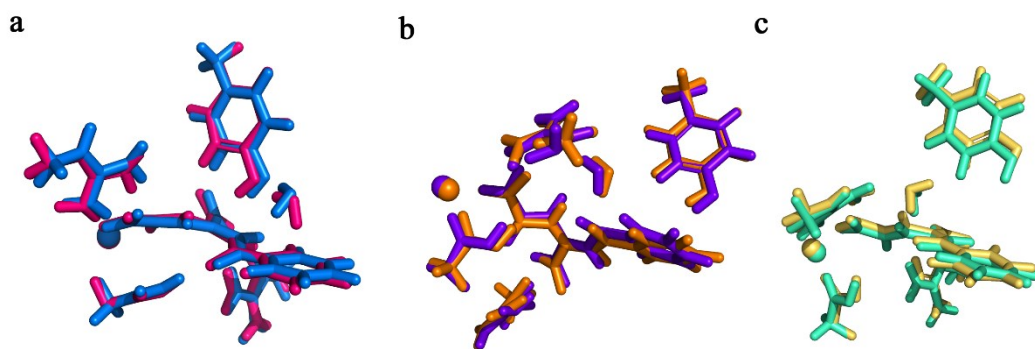
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104 Figure S13 Optimized structures for the reactant, transition states, intermediates and
 105 product among the whole catalytic reaction in SnA4 (calculated at B1 level).

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107

108 Figure S14 Superposition of QM/MM-optimized reactants and the MD results. And a

109 means the reactant of SnB3, b refers to the reactant of SnA3 and c is the reactant of

110 SnA4.

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112

113 **Part V. Cartesian Coordinates of the QM Region (SnB1-SnA4)**

114 **SnB1**

115 **R**

116	C	73.120363	53.466243	57.344363	135	H	62.589285	47.958628	59.427447
117	H	73.336140	52.473494	57.755626	136	H	62.556071	49.632457	60.103407
118	H	73.993398	54.092945	57.557782	137	N	60.182594	47.467558	60.064621
119	N	71.955589	54.030990	58.017518	138	H	60.719505	46.660953	59.758533
120	H	71.810191	55.044782	58.001911	139	H	59.333296	47.244158	60.590691
121	C	70.947904	53.336636	58.550983	140	C	65.852672	59.568351	61.296645
122	N	69.758938	53.929082	58.673665	141	H	65.830050	59.427177	62.385448
123	H	68.992647	53.354850	59.023663	142	H	65.263366	60.474849	61.102464
124	H	69.534304	54.710215	58.042930	143	C	65.211308	58.353434	60.666242
125	N	71.103192	52.065163	58.935929	144	C	65.245051	57.136435	61.359814
126	H	70.250772	51.622495	59.285393	145	H	65.770882	57.076002	62.315084
127	H	71.973435	51.834896	59.449907	146	C	64.613985	56.000987	60.873058
128	C	58.902164	49.722547	61.343323	147	H	64.617987	55.055442	61.417607
129	H	58.289105	48.936152	60.886947	148	C	63.904062	56.069680	59.673004
130	H	58.423644	50.679040	61.092022	149	O	63.234763	54.981988	59.205363
131	N	60.232984	49.697225	60.769227	150	H	63.216837	54.305104	59.919420
132	H	60.896665	50.449989	61.006860	151	C	64.537674	58.391350	59.440555
133	C	60.822881	48.638119	60.216179	152	H	64.513038	59.323959	58.872266
134	N	62.068339	48.783978	59.774485	153	C	63.883741	57.261574	58.943881

154	H	63.334917	57.303304	58.001074	176	O	65.868683	50.984701	61.776283
155	C	67.104895	46.902380	59.009107	177	O	68.262347	51.630564	59.321957
156	H	66.529204	46.852055	58.077667	178	O	68.493852	51.072514	61.449724
157	H	66.547539	46.404775	59.810607	179	O	64.688542	51.442726	56.745108
158	C	67.289777	48.339034	59.402253	180	H	63.836769	51.584007	54.573302
159	O	67.189846	48.719501	60.557006	181	O	63.446878	53.113996	61.451515
160	O	67.549656	49.151679	58.401227	182	O	62.566418	51.062105	61.283368
161	H	67.737618	50.079541	58.699316	183	H	65.997872	51.995237	58.629645
162	Zn	67.352242	49.809610	62.495814	184	H	62.135802	51.831862	58.799519
163	C	63.536172	51.563579	57.172527	185	H	62.090332	51.633186	52.768763
164	C	62.410293	51.533014	56.163324	186	H	59.678834	51.497932	53.392210
165	C	62.773164	51.554032	54.809538	187	H	59.024566	51.472221	55.797233
166	C	63.330079	51.998228	60.932949	188	H	60.735665	51.489882	57.542580
167	C	64.070769	51.806039	59.611791	189	O	65.084285	54.239431	56.999478
168	C	65.486019	51.796440	59.565299	190	H	65.194047	53.278555	56.952128
169	C	66.266513	51.423932	60.653955	191	H	64.495250	54.378127	57.758072
170	C	67.799459	51.408787	60.461417	192	h	72.984443	53.390165	56.265565
171	C	63.190874	51.766279	58.543820	193	h	58.922496	49.607066	62.426982
172	C	61.794799	51.561108	53.816824	194	h	66.879987	59.849204	61.064671
173	C	60.443640	51.515879	54.164971	195	h	68.047430	46.376886	58.855646
174	C	60.074505	51.498349	55.508682	196				
175	C	61.050313	51.512084	56.501258	197				

198 **IMI**

199	C	73.236231	53.597891	57.318644	220	N	60.297226	47.269574	60.022197
200	H	73.547839	52.650841	57.773208	221	H	60.771764	46.435584	59.688960
201	H	74.070292	54.295828	57.447482	222	H	59.455641	47.101459	60.580259
202	N	72.073901	54.132392	58.021696	223	C	65.873619	59.608676	61.337879
203	H	71.907486	55.143685	58.034108	224	H	65.844910	59.483717	62.427930
204	C	71.085561	53.406243	58.538647	225	H	65.289130	60.515352	61.130387
205	N	69.891392	53.979030	58.708449	226	C	65.215790	58.400942	60.711159
206	H	69.143618	53.390079	59.059772	227	C	65.260907	57.166819	61.371643
207	H	69.635328	54.764235	58.089412	228	H	65.847534	57.070197	62.287761
208	N	71.267590	52.116656	58.852889	229	C	64.552315	56.066079	60.905325
209	H	70.433331	51.640484	59.194178	230	H	64.554748	55.112349	61.436742
210	H	72.136308	51.889209	59.371719	231	C	63.742937	56.193097	59.771918
211	C	59.101802	49.635646	61.142294	232	O	62.937864	55.185922	59.375072
212	H	58.467628	48.872958	60.673760	233	H	62.925792	54.491608	60.069336
213	H	58.686705	50.608128	60.845746	234	C	64.477397	58.482823	59.525157
214	N	60.449670	49.521498	60.616821	235	H	64.457737	59.426181	58.974985
215	H	61.116296	50.297893	60.723216	236	C	63.748483	57.392570	59.053497
216	C	60.979117	48.423884	60.077053	237	H	63.148548	57.463526	58.145047
217	N	62.202887	48.496252	59.561943	238	C	67.104519	46.844696	59.045837
218	H	62.691829	47.628170	59.275467	239	H	66.521353	46.799829	58.117377
219	H	62.715422	49.379610	59.681224	240	H	66.546974	46.356896	59.853036

241	C	67.311651	48.281291	59.418423	263	H	64.196422	51.699976	54.470394
242	O	67.192062	48.700739	60.563472	264	O	63.129526	53.069457	61.206181
243	O	67.614130	49.069370	58.413665	265	O	62.856288	50.957481	60.528468
244	H	67.826530	49.986900	58.697254	266	H	66.389750	52.436336	58.664167
245	Zn	67.401134	49.731544	62.461828	267	H	62.780754	53.031428	58.213856
246	C	63.896658	51.552643	57.085607	268	H	62.406051	51.634659	52.700429
247	C	62.797859	51.519864	56.068766	269	H	60.008852	51.476411	53.383693
248	C	63.146286	51.538388	54.714932	270	H	59.407246	51.470581	55.793169
249	C	63.408283	52.080266	60.516448	271	H	61.195196	51.517436	57.516861
250	C	64.426336	52.312519	59.418001	272	O	65.222841	53.467545	55.521020
251	C	65.772757	52.167142	59.520275	273	H	65.723364	52.755507	55.927702
252	C	66.455592	51.548245	60.623071	274	H	64.377613	53.455921	57.550160
253	C	67.996327	51.382599	60.487400	275	h	73.053850	53.451007	56.254112
254	C	63.811968	52.680064	58.112257	276	h	59.052047	49.540026	62.226936
255	C	62.139162	51.539632	53.754954	277	h	66.900895	59.887090	61.102810
256	C	60.794898	51.493569	54.138027	278	h	68.040008	46.310285	58.880517
257	C	60.452829	51.488302	55.488329	279				
258	C	61.457405	51.512827	56.456227	280				
259	O	65.948713	51.045452	61.629741	281				
260	O	68.489397	51.577925	59.369745	282				
261	O	68.602584	50.974777	61.503499	283				
262	O	64.807944	50.763591	57.059970	284				

285 **SnB2**

286 **R**

287	C	72.957398	54.631626	57.638166	308	N	60.832385	47.044731	59.816650
288	H	73.191616	53.635321	58.028279	309	H	61.463177	46.325179	59.468202
289	H	73.738008	55.310537	58.001716	310	H	59.999933	46.709030	60.304138
290	N	71.665961	55.072667	58.154576	311	C	65.443289	60.404764	60.211815
291	H	71.423178	56.062508	58.041856	312	H	64.765022	61.016528	60.827870
292	C	70.685209	54.270634	58.588506	313	H	65.357552	60.776552	59.181872
293	N	69.431972	54.736015	58.589944	314	C	65.034170	58.945172	60.234846
294	H	68.705435	54.121108	58.955416	315	C	64.896823	58.206298	61.413873
295	H	69.176654	55.490403	57.940063	316	H	65.034315	58.711138	62.369696
296	N	70.925042	53.031147	58.997980	317	C	64.604263	56.843256	61.404126
297	H	70.100912	52.469409	59.241052	318	H	64.567585	56.292084	62.343425
298	H	71.831214	52.779557	59.428524	319	C	64.411763	56.174914	60.188266
299	C	59.353336	49.086047	61.241456	320	O	64.149960	54.862184	60.071657
300	H	58.819686	48.265073	60.747346	321	H	64.069611	54.258875	60.879517
301	H	58.770119	49.996241	61.048129	322	C	64.810099	58.269228	59.029203
302	N	60.675382	49.230340	60.655062	323	H	64.892811	58.817629	58.088718
303	H	61.268309	50.023856	60.958788	324	C	64.499230	56.915961	58.999463
304	C	61.362461	48.252209	60.069397	325	H	64.332977	56.411245	58.047542
305	N	62.618327	48.494520	59.705251	326	C	68.556849	47.914355	59.191022
306	H	63.159141	47.745609	59.234653	327	H	67.903231	47.306184	59.829167
307	H	63.030559	49.392745	59.948562	328	H	69.049879	48.655395	59.846467

329	C	67.729472	48.756252	58.252480	351	H	63.864068	50.976980	54.834167
330	O	68.128412	49.312605	57.261842	352	O	63.718417	52.950247	61.768421
331	O	66.482646	48.929719	58.703426	353	O	62.618703	51.017323	61.527420
332	H	66.013931	49.589584	58.148628	354	H	65.910806	52.029049	58.691075
333	Zn	67.659686	49.852726	62.475713	355	H	62.107041	51.509461	59.028869
334	C	63.517683	50.986364	57.447142	356	H	62.157567	50.837834	53.003244
335	C	62.417263	50.882526	56.410946	357	H	59.747750	50.669498	53.575144
336	C	62.801910	50.887949	55.061042	358	H	59.044102	50.603775	55.969128
337	C	63.429198	51.900673	61.167555	359	H	60.727689	50.741980	57.764441
338	C	64.070743	51.677577	59.791406	360	O	63.133773	54.246902	57.656026
339	C	65.480638	51.763310	59.653730	361	H	62.824314	53.346367	57.820122
340	C	66.365251	51.367716	60.639812	362	H	63.563261	54.451733	58.521046
341	C	67.869310	51.503308	60.344202	363	h	72.971649	54.606703	56.548559
342	C	63.165054	51.442973	58.771941	364	h	59.407711	48.910689	62.315867
343	C	61.847992	50.806579	54.048301	365	h	66.440491	60.701680	60.536614
344	C	60.491558	50.712359	54.371037	366	h	69.350687	47.303891	58.760648
345	C	60.099746	50.690120	55.709054	367				
346	C	61.054305	50.775539	56.724769	368				
347	O	66.074089	50.791607	61.745574	369				
348	O	68.259166	52.236093	59.445269	370				
349	O	68.639562	50.807821	61.098847	371				
350	O	64.657949	50.684008	57.100577	372				

373 **SnB3**

374 **R**

375	C	73.091979	54.669065	58.022328	395	H	62.580923	49.731382	59.732008
376	H	73.360203	53.685321	58.422924	396	N	60.646555	47.203496	59.508613
377	H	73.848433	55.370640	58.388304	397	H	61.329387	46.579829	59.068182
378	N	71.783340	55.082259	58.536517	398	H	59.820905	46.796287	59.953704
379	H	71.593706	56.076059	58.682200	399	C	64.870495	58.910071	62.054398
380	C	70.734170	54.265664	58.648029	400	H	64.915866	58.401007	63.028536
381	N	69.509260	54.791415	58.719994	401	H	64.101329	59.688526	62.159513
382	H	68.737160	54.148569	58.883441	402	C	64.456459	57.882537	61.021764
383	H	69.338927	55.698769	58.263837	403	C	64.680229	56.525755	61.287517
384	N	70.884385	52.937203	58.641958	404	H	65.192364	56.248661	62.209245
385	H	70.006265	52.423956	58.770267	405	C	64.238963	55.519126	60.431827
386	H	71.640798	52.546350	59.231093	406	H	64.373263	54.469125	60.711512
387	C	59.101511	49.001250	61.171381	407	C	63.563564	55.875575	59.265219
388	H	58.549039	48.187002	60.690082	408	O	63.071990	54.925066	58.400538
389	H	58.419779	49.861169	61.215606	409	H	63.305946	54.026860	58.702669
390	N	60.249893	49.365393	60.345660	410	C	63.780951	58.210308	59.840826
391	H	60.816162	50.164074	60.675622	411	H	63.585595	59.256921	59.603425
392	C	61.032476	48.459976	59.720614	412	C	63.346957	57.220261	58.959608
393	N	62.214537	48.870859	59.276772	413	H	62.828649	57.483773	58.035153
394	H	62.810033	48.165884	58.831253	414	C	68.556511	48.074400	59.102089

415	H	67.854810	47.441136	59.660296	437	O	68.750230	50.960903	61.002775
416	H	69.032820	48.752465	59.833416	438	O	65.030927	51.203910	57.031945
417	C	67.814138	49.016434	58.189300	439	H	64.770879	51.920864	54.792411
418	O	68.288545	49.623234	57.265042	440	O	63.581494	52.625204	61.915377
419	O	66.554049	49.213154	58.590024	441	O	62.422160	50.913581	61.048484
420	H	66.144855	49.942192	58.072957	442	H	66.023199	52.257704	58.806385
421	Zn	67.880623	50.012623	62.442085	443	H	62.291154	51.940308	58.698493
422	C	63.902514	51.645513	57.254348	444	H	63.491016	52.461759	52.700963
423	C	63.038976	51.948728	56.051175	445	H	61.018230	52.683753	52.801005
424	C	63.689114	52.054596	54.811825	446	H	59.841898	52.468221	54.986949
425	C	63.329560	51.802986	61.046384	447	H	61.117996	52.034082	57.050178
426	C	64.138249	51.852236	59.741097	448	O	63.411964	55.184738	55.560440
427	C	65.547061	51.950187	59.732861	449	H	63.947933	54.404583	55.379451
428	C	66.447251	51.528882	60.699679	450	H	63.204237	55.106308	56.507036
429	C	67.931517	51.638063	60.289817	451	h	73.125022	54.641328	56.933197
430	C	63.373331	51.879200	58.578007	452	h	59.377635	48.733886	62.191351
431	C	62.970571	52.338154	53.652813	453	h	65.809256	59.456561	61.964168
432	C	61.581828	52.476217	53.711093	454	h	69.365743	47.482042	58.675096
433	C	60.925519	52.359633	54.935924	455				
434	C	61.650501	52.117254	56.102712	456				
435	O	66.228665	50.959952	61.816752	457				
436	O	68.244166	52.320451	59.323574	458				

459 **TS1**

460	C	73.121327	54.723263	58.024991	481	N	60.676169	47.238798	59.458587
461	H	73.395936	53.738199	58.417516	482	H	61.357857	46.622392	59.003493
462	H	73.872299	55.427247	58.396895	483	H	59.857862	46.824302	59.911153
463	N	71.809302	55.122400	58.540956	484	C	64.794535	58.923515	61.894370
464	H	71.608442	56.114186	58.692526	485	H	64.777452	58.404275	62.863938
465	C	70.768509	54.295984	58.631689	486	H	64.039731	59.719938	61.971490
466	N	69.536952	54.804608	58.693723	487	C	64.414907	57.927386	60.818669
467	H	68.766678	54.160248	58.843602	488	C	64.567041	56.556431	61.065269
468	H	69.358716	55.717634	58.248727	489	H	64.999895	56.235532	62.016223
469	N	70.940838	52.967480	58.610024	490	C	64.155445	55.590698	60.154628
470	H	70.073918	52.435804	58.708127	491	H	64.237680	54.537895	60.428432
471	H	71.686319	52.582819	59.216873	492	C	63.572969	55.954260	58.920601
472	C	59.107222	49.044088	61.083724	493	O	63.146363	55.040001	58.056562
473	H	58.560497	48.237088	60.581227	494	H	63.368252	53.563903	58.404610
474	H	58.434062	49.911039	61.114609	495	C	63.833647	58.291551	59.598055
475	N	60.280074	49.395583	60.292418	496	H	63.677223	59.349283	59.375150
476	H	60.824211	50.213815	60.596286	497	C	63.440317	57.336994	58.660748
477	C	61.054825	48.500437	59.656039	498	H	62.997443	57.652945	57.712471
478	N	62.229063	48.918782	59.184532	499	C	68.610993	48.118499	59.118354
479	H	62.821052	48.198708	58.762382	500	H	67.892760	47.498977	59.671108
480	H	62.611424	49.761619	59.672612	501	H	69.107780	48.773564	59.856806

502	C	67.887383	49.085949	58.218794	524	H	64.786910	51.983791	54.781581
503	O	68.332403	49.633044	57.246285	525	O	63.613702	52.575370	61.978492
504	O	66.665451	49.383579	58.692951	526	O	62.554089	50.899426	60.929798
505	H	66.244038	50.074393	58.136438	527	H	66.077992	52.428495	58.809085
506	Zn	67.918487	50.012185	62.448755	528	H	62.373685	52.100295	58.727200
507	C	63.907689	51.824065	57.258538	529	H	63.501187	52.445613	52.680391
508	C	63.059700	52.094226	56.048278	530	H	61.034797	52.713820	52.787232
509	C	63.706901	52.130805	54.804624	531	H	59.870211	52.628604	54.986513
510	C	63.415544	51.827248	61.037330	532	H	61.155963	52.301983	57.064243
511	C	64.228199	52.063389	59.764994	533	O	63.472537	55.282741	55.474669
512	C	65.592804	52.106125	59.725926	534	H	64.141552	54.606273	55.336632
513	C	66.500936	51.597982	60.698250	535	H	63.298615	55.238550	56.461250
514	C	67.992239	51.630448	60.274985	536	h	73.153747	54.704022	56.935658
515	C	63.427972	52.360704	58.566979	537	h	59.355637	48.765979	62.107937
516	C	62.987968	52.380023	53.640549	538	h	65.744150	59.457834	61.866042
517	C	61.601911	52.543006	53.702900	539	h	69.401709	47.508775	58.681236
518	C	60.950985	52.498450	54.934662	540				
519	C	61.678714	52.303826	56.108316	541				
520	O	66.252878	51.038115	61.779697	542				
521	O	68.304979	52.268290	59.286552	543				
522	O	68.779535	50.946743	61.011430	544				
523	O	64.964681	51.234858	57.102453	545				

546 **IMI**

547	C	73.141296	54.767538	58.027005	568	N	60.716125	47.191239	59.419709
548	H	73.431180	53.790884	58.429428	569	H	61.366462	46.553882	58.946118
549	H	73.883939	55.485223	58.388889	570	H	59.911721	46.795084	59.912153
550	N	71.825674	55.156704	58.542637	571	C	64.822927	58.923906	61.990778
551	H	71.618914	56.145732	58.706973	572	H	64.887934	58.330850	62.914749
552	C	70.791570	54.322211	58.627949	573	H	64.063954	59.694780	62.185928
553	N	69.555782	54.818442	58.693568	574	C	64.388275	57.994517	60.876277
554	H	68.791887	54.167717	58.846126	575	C	64.506646	56.612512	61.066153
555	H	69.366588	55.733728	58.256967	576	H	64.931888	56.244975	62.002808
556	N	70.976882	52.994475	58.594982	577	C	64.084338	55.690221	60.116333
557	H	70.114945	52.455182	58.690180	578	H	64.155203	54.627069	60.349138
558	H	71.718537	52.613987	59.208572	579	C	63.497206	56.107881	58.898254
559	C	59.233284	49.046550	61.062390	580	O	63.058556	55.237204	58.012364
560	H	58.674931	48.252615	60.551765	581	H	63.348853	53.598227	58.499952
561	H	58.590587	49.936950	61.060610	582	C	63.806515	58.418681	59.674787
562	N	60.445735	49.341367	60.314434	583	H	63.675210	59.489898	59.497326
563	H	61.032776	50.127512	60.631028	584	C	63.386598	57.507872	58.705197
564	C	61.155789	48.431178	59.636596	585	H	62.944598	57.870026	57.773023
565	N	62.333629	48.805344	59.130495	586	C	68.629012	48.099376	59.147620
566	H	62.886853	48.065421	58.691279	587	H	67.942996	47.475007	59.734719
567	H	62.763590	49.633796	59.582927	588	H	69.148719	48.761645	59.863841

589	C	67.858247	49.058351	58.278788	611	H	64.911127	51.865216	54.919905
590	O	68.248092	49.591439	57.275845	612	O	63.581827	52.489459	62.096851
591	O	66.665272	49.370366	58.817213	613	O	62.726979	50.772157	60.929408
592	H	66.212372	50.043864	58.264335	614	H	66.103953	52.580830	58.891562
593	Zn	67.951643	50.019451	62.455995	615	H	62.420054	52.116139	58.832789
594	C	63.948758	51.888208	57.370216	616	H	63.721360	52.347451	52.764394
595	C	63.185779	52.240512	56.132841	617	H	61.298482	52.902888	52.804036
596	C	63.856459	52.136255	54.906262	618	H	60.100606	53.072359	54.975646
597	C	63.480966	51.778259	61.113291	619	H	61.319670	52.760910	57.100643
598	C	64.277150	52.155076	59.869246	620	O	63.374708	55.383664	55.449715
599	C	65.633927	52.226408	59.805958	621	H	63.963399	54.636250	55.318939
600	C	66.554582	51.669557	60.746657	622	H	63.216366	55.385068	56.444452
601	C	68.034511	51.645815	60.285606	623	h	73.170144	54.737054	56.937828
602	C	63.452859	52.461418	58.671829	624	h	59.432933	48.770377	62.097733
603	C	63.190222	52.400947	53.714604	625	h	65.764596	59.469282	61.928398
604	C	61.829877	52.719529	53.738543	626	h	69.408454	47.496227	58.682058
605	C	61.160326	52.824231	54.956056	627				
606	C	61.842107	52.622262	56.154647	628				
607	O	66.307761	51.113541	61.825915	629				
608	O	68.345235	52.276651	59.292775	630				
609	O	68.809752	50.927333	61.000171	631				
610	O	64.921407	51.162790	57.269889	632				

633 IM1'

634	C	73.197705	54.817536	58.031765	655	N	60.856100	46.805957	59.137034
635	H	73.507113	53.848861	58.438469	656	H	61.370532	46.107376	58.584682
636	H	73.931915	55.548935	58.382371	657	H	60.117903	46.469843	59.761995
637	N	71.878077	55.187988	58.552785	658	C	64.880537	58.977139	62.063660
638	H	71.657123	56.173228	58.725877	659	H	64.802050	58.725326	63.131258
639	C	70.855483	54.338655	58.608706	660	H	64.130993	59.764695	61.899413
640	N	69.609958	54.814192	58.673819	661	C	64.506881	57.734550	61.284997
641	H	68.859338	54.139426	58.774721	662	C	64.554914	56.500610	61.941195
642	H	69.409979	55.725688	58.232243	663	H	64.996204	56.447294	62.938691
643	N	71.066346	53.015921	58.544565	664	C	63.976718	55.363474	61.383316
644	H	70.217726	52.454063	58.617015	665	H	63.949191	54.412357	61.920547
645	H	71.805095	52.639605	59.163050	666	C	63.324465	55.457552	60.152477
646	C	59.704387	48.889335	60.783582	667	O	62.575238	54.434528	59.680222
647	H	59.093463	48.146060	60.258737	668	H	62.559418	53.709946	60.338626
648	H	59.253685	49.871693	60.583276	669	C	63.976583	57.766369	59.985771
649	N	61.050892	48.855179	60.246895	670	H	63.973904	58.706018	59.432334
650	H	61.755217	49.546807	60.543755	671	C	63.409935	56.634708	59.400643
651	C	61.522049	47.933446	59.411800	672	H	63.028261	56.626249	58.375061
652	N	62.693553	48.150279	58.805909	673	C	68.596545	48.008023	59.109466
653	H	63.090938	47.368758	58.285301	674	H	67.863310	47.379876	59.632101
654	H	63.272018	48.926157	59.146331	675	H	69.079681	48.644577	59.872502

676	C	67.901362	48.992660	58.204255	698	H	65.086663	51.678255	54.398850
677	O	68.367571	49.529183	57.236911	699	O	62.917895	52.156119	61.254645
678	O	66.679555	49.320328	58.662884	700	O	63.482397	50.123760	60.527696
679	H	66.275510	49.989070	58.065485	701	H	66.263766	52.610860	58.666914
680	Zn	67.918304	50.029541	62.400464	702	H	62.597313	51.897797	58.307457
681	C	64.187040	51.777134	56.896676	703	H	63.806487	52.096864	52.280123
682	C	63.428241	52.137636	55.672362	704	H	61.423014	52.773838	52.407472
683	C	64.040687	51.970904	54.420480	705	H	60.364869	53.158250	54.622630
684	C	63.554487	51.373848	60.540996	706	H	61.645415	52.861483	56.684129
685	C	64.402331	51.981342	59.444311	707	O	62.958986	55.317331	55.812870
686	C	65.738251	52.181756	59.516799	708	H	63.718531	54.729691	55.766801
687	C	66.594069	51.624669	60.531722	709	H	63.478987	53.381406	58.078974
688	C	68.099010	51.586748	60.171701	710	h	73.215945	54.779854	56.942585
689	C	63.620202	52.292265	58.204391	711	h	59.663523	48.695476	61.855410
690	C	63.331434	52.212685	53.252378	712	h	65.837902	59.488270	61.962348
691	C	61.990070	52.606175	53.323681	713	h	69.396921	47.407554	58.677145
692	C	61.396771	52.824105	54.558621	714				
693	C	62.122409	52.636481	55.732982	715				
694	O	66.272388	51.115234	61.611359	716				
695	O	68.466897	52.205416	59.192888	717				
696	O	68.825141	50.887286	60.952861	718				
697	O	65.195779	51.098125	56.847598	719				

720 **TS2**

721	C	73.166220	54.769684	58.034844	742	N	60.794314	47.244009	59.401214
722	H	73.453268	53.791099	58.434903	743	H	61.431705	46.621322	58.885694
723	H	73.916814	55.482336	58.390519	744	H	60.033496	46.817633	59.936157
724	N	71.858254	55.166969	58.562625	745	C	64.890858	58.936004	62.171651
725	H	71.658157	56.156467	58.729870	746	H	65.002929	58.285519	63.051848
726	C	70.816194	54.342809	58.649778	747	H	64.149661	59.700863	62.440748
727	N	69.587225	54.854140	58.732568	748	C	64.410629	58.106661	61.003665
728	H	68.820533	54.203739	58.872012	749	C	64.664696	56.730387	60.976577
729	H	69.402372	55.767857	58.289037	750	H	65.178838	56.272487	61.824091
730	N	70.985224	53.013622	58.604660	751	C	64.279941	55.933615	59.904398
731	H	70.118163	52.483465	58.702488	752	H	64.477420	54.861839	59.933741
732	H	71.727385	52.618869	59.208216	753	C	63.616890	56.491057	58.794624
733	C	59.350096	49.082145	61.102029	754	O	63.267738	55.752267	57.738830
734	H	58.813408	48.298574	60.554692	755	H	63.054995	53.528842	58.804672
735	H	58.742440	49.994431	61.033149	756	C	63.712607	58.653176	59.921012
736	N	60.635794	49.318695	60.474976	757	H	63.487248	59.722689	59.916278
737	H	61.233092	50.091670	60.810722	758	C	63.335900	57.868480	58.834342
738	C	61.288617	48.448835	59.708765	759	H	62.841893	58.314195	57.969321
739	N	62.470467	48.816529	59.202926	760	C	68.533571	48.163663	59.135515
740	H	63.002316	48.100346	58.708668	761	H	67.813774	47.530064	59.671237
741	H	62.923023	49.623084	59.661673	762	H	69.028096	48.794025	59.896538

763	C	67.807579	49.163133	58.265255	785	H	65.125188	52.440061	55.017173
764	O	68.228690	49.668666	57.260384	786	O	63.568292	52.588081	62.200065
765	O	66.632297	49.532132	58.801811	787	O	62.863428	50.772521	61.078913
766	H	66.187104	50.220113	58.245453	788	H	66.119739	52.626329	58.985805
767	Zn	67.966130	50.036415	62.478844	789	H	62.584483	51.820493	58.851342
768	C	64.147139	52.249890	57.437222	790	H	63.925047	52.749167	52.831779
769	C	63.344000	52.551448	56.187712	791	H	61.441783	52.965310	52.813501
770	C	64.043902	52.561993	54.974753	792	H	60.192625	52.971750	54.969321
771	C	63.527030	51.843165	61.235872	793	H	61.396487	52.738569	57.111537
772	C	64.300927	52.242718	59.986016	794	O	64.964129	54.083792	57.357293
773	C	65.653528	52.327831	59.918536	795	H	65.672180	54.248525	57.989599
774	C	66.577326	51.746232	60.841694	796	H	64.092489	54.933408	57.539095
775	C	68.047192	51.702407	60.349041	797	h	73.185780	54.738511	56.945481
776	C	63.451159	52.499239	58.778140	798	h	59.450482	48.804466	62.151259
777	C	63.371752	52.733621	53.771229	799	h	65.826244	59.485542	62.066166
778	C	61.976972	52.871415	53.760981	800	h	69.328197	47.566981	58.687623
779	C	61.278034	52.872605	54.966459	801				
780	C	61.961741	52.727957	56.179305	802				
781	O	66.338023	51.185709	61.918829	803				
782	O	68.350616	52.352844	59.367410	804				
783	O	68.823108	50.956381	61.033980	805				
784	O	65.028871	51.393312	57.332624	806				

807 **IM2**

808	C	73.178425	54.780126	58.035219	829	N	60.794490	47.241053	59.409642
809	H	73.470774	53.804886	58.439610	830	H	61.426858	46.618647	58.887002
810	H	73.926755	55.497735	58.385724	831	H	60.037470	46.816117	59.950493
811	N	71.869755	55.175080	58.562165	832	C	64.874563	58.888471	62.081701
812	H	71.669130	56.163471	58.734311	833	H	64.962793	58.232959	62.961002
813	C	70.829073	54.347439	58.645030	834	H	64.112111	59.640198	62.327541
814	N	69.598563	54.857302	58.722693	835	C	64.453764	58.065109	60.883348
815	H	68.831664	54.209614	58.877277	836	C	64.813086	56.713304	60.802020
816	H	69.414624	55.771860	58.283765	837	H	65.356416	56.258811	61.632114
817	N	71.002732	53.020319	58.596412	838	C	64.512634	55.938817	59.686447
818	H	70.137384	52.486855	58.699378	839	H	64.823321	54.893521	59.636077
819	H	71.747091	52.626269	59.197950	840	C	63.817421	56.508716	58.615974
820	C	59.349514	49.085985	61.096164	841	O	63.512883	55.794473	57.496977
821	H	58.813435	48.303738	60.545861	842	H	63.075172	53.482269	58.782011
822	H	58.744206	49.999884	61.023398	843	C	63.724622	58.607519	59.820542
823	N	60.638732	49.318832	60.476532	844	H	63.430054	59.658802	59.858518
824	H	61.231591	50.102208	60.797502	845	C	63.413612	57.844412	58.696588
825	C	61.290241	48.448300	59.708638	846	H	62.888035	58.290220	57.850502
826	N	62.466913	48.815199	59.195954	847	C	68.398603	48.228235	59.073694
827	H	62.995013	48.112494	58.680521	848	H	67.649367	47.586394	59.557629
828	H	62.914877	49.640835	59.625124	849	H	68.861496	48.833411	59.874762

850	C	67.716034	49.265458	58.192331	872	H	65.021344	52.207455	54.831956
851	O	68.225280	49.778661	57.227146	873	O	63.603111	52.607978	62.131561
852	O	66.527833	49.630701	58.662282	874	O	62.845499	50.814315	61.012156
853	H	66.042385	50.347643	58.097926	875	H	66.185217	52.655683	58.986143
854	Zn	67.982508	50.015138	62.463419	876	H	62.722537	51.750030	58.717577
855	C	64.325639	52.357435	57.367073	877	H	63.658754	52.407173	52.743851
856	C	63.360276	52.475154	56.150976	878	H	61.181846	52.684659	52.903673
857	C	63.946553	52.385744	54.880210	879	H	60.117206	52.845986	55.154695
858	C	63.549689	51.858122	61.169339	880	H	61.483221	52.740867	57.194470
859	C	64.359568	52.233884	59.935447	881	O	65.079865	53.656478	57.325584
860	C	65.711541	52.323782	59.901533	882	H	65.864018	53.461919	56.792292
861	C	66.615565	51.727391	60.827676	883	H	64.117716	55.010717	57.410243
862	C	68.095880	51.715283	60.368958	884	h	73.195229	54.743669	56.945974
863	C	63.544388	52.483676	58.704024	885	h	59.438408	48.807741	62.146280
864	C	63.181353	52.484057	53.722431	886	h	65.806051	59.450859	62.017535
865	C	61.792552	52.650204	53.809523	887	h	69.215717	47.637851	58.659161
866	C	61.198811	52.734017	55.068230	888				
867	C	61.978702	52.659434	56.227326	889				
868	O	66.357403	51.140367	61.888037	890				
869	O	68.407926	52.380260	59.399419	891				
870	O	68.872405	50.985168	61.069439	892				
871	O	65.135242	51.339694	57.241890	893				

894 TS3

895	C	73.017477	54.568170	58.018870	916	N	60.849781	47.247387	59.420880
896	H	73.223316	53.551114	58.370366	917	H	61.478499	46.619604	58.898031
897	H	73.801187	55.210196	58.435323	918	H	60.097945	46.830265	59.972816
898	N	71.722691	55.020868	58.533335	919	C	64.862213	58.902657	61.905079
899	H	71.564477	56.023932	58.647643	920	H	64.894575	58.227693	62.773663
900	C	70.646576	54.251431	58.700919	921	H	64.079708	59.644393	62.114724
901	N	69.447306	54.833816	58.777285	922	C	64.547675	58.097810	60.661340
902	H	68.652137	54.233643	58.984135	923	C	65.132021	56.833815	60.506031
903	H	69.302346	55.732291	58.292913	924	H	65.752099	56.439276	61.311672
904	N	70.727062	52.917628	58.758316	925	C	64.975412	56.100823	59.341006
905	H	69.827614	52.446794	58.886939	926	H	65.473815	55.142544	59.207346
906	H	71.479793	52.497467	59.333185	927	C	64.142162	56.569817	58.327828
907	C	59.396848	49.081177	61.083428	928	O	63.908451	55.805155	57.213090
908	H	58.848201	48.301939	60.539498	929	H	63.610217	54.175424	59.095892
909	H	58.774343	49.985946	61.061326	930	C	63.736575	58.567321	59.624536
910	N	60.652556	49.356886	60.415029	931	H	63.287436	59.559514	59.711844
911	H	61.268820	50.122009	60.774443	932	C	63.519297	57.809254	58.469204
912	C	61.322788	48.477295	59.673273	933	H	62.890657	58.185827	57.660902
913	N	62.485120	48.844319	59.133363	934	C	68.534879	48.246814	59.200254
914	H	63.009321	48.146926	58.611978	935	H	67.927760	47.589144	59.835480
915	H	62.922601	49.739406	59.394765	936	H	69.083326	48.914999	59.889120

937	C	67.632070	49.204465	58.456949	958	O	64.450981	50.998735	58.300277
938	O	67.890720	49.781384	57.431530	959	H	64.465803	53.128283	55.489726
939	O	66.515668	49.442927	59.146710	960	O	63.222362	52.270649	62.712502
940	H	65.902226	50.100678	58.715166	961	O	62.709855	50.868424	61.036642
941	Zn	67.843892	50.036641	62.493456	962	H	65.943278	53.487402	59.907565
942	C	64.157834	52.183238	58.008042	963	H	62.279657	53.018037	59.560618
943	C	63.072183	52.412604	56.960208	964	H	62.768071	53.289556	53.676102
944	C	63.424324	52.873803	55.687432	965	H	60.380265	52.746400	54.152863
945	C	63.298974	51.853437	61.563697	966	H	59.740143	51.919463	56.414171
946	C	64.095385	52.708730	60.600184	967	H	61.471060	51.650820	58.181289
947	C	65.483957	52.845889	60.646947	968	O	65.225959	53.044702	57.734098
948	C	66.384716	51.948502	61.217684	969	H	66.026994	52.652132	58.122818
949	C	67.752769	51.853641	60.496262	970	H	64.402837	54.968681	57.290336
950	C	63.353223	53.203822	59.505588	971	h	73.073082	54.596910	56.930684
951	C	62.463848	52.977855	54.677578	972	h	59.532889	48.785345	62.123641
952	C	61.133911	52.654225	54.935626	973	h	65.795054	59.466345	61.916482
953	C	60.775430	52.192707	56.206745	974	h	69.297864	47.676210	58.670792
954	C	61.740581	52.053451	57.203869	975				
955	O	66.215442	51.149917	62.179073	976				
956	O	67.942191	52.489820	59.459924	977				
957	O	68.594797	51.050712	61.016787	978				
					979				

980 P

981	C	72.957531	54.466893	58.039184	1002	N	60.767477	47.304465	59.472343
982	H	73.151238	53.441139	58.372103	1003	H	61.460427	46.716715	58.990478
983	H	73.739594	55.095021	58.479894	1004	H	60.003713	46.846210	59.974462
984	N	71.657915	54.918016	58.548811	1005	C	64.878724	58.840178	61.850005
985	H	71.502743	55.922925	58.645946	1006	H	64.918552	58.152757	62.708731
986	C	70.577251	54.155379	58.729445	1007	H	64.085605	59.568011	62.069303
987	N	69.378046	54.744050	58.791420	1008	C	64.565660	58.044940	60.597532
988	H	68.578127	54.138968	58.972230	1009	C	65.142980	56.779508	60.421354
989	H	69.242350	55.637801	58.296369	1010	H	65.778064	56.372955	61.209529
990	N	70.645153	52.823733	58.815442	1011	C	64.947391	56.045987	59.259905
991	H	69.743297	52.349314	58.912693	1012	H	65.430640	55.078256	59.130029
992	H	71.396187	52.400993	59.391599	1013	C	64.100403	56.531645	58.267543
993	C	59.201851	49.045209	61.184524	1014	O	63.826795	55.787232	57.141859
994	H	58.675468	48.241069	60.655403	1015	H	63.456860	53.960231	58.859184
995	H	58.532678	49.916597	61.193075	1016	C	63.733584	58.523667	59.581624
996	N	60.415146	49.396434	60.473266	1017	H	63.287722	59.515764	59.685159
997	H	60.991005	50.183682	60.846425	1018	C	63.489923	57.774517	58.427259
998	C	61.160147	48.551964	59.761172	1019	H	62.848761	58.159132	57.632755
999	N	62.328186	48.998956	59.286937	1020	C	68.825508	48.140886	59.203802
1000	H	62.935713	48.314330	58.839224	1021	H	68.234180	47.504901	59.872241
1001	H	62.710000	49.831779	59.781523	1022	H	69.397937	48.825170	59.854934

1023	C	67.913496	49.063423	58.443435	1045	H	65.069082	53.063576	54.845072
1024	O	68.194796	49.717730	57.469561	1046	O	63.051269	52.383982	62.743822
1025	O	66.730193	49.174603	59.050076	1047	O	62.482166	50.844453	61.227724
1026	H	66.164985	49.841446	58.596945	1048	H	65.614692	53.234968	59.579989
1027	Zn	67.710130	50.133255	62.423285	1049	H	61.940434	53.345915	59.749964
1028	C	64.881665	51.872013	57.290852	1050	H	63.199715	53.474115	53.238158
1029	C	63.769814	52.254321	56.363645	1051	H	60.851345	53.000323	53.927990
1030	C	64.038428	52.837885	55.123883	1052	H	60.380925	52.042329	56.168542
1031	C	63.070482	51.903054	61.621463	1053	H	62.282121	51.492329	57.714870
1032	C	63.794449	52.672805	60.533846	1054	O	65.817570	52.785468	57.399501
1033	C	65.234983	52.635188	60.395539	1055	H	66.538325	52.521094	58.069313
1034	C	66.170685	51.840523	60.987759	1056	H	64.341049	54.964548	57.163623
1035	C	67.529197	51.798004	60.297850	1057	h	73.029864	54.519081	56.952855
1036	C	63.028567	53.358439	59.661304	1058	h	59.400737	48.755524	62.216315
1037	C	62.987466	53.084378	54.236520	1059	h	65.802961	59.417423	61.875325
1038	C	61.674078	52.806566	54.616717	1060	h	69.559190	47.544222	58.661798
1039	C	61.409388	52.256030	55.874641	1061				
1040	C	62.456619	51.957155	56.742385	1062				
1041	O	66.055264	51.076519	62.030804	1063				
1042	O	67.714276	52.381089	59.200791	1064				
1043	O	68.435589	51.108203	60.860515	1065				
1044	O	64.893587	50.800973	57.853257	1066				

1067 **SnA1**

1068 **R**

1069	C	75.099334	55.340179	60.533749	1089	H	65.901607	47.079996	60.366169
1070	H	75.590024	54.407301	60.842652	1090	N	63.644920	45.956483	60.581152
1071	H	75.854760	56.125279	60.653600	1091	H	64.134080	45.632329	59.732914
1072	N	74.011745	55.636160	61.447456	1092	H	62.732280	45.563000	60.773483
1073	H	73.813893	56.607917	61.674942	1093	C	66.468615	59.534249	62.629174
1074	C	73.144904	54.754459	61.940683	1094	H	66.342167	58.715452	63.349954
1075	N	72.232002	55.205143	62.813215	1095	H	65.609823	60.206693	62.773878
1076	H	71.345704	54.722066	62.967523	1096	C	66.498601	58.986160	61.214541
1077	H	72.230618	56.211465	62.976269	1097	C	66.974601	57.692027	60.962353
1078	N	73.209353	53.469596	61.617161	1098	H	67.290004	57.060179	61.793956
1079	H	72.441526	52.830478	61.860338	1099	C	67.116152	57.192536	59.671775
1080	H	73.893581	53.095446	60.944855	1100	H	67.516835	56.187731	59.512019
1081	C	61.710517	47.567808	61.921587	1101	C	66.773912	58.002363	58.588144
1082	H	61.410787	46.923916	61.084805	1102	O	66.917772	57.590066	57.305285
1083	H	61.164426	48.506621	61.770116	1103	H	67.192177	56.661776	57.272303
1084	N	63.135268	47.857068	61.829105	1104	C	66.126122	59.762128	60.109275
1085	H	63.437028	48.829694	61.959355	1105	H	65.717235	60.765142	60.255630
1086	C	63.968079	47.170534	61.049225	1106	C	66.267434	59.285108	58.810702
1087	N	65.166616	47.677775	60.761605	1107	H	65.990932	59.898150	57.953714
1088	H	65.465669	48.553383	61.201786	1108	C	70.828011	46.956174	60.954744

1109	H	70.192732	47.000898	60.059916	1131	O	68.635908	50.163731	64.079773
1110	H	70.362554	46.318461	61.713466	1132	O	67.968209	53.825663	59.343020
1111	C	70.937560	48.341669	61.518230	1133	H	64.483750	54.563428	57.733144
1112	O	70.665591	48.616086	62.677037	1134	O	64.468320	50.402101	61.468097
1113	O	71.319244	49.267099	60.678731	1135	O	64.445941	50.410199	59.243144
1114	H	71.299689	50.162749	61.108743	1136	H	67.600341	52.782390	61.395268
1115	Zn	70.120784	49.051130	64.564954	1137	H	65.054865	52.556045	58.576775
1116	C	66.863734	53.628574	58.801446	1138	H	64.167881	55.593870	55.471748
1117	C	66.607468	54.298359	57.476440	1139	H	66.115037	55.890334	53.961756
1118	C	65.330547	54.696194	57.056314	1140	H	68.377540	55.181548	54.692954
1119	C	64.891050	50.778734	60.361852	1141	H	68.694530	54.207334	56.992575
1120	C	66.005809	51.837063	60.337817	1142	O	63.272536	54.011101	59.940358
1121	C	66.989439	51.887724	61.317955	1143	H	64.172104	53.654579	60.026214
1122	C	67.384905	50.781187	62.138181	1144	H	63.383754	54.916810	60.312334
1123	C	68.416999	51.102870	63.259193	1145	h	74.839780	55.279744	59.476845
1124	C	65.871495	52.738654	59.263299	1146	h	61.365123	47.121501	62.854100
1125	C	65.157956	55.276215	55.799320	1147	h	67.344908	60.107169	62.932389
1126	C	66.251776	55.447051	54.947472	1148	h	71.782768	46.522239	60.657752
1127	C	67.526492	55.056945	55.363003	1149				
1128	C	67.708571	54.502592	56.631240	1150				
1129	O	67.100343	49.595445	61.964121	1151				
1130	O	68.976298	52.197416	63.267854	1152				

1153 **IM1**

1154	C	75.085123	55.378207	60.514409	1175	N	63.572170	45.969268	60.600697
1155	H	75.597539	54.461031	60.835271	1176	H	64.046598	45.620014	59.751770
1156	H	75.817864	56.184810	60.630873	1177	H	62.684866	45.555944	60.861646
1157	N	73.981018	55.655042	61.415441	1178	C	66.435944	59.597725	62.682229
1158	H	73.761564	56.622588	61.646481	1179	H	66.300380	58.784681	63.406135
1159	C	73.130312	54.752758	61.895207	1180	H	65.591635	60.287172	62.833315
1160	N	72.181321	55.179279	62.741261	1181	C	66.438822	59.049329	61.268001
1161	H	71.330298	54.649618	62.911798	1182	C	66.859262	57.736985	61.013574
1162	H	72.140268	56.182822	62.906930	1183	H	67.145200	57.090099	61.844836
1163	N	73.235639	53.467661	61.582826	1184	C	66.959823	57.234002	59.719577
1164	H	72.491403	52.808712	61.849157	1185	H	67.312685	56.215334	59.549242
1165	H	73.935304	53.101253	60.921789	1186	C	66.629923	58.050169	58.637234
1166	C	61.658420	47.693896	61.866815	1187	O	66.713370	57.625664	57.354450
1167	H	61.348849	47.082034	61.008863	1188	H	66.827050	56.663812	57.307615
1168	H	61.167145	48.665952	61.730011	1189	C	66.092635	59.841711	60.165154
1169	N	63.096730	47.908294	61.803640	1190	H	65.725226	60.859987	60.315646
1170	H	63.445525	48.859373	61.966587	1191	C	66.195955	59.358341	58.866111
1171	C	63.903824	47.193813	61.022266	1192	H	65.928741	59.978793	58.011990
1172	N	65.087615	47.706317	60.675076	1193	C	70.858865	46.980839	60.990121
1173	H	65.306996	48.647016	61.010652	1194	H	70.232451	47.058133	60.090999
1174	H	65.843000	47.104165	60.328520	1195	H	70.377722	46.329427	61.727205

1196	C	70.978247	48.348768	61.594043	1218	H	63.868657	54.451727	58.213421
1197	O	70.673798	48.594230	62.752109	1219	O	64.539247	50.376757	61.593242
1198	O	71.399778	49.293063	60.795134	1220	O	65.101195	50.600061	59.451991
1199	H	71.377059	50.175832	61.250399	1221	H	67.449975	53.179027	61.987524
1200	Zn	70.164409	49.015967	64.654653	1222	H	64.355283	53.364769	59.799488
1201	C	66.434291	53.753713	59.086372	1223	H	63.364867	55.425232	55.956785
1202	C	66.012686	54.323843	57.772992	1224	H	65.165507	55.764755	54.283540
1203	C	64.683351	54.653632	57.477300	1225	H	67.501217	55.124578	54.802533
1204	C	65.107454	50.963615	60.646014	1226	H	68.044504	54.196271	57.068999
1205	C	65.863365	52.240710	60.951998	1227	O	62.678839	53.914569	59.524320
1206	C	66.922753	52.248929	61.783914	1228	H	65.387148	54.354233	60.778937
1207	C	67.488780	51.033520	62.375545	1229	H	63.011352	54.699915	59.979329
1208	C	68.535465	51.223224	63.499444	1230	h	74.832363	55.300747	59.456969
1209	C	65.421185	53.431070	60.160663	1231	h	61.276957	47.242999	62.782918
1210	C	64.396418	55.174746	56.209537	1232	h	67.327834	60.153043	62.972439
1211	C	65.401542	55.354476	55.262461	1233	h	71.808517	46.538729	60.688846
1212	C	66.722698	55.003575	55.556914	1234				
1213	C	67.027751	54.491262	56.810672	1235				
1214	O	67.289001	49.903702	61.978360	1236				
1215	O	69.128891	52.294853	63.579512	1237				
1216	O	68.722770	50.202544	64.213739	1238				
1217	O	67.629837	53.599286	59.289371	1239				

1240 **SnA2**

1241 **R**

1242	C	74.713759	54.351087	60.437783	1262	H	65.747402	46.604034	60.708186
1243	H	75.006702	53.355875	60.784776	1263	N	63.443358	45.475917	61.023393
1244	H	75.553653	55.025549	60.659927	1264	H	64.066879	44.841721	60.506996
1245	N	73.531546	54.803829	61.152750	1265	H	62.566158	45.082388	61.346252
1246	H	73.071577	55.660876	60.834009	1266	C	66.203698	59.694803	61.849137
1247	C	72.930876	54.214645	62.185933	1267	H	65.862423	58.976119	62.608084
1248	N	72.094098	54.921103	62.939753	1268	H	65.437225	60.481540	61.799637
1249	H	71.490972	54.402320	63.599235	1269	C	66.317389	58.998795	60.507282
1250	H	72.112641	55.945018	62.924250	1270	C	66.675751	57.645540	60.429342
1251	N	73.130800	52.928926	62.489650	1271	H	66.898133	57.090507	61.342131
1252	H	72.690883	52.580824	63.339638	1272	C	66.792944	56.978473	59.212923
1253	H	73.520961	52.242578	61.824241	1273	H	67.086425	55.924629	59.190033
1254	C	61.506722	47.196007	62.145338	1274	C	66.535104	57.675942	58.032659
1255	H	61.192108	46.528827	61.328808	1275	O	66.654946	57.088268	56.803898
1256	H	60.934531	48.123608	62.014319	1276	H	66.906245	56.157450	56.901104
1257	N	62.915179	47.510961	61.996990	1277	C	66.048648	59.667946	59.307927
1258	H	63.239138	48.489272	62.110698	1278	H	65.740749	60.716350	59.315699
1259	C	63.786748	46.726856	61.361948	1279	C	66.154586	59.016404	58.082534
1260	N	64.995747	47.207151	61.083288	1280	H	65.924046	59.537479	57.153640
1261	H	65.267746	48.128156	61.441465	1281	C	70.574600	46.478306	61.111402

1282	H	69.961567	46.448754	60.202135	1304	O	68.596429	50.002926	64.040880
1283	H	70.123378	45.867990	61.900995	1305	O	67.310284	53.485393	59.516585
1284	C	70.621144	47.898548	61.583826	1306	H	63.939604	53.790674	57.431766
1285	O	70.536951	48.231847	62.759385	1307	O	64.228436	49.939062	61.993851
1286	O	70.759455	48.798149	60.646483	1308	O	63.258314	50.501921	60.089218
1287	H	70.753471	49.720429	61.017409	1309	H	67.127517	52.431666	61.401338
1288	Zn	69.891892	48.696560	64.578910	1310	H	64.409617	52.075719	58.822094
1289	C	66.241142	53.170662	58.938256	1311	H	63.887546	54.554653	55.077551
1290	C	66.095741	53.673869	57.522722	1312	H	66.005184	54.868750	53.810020
1291	C	64.873723	53.923585	56.886770	1313	H	68.190555	54.438214	54.931572
1292	C	64.207367	50.555051	60.905628	1314	H	68.228964	53.688302	57.322687
1293	C	65.399355	51.495921	60.613341	1315	O	68.832922	51.137112	59.249885
1294	C	66.493474	51.552266	61.469551	1316	H	69.474004	51.200092	59.979046
1295	C	67.075458	50.477927	62.236838	1317	H	68.293711	51.937277	59.382411
1296	C	68.212383	50.890659	63.227738	1318	h	74.571502	54.325966	59.357413
1297	C	65.250874	52.316298	59.462685	1319	h	61.217508	46.754108	63.098830
1298	C	64.844354	54.357378	55.561608	1320	h	67.087324	60.200888	62.237918
1299	C	66.032084	54.540581	54.848423	1321	h	71.557774	46.070717	60.876227
1300	C	67.258086	54.300993	55.478748	1322				
1301	C	67.286840	53.883560	56.809673	1323				
1302	O	66.903229	49.273929	62.091553	1324				
1303	O	68.699852	52.025219	63.155373	1325				

1326 **IMI**

1327	C	74.669035	54.446506	60.368652	1348	N	63.408659	45.420530	61.056493
1328	H	75.021040	53.484140	60.753274	1349	H	64.023891	44.787788	60.524707
1329	H	75.468671	55.176885	60.559471	1350	H	62.547216	45.011625	61.410813
1330	N	73.469877	54.855725	61.077679	1351	C	66.169138	59.751017	61.843339
1331	H	72.971513	55.689495	60.757361	1352	H	65.801441	59.055718	62.611429
1332	C	72.869608	54.208005	62.075161	1353	H	65.428631	60.561340	61.774917
1333	N	71.970018	54.853419	62.816074	1354	C	66.280342	59.025645	60.516699
1334	H	71.372386	54.289462	63.435927	1355	C	66.592785	57.660366	60.480269
1335	H	71.958787	55.874871	62.834694	1356	H	66.757128	57.125216	61.414796
1336	N	73.149631	52.938350	62.372076	1357	C	66.746995	56.966757	59.283228
1337	H	72.620735	52.553288	63.151917	1358	H	66.988169	55.900500	59.289219
1338	H	73.497733	52.267191	61.667284	1359	C	66.590155	57.653898	58.080604
1339	C	61.510696	47.179534	62.193525	1360	O	66.779313	57.047856	56.872867
1340	H	61.208701	46.565137	61.332490	1361	H	67.039183	56.121093	56.983859
1341	H	61.005410	48.146430	62.071173	1362	C	66.081197	59.676431	59.294188
1342	N	62.942403	47.415957	62.135788	1363	H	65.798510	60.730932	59.269213
1343	H	63.282502	48.377245	62.288160	1364	C	66.236881	59.003317	58.086183
1344	C	63.784323	46.643966	61.443363	1365	H	66.087164	59.514836	57.136448
1345	N	64.992362	47.123645	61.152333	1366	C	70.588279	46.482429	61.156729
1346	H	65.290966	47.996102	61.594070	1367	H	69.938763	46.390113	60.276610
1347	H	65.738888	46.525421	60.755430	1368	H	70.190967	45.894464	61.991299

1369	C	70.587330	47.930071	61.546839	1391	H	64.156753	53.880663	57.319506
1370	O	70.464694	48.334629	62.700722	1392	O	64.253082	49.909624	62.142120
1371	O	70.693077	48.768847	60.556383	1393	O	63.251021	50.344845	60.209884
1372	H	70.616340	49.726481	60.828534	1394	H	67.590950	51.277731	60.566372
1373	Zn	69.902454	48.666298	64.578523	1395	H	64.698761	51.354317	58.488805
1374	C	66.174148	52.868831	58.944456	1396	H	64.467112	54.922736	55.073105
1375	C	66.257295	53.434839	57.554349	1397	H	66.726402	55.029382	54.056613
1376	C	65.148582	53.934968	56.868359	1398	H	68.686465	54.103862	55.267991
1377	C	64.244122	50.350002	60.971784	1399	H	68.329905	52.960404	57.534586
1378	C	65.565943	50.894301	60.439947	1400	O	68.449340	50.943705	58.452814
1379	C	66.741378	50.834118	61.102169	1401	H	69.093945	50.665849	59.116748
1380	C	67.137096	50.111714	62.335049	1402	H	66.462895	50.945321	58.538115
1381	C	68.206891	50.817766	63.214823	1403	h	74.523879	54.369792	59.291103
1382	C	65.624692	51.476436	59.058772	1404	h	61.138462	46.716671	63.107454
1383	C	65.323802	54.511237	55.608387	1405	h	67.065347	60.233891	62.232837
1384	C	66.595122	54.577115	55.039033	1406	h	71.568607	46.086966	60.890961
1385	C	67.699537	54.063623	55.728156	1407				
1386	C	67.536555	53.482089	56.986260	1408				
1387	O	66.820594	48.981767	62.602247	1409				
1388	O	68.469904	51.989507	62.948121	1410				
1389	O	68.738436	50.141942	64.139458	1411				
1390	O	66.649617	53.494983	59.865760	1412				

1413 **SnA3**

1414 **R**

1415	C	74.610280	54.314005	60.951778	1435	H	65.751270	46.211023	60.851458
1416	H	74.990299	53.368520	61.350990	1436	N	63.489425	45.101766	61.144896
1417	H	75.379152	55.074283	61.149195	1437	H	64.038795	44.523934	60.499450
1418	N	73.383522	54.681308	61.645912	1438	H	62.592094	44.719415	61.437699
1419	H	72.908104	55.544269	61.387355	1439	C	66.081129	60.454558	62.749403
1420	C	72.795648	54.007405	62.634832	1440	H	65.559236	59.900189	63.541599
1421	N	71.887166	54.617760	63.392489	1441	H	65.545233	61.408302	62.629388
1422	H	71.319174	54.029699	64.026262	1442	C	66.075805	59.650331	61.469722
1423	H	71.834561	55.638969	63.435847	1443	C	66.040740	58.253816	61.547471
1424	N	73.096444	52.735295	62.900299	1444	H	65.909633	57.777896	62.517936
1425	H	72.615264	52.323418	63.693339	1445	C	66.215480	57.448656	60.429323
1426	H	73.480395	52.085736	62.193500	1446	H	66.250874	56.361780	60.544388
1427	C	61.534118	46.840613	62.266557	1447	C	66.412425	58.054179	59.189642
1428	H	61.180724	46.016439	61.633906	1448	O	66.627850	57.314951	58.071285
1429	H	60.880197	47.695584	62.058673	1449	H	66.649985	56.371321	58.283226
1430	N	62.891388	47.210793	61.901367	1450	C	66.204502	60.234239	60.203221
1431	H	63.195833	48.210183	61.982853	1451	H	66.189509	61.320542	60.081953
1432	C	63.775745	46.397826	61.352214	1452	C	66.369778	59.445974	59.068262
1433	N	64.984774	46.877945	61.019256	1453	H	66.491837	59.907911	58.088984
1434	H	65.271952	47.771432	61.429653	1454	C	70.373909	46.615715	61.695269

1455	H	69.681635	46.443395	60.862860	1477	O	68.354089	49.703218	64.532132
1456	H	70.023491	46.083266	62.587355	1478	O	67.685402	52.448853	59.381926
1457	C	70.373304	48.083447	61.995618	1479	H	64.077342	53.923783	58.404469
1458	O	70.472996	48.553266	63.126652	1480	O	63.975148	49.690418	61.975828
1459	O	70.253165	48.844982	60.947872	1481	O	63.900453	49.686229	59.748114
1460	H	70.144450	49.822073	61.130232	1482	H	67.147911	52.030439	61.711739
1461	Zn	69.850356	48.607735	65.038489	1483	H	64.410292	52.108898	59.250132
1462	C	66.486871	52.687192	59.146384	1484	H	63.716838	55.439186	56.495571
1463	C	66.193800	53.658692	58.024936	1485	H	65.647478	56.162643	55.084945
1464	C	64.919700	54.189231	57.765215	1486	H	67.902425	55.229978	55.525125
1465	C	64.353067	50.073237	60.849027	1487	H	68.244119	53.629976	57.439658
1466	C	65.483901	51.108928	60.792786	1488	O	66.860875	54.522084	61.429384
1467	C	66.547573	51.125471	61.699213	1489	H	67.329767	54.496083	62.293215
1468	C	66.998802	50.080173	62.563334	1490	H	66.177639	53.841654	61.483751
1469	C	68.074715	50.526763	63.609080	1491	h	74.483600	54.221010	59.873181
1470	C	65.371659	52.048642	59.755911	1492	h	61.440829	46.574971	63.319552
1471	C	64.718231	55.061747	56.696301	1493	h	67.069634	60.730537	63.116500
1472	C	65.791490	55.447971	55.892892	1494	h	71.352487	46.222804	61.419458
1473	C	67.063948	54.930885	56.150859	1495				
1474	C	67.263523	54.043849	57.207509	1496				
1475	O	66.719264	48.885579	62.511498	1497				
1476	O	68.600560	51.640158	63.491186	1498				

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1500	C	74.596596	54.325662	60.945426	1521	N	63.400446	45.249007	61.253143
1501	H	75.008029	53.395031	61.347727	1522	H	63.939765	44.682990	60.587745
1502	H	75.344776	55.111037	61.126743	1523	H	62.518420	44.854048	61.577811
1503	N	73.363690	54.656114	61.646534	1524	C	66.046989	60.601504	62.880395
1504	H	72.830199	55.480824	61.369139	1525	H	65.485414	60.212982	63.741022
1505	C	72.885772	54.035033	62.727431	1526	H	65.602936	61.578466	62.631193
1506	N	72.043973	54.665680	63.534600	1527	C	65.951985	59.614426	61.744285
1507	H	71.462140	54.090745	64.171825	1528	C	65.774518	58.264576	62.063820
1508	H	71.899258	55.677161	63.478654	1529	H	65.544578	58.008599	63.098015
1509	N	73.253134	52.786921	63.034732	1530	C	65.926318	57.259471	61.123702
1510	H	72.897871	52.414327	63.908383	1531	H	65.841562	56.210383	61.399603
1511	H	73.566364	52.109760	62.320454	1532	C	66.260247	57.585260	59.798580
1512	C	61.461039	47.038600	62.300898	1533	O	66.502416	56.629641	58.893990
1513	H	61.155496	46.317244	61.530001	1534	H	66.656201	55.744359	59.407014
1514	H	60.915041	47.963372	62.085331	1535	C	66.179334	59.940592	60.404111
1515	N	62.882112	47.315453	62.170692	1536	H	66.275493	60.983765	60.091798
1516	H	63.208022	48.296293	62.215228	1537	C	66.321935	58.943215	59.442334
1517	C	63.728188	46.516769	61.528930	1538	H	66.519839	59.223903	58.409738
1518	N	64.930340	46.991774	61.183748	1539	C	70.388027	46.552620	61.710587
1519	H	65.183966	47.927638	61.502053	1540	H	69.688017	46.359791	60.889049
1520	H	65.693299	46.346752	60.929689	1541	H	70.055109	46.036098	62.618227

1542	C	70.384373	48.025601	61.973229	1564	H	63.907225	53.726675	57.999317
1543	O	70.481234	48.531342	63.088392	1565	O	64.191920	49.763251	61.962320
1544	O	70.264237	48.761230	60.905577	1566	O	64.013855	49.929257	59.742577
1545	H	70.211462	49.742524	61.097821	1567	H	67.231581	52.311768	61.601727
1546	Zn	69.899842	48.722334	64.998643	1568	H	64.326422	52.640330	59.593217
1547	C	66.279896	52.404323	58.708819	1569	H	63.670283	55.493980	56.324823
1548	C	66.015147	53.402031	57.612957	1570	H	65.669266	56.298611	55.043946
1549	C	64.778266	54.024282	57.417367	1571	H	67.844440	55.157335	55.337561
1550	C	64.490127	50.251933	60.850905	1572	H	68.063277	53.290536	56.999827
1551	C	65.545153	51.363917	60.846419	1573	O	67.006764	54.527545	60.263133
1552	C	66.644313	51.395002	61.639650	1574	H	67.680485	54.143416	59.687858
1553	C	67.177612	50.337561	62.506160	1575	H	65.992332	53.509743	60.204156
1554	C	68.209615	50.804756	63.582395	1576	h	74.468057	54.215484	59.868670
1555	C	65.368714	52.448229	59.859665	1577	h	61.131919	46.670060	63.272456
1556	C	64.647089	55.041706	56.475471	1578	h	67.062389	60.826304	63.206730
1557	C	65.752637	55.472309	55.748024	1579	h	71.368115	46.168818	61.427412
1558	C	66.985164	54.834555	55.920981	1580				
1559	C	67.111720	53.795038	56.834206	1581				
1560	O	66.995549	49.146567	62.354568	1582				
1561	O	68.670221	51.938080	63.455403	1583				
1562	O	68.523621	49.972281	64.482340	1584				
1563	O	67.345271	51.804266	58.699761	1585				

1586 **IMI**

1587	C	74.642978	54.309573	60.956485	1608	N	63.347588	45.198441	61.247748
1588	H	75.060151	53.378338	61.351314	1609	H	63.879794	44.636923	60.570821
1589	H	75.391448	55.096092	61.131008	1610	H	62.475613	44.796894	61.595303
1590	N	73.418834	54.638461	61.672626	1611	C	66.137194	60.403191	62.889837
1591	H	72.879227	55.461096	61.393244	1612	H	65.616257	59.932302	63.736405
1592	C	72.957209	54.023025	62.761549	1613	H	65.620334	61.358611	62.703983
1593	N	72.118458	54.655803	63.572594	1614	C	66.078753	59.485936	61.692778
1594	H	71.532037	54.084037	64.207570	1615	C	66.021400	58.102667	61.903811
1595	H	71.997778	55.672481	63.533465	1616	H	65.883740	57.751683	62.927301
1596	N	73.333625	52.778435	63.073635	1617	C	66.174740	57.186835	60.876748
1597	H	72.998734	52.413773	63.958140	1618	H	66.154660	56.116509	61.089777
1598	H	73.617004	52.092518	62.355548	1619	C	66.390759	57.610981	59.535223
1599	C	61.402637	46.995240	62.304973	1620	O	66.636483	56.767108	58.582056
1600	H	61.089074	46.262948	61.548229	1621	H	67.207553	55.543362	59.198738
1601	H	60.851347	47.915858	62.084472	1622	C	66.206167	59.922047	60.368415
1602	N	62.821730	47.271040	62.149193	1623	H	66.212621	60.990791	60.135261
1603	H	63.143692	48.246577	62.190992	1624	C	66.337641	59.019266	59.320500
1604	C	63.664686	46.471460	61.501052	1625	H	66.445244	59.399049	58.304103
1605	N	64.853068	46.958974	61.128127	1626	C	70.426832	46.693993	61.602733
1606	H	65.079354	47.912846	61.410219	1627	H	69.802559	46.643232	60.703314
1607	H	65.626926	46.324101	60.880172	1628	H	69.960051	46.135604	62.422302

1629	C	70.542254	48.125539	62.024025	1651	H	63.654408	53.826418	58.108658
1630	O	70.603631	48.487136	63.194893	1652	O	64.215672	49.716887	61.872679
1631	O	70.586923	48.987458	61.049455	1653	O	64.062334	50.034367	59.665250
1632	H	70.651060	49.936648	61.363943	1654	H	67.217015	52.383247	61.613986
1633	Zn	69.909774	48.723244	65.043483	1655	H	64.149584	52.608573	59.692414
1634	C	66.074191	52.570704	58.723746	1656	H	63.305613	55.532314	56.389879
1635	C	65.759201	53.562302	57.654842	1657	H	65.252527	56.412468	55.075114
1636	C	64.498996	54.142632	57.496645	1658	H	67.471557	55.375226	55.326318
1637	C	64.511489	50.287183	60.802422	1659	H	67.780271	53.468083	56.934697
1638	C	65.502823	51.444857	60.891616	1660	O	67.646865	54.686144	59.614695
1639	C	66.620443	51.470827	61.644192	1661	H	68.200247	54.365244	58.895460
1640	C	67.184608	50.382335	62.477020	1662	H	65.456927	53.563024	60.443767
1641	C	68.188354	50.823953	63.591459	1663	h	74.499810	54.204658	59.881049
1642	C	65.209217	52.595900	59.974788	1664	h	61.093914	46.641330	63.288591
1643	C	64.304482	55.129118	56.532716	1665	h	67.134536	60.689256	63.223815
1644	C	65.376625	55.593308	55.780266	1666	h	71.395387	46.246708	61.379341
1645	C	66.637013	55.001367	55.918386	1667				
1646	C	66.814923	53.963390	56.820209	1668				
1647	O	67.032290	49.201086	62.263211	1669				
1648	O	68.593847	51.982400	63.531737	1670				
1649	O	68.533813	49.944445	64.430750	1671				
1650	O	67.024020	51.828637	58.605645	1672				

1673 **TS2**

1674	C	74.646866	54.298265	60.955332	1695	N	63.356675	45.226921	61.253952
1675	H	75.062317	53.364969	61.346931	1696	H	63.888206	44.663232	60.579236
1676	H	75.396736	55.082856	61.133171	1697	H	62.484043	44.825209	61.597729
1677	N	73.421834	54.625599	61.670451	1698	C	66.133637	60.385713	62.862643
1678	H	72.874819	55.440711	61.385248	1699	H	65.617090	59.924140	63.716325
1679	C	72.959352	54.010471	62.759707	1700	H	65.607604	61.330444	62.655736
1680	N	72.114527	54.643242	63.564077	1701	C	66.091587	59.437765	61.687137
1681	H	71.535004	54.074429	64.208660	1702	C	66.059272	58.062023	61.941346
1682	H	71.992483	55.658897	63.520401	1703	H	65.925859	57.740560	62.973174
1683	N	73.342837	52.769888	63.078254	1704	C	66.248278	57.118414	60.943269
1684	H	73.001142	52.405212	63.960370	1705	H	66.287422	56.051257	61.161944
1685	H	73.623480	52.081985	62.360445	1706	C	66.459959	57.538640	59.619260
1686	C	61.407327	47.014026	62.301166	1707	O	66.726508	56.662273	58.647776
1687	H	61.102156	46.283016	61.539820	1708	H	66.961548	55.741920	59.059844
1688	H	60.849985	47.930862	62.081543	1709	C	66.215081	59.846579	60.355951
1689	N	62.825148	47.299152	62.151800	1710	H	66.205201	60.908296	60.096436
1690	H	63.147017	48.274952	62.200712	1711	C	66.383142	58.914502	59.335861
1691	C	63.672979	46.501477	61.507076	1712	H	66.495517	59.264001	58.311165
1692	N	64.861837	46.989140	61.140380	1713	C	70.433927	46.710067	61.599719
1693	H	65.084850	47.946521	61.417242	1714	H	69.811640	46.663185	60.698775
1694	H	65.634569	46.353379	60.891398	1715	H	69.962325	46.153048	62.417392

1716	C	70.551312	48.141191	62.022228	1738	H	63.777962	53.964026	58.209522
1717	O	70.604033	48.501562	63.194202	1739	O	64.257309	49.750961	61.895928
1718	O	70.607315	49.001781	61.048467	1740	O	64.087616	50.033956	59.688403
1719	H	70.659528	49.952551	61.359074	1741	H	67.258191	52.416331	61.561697
1720	Zn	69.901031	48.745780	65.035033	1742	H	64.241994	52.513703	59.553155
1721	C	66.255044	52.780367	58.834584	1743	H	63.330792	55.537984	56.387321
1722	C	65.874543	53.721175	57.717804	1744	H	65.205491	56.365958	54.947485
1723	C	64.596204	54.254231	57.551061	1745	H	67.460821	55.386321	55.196532
1724	C	64.546093	50.311621	60.816260	1746	H	67.866981	53.620251	56.938732
1725	C	65.542633	51.471271	60.877450	1747	O	67.374701	54.376881	59.707158
1726	C	66.666421	51.502373	61.623205	1748	H	68.113547	54.138174	59.132846
1727	C	67.227490	50.421288	62.459678	1749	H	65.260872	53.582897	60.542145
1728	C	68.215572	50.868707	63.582331	1750	h	74.504244	54.196718	59.879500
1729	C	65.244234	52.639406	59.981922	1751	h	61.095923	46.652266	63.281076
1730	C	64.345113	55.170574	56.527446	1752	h	67.129535	60.679343	63.194357
1731	C	65.377348	55.605669	55.705996	1753	h	71.401434	46.259188	61.379029
1732	C	66.654912	55.049732	55.848364	1754				
1733	C	66.887005	54.082438	56.816200	1755				
1734	O	67.081196	49.237394	62.250625	1756				
1735	O	68.621795	52.027895	63.526346	1757				
1736	O	68.552980	49.996298	64.434523	1758				
1737	O	67.129264	51.949184	58.635165	1759				

1760 **IM2**

1761	C	74.639881	54.283701	60.967114	1782	N	63.373782	45.284213	61.283821
1762	H	75.056897	53.349370	61.354293	1783	H	63.910950	44.710399	60.623207
1763	H	75.387552	55.068999	61.151200	1784	H	62.487410	44.897741	61.606110
1764	N	73.412016	54.602597	61.682536	1785	C	66.107472	60.428232	62.823031
1765	H	72.865462	55.419053	61.406569	1786	H	65.576669	59.974351	63.670568
1766	C	72.960035	53.988361	62.777876	1787	H	65.593018	61.376516	62.607255
1767	N	72.120488	54.621834	63.587848	1788	C	66.068287	59.476750	61.650461
1768	H	71.543482	54.052731	64.234926	1789	C	65.991475	58.104955	61.910752
1769	H	71.984477	55.634429	63.531320	1790	H	65.832236	57.782238	62.938751
1770	N	73.349718	52.750238	63.094297	1791	C	66.162196	57.157518	60.910921
1771	H	73.008391	52.380804	63.974661	1792	H	66.146082	56.089710	61.135866
1772	H	73.626765	52.063710	62.372457	1793	C	66.404742	57.580061	59.599858
1773	C	61.447501	47.090571	62.315409	1794	O	66.654171	56.694501	58.612786
1774	H	61.140847	46.394343	61.522010	1795	H	66.735440	55.796022	58.988018
1775	H	60.914017	48.026756	62.121124	1796	C	66.221405	59.882971	60.321130
1776	N	62.872026	47.353594	62.202264	1797	H	66.237724	60.943556	60.060377
1777	H	63.205715	48.330943	62.250268	1798	C	66.381414	58.948264	59.302543
1778	C	63.714624	46.548186	61.563292	1799	H	66.513847	59.279743	58.274020
1779	N	64.922631	47.011078	61.228168	1800	C	70.509400	46.673279	61.648083
1780	H	65.182912	47.947742	61.538777	1801	H	69.882826	46.643038	60.748715
1781	H	65.680431	46.357659	60.979084	1802	H	70.029356	46.123829	62.465572

1803	C	70.650221	48.103843	62.063217	1825	H	63.880006	53.977763	58.352844
1804	O	70.604333	48.481989	63.231474	1826	O	64.188385	49.817488	61.999304
1805	O	70.829896	48.942891	61.091824	1827	O	64.170420	49.867277	59.767854
1806	H	70.811348	49.899596	61.382026	1828	H	67.329525	52.292800	61.549038
1807	Zn	69.906546	48.713973	65.064724	1829	H	64.486904	52.158262	59.256725
1808	C	66.475068	52.944691	59.026669	1830	H	63.322997	55.428454	56.454213
1809	C	65.969223	53.781181	57.826255	1831	H	65.127033	56.238154	54.912885
1810	C	64.669836	54.265192	57.659791	1832	H	67.426523	55.371330	55.173948
1811	C	64.553236	50.260451	60.890183	1833	H	67.935328	53.699135	56.998384
1812	C	65.573722	51.402201	60.885283	1834	O	67.223838	54.005718	59.818219
1813	C	66.687347	51.423067	61.645897	1835	H	68.096807	53.923911	59.404856
1814	C	67.184598	50.369945	62.549940	1836	H	64.881574	53.391160	60.464902
1815	C	68.231974	50.831308	63.616149	1837	h	74.500707	54.185307	59.890538
1816	C	65.276386	52.517459	59.925133	1838	h	61.107086	46.702173	63.275268
1817	C	64.354510	55.109341	56.591200	1839	h	67.102478	60.714794	63.163490
1818	C	65.349198	55.537811	55.717125	1840	h	71.467063	46.210305	61.410168
1819	C	66.651776	55.047509	55.868195	1841				
1820	C	66.942922	54.141657	56.883452	1842				
1821	O	66.933222	49.190813	62.455397	1843				
1822	O	68.674743	51.976559	63.510370	1844				
1823	O	68.565368	49.988053	64.496066	1845				
1824	O	67.287500	52.000278	58.670692	1846				

1847 TS3

1848	C	74.594351	54.320792	60.937832	1869	N	63.382344	45.195062	61.284269
1849	H	74.993234	53.382693	61.335267	1870	H	63.917146	44.615208	60.627342
1850	H	75.352300	55.095089	61.125455	1871	H	62.491415	44.818028	61.604357
1851	N	73.365539	54.664349	61.641050	1872	C	66.002164	60.650382	62.860176
1852	H	72.853494	55.502210	61.373744	1873	H	65.444158	60.188965	63.685668
1853	C	72.874303	54.038566	62.712542	1874	H	65.545380	61.636126	62.680773
1854	N	72.032695	54.674409	63.519633	1875	C	65.937931	59.752486	61.649309
1855	H	71.487093	54.102894	64.190845	1876	C	65.651933	58.400029	61.848495
1856	H	71.915172	55.690242	63.485267	1877	H	65.285615	58.087864	62.824157
1857	N	73.223167	52.785985	63.013707	1878	C	65.841783	57.455794	60.849577
1858	H	72.843599	52.407418	63.874932	1879	H	65.647289	56.399274	61.032286
1859	H	73.546897	52.110642	62.301015	1880	C	66.331878	57.867812	59.605725
1860	C	61.423072	47.013381	62.253696	1881	O	66.648269	56.972722	58.641542
1861	H	61.111914	46.264177	61.511643	1882	H	66.732933	56.092049	59.046666
1862	H	60.866604	47.926621	62.015417	1883	C	66.294867	60.163891	60.359546
1863	N	62.837749	47.296526	62.099936	1884	H	66.462331	61.219877	60.132865
1864	H	63.168971	48.281559	62.109148	1885	C	66.489785	59.233631	59.344442
1865	C	63.698099	46.479010	61.507805	1886	H	66.809617	59.565215	58.358305
1866	N	64.901292	46.949081	61.158837	1887	C	70.392703	46.645292	61.676870
1867	H	65.143545	47.901001	61.446361	1888	H	69.704905	46.474310	60.840862
1868	H	65.673058	46.298075	60.956032	1889	H	70.027747	46.126231	62.571007

1890	C	70.404342	48.116406	61.962291	1912	H	64.169723	54.220320	58.677209
1891	O	70.515128	48.597024	63.087127	1913	O	64.153304	49.651153	61.890930
1892	O	70.294819	48.866643	60.905663	1914	O	64.147286	50.025865	59.695792
1893	H	70.195417	49.845233	61.085898	1915	H	66.828179	52.498127	62.298049
1894	Zn	69.911765	48.736129	64.995403	1916	H	64.141240	52.570020	59.786688
1895	C	66.775490	53.397311	59.562045	1917	H	63.677688	55.358116	56.550277
1896	C	66.255150	53.865099	58.207012	1918	H	65.513307	55.863787	54.941115
1897	C	64.966512	54.347052	57.945613	1919	H	67.791013	54.950070	55.358848
1898	C	64.508090	50.279190	60.863684	1920	H	68.245587	53.655516	57.459862
1899	C	65.351257	51.515990	61.156442	1921	O	66.938041	54.558501	60.318802
1900	C	66.406535	51.525394	62.061576	1922	H	67.613249	54.390636	61.013721
1901	C	67.136346	50.422590	62.593830	1923	H	64.969899	53.625664	61.049466
1902	C	68.239272	50.829336	63.612774	1924	h	74.464639	54.217894	59.860496
1903	C	64.971064	52.694135	60.483470	1925	h	61.118307	46.679883	63.245645
1904	C	64.692721	55.018217	56.753936	1926	h	67.014817	60.865847	63.201021
1905	C	65.711727	55.272964	55.835307	1927	h	71.370416	46.242527	61.412434
1906	C	66.989859	54.765326	56.075521	1928				
1907	C	67.250837	54.043888	57.240593	1929				
1908	O	67.065481	49.233622	62.275888	1930				
1909	O	68.778467	51.937761	63.485129	1931				
1910	O	68.543511	49.989973	64.513761	1932				
1911	O	67.669084	52.544703	59.647473	1933				

1934 P

1935	C	74.651205	54.303512	60.976928	1956	N	63.468000	45.203088	61.283043
1936	H	75.039144	53.359414	61.371150	1957	H	64.007525	44.626323	60.629875
1937	H	75.421084	55.065938	61.162859	1958	H	62.567478	44.831300	61.576238
1938	N	73.433407	54.665443	61.689918	1959	C	66.026467	60.558944	62.757468
1939	H	72.964355	55.535580	61.454772	1960	H	65.481934	60.013204	63.539872
1940	C	72.892181	54.009234	62.718433	1961	H	65.518776	61.528366	62.639737
1941	N	72.047303	54.640029	63.527864	1962	C	66.014804	59.769398	61.470088
1942	H	71.465753	54.063547	64.164081	1963	C	65.861543	58.381629	61.530284
1943	H	71.950360	55.658394	63.512824	1964	H	65.622496	57.919023	62.485357
1944	N	73.194300	52.736810	62.976840	1965	C	66.019626	57.579805	60.406756
1945	H	72.765308	52.328636	63.800402	1966	H	65.922156	56.495142	60.479664
1946	H	73.539457	52.081510	62.254754	1967	C	66.329103	58.178271	59.185158
1947	C	61.482846	46.993755	62.239085	1968	O	66.535249	57.435766	58.068348
1948	H	61.179427	46.229759	61.508433	1969	H	66.510041	56.494794	58.283218
1949	H	60.912419	47.896528	61.990511	1970	C	66.238881	60.354110	60.216329
1950	N	62.891183	47.298689	62.086654	1971	H	66.302349	61.439656	60.106695
1951	H	63.218421	48.305351	62.097388	1972	C	66.395893	59.569476	59.079589
1952	C	63.769233	46.494881	61.512190	1973	H	66.589760	60.027268	58.109808
1953	N	64.978187	46.970378	61.182858	1974	C	70.350746	46.633336	61.657298
1954	H	65.253621	47.912934	61.486406	1975	H	69.672385	46.473238	60.811861
1955	H	65.743031	46.310173	60.987690	1976	H	69.960909	46.127185	62.548059

1977	C	70.407701	48.103443	61.936387	1999	H	64.832191	54.056854	59.025803
1978	O	70.552888	48.585157	63.056446	2000	O	64.013013	49.650205	61.990569
1979	O	70.330225	48.854419	60.876531	2001	O	63.992234	49.981922	59.787103
1980	H	70.311255	49.834984	61.070564	2002	H	66.604036	52.516777	62.461613
1981	Zn	69.845946	48.765963	64.924388	2003	H	63.475669	52.630118	60.339124
1982	C	67.531519	53.766038	59.370866	2004	H	63.666624	54.966168	57.000710
1983	C	66.789242	54.190911	58.138382	2005	H	65.010831	55.752383	55.065557
1984	C	65.396172	54.351109	58.142221	2006	H	67.459735	55.452835	55.044944
1985	C	64.330209	50.282039	60.952840	2007	H	68.612039	54.397497	57.019145
1986	C	65.091556	51.570202	61.231647	2008	O	67.132679	54.441788	60.433535
1987	C	66.297989	51.562175	62.035726	2009	H	67.691885	54.233713	61.225335
1988	C	67.048293	50.449033	62.403359	2010	H	64.778950	53.681737	61.173261
1989	C	68.163563	50.750925	63.429191	2011	h	74.511790	54.206710	59.900239
1990	C	64.431029	52.693100	60.863566	2012	h	61.183886	46.670071	63.236039
1991	C	64.752098	54.864790	57.017565	2013	h	67.020136	60.806669	63.130725
1992	C	65.502292	55.282443	55.915899	2014	h	71.329871	46.221648	61.412565
1993	C	66.887510	55.110751	55.907714	2015				
1994	C	67.530754	54.534387	57.004985	2016				
1995	O	66.964182	49.258219	61.994283	2017				
1996	O	68.806541	51.815512	63.349585	2018				
1997	O	68.402088	49.869761	64.316954	2019				
1998	O	68.441950	52.976693	59.373714	2020				

2021 **SnA4**

2022 **R**

2023	C	73.467155	54.254865	56.684825	2043	H	65.709425	47.022491	57.077747
2024	H	73.915216	53.379120	57.161511	2044	N	63.477308	45.785305	57.021257
2025	H	74.031084	55.137068	57.020767	2045	H	64.225427	45.234853	56.575045
2026	N	72.075478	54.392930	57.083499	2046	H	62.522076	45.511830	56.800547
2027	H	71.597103	55.249570	56.777090	2047	C	65.610653	58.696883	59.430249
2028	C	71.358374	53.597664	57.878266	2048	H	65.604209	57.718129	59.931280
2029	N	70.104748	53.958113	58.168221	2049	H	64.750990	59.248795	59.840481
2030	H	69.501046	53.278616	58.629377	2050	C	65.396904	58.510339	57.940026
2031	H	69.631115	54.673490	57.629504	2051	C	65.929545	57.426786	57.227144
2032	N	71.848152	52.483414	58.419036	2052	H	66.576344	56.693706	57.713536
2033	H	71.198092	51.902243	58.950522	2053	C	65.654419	57.223417	55.875138
2034	H	72.688486	52.019061	58.048834	2054	H	66.073133	56.348135	55.373394
2035	C	61.506464	46.872635	58.633092	2055	C	64.820898	58.115829	55.195222
2036	H	61.594686	45.810492	58.903399	2056	O	64.497986	57.987019	53.887478
2037	H	60.966100	46.918916	57.674567	2057	H	65.015589	57.286688	53.430646
2038	N	62.823185	47.465167	58.488901	2058	C	64.549961	59.379484	57.239366
2039	H	62.994199	48.453764	58.711749	2059	H	64.076082	60.209640	57.765546
2040	C	63.753384	46.899029	57.709024	2060	C	64.269712	59.196511	55.889782
2041	N	64.970670	47.421378	57.673667	2061	H	63.597804	59.872513	55.364507
2042	H	65.254720	48.175273	58.311374	2062	C	70.396802	46.310616	57.319018

2063	H	69.704103	46.053720	56.508977	2085	O	68.669215	49.873754	60.419272
2064	H	70.095859	45.807711	58.243837	2086	O	67.506006	52.408681	55.192995
2065	C	70.293284	47.788228	57.514802	2087	H	63.851355	52.042237	53.454432
2066	O	70.281803	48.351283	58.606115	2088	O	63.978407	50.200685	58.606646
2067	O	70.175760	48.459969	56.404219	2089	O	63.380952	50.053867	56.477863
2068	H	69.989159	49.436024	56.521708	2090	H	67.351125	51.928480	57.429880
2069	Zn	69.920486	48.448061	60.596598	2091	H	64.254112	51.849394	55.327151
2070	C	66.281752	52.320160	54.895521	2092	H	63.432706	52.757288	51.137752
2071	C	65.921207	52.718623	53.481813	2093	H	65.229365	53.798446	49.799512
2072	C	64.656236	52.525159	52.899839	2094	H	67.514815	54.056634	50.767333
2073	C	64.166631	50.395440	57.402537	2095	H	67.920980	53.386499	53.165086
2074	C	65.432341	51.171912	56.961827	2096	O	67.429201	54.400050	57.029600
2075	C	66.606703	51.189175	57.698478	2097	H	67.599183	53.765762	56.300250
2076	C	67.026926	50.273827	58.734958	2098	H	66.697089	53.971385	57.492254
2077	C	68.394813	50.598207	59.417433	2099	h	73.560526	54.166306	55.602464
2078	C	65.256548	51.867143	55.733556	2100	h	60.871114	47.356894	59.374638
2079	C	64.415192	52.917471	51.583049	2101	h	66.483121	59.249072	59.779468
2080	C	65.434563	53.492491	50.821807	2102	h	71.387504	45.955801	57.034973
2081	C	66.704633	53.651276	51.376259	2103				
2082	C	66.942477	53.274963	52.698508	2104				
2083	O	66.520897	49.218871	59.064629	2105				
2084	O	69.134195	51.464070	58.947738	2106				

2107 **TS1**

2108	C	73.233840	54.303575	56.612590	2129	N	63.530829	45.820190	57.033087
2109	H	73.681635	53.399327	57.029186	2130	H	64.284637	45.269594	56.594872
2110	H	73.772310	55.165533	57.034373	2131	H	62.577604	45.596533	56.732405
2111	N	71.821146	54.374089	56.953845	2132	C	65.618554	58.697347	59.379034
2112	H	71.326905	55.218578	56.637295	2133	H	65.616994	57.712768	59.866050
2113	C	71.203253	53.672880	57.911098	2134	H	64.755691	59.237983	59.796046
2114	N	69.943926	53.957301	58.234908	2135	C	65.407598	58.528673	57.885069
2115	H	69.534543	53.342537	58.933362	2136	C	65.941180	57.452567	57.159122
2116	H	69.192969	54.403733	57.645388	2137	H	66.591765	56.694627	57.606659
2117	N	71.838586	52.704096	58.587012	2138	C	65.657547	57.271723	55.805679
2118	H	71.256862	52.099116	59.166119	2139	H	66.088170	56.409727	55.290110
2119	H	72.686089	52.259113	58.217612	2140	C	64.820326	58.169562	55.138844
2120	C	61.520963	47.062070	58.494119	2141	O	64.498653	58.052711	53.828286
2121	H	61.571673	45.984530	58.706372	2142	H	65.013446	57.349489	53.374839
2122	H	60.976000	47.183321	57.543888	2143	C	64.556641	59.405394	57.197854
2123	N	62.860730	47.602711	58.368880	2144	H	64.082286	60.228016	57.734947
2124	H	63.037239	48.601653	58.518631	2145	C	64.269355	59.240745	55.846945
2125	C	63.799768	46.981652	57.641896	2146	H	63.597569	59.925202	55.332451
2126	N	65.013219	47.508655	57.588746	2147	C	70.429822	46.291956	57.371812
2127	H	65.256602	48.330969	58.148101	2148	H	69.724773	46.060792	56.565001
2128	H	65.767012	47.089009	57.025011	2149	H	70.133848	45.772589	58.289374

2150	C	70.356612	47.767488	57.601633	2172	H	64.071903	52.181779	54.027632
2151	O	70.353360	48.305925	58.704507	2173	O	64.103621	50.340748	58.311545
2152	O	70.264744	48.466622	56.506638	2174	O	63.734161	50.882270	56.187463
2153	H	70.113163	49.445351	56.656478	2175	H	67.593322	52.289062	57.805750
2154	Zn	69.979957	48.398747	60.688701	2176	H	64.749658	53.171363	55.866719
2155	C	66.581195	52.526812	55.024268	2177	H	63.325505	52.572852	51.657318
2156	C	66.073492	52.884879	53.652472	2178	H	64.888306	53.564460	50.022114
2157	C	64.750589	52.611077	53.285553	2179	H	67.262196	53.998977	50.654601
2158	C	64.406815	50.909821	57.257614	2180	H	68.017543	53.514945	53.009202
2159	C	65.693809	51.744675	57.199790	2181	O	67.472661	54.570349	57.341839
2160	C	66.816322	51.532514	57.922284	2182	H	66.446257	53.734214	56.673206
2161	C	67.166515	50.413880	58.802249	2183	H	67.164533	54.483015	58.254392
2162	C	68.501035	50.568182	59.580433	2184	h	73.385163	54.274459	55.533554
2163	C	65.739650	52.835774	56.184916	2185	h	60.917556	47.524217	59.275392
2164	C	64.340506	52.828804	51.967164	2186	h	66.486454	59.248332	59.741294
2165	C	65.231959	53.362227	51.034470	2187	h	71.412771	45.933676	57.066016
2166	C	66.558605	53.617641	51.396732	2188				
2167	C	66.982356	53.359814	52.700784	2189				
2168	O	66.610204	49.347456	58.902281	2190				
2169	O	69.323379	51.396554	59.205838	2191				
2170	O	68.641164	49.742029	60.526752	2192				
2171	O	67.695166	52.024390	55.084254	2193				

2194 **IMI**

2195	C	73.345312	54.247294	56.627070	2216	N	63.529268	45.817242	57.029384
2196	H	73.801822	53.330670	57.011281	2217	H	64.279593	45.257367	56.595142
2197	H	73.905885	55.094730	57.057302	2218	H	62.574947	45.610459	56.719624
2198	N	71.939275	54.295494	56.975891	2219	C	65.617174	58.721028	59.377268
2199	H	71.447701	55.151911	56.706157	2220	H	65.615167	57.736765	59.864897
2200	C	71.359929	53.671379	58.041189	2221	H	64.757285	59.264004	59.797237
2201	N	70.160584	54.022093	58.400343	2222	C	65.402860	58.554717	57.884335
2202	H	69.865592	53.456042	59.192805	2223	C	65.968373	57.499336	57.152954
2203	H	68.742242	54.575877	57.840004	2224	H	66.645665	56.777446	57.618941
2204	N	72.073387	52.691714	58.677933	2225	C	65.689557	57.318974	55.798203
2205	H	71.526833	52.122039	59.317260	2226	H	66.148468	56.485947	55.260685
2206	H	72.776534	52.155739	58.160364	2227	C	64.823998	58.194354	55.136824
2207	C	61.521823	47.100010	58.471675	2228	O	64.510246	58.074217	53.825091
2208	H	61.549277	46.019068	58.669419	2229	H	65.030203	57.372369	53.375846
2209	H	60.979174	47.247738	57.523919	2230	C	64.525338	59.409509	57.203138
2210	N	62.872943	47.613066	58.355224	2231	H	64.032140	60.218174	57.744285
2211	H	63.059741	48.610980	58.493944	2232	C	64.240731	59.243323	55.851766
2212	C	63.808239	46.976293	57.636485	2233	H	63.552868	59.914248	55.340794
2213	N	65.027821	47.490471	57.589130	2234	C	70.457613	46.332729	57.371250
2214	H	65.273690	48.311227	58.146560	2235	H	69.751944	46.119209	56.560084
2215	H	65.781619	47.068937	57.025260	2236	H	70.151049	45.809750	58.283411

2237	C	70.404987	47.807417	57.620760	2259	H	63.965630	52.116080	54.063478
2238	O	70.386094	48.325436	58.731553	2260	O	64.100108	50.335925	58.273498
2239	O	70.343134	48.527837	56.536956	2261	O	63.788994	50.886632	56.140195
2240	H	70.197151	49.504023	56.703624	2262	H	67.588184	52.373078	57.852680
2241	Zn	69.987227	48.421860	60.705414	2263	H	64.656616	53.146388	55.892163
2242	C	66.509870	52.565200	54.991252	2264	H	63.148610	52.475199	51.715210
2243	C	65.948895	52.843234	53.623567	2265	H	64.649510	53.475296	50.026999
2244	C	64.619225	52.547607	53.300706	2266	H	67.038809	53.937615	50.582858
2245	C	64.428897	50.908389	57.232897	2267	H	67.868608	53.486873	52.915461
2246	C	65.690718	51.775718	57.216626	2268	O	67.737389	54.741350	57.741172
2247	C	66.813829	51.607423	57.941599	2269	H	66.186673	53.775841	56.635061
2248	C	67.178587	50.461608	58.803237	2270	H	67.418735	54.465025	58.609248
2249	C	68.504774	50.587060	59.599286	2271	h	73.475679	54.243137	55.544918
2250	C	65.671902	52.893545	56.206411	2272	h	60.931755	47.565475	59.261124
2251	C	64.169495	52.745502	51.992445	2273	h	66.488398	59.270127	59.734374
2252	C	65.025507	53.283339	51.029765	2274	h	71.434633	45.959240	57.064650
2253	C	66.360388	53.553891	51.346645	2275				
2254	C	66.827322	53.313775	52.638657	2276				
2255	O	66.618371	49.395432	58.834384	2277				
2256	O	69.332397	51.407276	59.245146	2278				
2257	O	68.613682	49.731438	60.530184	2279				
2258	O	67.638194	52.135888	55.072758	2280				

2281 **TS2**

2282	C	73.257327	54.215418	56.561619	2303	N	63.529808	45.807263	57.021266
2283	H	73.666408	53.269526	56.925348	2304	H	64.284202	45.250478	56.590201
2284	H	73.815767	55.028396	57.055021	2305	H	62.577801	45.603210	56.702753
2285	N	71.833783	54.289036	56.828012	2306	C	65.633976	58.710544	59.419394
2286	H	71.375245	55.158652	56.539783	2307	H	65.630403	57.722955	59.901166
2287	C	71.174992	53.670965	57.847215	2308	H	64.785713	59.258045	59.856303
2288	N	69.940930	54.013708	58.093860	2309	C	65.397158	58.559494	57.928348
2289	H	69.581263	53.483959	58.885319	2310	C	65.977621	57.529434	57.177578
2290	H	68.664156	54.627688	57.337336	2311	H	66.688871	56.831011	57.617756
2291	N	71.844567	52.725753	58.567611	2312	C	65.698936	57.346445	55.824563
2292	H	71.271664	52.174204	59.199919	2313	H	66.185201	56.524133	55.293993
2293	H	72.624435	52.212665	58.151779	2314	C	64.811205	58.211507	55.179610
2294	C	61.519004	47.076302	58.476568	2315	O	64.489107	58.104778	53.869315
2295	H	61.545453	45.996325	58.680321	2316	H	65.040526	57.443028	53.396546
2296	H	60.978708	47.219082	57.526589	2317	C	64.497931	59.402654	57.262195
2297	N	62.869290	47.590224	58.361723	2318	H	63.995441	60.199330	57.812198
2298	H	63.062354	48.584556	58.521998	2319	C	64.212191	59.241362	55.910413
2299	C	63.806211	46.959697	57.642104	2320	H	63.514470	59.906427	55.405558
2300	N	65.028097	47.470527	57.609822	2321	C	70.453610	46.337063	57.376404
2301	H	65.269513	48.286901	58.174205	2322	H	69.751684	46.127814	56.560876
2302	H	65.780813	47.069966	57.029520	2323	H	70.142828	45.810266	58.284838

2324	C	70.395845	47.810079	57.629690	2346	H	64.102813	52.147510	54.106678
2325	O	70.374307	48.328311	58.740667	2347	O	64.097617	50.275075	58.381853
2326	O	70.330871	48.530373	56.546288	2348	O	63.739982	50.834218	56.259727
2327	H	70.169756	49.504255	56.716838	2349	H	67.555141	52.369761	57.885656
2328	Zn	69.989062	48.409855	60.719780	2350	H	64.567272	53.017680	55.925596
2329	C	66.543752	52.686054	55.152482	2351	H	63.394781	52.456435	51.720958
2330	C	66.057512	52.989480	53.771611	2352	H	64.932146	53.533208	50.110571
2331	C	64.770323	52.614705	53.378805	2353	H	67.251700	54.139616	50.796042
2332	C	64.399160	50.860657	57.339306	2354	H	67.968840	53.766699	53.186702
2333	C	65.643320	51.754109	57.303917	2355	O	67.693931	54.903682	57.142409
2334	C	66.784144	51.603671	58.003432	2356	H	65.961194	53.810273	56.735342
2335	C	67.176295	50.448606	58.839674	2357	H	67.326112	54.871438	58.032435
2336	C	68.488733	50.588234	59.649121	2358	h	73.435858	54.247615	55.486837
2337	C	65.579786	52.870241	56.300376	2359	h	60.928992	47.548819	59.261857
2338	C	64.382413	52.784300	52.048084	2360	h	66.516374	59.251165	59.761693
2339	C	65.262278	53.365504	51.133519	2361	h	71.433060	45.967358	57.072987
2340	C	66.557253	53.722544	51.526736	2362				
2341	C	66.961030	53.522192	52.845588	2363				
2342	O	66.649210	49.365209	58.829241	2364				
2343	O	69.296951	51.437356	59.315812	2365				
2344	O	68.613548	49.716724	60.559770	2366				
2345	O	67.691160	52.338389	55.294872	2367				

2368 **IM2**

2369	C	73.150455	54.277870	56.482530	2390	N	63.577146	45.901652	57.046415
2370	H	73.551452	53.324649	56.834705	2391	H	64.328748	45.342028	56.615489
2371	H	73.698032	55.082835	57.001081	2392	H	62.624020	45.690997	56.735296
2372	N	71.720442	54.336104	56.709301	2393	C	65.677757	58.633915	59.475166
2373	H	71.251952	55.171843	56.357595	2394	H	65.710042	57.640435	59.944144
2374	C	71.050328	53.777485	57.760930	2395	H	64.814390	59.148149	59.922595
2375	N	69.785021	54.067038	57.906400	2396	C	65.438178	58.495154	57.982265
2376	H	69.419856	53.623114	58.748126	2397	C	66.021224	57.482967	57.203968
2377	H	68.787146	54.675167	56.691992	2398	H	66.737907	56.775711	57.630184
2378	N	71.747499	52.957724	58.595659	2399	C	65.737811	57.335705	55.845970
2379	H	71.187355	52.408605	59.241332	2400	H	66.240349	56.537592	55.292791
2380	H	72.596544	52.488702	58.277228	2401	C	64.836277	58.209246	55.229202
2381	C	61.560728	47.167422	58.484689	2402	O	64.505713	58.132057	53.919273
2382	H	61.596552	46.086113	58.679161	2403	H	65.047570	57.472801	53.431625
2383	H	61.020447	47.312773	57.535264	2404	C	64.531618	59.349069	57.339409
2384	N	62.908309	47.690952	58.373495	2405	H	64.030605	60.131980	57.911038
2385	H	63.085868	48.690244	58.514249	2406	C	64.234801	59.218001	55.987331
2386	C	63.850131	47.060178	57.657606	2407	H	63.527606	59.889267	55.503482
2387	N	65.067513	47.578915	57.616041	2408	C	70.453498	46.305372	57.402063
2388	H	65.306314	48.402768	58.172518	2409	H	69.740499	46.079227	56.600740
2389	H	65.821179	47.161825	57.048300	2410	H	70.164748	45.783740	58.320763

2411	C	70.387297	47.780536	57.641105	2433	H	64.162874	52.257314	54.041577
2412	O	70.383055	48.309939	58.747009	2434	O	64.110872	50.452563	58.293738
2413	O	70.298972	48.490349	56.552717	2435	O	63.840231	51.059463	56.170394
2414	H	70.144376	49.466491	56.720584	2436	H	67.636465	52.461569	57.932928
2415	Zn	69.989711	48.430547	60.719180	2437	H	64.733501	53.334381	55.958843
2416	C	66.616011	52.718144	55.123701	2438	H	63.515457	52.583477	51.628014
2417	C	66.141739	53.058995	53.745031	2439	H	65.105247	53.644564	50.062470
2418	C	64.853949	52.710307	53.324728	2440	H	67.409057	54.226596	50.805912
2419	C	64.452445	51.064183	57.279742	2441	H	68.056203	53.856884	53.234006
2420	C	65.708736	51.938517	57.309976	2442	O	68.280285	55.136654	55.945753
2421	C	66.824499	51.736799	58.035976	2443	H	66.223337	53.958313	56.722334
2422	C	67.173482	50.566173	58.872611	2444	H	68.891926	55.864139	55.762085
2423	C	68.510987	50.659012	59.655189	2445	h	73.354900	54.318717	55.412670
2424	C	65.732545	53.061330	56.307255	2446	h	60.963309	47.624291	59.273630
2425	C	64.499898	52.894249	51.984833	2447	h	66.543471	59.199446	59.819810
2426	C	65.409337	53.467092	51.092238	2448	h	71.431169	45.942477	57.084994
2427	C	66.696841	53.810463	51.519129	2449				
2428	C	67.068128	53.600285	52.847626	2450				
2429	O	66.597306	49.508900	58.891840	2451				
2430	O	69.323925	51.505207	59.326955	2452				
2431	O	68.637217	49.761349	60.540949	2453				
2432	O	67.692951	52.187552	55.245872	2454				

2455 **TS3**

2456	C	73.104056	54.345030	56.433623	2477	N	63.595099	45.951161	57.032885
2457	H	73.471554	53.382830	56.792739	2478	H	64.346658	45.388011	56.606990
2458	H	73.655747	55.142498	56.953296	2479	H	62.641951	45.745652	56.717764
2459	N	71.673413	54.447431	56.661587	2480	C	65.688977	58.624894	59.449157
2460	H	71.208645	55.278881	56.276647	2481	H	65.717424	57.632485	59.920573
2461	C	71.005200	53.849224	57.654758	2482	H	64.827602	59.142674	59.896559
2462	N	69.700253	54.097435	57.777899	2483	C	65.445921	58.485910	57.956615
2463	H	69.238191	53.634373	58.554745	2484	C	66.003038	57.459294	57.177891
2464	H	69.096138	54.459458	56.979141	2485	H	66.707875	56.731430	57.589813
2465	N	71.622683	53.037903	58.518945	2486	C	65.706767	57.309523	55.822716
2466	H	71.036073	52.469257	59.129836	2487	H	66.176615	56.476442	55.289630
2467	H	72.553218	52.656430	58.328004	2488	C	64.828273	58.206211	55.206863
2468	C	61.577964	47.225069	58.465954	2489	O	64.495771	58.135582	53.898092
2469	H	61.606941	46.140488	58.641778	2490	H	65.036423	57.476124	53.407689
2470	H	61.038148	47.390777	57.519771	2491	C	64.552375	59.355006	57.315521
2471	N	62.928939	47.740815	58.362679	2492	H	64.064370	60.145179	57.888374
2472	H	63.108207	48.742107	58.493592	2493	C	64.249415	59.228501	55.964633
2473	C	63.869782	47.107430	57.648155	2494	H	63.551453	59.910625	55.482860
2474	N	65.090195	47.620709	57.615089	2495	C	70.441730	46.286305	57.405033
2475	H	65.322673	48.449394	58.167836	2496	H	69.729671	46.051414	56.605292
2476	H	65.838687	47.215367	57.033122	2497	H	70.155499	45.770903	58.327826

2498	C	70.371685	47.762848	57.625218	2520	H	64.388840	52.366341	54.143056
2499	O	70.374721	48.312135	58.723296	2521	O	64.127140	50.473239	58.273054
2500	O	70.276587	48.455633	56.526985	2522	O	63.840522	51.138590	56.168819
2501	H	70.136390	49.435702	56.683491	2523	H	67.618359	52.475761	57.965598
2502	Zn	69.996175	48.434490	60.699054	2524	H	64.812232	53.417073	55.975422
2503	C	66.777109	52.913787	55.255651	2525	H	63.759786	52.582974	51.723514
2504	C	66.330994	53.263462	53.863467	2526	H	65.337675	53.619650	50.129768
2505	C	65.075303	52.828591	53.428078	2527	H	67.609333	54.300452	50.880364
2506	C	64.457730	51.117534	57.272375	2528	H	68.206334	54.122398	53.367316
2507	C	65.710789	51.990927	57.332218	2529	O	67.881146	54.898867	55.765648
2508	C	66.813004	51.750474	58.067296	2530	H	66.216478	54.050559	56.881321
2509	C	67.181810	50.588956	58.891693	2531	H	68.188601	55.734399	55.390627
2510	C	68.539477	50.716458	59.636548	2532	h	73.317981	54.373287	55.365211
2511	C	65.789446	53.161605	56.395989	2533	h	60.983682	47.671567	59.263158
2512	C	64.729563	52.941635	52.076021	2534	h	66.555965	59.188279	59.794114
2513	C	65.632103	53.497361	51.170777	2535	h	71.422222	45.929684	57.089561
2514	C	66.899430	53.904816	51.607986	2536				
2515	C	67.250454	53.794415	52.954322	2537				
2516	O	66.621996	49.523931	58.957305	2538				
2517	O	69.322621	51.591536	59.284778	2539				
2518	O	68.717781	49.837374	60.523983	2540				
2519	O	67.752356	52.200773	55.366601	2541				

2542 **IM3**

2543	C	73.231793	54.355179	56.552902	2564	N	63.601034	45.995130	57.019173
2544	H	73.620233	53.406013	56.923261	2565	H	64.356457	45.436289	56.594896
2545	H	73.801032	55.167614	57.026965	2566	H	62.648058	45.783661	56.707398
2546	N	71.815428	54.469067	56.858854	2567	C	65.625960	58.674252	59.449486
2547	H	71.343414	55.314710	56.509724	2568	H	65.630859	57.687289	59.933540
2548	C	71.161480	53.805237	57.812227	2569	H	64.770282	59.213451	59.882078
2549	N	69.855931	54.087085	57.995409	2570	C	65.397070	58.518245	57.957313
2550	H	69.362208	53.489978	58.657988	2571	C	65.959368	57.476602	57.205173
2551	H	69.303536	54.425515	57.208713	2572	H	66.635165	56.760025	57.678172
2552	N	71.748110	52.912088	58.599575	2573	C	65.701314	57.310505	55.843911
2553	H	71.139906	52.321985	59.172805	2574	H	66.180788	56.486034	55.307320
2554	H	72.667875	52.511901	58.377482	2575	C	64.838815	58.203626	55.197847
2555	C	61.584463	47.261225	58.459484	2576	O	64.531281	58.124221	53.886069
2556	H	61.618106	46.175455	58.626779	2577	H	65.041708	57.428117	53.412108
2557	H	61.041486	47.431350	57.515945	2578	C	64.523747	59.384258	57.285881
2558	N	62.933628	47.781098	58.355929	2579	H	64.029423	60.185594	57.836763
2559	H	63.111458	48.782355	58.486969	2580	C	64.249007	59.237532	55.931711
2560	C	63.874539	47.151258	57.636234	2581	H	63.562712	59.913298	55.425148
2561	N	65.093195	47.664405	57.605620	2582	C	70.421832	46.311923	57.370117
2562	H	65.321951	48.503258	58.146166	2583	H	69.724001	46.079109	56.557421
2563	H	65.836015	47.286207	56.998233	2584	H	70.116246	45.799035	58.288320

2585	C	70.354739	47.789383	57.589215	2607	H	64.589419	52.195900	54.305298
2586	O	70.370489	48.336971	58.689767	2608	O	64.206118	50.515899	58.243483
2587	O	70.253489	48.480358	56.492838	2609	O	63.844122	51.159395	56.147737
2588	H	70.131218	49.465766	56.639929	2610	H	67.726930	52.389388	57.807227
2589	Zn	69.996287	48.434694	60.665911	2611	H	64.910364	53.398316	55.888910
2590	C	67.046120	53.160601	55.255232	2612	H	63.716608	52.257346	51.983813
2591	C	66.421490	53.237161	53.835521	2613	H	65.021415	53.364886	50.181531
2592	C	65.181189	52.671051	53.519499	2614	H	67.318042	54.212850	50.674238
2593	C	64.512755	51.140665	57.220857	2615	H	68.172982	54.174167	53.013714
2594	C	65.793648	51.974943	57.222977	2616	O	67.754391	54.444070	55.473799
2595	C	66.900208	51.696335	57.942679	2617	H	66.129510	54.054847	56.988814
2596	C	67.239354	50.565831	58.810916	2618	H	68.622290	54.227182	55.109065
2597	C	68.574147	50.720983	59.594659	2619	h	73.392661	54.362999	55.474882
2598	C	65.879691	53.194415	56.353961	2620	h	60.989019	47.697578	59.261424
2599	C	64.690884	52.699637	52.207845	2621	h	66.501380	59.225905	59.792101
2600	C	65.434433	53.290265	51.185654	2622	h	71.407758	45.952371	57.075604
2601	C	66.705602	53.794274	51.475452	2623				
2602	C	67.185654	53.768757	52.785843	2624				
2603	O	66.674011	49.507050	58.924528	2625				
2604	O	69.362533	51.605279	59.264581	2626				
2605	O	68.743716	49.861079	60.500198	2627				
2606	O	67.899078	52.179607	55.310120	2628				

2629 **TS4**

2630	C	73.591329	54.333948	56.671826	2651	N	63.666747	46.076758	57.020334
2631	H	74.020276	53.435880	57.123068	2652	H	64.404766	45.496852	56.597480
2632	H	74.192183	55.193482	57.001399	2653	H	62.707416	45.866818	56.732012
2633	N	72.212966	54.502165	57.096144	2654	C	65.566723	58.730768	59.484873
2634	H	71.714863	55.326433	56.742870	2655	H	65.562830	57.743985	59.969229
2635	C	71.514028	53.735405	57.931190	2656	H	64.716954	59.277805	59.918939
2636	N	70.246299	54.099601	58.185591	2657	C	65.335368	58.578679	57.993691
2637	H	69.662449	53.486538	58.762622	2658	C	65.896293	57.538805	57.240107
2638	H	69.932259	55.008974	57.879167	2659	H	66.559312	56.816314	57.721207
2639	N	72.005730	52.652420	58.518282	2660	C	65.642547	57.382294	55.877200
2640	H	71.358247	52.105804	59.095695	2661	H	66.104820	56.558924	55.326769
2641	H	72.802403	52.134896	58.115560	2662	C	64.786560	58.280172	55.231103
2642	C	61.665396	47.369226	58.432322	2663	O	64.490223	58.207852	53.917043
2643	H	61.686896	46.280028	58.576521	2664	H	65.011658	57.524180	53.438099
2644	H	61.129986	47.563238	57.488838	2665	C	64.461200	59.445650	57.324696
2645	N	63.020937	47.875181	58.349002	2666	H	63.963171	60.241150	57.880074
2646	H	63.207103	48.879333	58.461382	2667	C	64.190728	59.306653	55.969546
2647	C	63.960053	47.231077	57.637427	2668	H	63.505132	59.983023	55.463906
2648	N	65.186064	47.722413	57.603881	2669	C	70.441544	46.325307	57.339165
2649	H	65.463188	48.568740	58.125077	2670	H	69.748659	46.105190	56.519256
2650	H	65.915715	47.280279	57.026452	2671	H	70.113299	45.821639	58.254206

2672	C	70.406307	47.803774	57.555030	2694	H	64.879837	51.963111	54.331730
2673	O	70.403216	48.354554	58.651590	2695	O	64.210755	50.598792	58.184469
2674	O	70.363335	48.500229	56.455732	2696	O	63.951069	51.111916	56.043343
2675	H	70.251028	49.481907	56.621709	2697	H	67.598250	52.732646	58.075404
2676	Zn	69.971024	48.501329	60.607328	2698	H	64.786967	53.524459	55.888146
2677	C	67.365394	53.001346	54.981881	2699	H	63.750254	52.102689	52.111017
2678	C	66.570559	53.152069	53.707919	2700	H	64.773975	53.415702	50.258939
2679	C	65.344975	52.508055	53.504041	2701	H	67.020023	54.440840	50.571284
2680	C	64.557225	51.190822	57.156376	2702	H	68.142438	54.302088	52.818445
2681	C	65.751043	52.152374	57.235960	2703	O	68.082119	54.140897	55.268809
2682	C	66.872348	51.918289	58.033939	2704	H	66.270031	54.178546	56.780708
2683	C	67.264651	50.740502	58.735108	2705	H	68.771676	53.849310	55.884997
2684	C	68.604182	50.844984	59.518968	2706	h	73.646131	54.248734	55.586560
2685	C	65.697692	53.312339	56.448117	2707	h	61.063929	47.786368	59.239971
2686	C	64.711827	52.599795	52.261697	2708	h	66.448274	59.276475	59.821235
2687	C	65.292752	53.319832	51.212009	2709	h	71.423692	45.946734	57.056082
2688	C	66.539202	53.917105	51.400147	2710				
2689	C	67.168636	53.842002	52.646567	2711				
2690	O	66.745010	49.631084	58.762858	2712				
2691	O	69.437404	51.709453	59.217019	2713				
2692	O	68.769939	49.963671	60.411883	2714				
2693	O	67.882166	51.918611	55.263422	2715				

2716 P

2717	C	73.613840	54.355837	56.706992	2738	N	63.730203	46.137373	57.034886
2718	H	74.068909	53.498650	57.211306	2739	H	64.458669	45.553225	56.605873
2719	H	74.192082	55.248346	56.982949	2740	H	62.768501	45.926156	56.759389
2720	N	72.235139	54.520584	57.138084	2741	C	65.554714	58.745206	59.475201
2721	H	71.724783	55.331643	56.771011	2742	H	65.545235	57.760821	59.963814
2722	C	71.517388	53.702313	57.903560	2743	H	64.707691	59.297843	59.907475
2723	N	70.222042	54.033256	58.118924	2744	C	65.322832	58.590543	57.984409
2724	H	69.684467	53.400744	58.732477	2745	C	65.881903	57.548989	57.231869
2725	H	70.000512	55.019283	58.096078	2746	H	66.541076	56.823584	57.713413
2726	N	71.997203	52.592526	58.440947	2747	C	65.626606	57.393438	55.869225
2727	H	71.359740	52.045150	59.032033	2748	H	66.082603	56.568204	55.316348
2728	H	72.805669	52.092777	58.037886	2749	C	64.774401	58.292893	55.221704
2729	C	61.736743	47.439878	58.429701	2750	O	64.482721	58.220073	53.905846
2730	H	61.755124	46.349859	58.567581	2751	H	65.010499	57.540212	53.429747
2731	H	61.205255	47.638195	57.484396	2752	C	64.448430	59.457167	57.315032
2732	N	63.093289	47.942702	58.356790	2753	H	63.949792	60.251786	57.870980
2733	H	63.285798	48.948587	58.467520	2754	C	64.178185	59.318954	55.959751
2734	C	64.031976	47.295893	57.646366	2755	H	63.492643	59.995397	55.454356
2735	N	65.258127	47.780508	57.598816	2756	C	70.435805	46.303249	57.336822
2736	H	65.575882	48.645451	58.081497	2757	H	69.742178	46.083684	56.517809
2737	H	65.974112	47.297938	57.038922	2758	H	70.107600	45.799614	58.251751

2759	C	70.405516	47.781315	57.553515	2781	H	65.025654	51.957802	54.366551
2760	O	70.410360	48.334454	58.647133	2782	O	64.211990	50.643194	58.266611
2761	O	70.368637	48.479688	56.452924	2783	O	64.025084	51.115623	56.108451
2762	H	70.253023	49.456213	56.637171	2784	H	67.418926	52.966778	58.479133
2763	Zn	69.938407	48.523057	60.589427	2785	H	64.622950	53.574709	56.047682
2764	C	67.615599	52.877071	54.850818	2786	H	63.811289	52.156107	52.236417
2765	C	66.749109	53.114089	53.656068	2787	H	64.750839	53.457504	50.336667
2766	C	65.494126	52.499997	53.534545	2788	H	67.016959	54.472890	50.531340
2767	C	64.573846	51.245663	57.248989	2789	H	68.274251	54.279217	52.698869
2768	C	65.692117	52.289557	57.369896	2790	O	68.269816	53.950948	55.288622
2769	C	66.830875	52.082600	58.221919	2791	H	66.196915	54.281619	56.775851
2770	C	67.300850	50.849892	58.678780	2792	H	68.797862	53.688651	56.068349
2771	C	68.592622	50.883362	59.522867	2793	h	73.663382	54.215918	55.627161
2772	C	65.502819	53.442097	56.673893	2794	h	61.128631	47.849158	59.236395
2773	C	64.789584	52.633127	52.334423	2795	h	66.439418	59.286335	59.810679
2774	C	65.321226	53.353101	51.259636	2796	h	71.417823	45.925585	57.052080
2775	C	66.582839	53.938275	51.378440	2797				
2776	C	67.286491	53.831540	52.582003					
2777	O	66.880744	49.699368	58.448934					
2778	O	69.479841	51.723314	59.287862					
2779	O	68.712953	49.959365	60.384961					
2780	O	67.838138	51.771740	55.272438					

2798	Residue Topology File (.rtf file)			2820	ATOM O6	GAO	-0.764331
2799	RESI MCP		-3.000	2821	ATOM H2	GAHA	0.132956
2800	GROUP			2822	ATOM H3	GAHA	0.138208
2801	ATOM C1	GAC	0.478382	2823	ATOM H4	GAHA	0.053973
2802	ATOM C2	GACA	-0.037593	2824	ATOM H5	GAHA	0.052472
2803	ATOM C3	GACA	-0.099564	2825	ATOM H6	GAHA	0.053973
2804	ATOM C4	GAC	0.747709	2826	ATOM H7	GAHA	0.076066
2805	ATOM C5	GACE	0.174351	2827	BOND C1	C2	
2806	ATOM C6	GACE	-0.374507	2828	BOND C1	C9	
2807	ATOM C7	GACF	0.346407	2829	BOND C1	O4	
2808	ATOM C8	GAC	0.617579	2830	BOND C2	C3	
2809	ATOM C9	GACF	-0.585627	2831	BOND C2	C13	
2810	ATOM C10	GACA	-0.163287	2832	BOND C3	C10	
2811	ATOM C11	GACA	-0.198686	2833	BOND C3	H1	
2812	ATOM C12	GACA	-0.163287	2834	BOND C4	C5	
2813	ATOM C13	GACA	-0.099564	2835	BOND C4	O5	
2814	ATOM O1	Y4	-0.545746	2836	BOND C4	O6	
2815	ATOM O2	GAO	-0.746895	2837	BOND C5	C6	
2816	ATOM O3	Y5	-0.746895	2838	BOND C5	C9	
2817	ATOM O4	GAO	-0.657830	2839	BOND C6	C7	
2818	ATOM H1	GAHA	0.076066	2840	BOND C6	H2	
2819	ATOM O5	GAO	-0.764331	2841	BOND C7	C8	

2842	BOND	C7	O1	2850	BOND	C12	C13	
2843	BOND	C8	O2	2851	BOND	C12	H6	
2844	BOND	C8	O3	2852	BOND	C13	H7	
2845	BOND	C9	H3	2853				
2846	BOND	C10	C11	2854	RESI ZN			2.000
2847	BOND	C10	H4	2855	GROUP			
2848	BOND	C11	C12	2856	ATOM ZN	M1		2.000
2849	BOND	C11	H5	2857				

2858 Parameter File (.prm file)

2859 BONDS

2860 GAC GACA 345.90 1.4910

2861 GAC GACF 354.50 1.4820

2862 GAC GAO 637.70 1.2180

2863 GACA GACA 461.10 1.3980

2864 GACA GAHA 345.80 1.0860

2865 GAC GACE 354.50 1.4820

2866 GACE GACE 382.80 1.4570

2867 GACE GACF 538.60 1.3510

2868 GACE GAHA 342.50 1.0880

2869 GACF Y4 401.60 1.3500

2870 GAC Y5 637.70 1.2180

2871 GACF GAHA 342.50 1.0880

2872 M1 Y4 83.70 1.9554

2873 M1 Y5 70.60 1.9939

2874 M1 NR2 21.40 2.2113

2875 ANGLES

2876 GAC GACA GACA 64.30 120.33

2877 GAC GACF GACE 63.80 126.41

2878 GAC GACF GAHA 46.50 116.46

2879 GACA GAC GACF 62.90 119.02

2880	GACA	GAC	GAO	68.70	122.60
2881	GACA	GACA	GACA	66.60	120.02
2882	GACA	GACA	GAHA	48.20	119.88
2883	GAC	GACE	GACE	63.10	120.98
2884	GAC	GACE	GACF	63.80	126.41
2885	GACE	GAC	GAO	68.80	123.20
2886	GACE	GACE	GACF	65.00	124.24
2887	GACE	GACE	GAHA	47.20	116.65
2888	GACE	GACF	GAHA	49.80	118.22
2889	GACE	GACF	Y4	70.60	121.69
2890	GACF	GACE	GAHA	49.80	118.22
2891	GACF	GAC	GAO	68.80	123.20
2892	GACF	GAC	Y5	68.80	123.20
2893	GAC	GACF	Y4	68.70	115.76
2894	GAO	GAC	Y5	77.90	130.25
2895	GAO	GAC	GAO	77.90	130.25
2896	CPH2	NR2	M1	51.16	114.61
2897	CPH1	NR2	M1	52.82	138.94
2898	GACF	Y4	M1	32.71	115.13
2899	GAC	Y5	M1	63.04	113.92
2900	NR2	M1	NR2	30.44	98.13
2901	NR2	M1	Y4	33.14	88.64

2902	NR2	M1	Y5	35.17	125.79		
2903	Y4	M1	Y5	60.17	82.69		
2904	DIHEDRALS						
2905	GAC	GACA	GACA	GACA	3.6250	2	180.00
2906	GAC	GACA	GACA	GAHA	3.6250	2	180.00
2907	GAC	GACE	GACF	GAC	6.6500	2	180.00
2908	GAC	GACF	GACE	GACE	6.6500	2	180.00
2909	GACA	GAC	GACF	GACE	2.1750	2	180.00
2910	GACA	GAC	GACF	GAHA	2.1750	2	180.00
2911	GACA	GACA	GACA	GACA	3.6250	2	180.00
2912	GACA	GACA	GACA	GAHA	3.6250	2	180.00
2913	GACA	GACA	GAC	GACF	1.0000	2	180.00
2914	GACA	GACA	GAC	GAO	1.0000	2	180.00
2915	GAC	GACE	GACE	GACF	1.0000	2	180.00
2916	GAC	GACE	GACE	GAHA	1.0000	2	180.00
2917	GAC	GACE	GACF	GAHA	6.6500	2	180.00
2918	GACE	GACE	GACF	Y4	6.6500	2	180.00
2919	GACE	GACF	GAC	GAO	2.1750	2	180.00
2920	GACE	GACE	GAC	GAO	2.1750	2	180.00
2921	GACE	GACE	GACF	GAHA	6.6500	2	180.00
2922	GACE	GACF	GAC	Y5	2.1750	2	180.00
2923	GACF	GACE	GACE	GACF	1.0000	2	180.00

2924	GAC	GACF	GACE	GAHA	6.6500	2	180.00
2925	GACF	GACE	GAC	GAO	2.1750	2	180.00
2926	GACF	GACE	GACE	GAHA	1.0000	2	180.00
2927	GAHA	GACE	GACF	Y4	6.6500	2	180.00
2928	GAO	GAC	GACF	Y4	2.1750	2	180.00
2929	Y4	GACF	GAC	Y5	2.1750	2	180.00
2930	GAHA	GACF	GAC	GAO	2.1750	2	180.00
2931	GAHA	GACA	GACA	GAHA	3.6250	2	180.00
2932	CPH1	CPH1	NR2	M1	0.0000	3	0.00
2933	CPH2	NR2	M1	Y4	0.0000	3	0.00
2934	CPH2	NR2	M1	Y5	0.0000	3	0.00
2935	HR1	CPH2	NR2	M1	0.0000	3	0.00
2936	HR3	CPH1	NR2	M1	0.0000	3	0.00
2937	GAC	GACF	Y4	M1	0.0000	3	0.00
2938	GACE	GACF	Y4	M1	0.0000	3	0.00
2939	GACF	GAC	Y5	M1	0.0000	3	0.00
2940	GAO	GAC	Y5	M1	0.0000	3	0.00
2941	M1	NR2	CPH2	NR1	0.0000	3	0.00
2942	CPH2	NR2	M1	NR2	0.0000	3	0.00
2943	GAC	Y5	M1	NR2	0.0000	3	0.00
2944	CPH1	NR2	M1	NR2	0.0000	3	0.00
2945	GACF	Y4	M1	NR2	0.0000	3	0.00

2946	CPH1	NR2	M1	Y4	0.0000	3	0.00
2947	CPH1	NR2	M1	Y5	0.0000	3	0.00
2948	GACF	Y4	M1	Y5	0.0000	3	0.00
2949	GAC	Y5	M1	Y4	0.0000	3	0.00
2950	IMPROPER						
2951	GAC	GACA	GACA	GACA	1.1000	2	180.00
2952	GAC	GACE	GACE	GACF	1.1000	2	180.00
2953	GAC	GACE	GACF	GAHA	1.1000	2	180.00
2954	GAC	GACE	GACF	Y4	1.1000	2	180.00
2955	GACA	GACA	GACA	GAHA	1.1000	2	180.00
2956	GACA	GACF	GAC	GAO	10.500	2	180.00
2957	GACE	GACF	GACE	GAHA	1.1000	2	180.00
2958	GACE	GAO	GAC	GAO	1.1000	2	180.00
2959	GACF	GAO	GAC	Y5	1.1000	2	180.00

2960 NONBONDED

2961	GAC	0.000000	-0.086000	1.908000	0.000000	-0.043000	1.908000
2962	GACA	0.000000	-0.086000	1.908000	0.000000	-0.043000	1.908000
2963	GACE	0.000000	-0.086000	1.908000	0.000000	-0.043000	1.908000
2964	GACF	0.000000	-0.086000	1.908000	0.000000	-0.043000	1.908000
2965	Y4	0.000000	-0.152000	1.768300	0.000000	-0.076000	1.768300
2966	GAO	0.000000	-0.210000	1.661200	0.000000	-0.105000	1.661200
2967	Y5	0.000000	-0.210000	1.661200	0.000000	-0.105000	1.661200

2968	GAHA	0.000000	-0.015000	1.459000	0.000000	-0.007500	1.459000
2969	M1	0.000000	-0.014917	1.395000	0.000000	-0.007458	1.395000
2970							