

Electronic Supplementary Information

Elucidating the Degradation Mechanism of A-234 by Various Detergents: A Theoretical Investigation

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1. Functional and basis set test.

Table S1. The relative Gibbs free energy (in kcal/mol) of key intermediates in path A at M06-2X/6-311++G(d,p) (*level 1*), M06-2X-D3/6-311++G(d,p) (*level 2*), B3LYP/6-311++G(d,p) (*level 3*), MN15/6-311++G(d,p) (*level 4*), ω B97X-D/6-311++G(d,p) (*level 5*) and PBE0/6-311++G(d,p) (*level 6*) level of theory.

Detergent	Species	<i>level 1</i>	<i>level 2</i>	<i>level 3</i>	<i>level 4</i>	<i>level 5</i>	<i>level 6</i>
H ₂ O ₂	^A IM1	-0.5	-0.8	0.6	-0.5	1.4	-0.2
	^A TS1	28.5	27.9	34.7	27.7	32.9	31.2
	^A IM2	11.2	10.9	20.8	11.2	17.0	15.9
	^A TS2	18.9	18.5	28.7	19.2	25.0	24.2
	^A IM3	13.4	13.0	22.7	13.5	19.1	18.1
	^A TS3	26.2	25.7	29.7	23.8	27.5	27.7
H ₂ O	P1	-0.7	-1.3	3.6	0.2	1.6	2.4
	^A IM1	-0.7	-1.1	2.1	-1.1	0.0	1.3
	^A TS1	33.2	32.9	39.0	32.7	36.4	35.2
	^A IM2	17.2	17.0	26.0	17.0	22.0	21.2
	^A TS2	24.6	24.5	33.3	25.0	29.4	28.9
	^A IM3	18.2	17.9	26.4	18.0	22.4	21.8
NH ₃	^A TS3	23.0	22.6	27.1	20.4	24.2	23.9
	P1	-3.6	-4.0	0.3	-3.1	-1.6	-1.5
	^A IM1	-0.6	2.5	5.2	2.8	3.5	4.3
	^A TS1	35.1	38.1	46.5	39.2	42.7	40.1
	^A IM2	20.3	23.4	32.7	23.9	28.1	27.1
	^A TS2	29.3	32.3	41.2	33.0	37.2	36.3
	^A IM3	19.2	22.2	30.7	22.7	26.0	25.7
	^A TS3	24.1	27.0	32.6	25.0	28.1	28.3
	P1	-3.1	-0.4	4.8	1.2	1.0	2.3

Table S2. The relative Gibbs free energies (in kcal/mol) of key intermediates involved in path A by using the single-point energy calculations at M06-2X/6-311++G(d,p)/SMD (*level A*), M06-2X/6-311++G(2d,2p)/SMD (*level B*), and M06-2X/def2-TZVP/SMD (*level C*) levels of theory, based on the optimized geometries at the M06-2X/6-311++G(d,p) level, as well as the full geometry optimizations and frequency calculations at the M06-2X/6-311++G(d,p)/SMD (*level D*) level of theory.

Detergent	Species	<i>level A</i>	<i>level B</i>	<i>level C</i>	<i>level D</i>
H ₂ O ₂	^AIM1	2.9	3.2	3.9	2.2
	^ATS1	31.3	32.2	33.1	32.2
	^AIM2	16.5	18.0	18.7	16.7
	^ATS2	21.5	23.7	24.5	23.1
	^AIM3	17.1	18.9	19.8	17.4
	^ATS3	27.5	29.2	31.6	27.2
H ₂ O	P1	6.1	7.5	9.9	5.9
	^AIM1	3.5	4.1	3.7	5.5
	^ATS1	38.8	39.6	39.3	41.1
	^AIM2	21.8	23.2	23.2	24.3
	^ATS2	27.6	29.6	29.7	31.2
	^AIM3	21.0	22.3	22.7	24.3
NH ₃	^ATS3	25.8	27.5	29.2	29.5
	P1	3.8	4.9	6.5	4.1
	^AIM1	4.2	4.7	4.6	6.5
	^ATS1	40.1	42.4	43.3	43.6
	^AIM2	27.0	29.9	31.9	29.4
	^ATS2	31.9	35.2	37.3	35.5
	^AIM3	24.4	27.5	29.8	27.9
	^ATS3	26.9	30.6	34.0	30.3
	P1	3.9	4.3	10.1	4.5

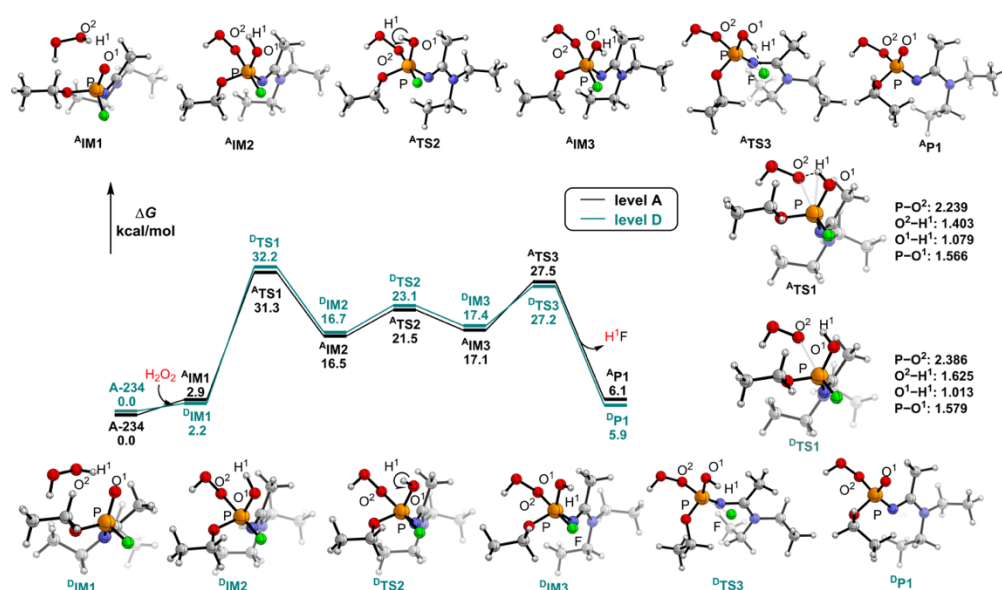


Fig. S1. Predicted relative free energy profiles (ΔG in kcal/mol) of the species involved in the perhydrolysis of A-234 by H_2O_2 through the path A at the M06-2X/6-311++G(d,p)/SMD// M06-2X/6-311++G(d,p) (*level A*) and M06-2X/6-311++G(d,p)/SMD (*level D*) levels of theory. The main transition-state structures and the selected key bond lengths (in Å) are given.

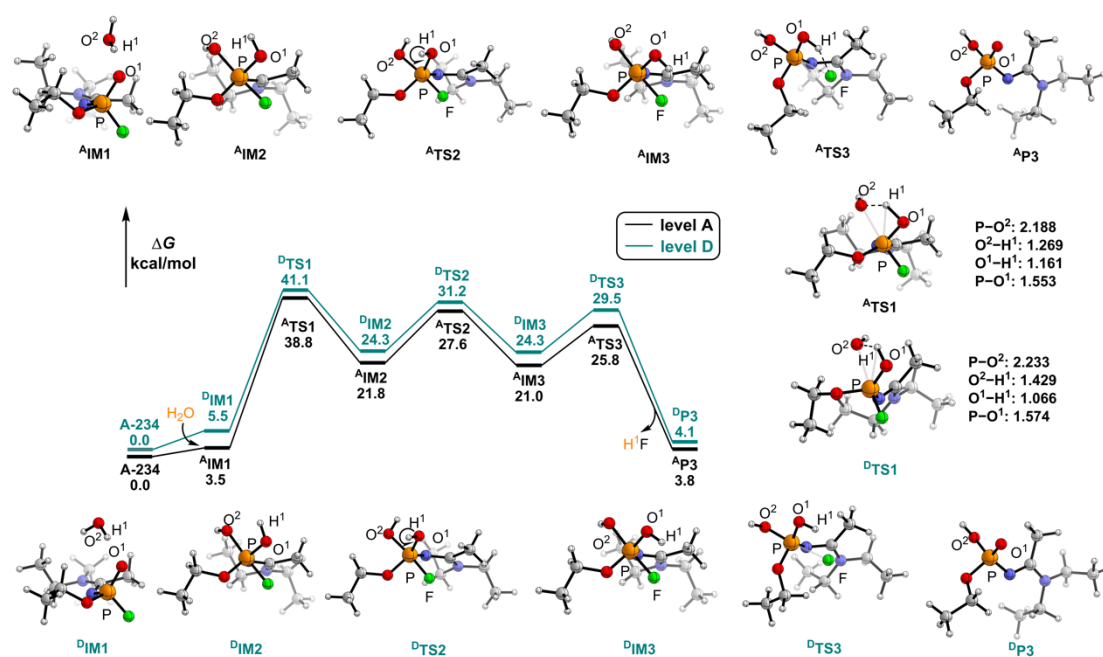


Fig. S2. Predicted relative free energy profiles (ΔG in kcal/mol) of the species involved in the perhydrolysis of A-234 by H_2O through the path A at the M06-2X/6-311++G(d,p)/SMD// M06-2X/6-311++G(d,p) (*level A*) and M06-2X/6-311++G(d,p)/SMD (*level D*) levels of theory. The main transition-state structures and the selected key bond lengths (in Å) are given.

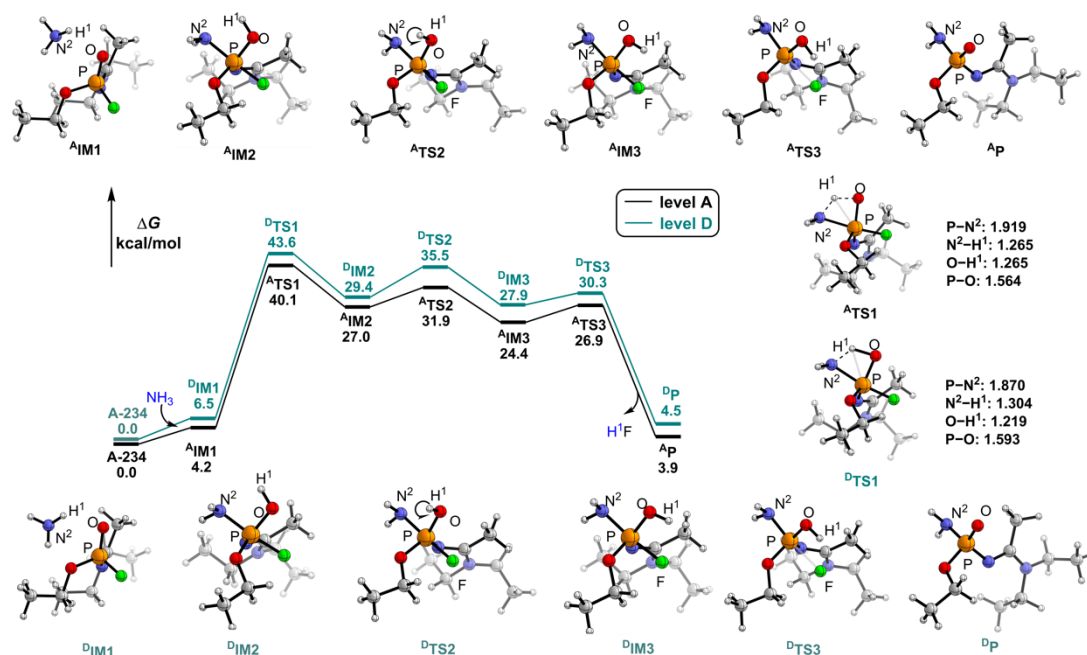


Fig. S3. Predicted relative free energy profiles (ΔG in kcal/mol) of the species involved in the perhydrolysis path A of A-234 by NH_3 at the M06-2X/6-311++G(d,p)/SMD//M06-2X/6-311++G(d,p) (*level A*) and M06-2X/6-311++G(d,p)/SMD (*level D*) levels of theory. The main transition-state structures and the selected key bond lengths (in Å) are given.

2. Energies of all structures.

Table S3. The calculated absolute electronic energy (E , in a.u.) and the thermal free energies (G , in a.u.) (calculated at 298.15 K and 1 atm).

Compound	E	G
A-234	-1016.8574	-1016.6319
H ₂ O ₂	-151.5510	-151.5463
H ₂ O	-76.4348	-76.4308
NH ₃	-56.5524	-56.5358
HF	-100.4510	-100.4578
Me(R ¹)C=NH ¹	-346.5052	-346.3387

Table S4. The calculated absolute electronic energy (E , in a.u.), thermal free energies (G , in a.u.) and the relative Gibbs free energies (ΔG , in kcal/mol) (calculated at 298.15 K and 1 atm).

Detergent	Compound	E	G	ΔG
Path A				
H ₂ O ₂	A¹IM1	-1168.4211	-1168.1694	2.9
	A¹TS1	-1168.3739	-1168.1241	31.3
	A¹IM2	-1168.4027	-1168.1477	16.5
	A¹TS2	-1168.3933	-1168.1398	21.5
	A¹IM3	-1168.4017	-1168.1468	17.1
	A¹TS3	-1168.3825	-1168.1302	27.5
H ₂ O	P1	-1067.9505	-1067.7106	6.1
	A¹IM1	-1093.3004	-1093.0528	3.5
	A¹TS1	-1093.2440	-1092.9967	38.8
	A¹IM2	-1093.2762	-1093.0237	21.8
	A¹TS2	-1093.2646	-1093.0144	27.6
	A¹IM3	-1093.2766	-1093.0250	21.0

NH ₃	^ATS3	-1093.2679	-1093.0174	25.8
	P2	-992.8360	-992.5987	3.8
	^AIM1	-1073.4160	-1073.1568	4.2
	^ATS1	-1073.3598	-1073.0996	40.1
	^AIM2	-1073.3854	-1073.1205	27.0
	^ATS2	-1073.3749	-1073.1126	31.9
	^AIM3	-1073.3879	-1073.1246	24.4
	^ATS3	-1073.3838	-1073.1206	26.9
	^AP	-972.9522	-972.7036	3.9
Path B				
H ₂ O ₂	^BIM1	-1168.4213	-1168.1682	3.6
	^BTS1	-1168.38024	-1168.1265	29.8
	^BIM2	-1168.40378	-1168.1459	17.6
	^BTS2	-1168.37972	-1168.1262	30.0
	^BIM3	-821.8818	-821.8181	13.4
	^BTS3	-973.3604	-973.2714	69.1
	P3	-872.9762	-872.8995	17.8
	^BIM1	-1093.29694	-1093.0510	4.7
	^BTS1	-1093.2471	-1092.9976	38.2
H ₂ O	^BIM2	-1093.27782	-1093.0237	21.8
	^BTS2	-1093.26885	-1093.0148	27.4
	^BIM3	-746.7742	-746.7125	7.1
	^BTS3	-823.152878	-823.0675	52.1
	P4	-722.758116	-722.6850	7.4
	^BIM1	-1073.4158	-1073.1584	3.2
	^BTS1	-1073.3562	-1073.0959	42.4
	^BP	-726.8962	-726.8239	3.2
Path C				
H ₂ O ₂	^CIM1	-1168.4203	-1168.1717	1.5

H ₂ O	^cTS1	-1168.3406	-1168.0889	53.4
	^cP1	-1067.9503	-1168.1692	5.6
	^cIM1	-1093.3027	-1093.0558	1.7
	^cTS1	-1093.2303	-1092.9807	48.8
	^cP2	-1093.2878	-1093.0579	3.0
NH ₃	^cIM1	-1073.3848	-1073.1211	26.6
	^cTS1	-1073.3791	-1073.1161	29.8
	P5	-1073.4039	-1073.1619	3.6
Detergent combinations				
H ₂ O ₂ /NH ₃	¹IM1	-1224.9892	-1224.7007	3.1
	¹TS1	-1224.9605	-1224.6729	20.5
	¹IM2	-1224.9684	-1224.6809	15.5
	¹TS2	-1224.9620	-1224.6751	19.2
	¹IM3	-1224.9692	-1224.6809	15.5
	¹TS3	-1224.9585	-1224.6720	21.1
H ₂ O ₂ /H ₂ O	P1	-1067.9505	-1067.7106	6.1
	²IM1	-1244.8689	-1244.5927	4.9
	²TS1	-1244.8241	-1244.5511	31.0
	²IM2	-1244.8446	-1244.5683	20.3
	²TS2	-1244.8352	-1244.5589	26.2
	²IM3	-1244.8427	-1244.5669	21.2
H ₂ O/NH ₃	²TS3	-1244.8271	-1244.5516	30.7
	P1	-1067.9505	-1067.7106	6.1
	³IM1	-1149.8637	-1149.5800	6.4
	³TS1	-1149.8264	-1149.5437	29.1
	³IM2	-1149.8404	-1149.5561	21.4
	³TS2	-1149.8325	-1149.5485	26.1
	³IM3	-1149.8414	-1149.5567	21.0
	³TS3	-1149.8328	-1149.5485	26.1

	P2	-992.8360	-992.5987	3.8
	⁴IM1	-1169.7461	-1169.4750	6.4
	⁴TS1	-1169.6986	-1169.4288	35.4
	⁴IM2	-1169.7188	-1169.4449	25.2
H ₂ O/H ₂ O	⁴TS2	-1169.7077	-1169.4346	31.7
	⁴IM3	-1169.7186	-1169.4458	24.7
	⁴TS3	-1169.7102	-1169.4375	29.9
	P2	-992.8360	-992.5987	3.8

3. Imaginary frequencies of the transition states.

Table S5. Calculated imaginary frequencies (in cm^{-1}) of transition states at the M06-2X/6-311++G(d,p) level of theory.

Detergent	Species	Imaginary frequencies
Path A		
H ₂ O ₂	^A TS1	595.5729i
	^A TS2	496.3955i
	^A TS3	375.4384i
H ₂ O	^A TS1	1139.6313i
	^A TS2	463.7079i
	^A TS3	317.3718i
NH ₃	^A TS1	1453.9177i
	^A TS2	531.1805i
	^A TS3	280.9746i
Path B		
H ₂ O ₂	^B TS1	777.3362i
	^B TS2	85.5827i
	^B TS3	494.8560i
H ₂ O	^B TS1	955.0077i
	^B TS2	93.5431i
	^B TS3	580.7424i
NH ₃	^B TS1	1196.9009i
Path C		
H ₂ O ₂	^C TS1	491.3771i
H ₂ O	^C TS1	463.6405i
NH ₃	^C TS1	324.3424i
Detergent combinations		
H ₂ O ₂ /NH ₃	^I TS1	387.9567i

	¹TS2	66.5424i
	¹TS3	501.0190i
	²TS1	1282.6712i
H ₂ O ₂ /H ₂ O	²TS2	371.2463i
	²TS3	347.9754i
	³TS1	574.4398i
H ₂ O/NH ₃	³TS2	94.0707i
	³TS3	187.7111i
	⁴TS1	1297.5479i
H ₂ O/H ₂ O	⁴TS2	386.3065i
	⁴TS3	278.7429i

4. Reaction rate constants of selected rate-determining steps.

Table S6. Reaction rate constants of the rate-determining steps estimated at M06-2X/6-311++G(d,p) level of theory at 298.15 K and 1 atm, based on Arrhenius equation $k = AT^n \exp(-E_a/RT)$ (k in s^{-1} , A in s^{-1} , and E_a in kcal/mol, respectively).

Detergent	steps (ΔG , in kcal/mol)	k (s^{-1})	A (s^{-1})	n	E_a (kcal/mol)
Path A					
H ₂ O ₂	^A IM1 $\rightarrow$ ^A TS1 (28.5)	5.05E-09	1.66E+11	2.09E-01	27.3
H ₂ O	^A IM1 $\rightarrow$ ^A TS1 (33.2)	1.86E-12	2.10E+13	-7.93E-01	31.5
NH ₃	^A IM1 $\rightarrow$ ^A TS1 (38.4)	1.37E-13	1.50E+15	-1.58E+00	32.9
Path B					
H ₂ O ₂	^B IM1 $\rightarrow$ ^B TS1 (30.6)	2.41E-10	1.15E+11	-5.57E-02	28.0
H ₂ O	^B IM1 $\rightarrow$ ^B TS1 (40.3)	1.28E-15	2.91E+12	-9.81E-01	34.0
NH ₃	^B IM1 $\rightarrow$ ^B TS1 (49.9)	2.83E-21	3.12E+13	-1.30E+00	42.0
Path C					
H ₂ O ₂	^C IM1 $\rightarrow$ ^C TS1 (53.8)	2.73E-27	1.78E+10	-5.87E-03	50.2
H ₂ O	^C IM1 $\rightarrow$ ^C TS1 (51.7)	1.03E-25	3.25E+12	-3.85E-01	49.8
NH ₃	^C IM1 $\rightarrow$ ^C TS1 (4.5)	3.62E+09	3.42E+11	3.50E-01	3.9
Detergent combinations					
H ₂ O ₂ /NH ₃	¹ IM1 $\rightarrow$ ¹ TS1 (24.2)	1.34E-05	2.26E+13	-6.99E-01	22.5
H ₂ O ₂ /H ₂ O	² IM1 $\rightarrow$ ² TS1 (26.0)	1.30E-06	1.41E+15	-1.49E+00	23.6
H ₂ O/NH ₃	³ IM1 $\rightarrow$ ³ TS1 (26.9)	1.63E-07	1.05E+15	-1.31E+00	25.3
H ₂ O/H ₂ O	⁴ IM1 $\rightarrow$ ⁴ TS1 (28.2)	3.29E-08	1.79E+17	-2.37E+00	25.7

5. IRC analysis for key transition states (^ATS1, ^BTS1, and ^CTS1) of A-234 degraded by H₂O₂ and NH₃.

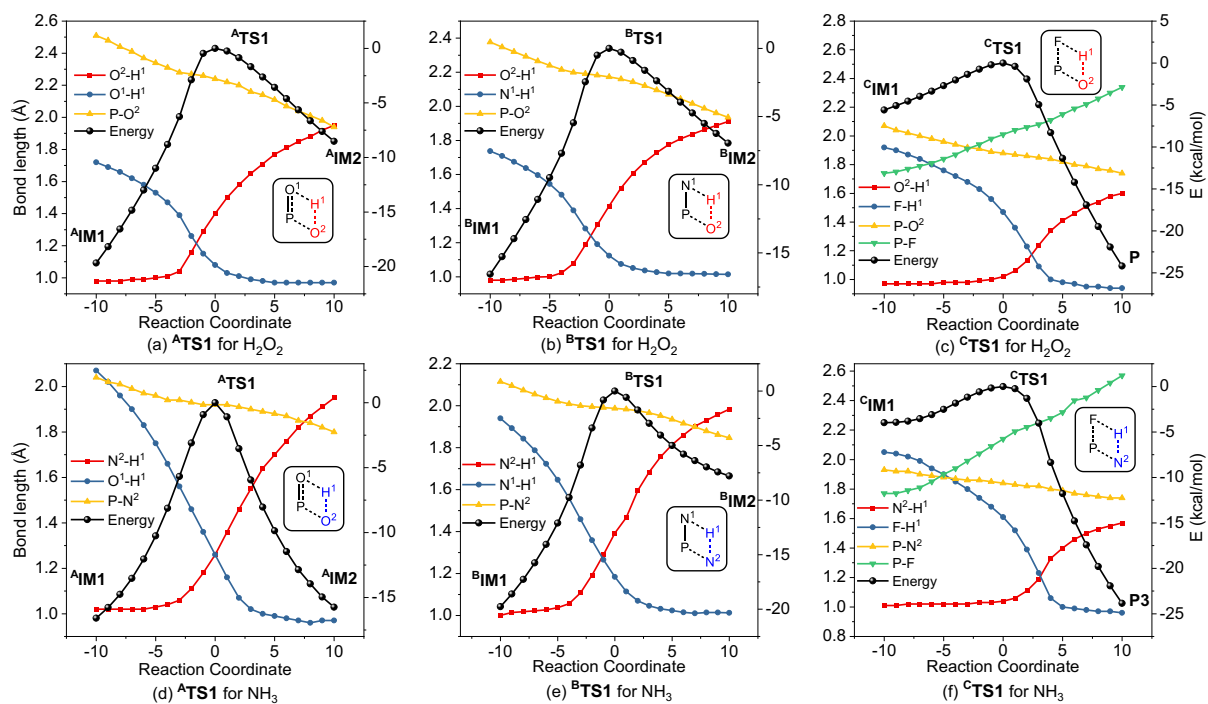


Fig. S4. IRC analysis for the key transition states. (a) ^ATS1 for H₂O₂, (b) ^BTS1 for H₂O₂, (c) ^CTS1 for H₂O₂, (d) ^ATS1 for NH₃, (e) ^BTS1 for NH₃, and (f) ^CTS1 for NH₃.

6. Atomic cartesian coordinates (in Å) of all optimized species.

Perhydrolysis by H₂O₂

Perhydrolysis path A

^AIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.13167000	-0.81030800	-0.71412100
N	0.33975500	-0.17337300	-0.77716600
O	-1.49690200	-1.94840200	0.16079300
C	1.38900800	-0.47549000	-0.05808100
F	-1.46664900	-1.15585600	-2.22252600
C	1.50509600	-1.67816100	0.84706300
H	0.69153900	-2.37109400	0.65224200
H	2.45876000	-2.18528100	0.69971600
H	1.43470400	-1.35084600	1.88757400
N	2.44677500	0.34392500	-0.14133600
O	-2.06573800	0.47270200	-0.47558200
C	-3.49375900	0.25952300	-0.36320800
H	-3.67236800	-0.48157300	0.41890900
H	-3.85643700	-0.13219500	-1.31692200
C	-4.13092800	1.58878500	-0.03138400
H	-5.21513200	1.47391400	0.01865600
H	-3.78444300	1.95168600	0.93815200
H	-3.89181300	2.32936500	-0.79545300
C	2.37238100	1.53895200	-0.98962200
H	1.85296000	1.27216000	-1.90864200
H	3.39839400	1.81578900	-1.24127100
C	1.65432900	2.68275600	-0.28238000
H	1.64042900	3.57033300	-0.91750600
H	0.62550900	2.39240300	-0.06666900
H	2.15414700	2.93863100	0.65474100
C	3.67734500	0.16823200	0.62861900
C	4.76510100	-0.54255900	-0.17100400
H	5.68261000	-0.61492100	0.41579600
H	4.44924000	-1.55082500	-0.44529800
H	4.98938700	0.00201200	-1.09028600
H	4.01272800	1.16632000	0.92152400
H	3.45875600	-0.36616000	1.55107300

O	-0.77810300	-0.35095000	2.39089000
H	-1.20478300	-1.12169900	1.97497100
O	-1.81892200	0.61906600	2.39697800
H	-1.70912800	1.03389100	1.52810700

^ATS1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.12254100	-0.50207900	-0.66694600
N	0.38038100	0.04004800	-0.66961400
O	-1.60907100	-1.97336500	-0.44154200
C	1.44863300	-0.43474800	-0.09165200
F	-1.44544500	-0.42547400	-2.23077100
C	1.57581100	-1.83598100	0.45299500
H	0.78388600	-2.46095400	0.04835900
H	2.53852700	-2.27668200	0.19514800
H	1.45613600	-1.80873200	1.53775100
N	2.51528700	0.37201500	-0.00458800
O	-2.09745200	0.64919900	-0.17743300
C	-3.52704300	0.45640900	-0.29702400
H	-3.79693200	-0.45596200	0.23806400
H	-3.77140300	0.34632100	-1.35619200
C	-4.19294900	1.66889600	0.30882800
H	-5.27676800	1.57775500	0.21803400
H	-3.94290700	1.75006200	1.36789600
H	-3.87270000	2.57757100	-0.20223900
C	2.42467100	1.74647700	-0.50953900
H	1.86225200	1.72885000	-1.44200600
H	3.44320300	2.07457100	-0.72796900
C	1.75584400	2.67160100	0.50094600
H	1.72373400	3.69202800	0.11475900
H	0.73497000	2.33607300	0.68715700
H	2.30383500	2.67938000	1.44610100
C	3.77265200	-0.00700700	0.63793800
C	4.81356900	-0.49655800	-0.36424900
H	5.75247500	-0.72518000	0.14331600
H	4.46761300	-1.39721800	-0.87491000
H	5.01077600	0.26500100	-1.12127100
H	4.13892700	0.87929300	1.16215500
H	3.58024800	-0.75840600	1.40164900
O	-0.88233600	-0.98321900	1.50663100
H	-1.41649600	-1.92968700	0.61971000
O	-1.99508300	-0.52559300	2.27607400

H	-1.89752800	0.43121500	2.20574200
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^AIM2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.16162100	-0.49364900	-0.36114100
N	0.34142900	0.14180300	-0.42132100
O	-1.60848600	-2.00735600	-0.71467800
C	1.46770600	-0.39934300	-0.08826600
F	-1.44137900	-0.09998500	-1.93302700
C	1.67297100	-1.87914400	0.14402700
H	0.82956800	-2.43313500	-0.25893300
H	2.58682700	-2.23449800	-0.33229700
H	1.72847200	-2.07606700	1.21669500
N	2.54863700	0.40372000	0.03447800
O	-2.36281600	0.44828200	0.16769700
C	-3.30295000	1.12958100	-0.68025600
H	-3.77723800	0.40710300	-1.34650200
H	-2.76706200	1.85770200	-1.29007000
C	-4.31106000	1.79695100	0.22883400
H	-5.04474100	2.34333000	-0.36698600
H	-4.83955700	1.05379000	0.82884100
H	-3.81423400	2.49882500	0.90018400
C	2.38801500	1.84543100	-0.15920400
H	1.70634800	2.00010700	-0.99502300
H	3.36615700	2.24649700	-0.43529000
C	1.85377700	2.52634400	1.09667100
H	1.74782500	3.60056000	0.93227900
H	0.87741400	2.11212400	1.35149000
H	2.53118300	2.37436700	1.94062300
C	3.87522300	-0.06395000	0.42174800
C	4.78444300	-0.30980500	-0.77945100
H	5.78100600	-0.61196900	-0.45116800
H	4.37679000	-1.09479800	-1.41937200
H	4.88221300	0.59609500	-1.38106300
H	4.30837800	0.70215400	1.07070400
H	3.78613100	-0.96283700	1.03006800
O	-0.85039500	-0.91287700	1.31154300
H	-1.77892300	-2.50069400	0.09971100
O	-1.96568000	-1.58036800	1.89816000
H	-2.59003800	-0.85054900	2.02197000

^ATS2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.15300400	-0.50394000	-0.35859300
N	0.34277500	0.13348700	-0.44523600
O	-1.42524200	-2.05088200	-0.77163500
C	1.46278300	-0.39840800	-0.06617200
F	-1.47621400	-0.01933900	-1.92164900
C	1.66490800	-1.86818000	0.22185600
H	0.80435100	-2.43718100	-0.11809700
H	2.56357700	-2.24463400	-0.26826500
H	1.75704900	-2.01702800	1.29972100
N	2.53948200	0.40967000	0.04708500
O	-2.42830800	0.34684800	0.16796900
C	-3.29573500	1.16747600	-0.63132900
H	-3.77549600	0.55586800	-1.39695500
H	-2.70192100	1.93210000	-1.13283900
C	-4.31055500	1.77631800	0.31141800
H	-4.99690700	2.41787200	-0.24474800
H	-4.89172400	0.99672600	0.80726000
H	-3.81172600	2.37711800	1.07323800
C	2.38503600	1.84377100	-0.20070000
H	1.71059700	1.96985500	-1.04706000
H	3.36668700	2.23219900	-0.48223500
C	1.84310900	2.57060400	1.02567700
H	1.74085600	3.63850200	0.82235400
H	0.86414000	2.16750000	1.28811900
H	2.51340200	2.44715000	1.87986100
C	3.86502000	-0.04740200	0.45081200
C	4.77669900	-0.32576000	-0.74149600
H	5.77204600	-0.62004100	-0.40258800
H	4.36967900	-1.12763700	-1.36043700
H	4.87724600	0.56339200	-1.36717400
H	4.29647500	0.73603100	1.07991100
H	3.77341900	-0.93022800	1.08134400
O	-0.85122000	-0.92231400	1.29131200
H	-2.35350300	-2.29592400	-0.81383700
O	-1.95702300	-1.60786800	1.86582100
H	-2.52631400	-0.86737600	2.11509300

^AIM3

Coordinates (Angstroms)			
	X	Y	Z
P	-1.16923800	-0.54164000	-0.32987700
N	0.31657900	0.13807200	-0.38435100
O	-1.50629400	-2.06338200	-0.77352300
C	1.44361900	-0.39667700	-0.03511600
F	-1.46189800	-0.07352500	-1.93292500
C	1.65378700	-1.86478800	0.26050300
H	0.79362900	-2.44156800	-0.06715200
H	2.55205500	-2.24072600	-0.23036600
H	1.75117000	-2.00698700	1.33892400
N	2.52627900	0.41008300	0.04927700
O	-2.39149500	0.37820700	0.17857500
C	-3.20784500	1.23980000	-0.62912800
H	-3.72380400	0.64668900	-1.38534700
H	-2.56851900	1.96194600	-1.13837900
C	-4.18524200	1.91846200	0.30507200
H	-4.83267600	2.59213400	-0.25971900
H	-4.81068800	1.17921000	0.80844900
H	-3.65257100	2.49805800	1.06038600
C	2.37355700	1.84108800	-0.21571600
H	1.68321500	1.95854900	-1.05032900
H	3.35137000	2.22002900	-0.52276800
C	1.85994800	2.59067900	1.00914400
H	1.76605300	3.65675800	0.79259200
H	0.88101600	2.20235100	1.29253900
H	2.54294100	2.47211500	1.85392800
C	3.85348200	-0.04226900	0.45268000
C	4.75939500	-0.34101900	-0.73917200
H	5.75642600	-0.62954600	-0.40022600
H	4.34981900	-1.15333700	-1.34268800
H	4.85702300	0.53744100	-1.38023400
H	4.28986400	0.75057400	1.06654600
H	3.76507200	-0.91440200	1.09845600
O	-0.91092600	-1.04469000	1.27661200
H	-1.74837500	-2.09913400	-1.70440900
O	-2.05503100	-1.64990400	1.86309400
H	-2.60159200	-0.87441300	2.05213000

^ATS3

Coordinates (Angstroms)			
	X	Y	Z
P	1.46989900	-0.48996300	-0.15148900
N	0.00677800	-0.01421800	-0.58362400
O	1.93359900	-1.96734000	0.10090600
C	-1.12720800	-0.65597100	-0.44410500
F	0.43725600	-1.26547600	1.72119400
C	-1.25816400	-2.15626300	-0.39775600
H	-0.27980100	-2.62025300	-0.45088200
H	-1.73732100	-2.46562300	0.53104000
H	-1.85198400	-2.50116500	-1.24716000
N	-2.24871000	0.07068100	-0.40297200
O	2.17599800	0.53348200	0.82782100
C	1.45476000	1.36140700	1.76800900
H	2.05763200	1.35778100	2.67533200
H	0.50195400	0.88213500	1.98936200
C	1.30865400	2.75326500	1.18848300
H	0.75574400	3.39092800	1.88237600
H	2.28601700	3.20532600	1.01056500
H	0.76896000	2.71266600	0.23936500
C	-2.16597200	1.53574300	-0.39178700
H	-1.33630500	1.82166600	0.25459600
H	-3.08934200	1.90289200	0.06020800
C	-1.98320600	2.11016400	-1.79125200
H	-1.95667600	3.20081900	-1.74892000
H	-1.04739000	1.75258300	-2.22080600
H	-2.80896600	1.81395300	-2.44239600
C	-3.58291600	-0.50789700	-0.24415200
C	-4.00393600	-0.56786200	1.22168400
H	-5.00411700	-0.99552400	1.31145500
H	-3.30630700	-1.17928800	1.79669200
H	-4.01891000	0.43014400	1.66389200
H	-4.27371100	0.11366000	-0.81931800
H	-3.60639100	-1.49933700	-0.69101500
O	2.27089600	-0.13361400	-1.53756000
H	1.45595200	-2.12284700	0.98144600
O	3.67559700	-0.26681400	-1.34234500
H	3.89990000	0.58175300	-0.93341000

P1

	X	Y	Z
P	1.47857100	-0.31489200	-0.15185600
N	0.01272100	0.23712400	-0.53646400
O	1.61838700	-1.01922900	1.15700600
C	-1.08688500	-0.47336400	-0.45102900
F	-0.57889300	-1.14160200	2.38124800
C	-1.12950600	-1.98300700	-0.42155600
H	-0.13021800	-2.39426900	-0.30389400
H	-1.74446500	-2.33823800	0.40410100
H	-1.53960100	-2.35146300	-1.36517000
N	-2.25378200	0.18003500	-0.43787600
O	2.51023700	0.89099500	-0.29328700
C	2.91481800	1.62191000	0.88342700
H	3.72384600	2.26519700	0.54057900
H	3.30380600	0.91062500	1.61448300
C	1.76838800	2.43115100	1.45764200
H	2.13122600	3.04492900	2.28466400
H	1.34246300	3.08305000	0.69302700
H	0.98198000	1.77576200	1.83919900
C	-2.26411400	1.64627900	-0.43063000
H	-1.43066600	1.98836400	0.18202000
H	-3.19341400	1.95740600	0.05069100
C	-2.16363000	2.21572800	-1.84065700
H	-2.19938800	3.30646500	-1.81177400
H	-1.22154600	1.90901200	-2.29565000
H	-2.98960900	1.86262400	-2.46261800
C	-3.54753700	-0.48645100	-0.29240100
C	-3.95874000	-0.60650300	1.17289900
H	-4.91845700	-1.11984500	1.25735100
H	-3.20560200	-1.15708100	1.73978200
H	-4.05851100	0.38089100	1.62800800
H	-4.27693500	0.10318800	-0.85334100
H	-3.50759800	-1.46527100	-0.76705800
O	1.91028500	-1.20614800	-1.45653300
H	0.30697800	-1.14367600	2.01749500
O	3.26273400	-1.64289100	-1.33527900
H	3.73471500	-0.91624600	-1.76633400

Perhydrolysis path B

^BIM1

Coordinates (Angstroms)

	X	Y	Z
P	-1.19864600	-1.02512400	0.11314100
N	0.14746000	-0.23242500	-0.34969500
O	-1.57517700	-0.96609100	1.54356000
C	1.35269200	-0.54140500	0.06179700
F	-1.00105000	-2.53803800	-0.34170700
C	1.62838300	-1.79807800	0.85300300
H	1.37958100	-2.65785400	0.22831500
H	2.65279500	-1.89924500	1.19438900
H	0.95840000	-1.81710800	1.71590000
N	2.36676000	0.27638000	-0.25294100
O	-2.29932800	-0.52763500	-0.90041100
C	-3.62401000	-0.13472400	-0.46666200
H	-3.58169200	0.14291900	0.58691400
H	-4.27532200	-1.00251000	-0.58648200
C	-4.06314000	1.02530200	-1.32833800
H	-5.08391600	1.31120700	-1.06637900
H	-3.40852500	1.88092800	-1.15981800
H	-4.03724200	0.75162500	-2.38406000
C	2.10565400	1.50251700	-1.01695500
H	1.23877000	1.32404800	-1.64931600
H	2.96967200	1.66776000	-1.66569200
C	1.87927400	2.69436200	-0.09147000
H	1.62917600	3.58283800	-0.67400500
H	1.06671700	2.49379300	0.60983800
H	2.77780500	2.91429300	0.49023300
C	3.75766300	0.06273300	0.15491100
C	4.49591300	-0.89145100	-0.77726600
H	5.54144600	-0.98495200	-0.47771200
H	4.04168500	-1.88395200	-0.76103500
H	4.46353300	-0.52172000	-1.80408200
H	4.23562600	1.04351600	0.14249900
H	3.79808100	-0.27685400	1.18936500
O	-0.88816500	1.75096700	1.88673600
H	-1.18924300	0.84641800	2.09678300
O	-1.50531000	1.97405800	0.62408100
H	-0.83848100	1.63043900	0.00519500

^BTS1

Coordinates (Angstroms)			
	X	Y	Z

P	-1.32645900	-0.88245300	0.19145900
N	0.15127000	-0.14968500	-0.32367000
O	-1.56201100	-1.14322500	1.62901300
C	1.37634300	-0.54521000	-0.02035900
F	-0.96200200	-2.32861500	-0.43833700
C	1.61919000	-1.93242700	0.50038600
H	1.34278700	-2.64502400	-0.27716900
H	2.64750200	-2.10391300	0.79791600
H	0.95354900	-2.11147100	1.34791200
N	2.38323500	0.30519900	-0.20437600
O	-2.46648300	-0.59156200	-0.86142100
C	-3.68412600	0.12275900	-0.54099700
H	-3.68190400	0.38437900	0.51638200
H	-4.48922400	-0.58585900	-0.74009900
C	-3.78728500	1.35061700	-1.41530900
H	-4.74458300	1.84640800	-1.23893300
H	-2.98189800	2.04239600	-1.17008600
H	-3.72932800	1.07345900	-2.46937300
C	2.13691600	1.64193200	-0.77025700
H	1.32947900	1.56215300	-1.49774900
H	3.04073600	1.91804800	-1.31764100
C	1.81521100	2.66956200	0.31060500
H	1.64387000	3.64395000	-0.14984500
H	0.92337300	2.39219100	0.87734800
H	2.65007800	2.76625100	1.00890200
C	3.77445400	0.01805700	0.16686900
C	4.52140200	-0.73011400	-0.93027600
H	5.56468400	-0.87708100	-0.64569300
H	4.07137700	-1.70771800	-1.11250000
H	4.49643600	-0.16574600	-1.86457600
H	4.24355800	0.98471300	0.35652500
H	3.80117600	-0.52124000	1.11237800
O	-0.95630500	1.48479000	1.85737900
H	-1.25064300	0.67233000	2.30540300
O	-1.44000300	1.26039200	0.53305900
H	-0.25186400	0.88329000	-0.13784300

^BIM2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.38040600	-0.71283400	0.24591500
N	0.20520900	-0.00681600	-0.27982500

O	-1.40664500	-1.25006900	1.63950100
C	1.41469000	-0.46877300	-0.02135700
F	-0.88440900	-2.07780300	-0.56152000
C	1.57670600	-1.87504000	0.47001100
H	1.38281000	-2.55219500	-0.36259900
H	2.56590800	-2.06278300	0.87210300
H	0.81328300	-2.07749600	1.22373300
N	2.47698700	0.32123500	-0.20183100
O	-2.58957300	-0.63758700	-0.80784300
C	-3.83807200	0.04741200	-0.60525000
H	-3.99056800	0.23923800	0.45645200
H	-4.59448200	-0.65957900	-0.95042700
C	-3.88638700	1.32735900	-1.41268900
H	-4.87787500	1.77905600	-1.33051700
H	-3.14588200	2.03400100	-1.03919600
H	-3.69005400	1.11543500	-2.46551200
C	2.32100100	1.67926500	-0.74259000
H	1.57655200	1.65752900	-1.54131800
H	3.26785200	1.93762700	-1.21903100
C	1.96551000	2.69439700	0.34222900
H	1.85055000	3.68563700	-0.09924800
H	1.03872500	2.43153800	0.85929000
H	2.76279800	2.74364800	1.08703100
C	3.84967500	-0.07132800	0.14828400
C	4.52140900	-0.87462100	-0.95772100
H	5.55382600	-1.10220900	-0.68681700
H	3.99404300	-1.81424500	-1.13074600
H	4.52765600	-0.31044800	-1.89261800
H	4.39351400	0.85673500	0.33116000
H	3.85008000	-0.61118200	1.09343400
O	-1.00336500	1.35549400	1.80464000
H	-1.16953100	0.58582800	2.38134400
O	-1.73525900	0.97868200	0.64296000
H	0.11273900	0.99147400	-0.40953000

^BTS2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.60301600	-0.45826700	0.07823600
N	0.54252500	0.27027500	-0.08900900
O	-1.41385500	-0.70929100	1.52201400
C	1.63605100	-0.35813800	0.18260000

F	-0.95513500	-1.41156000	-1.00571100
C	1.51321800	-1.74832600	0.75137500
H	1.42284000	-2.45277700	-0.07910500
H	2.36216900	-2.04317500	1.36205500
H	0.60365500	-1.80063800	1.34677200
N	2.87765700	0.14985000	-0.06317900
O	-3.07226400	-0.88745300	-0.42477300
C	-4.23185400	-0.35537000	0.23057700
H	-3.93968200	0.16709900	1.14551400
H	-4.83907500	-1.21591600	0.51603900
C	-4.98028900	0.55957000	-0.71614700
H	-5.89512800	0.92332100	-0.24274300
H	-4.35651500	1.41263800	-0.98481000
H	-5.24953000	0.01956100	-1.62523500
C	3.02221600	1.42161400	-0.76620500
H	2.28027100	1.47248700	-1.56710300
H	3.99767700	1.41071300	-1.25738100
C	2.91254100	2.62951300	0.16276400
H	3.03950500	3.55694700	-0.39888600
H	1.94001300	2.65780100	0.65802300
H	3.68457400	2.58696800	0.93420200
C	4.11997600	-0.49802100	0.35819400
C	4.61611400	-1.53972100	-0.63913500
H	5.57390500	-1.95408800	-0.31744600
H	3.89996800	-2.35778300	-0.73213600
H	4.74925300	-1.09138400	-1.62617300
H	4.86312300	0.29444100	0.47327900
H	3.99738200	-0.93389300	1.34913800
O	-1.21437300	2.03179200	0.62335800
H	-1.19120100	1.52867400	1.45876300
O	-1.86656000	1.13760500	-0.27015100
H	0.64555000	1.20822600	-0.45732700

^BIM3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.41902200	-0.25262100	-0.12779600
N	1.13418600	1.73642500	0.25808100
O	-0.82015800	-0.94749500	1.00941500
C	1.76559700	0.70600200	0.73082400
F	-0.47904700	-0.22421700	-1.39088000
C	1.58368700	0.39260400	2.19336600

H	1.29304700	-0.64526000	2.34657500
H	2.51187000	0.59699400	2.73331700
H	0.79492800	1.02721600	2.58869400
N	2.59362600	-0.09292800	0.01101800
O	-2.69905900	-0.85796900	-0.81627100
C	-3.93844200	-0.94448900	-0.06639700
H	-3.71911500	-0.89137500	1.00335600
H	-4.33589000	-1.93403100	-0.28715500
C	-4.87754400	0.15622500	-0.50638200
H	-5.82794500	0.06100200	0.02284200
H	-4.44736900	1.13377900	-0.28724600
H	-5.06590600	0.08356500	-1.57823900
C	2.78362700	0.13089700	-1.41955200
H	1.82549100	0.38441000	-1.87956400
H	3.08490300	-0.82147500	-1.85958900
C	3.84058600	1.19623900	-1.70169000
H	3.95703500	1.34691700	-2.77675600
H	3.56676600	2.14980500	-1.24621600
H	4.80510700	0.89186300	-1.28992400
C	3.17363300	-1.31947100	0.55836000
C	2.27012200	-2.52993700	0.33799300
H	2.73002200	-3.43145000	0.74857000
H	1.29931000	-2.37311800	0.81304600
H	2.09654100	-2.69170800	-0.72864000
H	4.14230500	-1.46479200	0.07230700
H	3.37996400	-1.17910700	1.61809000
O	-1.27523600	1.94922800	1.18932100
H	-0.30377200	2.04704400	0.87471900
O	-1.85588300	1.27772600	0.07123700
H	1.30987300	1.91218200	-0.72576400

^BTS3

	Coordinates (Angstroms)		
	X	Y	Z
P	-0.33479300	-0.22697300	0.09198700
O	-0.16954300	0.12505900	1.50613600
F	-1.89027000	1.11912500	-0.44803100
O	0.76900900	-0.99645800	-0.71802200
C	2.17312500	-0.62913700	-0.76041200
H	2.25286500	0.42263800	-1.03574000
H	2.57022100	-1.23709500	-1.57070300

C	2.85577200	-0.93180700	0.55626900
H	3.92191100	-0.71695500	0.46172100
H	2.44964400	-0.32137700	1.36379900
H	2.73304000	-1.98353200	0.81727600
O	-2.68656500	-1.11794400	0.36105500
H	-3.03457800	-0.29747700	-0.03152300
O	-1.47503100	-1.27731900	-0.35065400
O	0.24727200	1.45498600	-0.66468800
H	-0.79001300	1.74608400	-0.68246900
O	0.95419000	2.21914100	0.29324700
H	0.64320300	1.82612100	1.13838200

P2

	Coordinates (Angstroms)		
	X	Y	Z
P	-0.27263500	0.02816500	0.11127000
O	-0.19873500	0.19010300	1.56229700
O	0.90116200	0.61859100	-0.74866900
C	2.20416200	0.85048100	-0.15072200
H	2.06080900	1.40897100	0.77544400
H	2.71960900	1.47666800	-0.87577700
C	2.92831700	-0.45619500	0.08946000
H	3.93162100	-0.25347000	0.46907100
H	2.40127300	-1.06106700	0.83048700
H	3.01176400	-1.02407200	-0.83804200
O	-1.40319800	-2.19203500	0.11724800
H	-2.01432200	-2.28148900	-0.62708800
O	-0.33640400	-1.47410300	-0.50278800
O	-1.63485900	0.59778700	-0.57056200
O	-1.88826400	1.91138300	-0.08198000
H	-2.33371900	1.73245000	0.76005700

Perhydrolysis path C

^cIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-0.88909900	-0.54692600	-0.53881000
N	0.57596300	0.14578900	-0.40182600
O	-1.34510100	-1.39840100	0.58548800
C	1.64788300	-0.47572300	0.00656600
F	-0.86199600	-1.37130500	-1.88875500
C	1.71013700	-1.95366200	0.32099700
H	0.91085500	-2.48368700	-0.19103800
H	2.66435500	-2.39139400	0.03329300
H	1.55842800	-2.10045100	1.39353500
N	2.77183600	0.24414400	0.16753200
O	-1.87650400	0.60047000	-0.97939500
C	-2.30719500	1.57597300	-0.00367600
H	-1.45835400	2.23413200	0.20481100
H	-2.60610300	1.05791700	0.91030800
C	-3.47225700	2.32821400	-0.59901700
H	-3.80919500	3.09652100	0.09955400
H	-3.18180400	2.80598100	-1.53585400
H	-4.29429400	1.63687700	-0.78162800
C	2.75854100	1.67903700	-0.13139100
H	2.12284100	1.83562400	-1.00128800
H	3.78034100	1.96145400	-0.39527300
C	2.25542000	2.49802400	1.05198000
H	2.27440100	3.56257100	0.81140500
H	1.23035500	2.21166200	1.28920800
H	2.87863300	2.33711800	1.93489100
C	4.02031500	-0.29498200	0.70442000
C	4.99433000	-0.71535700	-0.39215700
H	5.93170000	-1.06521400	0.04424500
H	4.57398100	-1.51862700	-1.00017000
H	5.21753400	0.12440700	-1.05308300
H	4.46427300	0.49013800	1.32171700
H	3.80377500	-1.12489700	1.37541700
O	-3.74105100	-1.09639200	1.78234000
H	-2.83450500	-1.30016800	1.46789100
O	-4.33707100	-0.60835600	0.58481500
H	-4.81257700	-1.38156400	0.26073700

cTS1

Coordinates (Angstroms)			
	X	Y	Z
P	1.19245500	0.61701600	0.26959900
N	-0.18466900	-0.19618300	0.00024800
O	1.69083000	1.23869300	1.50974900
C	-1.35489200	0.18143900	0.45914300
F	0.24442900	2.30014300	-0.27902800
C	-1.57411600	1.19590500	1.55520800
H	-0.64246000	1.69221700	1.80791900
H	-2.29846100	1.94892300	1.24347700
H	-1.95842300	0.68749800	2.44349000
N	-2.43528200	-0.43306300	-0.04491000
O	2.27041900	-0.58574600	-0.10740400
C	2.49523500	-1.59237400	0.88317600
H	1.54912000	-2.11284000	1.06767900
H	2.81899600	-1.11126400	1.80967600
C	3.54262600	-2.54661400	0.35196200
H	3.72696800	-3.34264600	1.07586300
H	3.20937200	-2.99593900	-0.58471100
H	4.48344200	-2.02188000	0.17415700
C	-2.27843100	-1.42081900	-1.11734600
H	-1.47836200	-1.08274600	-1.77348000
H	-3.21166000	-1.42948900	-1.68474700
C	-1.96568000	-2.80660200	-0.56478000
H	-1.88625900	-3.52953300	-1.37878900
H	-1.01719200	-2.78017000	-0.02771400
H	-2.75061800	-3.14393300	0.11647300
C	-3.80242800	-0.17724700	0.40474600
C	-4.51160400	0.85583600	-0.46662700
H	-5.53875100	0.99842500	-0.12578800
H	-3.99425100	1.81579500	-0.42535800
H	-4.53960100	0.53250800	-1.50892600
H	-4.33448400	-1.13170300	0.37252900
H	-3.79229200	0.14006200	1.44547000
O	1.80273400	1.28876300	-1.37886200
H	1.37173200	2.20281700	-1.21934500
O	3.21005200	1.36880400	-1.51502300
H	3.43961800	0.49083700	-1.14855600

cP1

Coordinates (Angstroms)			
	X	Y	Z
P	-1.33634500	-0.31066400	0.44618700
N	0.06567800	0.42739400	0.10826300
O	-1.74365500	-0.60859200	1.82919900
C	1.23490000	0.03576500	0.55337100
F	1.29089800	-2.28486600	-1.26882900
C	1.45185000	-1.08573000	1.54295400
H	0.52030400	-1.60702300	1.74795200
H	2.18369000	-1.79712200	1.16153200
H	1.81217500	-0.67326500	2.48843600
N	2.31898900	0.68612800	0.11064000
O	-2.46639600	0.43545200	-0.40816600
C	-3.32816400	1.39046000	0.24050100
H	-2.74833400	2.29600800	0.44061300
H	-3.66442800	0.96990700	1.19031800
C	-4.48237900	1.67507300	-0.69286300
H	-5.15062300	2.41233400	-0.24409200
H	-4.11842400	2.06603800	-1.64387800
H	-5.05098800	0.76330200	-0.88234800
C	2.16826000	1.75518700	-0.88082600
H	1.37288200	1.46962100	-1.56799500
H	3.10430600	1.80819800	-1.44037600
C	1.85394200	3.09291500	-0.22158700
H	1.77009400	3.87696400	-0.97660400
H	0.90856200	3.02473600	0.31733200
H	2.64126500	3.37641600	0.48091900
C	3.68745400	0.31133800	0.46476900
C	4.28637900	-0.67190700	-0.53756100
H	5.30620800	-0.93353700	-0.24894200
H	3.68477100	-1.58063600	-0.59223900
H	4.31555000	-0.23503000	-1.53767200
H	4.27285600	1.23372100	0.49792500
H	3.70294700	-0.10241900	1.47142400
O	-1.16803300	-1.64373700	-0.54246800
H	0.37574700	-2.16085900	-1.11716900
O	-2.35658600	-2.41690200	-0.61387900
H	-2.86024600	-1.92661400	-1.28085800

Hydrolysis by H₂O

Hydrolysis path A

^AIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.46714800	-0.89355500	-0.12548400
N	-0.14119600	-0.04802600	-0.49687700
O	-1.57369200	-1.38640800	1.26789400
C	1.08632500	-0.45301900	-0.29654600
F	-1.61423000	-2.08438000	-1.15905700
C	1.46619200	-1.89110100	-0.03680400
H	0.66126400	-2.55376200	-0.34708200
H	2.37240200	-2.17196300	-0.57266700
H	1.62694800	-2.01415200	1.03709100
N	2.06758300	0.45730100	-0.33037100
O	-2.68969700	-0.01533100	-0.62786100
C	-2.94877600	1.23524700	0.03439800
H	-2.08808800	1.89208400	-0.12265400
H	-3.06154500	1.04783900	1.10600700
C	-4.21031000	1.81464400	-0.56272400
H	-4.44100500	2.77130300	-0.09025200
H	-4.08333900	1.97345300	-1.63422000
H	-5.04878800	1.13498000	-0.40745300
C	1.72916300	1.87271900	-0.49885900
H	0.91607600	1.93979200	-1.21986600
H	2.60661400	2.36577600	-0.92439000
C	1.32740400	2.50651400	0.82879100
H	1.04682900	3.55137900	0.68048900
H	0.48708400	1.96001700	1.25813300
H	2.15078400	2.46949300	1.54563000
C	3.46003200	0.15572300	-0.00597600
C	4.31219300	-0.06484900	-1.25193300
H	5.35399700	-0.23913400	-0.97616700
H	3.95581600	-0.92620600	-1.82012200
H	4.27287900	0.80859900	-1.90604700
H	3.84129200	1.00411200	0.56749800
H	3.50104300	-0.70385200	0.66078800
O	0.66656400	-0.45038700	2.62430900
H	-0.18375600	-0.81302800	2.31214600
H	0.60533900	-0.43717700	3.58084700

^ATS1

	Coordinates (Angstroms)		
	X	Y	Z

P	-1.35430400	-0.85630800	0.00520600
N	0.02741000	0.02149100	0.07173000
O	-1.64883300	-2.08270800	0.91111300
C	1.22671500	-0.47487000	0.10012500
F	-1.09068100	-1.67212200	-1.35793100
C	1.55298200	-1.94523400	0.24313700
H	0.66402400	-2.55344500	0.10345000
H	2.30819700	-2.25100700	-0.48115800
H	1.94094600	-2.13899900	1.24643100
N	2.26799800	0.38359100	0.02867600
O	-2.53267600	0.00032600	-0.59665900
C	-2.91858500	1.31532000	-0.15566900
H	-2.01558800	1.87778500	0.09337500
H	-3.51889300	1.21070600	0.74555800
C	-3.68368600	1.95240600	-1.29369000
H	-4.01808200	2.94932600	-0.99904200
H	-3.05579000	2.03933400	-2.18137100
H	-4.55910500	1.35244300	-1.54561100
C	2.00783600	1.81471600	-0.13669900
H	1.16622900	1.93115100	-0.81887200
H	2.89140800	2.25051700	-0.60850900
C	1.71328700	2.50132800	1.19262000
H	1.56659900	3.57276300	1.04305000
H	0.80481300	2.08503300	1.62921500
H	2.53909700	2.36424700	1.89484000
C	3.66869500	-0.02043300	0.11223700
C	4.30967000	-0.20137600	-1.26131900
H	5.36511900	-0.46093200	-1.15897900
H	3.81015200	-0.99435200	-1.82093800
H	4.23948200	0.71781700	-1.84617800
H	4.19433800	0.75673100	0.67394500
H	3.75351100	-0.93338400	0.69936300
O	-1.86026100	-0.08412000	1.91141200
H	-1.82696200	-1.34571400	1.79048800
H	-1.11398000	0.30901100	2.37001300

^AIM2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.35662200	-0.64040300	-0.25548300
N	-0.12679500	0.10624400	-0.31463300
O	1.74409800	-2.06183800	-0.93889200
C	-1.28609300	-0.45237100	-0.17396200
F	0.95001600	-1.52152800	1.09075600
C	-1.54628400	-1.94026200	-0.25503700
H	-0.61179300	-2.49081100	-0.28593600
H	-2.12423700	-2.28303100	0.60418700
H	-2.11510300	-2.16176300	-1.16150100
N	-2.36752900	0.34712600	-0.00063100
O	2.46131000	0.08344000	0.65692900
C	3.29995400	1.17038900	0.25716000
H	2.67894300	2.01022400	-0.06661200
H	3.92373800	0.86526900	-0.58327800
C	4.13193200	1.54409200	1.46530000
H	4.79661200	2.37478900	1.21889900
H	3.48848800	1.84052500	2.29456400
H	4.73551800	0.69376900	1.78500000
C	-2.18282400	1.79338300	0.10389200
H	-1.24951800	1.97890700	0.63374600
H	-3.00251800	2.18474300	0.71138300
C	-2.16265300	2.46456000	-1.26567600
H	-2.03533200	3.54402500	-1.16223600
H	-1.33570000	2.07007200	-1.85722500
H	-3.09501200	2.28115800	-1.80517000
C	-3.73909000	-0.14041700	0.09925900
C	-4.19087000	-0.32786400	1.54585900
H	-5.23234500	-0.65382400	1.58208200
H	-3.57508200	-1.07520400	2.04936800
H	-4.10654400	0.60717200	2.10314800
H	-4.38038600	0.58968600	-0.40285000
H	-3.84149900	-1.07159700	-0.45528800
O	1.84505300	0.12779600	-1.70446100
H	2.04198400	-1.89648800	-1.83987100
H	1.25245800	0.85433900	-1.90950400

^ATS2

	Coordinates (Angstroms)		
	X	Y	Z

P	1.33015100	-0.53841600	-0.32084600
N	-0.17103400	0.13696300	-0.39208400
O	1.53660800	-1.94613200	-1.13975200
C	-1.31674700	-0.44567700	-0.20997300
F	0.90770800	-1.44795400	1.03940000
C	-1.56348000	-1.93241600	-0.32610900
H	-0.62158500	-2.46615800	-0.39065000
H	-2.12144800	-2.30265400	0.53488300
H	-2.14653100	-2.13630100	-1.22792200
N	-2.39274600	0.33657600	0.03242500
O	2.53031000	-0.00037000	0.60876100
C	3.44581900	1.06227100	0.30274000
H	2.88353000	1.95835100	0.03853300
H	4.05550600	0.78358400	-0.55722900
C	4.28677300	1.27253300	1.54370900
H	5.00728800	2.07522200	1.37230100
H	3.65519900	1.54117400	2.39141500
H	4.83133400	0.36150500	1.79600700
C	-2.21438200	1.78208300	0.17600500
H	-1.27279600	1.95756900	0.69395700
H	-3.02696400	2.14746600	0.80860300
C	-2.21839300	2.49268200	-1.17324700
H	-2.11830700	3.57118600	-1.03589400
H	-1.38054900	2.13891100	-1.77439500
H	-3.14924300	2.30222400	-1.71326600
C	-3.75933400	-0.16238000	0.14646600
C	-4.17591700	-0.39797800	1.59642300
H	-5.21432000	-0.73176200	1.64626800
H	-3.54379300	-1.15658200	2.06135300
H	-4.08397500	0.51972500	2.18060800
H	-4.41530600	0.57960700	-0.31779400
H	-3.86750800	-1.07647900	-0.43467200
O	1.90302900	0.39449000	-1.60169800
H	2.42690000	-2.30011500	-1.05593000
H	1.26177500	0.41595300	-2.31505600

^AIM3

Coordinates (Angstroms)			
	X	Y	Z
P	1.36118000	-0.59676800	-0.31370200
N	-0.14308300	0.10370300	-0.35537200
O	1.82806200	-2.00480300	-0.97416200

C	-1.30160500	-0.45247000	-0.21574400
F	0.91392400	-1.51245000	1.07153500
C	-1.57027400	-1.93437200	-0.34565000
H	-0.63752500	-2.47717000	-0.44598900
H	-2.10624400	-2.31441100	0.52502100
H	-2.17558800	-2.12223900	-1.23528500
N	-2.37672600	0.34414600	0.00109700
O	2.43132900	0.10850800	0.65402000
C	3.33768000	1.14293200	0.25373700
H	2.76905400	2.00960500	-0.09253600
H	3.95519200	0.79047800	-0.57279700
C	4.16921400	1.48543200	1.47114600
H	4.88047100	2.27721200	1.22679000
H	3.52982300	1.82517600	2.28694900
H	4.72293300	0.60873000	1.80960100
C	-2.18214200	1.78490900	0.15672700
H	-1.24021700	1.94466300	0.67972200
H	-2.99103900	2.15742900	0.78994100
C	-2.17696700	2.50634900	-1.18704600
H	-2.04325700	3.58055000	-1.04469200
H	-1.35944900	2.13161200	-1.80385300
H	-3.11718700	2.34722300	-1.72056500
C	-3.74872200	-0.14095200	0.10575400
C	-4.17784800	-0.37802800	1.55204000
H	-5.21999100	-0.70117000	1.59354200
H	-3.55718500	-1.14500200	2.01877400
H	-4.08046800	0.53618100	2.14078500
H	-4.39465200	0.60888600	-0.35986500
H	-3.86479600	-1.05152500	-0.47953700
O	1.84189900	0.17157900	-1.71224700
H	1.83085500	-2.69011800	-0.29783700
H	1.18857500	0.82743800	-1.96320400

^ATS3

	Coordinates (Angstroms)		
	X	Y	Z
P	1.53362000	-0.60815300	-0.52198700
N	0.00986400	-0.15093900	-0.70667700
O	2.03720300	-2.06445800	-0.13964300
C	-1.08692000	-0.64440400	-0.20443800
F	0.95632500	-1.02063300	1.62105100
C	-1.24736900	-2.06115200	0.28468300

H	-0.31555600	-2.60182700	0.17056500
H	-1.51847900	-2.07014100	1.34039100
H	-2.02128800	-2.56680900	-0.29687500
N	-2.17161000	0.14677000	-0.18691400
O	2.42841700	0.53230700	0.10743500
C	2.08938200	1.32603600	1.26369300
H	2.35573300	0.75915500	2.15244800
H	1.00863200	1.47727600	1.27649400
C	2.84947100	2.62728500	1.14034600
H	2.64078200	3.25809700	2.00703900
H	3.92374900	2.44078700	1.10021300
H	2.55684600	3.16393100	0.23652700
C	-2.06829800	1.52998900	-0.66216300
H	-1.10389300	1.92756800	-0.34795300
H	-2.85373500	2.10115500	-0.16276800
C	-2.21115700	1.61618300	-2.17722500
H	-2.15798400	2.65653700	-2.50364200
H	-1.40507600	1.05887700	-2.65503300
H	-3.16992400	1.20419800	-2.50123700
C	-3.46434600	-0.25745500	0.36170000
C	-3.61020000	0.13855300	1.82867800
H	-4.59085200	-0.15650600	2.20677200
H	-2.84090100	-0.34420500	2.43394200
H	-3.50753900	1.21847000	1.95208800
H	-4.23668200	0.22316200	-0.24437600
H	-3.59576000	-1.33069300	0.24190200
O	2.04935800	-0.56102900	-2.04455200
H	1.78469000	-2.08590000	0.82939100
H	2.94503200	-0.90072900	-2.13796700

P3

	Coordinates (Angstroms)		
	X	Y	Z
P	1.46035500	-0.69319500	-0.45862700
N	0.13735900	0.24041800	-0.45881000
O	1.47458200	-1.81562300	0.53410000
C	-1.08709800	-0.21400800	-0.53414300
F	-0.68105700	-2.03031800	1.80303900
C	-1.46045800	-1.59537200	-1.02038400
H	-0.57463800	-2.21325100	-1.13845600
H	-2.12563200	-2.08940100	-0.31377300
H	-1.95449100	-1.51631500	-1.99195000

N	-2.08915900	0.61389200	-0.20582300
O	2.69407300	0.29736200	-0.26372000
C	2.85754000	0.94767700	1.00884700
H	2.86321100	0.18657700	1.79375100
H	2.00351800	1.61273200	1.16632500
C	4.15854400	1.71587000	0.96762000
H	4.31570600	2.23389900	1.91553400
H	4.99442100	1.03612800	0.79796400
H	4.13869000	2.45285800	0.16385700
C	-1.78348300	1.95545000	0.29816900
H	-0.89926200	1.88752400	0.93102200
H	-2.62555400	2.26414600	0.92087800
C	-1.55632000	2.94543700	-0.83822800
H	-1.35351700	3.94119800	-0.43899700
H	-0.70277500	2.62831300	-1.43788900
H	-2.43766900	3.00733500	-1.48097600
C	-3.49294200	0.20607500	-0.17850300
C	-3.89761900	-0.33478300	1.19077500
H	-4.94355000	-0.64759600	1.18309400
H	-3.27058800	-1.18420600	1.46879200
H	-3.77611300	0.43138700	1.95915000
H	-4.08821400	1.08462900	-0.43975800
H	-3.67295000	-0.53305300	-0.95716200
O	1.70057900	-1.20625100	-1.96162300
H	0.18749600	-2.01668100	1.39498100
H	2.42584000	-1.83759500	-2.02686100

Hydrolysis path B

^BIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.25190400	-0.89048000	0.08226000
N	0.11295400	-0.07688600	-0.26458400
O	-1.64397300	-1.05284600	1.49703100
C	1.30242400	-0.46285000	0.11983400
F	-1.10121200	-2.31734000	-0.61620900
C	1.53045900	-1.78622200	0.81190800
H	1.21942000	-2.58231100	0.13245200
H	2.55619100	-1.96835600	1.11387500
H	0.87855800	-1.83452400	1.68741800
N	2.34677000	0.34128600	-0.13182300

O	-2.32451200	-0.17698500	-0.83325100
C	-3.71085100	-0.06266500	-0.43777700
H	-3.78702000	-0.22915400	0.63836500
H	-4.26198900	-0.84656500	-0.96099500
C	-4.18936200	1.31863200	-0.82167000
H	-5.24928000	1.42149200	-0.57948700
H	-3.62598000	2.07126300	-0.26880300
H	-4.05932000	1.48356800	-1.89225100
C	2.13343800	1.61016400	-0.83796300
H	1.28018800	1.48477100	-1.50085600
H	3.02090300	1.78920100	-1.45045200
C	1.90141200	2.76157200	0.13431800
H	1.73973000	3.69152000	-0.41370000
H	1.02566700	2.56988900	0.75649100
H	2.76305700	2.90182200	0.79157800
C	3.72467100	0.05982000	0.27598400
C	4.45772600	-0.82781800	-0.72396200
H	5.49569900	-0.97181300	-0.41811700
H	3.98033500	-1.80658100	-0.80021100
H	4.45142200	-0.37104100	-1.71564600
H	4.22566600	1.02609200	0.35751400
H	3.73865800	-0.37041800	1.27679000
O	-1.54836900	2.01509800	1.42235400
H	-1.05063300	1.78333900	0.63040600
H	-1.63455400	1.17434800	1.88935700

^BTS1

Coordinates (Angstroms)			
	X	Y	Z
P	-1.43082200	-0.77333500	0.31295800
N	0.09077900	0.00435800	-0.02115700
O	-1.71995800	-1.30082300	1.66233900
C	1.30616400	-0.48667300	0.06297400
F	-1.01199400	-2.09979000	-0.54690700
C	1.54613100	-1.95503800	0.27651500
H	1.30138900	-2.48389800	-0.64536500
H	2.56943600	-2.17793400	0.55953600
H	0.86072900	-2.32040400	1.04197300
N	2.34034000	0.35626500	-0.05285400
O	-2.52985600	-0.38446100	-0.76665300
C	-3.72506700	0.35825300	-0.47007200
H	-3.81380600	0.50086100	0.60620800

H	-4.54495300	-0.27512500	-0.81345100
C	-3.70145100	1.67973700	-1.20538900
H	-4.64565400	2.20761800	-1.05111300
H	-2.88454400	2.29198000	-0.82537800
H	-3.56940100	1.51366300	-2.27616800
C	2.10654700	1.77107400	-0.37153300
H	1.23596300	1.83626300	-1.02382400
H	2.97244900	2.11191600	-0.94318700
C	1.92002700	2.62342500	0.87967700
H	1.79402100	3.67098600	0.60152700
H	1.03481000	2.31332100	1.43739300
H	2.78967100	2.54544200	1.53611800
C	3.74405300	-0.03795900	0.11050900
C	4.33660000	-0.62088400	-1.16680300
H	5.39469000	-0.84825100	-1.02521900
H	3.82068400	-1.53937600	-1.45185800
H	4.24491500	0.08965300	-1.99079400
H	4.28313500	0.86556700	0.40077100
H	3.84159200	-0.72813700	0.94727200
O	-1.54980700	1.21604300	0.93756200
H	-0.32792100	0.98973200	0.40364800
H	-1.60581900	1.17221100	1.89653400

^BIM2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.51225100	-0.72439800	0.32283400
N	0.09363900	0.10501400	0.08786100
O	-1.62964800	-1.70715700	1.43889600
C	1.29968200	-0.41857500	0.10566700
F	-0.91746500	-1.79023500	-0.84155400
C	1.46536000	-1.89906800	0.27984400
H	1.36994900	-2.37524300	-0.69693200
H	2.42848000	-2.14804700	0.71530000
H	0.65640700	-2.28339900	0.90160400
N	2.37454700	0.37384800	-0.01809600
O	-2.58833400	-0.31904700	-0.81161600
C	-3.76219400	0.47225600	-0.61299400
H	-4.09358200	0.41274700	0.42302000
H	-4.51656000	0.00622000	-1.24983900
C	-3.52324700	1.90983700	-1.03015900
H	-4.45501200	2.47811800	-0.97443600

H	-2.79128800	2.37134500	-0.36708800
H	-3.15859500	1.94588500	-2.05883500
C	2.22564400	1.80066800	-0.32565700
H	1.38598800	1.92647300	-1.01218700
H	3.11903900	2.09996400	-0.87642600
C	2.06354200	2.65704200	0.92819400
H	1.97482200	3.70967400	0.65518500
H	1.17548000	2.37491600	1.49776000
H	2.93108100	2.54473700	1.58160400
C	3.75665400	-0.10656200	0.11539800
C	4.28818100	-0.71959100	-1.17394100
H	5.33437200	-1.00599200	-1.05279900
H	3.71666400	-1.60766700	-1.44711200
H	4.22090800	-0.00427300	-1.99629800
H	4.35473900	0.76124000	0.39919400
H	3.82691800	-0.80558200	0.94698400
O	-1.87566800	0.71482900	1.22251200
H	0.00451700	1.10562100	0.19968300
H	-1.95321800	0.43428600	2.13829200

^BTS2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.52767100	-0.45985200	0.26503600
N	0.27410200	0.27889200	0.07132600
O	-1.48863900	-1.20485200	1.54840300
C	1.42220400	-0.33698700	0.18019500
F	-0.91109200	-1.47810700	-0.88189500
C	1.42411200	-1.79094700	0.55350900
H	2.33271200	-2.08306600	1.07194800
H	0.55182200	-1.99966300	1.17299500
H	1.32697800	-2.37707800	-0.36231800
N	2.58729900	0.30154400	-0.04671000
O	-2.88981000	-0.52922800	-0.62282200
C	-4.13254200	-0.00389000	-0.15298400
H	-4.09286400	0.16109400	0.92533400
H	-4.86693600	-0.78777000	-0.35129400
C	-4.49478400	1.26792400	-0.89412200
H	-5.48515900	1.61370800	-0.58727600
H	-3.76383900	2.04690100	-0.67888000
H	-4.51195000	1.08161600	-1.96970400
C	2.60584200	1.66820700	-0.57204800

H	1.79014000	1.78469900	-1.28887900
H	3.52884900	1.77706400	-1.14478900
C	2.54044900	2.72314900	0.52963300
H	2.56411700	3.72508500	0.09802800
H	1.62826900	2.62420400	1.12097800
H	3.39104900	2.62137300	1.20662100
C	3.90297700	-0.30673200	0.18473600
C	4.37570000	-1.14906600	-0.99387000
H	5.38180900	-1.52981200	-0.80858900
H	3.71007000	-1.99783300	-1.15641700
H	4.39743800	-0.55291000	-1.90865800
H	4.59588100	0.51802300	0.36342800
H	3.88563900	-0.88850400	1.10469200
O	-1.86055800	1.15689900	0.64522800
H	0.27945500	1.27055200	-0.12252400
H	-1.51008600	1.31750900	1.52774500

^BIM3

	Coordinates (Angstroms)		
	X	Y	Z
P	2.37087900	0.24619100	0.65366800
N	-0.98994200	0.99108200	-0.14560300
O	1.91425300	-1.13800300	0.87469200
C	-1.73239200	-0.06711800	-0.23715700
F	2.50630300	1.04738800	2.00745900
C	-1.05062300	-1.38287900	-0.49913500
H	-1.20448100	-1.67695300	-1.54064300
H	0.01572900	-1.28975400	-0.30130800
H	-1.44442300	-2.17123700	0.14239300
N	-3.08398100	-0.05660200	-0.12296800
O	3.86776700	0.37808400	0.13555500
C	4.42512500	-0.66728800	-0.67912000
H	4.27561600	-1.62355100	-0.17303100
H	5.49083700	-0.44686100	-0.71994000
C	3.81007200	-0.67800500	-2.06525200
H	4.31490900	-1.41906100	-2.68874400
H	2.75019100	-0.93718000	-2.01592100
H	3.90655300	0.30322400	-2.53199800
C	-3.80100900	1.18171000	0.16670200
H	-3.24984800	1.75004600	0.92051900
H	-4.74903400	0.90556500	0.63226800
C	-4.05539400	2.01816300	-1.08577700

H	-4.59107200	2.93475000	-0.83229600
H	-3.11884100	2.28888700	-1.57642100
H	-4.65885700	1.45587600	-1.80134800
C	-3.90885100	-1.25452900	-0.28285500
C	-4.24555800	-1.91819300	1.04906500
H	-4.89349700	-2.78256200	0.89138900
H	-3.33799500	-2.25259400	1.55472200
H	-4.76322100	-1.22197900	1.71227600
H	-4.82482300	-0.94923500	-0.79654900
H	-3.40521600	-1.95496500	-0.94642000
O	1.50635400	1.15045400	-0.24936700
H	-1.48492200	1.86321300	-0.00227500
H	0.41472600	1.04822000	-0.20471200

^BTS3

	Coordinates (Angstroms)		
	X	Y	Z
P	0.41918400	0.05359400	0.12336600
O	0.26742900	0.14152900	1.57815900
F	2.33816300	0.58912700	0.19872400
O	-0.81070000	-0.81415200	-0.47637100
C	-2.11239300	-0.70088600	0.12921400
H	-2.02214300	-0.92426600	1.19414100
H	-2.70452600	-1.47760200	-0.35356700
C	-2.72276500	0.66921200	-0.09119600
H	-3.74471900	0.68031800	0.29326900
H	-2.15494200	1.43857500	0.43591600
H	-2.74186100	0.91398900	-1.15406300
O	0.34739800	1.24920400	-0.91701600
H	1.12284000	1.81926600	-0.81941700
O	1.48604100	-1.25130900	-0.55509100
H	2.35405000	-0.82255800	-0.22652100
H	1.24967800	-2.14589600	-0.27430700

P4

Coordinates (Angstroms)			
	X	Y	Z
P	0.71387500	0.00875500	0.10699000
O	0.69643800	-0.10766800	1.57195800
O	-0.46692100	-0.71939200	-0.65592000
C	-1.77422200	-0.80807600	-0.04641100
H	-1.65943100	-1.22556800	0.95607500
H	-2.31444500	-1.51681000	-0.67140200
C	-2.46600900	0.53914200	-0.00789400
H	-3.48562300	0.41445700	0.36210400
H	-1.94417200	1.22799000	0.65893200
H	-2.50353500	0.97816500	-1.00570600
O	0.64669300	1.49528500	-0.47204400
H	1.15986000	2.12465000	0.04559100
O	2.01752800	-0.56002700	-0.61768200
H	2.33070800	-1.38617900	-0.23511100

Hydrolysis path C**^cIM1**

Coordinates (Angstroms)			
	X	Y	Z
P	1.28723100	-1.17997100	0.12242100
N	-0.02904000	-0.20515700	0.20883500
O	1.39549000	-2.13896600	-0.98650300
C	-1.23820900	-0.58357200	-0.12981300
F	1.36256000	-1.87957800	1.53903200
C	-1.58347000	-1.99155600	-0.56005700
H	-0.92185900	-2.70435700	-0.07359200
H	-2.61309100	-2.25157400	-0.32750500
H	-1.41445600	-2.09212100	-1.63506900

N	-2.22469200	0.32344600	-0.09966000
O	2.51409400	-0.18191900	0.30234300
C	2.97392500	0.53871600	-0.86170600
H	2.16477900	1.18878100	-1.20878400
H	3.21626500	-0.18663000	-1.64158300
C	4.17936400	1.35081500	-0.45253200
H	4.58110300	1.87668400	-1.32060600
H	3.90103800	2.09091800	0.29841800
H	4.95464000	0.70024200	-0.04618400
C	-1.95452000	1.69492500	0.35086700
H	-1.27317500	1.65704400	1.19840200
H	-2.90343100	2.10087300	0.70854200
C	-1.38445700	2.56334400	-0.76464600
H	-1.15872600	3.55911000	-0.38158100
H	-0.45649100	2.13274800	-1.14163200
H	-2.09395400	2.65331200	-1.59105900
C	-3.58157300	0.06928700	-0.58752900
C	-4.53948800	-0.32602600	0.53162500
H	-5.55016600	-0.45446500	0.13987700
H	-4.22794000	-1.26111100	1.00078600
H	-4.56777000	0.44430600	1.30465000
H	-3.91936000	0.99290800	-1.06368200
H	-3.55655100	-0.68574800	-1.37155100
O	1.11896100	2.38049900	1.07237000
H	1.84283300	2.12350200	1.64864500
H	0.74314000	1.53081700	0.78875000

^cTS1

Coordinates (Angstroms)			
	X	Y	Z
P	1.36561100	-0.80698200	-0.00345100
N	0.02239200	0.10825400	0.11382000
O	1.87586800	-1.57175300	-1.16014200
C	-1.13268800	-0.22848800	-0.40144200
F	0.27785700	-2.35285700	0.62113400
C	-1.34981900	-1.32017000	-1.42182200
H	-0.44144200	-1.89775600	-1.56039500
H	-2.14744300	-1.99154700	-1.10209800
H	-1.63410400	-0.86917900	-2.37632600
N	-2.20299100	0.50028500	-0.03748000
O	2.48706500	0.36552500	0.30086600

C	2.75382200	1.29012400	-0.75100800
H	1.82909500	1.82594100	-0.99527000
H	3.08169400	0.73908600	-1.63729300
C	3.82041000	2.25066200	-0.26978700
H	4.04772800	2.98305100	-1.04708200
H	3.48071700	2.77971400	0.62197400
H	4.73558100	1.70874800	-0.02548300
C	-2.05181200	1.56897300	0.95348000
H	-1.32805400	1.24060700	1.69747700
H	-3.02018400	1.69320500	1.44365200
C	-1.59778700	2.87450000	0.31029100
H	-1.52398500	3.66269300	1.06205800
H	-0.61753300	2.73413900	-0.14595300
H	-2.30401900	3.19949700	-0.45770100
C	-3.54762800	0.29750000	-0.57078000
C	-4.39557000	-0.60107500	0.32577400
H	-5.40312600	-0.70356100	-0.08185000
H	-3.94986900	-1.59385000	0.40769000
H	-4.47485800	-0.18333000	1.33130900
H	-4.00940300	1.28420300	-0.66433300
H	-3.48560600	-0.11417900	-1.57613200
O	1.90988900	-1.37140600	1.68170700
H	1.39452300	-2.23528400	1.65774500
H	2.87346500	-1.41261400	1.74751900

cP

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.46664100	-0.80745400	0.30248400
N	-0.18044400	0.17334000	0.12523500
O	-1.84686900	-1.33605000	1.62875200
C	1.02836800	-0.10327300	0.53808100
F	1.34874200	-2.08670900	-1.60973100
C	1.40371200	-1.30849600	1.36990000
H	0.54207600	-1.95281600	1.52363000
H	2.19814300	-1.87527800	0.88419500
H	1.74825800	-0.98270700	2.35390600
N	2.01250700	0.75004300	0.21336400
O	-2.65130000	-0.05760200	-0.46468400
C	-3.21841300	1.10948000	0.15265500
H	-2.43775400	1.87298000	0.23003100

H	-3.55766800	0.84618200	1.15828100
C	-4.36298800	1.57855000	-0.71634600
H	-4.81909600	2.47127200	-0.28428300
H	-4.00473500	1.81677600	-1.71858700
H	-5.12277600	0.79983900	-0.79325700
C	1.71000800	1.91019800	-0.62876000
H	0.97084400	1.60760800	-1.36975200
H	2.63060200	2.17847800	-1.15101300
C	1.19410700	3.08410200	0.19535600
H	0.98991300	3.94079200	-0.44997800
H	0.27152700	2.80028400	0.70270100
H	1.92890600	3.38689300	0.94512200
C	3.42136900	0.51539100	0.52331400
C	4.13822600	-0.22431100	-0.60364000
H	5.18642200	-0.38694900	-0.34511600
H	3.66235900	-1.18749700	-0.79521900
H	4.09993500	0.35198100	-1.53012900
H	3.87933500	1.49283100	0.69559300
H	3.50254000	-0.03409300	1.45943300
O	-1.15296500	-2.01107300	-0.76886300
H	0.43057000	-2.08232900	-1.42194000
H	-1.74017800	-2.76778600	-0.65848000

Ammonolysis by NH₃

Ammonolysis path A

^AIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.42450100	-1.03556300	-0.42963600
N	-0.01836400	-0.25648000	-0.61950000
O	-1.54530500	-2.29642400	0.31680300
C	1.14040800	-0.55769100	-0.10511800
F	-1.92973900	-1.17509800	-1.93026100
C	1.48943300	-1.87678300	0.53755300
H	0.71089600	-2.60664900	0.33637500
H	2.44879300	-2.24663400	0.17426900
H	1.54332900	-1.72966800	1.61866400
N	2.10464700	0.37960700	-0.16025100
O	-2.44239400	0.06720000	0.12005300
C	-2.62606400	1.32131400	-0.55797200

H	-3.31537700	1.15953600	-1.39006800
H	-1.66479600	1.65740700	-0.95651000
C	-3.18375100	2.30808100	0.44314100
H	-3.37455800	3.26765100	-0.04139700
H	-4.11923200	1.93593900	0.86281200
H	-2.47413400	2.46550900	1.25785400
C	1.79025100	1.69880500	-0.71287100
H	1.16006200	1.56025100	-1.59017700
H	2.73152200	2.14871600	-1.03659700
C	1.09073400	2.57711300	0.32024800
H	0.83342400	3.54689100	-0.11098600
H	0.17856100	2.08402300	0.66054000
H	1.73323900	2.74606400	1.18746000
C	3.44036600	0.21118600	0.40601500
C	4.46706800	-0.20752900	-0.64238700
H	5.46147300	-0.27753800	-0.19726900
H	4.20948900	-1.17842000	-1.06981600
H	4.50722200	0.51878600	-1.45674700
H	3.72261200	1.16968600	0.84963200
H	3.40386800	-0.50639300	1.22335100
N	-0.62875400	-0.52239200	2.68684200
H	-0.96527300	-1.44241100	2.40807900
H	-1.36268700	0.12414100	2.41112100
H	-0.58504300	-0.50589200	3.70016700

^ATS1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.37305900	-0.56700500	0.39675900
N	0.12246600	0.15461500	0.36727600
O	-1.68451200	-1.93574600	1.08542200
C	1.23206600	-0.46317600	0.11131700
F	-1.22630800	-1.22206800	-1.12635400
C	1.39404600	-1.96461800	0.01028400
H	0.42743000	-2.45841500	0.03016900
H	1.91402400	-2.23712400	-0.90913100
H	1.98229100	-2.32791100	0.85662300
N	2.35634100	0.28282500	-0.03994000
O	-2.55387400	0.43641800	-0.05941200
C	-2.99157600	0.61333200	-1.41568600
H	-3.37352900	-0.33318600	-1.79970200
H	-2.14041600	0.91363300	-2.03025400

C	-4.06419700	1.68019200	-1.39453200
H	-4.43501600	1.85580800	-2.40643300
H	-4.90030100	1.36719900	-0.76733300
H	-3.66533100	2.61638400	-1.00109600
C	2.26537500	1.74001100	0.03259700
H	1.32781200	2.04631100	-0.42952200
H	3.08808700	2.14816600	-0.55966700
C	2.33609300	2.24480900	1.47010800
H	2.29250300	3.33550400	1.49611600
H	1.49321700	1.84919300	2.03761400
H	3.26474100	1.92789500	1.95107600
C	3.68459800	-0.27418500	-0.26995200
C	4.05559700	-0.31679300	-1.75075400
H	5.07005800	-0.69928800	-1.88071600
H	3.36840500	-0.96077300	-2.30253800
H	4.00826600	0.68110600	-2.19133900
H	4.39755300	0.34935600	0.27736400
H	3.74876500	-1.26908800	0.16709400
N	-1.70079600	0.03277800	2.18949500
H	-1.81791400	-1.22448800	2.11179200
H	-2.52550000	0.61126000	2.30186600
H	-0.90349200	0.45781400	2.64761200

^AIM2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.37154000	-0.27330600	-0.60863000
N	-0.17978100	0.28435700	-0.40249300
O	1.76062500	-1.61418800	-1.45426700
C	-1.25281000	-0.41894100	-0.23874900
F	1.18906700	-1.33867700	0.70729400
C	-1.36674700	-1.90713500	-0.48510300
H	-0.38478900	-2.34421800	-0.63217300
H	-1.84859400	-2.40525300	0.35724600
H	-1.97058900	-2.08433100	-1.37881200
N	-2.38923600	0.22578700	0.12965100
O	2.57733900	0.47188600	0.18026800
C	3.09000400	0.12557400	1.47559200
H	3.44008100	-0.90730500	1.46280000
H	2.28956600	0.20369500	2.21258300
C	4.21573600	1.09309100	1.77218100
H	4.64252200	0.87896600	2.75431400

H	5.00435600	1.00381800	1.02336900
H	3.84830000	2.12043500	1.76756300
C	-2.34690700	1.66487700	0.38258200
H	-1.39466800	1.89891100	0.85645200
H	-3.14667600	1.89586700	1.09070400
C	-2.51361200	2.47198900	-0.90106500
H	-2.48933900	3.54242300	-0.68700500
H	-1.70300900	2.23403700	-1.59070100
H	-3.46523500	2.24248600	-1.38683500
C	-3.69029400	-0.41901800	0.26548300
C	-3.99720200	-0.82286800	1.70591900
H	-4.99418600	-1.26267300	1.77670300
H	-3.26907900	-1.55218300	2.06564900
H	-3.95890200	0.04464500	2.36782000
H	-4.44305100	0.28871000	-0.09384800
H	-3.74474100	-1.28462800	-0.39254000
N	1.62249900	0.74072300	-2.01659000
H	1.86651000	-1.34059200	-2.37271400
H	2.56458300	1.11378600	-2.05717900
H	0.97513700	1.51803000	-2.02261100

^ATS2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.37032800	-0.41224900	-0.55785800
N	-0.16166700	0.18334300	-0.40247700
O	1.72776400	-1.90570400	-1.14258100
C	-1.25187700	-0.45704200	-0.14930800
F	1.19437300	-1.18733300	0.98179100
C	-1.38954000	-1.96215600	-0.16262600
H	-0.40956900	-2.42883500	-0.17210200
H	-1.93665400	-2.31438700	0.71260700
H	-1.93474600	-2.27040400	-1.05846700
N	-2.37849100	0.26248500	0.09384100
O	2.62225900	0.42388800	0.06138500
C	3.02152300	0.47714100	1.44057500
H	3.34685000	-0.51158200	1.76589200
H	2.16513100	0.76635100	2.05122500
C	4.13995700	1.49325600	1.53203500
H	4.48570500	1.57558600	2.56467100
H	4.98266100	1.19399700	0.90656900
H	3.79502000	2.47348200	1.19973100

C	-2.30525500	1.72179400	0.09308600
H	-1.36681700	2.01632000	0.56161100
H	-3.12483600	2.09039800	0.71515200
C	-2.39636400	2.29351800	-1.31875700
H	-2.34498600	3.38409000	-1.29508800
H	-1.56967700	1.91409700	-1.92072000
H	-3.33727400	2.00688600	-1.79508900
C	-3.69933400	-0.32505600	0.28131900
C	-4.06555100	-0.48757200	1.75482100
H	-5.07691100	-0.88643800	1.85804200
H	-3.37090000	-1.16735600	2.25183400
H	-4.02252500	0.47335500	2.27165000
H	-4.42103900	0.33126300	-0.21396300
H	-3.75446400	-1.28305000	-0.23345600
N	1.54252500	0.31992200	-2.11637800
H	2.67114400	-2.05592500	-1.24549200
H	2.47306400	0.22756500	-2.50868400
H	1.30843700	1.30530700	-2.08636600

^AIM3

	Coordinates (Angstroms)		
	X	Y	Z
P	1.44086200	-0.62930400	-0.42973600
N	-0.07738600	0.02476600	-0.39080900
O	1.94853400	-2.17347900	-0.58649100
C	-1.19873700	-0.51362800	-0.06278700
F	1.26224000	-1.06759500	1.28962200
C	-1.39647700	-1.98249200	0.23447100
H	-0.43493800	-2.46874500	0.35745400
H	-1.97962800	-2.12790100	1.14434900
H	-1.92386000	-2.45819500	-0.59602000
N	-2.30641400	0.27434700	-0.01753700
O	2.56354000	0.45303100	-0.00904300
C	2.69480600	1.04522700	1.29087900
H	3.08775700	0.30502300	1.98821200
H	1.70833900	1.35355100	1.64468700
C	3.62900600	2.22712200	1.14458800
H	3.77374600	2.71116400	2.11282400
H	4.60048600	1.90059900	0.77019600
H	3.21734500	2.95711700	0.44602500
C	-2.17771800	1.69846700	-0.31704700
H	-1.24137700	2.05352100	0.11259600

H	-2.99919300	2.21414400	0.18669900
C	-2.20824400	1.96832400	-1.81848300
H	-2.11369400	3.03770500	-2.01827600
H	-1.38152300	1.44540100	-2.30083300
H	-3.14656500	1.62080100	-2.25784400
C	-3.65226600	-0.21980600	0.24528900
C	-4.06452800	-0.05624400	1.70657000
H	-5.09183800	-0.39495300	1.85654900
H	-3.40862700	-0.63487600	2.35985000
H	-4.00201100	0.99062700	2.01058700
H	-4.33610600	0.33807100	-0.40121100
H	-3.72969900	-1.26280700	-0.05847200
N	1.60972600	-0.43581800	-2.11801100
H	2.05907200	-2.57076900	0.28307600
H	2.50079300	-0.75686900	-2.47534600
H	1.43530500	0.51401800	-2.41776100

^ATS3

	Coordinates (Angstroms)		
	X	Y	Z
P	1.55591500	-0.61761700	-0.50484900
N	0.01920200	-0.14149500	-0.67102800
O	2.08783500	-2.06512000	-0.11594200
C	-1.07480200	-0.64259200	-0.18041300
F	0.98775400	-0.99785500	1.62378500
C	-1.22082400	-2.05314700	0.33168500
H	-0.28039100	-2.58224800	0.23739300
H	-1.50354900	-2.04913400	1.38442200
H	-1.98169000	-2.57887800	-0.24936500
N	-2.17923900	0.12981400	-0.19132600
O	2.42153900	0.56618700	0.11478700
C	2.07109200	1.34615700	1.27521900
H	2.36235300	0.78887700	2.16233500
H	0.98672400	1.46721100	1.30079900
C	2.79270800	2.66980400	1.14835800
H	2.57680400	3.29226300	2.01940900
H	3.87147800	2.51487800	1.09400200
H	2.47397500	3.20272900	0.25070100
C	-2.09409700	1.50623400	-0.68258500
H	-1.13270500	1.91866200	-0.37758200
H	-2.88285500	2.07734800	-0.18799400
C	-2.24655300	1.57300000	-2.19811900

H	-2.19210100	2.60781500	-2.54200900
H	-1.44778400	1.00251600	-2.67317000
H	-3.20793600	1.15859600	-2.51082900
C	-3.46793400	-0.28672800	0.35568200
C	-3.63184100	0.12590300	1.81643700
H	-4.61067200	-0.17942500	2.19141000
H	-2.85993700	-0.33674200	2.43395400
H	-3.54686700	1.20884400	1.92668700
H	-4.24515300	0.17255700	-0.26097400
H	-3.58254400	-1.36341700	0.24977400
N	2.06823900	-0.65177400	-2.09485400
H	1.86209300	-2.09688500	0.85097600
H	3.01709600	-0.97870700	-2.22184500
H	1.89624800	0.20195400	-2.60731100

^AP

Coordinates (Angstroms)			
	X	Y	Z

P	-1.48559600	0.71798000	-0.47638400
N	-0.14924600	-0.22033400	-0.51058800
O	-1.47247700	1.83679000	0.52316100
C	1.06917600	0.25476000	-0.54211300
F	0.60740800	1.93253000	1.90533700
C	1.43705100	1.66786000	-0.93443600
H	0.54616200	2.27318500	-1.07299900
H	2.05090400	2.13381200	-0.16464100
H	1.98950800	1.65032900	-1.87714800
N	2.07980200	-0.58039200	-0.24922200
O	-2.67135900	-0.33062300	-0.21304700
C	-2.67010500	-1.07980400	1.01315300
H	-2.52642700	-0.38927300	1.84940300
H	-1.83053200	-1.77963700	0.98655800
C	-3.99526600	-1.80069900	1.11530900
H	-4.02921100	-2.39322200	2.03159200
H	-4.81666300	-1.08341200	1.13188300
H	-4.13135500	-2.46764500	0.26270800
C	1.78314200	-1.94840100	0.18244500
H	0.89228800	-1.92125200	0.80937600
H	2.62227400	-2.28145300	0.79650600
C	1.57654600	-2.88390900	-1.00292100
H	1.38157600	-3.90048500	-0.65533500
H	0.72410900	-2.54672600	-1.59305300

H	2.46354800	-2.90408200	-1.64057400
C	3.47323800	-0.14944600	-0.14780600
C	3.82064800	0.31301500	1.26551000
H	4.85882000	0.64765800	1.31289500
H	3.16518100	1.12984300	1.57405800
H	3.69206700	-0.50201300	1.98066200
H	4.09552500	-0.99846700	-0.44205600
H	3.66426200	0.64064800	-0.87165500
N	-1.80248400	1.31680200	-1.99826000
H	-0.23645700	1.95588600	1.44209000
H	-2.50446400	2.04633700	-2.01312800
H	-1.96624200	0.62538200	-2.71868800

Ammonolysis path B

^BIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.15418500	-0.84110200	0.05592800
N	0.22889000	-0.06356000	-0.28681000
O	-1.49810800	-1.16264900	1.45393400
C	1.39724600	-0.44117000	0.14818000
F	-1.10826600	-2.18742300	-0.80676900
C	1.64190600	-1.69212500	0.96281800
H	0.83952500	-2.40877600	0.80458600
H	2.58895200	-2.16547700	0.70936100
H	1.64520400	-1.43511300	2.02527100
N	2.45684900	0.34052000	-0.12938600
O	-2.23060000	0.01652600	-0.72896700
C	-3.63828600	-0.20966800	-0.47985900
H	-3.79402600	-0.28355000	0.59765900
H	-3.91739500	-1.15477600	-0.95363300
C	-4.39544800	0.95900900	-1.06319700
H	-5.46837400	0.79931600	-0.93850900
H	-4.11596800	1.87241400	-0.53779000
H	-4.17847600	1.06508100	-2.12713000
C	2.26024100	1.56654400	-0.90790400
H	1.50851800	1.36533400	-1.66930900
H	3.20713200	1.78662600	-1.40646800
C	1.82484100	2.73042200	-0.02439700
H	1.69845100	3.63447300	-0.62285100
H	0.87406100	2.49237300	0.45383300

H	2.56773500	2.93508400	0.75039700
C	3.80854500	0.09663500	0.36957700
C	4.67774800	-0.64933200	-0.63854000
H	5.69189600	-0.76988300	-0.25301300
H	4.26720600	-1.63851500	-0.84982100
H	4.73303900	-0.10059300	-1.58073300
H	4.24524800	1.07348700	0.59277200
H	3.76043800	-0.43927500	1.31645400
N	-2.43865700	1.88022900	1.68168600
H	-2.17413700	0.97264600	2.05812700
H	-2.16472100	2.58735200	2.35400400
H	-1.88780900	2.02187000	0.84055600

^BTs1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.39324400	-0.56665400	0.37123300
N	0.17841700	0.12362700	-0.01680600
O	-1.67844100	-1.16860000	1.69943300
C	1.35923400	-0.43859000	0.08800500
F	-0.97948300	-1.92382000	-0.50299200
C	1.51814800	-1.89796400	0.41545200
H	1.30878600	-2.47920500	-0.48344200
H	2.51194300	-2.13851900	0.78034900
H	0.76890900	-2.18152900	1.15475700
N	2.44653300	0.32621600	-0.10243500
O	-2.52253500	-0.24306900	-0.74891900
C	-3.84869900	0.09456100	-0.33874300
H	-3.85311300	0.42516200	0.70375300
H	-4.45276000	-0.81363800	-0.39983700
C	-4.38398600	1.16637200	-1.26594300
H	-5.41963700	1.40459000	-1.01458700
H	-3.78930700	2.07988100	-1.19163800
H	-4.34530800	0.82070800	-2.29985400
C	2.29490000	1.72358400	-0.52148500
H	1.41549200	1.79420700	-1.16116100
H	3.16778500	1.96948900	-1.13047700
C	2.18519400	2.67446600	0.66661900
H	2.10605500	3.70528000	0.31670900
H	1.30170800	2.44855800	1.26637200
H	3.06633100	2.59832400	1.30792900
C	3.82389600	-0.14349000	0.07686900

C	4.35218500	-0.88213800	-1.14722800
H	5.39612000	-1.16500700	-0.99968000
H	3.77199000	-1.78687600	-1.33545100
H	4.28935500	-0.24761800	-2.03368100
H	4.42792000	0.74437800	0.27254400
H	3.89461900	-0.75861500	0.97298800
N	-1.48852600	1.32806600	0.96317200
H	-1.60962300	1.36693000	1.96953900
H	-2.16605500	1.93770200	0.51805700
H	-0.22960000	1.15716300	0.39233900

Bp

Coordinates (Angstroms)			
	X	Y	Z
P	-1.48796600	0.45516900	0.13065400
N	1.51389800	1.82440700	0.43092700
O	-1.01010600	-0.65906200	0.96583900
C	1.88665400	0.64385000	0.80259700
F	-0.72864100	0.42424500	-1.26450800
C	1.67816400	0.27578700	2.25004200
H	1.08993500	-0.63712700	2.34414400
H	2.63849400	0.14618500	2.75520000
H	1.14176600	1.09259900	2.72690200
N	2.46418700	-0.29493200	-0.00453400
O	-3.02259500	0.36033200	-0.27274700
C	-3.65326600	-0.93389100	-0.37787300
H	-3.41388200	-1.51379000	0.51539300
H	-3.23934500	-1.44886200	-1.24880000
C	-5.13889800	-0.70378500	-0.52783300
H	-5.65386300	-1.66149000	-0.62334400
H	-5.53272700	-0.18158700	0.34505500
H	-5.34552200	-0.10526400	-1.41568500
C	2.62455500	-0.03787900	-1.43099200
H	1.73080900	0.46243700	-1.81382800
H	2.66578100	-1.00579600	-1.93444300
C	3.88932100	0.76160200	-1.73961100
H	3.97788200	0.94546700	-2.81245900
H	3.88044100	1.72309800	-1.22286300
H	4.77395100	0.21228000	-1.41018100
C	2.76512300	-1.65266900	0.44422800
C	1.61827700	-2.62619300	0.18308900
H	1.88423000	-3.62908600	0.52555700

H	0.71265300	-2.29392300	0.69371900
H	1.39440400	-2.68090000	-0.88522900
H	3.67097900	-1.97488500	-0.07859000
H	3.01512700	-1.63391300	1.50370600
N	-1.34396000	2.02489900	0.55827400
H	-0.37483900	2.30223700	0.75739300
H	-2.04437800	2.38328000	1.19109300
H	1.70852200	2.00156900	-0.55127000

Ammonolysis path C

^cIM1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.42242400	-0.89077600	0.03662300
N	0.01760900	-0.02535100	0.25519900
O	1.95858700	-1.51431500	-1.20082000
C	-1.09974300	-0.31178900	-0.33678000
F	0.60953400	-2.33496500	0.63678800
C	-1.26674300	-1.32906700	-1.44361000
H	-0.37368200	-1.94053900	-1.53539200
H	-2.12446900	-1.97427800	-1.24969900
H	-1.43069400	-0.81391600	-2.39381600
N	-2.20664200	0.38394800	0.02845900
O	2.40414900	0.49620800	0.18969400
C	2.41871200	1.38975000	-0.90968700
H	1.39043800	1.68839300	-1.15151200
H	2.83830700	0.87940400	-1.78185100
C	3.24380300	2.60289600	-0.52808100
H	3.28399900	3.31375000	-1.35635400
H	2.80764700	3.10211100	0.33954000
H	4.26410600	2.30409200	-0.27972400
C	-2.10949500	1.37754100	1.09600500
H	-1.45291900	0.98294100	1.87049500
H	-3.10874100	1.49339100	1.52320300
C	-1.58032300	2.71576500	0.58954300
H	-1.56119400	3.44958400	1.39816000
H	-0.56629700	2.58625200	0.21005300
H	-2.21293700	3.10684800	-0.21122200
C	-3.50616800	0.25286800	-0.62047500
C	-4.44451800	-0.68894000	0.13070300
H	-5.41973300	-0.73002000	-0.35891800

H	-4.03000400	-1.69811600	0.16553200
H	-4.59250600	-0.35017100	1.15820800
H	-3.94477800	1.25360900	-0.67654300
H	-3.37272200	-0.08196000	-1.64762300
H	2.60728500	-2.20629000	1.68597100
N	2.28883600	-1.23953700	1.70904900
H	3.04905200	-0.57475800	1.83667400
H	1.59401400	-1.15670500	2.44873500

^cTS1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.37824000	-0.82812600	0.01450400
N	0.05027900	0.11621100	0.12323200
O	1.86156100	-1.64499100	-1.11678600
C	-1.10011100	-0.18926400	-0.42241600
F	0.04119100	-2.38873200	0.61288000
C	-1.30862500	-1.23812500	-1.48648200
H	-0.40453600	-1.82209200	-1.62347800
H	-2.11343400	-1.91500700	-1.19959700
H	-1.57420600	-0.74822200	-2.42765600
N	-2.17012400	0.53832100	-0.05259400
O	2.51626200	0.34626100	0.29075400
C	2.76586300	1.27367400	-0.76105300
H	1.84460900	1.82920600	-0.97203700
H	3.05313300	0.72244400	-1.66167300
C	3.86976100	2.20922200	-0.31517400
H	4.08777000	2.93821100	-1.09829100
H	3.57283000	2.74571500	0.58773000
H	4.77977100	1.64596800	-0.10207000
C	-2.03109900	1.57077400	0.97547300
H	-1.33050800	1.21008200	1.72675400
H	-3.00889900	1.69120200	1.44749000
C	-1.54689500	2.89196100	0.38832000
H	-1.48110600	3.65433300	1.16722000
H	-0.55896700	2.75445700	-0.05206100
H	-2.23235700	3.25017500	-0.38359300
C	-3.51034900	0.34916700	-0.60203800
C	-4.35980500	-0.58146600	0.25969300
H	-5.36149400	-0.68314400	-0.16250200
H	-3.90288700	-1.57062500	0.32047200
H	-4.45547200	-0.19167700	1.27513900

H	-3.97500600	1.33685100	-0.66802900
H	-3.43858800	-0.03065300	-1.61903100
H	1.14062700	-2.21456300	1.77660600
N	1.84333700	-1.44617600	1.68495600
H	2.81209800	-1.75956600	1.65893900
H	1.74283100	-0.70691900	2.37734100

P5

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.45272800	-0.88112100	0.13216300
N	-0.19200200	0.15544000	0.04180500
O	-1.73299900	-1.64582100	1.36798400
C	0.99367800	-0.03060100	0.55950500
F	1.41316700	-2.33808800	-1.20821900
C	1.34260000	-1.09352800	1.57484800
H	0.48295200	-1.72953300	1.76649600
H	2.17296900	-1.70111600	1.21483700
H	1.63037100	-0.62036700	2.51671100
N	1.97903200	0.80306300	0.18127000
O	-2.68778100	0.00231700	-0.40171400
C	-3.12155700	1.11062300	0.40025000
H	-2.29855800	1.82844100	0.47355800
H	-3.36352400	0.74691800	1.40308700
C	-4.33018800	1.72323300	-0.27089000
H	-4.68932100	2.57547000	0.30914200
H	-4.07369000	2.06605900	-1.27430200
H	-5.13323800	0.98913400	-0.34722300
C	1.71143500	1.82994000	-0.82753100
H	1.02664800	1.41340100	-1.56510500
H	2.65850200	2.05039400	-1.32441700
C	1.12256900	3.09048100	-0.20463600
H	0.94649100	3.84833400	-0.97069600
H	0.17355900	2.85233800	0.27668800
H	1.80088600	3.50893700	0.54271500
C	3.36946500	0.65303800	0.60541700
C	4.16890200	-0.21577100	-0.36292200
H	5.20046400	-0.31842400	-0.02020400
H	3.71920300	-1.20645600	-0.44946500
H	4.18297600	0.22882500	-1.36012400
H	3.79797300	1.65686800	0.66701200
H	3.40185400	0.23926800	1.61133600

H	0.46190700	-2.27113400	-1.22689100
N	-1.21456400	-1.94220400	-1.18816700
H	-1.79632400	-2.76957000	-1.08905300
H	-1.41213400	-1.49872600	-2.08134900

Detergent combinations

H₂O₂/NH₃

¹IM1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.29247800	-0.40104000	-1.18726800
N	0.17732900	0.24039700	-1.09416300
O	-1.56715900	-1.84199600	-1.04540900
C	1.25778600	-0.32239900	-0.61895700
F	-1.82356900	0.16290200	-2.57082700
C	1.50191800	-1.81198500	-0.59605400
H	0.71781100	-2.32341200	-1.14648800
H	2.47331100	-2.04919900	-1.03279200
H	1.48805400	-2.16914100	0.43636800
N	2.22511300	0.47596700	-0.15349700
O	-2.20464800	0.45080800	-0.17060600
C	-2.28917500	1.88850000	-0.29580600
H	-2.95165100	2.11033600	-1.13487800
H	-1.29224200	2.27931700	-0.51592000
C	-2.82732200	2.44062300	1.00520900
H	-2.95279300	3.52187100	0.92210700
H	-3.79726900	1.99662400	1.23525500
H	-2.14052300	2.23413900	1.82864700
C	1.96907800	1.91527100	-0.03498900
H	1.43264900	2.23925000	-0.92522800
H	2.93957100	2.41643700	-0.02081600
C	1.16970500	2.22074900	1.22852900
H	0.93721900	3.28666100	1.28402200
H	0.24217600	1.64592500	1.23388200
H	1.72915100	1.94188400	2.12404100
C	3.47190900	-0.01163200	0.43193900
C	4.62923100	0.02905600	-0.56121000
H	5.55518400	-0.29417100	-0.08184300
H	4.43263700	-0.62609600	-1.41215100
H	4.77642400	1.04151900	-0.94260700

H	3.68705800	0.62367300	1.29451100
H	3.32604700	-1.01674200	0.82220200
O	-0.07221000	-0.83785900	1.85419000
H	-1.47349400	-3.05582300	0.52891300
N	-1.15999100	-3.31807700	1.46571100
H	-1.98014600	-3.40711600	2.05616100
H	-0.34146800	-1.79408900	1.83765200
H	-0.72260000	-4.23102800	1.41538000
O	-1.22175800	-0.23017000	2.43785400
H	-1.75554800	-0.02470600	1.65348700

¹TS1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.17656100	-0.38757000	-0.72434900
N	0.36673800	0.16768900	-0.62138500
O	-1.68569100	-1.78115500	-1.04990000
C	1.40733400	-0.47784300	-0.21302100
F	-1.39383900	0.26145800	-2.22020100
C	1.46210400	-1.96966700	0.02222000
H	0.59245300	-2.43917300	-0.43025000
H	2.36962000	-2.40358500	-0.39952700
H	1.43431900	-2.16387500	1.09659300
N	2.54668000	0.22494800	0.00358900
O	-2.18448700	0.69725600	-0.03088300
C	-2.35995600	2.01087200	-0.58513400
H	-3.00318200	1.94408700	-1.46328100
H	-1.38785200	2.39832300	-0.90020000
C	-2.97414300	2.87452400	0.49558300
H	-3.15702800	3.88063600	0.11291700
H	-3.92385700	2.45337500	0.83022200
H	-2.30473800	2.95416700	1.35563100
C	2.52602300	1.67605900	-0.17399500
H	1.93540000	1.89961000	-1.06189700
H	3.55453500	1.99764500	-0.35662600
C	1.94115000	2.38166000	1.04594600
H	1.91035800	3.46180100	0.88670500
H	0.92948300	2.01472700	1.22549300
H	2.54253900	2.18277000	1.93654800
C	3.78353700	-0.35823400	0.50717400
C	4.77885100	-0.67662600	-0.60610700
H	5.70993600	-1.06793000	-0.19052000

H	4.36547700	-1.41823200	-1.29246900
H	5.01186300	0.22069100	-1.18311200
H	4.21977000	0.36171100	1.20563200
H	3.55997600	-1.25018500	1.09055400
O	-1.05027400	-1.04518900	1.13086700
H	-2.49592900	-2.55324500	-0.04751600
N	-2.82258400	-2.77014600	0.97563100
H	-3.79887400	-2.54441900	1.12920900
H	-2.12143600	-2.01366000	1.39005900
H	-2.62041300	-3.71805600	1.27164700
O	-0.79553800	-0.05703600	2.11590800
H	-1.42675500	0.63033100	1.85245400

¹IM2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.24807100	0.28014300	-0.57885200
N	-0.31376700	-0.21990900	-0.62130800
O	1.81696300	1.66997500	-1.10598000
C	-1.36496400	0.41050700	-0.21505600
F	1.54391700	-0.35419100	-2.07041600
C	-1.42804200	1.89667000	0.05990700
H	-0.58641800	2.39177800	-0.41733500
H	-2.35410300	2.33336700	-0.31383000
H	-1.35748000	2.06506200	1.13731400
N	-2.50595600	-0.29818000	-0.04493700
O	2.20701000	-0.82454600	0.12944700
C	2.45629900	-2.11557400	-0.44735800
H	3.15649100	-2.00539200	-1.27580100
H	1.51990500	-2.51912400	-0.83998800
C	3.01932700	-2.99011100	0.65184800
H	3.24849400	-3.98318400	0.26018400
H	3.93557600	-2.55561900	1.05492200
H	2.29749300	-3.09967300	1.46439600
C	-2.47551600	-1.74442900	-0.26277600
H	-1.87121700	-1.93976000	-1.14805600
H	-3.50001000	-2.06453000	-0.46806800
C	-1.90356900	-2.48121900	0.94458000
H	-1.87481700	-3.55699700	0.75882200
H	-0.89101100	-2.12443700	1.13930200
H	-2.51198700	-2.30231600	1.83461200
C	-3.75291300	0.26445900	0.46010100

C	-4.72980400	0.62364900	-0.65656100
H	-5.66911600	0.99523800	-0.24170300
H	-4.30844200	1.39291300	-1.30674400
H	-4.94943200	-0.25117700	-1.27197800
H	-4.19815700	-0.48360900	1.12198400
H	-3.54054300	1.13189800	1.08352000
O	1.15588300	1.05294000	1.01114500
H	1.94088000	2.40522900	-0.44347300
N	2.16269100	3.67867900	0.72102300
H	3.12196900	3.95529100	0.89762200
H	1.84632900	3.09874400	1.49433400
H	1.59805800	4.51992800	0.69182400
O	0.65208700	0.19532900	2.02110200
H	1.34998100	-0.47548600	2.06739200

¹TS2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.07810100	-0.54982700	-0.30276600
N	0.45276100	-0.07174200	-0.58783600
O	-1.57664500	-2.06232000	-0.44903700
C	1.53331000	-0.57406000	-0.07494400
F	-1.51410900	-0.23612300	-1.88750000
C	1.63240200	-1.95054500	0.54038600
H	0.76584400	-2.54390500	0.26106500
H	2.54069200	-2.46224700	0.22117300
H	1.63286300	-1.85669700	1.62902500
N	2.65845700	0.16974000	-0.12416700
O	-2.09522500	0.64175700	0.18395100
C	-2.37354300	1.79515400	-0.62592900
H	-3.10119300	1.52798000	-1.39378300
H	-1.45586700	2.11220300	-1.12602600
C	-2.89975300	2.87155700	0.29912000
H	-3.14762400	3.76853000	-0.27196800
H	-3.79955200	2.53208700	0.81601400
H	-2.14889100	3.13649000	1.04664400
C	2.58832200	1.52489500	-0.67186100
H	1.94484300	1.50066700	-1.55069700
H	3.59670700	1.80007500	-0.99034400
C	2.04917400	2.51442700	0.35656300
H	1.98268100	3.51588600	-0.07400500
H	1.05724900	2.19513300	0.68037800

H	2.70072100	2.55943100	1.23271900
C	3.94050400	-0.24986600	0.43139800
C	4.86812200	-0.84521300	-0.62444400
H	5.83333800	-1.10535800	-0.18513500
H	4.43020400	-1.74569600	-1.05938200
H	5.04070700	-0.13173400	-1.43285900
H	4.39994100	0.63469100	0.88103000
H	3.77504200	-0.95440700	1.24481000
O	-0.88387900	-0.91980800	1.39544200
H	-2.56576200	-2.12519800	-0.35318800
N	-4.22700000	-1.71005500	0.06225600
H	-4.85108700	-1.53646900	-0.71805000
H	-4.05926300	-0.82372200	0.53295400
H	-4.70134800	-2.32585000	0.71326400
O	-0.34356900	0.17611500	2.12426500
H	-1.09795500	0.78097900	2.15488100

¹IM3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.24250500	-0.37782000	0.27554300
N	0.24867900	-0.14548800	-0.36658500
O	-1.84913100	-1.77285500	0.74009600
C	1.37445700	-0.52505400	0.14915500
F	-1.87735700	-0.64686200	-1.28969100
C	1.52449200	-1.58240100	1.21953900
H	0.61175600	-2.16709200	1.29544100
H	2.36438800	-2.24428400	1.00695300
H	1.68275000	-1.09565700	2.18503500
N	2.50742400	0.04450700	-0.32255700
O	-2.08198400	1.00655900	0.36210000
C	-2.36040000	1.82135300	-0.78450800
H	-3.22066100	1.40885800	-1.31311100
H	-1.50009400	1.80011000	-1.45786200
C	-2.63318300	3.22146600	-0.27821700
H	-2.88130400	3.88110900	-1.11232200
H	-3.46890300	3.21823200	0.42347100
H	-1.75319700	3.62356800	0.22867600
C	2.39938700	1.11026000	-1.31890800
H	1.63445000	0.82320000	-2.03969100
H	3.35854500	1.16810000	-1.83941700
C	2.04550600	2.44636200	-0.67249500

H	1.95135200	3.22643600	-1.43110000
H	1.09917200	2.34997500	-0.13771300
H	2.81658000	2.75087400	0.03952500
C	3.84151300	-0.23744500	0.19523800
C	4.59782300	-1.25325100	-0.65691300
H	5.60780900	-1.40430900	-0.27019900
H	4.08041600	-2.21466000	-0.66118000
H	4.67456400	-0.90841300	-1.69022700
H	4.38450600	0.71151900	0.21861000
H	3.77208700	-0.57331300	1.22863800
O	-0.83706700	-0.18527400	1.94207000
H	-2.30528000	-2.30899100	0.03306500
N	-3.07963100	-3.18878400	-1.24107800
H	-2.85660000	-2.51395000	-1.96758100
H	-4.08866500	-3.26413400	-1.17729300
H	-2.71772800	-4.09385100	-1.51898900
O	-0.14659900	1.03388300	2.16987000
H	-0.86677800	1.67783800	2.11245500

¹TS3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.24889700	-0.43751400	0.41629100
N	0.20806300	-0.07077000	-0.24101300
O	-1.78380000	-1.82968100	0.69063400
C	1.34204500	-0.48473000	0.22186400
F	-1.77573800	-0.76539800	-1.56442600
C	1.51012800	-1.54130900	1.29140000
H	0.59728000	-2.12518500	1.38427300
H	2.34466700	-2.20657900	1.06972000
H	1.68716000	-1.05255000	2.25294300
N	2.47005100	0.06723600	-0.28968600
O	-2.22302800	0.82565900	0.25519700
C	-2.25153800	1.68230200	-0.89814000
H	-3.06006500	1.34846500	-1.54761100
H	-1.31205200	1.58125800	-1.44205600
C	-2.46507800	3.09663100	-0.40101800
H	-2.54727400	3.78251300	-1.24713500
H	-3.38044900	3.16533700	0.18985700
H	-1.62282100	3.41681200	0.21718100
C	2.34169900	1.12331400	-1.29360200
H	1.54337100	0.84063600	-1.97939800

H	3.28020700	1.15710300	-1.85283700
C	2.03740500	2.47449800	-0.65281300
H	1.92602800	3.24549800	-1.41839700
H	1.11122300	2.40351600	-0.08017000
H	2.84199400	2.77643700	0.02245900
C	3.81347800	-0.21354500	0.20183500
C	4.54724000	-1.24475100	-0.65190800
H	5.56549500	-1.39365900	-0.28638000
H	4.02659500	-2.20420900	-0.63018900
H	4.60090000	-0.91541900	-1.69169000
H	4.36242400	0.73247600	0.20027900
H	3.76648800	-0.53544000	1.24125000
O	-0.95589000	-0.11634700	2.05833800
H	-2.40976800	-2.64390000	-0.27662000
N	-2.79796100	-2.95807700	-1.28276100
H	-2.43646600	-2.03682000	-1.73089100
H	-3.80644000	-3.04872000	-1.31569400
H	-2.35033000	-3.78753900	-1.65370400
O	-0.43599000	1.19480000	2.24923300
H	-1.23674600	1.73260800	2.17157700

H₂O₂/H₂O

²IM1

Coordinates (Angstroms)			
	X	Y	Z

P	1.02205800	-0.98433300	0.73859700
N	-0.48568100	-0.46109100	0.83544700
O	1.51757600	-1.92709700	-0.29705800
C	-1.43944800	-0.56284800	-0.05710300
F	1.29733100	-1.60432200	2.16939700
C	-1.37566200	-1.41934300	-1.29734800
H	-0.51359500	-2.07794200	-1.25037200
H	-2.28400300	-2.01282700	-1.40599600
H	-1.26736100	-0.76844800	-2.16716600
N	-2.56434200	0.12791100	0.16060000
O	1.89879400	0.35667300	0.81325300
C	3.34559400	0.26957600	0.84103900
H	3.65676200	-0.62478700	0.29732500
H	3.64478200	0.17932700	1.88735300
C	3.89925800	1.51705700	0.19321600
H	4.98970200	1.50442900	0.24622700

H	3.59765900	1.55719800	-0.85392900
H	3.53964900	2.41040200	0.70778500
C	-2.67816600	0.99385900	1.33958900
H	-2.16590500	0.50661200	2.16692500
H	-3.74083200	1.06158500	1.58434300
C	-2.08600900	2.37262000	1.07482800
H	-2.18335800	3.00147400	1.96182800
H	-1.03117200	2.28087400	0.81701200
H	-2.59538600	2.86761600	0.24488200
C	-3.69286600	0.15461700	-0.76860700
C	-4.78768100	-0.83511200	-0.38104800
H	-5.63287800	-0.75378200	-1.06702900
H	-4.41478100	-1.86053000	-0.41194600
H	-5.14883200	-0.63817400	0.63023300
H	-4.08438600	1.17470000	-0.75982100
H	-3.33798300	-0.02994600	-1.78046400
O	0.39859400	0.97384000	-1.76991000
H	1.22550600	0.64222300	-2.16952100
O	0.81531400	2.14718700	-1.08277700
H	1.13341300	1.77494200	-0.24347200
O	2.67204100	-0.48721100	-2.28337900
H	3.08548600	-0.91999700	-3.03228300
H	2.34214300	-1.18848900	-1.68620500

²TS1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.10177900	-0.01216500	-0.55780800
N	-0.46612500	-0.40980200	-0.51423500
O	1.73459400	1.30715000	-1.04193500
C	-1.49334800	0.36170400	-0.32107900
F	1.43763200	-0.88284900	-1.88518100
C	-1.46483100	1.86967900	-0.39773500
H	-0.52543800	2.19755000	-0.83424000
H	-2.29178600	2.24633700	-1.00092700
H	-1.53517900	2.28386500	0.60965000
N	-2.67819000	-0.22442400	-0.06625100
O	1.99009600	-0.91590200	0.43838200
C	3.06895300	-1.76611600	-0.00594200
H	2.68598500	-2.47059500	-0.74366500
H	3.35858600	-2.31310400	0.89129700
C	4.22354900	-0.95038500	-0.55192500

H	5.06247400	-1.61053400	-0.78232100
H	3.92883000	-0.43045700	-1.46447200
H	4.54711600	-0.21203400	0.18414100
C	-2.74340100	-1.68249600	0.06187500
H	-2.08850800	-2.11757100	-0.69165200
H	-3.77050200	-1.98126900	-0.16060100
C	-2.32882700	-2.13437800	1.45808900
H	-2.36317200	-3.22316000	1.53150300
H	-1.31368400	-1.79382500	1.66616800
H	-2.99560000	-1.71789100	2.21704100
C	-3.91688800	0.50973800	0.17362500
C	-4.77796300	0.62628300	-1.08116300
H	-5.71535400	1.13856000	-0.85565400
H	-4.25511000	1.18597300	-1.85910100
H	-5.01540300	-0.36190700	-1.48011000
H	-4.45988400	-0.02775400	0.95550100
H	-3.68867200	1.49350500	0.58017500
O	0.78195900	1.03947800	1.19886400
H	1.76356000	1.80279200	1.29133900
O	0.55743700	0.24284400	2.34648400
H	1.20657000	-0.46565300	2.21587800
O	2.65829000	2.40458900	0.85592900
H	2.54310600	3.35285300	0.94786800
H	2.28440800	1.96257100	-0.21691200

²IM2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.21522400	0.12144100	-0.40960200
N	-0.33930300	-0.38393000	-0.47048700
O	1.83005100	1.39886700	-1.15159400
C	-1.41774900	0.30557800	-0.28765600
F	1.61193200	-0.76842200	-1.73358900
C	-1.49186400	1.81603300	-0.32161300
H	-0.60879200	2.21563200	-0.81306900
H	-2.37767700	2.16006400	-0.85511700
H	-1.51748500	2.19774200	0.70196700
N	-2.57296600	-0.36447800	-0.07882000
O	2.13798300	-0.78279300	0.56470000
C	2.63651900	-2.09285900	0.23899600
H	1.90867600	-2.61767200	-0.38007200
H	2.71116100	-2.60209400	1.20146200

C	3.98960500	-2.00632600	-0.43578300
H	4.38356800	-3.01090400	-0.60620400
H	3.90175000	-1.49597900	-1.39449500
H	4.69203800	-1.46074100	0.19666600
C	-2.54044200	-1.82585200	-0.00690900
H	-1.85800700	-2.18624200	-0.77576300
H	-3.54514300	-2.18497000	-0.24264600
C	-2.09535600	-2.30900700	1.36961300
H	-2.06800500	-3.40011900	1.40129400
H	-1.09903100	-1.92078700	1.58533900
H	-2.78068400	-1.95998600	2.14597200
C	-3.85616600	0.27682200	0.18747000
C	-4.72146700	0.39955700	-1.06395400
H	-5.69080700	0.83861000	-0.81926800
H	-4.23432400	1.02801000	-1.81208600
H	-4.89311700	-0.58157200	-1.51126900
H	-4.36731700	-0.33036800	0.93954300
H	-3.69390200	1.25176500	0.64485100
O	0.99198400	1.19094100	0.99415400
H	1.59341600	2.99409900	1.15112400
O	0.43251000	0.53535600	2.11662800
H	1.14054700	-0.08462800	2.34775900
O	2.04751100	3.59105000	0.53638700
H	1.56994800	4.42240100	0.53985300
H	1.94453100	2.20972500	-0.61755000

²TS2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.03260200	0.19543100	-0.41184500
N	-0.51879600	-0.26284300	-0.53208600
O	1.55684100	1.58084300	-1.06706100
C	-1.57564300	0.43409600	-0.23876500
F	1.45777200	-0.62704500	-1.79208100
C	-1.60882800	1.94074800	-0.12673800
H	-0.71922200	2.36722200	-0.58176700
H	-2.49425500	2.35329400	-0.61047200
H	-1.60993900	2.22144700	0.92921900
N	-2.73435100	-0.22857000	-0.05766200
O	2.00345100	-0.74310500	0.47952300
C	2.78248500	-1.86718400	0.03144400
H	2.19093000	-2.47670500	-0.65058900

H	2.97233200	-2.43538800	0.94313600
C	4.08094400	-1.40262700	-0.59595700
H	4.73241200	-2.25971200	-0.78115300
H	3.88671600	-0.90711600	-1.54812600
H	4.58568100	-0.70288200	0.07197600
C	-2.73741700	-1.69159500	-0.12107400
H	-2.08020200	-1.99564700	-0.93463500
H	-3.75586100	-2.00327000	-0.36489700
C	-2.27591300	-2.30634900	1.19604500
H	-2.27426700	-3.39609300	1.12878900
H	-1.26615900	-1.96170500	1.42288100
H	-2.93606100	-2.01335400	2.01608500
C	-3.99638800	0.41354900	0.29760200
C	-4.88395500	0.66797300	-0.91756100
H	-5.83683700	1.10434600	-0.61154500
H	-4.39745900	1.35154700	-1.61601700
H	-5.08875500	-0.26430800	-1.44776300
H	-4.50390600	-0.24998700	1.00281200
H	-3.79925700	1.33852300	0.83689700
O	0.86431900	1.17257500	1.04800100
H	2.81585400	1.66266600	1.12127000
O	0.29120500	0.43909300	2.12111600
H	0.98889300	-0.20307300	2.31866000
O	3.71968900	1.72002200	0.77286200
H	4.05636200	2.56462800	1.07830500
H	2.50029900	1.57030200	-1.27392400

²IM3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.03284700	-0.14628000	-0.43159500
N	0.52689900	0.30044600	-0.52202600
O	-1.67040800	-1.44952400	-1.17406700
C	1.57403400	-0.42078900	-0.24874500
F	-1.41800100	0.74667900	-1.80520700
C	1.59319700	-1.93138600	-0.19573200
H	0.70816800	-2.33294900	-0.68097000
H	2.48390800	-2.33229900	-0.67908300
H	1.57184400	-2.25507600	0.84769500
N	2.73736800	0.22180800	-0.03315000
O	-1.95374100	0.78969600	0.49587500
C	-2.78658400	1.88913900	0.08636000

H	-2.24062100	2.52273100	-0.61151500
H	-2.96383100	2.44342800	1.00847200
C	-4.08715400	1.37688200	-0.49785000
H	-4.77745200	2.20805700	-0.65783000
H	-3.90720100	0.89141700	-1.45834400
H	-4.54080800	0.65589400	0.18451400
C	2.75737100	1.68658000	-0.04263000
H	2.11476800	2.02801300	-0.85298200
H	3.78262000	1.99423300	-0.26136000
C	2.28548800	2.25906500	1.28963200
H	2.30751000	3.35031100	1.26475100
H	1.26443400	1.92934700	1.48571700
H	2.92519800	1.92099800	2.10846000
C	3.98799600	-0.44601800	0.31744000
C	4.89124800	-0.66609800	-0.89269400
H	5.83531500	-1.12181700	-0.58784000
H	4.40989100	-1.32062100	-1.62189300
H	5.11265100	0.28210300	-1.38671600
H	4.49103900	0.18710900	1.05302100
H	3.77376700	-1.38713300	0.82104200
O	-0.90832500	-1.23942700	0.91548200
H	-2.82898600	-1.76013300	1.24328000
O	-0.31437600	-0.60907100	2.03804100
H	-1.00775200	0.01002700	2.31236800
O	-3.75455000	-1.88773400	0.99633100
H	-3.68084800	-2.18707300	0.08697600
H	-1.91114600	-1.22403800	-2.07873100

²TS3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.07032700	0.15177900	-0.69274700
N	0.37510200	-0.19163700	-0.11285900
O	-1.36496200	0.99823300	-1.98477400
C	1.56589600	0.22658100	-0.44545600
F	-0.65614100	2.32844000	-0.23216000
C	1.79234200	1.28705700	-1.48836900
H	1.21202900	2.15607600	-1.16839800
H	2.83288000	1.56465600	-1.62106300
H	1.38249000	0.94497600	-2.44094200
N	2.60676700	-0.31656600	0.20133100

O	-2.12977400	0.29785700	0.47976500
C	-1.87028100	0.95974000	1.74770100
H	-0.82111500	1.24564500	1.78073800
H	-2.07753100	0.20219800	2.50576200
C	-2.77304900	2.16342100	1.87370800
H	-2.62935100	2.62459400	2.85354300
H	-2.51371500	2.88291400	1.09849000
H	-3.82180000	1.87291900	1.78263100
C	2.35584400	-1.29455500	1.26881000
H	1.48920200	-0.95942700	1.83690800
H	3.22696800	-1.27279600	1.92752300
C	2.11647700	-2.69418100	0.71419600
H	1.99068200	-3.40445800	1.53363600
H	1.21068000	-2.70241000	0.10669300
H	2.96318000	-3.02227700	0.10597000
C	4.00965600	-0.05576100	-0.12385500
C	4.57658700	1.12558100	0.65554400
H	5.63525200	1.26220000	0.42689000
H	4.04405700	2.04513300	0.40551100
H	4.47570400	0.95915800	1.72998500
H	4.55862000	-0.96856300	0.11744600
H	4.11925100	0.08802500	-1.19773600
O	-1.61784500	-1.24305200	-1.35560700
H	-3.66356700	-0.86779400	0.39409200
O	-1.47344400	-2.33331700	-0.45244100
H	-2.39490200	-2.41379000	-0.12929700
O	-4.02243900	-1.76732800	0.37417400
H	-4.73544100	-1.75569800	-0.26827600
H	-1.16961000	1.91705300	-1.62137400

H₂O/NH₃

³IM1

	Coordinates (Angstroms)		
	X	Y	Z
P	1.41989200	0.41556700	-0.99289900
N	-0.06481300	-0.20688500	-0.91867200
O	1.70343800	1.85608500	-0.86607800
C	-1.14622200	0.36881100	-0.46493300
F	1.95292700	-0.16638800	-2.36897600
C	-1.32262400	1.85823800	-0.30248100

H	-2.29108900	2.18253500	-0.68379700
H	-1.25408600	2.10157000	0.76054900
H	-0.52834600	2.38309400	-0.82526600
N	-2.18279900	-0.41789200	-0.14069200
O	2.30247000	-0.43238600	0.04243300
C	2.37219400	-1.86891700	-0.04557400
H	3.11956300	-2.12337200	-0.80020200
H	1.40043900	-2.25464400	-0.36609400
C	2.75371500	-2.39741000	1.31898800
H	2.85399800	-3.48397700	1.28402100
H	3.70407500	-1.96931600	1.64057800
H	1.98961400	-2.14527100	2.05762600
C	-2.02635300	-1.87355600	-0.19525000
H	-1.44159700	-2.11961300	-1.07987600
H	-3.02380100	-2.30292600	-0.31496600
C	-1.34902800	-2.39705700	1.06736900
H	-1.19486300	-3.47616100	1.00073500
H	-0.38643700	-1.90107900	1.19823200
H	-1.95306800	-2.18770600	1.95277600
C	-3.42866600	0.07775200	0.44034800
C	-4.52880700	0.24406900	-0.60358200
H	-5.45825900	0.56723400	-0.13085100
H	-4.24470300	0.98602500	-1.35229200
H	-4.71749500	-0.69939400	-1.11989900
H	-3.73407900	-0.64594400	1.20009400
H	-3.24160700	1.01145400	0.96703000
O	0.33803500	0.60045600	2.14830400
H	0.62704100	4.09856200	1.58616700
N	1.23175700	3.29063100	1.68627800
H	2.04983900	3.59727200	2.20156700
H	1.53767600	3.01028200	0.75214400
H	0.58570000	1.54647500	2.16441900
H	1.14095000	0.16310200	1.84659200

³TS1

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.22803100	0.35484600	0.48560000
N	0.30066700	-0.26856600	0.31519800
O	-1.61487300	1.75735600	0.93377500
C	1.37846600	0.38970700	0.07508300
F	-1.38401200	-0.34115400	1.98097800

C	1.47155000	1.89555600	-0.03518400
H	2.35802900	2.28122300	0.46875300
H	1.51231100	2.17561800	-1.09058100
H	0.58558800	2.34535100	0.40572700
N	2.53545400	-0.31176400	-0.09789800
O	-2.32137400	-0.65995800	-0.16783100
C	-2.73954600	-1.87511400	0.46767600
H	-3.30647900	-1.63907100	1.36898700
H	-1.85796700	-2.44947900	0.76150600
C	-3.58270100	-2.63088600	-0.53730100
H	-3.93909700	-3.56572300	-0.09945900
H	-4.44720800	-2.03489200	-0.83483400
H	-2.99920700	-2.86486500	-1.42956800
C	2.50453100	-1.76706500	0.01739600
H	1.82337400	-2.02686300	0.82754100
H	3.50948000	-2.09514900	0.29589200
C	2.05965500	-2.43601900	-1.27982400
H	2.06689900	-3.52305700	-1.17393300
H	1.04627700	-2.11531600	-1.52460000
H	2.72416800	-2.16835100	-2.10541800
C	3.81378900	0.29212400	-0.44688900
C	4.70392700	0.54086100	0.76924400
H	5.66972100	0.94963500	0.46399700
H	4.23027500	1.24364900	1.45744100
H	4.88241300	-0.38947600	1.31234200
H	4.31553800	-0.38738700	-1.14250500
H	3.64711300	1.21843100	-0.99558300
O	-1.11942600	1.00698400	-1.33331000
H	-2.03765400	3.95264500	-1.27827800
N	-2.45161700	3.05846100	-1.04374700
H	-3.44839000	3.06696300	-1.22475300
H	-2.20753900	2.71417200	-0.02636300
H	-1.90247800	2.15208100	-1.47050100
H	-1.25275500	0.27058900	-1.93576000

³IM2

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.27705900	0.29769000	0.33513100
N	0.26459000	-0.31135600	0.25263100
O	-1.67095200	1.71420600	0.95920400
C	1.35888300	0.33360500	0.05774800

F	-1.44369200	-0.32646800	1.86844200
C	1.47442600	1.84063500	-0.03119800
H	2.35655400	2.20886100	0.49219300
H	1.53775900	2.13838700	-1.08087200
H	0.59315300	2.30478300	0.40258800
N	2.51328800	-0.37798200	-0.08137100
O	-2.37058900	-0.75320600	-0.23867700
C	-2.79982500	-1.93325400	0.45504900
H	-3.36826900	-1.64499300	1.33943900
H	-1.92301700	-2.49656100	0.78149000
C	-3.64459500	-2.73062800	-0.51531200
H	-4.01030900	-3.63910400	-0.03219700
H	-4.50212500	-2.14258200	-0.84605600
H	-3.05949100	-3.01383700	-1.39196900
C	2.46376700	-1.83406200	0.02121700
H	1.74709800	-2.09207900	0.80069700
H	3.45305700	-2.17332000	0.33920900
C	2.06772300	-2.49044400	-1.29786000
H	2.06336000	-3.57805900	-1.19919600
H	1.06735400	-2.16246800	-1.58288100
H	2.76742100	-2.22250900	-2.09368000
C	3.80976400	0.21456000	-0.38281000
C	4.66011200	0.44700000	0.86438600
H	5.63974400	0.84716700	0.59423400
H	4.17142700	1.15077400	1.54098800
H	4.81061900	-0.48827100	1.40734400
H	4.32722800	-0.46709600	-1.06439100
H	3.67229500	1.14494000	-0.93288600
O	-1.24164100	1.01192200	-1.23303300
H	-1.34312200	4.55849500	-0.92065400
N	-1.95547000	3.75186400	-0.89048600
H	-1.67677600	3.09268600	-1.61335400
H	-2.89794900	4.06803600	-1.08818500
H	-1.80083900	2.45175300	0.31057800
H	-1.30898700	0.32233100	-1.89807900

³TS2

	Coordinates (Angstroms)		
	X	Y	Z
P	1.08032700	-0.48297000	0.03143500
N	-0.44729600	0.10873000	0.22318900
O	1.41618700	-2.03191700	0.29916300

C	-1.54683800	-0.47630200	-0.11347000
F	1.39300200	-0.17092800	1.66595700
C	-1.65584100	-1.90138000	-0.60845900
H	-2.48695600	-2.42309500	-0.13315800
H	-1.81445800	-1.89770400	-1.68953100
H	-0.73380000	-2.44094000	-0.41142300
N	-2.70369600	0.23133800	-0.01329700
O	2.21399000	0.64060000	-0.34434900
C	2.67931900	1.66226100	0.54871000
H	3.27499400	1.20987000	1.34311000
H	1.82271200	2.15429900	1.01294900
C	3.49799900	2.63040400	-0.27919700
H	3.88759800	3.42876800	0.35587300
H	4.34142900	2.11949600	-0.74817800
H	2.88692400	3.07679800	-1.06522700
C	-2.65674400	1.60592200	0.47940500
H	-1.91134100	1.65416800	1.27306300
H	-3.63460500	1.83169200	0.91227600
C	-2.31585300	2.59937800	-0.62698000
H	-2.31122100	3.61992900	-0.23822200
H	-1.32672400	2.37446400	-1.02783700
H	-3.04561400	2.54582000	-1.43880200
C	-4.01352200	-0.28664800	-0.38821200
C	-4.78881600	-0.85066300	0.80055600
H	-5.78004100	-1.18662500	0.48871300
H	-4.25827000	-1.69647200	1.24192000
H	-4.91322700	-0.09178300	1.57574300
H	-4.57097000	0.53927600	-0.83969300
H	-3.90236600	-1.04035300	-1.16647500
O	0.96388800	-0.81229000	-1.62787200
H	4.73181300	-2.45043700	-0.48707100
N	4.15256800	-1.79178200	0.02120800
H	4.04271700	-0.95880800	-0.55306600
H	4.64960300	-1.52367600	0.86381900
H	2.39486100	-2.17602300	0.28798400
H	0.95324600	0.00725600	-2.12925200

³IM3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.24563800	-0.34009500	0.46991600
N	0.24034700	0.13518300	-0.09429800

O	-1.61912500	-1.86681700	0.75846500
C	1.38033500	-0.28922400	0.33390000
F	-1.73027200	-0.61178300	-1.17379700
C	1.57907700	-1.41533700	1.32580400
H	2.38970300	-2.07620200	1.01719800
H	1.81897100	-0.99650600	2.30587500
H	0.66395400	-1.99029300	1.43480600
N	2.50527100	0.31151300	-0.14385700
O	-2.28795400	0.90215000	0.52414000
C	-2.77005700	1.62185800	-0.61707800
H	-3.49248000	1.00553400	-1.15273600
H	-1.93510600	1.83186800	-1.28905100
C	-3.40354200	2.89542700	-0.09862200
H	-3.80967800	3.47592300	-0.92976500
H	-4.21453700	2.66318000	0.59339600
H	-2.66592100	3.50614000	0.42482400
C	2.37390700	1.39759200	-1.11212800
H	1.56369400	1.14403700	-1.79544800
H	3.30493900	1.44022800	-1.68332800
C	2.09404700	2.73738500	-0.43797700
H	2.02749100	3.53449100	-1.18159300
H	1.14805900	2.68349800	0.10218800
H	2.88878500	2.99364700	0.26721800
C	3.85586600	-0.00903000	0.29997100
C	4.56972800	-0.98435700	-0.63361000
H	5.59287000	-1.16221400	-0.29558400
H	4.04441400	-1.94079300	-0.66792300
H	4.60963500	-0.58665200	-1.64980700
H	4.41226400	0.93156200	0.35204100
H	3.82758800	-0.40172300	1.31540600
O	-0.95523200	-0.15089700	2.10664200
H	-1.71537700	-4.09675200	-1.81238600
N	-2.30961200	-3.34742200	-1.47725400
H	-3.27032600	-3.66666100	-1.52865900
H	-2.20505500	-2.54890000	-2.09741700
H	-1.86622700	-2.39678000	-0.04178500
H	-1.09034900	0.76456000	2.36030800

³TS3

	Coordinates (Angstroms)		
	X	Y	Z
P	-1.39584200	-0.20792900	-0.82538400

N	0.21093200	-0.39843200	-0.76392300
O	-2.13963100	1.08154200	-1.23786700
C	1.13164700	0.48610000	-0.50846900
F	-0.90541500	1.12273200	1.04792700
C	0.97871700	1.97042400	-0.72227200
H	1.20869300	2.51403700	0.19316100
H	1.65471700	2.29252400	-1.51919100
H	-0.04200200	2.19532600	-1.00779400
N	2.33881500	0.04123900	-0.11237600
O	-2.10458800	-1.08400200	0.29038400
C	-1.64548800	-1.29574700	1.63782500
H	-2.06731300	-0.51455400	2.26566200
H	-0.56120000	-1.18556400	1.66564600
C	-2.09755800	-2.68171400	2.04484300
H	-1.80464300	-2.87651900	3.07898200
H	-3.18258600	-2.76978700	1.96983000
H	-1.64540400	-3.44223500	1.40541500
C	2.55029500	-1.38967500	0.10926100
H	1.63297300	-1.80971400	0.51999300
H	3.33782000	-1.49006200	0.85957000
C	2.93601000	-2.10781300	-1.17907700
H	3.10262000	-3.17014600	-0.98970000
H	2.13519100	-2.00280100	-1.91172600
H	3.85276200	-1.68770900	-1.59970400
C	3.45637400	0.92211400	0.21602100
C	3.48330800	1.27939900	1.70020600
H	4.32882500	1.93405500	1.92071200
H	2.55944300	1.78455300	1.98779400
H	3.57794200	0.38122100	2.31379800
H	4.37471800	0.40223600	-0.06989600
H	3.40581100	1.82203700	-0.39373200
O	-1.77958000	-1.08304500	-2.12847400
H	-2.54371600	3.80791100	0.32543900
N	-2.75070000	2.83264600	0.50295900
H	-3.65893000	2.76844000	0.94665600
H	-2.02090000	2.40045300	1.09873800
H	-2.43273700	1.82733000	-0.53325700
H	-1.28848300	-1.90934400	-2.14596500

H₂O/H₂O

⁴IM1

Coordinates (Angstroms)

	X	Y	Z
P	1.15241500	-0.07229100	-1.16081200
N	-0.38987500	-0.43144000	-0.93408500
O	1.66111100	1.31402000	-1.32495200
C	-1.32152100	0.35210600	-0.44846600
F	1.55278000	-0.93035700	-2.42672800
C	-1.23433500	1.85704400	-0.39602900
H	-0.44479100	2.20282700	-1.05709500
H	-2.17967300	2.31677800	-0.68324700
H	-0.98578800	2.15087300	0.62646800
N	-2.43497500	-0.22709600	0.01094400
O	1.89723600	-0.85804800	0.01889700
C	3.33106700	-0.75566300	0.17489700
H	3.66565300	0.20698500	-0.21785700
H	3.78314200	-1.56050300	-0.40907700
C	3.64489100	-0.87819900	1.64817900
H	4.72634800	-0.86973400	1.79856400
H	3.21173600	-0.03623600	2.18998700
H	3.24690100	-1.81279200	2.04752600
C	-2.54801300	-1.68978600	0.00738700
H	-2.15454500	-2.05962200	-0.93828200
H	-3.61400500	-1.92386800	0.05109700
C	-1.80080400	-2.31693300	1.17927800
H	-1.98669200	-3.39218400	1.21188800
H	-0.72950600	-2.15290200	1.06081400
H	-2.12000400	-1.87920300	2.12764600
C	-3.50382800	0.50353900	0.69024500
C	-4.67650200	0.81143300	-0.23531700
H	-5.47514500	1.31158500	0.31567000
H	-4.36414300	1.45925800	-1.05658700
H	-5.08148000	-0.10650500	-0.66619500
H	-3.83184700	-0.12254800	1.52370500
H	-3.09850800	1.41123600	1.13270800
O	0.21176000	0.51040500	2.10219800
H	0.90344500	1.18043000	1.98363400
O	2.27426500	2.22313800	1.16464500
H	2.59099300	3.11928800	1.28882300
H	2.12446800	2.10042300	0.20651600
H	0.62544700	-0.29363200	1.77067700

⁴TS1

Coordinates (Angstroms)

	X	Y	Z
P	1.21340200	0.03741600	-0.29467300
N	-0.35431800	-0.42452500	-0.24570700
O	1.75968900	1.35684700	-0.87706600
C	-1.40231300	0.32286600	-0.13117300
F	1.53317400	-0.84570600	-1.63016100
C	-1.39764200	1.83456500	-0.15736500
H	-0.46241400	2.19014000	-0.58146900
H	-2.22332600	2.22643600	-0.75084400
H	-1.47871700	2.21143000	0.86448600
N	-2.60274900	-0.28700700	0.01094400
O	2.15560700	-0.84726400	0.66648600
C	3.11195700	-1.81625500	0.19426400
H	2.62151000	-2.50670600	-0.49098500
H	3.40203000	-2.35673600	1.09548000
C	4.30646900	-1.14221300	-0.45054500
H	5.04695100	-1.89416700	-0.73223800
H	4.00162400	-0.60013000	-1.34641000
H	4.76847200	-0.44074300	0.24636800
C	-2.66262000	-1.74885000	0.03496100
H	-1.94603000	-2.12810200	-0.69269400
H	-3.66583800	-2.03744400	-0.28807000
C	-2.35734000	-2.30678100	1.42109900
H	-2.42958900	-3.39623600	1.41813200
H	-1.34548800	-2.02459600	1.71395100
H	-3.06097000	-1.91941000	2.16220500
C	-3.86298400	0.42214900	0.20352600
C	-4.63949900	0.60774300	-1.09772900
H	-5.59584400	1.09900600	-0.90715100
H	-4.07194600	1.21528800	-1.80523500
H	-4.83855900	-0.35674600	-1.56910800
H	-4.45503100	-0.16311000	0.91265800
H	-3.67656900	1.38207500	0.68308100
O	0.89573800	1.01767400	1.43846800
H	1.46152200	2.07399900	1.35030600
O	2.08975500	2.95995500	0.84363900
H	1.61863200	3.79284700	0.78154400
H	1.99285700	2.25108900	-0.15046300
H	1.25411100	0.47563600	2.14690000

⁴IM2

Coordinates (Angstroms)

	X	Y	Z
P	1.26429700	0.12497100	-0.15650600
N	-0.29922700	-0.40872900	-0.14937800
O	1.77939100	1.42319200	-0.94711300
C	-1.37795500	0.29217600	-0.11045300
F	1.55933200	-0.72713900	-1.54769000
C	-1.43487800	1.80213500	-0.20436700
H	-0.50814200	2.18236700	-0.62513700
H	-2.26260100	2.13626200	-0.82929900
H	-1.55684700	2.22231900	0.79710900
N	-2.56508300	-0.35848300	0.01853000
O	2.27249600	-0.81308200	0.68925300
C	2.93523600	-1.99436300	0.20770000
H	2.24949200	-2.57551300	-0.40775200
H	3.16311400	-2.55793800	1.11354600
C	4.20168200	-1.64153900	-0.54548500
H	4.72761200	-2.55430400	-0.83492900
H	3.96116300	-1.07531000	-1.44522000
H	4.86291900	-1.04572600	0.08626400
C	-2.57007100	-1.81824900	0.09162900
H	-1.80890600	-2.19192100	-0.59279200
H	-3.54657900	-2.15880600	-0.26197500
C	-2.30252300	-2.32201700	1.50632100
H	-2.33664500	-3.41299800	1.53700900
H	-1.31356600	-1.99551500	1.82986100
H	-3.04842900	-1.93709600	2.20635100
C	-3.85577600	0.30786900	0.14250000
C	-4.59513700	0.41884000	-1.18898900
H	-5.57513900	0.87947700	-1.04776700
H	-4.02681100	1.02194700	-1.89973300
H	-4.74194500	-0.56853700	-1.63126300
H	-4.45159900	-0.27274300	0.85264500
H	-3.72290200	1.29101800	0.59271900
O	1.08836000	1.08076300	1.28579700
H	1.41236300	2.89098200	1.33665500
O	1.77474300	3.61014600	0.79183900
H	1.14704400	4.33417600	0.81455200
H	1.88262300	2.22736600	-0.40616400
H	1.22211200	0.52340000	2.05671000

⁴TS2

Coordinates (Angstroms)

	X	Y	Z
P	1.10199200	0.33016700	-0.11324400
N	-0.44147500	-0.22323500	-0.16766600
O	1.46016400	1.77270500	-0.76679400
C	-1.52650800	0.46095700	-0.00153500
F	1.43718600	-0.36998200	-1.60645000
C	-1.59327900	1.96688500	0.12073000
H	-0.65200800	2.41535700	-0.18264200
H	-2.39874800	2.37587400	-0.48964700
H	-1.77183900	2.23898200	1.16378400
N	-2.69976800	-0.21505100	0.06116600
O	2.16458900	-0.69715700	0.57678800
C	2.65058300	-1.92250500	-0.00136000
H	1.88161900	-2.36244100	-0.63448900
H	2.81821500	-2.57471400	0.85746000
C	3.93883700	-1.69380500	-0.76503600
H	4.32157400	-2.64507500	-1.14161400
H	3.76495100	-1.02932900	-1.61109600
H	4.70121100	-1.25852400	-0.11452400
C	-2.69404600	-1.67149700	-0.07114600
H	-1.94697000	-1.93956300	-0.81775000
H	-3.67644100	-1.96784200	-0.44659200
C	-2.39256600	-2.36404400	1.25385500
H	-2.42075200	-3.44889400	1.13334800
H	-1.39829500	-2.07844300	1.59928100
H	-3.12455500	-2.08558800	2.01602700
C	-3.99762900	0.41755300	0.27125000
C	-4.74185200	0.68368200	-1.03506000
H	-5.72474300	1.11509800	-0.83501800
H	-4.18127200	1.37547300	-1.66652100
H	-4.88309100	-0.24261100	-1.59551000
H	-4.58332600	-0.25312200	0.90627700
H	-3.87057900	1.33942200	0.83672800
O	1.00764900	1.11783100	1.39745200
H	2.97739200	1.99327200	1.23774900
O	3.81355400	1.80733500	0.78751300
H	3.94195000	0.87062600	0.96548500
H	2.40060000	1.86967700	-0.96984800
H	0.92037400	0.46863200	2.10145000

⁴IM3

Coordinates (Angstroms)

	X	Y	Z
P	1.08515100	-0.34833700	0.13931700
N	-0.45794100	0.22189700	0.17138600
O	1.55979500	-1.74601100	0.82390500
C	-1.54179700	-0.46358400	0.00058900
F	1.37479600	0.36912600	1.66184100
C	-1.61013900	-1.97177200	-0.10267400
H	-0.67207600	-2.41871200	0.21278700
H	-2.42301600	-2.37153900	0.50401800
H	-1.77665000	-2.25920500	-1.14344200
N	-2.71410200	0.21120900	-0.08316400
O	2.13029600	0.68114200	-0.54562700
C	2.64400300	1.89757000	0.03280900
H	1.87913900	2.35396900	0.65955700
H	2.82926100	2.54197200	-0.82770400
C	3.92308500	1.63379500	0.79966800
H	4.35082200	2.57963200	1.13980900
H	3.72280000	1.00831500	1.66898500
H	4.65473800	1.13088500	0.16453900
C	-2.70963000	1.66978100	0.02791500
H	-1.97195600	1.94851300	0.77985400
H	-3.69676900	1.97102000	0.38665000
C	-2.39106600	2.34289400	-1.30300000
H	-2.42197200	3.42928100	-1.19858100
H	-1.39209100	2.05361400	-1.63117800
H	-3.11273400	2.05284300	-2.07064900
C	-4.00846500	-0.42264500	-0.31176000
C	-4.77841800	-0.67378600	0.98249000
H	-5.75837500	-1.10470800	0.76775400
H	-4.23250000	-1.36093200	1.63172500
H	-4.92806400	0.25846500	1.53070800
H	-4.58088900	0.24178700	-0.96507900
H	-3.87192200	-1.35060600	-0.86495500
O	1.01029200	-1.21120200	-1.29578900
H	3.30319900	-2.13994000	-0.87844500
O	4.05850300	-1.57707500	-1.07950800
H	3.64415000	-0.71890200	-1.21336300
H	1.77045400	-1.60664000	1.75283100
H	1.00180600	-0.61628700	-2.04977000

⁴TS3

Coordinates (Angstroms)

	X	Y	Z
P	1.33979400	-0.12231100	-0.82422000
N	-0.15202900	0.40317900	-0.52174200
O	1.73074700	-1.26462300	-1.84316800
C	-1.30912700	-0.17770600	-0.65312000
F	0.60007600	-2.05558500	0.02553900
C	-1.58502400	-1.34555300	-1.56543800
H	-0.67614100	-1.64283500	-2.07432000
H	-1.95102400	-2.19802700	-0.99303400
H	-2.32919600	-1.06251400	-2.31314100
N	-2.34818600	0.34300700	0.02345500
O	2.20766200	-0.06746900	0.51913700
C	1.75822000	-0.50472200	1.82539500
H	0.68853100	-0.69930600	1.78576900
H	1.95588800	0.34336400	2.48664100
C	2.52529200	-1.73701900	2.24426100
H	2.24843600	-2.01071600	3.26526500
H	2.27084300	-2.55651700	1.57424200
H	3.60058200	-1.55043200	2.21617400
C	-2.13067800	1.48001200	0.92253800
H	-1.16692800	1.34751400	1.41309100
H	-2.91185500	1.44200700	1.68491600
C	-2.16684700	2.80672400	0.17292100
H	-2.02360200	3.63763800	0.86620700
H	-1.36890000	2.83154400	-0.56951000
H	-3.12618100	2.94265300	-0.33225000
C	-3.70395200	-0.19898500	-0.02324200
C	-3.96229300	-1.19508800	1.10438600
H	-4.98858700	-1.56441800	1.05855400
H	-3.28085100	-2.04436500	1.02936500
H	-3.81134300	-0.72685500	2.07906700
H	-4.39278400	0.64686600	0.04833200
H	-3.88139600	-0.66455300	-0.99043800
O	2.03162000	1.07134300	-1.62582600
H	3.66414900	3.12783900	0.53656000
O	2.82740300	2.65985400	0.49922900
H	3.01057200	1.74382400	0.75086300
H	1.40624800	-2.07062300	-1.36523700
H	2.13444500	1.88072000	-1.09685000

