

Supporting information for:

The Origin of Experimental Regioselectivity in Ring-Closing Reaction of pyrido[1,2-e]purine Systems and Comparison the Aromaticity Character of Probable Products; A Mechanistic Study Based on the DFT Insights

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Table 1(S). Absolute energy values of the involved species							
M06-2X/ def2svp							M06-2X/def2tzvp
	species	G (a.u)	H (a.u)	S (cal.mol ⁻¹ .K ⁻¹)	E (a.u)	E (a.u)	
H	Triethyl orthoformate	-501.24108	-501.186693	114.466	-501.4329161	-502.0165008	
	(2)	-714.620387	-714.567052	112.251	-714.7857728	-715.5818295	
	In1	-1215.856901	-1215.769522	183.905	-1216.237153	-1217.6104286	
	In2	-1061.06581	-1060.992061	155.218	-1061.371233	-1062.563457	
	In3	-906.277883	-906.212816	136.945	-906.5020799	-907.5152981	
	In4(1)	-906.25389	-906.192375	129.468	-906.4823198	-907.4951235	
	Product	-906.277168	-906.212552	135.996	-906.5005672	-907.51832	
	TS1	-1215.821742	-1215.735412	181.697	-1216.200203	-1217.5763216	
	TS2	-1061.035641	-1060.962404	154.14	-1061.338378	-1062.5314059	
	TS3	-906.221504	-906.161427	126.444	-906.448398	-907.464166	
	TS4	-906.226486	-906.164388	130.697	-906.4515584	-907.4667894	
		(2)	-714.619268	-714.565515	113.134	-714.7841545	-715.5801443
		In1	-1215.852929	-1215.761164	193.135	-1216.228345	-1217.6025359
		In2	-1061.065372	-1060.990726	157.104	-1061.369717	-1062.5619094
		In3	-906.277091	-906.211493	138.062	-906.5005704	-907.5136685
		In4(2)	-906.258098	-906.197037	128.514	-906.4869562	-907.5002493
		Product	-906.229665	-906.168376	128.992	-906.5057242	-907.5244821
		TS1	-1215.820252	-1215.733458	182.675	-1216.198244	-1217.5745523
		TS2	-1061.033589	-1060.961167	152.424	-1061.337161	-1062.5299702
	TS3	-906.223804	-906.163283	127.376	-906.4513942	-907.4670036	
	TS4	-906.229665	-906.168376	128.992	-906.455311	-907.4706269	
Me	Triethyl orthoacetate	-540.480037	-540.424141	117.643	-540.6989464	-541.3247782	
	In1	-1255.102023	-1255.012457	188.508	-1255.508495	-1256.9233119	
	In2	-1100.304012	-1100.228057	159.861	-1100.635699	-1101.8698464	
	In3	-945.519865	-945.45055	145.885	-945.7691436	-946.8261456	
	In4(1)	-945.502507	-945.437845	136.094	-945.7563207	-946.8100188	
	Product	-945.520878	-945.450643	147.821	-945.7692596	-946.8297875	
	TS1	-1255.070363	-1254.980968	188.146	-1255.474436	-1256.8918913	
	TS2	-1100.278996	-1100.203509	158.876	-1100.608523	-1101.8450633	
	TS3	-945.470332	-945.40523	137.019	-945.7222282	-946.781162	
	TS4	-945.47036	-945.404984	137.596	-945.7213481	-946.7770131	
		In1	-1255.095783	-1255.003381	194.478	-1255.499055	-1256.9149734
		In2	-1100.310224	-1100.233423	161.642	-1100.641201	-1101.8741671
		In3	-945.51862	-945.449018	146.491	-945.7674538	-946.8243744
		In4(1)	-945.495352	-945.433585	130.000	-945.752952	-946.8084141
		Product	-945.5295	-945.461062	144.04	-945.77969	-946.8383958
		TS1	-1255.068848	-1254.980718	185.485	-1255.474446	-1256.8922726
	TS2	-1100.277211	-1100.202466	157.315	-1100.607372	-1101.8437147	
	TS3	-945.472327	-945.408237	134.889	-945.725506	-946.784 1272	
	TS4	-945.470594	-945.408146	131.433	-945.7244007	-946.7819982	

Table 1(S). Continued							
M06-2X/ def2svp							M06-2X/def2tzvp
	species	G (a.u)	H (a.u)	S (cal.mol ⁻¹ .K ⁻¹)	E (a.u)	E (a.u)	
Et	Triethyl orthopropionate	-579.713485	-579.655095	122.893	-579.9599054	-580.6290839	
	In1	-1294.336745	-1294.242366	198.638	-1294.768341	-1296.2262269	
	In2	-1139.539562	-1139.463046	161.04	-1139.899805	-1141.1765908	
	In3	-984.754481	-984.682521	151.453	-985.0312357	-986.1315761	
	In4(1)	-984.741187	-984.672952	143.613	-985.0211995	-986.1177396	
	Product	-984.754793	-984.681933	153.348	-985.0306378	-986.1348968	
	TS1	-1294.30729	-1294.214875	194.502	-1294.738398	-1296.1983388	
	TS2	-1139.516165	-1139.437919	164.683	-1139.8 73061	-1141.1524828	
	TS3	-984.712319	-984.644175	143.42	-984.9913017	-986.0933512	
	TS4	-984.709151	-984.639488	146.617	-984.9859279	-986.0847775	
		In1	-1294.330445	-1294.236469	197.79	-1294.762575	-1296.2217513
		In2	-1139.538718	-1139.45897	167.845	-1139.896461	-1141.1714034
		In3	-984.752685	-984.680986	150.903	-985.0295876	-986.1299606
		In4(2)	-984.7338	-984.668758	136.892	-985.0178743	-986.1161398
		Product	-984.761029	-984.689278	151.011	-985.0375216	-986.1434799
		TS1	-1294.303252	-1294.214739	186.291	-1294.738637	-1296.1994276
		TS2	-1139.514631	-1139.436884	163.633	-1139.8 71885	-1141.1510154
	TS3	-984.690442	-984.637683	138.611	-984.984851	-986.0870275	
	TS4	-984.70904	-984.643128	138.724	-984.9891274	-986.0897466	

Table 2(S). Calculated thermodynamic and kinetic parameters of the step 4 as RDS of the reaction in wb97xd/6-31+g(d,p) level

wb97xd/6-31+g(d,p)						
Route	R	Step	ΔG^1	ΔH^1	ΔS^2	ΔG^{*1}
Route 1	H	4(1)	14.07	11.06	-10.102	31.77
	Me	4(1)	9.26	8.16	-3.696	27.09
	Et	4(1)	7.38	4.46	-9.79	24.40
Route 2	H	4(2)	10.90	7.06	-12.858	31.02
	Me	4(2)	11.85	8.53	-11.117	25.96
	Et	4(2)	10.45	6.67	-12.667	30.80

1) kcal.mol⁻¹

2) cal.mol⁻¹K⁻¹

Table 3(S). Absolute energy values of the involved species correspond to step 4 in wb97xd/6-31+g(d,p) level

			wb97xd/6-31+g(d,p)		
Route	R	Step	G (a.u)	H (a.u)	S (cal.mol⁻¹.K⁻¹)
Route 1	H	In3	-907.066255	-907.000782	137.800
		In4(1)	-907.043829	-906.983156	127.698
		TS3	-907.015628	-906.953816	130.094
	Me	In3	-946.348173	-946.282632	137.943
		In4(1)	-946.33341	-946.269625	134.247
		TS3	-946.305009	-946.240598	135.564
	Et	In3	-985.62681	-985.555624	149.823
		In4(1)	-985.615055	-985.548521	140.033
		TS3	-985.587922	-985.521007	140.833
Route 2	H	In3	-907.066232	-906.999345	140.775
		In4(1)	-907.048865	-906.988087	127.917
		TS3	-907.016801	-906.956127	127.699
	Me	In3	-946.347619	-946.27978	142.781
		In4(1)	-946.328742	-946.266184	131.664
		TS3	-946.306256	-946.242957	133.222
	Et	In3	-985.62482	-985.553811	149.451
		In4(1)	-985.608172	-985.543182	136.784
		TS3	-985.57574	-985.514955	138.457
1) kcal.mol ⁻¹					
2) cal.mol ⁻¹ K ⁻¹					

Cartesian coordinate of species

Route 1

H:

Triethyl orthoformate

O 1

C	-0.13221600	-0.15919500	0.25758700
H	-0.17851800	-0.12400400	1.37288600
O	-1.34124200	0.23206800	-0.27740500
O	0.14631900	-1.44225100	-0.16524300
O	0.85186900	0.69495300	-0.19760400
C	0.80009700	1.99380000	0.36758300
H	-0.15217400	2.47725500	0.09589300
H	0.83005500	1.91517800	1.46981900
C	1.27224400	-2.05574600	0.44568500
H	1.00095900	-3.10765200	0.61737400
H	1.45487200	-1.59703600	1.43290300
C	-2.46745100	-0.41466400	0.28985900
H	-2.45712800	-0.27577300	1.38654600
H	-2.40875000	-1.49738800	0.09310700
C	1.97868200	2.78878600	-0.14680800
H	1.94149700	2.86244100	-1.24241700
H	1.96467100	3.80397500	0.27119400
H	2.92349900	2.30585800	0.13885400
C	2.51122800	-1.96527000	-0.42569000
H	2.80282300	-0.91754100	-0.57053800
H	3.34454200	-2.50794800	0.04230500
H	2.31500900	-2.41499400	-1.40918100
C	-3.71803600	0.18040200	-0.31597100
H	-4.61062600	-0.30589000	0.09901700
H	-3.77449200	1.25689500	-0.10353900
H	-3.71908900	0.03979100	-1.40567500

(2)

O 1

C	3.30996600	-1.76224800	0.00210700
C	4.05657300	-0.53562900	0.00034600
C	3.42904900	0.67681400	-0.00131400
C	2.00113300	0.72771200	-0.00135100
N	1.32258800	-0.50608400	0.00024000
C	1.95225600	-1.72616700	0.00190800
N	1.18008600	1.75674700	-0.00291600
C	-0.07341100	1.19712100	-0.00232300

C	-0.02141800	-0.20261700	-0.00056500
C	-1.37708100	1.74482500	-0.00262900
N	-2.41343000	0.92624800	-0.00307000
C	-2.21767800	-0.42246800	-0.00152400
N	-1.04358000	-1.04772200	0.00016300
C	-1.59637600	3.22527700	0.00499100
N	-3.37472900	-1.14099200	-0.00220900
N	-3.39771900	-2.52179900	0.00188700
H	3.82233100	-2.72265500	0.00366300
H	5.14615100	-0.58043500	0.00045500
H	3.97749500	1.61789000	-0.00258200
H	1.29675600	-2.59695700	0.00328000
H	-1.19208700	3.65914300	0.93160000
H	-1.05837100	3.69401500	-0.83117500
H	-2.66571800	3.45055800	-0.06689900
H	-3.89225800	-2.86031600	0.82619500
H	-3.89337600	-2.86505000	-0.81975200
H	-4.23150400	-0.59669800	-0.00132400

In1

O 1

C	5.91352400	-1.75245800	0.19525800
C	6.59939900	-0.77634800	-0.60386800
C	5.97407200	0.36169500	-1.02467600
C	4.61069600	0.58775900	-0.66231600
N	3.98991900	-0.40207100	0.12334200
C	4.61741300	-1.54809100	0.54613500
N	3.80635300	1.59212100	-0.94043900
C	2.62356000	1.26587700	-0.32510100
C	2.70175700	0.03659400	0.34230200
C	1.36928300	1.91255000	-0.23800400
N	0.39790900	1.33178800	0.44267100
C	0.61020400	0.12710700	1.04846500
N	1.74566200	-0.56782700	1.03463100
C	1.12961800	3.23005300	-0.90640900
N	-0.47552900	-0.34299900	1.72262600
N	-0.54995000	-1.66332600	2.15019300
H	6.42319800	-2.65655800	0.52367800
H	7.64057100	-0.95393900	-0.87549100
H	6.47611300	1.11473500	-1.63065500
H	4.01100100	-2.22458700	1.14843500
H	1.83152100	3.98262500	-0.51866900
H	1.31500500	3.14380200	-1.98683700
H	0.10044400	3.56283700	-0.73428200
H	-0.79133700	-1.68122200	3.14000400
H	-1.31195100	-2.11516900	1.64003200
H	-1.34572300	0.16552300	1.56332200
C	-3.76591900	-0.71743100	0.41720200
H	-4.37253900	-1.36179200	1.08473300

O	-2.72008200	-1.50151700	-0.02630100
O	-3.24760000	0.36656100	1.10807800
O	-4.54708900	-0.23434000	-0.62031300
C	-5.33344600	-1.22795900	-1.25932300
H	-4.67972400	-2.04080100	-1.61876400
H	-6.03647700	-1.66494400	-0.52771800
C	-4.20278100	1.25511000	1.68172200
H	-3.85269900	1.47545900	2.70049000
H	-5.17563600	0.74441300	1.76497600
C	-1.91504800	-0.92602300	-1.05827800
H	-1.57778500	0.07572300	-0.74798100
H	-2.52202800	-0.81172800	-1.97064800
C	-6.07498200	-0.58510800	-2.40851400
H	-5.36521000	-0.16463600	-3.13445300
H	-6.69854600	-1.32904300	-2.92122300
H	-6.72354500	0.22336400	-2.04400000
C	-4.32332400	2.52691600	0.86709600
H	-4.69905000	2.29858500	-0.13838400
H	-5.01128500	3.23070500	1.35598900
H	-3.34001800	3.01009900	0.77559400
C	-0.74192100	-1.84751600	-1.30456800
H	-0.09372200	-1.42776900	-2.08644300
H	-0.14447100	-1.97586400	-0.39091800
H	-1.09111600	-2.83559200	-1.63640300

H	-2.75067600	0.20255900	-2.46420000
H	-1.84914600	2.19238900	-1.31577100
C	-3.21197400	0.03299100	-0.49251500
H	-3.73793600	0.99013900	-0.26412400
O	-2.53606800	-0.37998500	0.64880200
O	-4.11933400	-0.90650200	-0.94403000
C	-2.73963000	0.35405300	1.84564400
H	-2.64561200	-0.36944600	2.66831200
H	-3.76860100	0.75261900	1.88044300
C	-1.72427100	1.46941800	2.00236300
H	-1.83858100	2.22547700	1.21227100
H	-1.84476700	1.96438200	2.97626500
H	-0.70435400	1.06157200	1.93877500
C	-5.26257900	-1.10123600	-0.12652200
H	-6.09149300	-1.33316100	-0.81011700
H	-5.51829400	-0.15754200	0.38700300
C	-5.07861500	-2.23197300	0.87027800
H	-6.01574400	-2.40843200	1.41639000
H	-4.80704800	-3.15614500	0.34118700
H	-4.28581900	-2.00320400	1.59375600

In3

O 1

C	3.40641100	-3.01571100	-0.01153200
C	4.67828200	-2.35636700	0.08223400
C	4.76994100	-0.99528900	0.13363800
C	3.57695200	-0.21052000	0.09241700
N	2.35962000	-0.91099200	0.00169500
C	2.26550200	-2.28025400	-0.05061100
N	3.40862600	1.09561200	0.12332200
C	2.05040400	1.26963300	0.05004700
C	1.37035500	0.04637700	-0.02639300
C	1.22363700	2.41686700	0.03340200
N	-0.08528000	2.25668900	-0.05186000
C	-0.61045900	1.00529100	-0.11922200
N	0.05967300	-0.14129300	-0.11037000
C	1.80372200	3.79334500	0.11498500
N	-1.97530700	0.99467900	-0.20694800
N	-2.68591600	-0.15416200	-0.26559000
H	3.34699300	-4.10180900	-0.05232200
H	5.58530400	-2.96117100	0.11114000
H	5.72469800	-0.47593300	0.20444100
H	1.25535800	-2.68335400	-0.12258600
H	2.30729600	3.93040800	1.08339000
H	2.56460700	3.93128000	-0.66615700
H	1.01520900	4.54530200	0.00489000
H	-2.43114600	1.90496400	-0.21350100
C	-3.94614200	-0.05255200	-0.35388800
H	-4.48951800	0.90824200	-0.37306200
O	-4.68960500	-1.15890000	-0.46118300

In2

O 1

C	3.47106200	-3.15597600	-0.18734400
C	4.68804100	-2.61099300	0.34478200
C	4.82108800	-1.27369500	0.58435600
C	3.72864700	-0.39862100	0.29913400
N	2.56228000	-0.98799800	-0.22262100
C	2.42596900	-2.33327900	-0.46244700
N	3.61773700	0.90577000	0.44219800
C	2.34969300	1.19309400	0.00555200
C	1.66742500	0.04214900	-0.41325500
C	1.61812400	2.39683600	-0.11065000
N	0.38404200	2.34650500	-0.58073600
C	-0.15906800	1.15460200	-0.94139900
N	0.43170300	-0.03203500	-0.89062000
C	2.21092300	3.71078600	0.28973800
N	-1.43855900	1.26707900	-1.42533100
N	-2.26226600	0.17621700	-1.57169000
H	3.37658400	-4.22440100	-0.37264200
H	5.51834500	-3.28440800	0.56025400
H	5.73487100	-0.84030300	0.98870100
H	1.46325500	-2.64781000	-0.86549700
H	2.49382000	3.68850200	1.35227200
H	3.12917700	3.90280200	-0.28395000
H	1.49166900	4.51860900	0.11781500

C	-6.09842000	-0.98327800	-0.32456400
H	-6.54753000	-1.87290400	-0.78232400
H	-6.41493700	-0.10597100	-0.91221300
C	-6.50944700	-0.85067600	1.12766900
H	-7.60206900	-0.76703200	1.20248100
H	-6.18598300	-1.73132200	1.69921900
H	-6.06578900	0.04558500	1.58524100

C	-5.15513000	-0.29966700	0.27473800
C	-4.46243700	0.87324500	0.19049700
C	-3.04437400	0.84314100	0.07162900
N	-2.41532300	-0.42223700	0.04353900
C	-3.11997900	-1.60588100	0.13174300
N	-2.17812000	1.83317100	-0.02034000
C	-0.96156100	1.23420000	-0.11068800
C	-1.08689800	-0.14849300	-0.07430100
C	0.35197000	1.81930900	-0.22733000
N	1.40354200	1.05020500	-0.29918800
C	1.25385800	-0.29562600	-0.26461100
N	0.02517700	-0.94492600	-0.15418600
C	0.49223900	3.30483800	-0.26113700
N	2.20282200	-1.20991100	-0.32913300
N	1.62662400	-2.42450800	-0.26568500
H	-5.02708400	-2.49098200	0.31622900
H	-6.24103300	-0.28669600	0.36667000
H	-4.94936100	1.84707400	0.21177900
H	-2.54819200	-2.53035600	0.10776300
H	-0.08361900	3.71643000	-1.10258200
H	0.07232700	3.73924200	0.65765300
H	1.54653200	3.58391300	-0.35774300
H	4.05742700	-1.12810800	-0.45294200
C	0.33152800	-2.28004800	-0.16173200
H	-0.39393000	-3.08463700	-0.09381400
O	5.02866600	-1.11234400	-0.33349100
C	5.27484700	-0.28712800	0.77619500
H	6.31994400	-0.44994200	1.08645700
H	4.64323400	-0.58008200	1.63741000
C	5.05378600	1.18552900	0.46383700
H	5.27759400	1.81675200	1.33658800
H	5.70295000	1.49791700	-0.36750000
H	4.00724600	1.35722000	0.16883500

In4

O 1

C	-1.93135700	-2.93865700	-0.47929200
C	-3.25382400	-2.53809200	-0.09609000
C	-3.53317800	-1.23165700	0.18295500
C	-2.50001500	-0.25500200	0.09620900
N	-1.20804400	-0.70187500	-0.28236800
C	-0.93194700	-2.02448800	-0.56868200
N	-2.52285800	1.04123300	0.31972400
C	-1.24266800	1.46116800	0.10424500
C	-0.42355500	0.40674100	-0.26366200
C	-0.66082300	2.78536000	0.19934200
N	0.60980900	2.96585100	0.00070900
C	1.41209300	1.89123700	-0.29945400
N	0.89049700	0.60226300	-0.59083700
C	-1.54311500	3.94013100	0.54661400
N	2.69562400	1.90416100	-0.34085300
N	3.07145500	0.62122800	-0.74134800
H	-1.71268600	-3.98083300	-0.70718100
H	-4.03958100	-3.29069100	-0.03046200
H	-4.52676900	-0.89548400	0.47683900
H	0.08900300	-2.26436800	-0.85754800
H	-2.34749900	4.03404000	-0.19754000
H	-2.02649100	3.75914700	1.51782200
H	-0.95932500	4.86560800	0.58577900
C	1.99540200	-0.32043300	-0.49736000
H	1.98940500	-1.10384800	-1.27344800
O	1.94875300	-0.90453500	0.77825100
C	2.86711900	-1.96983300	0.99476100
H	3.01975000	-2.01331700	2.08088500
H	3.84524300	-1.72658800	0.54498400
C	2.35458300	-3.30274500	0.47977400
H	3.06426200	-4.10015400	0.73964500
H	1.38378500	-3.54202200	0.93615800
H	2.24226900	-3.30789200	-0.61468400
H	3.98094600	0.35026800	-0.37859200

Product

O 1

C	-4.47225300	-1.55701000	0.24584000
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TS1 (v = 154.17 i(cm⁻¹))

O 1

C	-5.89759800	-1.84071800	-0.24091100
C	-6.59756800	-0.93216900	0.62301300
C	-5.99864300	0.19882500	1.09800600
C	-4.64877600	0.48607200	0.72752700
N	-4.01345400	-0.43984400	-0.12133000
C	-4.61416000	-1.57852300	-0.59910500
N	-3.86930800	1.49777100	1.04757600
C	-2.68860400	1.24172000	0.39618800
C	-2.74325600	0.04840400	-0.33646900
C	-1.45573100	1.92973800	0.32414400
N	-0.48085200	1.41565600	-0.40479400
C	-0.67180200	0.24332600	-1.07421600
N	-1.78329800	-0.48777600	-1.07815000
C	-1.24066300	3.21766000	1.05501400

N	0.41458500	-0.15347300	-1.79636600
N	0.50997200	-1.42685100	-2.33593300
H	-6.38586800	-2.73954300	-0.61328200
H	-7.62831600	-1.15607100	0.90040100
H	-6.51206500	0.90087800	1.75360600
H	-3.99825500	-2.20206900	-1.24716300
H	-1.95231100	3.97586500	0.69669200
H	-1.43069700	3.07980700	2.12904400
H	-0.21660300	3.57495500	0.90250900
H	0.72628100	-1.36237700	-3.32930000
H	1.27844200	-1.92048100	-1.87930900
H	1.25677500	0.40100500	-1.65202700
C	3.66107300	-0.56707000	-0.60862500
H	4.31470900	-1.07572800	-1.33234500
O	2.69561100	-1.37473700	-0.17453700
O	3.22852800	0.65155000	-0.95822600
O	4.77987700	-0.27724200	0.71873300
C	5.34652300	-1.49852400	1.09459300
H	4.57204100	-2.20568900	1.45499600
H	5.84551200	-1.99415000	0.23568800
C	4.21901500	1.57101500	-1.43808900
H	3.81173200	2.00490800	-2.36115000
H	5.13288500	1.01293500	-1.68965300
C	1.88595600	-0.88811900	0.91233700
H	1.49934900	0.10897000	0.65854400
H	2.53872100	-0.79523400	1.79225100
C	6.36434300	-1.25628600	2.19552700
H	5.87947400	-0.79290100	3.06670700
H	6.82902900	-2.19955900	2.51526700
H	7.15401400	-0.57845800	1.84143600
C	4.49391700	2.63538600	-0.39923400
H	4.89883100	2.16633700	0.50543700
H	5.21939400	3.36155200	-0.79117200
H	3.56802100	3.17121900	-0.14769900
C	0.76651400	-1.87732900	1.12988400
H	0.12539500	-1.53360100	1.95322100
H	0.14831100	-1.97063000	0.22518300
H	1.16632900	-2.86733900	1.38984600

TS2 (v = 241.14 i(cm⁻¹))

0 1			
C	2.87323100	-3.18395400	0.00058000
C	4.17714900	-2.75797900	0.42286900
C	4.47787100	-1.43475000	0.57269300
C	3.47567700	-0.45420500	0.30095000
N	2.21822600	-0.92966100	-0.11326900
C	1.91237400	-2.26042400	-0.26075500
N	3.52390200	0.86101000	0.36969300
C	2.27161100	1.27118100	-0.00570100
C	1.43767000	0.18677400	-0.31107200

C	1.68336700	2.54727800	-0.16613100
N	0.41822900	2.62138000	-0.54556600
C	-0.27900900	1.48472900	-0.77540300
N	0.17319700	0.24209000	-0.71078700
C	2.46244500	3.79934000	0.08268700
N	-1.60033500	1.69018500	-1.11822700
N	-2.40150100	0.62748500	-1.45776700
H	2.64551300	-4.24244800	-0.11158100
H	4.93830100	-3.51204000	0.62605000
H	5.46008200	-1.09070100	0.89375300
H	0.89379400	-2.48036400	-0.58068900
H	2.82585600	3.81684600	1.12042400
H	3.34746800	3.82895200	-0.56922500
H	1.83595700	4.67800000	-0.10363800
H	-1.90299700	-0.13382700	-1.92008700
H	-1.79359000	2.56653900	-1.59324200
C	-3.26672800	0.19062900	-0.46740900
H	-3.80950900	1.00508700	0.03878300
O	-2.37215900	-0.41777800	0.95866600
O	-3.97406600	-0.84971400	-0.90020200
C	-2.55526100	0.37248500	2.08975800
H	-2.51382600	-0.28758500	2.97781600
H	-3.56958400	0.83040000	2.11650800
C	-1.51532500	1.47781400	2.24110500
H	-1.62747900	2.23025200	1.44790200
H	-1.60942200	1.98049500	3.21555400
H	-0.50216000	1.05242100	2.16268400
C	-4.92941800	-1.39714600	0.01334000
H	-5.87647800	-1.47568300	-0.53853200
H	-5.07519000	-0.69624100	0.84882600
C	-4.46667800	-2.74958500	0.50943300
H	-5.21489100	-3.17783000	1.19067200
H	-4.32975700	-3.44065400	-0.33374400
H	-3.51271200	-2.63044500	1.03699400

TS3 (v = 332.94 i(cm⁻¹))

0 1			
C	-2.95956100	-2.10421300	-0.71349900
C	-4.04581000	-1.24588100	-0.33033300
C	-3.82690500	0.05661100	0.01314300
C	-2.49731200	0.57684000	-0.00149700
N	-1.46492900	-0.31404400	-0.37903400
C	-1.68970100	-1.62471100	-0.73467800
N	-2.04042400	1.77498900	0.28400800
C	-0.68446200	1.68733200	0.09256700
C	-0.29932000	0.40783200	-0.31475600
C	0.37637500	2.62090000	0.27813200
N	1.61226100	2.26902600	0.02319900
C	1.89653600	0.99218500	-0.41421700
N	0.95365700	0.01192700	-0.53850100

C	0.08336600	4.00426100	0.77139900
N	3.16486600	0.71906700	-0.71108500
N	3.18660600	-0.57763600	-1.26296800
H	-3.14377600	-3.13985200	-0.99380600
H	-5.05946300	-1.64733500	-0.31895700
H	-4.63498000	0.72712400	0.30318800
H	-0.81341200	-2.20300300	-1.02694200
H	-0.62112300	4.50605300	0.09227400
H	-0.39996200	3.95723000	1.75824000
H	1.00947700	4.58486200	0.84009900
H	3.18625600	-0.59325300	-2.28237200
C	2.37816000	-1.47513100	-0.71378300
H	1.95177800	-2.25443900	-1.35743900
O	2.48445900	-1.71634000	0.56225600
C	1.61891300	-2.69657500	1.15817300
H	2.28186300	-3.40675000	1.66817400
H	1.08578100	-3.23845600	0.36226700
C	0.66819600	-2.04527000	2.13762400
H	0.09492800	-2.82623200	2.65505500
H	1.22913700	-1.47248900	2.88798200
H	-0.03728400	-1.37111700	1.63520500

O	-2.22414000	-0.13520000	0.58915200
C	-3.57041900	0.14860100	0.42186600
H	-4.19240800	-0.77418600	0.42064800
H	-3.77131900	0.64493700	-0.55797500
C	-4.05692100	1.06741200	1.53342800
H	-5.12687700	1.29682900	1.42458900
H	-3.89765300	0.59188300	2.51209900
H	-3.49139600	2.01082100	1.51772900
H	-2.82069700	-2.81467900	-1.09614300

Route 2

H:

(2)

0 1

C	3.53037200	-1.62242800	0.00233100
C	4.18005900	-0.34165200	0.00024100
C	3.46147300	0.81850900	-0.00172200
C	2.03364600	0.75994400	-0.00158400
N	1.45154500	-0.52278700	0.00030100
C	2.17405900	-1.69097400	0.00225200
N	1.13857000	1.72406500	-0.00295700
C	-0.07033600	1.07199400	-0.00211500
C	0.08801300	-0.32203500	-0.00032100
C	-1.40822100	1.51888300	-0.00235300
N	-2.38829000	0.62829200	-0.00273000
C	-2.09631800	-0.69344200	-0.00098200
N	-0.87114400	-1.23262300	0.00070800
C	-1.73537300	2.97969800	0.00430600
N	-3.12412900	-1.58913700	-0.00104400
N	-4.45537700	-1.22203700	0.00031000
H	4.11525300	-2.54049300	0.00392200
H	5.26986000	-0.30282700	0.00019500
H	3.93508600	1.79929700	-0.00341300
H	1.58771900	-2.60981600	0.00369100
H	-1.36488400	3.44299000	0.93084900
H	-1.23275500	3.48654700	-0.83181000
H	-2.81844200	3.12475400	-0.06826100
H	-4.92200000	-1.60218600	-0.82195100
H	-4.92035300	-1.60218400	0.82351100
H	-2.85194800	-2.56747200	0.00083800

ln1

0 1

C	6.54267400	-2.28345800	-0.68863000
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TS4 ($\nu = 262.45 \text{ i}(\text{cm}^{-1})$)

0 1

C	-0.26753200	3.44553200	-0.62863300
C	1.01353700	3.95962400	-0.24393100
C	2.03103600	3.11618300	0.09745900
C	1.81928100	1.70856900	0.05899800
N	0.54693300	1.25098300	-0.36270600
C	-0.49044500	2.10710400	-0.67968200
N	2.62611700	0.71295000	0.36581900
C	1.89403100	-0.41615900	0.15148700
C	0.62448900	-0.10302100	-0.30529900
C	2.22823000	-1.80750000	0.37750400
N	1.34079800	-2.74274900	0.19547800
C	0.09153900	-2.41097600	-0.24296300
N	-0.26283800	-1.09600800	-0.61218300
C	3.60207600	-2.15363900	0.84916400
N	-0.91589300	-3.21225000	-0.39131500
N	-1.91927700	-2.41419100	-0.87131800
H	-1.08317700	4.12272000	-0.87662800
H	1.16681900	5.03842100	-0.21629600
H	3.01117700	3.47408900	0.40965000
H	-1.44627400	1.64616600	-0.91771600
H	3.82531900	-1.60911800	1.77799200
H	3.68604800	-3.23241900	1.01509700
H	4.34298000	-1.83011100	0.10335700
C	-1.62544300	-1.08516600	-0.86849300
H	-2.08104300	-0.43428700	-1.62147800

C	7.49090100	-1.32342000	-0.19644600
C	7.09173500	-0.09799900	0.25254400
C	5.70279100	0.23850800	0.23378000
N	4.81975400	-0.74123300	-0.26052200
C	5.22055000	-1.97472300	-0.71216600
N	5.08388900	1.33657900	0.61043100
C	3.75578100	1.08589700	0.36375200
C	3.55734900	-0.19352400	-0.17663100
C	2.57988300	1.84369900	0.54403500
N	1.41253200	1.31896500	0.20479700
C	1.35989200	0.06668700	-0.30826100
N	2.40566400	-0.74222400	-0.52449500
C	2.63277100	3.22808800	1.11157500
N	0.14678100	-0.45006600	-0.64712000
N	-1.04503500	0.23184900	-0.49820400
H	6.87358900	-3.25800600	-1.04323100
H	8.54958700	-1.58520100	-0.18348400
H	7.79457900	0.64309300	0.63099100
H	4.42540500	-2.63206000	-1.06395400
H	3.10735300	3.21224900	2.10343500
H	3.24869600	3.87615800	0.47106900
H	1.62244200	3.64303400	1.19205800
H	-1.49247700	0.38807700	-1.40117300
H	-1.70481600	-0.31190700	0.06035300
H	0.16800000	-1.38278100	-1.04839400
C	-4.41142100	-0.54395900	-0.48613600
H	-4.38497700	-1.20025900	-1.37966000
O	-3.87926700	0.66321500	-0.88571500
O	-3.63511300	-1.06130200	0.53635800
O	-5.71535000	-0.42793900	-0.02397800
C	-6.65524800	-0.09173600	-1.03076700
H	-6.39913300	0.89013300	-1.46404300
H	-6.60168600	-0.83606200	-1.84590100
C	-3.98108500	-2.37265200	0.97025900
H	-3.03301000	-2.90934300	1.11892300
H	-4.53474000	-2.89074600	0.16965200
C	-3.90570700	1.70183400	0.09215400
H	-3.42119800	1.34787500	1.01538600
H	-4.95291300	1.94664800	0.33327400
C	-8.03307800	-0.06763000	-0.41027300
H	-8.07877500	0.68069000	0.39300700
H	-8.78713500	0.18624400	-1.16682400
H	-8.27957800	-1.05075200	0.01403400
C	-4.78527200	-2.34657600	2.25525100
H	-5.74378200	-1.83691700	2.09684600
H	-4.97729100	-3.37179900	2.60182100
H	-4.22830900	-1.81621300	3.04046400
C	-3.17971900	2.89815200	-0.47928000
H	-3.22263000	3.73830800	0.22675800
H	-2.12730100	2.64369700	-0.66327700
H	-3.64394700	3.21383000	-1.42421800

In2

0 1

C	-4.97886400	-2.03803900	-0.21035900
C	-5.77482200	-1.04925900	0.46067700
C	-5.26546800	0.17684000	0.77676900
C	-3.91303300	0.48466500	0.43203500
N	-3.18169100	-0.52235300	-0.22571200
C	-3.69250600	-1.75714600	-0.54260500
N	-3.20909200	1.57955300	0.62733800
C	-1.97834300	1.29885700	0.08816400
C	-1.92750400	0.00328400	-0.44852600
C	-0.78675400	2.04317000	-0.03719000
N	0.26487400	1.48494700	-0.61938000
C	0.18316200	0.21835100	-1.07605100
N	-0.88876800	-0.57566800	-1.02877700
C	-0.69676000	3.45249300	0.45874300
N	1.28512600	-0.33343400	-1.68530500
N	2.54348000	0.20575700	-1.55997300
H	-5.39658800	-3.01290100	-0.45532800
H	-6.80652000	-1.28940700	0.72048900
H	-5.85172800	0.94023400	1.28642500
H	-3.00874800	-2.43722200	-1.05061200
H	-1.32468400	4.10797200	-0.16358800
H	-1.07777200	3.52161400	1.48700200
H	0.34013900	3.80266700	0.41691200
H	3.02975000	0.21355300	-2.45368600
H	1.19267500	-1.32504500	-1.89883800
C	3.35330400	-0.44954500	-0.55955500
H	3.34262400	-1.56025600	-0.66632900
O	2.86153100	-0.12440100	0.69888900
O	4.63105500	0.03100100	-0.77539800
C	2.59800700	-1.18656700	1.60202500
H	2.75952100	-0.77737300	2.60968700
H	3.33185600	-1.99930100	1.46086300
C	1.18136600	-1.70939900	1.46377100
H	1.01746900	-2.15670000	0.47264800
H	0.97910100	-2.47386900	2.22708900
H	0.46028000	-0.88781500	1.58770900
C	5.65727900	-0.58118000	-0.01029900
H	6.55424300	-0.58013900	-0.64574500
H	5.39741700	-1.63696100	0.18355300
C	5.93747100	0.15756700	1.28645700
H	6.79594400	-0.29777200	1.79968400
H	6.17788300	1.20880100	1.07456800
H	5.06973000	0.13093900	1.95789800

In3

0 1

C	-4.53427200	-2.34818200	0.00016200
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C	-5.49847500	-1.29150600	0.12627800
C	-5.11479100	0.01704100	0.18286700
C	-3.72520700	0.34382400	0.11550500
N	-2.82654800	-0.73282400	-0.00796500
C	-3.21116300	-2.04994500	-0.06516000
N	-3.11774700	1.51116900	0.15049100
C	-1.78295300	1.20903500	0.04813700
C	-1.56819200	-0.17449400	-0.05239600
C	-0.61377600	1.99842700	0.02836600
N	0.56546100	1.40267400	-0.07972200
C	0.62668200	0.05750500	-0.17133700
N	-0.40370300	-0.79219000	-0.16307100
C	-0.68410100	3.49029900	0.11798300
N	1.85761000	-0.53089200	-0.28682800
N	3.01088900	0.17484900	-0.28814000
H	-4.85356300	-3.38789200	-0.04386600
H	-6.55766000	-1.54628300	0.17706600
H	-5.83072300	0.83218900	0.27847800
H	-2.40438600	-2.77637800	-0.16166800
H	-1.15608000	3.89736800	-0.78884900
H	-1.30856600	3.79232400	0.97031000
H	0.32161000	3.91139300	0.22107200
H	1.86291900	-1.54751700	-0.34371600
C	4.08939200	-0.48467200	-0.37795000
H	4.13667900	-1.58590400	-0.44130900
O	5.25801900	0.16490200	-0.43143600
C	6.42517700	-0.63773400	-0.26765600
H	7.25122900	-0.02984400	-0.65582100
H	6.34271500	-1.53680100	-0.90058900
C	6.65490000	-1.00711000	1.18387900
H	7.58782600	-1.57821100	1.28290500
H	6.73051200	-0.10181500	1.80161200
H	5.83227200	-1.62626300	1.57044600

N	-1.12497000	1.56887300	-1.28332300
N	-1.56893000	2.88962400	-1.05082100
H	3.43856000	-3.79370800	0.94970600
H	5.03956600	-2.84374800	2.64714600
H	4.90058400	-0.45371100	3.31554000
H	1.69121600	-2.26832400	-0.06179700
H	2.37031100	3.89276900	2.42848900
H	1.77769100	4.73281800	0.95688100
H	0.65323000	4.38114000	2.28938100
H	-1.88143800	3.32052800	-1.91646600
C	-0.53192500	3.65749800	-0.38854400
O	0.34715500	4.34931100	-1.23035300
C	0.06908300	5.73397400	-1.39013700
H	0.94314800	6.15036600	-1.90675000
H	0.00953300	6.21329600	-0.39609100
C	-1.19794000	5.99901700	-2.18335900
H	-1.31938200	7.07801500	-2.34965200
H	-1.14975700	5.50007200	-3.16197700
H	-2.09187300	5.64426400	-1.64755600
H	-0.95183400	4.35883300	0.35343100

Product

0 1

C	3.32092600	-2.82940000	1.42577300
C	3.97102700	-2.42429800	2.64126300
C	3.87484300	-1.14885600	3.11540000
C	3.10742000	-0.18891700	2.38378000
N	2.49369500	-0.64294200	1.20469400
C	2.58976800	-1.92649100	0.72537800
N	2.87780400	1.07889900	2.63892200
C	2.08311600	1.50976900	1.60452500
C	1.81820600	0.43953100	0.67211900
C	1.53578300	2.74173000	1.33879400
N	0.78593300	2.78071400	0.18319400
C	0.58086000	1.68040900	-0.66594900
N	1.11287300	0.46980400	-0.41757300
C	1.68661600	3.96801100	2.16213100
N	-0.17987500	2.04863400	-1.68010800
N	-0.46845500	3.35095600	-1.50605000
H	3.40920700	-3.85110600	1.06199900
H	4.55519700	-3.16041300	3.19486400
H	4.36152500	-0.82595400	4.03424400
H	2.05809900	-2.12611100	-0.20503600
H	2.31162300	3.74254700	3.03236100
H	2.15637900	4.77154600	1.57529200
H	0.70435500	4.32727100	2.50387800
H	-1.45564400	4.16697100	-2.85304400
C	0.09389900	3.79990100	-0.41261000
O	-1.80896100	4.67300700	-3.61257300
C	-1.18182200	5.92868100	-3.57065300

In4

0 1

C	3.37261600	-2.74620800	1.23720200
C	4.28292000	-2.19273200	2.20732100
C	4.21915800	-0.88541300	2.58392700
C	3.22284700	-0.03364100	2.00167100
N	2.36131600	-0.63264100	1.05692500
C	2.42631400	-1.95281500	0.67891000
N	2.97145100	1.23307100	2.19892700
C	1.90513000	1.51572400	1.36534400
C	1.49353700	0.35269800	0.62621100
C	1.21926300	2.68449400	1.11926300
N	0.19626300	2.57035500	0.23295300
C	-0.14255000	1.38252700	-0.47424700
N	0.54602300	0.22575300	-0.25417700
C	1.52685600	4.00187200	1.73923900

H	-1.34055200	6.41429100	-4.54704900
H	-0.08649600	5.82335500	-3.44687400
C	-1.73488700	6.81532500	-2.46462800
H	-1.25387800	7.80414000	-2.46298000
H	-2.81812800	6.95247900	-2.59484600
H	-1.56988700	6.35217100	-1.47958100
H	0.03472800	4.81112900	-0.02026200

C	4.71468500	3.36839600	-1.58332100
H	4.87956000	2.81986900	-2.52187700
H	4.42932800	4.40132700	-1.82812300
H	5.66300700	3.39003500	-1.02732200
C	5.70636000	-0.92588100	0.76295000
H	5.83772600	-0.14332600	0.00599300
H	6.60194000	-0.97814500	1.39743700
H	5.57907000	-1.89651300	0.26359200
C	0.48485300	0.15126100	-2.18195200
H	0.36907000	-0.54470600	-3.02380200
H	-0.44945800	0.15039700	-1.60153400
H	0.64563800	1.16244000	-2.58048400

TS1 ($\nu = 164.92 \text{ i}(\text{cm}^{-1})$)

O 1			
C	-4.34719900	2.58830300	1.59799000
C	-5.36919900	2.45518800	0.59726400
C	-5.32086200	1.46229700	-0.33723600
C	-4.23285300	0.53610600	-0.32153700
N	-3.26038500	0.71388700	0.68204600
C	-3.30861500	1.71341400	1.62345200
N	-3.97421600	-0.48668900	-1.10616700
C	-2.80169400	-1.00853100	-0.61707800
C	-2.33120000	-0.28739100	0.49212300
C	-1.99250300	-2.09343400	-1.00815000
N	-0.89048400	-2.36014000	-0.32242600
C	-0.55062500	-1.58569500	0.73384800
N	-1.23163700	-0.52462500	1.18667400
C	-2.33049900	-2.92345100	-2.20693300
N	0.57669600	-1.89975200	1.43393300
N	1.44910000	-2.90137800	1.05054800
H	-4.39746700	3.38507100	2.33792700
H	-6.19749600	3.16449800	0.59011700
H	-6.08494300	1.34249400	-1.10412200
H	-2.48633200	1.73040100	2.33877800
H	-3.41526900	-2.95421100	-2.36717900
H	-1.87219300	-2.47192300	-3.10126000
H	-1.92864800	-3.93698300	-2.09411900
H	2.35787200	-2.48472100	0.84732500
H	1.56414100	-3.56841000	1.81165600
H	0.83935900	-1.23606100	2.15655500
C	2.79786900	0.62066700	0.52495900
H	2.73589200	1.33297500	1.36069300
O	1.66949700	0.58804900	-0.16941500
O	3.30537500	-0.58397600	0.81254000
O	4.03593300	1.38045400	-0.46878300
C	3.63642800	2.68648800	-0.75907500
H	2.67984800	2.69858400	-1.31941300
H	3.46006600	3.27154500	0.16881100
C	4.49497100	-0.60619200	1.61154600
H	4.32841800	-1.37440000	2.37940700
H	4.60656000	0.36608400	2.11484000
C	1.64298900	-0.27925800	-1.31377000
H	1.51790200	-1.31864000	-0.97429700
H	2.60816400	-0.18439600	-1.83238300

TS2 ($\nu = 241.91 \text{ i}(\text{cm}^{-1})$)

O 1			
C	-5.25202400	-1.67722800	0.04839400
C	-5.90565300	-0.48355600	0.50562900
C	-5.22936800	0.69605700	0.62336600
C	-3.84254900	0.74548300	0.28280100
N	-3.25619800	-0.45366300	-0.16223200
C	-3.93441400	-1.64222200	-0.27797900
N	-2.99062200	1.74910900	0.31220800
C	-1.80648000	1.20921000	-0.12105300
C	-1.93623700	-0.15706900	-0.42233700
C	-0.52726300	1.75579900	-0.34949500
N	0.43759100	0.95789400	-0.78853900
C	0.18493400	-0.34862600	-0.99089300
N	-0.98445400	-0.96883000	-0.85409500
C	-0.24617600	3.20743800	-0.12418600
N	1.24007600	-1.14088800	-1.39809100
N	2.48602300	-0.60214200	-1.61210100
H	-5.80219700	-2.61242800	-0.03839600
H	-6.96450500	-0.52717800	0.76307000
H	-5.70647200	1.61184300	0.96965100
H	-3.34801200	-2.49036000	-0.63126600
H	-0.88880400	3.82312400	-0.77032400
H	-0.47949800	3.47941700	0.91545100
H	0.80600600	3.42572000	-0.33550700
H	2.45845800	0.36122400	-1.94795900
H	0.99556300	-1.94343200	-1.96924900
C	3.39433900	-0.78687800	-0.58148300
H	3.42354800	-1.81815100	-0.19375900
O	2.83713400	0.01474600	0.91885900
O	4.55374600	-0.20584900	-0.87865400
C	2.57286800	-0.88607100	1.94630400
H	2.82136900	-0.39323100	2.90634400
H	3.23627600	-1.77851100	1.89862300
C	1.12296100	-1.35563300	1.98575600
H	0.88387400	-1.95739000	1.09734200

H	0.92361000	-1.96074400	2.88310100
H	0.44775900	-0.48500300	1.99458900
C	5.59563500	-0.32189700	0.09442800
H	6.49267900	-0.64584800	-0.45147200
H	5.33130900	-1.10742500	0.81844200
C	5.82259900	1.00521800	0.78527900
H	6.64517600	0.91775700	1.50851100
H	6.08784800	1.77731100	0.04967200
H	4.90304300	1.30163600	1.30426200

C	-4.85085300	-1.03647400	0.56035900
C	-5.22057600	0.35143400	0.46226200
C	-4.30124300	1.32051400	0.19523000
C	-2.92905600	0.95253800	0.00658500
N	-2.62721800	-0.42007400	0.11618500
C	-3.55605400	-1.39784900	0.38497800
N	-1.88552900	1.69525400	-0.25757700
C	-0.83071400	0.80874900	-0.33544300
C	-1.26858900	-0.54565800	-0.09989300
C	0.50650800	1.00915600	-0.57557400
N	1.25286300	-0.13947900	-0.59414500
C	0.74537200	-1.43920200	-0.32663100
N	-0.57180200	-1.64125400	-0.07662900
C	1.16890700	2.32010600	-0.79249000
N	1.69160600	-2.32417600	-0.37096000
N	2.81324400	-1.60176300	-0.71192700
H	-5.60031300	-1.79656400	0.77180900
H	-6.26612500	0.62675000	0.60627500
H	-4.56490300	2.37408900	0.11764600
H	-3.16874700	-2.41547200	0.43788700
H	0.42938700	3.12315800	-0.71205700
H	1.95807800	2.43938000	-0.03593600
H	1.63941000	2.35439600	-1.78647200
H	3.70776900	-2.07034700	-0.75943600
C	2.64433300	-0.25445300	-0.65654100
O	3.13954400	0.51109300	0.91861200
C	4.40970400	1.05937400	0.81896800
H	4.51288800	1.85906100	1.57819500
H	4.56208400	1.57111900	-0.16136100
C	5.52950800	0.04128500	1.01717100
H	6.51738100	0.52545800	1.02558100
H	5.38904400	-0.48802700	1.97101600
H	5.53126100	-0.70873700	0.21151100
H	3.24080900	0.40030200	-1.30206700

TS3 ($\nu = 315.01 \text{ i}(\text{cm}^{-1})$)

O 1			
C	4.56237700	-1.09417500	0.74103400
C	5.01595800	0.22941100	0.40743600
C	4.15681400	1.17617500	-0.06710400
C	2.77389000	0.84952300	-0.23688600
N	2.38731200	-0.46289800	0.10651800
C	3.25317100	-1.41647600	0.58365300
N	1.77213700	1.57803000	-0.66830500
C	0.68338300	0.73572600	-0.61537100
C	1.02914000	-0.54606000	-0.13358400
C	-0.67753500	0.91826600	-0.90383800
N	-1.48655200	-0.11338800	-0.70923800
C	-1.04535200	-1.35627500	-0.27902300
N	0.25225800	-1.59109800	0.04313400
C	-1.22350300	2.23345200	-1.36425500
N	-1.93413000	-2.34347200	-0.17014100
N	-3.15914700	-1.88368800	-0.69933100
H	5.25929100	-1.83993600	1.11927800
H	6.07078700	0.47344500	0.53896900
H	4.48151500	2.18324200	-0.32577500
H	2.80907500	-2.38726700	0.80481300
H	-1.53110600	2.83331200	-0.49266500
H	-0.44835600	2.79809900	-1.89631800
H	-2.09554400	2.08827500	-2.01384400
H	-3.32420400	-2.16079300	-1.66617500
C	-3.46678100	-0.61658000	-0.44638700
H	-4.03344600	-0.05219800	-1.19702700
O	-3.53635700	-0.23505300	0.80307700
C	-3.72493200	1.16496600	1.06750300
H	-4.74005700	1.28338900	1.47027000
H	-3.65939300	1.72166400	0.12122900
C	-2.68019300	1.62543700	2.05771600
H	-2.82946100	2.68977700	2.28314900
H	-2.76236900	1.05670000	2.99337800
H	-1.66763600	1.48798100	1.65227200

TS4 ($\nu = 303.31 \text{ i}(\text{cm}^{-1})$)

O 1

Route 1

Me:

Triethyl orthoacetate

O 1			
C	-0.11295300	-0.02194700	-1.12263400
O	1.27210200	-0.05441800	-0.98688900
O	-0.58959200	-1.23476100	-0.63093100
O	-0.57319500	0.97153600	-0.26437600
C	-0.27135200	2.31238000	-0.61098300
H	0.78186400	2.38462700	-0.92717600
H	-0.90345500	2.63808100	-1.45499100
C	-1.98741900	-1.35122100	-0.40461200

H	-2.31737300	-2.29113400	-0.87349200
H	-2.52749800	-0.52761300	-0.89438700
C	1.98202800	-0.96074400	-1.81350400
H	2.04772000	-0.56674200	-2.84251100
H	1.44905900	-1.92448500	-1.85149600
C	-0.52717200	3.17805100	0.60285600
H	0.11976800	2.86971400	1.43547600
H	-0.32361800	4.23190700	0.37082400
H	-1.57439500	3.08814400	0.92391600
C	-2.28522000	-1.36050500	1.08229800
H	-1.97926300	-0.40498300	1.52838700
H	-3.35903800	-1.51183100	1.26149700
H	-1.73301700	-2.17209400	1.57692100
C	3.36657400	-1.13949800	-1.22952200
H	3.96327200	-1.81483200	-1.85702000
H	3.88421200	-0.17188900	-1.16901700
H	3.30186700	-1.56268200	-0.21779300
C	-0.54382500	0.20790600	-2.57249400
H	0.00116000	1.05497500	-3.00915200
H	-1.61967400	0.41875100	-2.62186700
H	-0.33531600	-0.69030700	-3.16689800

In1

O 1

C	-5.98992500	-1.87677600	0.11750500
C	-6.70763700	-0.79610900	0.73439500
C	-6.11926700	0.41726700	0.94429300
C	-4.76265300	0.61826300	0.54292100
N	-4.10903700	-0.47594000	-0.05583000
C	-4.69997800	-1.69766100	-0.26751000
N	-3.99156700	1.67984200	0.63748900
C	-2.79467400	1.28699400	0.09020300
C	-2.83298200	-0.04500300	-0.34875800
C	-1.56209000	1.94457100	-0.11375400
N	-0.57066900	1.28122500	-0.68340400
C	-0.74067300	-0.01636200	-1.06110200
N	-1.85616100	-0.73313300	-0.92076000
C	-1.34450900	3.36136900	0.31961100
N	0.36171500	-0.56694500	-1.64100900
N	0.47787000	-1.93924400	-1.82575700
H	-6.46993500	-2.84034000	-0.04424600
H	-7.74284500	-0.95516600	1.03830300
H	-6.64496300	1.24909400	1.41139800
H	-4.07117400	-2.45159300	-0.74112100
H	-2.30082100	3.86010700	0.51562700
H	-0.74807200	3.37531200	1.24459200
H	-0.78215900	3.90944400	-0.44702300
H	0.74281600	-2.12835000	-2.79123600
H	1.23069100	-2.27766600	-1.22238100
H	1.21555800	-0.01218300	-1.56549500

C	3.64201300	-0.63735000	-0.32813300
O	2.60153700	-1.34297100	0.26487600
O	3.06426000	0.38391300	-1.09191600
O	4.44129800	-0.01076100	0.62741700
C	5.15986100	-0.85851900	1.51021900
H	4.51221100	-1.69198100	1.83084800
H	6.03293900	-1.28973700	0.99189800
C	3.88092300	1.47275200	-1.51132900
H	3.65673000	1.64178800	-2.57481000
H	4.94295800	1.20060000	-1.42890300
C	1.81347300	-0.62158100	1.21011900
H	1.45642200	0.31602700	0.75513900
H	2.43617500	-0.35891600	2.08073500
C	5.60152400	-0.03254400	2.69815600
H	4.73045000	0.37280300	3.23165000
H	6.18328000	-0.65021500	3.39499600
H	6.22962500	0.80680600	2.36914200
C	3.57635500	2.71129000	-0.69250900
H	3.82963600	2.53522800	0.36133600
H	4.15420600	3.57052100	-1.06098900
H	2.50645800	2.95512600	-0.76198700
C	0.65725100	-1.50575700	1.62288700
H	0.01640700	-0.97430800	2.34012500
H	0.04602600	-1.78454600	0.75222300
H	1.02517700	-2.42529500	2.09999200
C	4.39799900	-1.61629600	-1.21037100
H	3.70563600	-1.99395700	-1.97331000
H	5.23893100	-1.10939300	-1.70160100
H	4.77575100	-2.46258500	-0.62409500

In2

O 1

C	-3.50545000	3.16174500	-0.22279300
C	-4.75399800	2.63893900	0.25619800
C	-4.92549600	1.30269900	0.47645300
C	-3.84235300	0.40590600	0.22457800
N	-2.64355800	0.97444200	-0.24456800
C	-2.46861100	2.31856400	-0.46501000
N	-3.76568100	-0.90191400	0.35709100
C	-2.48747700	-1.21289100	-0.03249100
C	-1.76417200	-0.07316500	-0.41095500
C	-1.77870800	-2.43148100	-0.13737700
N	-0.52639400	-2.40367300	-0.55749800
C	0.05916000	-1.21891300	-0.87701000
N	-0.50876500	-0.02030500	-0.83653200
C	-2.41728900	-3.73667300	0.21933100
N	1.35880300	-1.35155000	-1.28754100
N	2.19032400	-0.27385800	-1.45678300
H	-3.38043400	4.22946700	-0.39365600
H	-5.57693700	3.32897800	0.44567400

H	-5.86374000	0.88625100	0.84082700
H	-1.48413600	2.61532700	-0.82674200
H	-3.32497900	-3.89157400	-0.38156000
H	-1.71546400	-4.56014000	0.04992900
H	-2.72725000	-3.72792200	1.27457100
H	2.67816800	-0.31752900	-2.34955900
H	1.73166100	-2.29610900	-1.23595200
C	3.14923200	-0.07245500	-0.37208600
O	2.42817600	0.38847900	0.72923200
O	3.95337900	0.95607000	-0.87524700
C	2.43936500	-0.25349400	1.99284000
H	2.30070200	0.55212100	2.72836700
H	3.41953600	-0.70744200	2.20316800
C	1.32514900	-1.27537000	2.13239700
H	1.45811700	-2.11892100	1.44039000
H	1.29853600	-1.66909500	3.15828700
H	0.35379600	-0.80685000	1.91260300
C	4.75305100	1.65538800	0.06529600
H	5.75720000	1.75347800	-0.37437500
H	4.85777300	1.07352900	0.99510600
C	4.16363400	3.02048000	0.36446400
H	4.04745200	3.59419100	-0.56590000
H	3.17648300	2.90627800	0.83171800
H	4.81873100	3.58643400	1.04175300
C	4.00449100	-1.31128000	-0.09817100
H	4.81297100	-1.09474400	0.61159900
H	3.41363200	-2.14691400	0.29871000
H	4.45946000	-1.61519700	-1.05000100

In3

O 1			
C	3.34594700	-3.03037000	0.19242600
C	4.64036000	-2.41189100	0.13504900
C	4.77549400	-1.05699000	0.03802500
C	3.60648300	-0.23747600	-0.00725200
N	2.36525400	-0.89848800	0.05049500
C	2.22736200	-2.26145900	0.14866300
N	3.48019600	1.07054600	-0.09806800
C	2.12640300	1.28619700	-0.10192000
C	1.40555700	0.08730300	-0.01207300
C	1.33637200	2.45679400	-0.17647500
N	0.02073600	2.33708000	-0.16223400
C	-0.54653300	1.10568800	-0.07138400
N	0.08681600	-0.05847900	0.00993400
C	1.96192000	3.81276600	-0.26393800
N	-1.91559400	1.14195900	-0.05619800
N	-2.66077100	0.01328300	-0.07693800
H	3.25138500	-4.11202200	0.26961100
H	5.52915500	-3.04291600	0.16821600
H	5.74769900	-0.56818500	-0.00823200

H	1.20314900	-2.63259100	0.18461100
H	2.53481700	4.02061200	0.65191000
H	2.67078100	3.85050100	-1.10304600
H	1.19037000	4.57926900	-0.39250400
H	-2.32571000	2.06472200	-0.17257900
C	-3.92896700	0.13242300	-0.01474700
O	-4.61118900	-1.03171700	0.01830800
C	-5.93498500	-1.10257600	-0.50707300
H	-5.95733500	-1.99288800	-1.15122300
H	-6.14231500	-0.23387400	-1.14906400
C	-6.95404500	-1.23251300	0.60646200
H	-7.95752800	-1.37954000	0.18446600
H	-6.71119100	-2.09779600	1.23817200
H	-6.97281600	-0.33642700	1.24279300
C	-4.66387900	1.44122600	0.07820800
H	-4.64556900	1.97956600	-0.88192500
H	-5.70708400	1.30443300	0.37815700
H	-4.17782800	2.07844300	0.83186600

In4

O 1			
C	-2.78347800	-2.32639200	-0.35758900
C	-3.94918400	-1.53254300	-0.10368700
C	-3.83753800	-0.18829800	0.10160500
C	-2.55796700	0.43329400	0.03762400
N	-1.44043400	-0.38130400	-0.28719300
C	-1.55455300	-1.75434500	-0.43604500
N	-2.21072600	1.68454000	0.24257500
C	-0.86147900	1.71406900	0.05412600
C	-0.37124900	0.46399300	-0.29805400
C	0.07742900	2.80161300	0.23620200
N	1.35518300	2.59916600	0.12617200
C	1.82020100	1.35164900	-0.21358800
N	0.95688400	0.29164800	-0.57780100
C	-0.44553400	4.15635100	0.58904000
N	3.05757500	1.00665700	-0.26478600
N	3.07647400	-0.28815800	-0.76930900
H	-2.86349100	-3.40652200	-0.46986200
H	-4.92484700	-2.01579200	-0.05274700
H	-4.69487900	0.44462400	0.32780200
H	-0.62752700	-2.30968300	-0.55515700
H	-1.11218600	4.51796000	-0.20759600
H	-1.04801300	4.09781400	1.50709400
H	0.38277200	4.85860700	0.72827400
C	1.75580300	-0.91443900	-0.79545300
O	1.52961200	-1.87256100	0.20198300
C	1.67834500	-1.43725000	1.54912900
H	0.87657900	-0.72016500	1.80054700
H	2.64154300	-0.91301400	1.66621300
C	1.60876800	-2.65104700	2.44784900

H	1.71620800	-2.34983200	3.49805500	O 1			
H	0.64305100	-3.16125600	2.32832200	C	-5.83653300	-1.73577900	-0.16470800
H	2.41221300	-3.35777400	2.20062300	C	-6.49684600	-0.79606500	0.69778300
H	3.82095300	-0.86740600	-0.39052000	C	-5.85852200	0.32279300	1.14857900
C	1.51427800	-1.60174200	-2.12960600	C	-4.50696100	0.56641200	0.75334100
H	2.23188600	-2.42732600	-2.22638700	N	-3.91124900	-0.38803100	-0.09320000
H	1.68272400	-0.88020300	-2.93618400	C	-4.55191500	-1.51547200	-0.54593600
H	0.49838100	-2.00686600	-2.21126700	N	-3.69621400	1.56004200	1.04756000

Product

O 1				C	-2.53269900	1.26484400	0.38072400
C	-4.43989300	-1.78545900	-0.37327700	C	-2.63188500	0.06271900	-0.33565300
C	-5.10230400	-0.52052900	-0.29636100	C	-1.28565400	1.91890200	0.27545000
C	-4.37479100	0.63022300	-0.22961500	N	-0.33957700	1.37280400	-0.46968700
C	-2.95263000	0.56673400	-0.23945500	C	-0.57067700	0.19697500	-1.11659400
N	-2.33492000	-0.70189400	-0.32555900	N	-1.70051600	-0.50758900	-1.08651100
C	-3.08437600	-1.86105100	-0.38591100	C	-1.00206400	3.19465900	1.00592300
N	-2.07607000	1.54655200	-0.17672800	N	0.48934700	-0.23453800	-1.85758200
C	-0.86430900	0.93954300	-0.22082300	N	0.54869500	-1.52265600	-2.36887600
C	-0.98919300	-0.44454700	-0.31542100	H	-6.35646800	-2.62520500	-0.51624300
C	0.43949700	1.54965700	-0.17039900	H	-7.52907400	-0.98662600	0.99370500
N	1.50283900	0.80157500	-0.21595700	H	-6.34022600	1.04787800	1.80323000
C	1.36774200	-0.54253000	-0.31523400	H	-3.96380500	-2.16491100	-1.19436400
N	0.14705300	-1.23048100	-0.37326200	H	-1.93380400	3.71225400	1.26290700
C	0.55143000	3.03395900	-0.06080000	H	-0.46616800	2.96972400	1.94093300
N	2.34871600	-1.41459800	-0.37954300	H	-0.36011100	3.84485800	0.39906000
N	1.81419900	-2.64208400	-0.48173900	H	0.76475200	-1.48666400	-3.36372300
H	-5.01203000	-2.71048300	-0.42042100	H	1.30198000	-2.02953800	-1.90072300
H	-6.19146900	-0.48495600	-0.28881000	H	1.35040100	0.29366500	-1.72172200
H	-4.83200900	1.61651200	-0.16498300	C	3.74138000	-0.65266400	-0.77930200
H	-2.54311300	-2.79742700	-0.43964500	O	2.79261400	-1.45858700	-0.27871800
H	0.05542100	3.51158000	-0.91811100	O	3.24497200	0.57309100	-1.06915000
H	0.03153800	3.38105700	0.84373500	O	4.86559400	-0.29850100	0.52772200
H	1.60438100	3.33220100	-0.02504400	C	5.43119200	-1.46417000	1.05077400
H	4.19632400	-1.26302100	-0.29844200	H	4.67610000	-2.27222300	1.13202400
C	0.50604600	-2.56232600	-0.48181100	H	6.24258600	-1.85146000	0.40157400
O	5.14993300	-1.23551500	-0.07761300	C	4.14341000	1.66844700	-1.27914600
C	5.25633800	-0.51121500	1.12092800	H	3.91611400	2.08264800	-2.27162800
H	6.26445400	-0.68935600	1.52979700	H	5.17568900	1.29828500	-1.27415000
H	4.54050900	-0.88729800	1.87762100	C	2.03276300	-0.97040600	0.83889800
C	5.03979800	0.98095700	0.91667600	H	1.65715200	0.03706400	0.61133800
H	5.15593100	1.53475800	1.86009800	H	2.71285000	-0.89983400	1.70034900
H	5.76753200	1.37247400	0.19052700	C	5.99415400	-1.16149000	2.42978600
H	4.02736800	1.16516300	0.52610800	H	5.19314500	-0.82896800	3.10590000
C	-0.37232100	-3.75826100	-0.59247400	H	6.47117300	-2.05172500	2.86345100
H	-1.01457600	-3.71878900	-1.48197500	H	6.74423700	-0.36011200	2.36566300
H	0.29394200	-4.62205400	-0.69065600	C	3.93580700	2.69232300	-0.18480200
H	-0.98709600	-3.90474500	0.30533700	H	4.20228700	2.24588700	0.78202200
				H	4.56574400	3.57471100	-0.36276400
				H	2.88441400	3.01204600	-0.15606000
				C	0.90184100	-1.94100200	1.08567200
				H	0.30643000	-1.60377100	1.94526000
				H	0.23967800	-2.00146500	0.20973000

TS1 (v = 144.25 i(cm-1))

H	1.29054500	-2.94532500	1.30498800
C	4.52680000	-1.33485000	-1.86008700
H	5.35926800	-0.70357200	-2.19029900
H	4.91188600	-2.29505500	-1.49905800
H	3.84929500	-1.51679000	-2.70685800

C	-4.07408700	1.50696000	0.25385100
H	-3.46080700	2.34695000	0.59863400
H	-4.71654000	1.16747300	1.07311800
H	-4.70576900	1.84225900	-0.58130800

TS2 (v = 225.65 i(cm-1))

0 1			
C	2.88288700	-3.20621200	0.13935600
C	4.22078400	-2.82301200	0.49083600
C	4.58038000	-1.50982000	0.58947900
C	3.60679100	-0.49645500	0.33478500
N	2.31408100	-0.93058600	-0.01163800
C	1.94888100	-2.25131900	-0.10636200
N	3.70997200	0.81686300	0.36635800
C	2.45932800	1.26817500	0.03456900
C	1.57082400	0.21149100	-0.20631900
C	1.91494400	2.56283700	-0.13292800
N	0.63845700	2.67951300	-0.45881800
C	-0.11332000	1.56673700	-0.63059100
N	0.29308900	0.30834900	-0.55179400
C	2.75633600	3.78751600	0.03606600
N	-1.43598100	1.81663600	-0.92839600
N	-2.27917200	0.77531900	-1.24430600
H	2.60788900	-4.25708600	0.06902500
H	4.95990100	-3.60168400	0.68216300
H	5.58912600	-1.19826100	0.85693900
H	0.90876300	-2.43793300	-0.37384100
H	3.30908000	3.74282300	0.98460100
H	3.50261900	3.84107300	-0.77081800
H	2.12934200	4.68504900	0.00769200
H	-1.76973600	-0.03792600	-1.59266600
H	-1.60283500	2.68925600	-1.41992000
C	-3.19966600	0.39894700	-0.25411400
O	-2.27859000	-0.21416400	1.15294500
O	-3.79685600	-0.72555100	-0.69067300
C	-2.25129800	0.51446500	2.33809300
H	-2.06514400	-0.20913500	3.15619500
H	-3.23073400	0.97290600	2.58183400
C	-1.17217500	1.59079200	2.39454600
H	-1.35689900	2.38277800	1.65465500
H	-1.13033300	2.05033200	3.39373000
H	-0.18732600	1.14917500	2.17483600
C	-4.79101200	-1.31371600	0.14308900
H	-5.73440400	-0.75339600	0.03992000
H	-4.45121300	-1.25216500	1.18678600
C	-4.96667700	-2.75081400	-0.28978500
H	-5.74274600	-3.23483200	0.31745300
H	-5.26591200	-2.80385000	-1.34563200
H	-4.02528600	-3.30234000	-0.16347700

TS3 (v = 236.73 i(cm-1))

0 1			
C	-2.67929700	-2.61768300	-0.50112600
C	-3.90644300	-1.97467700	-0.12232200
C	-3.94276300	-0.63830000	0.15068900
C	-2.74378000	0.13279900	0.07034000
N	-1.55823100	-0.55394100	-0.28397400
C	-1.53115300	-1.89813300	-0.58089800
N	-2.53552500	1.41374000	0.27106500
C	-1.19413300	1.58915100	0.04429200
C	-0.55954200	0.38967000	-0.29232000
C	-0.35198100	2.73493300	0.12683800
N	0.92282500	2.63145300	-0.15294900
C	1.46058700	1.41306200	-0.51318400
N	0.74642500	0.24494700	-0.52977500
C	-0.92131200	4.05939100	0.53311400
N	2.74844600	1.39557200	-0.83677200
N	3.04641100	0.09349200	-1.27736000
H	-2.65933900	-3.68027000	-0.73686200
H	-4.81958500	-2.56766300	-0.06440400
H	-4.86161000	-0.12325200	0.42869800
H	-0.56807900	-2.30333000	-0.88588800
H	-1.69576600	4.37223200	-0.18257000
H	-1.40774500	3.97615600	1.51577600
H	-0.12958000	4.81512700	0.57288000
H	3.06806700	-0.00662500	-2.29088900
C	2.45600800	-0.91179900	-0.63242100
O	2.63230900	-0.91009400	0.67329200
C	1.87291600	-1.79630600	1.50205200
H	2.27044800	-2.81662800	1.39808800
H	0.82543500	-1.78162500	1.16174900
C	1.98537000	-1.30053100	2.92323200
H	1.42640500	-1.96733100	3.59213200
H	3.03570900	-1.28265300	3.24312500
H	1.57011000	-0.28717300	3.00797200
C	2.19591500	-2.19404800	-1.35526100
H	3.15270100	-2.73032400	-1.44585100
H	1.51021200	-2.83813700	-0.79712500
H	1.78933600	-1.99976000	-2.35294800

TS4 (v = 247.31 i(cm-1))

0 1			
C	-1.61141900	3.20986100	0.30591000
C	-3.01058900	2.99438000	0.08942000

C	-3.49319700	1.73484400	-0.11873900
C	-2.60202800	0.62516200	-0.07839000
N	-1.24626900	0.87965300	0.24661200
C	-0.74491900	2.16542700	0.36657600
N	-2.82497600	-0.65251100	-0.30643200
C	-1.62081000	-1.26029400	-0.12171600
C	-0.64896400	-0.34419400	0.25473000
C	-1.23168100	-2.63117700	-0.37627800
N	0.01433700	-2.99340100	-0.28433700
C	0.94858300	-2.08956800	0.13307500
N	0.62178200	-0.77484400	0.53275900
C	-2.27397900	-3.61440000	-0.79740300
N	2.21722200	-2.30802100	0.26581100
N	2.71541400	-1.13710200	0.76688700
H	-1.21568700	4.22072000	0.39228100
H	-3.68467600	3.85045400	0.05982300
H	-4.54285600	1.53410200	-0.32949000
H	0.34064600	2.25056800	0.40792400
H	-2.80076200	-3.24241200	-1.68783900
H	-1.81407300	-4.58505900	-1.00947300
H	-3.02647200	-3.72330400	-0.00250000
C	1.80680400	-0.12034100	0.89328900
O	1.93543800	1.14049500	-0.44063100
C	3.20690500	1.12663400	-0.99214300
H	3.44517600	0.14203500	-1.44910600
H	3.99531500	1.29879500	-0.22381100
C	3.32226400	2.20599700	-2.05886200
H	4.31442900	2.19380700	-2.53297100
H	2.56015700	2.04810600	-2.83581600
H	3.15793700	3.19952800	-1.61686000
H	3.66864900	-1.10183000	1.10439700
C	1.91540700	0.77987200	2.08951100
H	2.88603600	1.29160200	2.05950600
H	1.12466600	1.53488100	2.10201900
H	1.85118900	0.17441900	3.00399100

Route 2

Me:

In1

O 1			
C	6.38397400	-2.33932700	-1.05108100
C	7.37998500	-1.44201500	-0.53568100
C	7.03623000	-0.24465500	0.02192600
C	5.65777800	0.12593800	0.09463400
N	4.72646300	-0.79249500	-0.42740700
C	5.07118400	-1.99791400	-0.98785900

N	5.08718900	1.20814000	0.57855800
C	3.74295000	1.00967200	0.37507700
C	3.48512100	-0.22081500	-0.24747300
C	2.59773200	1.78262600	0.66055500
N	1.40273000	1.31455100	0.33470800
C	1.29280400	0.10526200	-0.26562500
N	2.30474100	-0.71236700	-0.58448800
C	2.71281300	3.12057100	1.32270400
N	0.05210000	-0.35275200	-0.59034900
N	-1.11103800	0.35242300	-0.35304300
H	6.67123200	-3.29202900	-1.49246100
H	8.43043300	-1.72944800	-0.59361400
H	7.77590800	0.44945400	0.41886400
H	4.24216100	-2.60702400	-1.34821900
H	3.19163500	3.01565800	2.30732100
H	3.35123500	3.78564300	0.72324400
H	1.72092200	3.56947500	1.44223700
H	-1.57644200	0.60662800	-1.22396000
H	-1.77531100	-0.20914700	0.18217300
H	0.03121200	-1.24750100	-1.07048000
C	-4.38171000	-0.60842200	-0.55291600
O	-3.95499500	0.68058800	-0.84234800
O	-3.68620500	-1.02499400	0.58774300
O	-5.73689600	-0.63269400	-0.21919400
C	-6.65210500	-0.27639600	-1.24242500
H	-6.26957600	0.60030300	-1.79255600
H	-6.75763500	-1.10598000	-1.96194900
C	-4.15882100	-2.17334300	1.28250600
H	-3.27256000	-2.77820300	1.52501900
H	-4.80543400	-2.77436900	0.62640400
C	-4.27542700	1.67231100	0.12873200
H	-4.07172600	1.27760700	1.13580000
H	-5.35173900	1.90628900	0.07113800
C	-7.98298000	0.03392500	-0.59343800
H	-7.88465300	0.87758100	0.10391500
H	-8.72756800	0.29448100	-1.35722400
H	-8.34786900	-0.83875900	-0.03408300
C	-4.89834800	-1.78165300	2.54682100
H	-5.79718000	-1.20375600	2.29533800
H	-5.19500400	-2.67769500	3.11030100
H	-4.25238700	-1.16773300	3.19072700
C	-3.43661800	2.89808600	-0.15843500
H	-3.68205600	3.69953000	0.55136300
H	-2.36917700	2.65494000	-0.06696200
H	-3.62895600	3.26589300	-1.17635200
C	-4.03438300	-1.47287800	-1.75440700
H	-2.94456100	-1.46038400	-1.88005500
H	-4.50062600	-1.08165700	-2.66676900
H	-4.36966100	-2.50488600	-1.58885500

In2

0 1
 C -5.20457300 -1.37836700 -0.50789100
 C -5.86978800 -0.29757700 0.16426400
 C -5.18800200 0.81269900 0.56994900
 C -3.78358400 0.90310500 0.32155600
 N -3.18542400 -0.18496200 -0.34203100
 C -3.87046900 -1.30333500 -0.75020700
 N -2.92445200 1.85613200 0.61345300
 C -1.72293300 1.39696300 0.13349100
 C -1.85055100 0.13385200 -0.46606400
 C -0.41840500 1.93151500 0.12300500
 N 0.55934000 1.23641100 -0.44012300
 C 0.30039600 0.02639900 -0.97595900
 N -0.88535100 -0.58442000 -1.01667800
 C -0.11066300 3.25512700 0.75071900
 N 1.32838200 -0.65208400 -1.59470600
 N 2.63477000 -0.37510700 -1.26037300
 H -5.76011200 -2.25928700 -0.82463900
 H -6.94161100 -0.37215000 0.35103000
 H -5.67393100 1.64292700 1.08077500
 H -3.27623100 -2.06727600 -1.25153200
 H -1.00273900 3.89288900 0.77294400
 H 0.22100600 3.09946200 1.78927500
 H 0.70257900 3.75228500 0.20832800
 H 3.22999800 -0.40056300 -2.08519700
 H 1.08302100 -1.61479200 -1.82169400
 C 3.21533400 -1.19544800 -0.19660500
 O 2.24942300 -1.18714800 0.81234300
 O 4.40621500 -0.59732900 0.20501400
 C 2.58730400 -1.82694300 2.03406600
 H 2.36693500 -1.11104100 2.84099500
 H 3.67004100 -2.02411900 2.06974200
 C 1.78155300 -3.09741700 2.22707500
 H 2.02343500 -3.84324000 1.45717100
 H 1.98892400 -3.53698100 3.21271300
 H 0.70680700 -2.87571600 2.16594800
 C 4.30085700 0.74045800 0.69120400
 H 4.73547700 0.75295500 1.70358000
 H 3.24137700 1.02233300 0.76642800
 C 5.04574400 1.69171400 -0.22283200
 H 5.04340300 2.70846500 0.19486800
 H 6.08977900 1.37132500 -0.34764100
 H 4.56568300 1.71789200 -1.21079500
 C 3.57270500 -2.60369500 -0.65439200
 H 4.32325300 -2.54611800 -1.45328600
 H 2.67636500 -3.11544100 -1.03096000
 H 3.99322900 -3.19129400 0.17241500

In3

0 1

C -4.70458000 -2.25023200 -0.33246800
 C -5.63407100 -1.16652100 -0.17997200
 C -5.20526800 0.11752200 -0.00563400
 C -3.80297200 0.39021300 0.02595400
 N -2.93934600 -0.71098400 -0.12850400
 C -3.36957100 -2.00334500 -0.30404600
 N -3.15597800 1.52628400 0.17993400
 C -1.82974900 1.17775900 0.12770300
 C -1.66052400 -0.20285200 -0.06235400
 C -0.63345100 1.91892600 0.22451800
 N 0.52728900 1.28485800 0.13829600
 C 0.54579600 -0.05174000 -0.04878200
 N -0.51472800 -0.85637100 -0.16032300
 C -0.65460500 3.40237500 0.41960400
 N 1.75991600 -0.68519700 -0.11674300
 N 2.92729800 -0.00062400 -0.20140700
 H -5.05969600 -3.26989000 -0.47025100
 H -6.70319800 -1.38021400 -0.20470300
 H -5.89456300 0.95259200 0.11127500
 H -2.58655800 -2.75391700 -0.41125700
 H -1.13664600 3.88823000 -0.44163800
 H -1.24840700 3.66058800 1.30812700
 H 0.36580700 3.78416100 0.53013700
 H 1.71237400 -1.67956300 -0.32255700
 C 4.01560000 -0.66618400 -0.19784800
 O 5.13095600 0.08906800 -0.29505700
 C 6.40099500 -0.49284300 -0.56474700
 H 6.92703800 0.24017400 -1.19084200
 H 6.28948300 -1.40808900 -1.16452700
 C 7.18162600 -0.74364400 0.71078200
 H 8.19090100 -1.10453900 0.47016900
 H 7.27228200 0.18927100 1.28368100
 H 6.69071300 -1.49168100 1.34903900
 C 4.10816800 -2.16312900 -0.09147900
 H 3.92594900 -2.64176800 -1.06629600
 H 5.08493000 -2.49485200 0.27219000
 H 3.34930400 -2.52713200 0.61483800

In4

0 1

C 3.39425200 -2.73723100 1.09413300
 C 4.34369700 -2.22033000 2.04670300
 C 4.30497300 -0.92461000 2.46416800
 C 3.29507300 -0.04824600 1.94533500
 N 2.39189600 -0.61260700 1.01821000
 C 2.43340600 -1.92058100 0.59684800
 N 3.06279600 1.21377000 2.18925200
 C 1.96427200 1.52787100 1.40922100
 C 1.51696700 0.39334800 0.65345900
 C 1.27925400 2.71128600 1.23641200

N	0.20574000	2.64359000	0.40316200
C	-0.14094200	1.48314000	-0.35325500
N	0.53857000	0.31043500	-0.19596500
C	1.67924600	3.97895700	1.90984800
N	-1.12515700	1.69734900	-1.15105900
N	-1.57610500	2.99824500	-0.86428700
H	3.44179200	-3.77557800	0.77175600
H	5.10994800	-2.88999800	2.43934300
H	5.01571000	-0.51990900	3.18328300
H	1.66819200	-2.20806400	-0.12454100
H	2.64421300	3.82107800	2.40281400
H	1.76101700	4.79179600	1.17550900
H	0.93754100	4.26755100	2.66824100
H	-1.89690400	3.46019400	-1.70984200
C	-0.54639500	3.76483100	-0.16851300
O	0.37897600	4.41081000	-1.01731800
C	0.09359300	5.71274200	-1.50671200
H	1.01778800	6.02374300	-2.01139200
H	-0.06935600	6.41304200	-0.67142100
C	-1.06664500	5.76892700	-2.48696200
H	-1.11234300	6.76545900	-2.94714900
H	-0.92954500	5.02648300	-3.28653300
H	-2.03647600	5.59258800	-1.99815800
C	-1.19534200	4.70217600	0.84088600
H	-0.48261500	5.40499400	1.28576000
H	-1.98250500	5.27604300	0.33313300
H	-1.67055200	4.10328700	1.62599400

H	3.01187700	3.69835500	3.02080400
H	3.26025900	4.78624000	1.62742300
H	1.67697500	4.73120300	2.44300200
H	-0.17052900	5.38657700	-2.74569900
C	1.14611400	4.35790400	-0.65547100
O	-0.73219100	6.17031300	-2.92165100
C	-1.95985300	5.89596800	-2.28964600
H	-2.58969900	6.79385900	-2.38937900
H	-1.81607600	5.72919500	-1.20360400
C	-2.66346100	4.69316800	-2.89906100
H	-3.63416400	4.51135300	-2.41546400
H	-2.83239000	4.85585000	-3.97349600
H	-2.04304800	3.79145500	-2.78060800
C	1.28059600	5.77432400	-0.21236200
H	2.32947600	6.07596000	-0.09705500
H	0.81715400	6.38744300	-0.99574700
H	0.75376700	5.95846800	0.73244500

TS1 (v = 164.70 i(cm-1))

0 1

C	-3.25986700	2.48682900	2.54835900
C	-4.21061300	2.75436800	1.50590200
C	-4.23827800	2.00894900	0.36339200
C	-3.30289000	0.94149600	0.19923600
N	-2.39546100	0.72292700	1.25404500
C	-2.36801800	1.47237600	2.40517600
N	-3.13648400	0.10022300	-0.79823900
C	-2.09277500	-0.69954000	-0.40405500
C	-1.60933500	-0.34034100	0.86364300
C	-1.43455700	-1.79019800	-1.00508000
N	-0.41936900	-2.36024100	-0.37256400
C	-0.02971000	-1.89225600	0.83166900
N	-0.60585600	-0.89962200	1.51720400
C	-1.87740100	-2.33719000	-2.32701800
N	1.03712700	-2.49282500	1.45654600
N	1.98029300	-3.19384400	0.71551300
H	-3.24924400	3.08771800	3.45592600
H	-4.92351600	3.56910900	1.63672000
H	-4.95193900	2.19328000	-0.43841800
H	-1.61583000	1.18700900	3.14101500
H	-2.33747300	-1.55098600	-2.93901300
H	-1.02859400	-2.78778200	-2.85551600
H	-2.63401700	-3.12113500	-2.16588700
H	2.77747800	-2.58615400	0.51759200
H	2.30366000	-3.99441700	1.25329400
H	1.36977100	-1.94804900	2.24951000
C	2.22388500	0.71917800	0.33475000
O	1.38799900	0.33710500	-0.63591000
O	2.94636100	-0.31900900	0.81465800
O	3.47988600	1.68246000	-0.43476300

Product

0 1

C	2.43117500	-2.83280700	1.53823300
C	3.04737500	-2.56450100	2.80851500
C	3.23570300	-1.29139200	3.25964000
C	2.80786200	-0.19311000	2.44843700
N	2.21154700	-0.51671100	1.21757200
C	2.02237500	-1.79845900	0.76145900
N	2.88184400	1.09809200	2.67065000
C	2.31836300	1.68182000	1.55957400
C	1.88353900	0.68421900	0.61521500
C	2.12554500	3.00518600	1.24487400
N	1.51545400	3.21386300	0.02216400
C	1.13208300	2.16219800	-0.84021300
N	1.31828800	0.86287500	-0.53781500
C	2.53969900	4.12798200	2.13075600
N	0.59116300	2.66245400	-1.92957600
N	0.61156900	4.00119300	-1.79823700
H	2.29052900	-3.85541700	1.19404000
H	3.37026000	-3.40563900	3.42331600
H	3.70176300	-1.07206000	4.21880600
H	1.54655400	-1.88924600	-0.21515100

C	2.95527900	2.82278800	-1.04313300	H	0.71174800	3.39469900	-0.07625000
H	1.97271900	2.60920600	-1.51082600	H	2.38993200	0.40550800	-1.59278600
H	2.78433300	3.63724100	-0.30834600	H	0.94970900	-1.91490700	-1.86712300
C	3.87617000	-0.04187500	1.86280600	C	3.35162100	-0.86718500	-0.37749400
H	3.32398100	0.19163400	2.78753800	O	2.75301200	-0.08844600	1.11894700
H	4.46842900	0.83732100	1.57419900	O	4.44865800	-0.13232600	-0.64061900
C	1.92964900	-0.50777300	-1.66323600	C	2.30941500	-0.87157000	2.18017400
H	1.81547600	-1.55594600	-1.34895500	H	2.42590900	-0.26331500	3.09890000
H	2.99644300	-0.27136000	-1.77223100	H	2.94391600	-1.76509300	2.34804800
C	3.91976300	3.30830100	-2.11358900	C	0.85225600	-1.31019400	2.07781200
H	4.04693800	2.53923100	-2.88966200	H	0.69716500	-1.99375400	1.23085900
H	3.55193800	4.22905400	-2.58856700	H	0.53289300	-1.82057200	2.99914100
H	4.90552300	3.51441000	-1.67175700	H	0.20374200	-0.43305400	1.92449700
C	4.74453000	-1.26356000	2.05304300	C	5.54878800	-0.23752600	0.25755800
H	5.28794400	-1.49767600	1.12713200	H	6.06948900	-1.19439800	0.09108100
H	5.47623800	-1.08328700	2.85126900	H	5.16104000	-0.21707500	1.28636300
H	4.13783700	-2.13598300	2.33508100	C	6.47251500	0.92921800	-0.00502900
C	1.16565900	-0.22904800	-2.93698100	H	7.34591500	0.87509600	0.65791500
H	1.49157000	-0.91594200	-3.72977700	H	6.82341700	0.91819900	-1.04611700
H	0.08696000	-0.36887600	-2.77801900	H	5.95039500	1.87791900	0.17863200
H	1.33495600	0.80278300	-3.27568900	C	3.54172500	-2.32108100	-0.05976800
C	1.55710300	1.62545800	1.32901100	H	2.57594500	-2.79431200	0.14875600
H	0.92312900	1.00903400	1.98231600	H	4.20524300	-2.45868600	0.80009700
H	2.30207000	2.16756900	1.92164700	H	3.99394200	-2.79933000	-0.94054900
H	0.92579400	2.34470400	0.79454300				

TS3 (v = 235.83 i(cm-1))

O 1			
C	4.85251800	-1.14708900	0.63166300
C	5.31245700	0.19994700	0.42373500
C	4.45528700	1.19401300	0.05336200
C	3.06793300	0.89464400	-0.13204700
N	2.67541700	-0.44296000	0.08697100
C	3.53930500	-1.44391200	0.45827200
N	2.06745300	1.66721300	-0.48027000
C	0.97229900	0.83040500	-0.49766900
C	1.31480000	-0.49462700	-0.14906600
C	-0.39103500	1.04998500	-0.74648100
N	-1.20965000	0.01085500	-0.64640700
C	-0.76274600	-1.27722400	-0.38064700
N	0.53437100	-1.54864000	-0.08065400
C	-0.91913900	2.40613900	-1.10165700
N	-1.64468300	-2.27182500	-0.41913500
N	-2.86354300	-1.75010800	-0.90249900
H	5.54739400	-1.93129100	0.92661200
H	6.37033000	0.42352400	0.56687400
H	4.78531200	2.21941900	-0.10841200
H	3.09098800	-2.42907100	0.58868400
H	-0.08945900	3.07000100	-1.37043000
H	-1.62298900	2.33682100	-1.94151700
H	-1.44912500	2.85413100	-0.24762300

TS2 (v = 229.81 i(cm-1))

O 1			
C	-5.37620600	-1.68535500	-0.11955400
C	-6.03958900	-0.50993300	0.36996400
C	-5.36140200	0.65789700	0.56804000
C	-3.96265200	0.71318700	0.28175300
N	-3.36665100	-0.46834500	-0.19668300
C	-4.04697500	-1.64468100	-0.39466900
N	-3.10663600	1.70761200	0.39112800
C	-1.90937400	1.17865200	-0.01923800
C	-2.03524300	-0.17098000	-0.38949800
C	-0.61924100	1.72573800	-0.17338100
N	0.35911500	0.93900300	-0.60221900
C	0.10856000	-0.35689200	-0.86993600
N	-1.07201100	-0.97027700	-0.81842500
C	-0.34049300	3.16502900	0.12245300
N	1.17691600	-1.14041200	-1.25183400
N	2.43272500	-0.59666200	-1.40393200
H	-5.92772600	-2.61117300	-0.27264100
H	-7.10734300	-0.55787400	0.58642100
H	-5.84567200	1.55970400	0.94006000
H	-3.45262000	-2.47934500	-0.76621600
H	-0.98443800	3.81038800	-0.49229300
H	-0.57333800	3.38507800	1.17459100

H	-2.99156000	-1.88273900	-1.90424200
C	-3.19136400	-0.52539900	-0.47656400
O	-3.23460000	-0.39984000	0.83621900
C	-3.46648700	0.88324600	1.42309100
H	-4.48460300	1.21801700	1.17548500
H	-2.74444800	1.59623300	0.99705800
C	-3.28011200	0.74310900	2.91424500
H	-3.45377200	1.71111100	3.40131200
H	-3.98971800	0.01189200	3.32368600
H	-2.25820300	0.41262100	3.14280000
C	-4.01464200	0.37552900	-1.33823200
H	-3.81093400	0.18332400	-2.39662000
H	-3.79369900	1.42516200	-1.11663600
H	-5.07872000	0.19522300	-1.12485000

C	3.47710800	0.82765600	-1.74594400
H	3.48838500	1.88289400	-1.46212600
H	4.51125200	0.45853400	-1.74535700
H	3.07209800	0.71175300	-2.76033800

Route 1

Et:

In1

O 1

C	5.84757100	-1.76600600	0.07781800
C	6.53984300	-0.72605600	-0.63024300
C	5.91873100	0.44552600	-0.95445300
C	4.55363900	0.64208100	-0.58224200
N	3.92659100	-0.40993800	0.11239600
C	4.54998500	-1.58934100	0.43834900
N	3.75209600	1.66756600	-0.77942800
C	2.56474700	1.29172400	-0.20265300
C	2.63738500	0.01076400	0.35971100
C	1.30962800	1.92969300	-0.07254100
N	0.33356300	1.29614600	0.55145700
C	0.54142100	0.04649700	1.06058400
N	1.67616000	-0.64724000	0.99388700
C	1.07457100	3.29616600	-0.63579900
N	-0.54670200	-0.47198200	1.69360300
N	-0.61992800	-1.81946100	2.02528300
H	6.35376200	-2.69621300	0.32959000
H	7.58216100	-0.88168200	-0.91064100
H	6.42563500	1.24699200	-1.49040000
H	3.93959200	-2.31436300	0.97672000
H	1.80749100	4.00584800	-0.22591200
H	1.21519200	3.28252200	-1.72650700
H	0.05979100	3.63564600	-0.40187000
H	-0.87138000	-1.91103700	3.00845100
H	-1.36864500	-2.24080300	1.47111400
H	-1.41769000	0.04492500	1.56218400
C	-3.82586800	-0.80704700	0.47658400
O	-2.76991400	-1.51157600	-0.08165400
O	-3.28113700	0.32839800	1.09512600
O	-4.69002700	-0.31988200	-0.50283600
C	-5.43169900	-1.25957100	-1.26094700
H	-4.79180700	-2.11964600	-1.52150400
H	-6.28076900	-1.63500300	-0.66483100
C	-4.14982100	1.39970500	1.45052000
H	-3.87236200	1.70187700	2.47117500
H	-5.19137200	1.04875400	1.47458600
C	-2.03378300	-0.84684400	-1.10688200
H	-1.70152500	0.13780200	-0.74215400

TS4 (v = 235.83 i(cm-1))

O 1

C	-4.76118300	-1.10295100	0.70326200
C	-5.19331900	0.26757200	0.61186600
C	-4.32714800	1.27243700	0.30242100
C	-2.94867200	0.96118500	0.06177000
N	-2.58539600	-0.39765600	0.16458500
C	-3.46046700	-1.41092500	0.47755300
N	-1.94787800	1.74478900	-0.24403900
C	-0.86036700	0.90088800	-0.36028800
C	-1.23116400	-0.46494600	-0.10079400
C	0.45891200	1.16462000	-0.64123500
N	1.26306000	0.05579500	-0.70190500
C	0.81867100	-1.25973300	-0.37650700
N	-0.47991000	-1.52243500	-0.08261800
C	0.99864200	2.53667600	-0.83504000
N	1.79445200	-2.10816000	-0.41411700
N	2.87517900	-1.36180400	-0.82199800
H	-5.46822200	-1.89224000	0.95074500
H	-6.24302000	0.49983900	0.79622000
H	-4.63850900	2.31333300	0.23018000
H	-3.02937900	-2.41122600	0.52168800
H	0.19868700	3.25747600	-0.63660900
H	1.83518400	2.68638000	-0.13841800
H	1.36229500	2.67987000	-1.86220400
H	3.79223000	-1.78738700	-0.81156200
C	2.67393900	-0.00750600	-0.79195700
O	3.04592400	0.70755200	0.83982800
C	4.38107600	0.98219900	1.09988200
H	4.43063300	1.47345200	2.09158700
H	4.80810300	1.72307800	0.38875000
C	5.29234000	-0.24452400	1.13584000
H	6.28004700	0.01306300	1.54545600
H	4.84415700	-1.02682000	1.76661100
H	5.46113600	-0.66680300	0.13302300

H	-2.68890100	-0.68336000	-1.97761400
C	-5.92974200	-0.56293800	-2.50827600
H	-5.08456400	-0.21750100	-3.11989900
H	-6.54028500	-1.24873700	-3.11041700
H	-6.54447500	0.30751200	-2.23970900
C	-3.99341700	2.55722500	0.48475700
H	-4.29858100	2.24763700	-0.52338800
H	-4.61087400	3.40996800	0.80052000
H	-2.94331600	2.88215400	0.45248100
C	-0.85439100	-1.72201600	-1.47026300
H	-0.24736400	-1.23194500	-2.24409900
H	-0.21730500	-1.90332900	-0.59213400
H	-1.19687000	-2.69162100	-1.85907000
C	-4.47641000	-1.71100800	1.53485600
H	-3.81019200	-1.64028600	2.40759300
H	-5.43213300	-1.24820600	1.82553600
C	-4.66164500	-3.18416300	1.18313000
H	-4.98307500	-3.73488800	2.07771300
H	-5.41705600	-3.35082100	0.40595600
H	-3.71500100	-3.62042100	0.83770200

O	-4.22882600	-0.74888900	-0.87936500
C	-2.65671000	0.50060300	1.94262100
H	-2.56354700	-0.28369600	2.70780400
H	-3.60907500	1.01675900	2.13432700
C	-1.48534700	1.46111400	2.04757000
H	-1.56821000	2.28581700	1.32554300
H	-1.43658500	1.89002400	3.05849100
H	-0.54243500	0.92974500	1.84817500
C	-5.06162700	-1.36242800	0.09192500
H	-6.07274200	-1.41789100	-0.33925400
H	-5.12568800	-0.73939000	0.99822300
C	-4.55123300	-2.74656100	0.44374200
H	-4.48179300	-3.36706200	-0.46085100
H	-3.55362800	-2.67145500	0.89639700
H	-5.23089500	-3.24056600	1.15241000
C	-4.14686800	1.56228900	-0.21010100
H	-4.93583700	1.38023200	0.53380600
H	-3.48561500	2.32691200	0.22294800
C	-4.77639800	2.07032600	-1.50226900
H	-5.42330200	2.93395000	-1.30175700
H	-4.01857000	2.38881600	-2.23373600
H	-5.38485800	1.28222200	-1.96666600

In2

O 1

C	3.14952300	-3.20133800	0.07421800
C	4.39885300	-2.69146300	0.56485300
C	4.60998800	-1.35050800	0.70890300
C	3.56850600	-0.43572800	0.36379900
N	2.36690100	-0.99208300	-0.11235700
C	2.15213400	-2.34075500	-0.25669400
N	3.53399500	0.87982400	0.41325400
C	2.28154400	1.20836500	-0.03942000
C	1.53154500	0.07204400	-0.37383200
C	1.61910300	2.44091200	-0.24001700
N	0.37885200	2.42857300	-0.69596900
C	-0.23743600	1.24662900	-0.96136600
N	0.28907600	0.03513900	-0.83688400
C	2.29242900	3.74326900	0.05827200
N	-1.52235700	1.39519000	-1.41610600
N	-2.39071600	0.33790700	-1.51001800
H	2.99229700	-4.27291600	-0.03482600
H	5.19034900	-3.39465000	0.82626400
H	5.54952600	-0.94353600	1.08054300
H	1.17055600	-2.62668300	-0.63479200
H	2.57531900	3.78547300	1.12024800
H	3.21962300	3.83221400	-0.52598100
H	1.62445100	4.57836000	-0.17766700
H	-2.85604600	0.30763200	-2.41451800
H	-1.86760600	2.35250300	-1.40866500
C	-3.36496500	0.25491700	-0.42549000
O	-2.67846000	-0.19095100	0.70469300

In3

O 1

C	3.34780100	-3.03376800	0.10358200
C	4.64157100	-2.41606500	0.02703000
C	4.77671600	-1.05995900	-0.05162600
C	3.60828400	-0.23843100	-0.05730300
N	2.36767600	-0.89868700	0.01811700
C	2.22977500	-2.26288200	0.09758500
N	3.48216900	1.07121700	-0.12319700
C	2.12916800	1.28872100	-0.09133200
C	1.40861600	0.08933700	-0.00463400
C	1.33955700	2.46135300	-0.12878300
N	0.02436100	2.34288300	-0.08311100
C	-0.54201000	1.11115300	0.00098000
N	0.09043000	-0.05504300	0.04384100
C	1.96455800	3.81781300	-0.21120800
N	-1.91130400	1.14976200	0.04835100
N	-2.65596800	0.02352600	0.07555100
H	3.25325100	-4.11637400	0.16582300
H	5.52989800	-3.04858500	0.03156600
H	5.74847500	-0.57175700	-0.11168100
H	1.20606200	-2.63327000	0.15126300
H	2.54760400	4.01722400	0.70015800
H	2.66397000	3.86292200	-1.05777400
H	1.19178300	4.58565100	-0.32349500
H	-2.32143000	2.07727500	-0.02329300
C	-3.92699200	0.12546400	0.07557300

O	-4.58888800	-1.04308200	0.24521200
C	-5.83820500	-1.26278500	-0.40745200
H	-5.81494000	-2.31046200	-0.73735900
H	-5.91082000	-0.64142600	-1.31325300
C	-7.00820300	-1.03876200	0.52953100
H	-7.94578800	-1.32803700	0.03535200
H	-6.88789500	-1.65275400	1.43270000
H	-7.09175700	0.01341300	0.83599100
C	-4.70580900	1.41562000	0.05955000
H	-4.20880100	2.13929200	-0.60351300
H	-5.69850800	1.25211600	-0.37705100
C	-4.84298100	1.98390100	1.47782800
H	-3.85724200	2.19545700	1.91622700
H	-5.42396400	2.91514400	1.46793000
H	-5.35341700	1.26263200	2.13128400

In4

O 1			
C	-2.67727200	-2.49939600	-0.31132400
C	-3.91285900	-1.78178300	-0.20168600
C	-3.91331700	-0.42620700	-0.04683200
C	-2.67848600	0.28248900	-0.02029800
N	-1.48314300	-0.46190500	-0.20896300
C	-1.48797000	-1.84440000	-0.30482600
N	-2.43680600	1.56175000	0.16267800
C	-1.08097600	1.68092800	0.09301000
C	-0.47781600	0.45685200	-0.16188900
C	-0.23709600	2.83621100	0.31901700
N	1.05618600	2.72125100	0.32601200
C	1.63376100	1.50106300	0.06895800
N	0.87830500	0.36692900	-0.30781100
C	-0.87980100	4.15965900	0.58211400
N	2.89407500	1.24942900	0.11153600
N	3.04143500	-0.05393400	-0.34460800
H	-2.67343300	-3.58603200	-0.38071400
H	-4.85344000	-2.33220300	-0.22082700
H	-4.82984600	0.15100400	0.06920300
H	-0.51689100	-2.33468500	-0.31507300
H	-1.49103700	4.45609700	-0.28301000
H	-1.56077300	4.08054600	1.44184500
H	-0.11614000	4.91994100	0.77600600
C	1.77640900	-0.77667100	-0.45394900
O	1.55764100	-1.74402300	0.53443700
C	1.56577800	-1.28972000	1.88332600
H	0.67430300	-0.66537700	2.07215000
H	2.45449400	-0.66103200	2.05998500
C	1.57027700	-2.50119500	2.78830200
H	1.57088300	-2.18789900	3.84051400
H	0.67850800	-3.11717900	2.60786200
H	2.46283100	-3.11366600	2.60246200

H	3.79756000	-0.56718100	0.10032700
C	1.68273700	-1.50052700	-1.79899100
H	0.76744400	-2.10758000	-1.83114700
H	2.52874100	-2.20465900	-1.81577900
C	1.73911000	-0.55241500	-2.98566900
H	1.75364800	-1.11576900	-3.92766500
H	0.86402500	0.11352400	-3.00130700
H	2.64276200	0.07037600	-2.93779400

Product

O 1			
C	-4.45364400	-1.75558700	-0.63531400
C	-5.11681500	-0.50463800	-0.43811400
C	-4.38893200	0.62966800	-0.23332500
C	-2.96759000	0.55995900	-0.20469400
N	-2.34902200	-0.70273300	-0.35735300
C	-3.09891500	-1.83891900	-0.59888600
N	-2.09192300	1.53184400	-0.06069000
C	-0.88036900	0.92618500	-0.11136800
C	-1.00338400	-0.45212200	-0.27293400
C	0.42210100	1.54088900	-0.07531700
N	1.48635200	0.80244000	-0.19465100
C	1.35431100	-0.54079100	-0.30909500
N	0.13574400	-1.23497100	-0.33292700
C	0.53041900	3.02170200	0.07628700
N	2.33834500	-1.40915700	-0.37765200
N	1.80921200	-2.64223700	-0.42417500
H	-5.02307400	-2.66262600	-0.83080900
H	-6.20545500	-0.46367200	-0.46582200
H	-4.84544700	1.60884800	-0.09578300
H	-2.56117300	-2.76323400	-0.76948700
H	0.00455500	3.52201700	-0.74979100
H	0.03863600	3.33855000	1.00721000
H	1.58259000	3.32465100	0.08655200
H	4.18774700	-1.26625100	-0.35952700
C	0.50084000	-2.56937800	-0.39283500
O	5.14854100	-1.24262700	-0.17237600
C	5.29999300	-0.50728400	1.01455300
H	6.32445400	-0.67841000	1.38366900
H	4.61669300	-0.87930500	1.80273400
C	5.06907100	0.98224200	0.80685000
H	5.22116400	1.54421400	1.74028400
H	5.76532500	1.37079500	0.04896000
H	4.04076200	1.15946200	0.45662300
C	-0.37278400	-3.77468200	-0.29818600
H	-1.08711300	-3.81216100	-1.13209800
H	0.30644700	-4.62201500	-0.45597200
C	-1.05255300	-3.90585400	1.06768100
H	-1.70435400	-4.78910600	1.08839400
H	-0.29436800	-4.01461800	1.85471600

H -1.66556200 -3.02743800 1.31822600

H 4.37344300 3.64055600 -0.12070900

TS1 (v = 129.66 i(cm-1))

H 2.71645000 2.99252800 0.02609600

0 1

C 0.93752700 -2.16730500 0.91301300

C -5.80223100 -1.70075800 0.06706700

H 0.33896200 -1.93244500 1.80382400

C -6.41675700 -0.70656300 0.90187600

H 0.25785600 -2.22250100 0.05083900

C -5.75314300 0.43308300 1.25290800

H 1.40743900 -3.14988100 1.06077300

C -4.42103300 0.64276200 0.78090100

C 4.65566100 -1.14067700 -1.84562800

N -3.86949600 -0.36479000 -0.03405700

H 5.58992900 -0.56383400 -1.84387400

C -4.53627300 -1.51263500 -0.38724400

H 4.90510600 -2.17127400 -1.56045600

N -3.59231100 1.64498300 0.97991500

C 3.99294900 -1.09681000 -3.21955000

C -2.46104000 1.30046700 0.28287300

H 3.81967600 -0.05995800 -3.54069500

C -2.59859800 0.05947100 -0.35691000

H 4.62799000 -1.58562400 -3.96898500

C -1.21412000 1.93396300 0.09162400

H 3.02320200 -1.61158600 -3.20498700

N -0.30162900 1.33506600 -0.65476400

TS2 (v = 206.50 i(cm-1))

C -0.56648400 0.12641900 -1.22100600

0 1

N -1.70043900 -0.56277600 -1.10710800

C 2.89203300 -3.18579500 0.20780200

C -0.89279000 3.24643500 0.73594000

C 4.22882800 -2.79331500 0.55317600

N 0.46103300 -0.36346400 -1.97498500

C 4.58608600 -1.47787200 0.62633600

N 0.46534000 -1.67164100 -2.43277800

C 3.61100600 -0.47139100 0.35086900

H -6.34226400 -2.60589000 -0.20505100

N 2.31995900 -0.91465100 0.00997000

H -7.43381700 -0.87164400 1.25915500

C 1.95683300 -2.23757200 -0.05849600

H -6.19988400 1.19888800 1.88559100

N 3.71088300 0.84255600 0.35965300

H -3.98297100 -2.20473200 -1.02200200

C 2.45946100 1.28489500 0.01886000

H -1.80978500 3.77569000 1.02048200

C 1.57418900 0.22195500 -0.20582000

H -0.30038900 3.07073500 1.64716700

C 1.91079300 2.57512000 -0.16765200

H -0.29071700 3.86526900 0.05922100

N 0.63313400 2.68266700 -0.49231400

H 0.61681400 -1.68846300 -3.43976600

C -0.11496300 1.56497200 -0.64675000

H 1.22517800 -2.18404300 -1.98220700

N 0.29615200 0.30941700 -0.55259200

H 1.33755700 0.15005500 -1.88629200

C 2.74861100 3.80500500 -0.02003600

C 3.74652000 -0.58318700 -0.77757300

N -1.44001300 1.80674400 -0.94269200

O 2.81072800 -1.46942000 -0.39875300

N -2.28059300 0.76039900 -1.24521400

O 3.19659100 0.62904400 -1.01637100

H 2.61878500 -4.23836200 0.15889000

O 4.76502800 -0.26858600 0.62288000

H 4.96885800 -3.56689900 0.76093100

C 5.37730700 -1.43760600 1.08253300

H 5.59377600 -1.15941300 0.88960700

H 4.66775300 -2.28982500 1.07161500

H 0.91709900 -2.43099900 -0.32265400

H 6.23346800 -1.73008400 0.44107200

H 3.31343200 3.77181400 0.92175000

C 4.04792700 1.77178900 -1.14866800

H 3.48427800 3.85412500 -0.83694600

H 3.81503200 2.23318200 -2.11924400

H 2.11737700 4.69952800 -0.04966500

H 5.09664500 1.44977500 -1.15168100

H -1.77842800 -0.05109900 -1.60728400

C 1.98624400 -1.09737300 0.72061600

H -1.61071700 2.67379100 -1.44321600

H 1.53388200 -0.11463800 0.52657800

C -3.19525800 0.38771600 -0.25020800

H 2.64339700 -1.00499800 1.59700000

O -2.26870700 -0.24589900 1.14411500

C 5.86835400 -1.21100400 2.50315100

O -3.81182600 -0.72592400 -0.69300900

H 5.02396200 -0.97769800 3.16797700

C -2.21940500 0.47010800 2.33676800

H 6.38112600 -2.10362900 2.88848800

H -2.02048000 -0.26385000 3.14248900

H 6.57077100 -0.36573000 2.53211400

H -3.19312200 0.92741400 2.60324600

C 3.78154300 2.72258700 -0.00241900

C -1.13651900 1.54309500 2.38783600

H 4.05393200 2.23424900 0.94203700

H -1.32860500 2.34203500 1.65710600

H -1.08162300 1.99449100 3.39009500

H	-0.15537200	1.10130500	2.15288700
C	-4.78712500	-1.32462700	0.15547400
H	-5.70349200	-0.71155000	0.15525900
H	-4.38249300	-1.35844000	1.17698900
C	-5.07114200	-2.71128100	-0.37326000
H	-5.82890300	-3.20267100	0.25091800
H	-5.44681000	-2.66322800	-1.40453000
H	-4.15695400	-3.32008600	-0.36099300
C	-4.06257600	1.50240700	0.27398300
H	-3.41022100	2.29110800	0.67073700
H	-4.65918900	1.12169800	1.11292000
C	-4.96987100	2.04858800	-0.82697300
H	-4.37714900	2.48174200	-1.64410000
H	-5.59483600	1.25083800	-1.25343900
H	-5.63226600	2.82734600	-0.42778200

TS3 (v = 167.11 i(cm-1))

O 1			
C	-1.77450600	-2.69640500	1.65134400
C	-3.17197400	-2.36034200	1.66357000
C	-3.62426100	-1.18776000	1.13022000
C	-2.69418800	-0.27265000	0.54885900
N	-1.33349800	-0.65383600	0.57250300
C	-0.87655400	-1.83730500	1.10497900
N	-2.87383500	0.89637300	-0.02572400
C	-1.61327000	1.30493100	-0.38951200
C	-0.64528200	0.36635500	-0.02833200
C	-1.12310400	2.44970200	-1.08376700
N	0.16226200	2.58218800	-1.31497500
C	1.04598500	1.61373200	-0.88858500
N	0.65989000	0.47296900	-0.25609300
C	-2.07436400	3.50500300	-1.55799600
N	2.34143300	1.79595300	-1.14142300
N	3.04887000	0.77842100	-0.46602000
H	-1.42610500	-3.63720400	2.07435000
H	-3.87975700	-3.06206100	2.10601600
H	-4.67991100	-0.91845800	1.12769600
H	0.20047200	-2.00281400	1.04232100
H	-1.53201100	4.29025800	-2.09537200
H	-2.83509000	3.05990500	-2.21557200
H	-2.60721700	3.94396800	-0.70166200
H	3.44416600	1.09776300	0.41726800
C	2.50055800	-0.44482300	-0.45820500
O	2.72633900	-1.27723600	0.52896200
C	3.04012800	-0.77615700	1.83986600
H	2.31493700	0.01842900	2.07944100
H	4.05473100	-0.35091500	1.82626800
C	2.95700900	-1.93058100	2.80798500
H	3.22672200	-1.58181000	3.81288100
H	1.93940100	-2.34122600	2.84489800

H	3.65332200	-2.72740500	2.51586500
C	2.17935700	-1.13452200	-1.75269400
H	1.33706600	-1.81469700	-1.57305700
H	1.86968800	-0.37466400	-2.47937600
C	3.40696700	-1.89761400	-2.25364100
H	3.71420200	-2.66560500	-1.53170400
H	3.17569300	-2.39053300	-3.20638600
H	4.25075100	-1.21294400	-2.41522600

TS4 (v = 241.16 i(cm-1))

O 1			
C	-0.03157100	3.67389100	-0.57764400
C	1.32874900	4.07885000	-0.38581100
C	2.29609900	3.15381600	-0.11926600
C	1.95403200	1.77243000	-0.07497100
N	0.61839700	1.41436200	-0.38306100
C	-0.37770900	2.36045700	-0.55893500
N	2.69234600	0.72297500	0.22118300
C	1.85649100	-0.34386600	0.09698300
C	0.59122800	0.05446500	-0.31117900
C	2.07804700	-1.73228700	0.44219300
N	1.10297000	-2.59154500	0.38897700
C	-0.11752200	-2.19560800	-0.07705600
N	-0.37986000	-0.88626200	-0.53556100
C	3.43231000	-2.15357800	0.91052900
N	-1.15892900	-2.95025400	-0.22222400
N	-2.09805600	-2.13301200	-0.79009500
H	-0.81538800	4.41868500	-0.70698900
H	1.58001100	5.13907100	-0.41954100
H	3.33243900	3.42522300	0.07768200
H	-1.39609300	1.97179600	-0.57265800
H	3.73505400	-1.54308700	1.77344400
H	3.42636200	-3.21390900	1.18299100
H	4.17263900	-1.97544100	0.11687100
C	-1.71221800	-0.82977800	-0.96204800
O	-2.42411000	0.28981400	0.31283400
C	-3.78930500	0.09861000	0.46394600
H	-4.06020200	-0.97133900	0.32166400
H	-4.37994000	0.66788200	-0.28696400
C	-4.23050000	0.51758800	1.86065200
H	-5.30920800	0.35733400	2.00366800
H	-3.68411200	-0.06469200	2.61666100
H	-4.01236300	1.58253700	2.02786200
H	-2.93403100	-2.54152400	-1.18802300
C	-2.12564000	-0.13556500	-2.23569400
H	-3.22279200	-0.19874900	-2.29303300
H	-1.87719300	0.92928100	-2.17444000
C	-1.47280600	-0.77442600	-3.45881100
H	-1.74574200	-1.83487100	-3.54786300
H	-1.79308200	-0.25896700	-4.37313800

H -0.37690900 -0.70825500 -3.39566500

Route 2

Et:

In1

O 1

C	6.47689600	-2.15741000	-1.27308600
C	7.44161000	-1.25391300	-0.71083900
C	7.05523700	-0.11895800	-0.05859300
C	5.66315400	0.17870000	0.06802600
N	4.76385600	-0.74381600	-0.50077000
C	5.15127100	-1.88569700	-1.15793700
N	5.05420600	1.19610400	0.63822400
C	3.71636200	0.94899700	0.44612500
C	3.50185300	-0.24607700	-0.25656800
C	2.54354600	1.64789700	0.80181600
N	1.36446400	1.14819000	0.46494900
C	1.29711500	-0.02226500	-0.21300200
N	2.33815900	-0.76721300	-0.60696500
C	2.61159500	2.94066900	1.55385000
N	0.07075800	-0.52194200	-0.53408000
N	-1.11176800	0.15003500	-0.29439500
H	6.79723800	-3.05880400	-1.79255800
H	8.50274400	-1.48451100	-0.81170000
H	7.77125000	0.57952000	0.37260100
H	4.34361700	-2.50485200	-1.54836600
H	3.06059800	2.77737900	2.54487500
H	3.25611300	3.65561500	1.02279300
H	1.60768800	3.36200600	1.67329500
H	-1.55788600	0.44282800	-1.16350500
H	-1.77935200	-0.44978100	0.19256800
H	0.08282700	-1.36478100	-1.10077100
C	-4.38070600	-0.75670800	-0.61510000
O	-3.92027200	0.53506500	-0.85346300
O	-3.71017000	-1.25513600	0.51133200
O	-5.74251900	-0.76306600	-0.32105200
C	-6.61321000	-0.29760000	-1.34030000
H	-6.18004200	0.59821100	-1.81513400
H	-6.72852200	-1.07088200	-2.11923300
C	-4.39373000	-2.04382600	1.48087700
H	-3.64599900	-2.75855600	1.85423000
H	-5.19935400	-2.61596200	1.00251600
C	-4.19321600	1.49043700	0.16420100
H	-3.91480500	1.06994300	1.14317600
H	-5.27475700	1.70753000	0.18651100
C	-7.94894200	0.01927600	-0.70511300
H	-7.83679000	0.80540300	0.05484200

H	-8.65912500	0.36713800	-1.46685300
H	-8.36605100	-0.87538700	-0.22261600
C	-4.93669500	-1.20112000	2.61828500
H	-5.69951400	-0.50444800	2.24552500
H	-5.39012300	-1.84653400	3.38424700
H	-4.12802000	-0.62415700	3.09027900
C	-3.39364900	2.73970900	-0.13529400
H	-3.60882600	3.51508700	0.61231100
H	-2.31892800	2.51318100	-0.11137400
H	-3.65178600	3.13381800	-1.12836000
C	-4.01870800	-1.57759400	-1.85007600
H	-2.92632100	-1.50382200	-1.95410900
H	-4.45779600	-1.09181700	-2.73365800
C	-4.45510700	-3.03077300	-1.74261900
H	-5.54080800	-3.10870400	-1.58270400
H	-4.20582200	-3.58030000	-2.65979600
H	-3.95086300	-3.52994200	-0.90304200

In2

O 1

C	-5.16145400	-1.47662600	-0.64878100
C	-5.86841800	-0.42574800	0.02837800
C	-5.21470100	0.66558800	0.52304900
C	-3.79792900	0.76617600	0.36466200
N	-3.15898600	-0.29322000	-0.30693200
C	-3.81522200	-1.39195600	-0.80515000
N	-2.95872700	1.70468500	0.74848800
C	-1.72970800	1.26260600	0.32450700
C	-1.81898500	0.02645200	-0.33302700
C	-0.42766700	1.79941300	0.40902100
N	0.58638700	1.12063000	-0.10847800
C	0.36134400	-0.07110000	-0.70388500
N	-0.82364500	-0.66976500	-0.85639000
C	-0.17754900	3.11889700	1.06989000
N	1.42486200	-0.76591500	-1.21124400
N	2.72675200	-0.35810000	-1.08674400
H	-5.69430600	-2.34190300	-1.03902200
H	-6.94949700	-0.50768900	0.14625000
H	-5.73245900	1.47286100	1.03945500
H	-3.18907300	-2.13296800	-1.30209600
H	-0.73865200	3.91207500	0.55436200
H	-0.53620100	3.09487200	2.10909600
H	0.89162400	3.35622000	1.05424600
H	3.17401100	-0.25271300	-1.99612400
H	1.19383300	-1.64646300	-1.66461200
C	3.57279700	-1.19743600	-0.22655500
O	3.18415600	-0.98053800	1.09459400
O	4.87535800	-0.73200200	-0.42182000
C	2.55396600	-1.94699600	1.91950000
H	2.83530200	-1.66458500	2.94430500

H	2.96135800	-2.95306600	1.74749500
C	1.04169600	-1.95773100	1.79276700
H	0.71340500	-2.35360200	0.82241800
H	0.61012200	-2.58625700	2.58481300
H	0.64308900	-0.93794500	1.89981400
C	5.33646300	0.37482300	0.34149700
H	6.41362300	0.41735200	0.12805200
H	5.21500800	0.15649200	1.41240100
C	4.68146200	1.70054900	-0.00436700
H	5.18169900	2.50901400	0.54889900
H	4.77438600	1.90726300	-1.08065800
H	3.61480300	1.68934200	0.24962800
C	3.57416000	-2.67085000	-0.65904700
H	3.63199400	-2.67281400	-1.75829400
H	2.60503700	-3.12215800	-0.39976800
C	4.73563700	-3.48512100	-0.09857500
H	4.62101800	-4.54759400	-0.35270600
H	5.68371400	-3.12572500	-0.51649500
H	4.80959500	-3.40306700	0.99484000

In3

O 1			
C	-4.70212100	-2.26612800	-0.27573400
C	-5.63760500	-1.17931000	-0.20226100
C	-5.21632500	0.11410300	-0.09020400
C	-3.81574200	0.39363600	-0.04376500
N	-2.94628300	-0.71094300	-0.11857700
C	-3.36874400	-2.01276800	-0.23250000
N	-3.17522500	1.53887100	0.06284300
C	-1.84742800	1.19309700	0.05967500
C	-1.67072700	-0.19518500	-0.05141100
C	-0.65547100	1.94255900	0.14659700
N	0.50861700	1.30897300	0.11933000
C	0.53352300	-0.03528900	0.00831100
N	-0.52126700	-0.84906900	-0.08281200
C	-0.68480300	3.43362200	0.26772400
N	1.75050800	-0.66825300	-0.00681900
N	2.91949400	0.00792300	0.03182200
H	-5.05137000	-3.29311300	-0.36577300
H	-6.70536200	-1.39836100	-0.23729900
H	-5.90974500	0.95199000	-0.03356800
H	-2.58105700	-2.76452100	-0.28220800
H	-1.15946900	3.87498700	-0.62096000
H	-1.28925000	3.73102800	1.13670600
H	0.33269300	3.82495200	0.37144600
H	1.71194800	-1.67921800	-0.10810900
C	4.01099200	-0.65116000	0.01629300
O	5.12502900	0.09838100	0.19332200
C	6.35380300	-0.27772100	-0.42354500
H	6.82404600	0.66555000	-0.73324500

H	6.16110500	-0.85729200	-1.33947100
C	7.26270900	-1.02010600	0.53593400
H	8.24726100	-1.17805300	0.07465900
H	7.39974000	-0.43083100	1.45305800
H	6.85289700	-2.00126600	0.81409100
C	4.12922000	-2.15348300	-0.02650200
H	3.36873400	-2.56362300	-0.70757200
H	5.09387600	-2.44627300	-0.45774000
C	3.97880500	-2.75211500	1.37802200
H	2.99894300	-2.50593900	1.81129700
H	4.07661000	-3.84494700	1.34554500
H	4.75211400	-2.35373600	2.04959900

In4

O 1			
C	3.38777600	-2.74738500	1.11707600
C	4.34267700	-2.22414400	2.06065800
C	4.30966600	-0.92436300	2.46575300
C	3.30036600	-0.04994400	1.94252100
N	2.39163300	-0.62055500	1.02479300
C	2.42736500	-1.93262300	0.61590700
N	3.07338400	1.21526300	2.17485200
C	1.97271100	1.52552700	1.39640000
C	1.51874600	0.38478800	0.65305300
C	1.28856900	2.70818400	1.21755200
N	0.21163300	2.63514000	0.38789600
C	-0.13667000	1.47149800	-0.36112900
N	0.53817600	0.29716100	-0.19282200
C	1.69457300	3.98129900	1.87732500
N	-1.11583200	1.68319900	-1.16561700
N	-1.56180400	2.98915300	-0.89684600
H	3.43079200	-3.78898500	0.80470600
H	5.10856300	-2.89234500	2.45650400
H	5.02453600	-0.51502600	3.17811500
H	1.65827400	-2.22474700	-0.09946000
H	2.65800700	3.82342700	2.37330600
H	1.78017900	4.78502300	1.13365600
H	0.95532200	4.28468200	2.63301100
H	-1.85759900	3.44988900	-1.75210100
C	-0.54924500	3.75398200	-0.17368100
O	0.37364800	4.42935500	-1.00167900
C	0.07907300	5.73447400	-1.47880900
H	1.00259700	6.05602300	-1.97811400
H	-0.09077800	6.42666600	-0.63852400
C	-1.07827700	5.79101300	-2.46236300
H	-1.13596900	6.79450100	-2.90572000
H	-0.92869500	5.06448400	-3.27421100
H	-2.04686600	5.59293400	-1.97941600
C	-1.21977000	4.67042700	0.85373900
H	-0.48448100	5.37243800	1.26887300

H	-1.95149800	5.27575900	0.29663500
C	-1.93509700	3.90242600	1.95561700
H	-1.22823600	3.34026700	2.58350400
H	-2.49058200	4.59198000	2.60433600
H	-2.64291900	3.18583000	1.51780800

TS1 (v = 159.81 i(cm-1))

0 1

C	-2.93657600	2.27487900	2.98019000
C	-3.86613900	2.70610600	1.97462900
C	-3.95217300	2.07220100	0.76838700
C	-3.09550400	0.96190300	0.49746600
N	-2.21078700	0.57983700	1.52254000
C	-2.12301800	1.21477900	2.73679400
N	-2.96963500	0.22093600	-0.58442400
C	-1.96711900	-0.66601400	-0.28042500
C	-1.47310000	-0.46661500	1.01588500
C	-1.33634700	-1.70109000	-1.00374300
N	-0.32885500	-2.35500100	-0.44622800
C	0.07583200	-2.03133700	0.80082000
N	-0.47279800	-1.11042900	1.59476400
C	-1.81098000	-2.08968400	-2.36940500
N	1.12654700	-2.72887100	1.35467900
N	2.11320400	-3.25007200	0.52450800
H	-2.87874800	2.78731900	3.93876400
H	-4.51352900	3.55793700	2.18583400
H	-4.64804500	2.38610400	-0.00836300
H	-1.39069900	0.80855700	3.43511600
H	-2.02473200	-1.19662000	-2.97263600
H	-1.06650400	-2.71981700	-2.86865400
H	-2.75216600	-2.65494800	-2.28472400
H	2.86729700	-2.56880600	0.41408000
H	2.49265100	-4.09600700	0.94202500
H	1.43158000	-2.29761500	2.22548100
C	1.90738200	0.81852700	0.08628800
O	1.29680700	0.36257800	-1.00816900
O	2.51546800	-0.17741400	0.77106000
O	3.31481200	1.72737500	-0.45291200
C	2.99042000	2.76455400	-1.32528200
H	2.18833400	2.46009000	-2.02767800
H	2.61364900	3.65669300	-0.78076600
C	3.17878100	0.17551600	1.98373600
H	2.42939900	0.29684400	2.78346700
H	3.69428900	1.13384700	1.83199500
C	2.03402900	-0.55356500	-1.83285100
H	1.93037600	-1.56400100	-1.41247700
H	3.09056800	-0.25306700	-1.80830900
C	4.22628600	3.15426200	-2.12200800
H	4.57526000	2.30278800	-2.72456000
H	4.01229100	3.99591700	-2.79625500
H	5.03937100	3.45025600	-1.44349700
C	4.16277800	-0.92091600	2.32228600
H	4.91078900	-1.02328200	1.52401000
H	4.68159800	-0.68440400	3.26035400
H	3.65560600	-1.88846000	2.44873800
C	1.45915000	-0.48025500	-3.22777800

Product

0 1

C	3.22685200	-2.90950800	1.40321600
C	3.86809500	-2.57143700	2.64384800
C	3.82505400	-1.30650300	3.15251000
C	3.12360500	-0.28847300	2.43234100
N	2.51457800	-0.67905600	1.22784400
C	2.55846400	-1.95156000	0.71349800
N	2.95274100	0.98154600	2.71703800
C	2.20033100	1.48003300	1.67852400
C	1.90747400	0.45198200	0.71356700
C	1.73766500	2.75193000	1.44012600
N	1.00062900	2.88036800	0.27540500
C	0.77938900	1.80429100	-0.61409100
N	1.24440000	0.55975800	-0.39475500
C	2.04710900	3.90237500	2.33294800
N	0.07855500	2.22269100	-1.64476400
N	-0.16786100	3.53023200	-1.44908100
H	3.27349100	-3.92390200	1.01225300
H	4.40258100	-3.35121700	3.18791800
H	4.30782500	-1.03437000	4.08962000
H	2.04071700	-2.09812300	-0.23450400
H	2.57422000	3.51296800	3.21051100
H	2.70049300	4.62445800	1.82188300
H	1.14085200	4.42674400	2.66194000
H	-1.01014100	4.21218300	-2.94951200
C	0.36332200	3.94954100	-0.32512900
O	-1.31923700	4.66932100	-3.75808200
C	-1.18956000	6.04144600	-3.49291400
H	-1.26100200	6.57818700	-4.45261700
H	-0.18724600	6.27360800	-3.08085600
C	-2.26390000	6.54804700	-2.54162800
H	-2.15516000	7.62462100	-2.34503500
H	-3.26226400	6.36692900	-2.96542200
H	-2.20428600	6.01382200	-1.58068400
C	0.16673600	5.32732200	0.22044100
H	1.08302700	5.69817900	0.69391500
H	-0.01370700	5.96974200	-0.65256500
C	-1.02578900	5.41704900	1.17743800
H	-1.15441300	6.44840100	1.53169700
H	-1.94871600	5.10653100	0.66783600
H	-0.89786400	4.76684500	2.05439600

H	1.97302700	-1.19769300	-3.88167800
H	0.38905200	-0.72910500	-3.21802900
H	1.58041300	0.52683600	-3.65090200
C	1.04526000	1.77737100	0.88843300
H	0.58569600	1.17237300	1.68478400
H	1.71311900	2.49786200	1.38029400
C	-0.04304300	2.49074900	0.09197200
H	-0.65735800	1.77266800	-0.46868500
H	-0.69793100	3.04782500	0.77856500
H	0.37694200	3.20355400	-0.62885900

H	5.14525600	-0.17161400	1.28852500
C	6.49491300	0.90370300	-0.02699600
H	7.35738200	0.85802100	0.65075800
H	6.86089100	0.84573200	-1.06129700
H	5.98958500	1.86890900	0.11236100
C	3.53577000	-2.32650600	-0.07516900
H	2.56114900	-2.74796900	0.20311000
H	4.19288000	-2.42348000	0.79845100
C	4.12468700	-3.06443000	-1.27581700
H	3.44228800	-3.02095200	-2.13553700
H	5.07947900	-2.61502400	-1.58438500
H	4.30454900	-4.11849300	-1.02859100

TS2 (v = 212.40 i(cm-1))

0 1

C	-5.37201600	-1.69517800	-0.13322800
C	-6.03764100	-0.52512000	0.36598200
C	-5.36189300	0.64260400	0.57285300
C	-3.96342400	0.70315900	0.28630900
N	-3.36510500	-0.47330700	-0.20156200
C	-4.04300300	-1.64947700	-0.40865400
N	-3.10950300	1.69856400	0.40316100
C	-1.91127400	1.17543100	-0.01171900
C	-2.03443800	-0.17150400	-0.39257000
C	-0.62238200	1.72647600	-0.16202700
N	0.35760100	0.94519600	-0.59724300
C	0.10958800	-0.34896700	-0.87477500
N	-1.06955100	-0.96528700	-0.82794900
C	-0.34656100	3.16395200	0.14504900
N	1.17958300	-1.12742300	-1.26348400
N	2.43434900	-0.58045400	-1.40783900
H	-5.92168400	-2.62086100	-0.29360900
H	-7.10516600	-0.57710900	0.58262900
H	-5.84787200	1.54040000	0.95224700
H	-3.44707800	-2.47978500	-0.78737100
H	-0.99315500	3.81275800	-0.46323600
H	-0.57787500	3.37486400	1.19938700
H	0.70479000	3.39765800	-0.05368900
H	2.39557700	0.42143500	-1.59791300
H	0.95372400	-1.89560000	-1.88756800
C	3.35084100	-0.86311000	-0.38412400
O	2.75910800	-0.08558400	1.11567800
O	4.45622300	-0.13807400	-0.64724500
C	2.31040000	-0.86419900	2.17872800
H	2.42986900	-0.25338900	3.09534600
H	2.93945800	-1.76066200	2.34965000
C	0.85038600	-1.29312500	2.07635800
H	0.69055300	-1.97540200	1.22921000
H	0.52781500	-1.80182200	2.99749300
H	0.20762500	-0.41169100	1.92360100
C	5.54479900	-0.23425100	0.26632500
H	6.04927100	-1.20628400	0.13926500

TS3 (v = 209.72 i(cm-1))

0 1

C	4.56069400	-0.93002100	0.81374100
C	5.05647400	0.28492400	0.22498500
C	4.22884900	1.14059600	-0.44140000
C	2.83788900	0.82591100	-0.55923100
N	2.40937800	-0.37694300	0.04148900
C	3.24293200	-1.23900500	0.71024200
N	1.85987500	1.47534700	-1.14532700
C	0.74709900	0.69122400	-0.93195200
C	1.05238000	-0.47317200	-0.19907000
C	-0.60599200	0.84599400	-1.27817900
N	-1.45343000	-0.09256200	-0.88281600
C	-1.03451500	-1.26033700	-0.24857400
N	0.24754700	-1.45237400	0.15112500
C	-1.06531500	2.02219600	-2.08282800
N	-1.93838900	-2.21140300	-0.03358200
N	-3.14039900	-1.80824700	-0.65761300
H	5.23231200	-1.60427600	1.34209000
H	6.11747300	0.52038200	0.31635300
H	4.58717700	2.06477600	-0.89335100
H	2.76891300	-2.13167600	1.11881900
H	-0.85878500	2.95945600	-1.54651900
H	-0.49403000	2.05778700	-3.02136500
H	-2.13298600	1.95685300	-2.31729500
H	-3.22629100	-2.14871200	-1.61532700
C	-3.44226500	-0.50516600	-0.53946000
O	-3.48028600	-0.08184100	0.70670300
C	-3.92469000	1.22855200	1.08023900
H	-4.19689400	1.11585400	2.13592400
H	-4.83803900	1.48762800	0.52722200
C	-2.84685300	2.27688000	0.91507100
H	-3.18572000	3.21359200	1.37770700
H	-1.91877700	1.95664200	1.40869400
H	-2.63385400	2.47754500	-0.14131700
C	-4.27809700	0.14556100	-1.60240900
H	-3.86052000	-0.13463200	-2.57774500

H	-4.19000900	1.23595000	-1.51672100
C	-5.74289700	-0.29087500	-1.48866500
H	-6.16280100	-0.03407600	-0.50669300
H	-6.33979200	0.20986000	-2.26079100
H	-5.83812100	-1.37607700	-1.62459100

wb97xd/6-31+g(d,p)

Route 1

H:

In 3

TS4 (v = 293.35 i(cm-1))

0 1			
C	-4.77402000	-1.09930700	0.68498900
C	-5.20055800	0.27340800	0.60145900
C	-4.32956600	1.27706600	0.30171000
C	-2.95154200	0.96217900	0.06361200
N	-2.59391000	-0.39861200	0.15802800
C	-3.47371300	-1.41065200	0.46137300
N	-1.94676500	1.74424900	-0.23330100
C	-0.86217300	0.89727100	-0.35309100
C	-1.23895000	-0.46921200	-0.10342200
C	0.45890200	1.15853300	-0.62698700
N	1.25924500	0.04586300	-0.69473300
C	0.80958800	-1.26897900	-0.37322800
N	-0.49106900	-1.52872400	-0.08565600
C	1.00460100	2.53182900	-0.79577200
N	1.78316500	-2.11995400	-0.40734400
N	2.86795500	-1.37597500	-0.80793300
H	-5.48492800	-1.88752200	0.92467400
H	-6.24998100	0.50841300	0.78390700
H	-4.63670500	2.31961100	0.23543800
H	-3.04652000	-2.41284800	0.50007200
H	0.20441200	3.25157400	-0.59446600
H	1.83534800	2.66605000	-0.08913200
H	1.37965600	2.69338900	-1.81651400
H	3.78385500	-1.80433400	-0.79645800
C	2.66951400	-0.02044400	-0.78794900
O	3.05818600	0.71245900	0.83198600
C	4.39438300	0.99981500	1.07519300
H	4.44922900	1.50336100	2.06040400
H	4.80868300	1.73491500	0.35118600
C	5.31324500	-0.22061300	1.11865900
H	6.30522200	0.05010400	1.50909100
H	4.87938900	-0.99431600	1.76960300
H	5.46956700	-0.65952800	0.12094800
C	3.46233500	0.80286500	-1.77024900
H	3.44767300	1.85636000	-1.47189800
H	4.50791900	0.47102400	-1.68213500
C	2.97017800	0.60856100	-3.20139200
H	1.92735500	0.93956300	-3.31489100
H	3.58928300	1.18698700	-3.89877500
H	3.01939800	-0.45081200	-3.48742700

0 1			
C	3.39818900	-3.01256700	-0.04115500
C	4.66260200	-2.35812500	0.11918800
C	4.75055200	-0.99976900	0.20530800
C	3.56156700	-0.21881500	0.13461700
N	2.34992900	-0.91077100	-0.02181800
C	2.25920500	-2.27997100	-0.10921900
N	3.39756000	1.09220400	0.19170000
C	2.03510800	1.26706000	0.06805300
C	1.36464200	0.05156900	-0.06421800
C	1.22047900	2.41508600	0.05353300
N	-0.09188200	2.26579100	-0.08123900
C	-0.61272900	1.01431400	-0.20033300
N	0.05344000	-0.13880500	-0.19932200
C	1.78950600	3.79095700	0.19075500
N	-1.97281000	1.01260600	-0.34711200
N	-2.68941700	-0.15225900	-0.38322300
H	3.34135200	-4.09136500	-0.11033800
H	5.56325300	-2.95997900	0.17139200
H	5.69784500	-0.48849500	0.32667000
H	1.26275400	-2.68508300	-0.23009300
H	2.28264100	3.89932500	1.16187100
H	2.54884000	3.96570600	-0.57730200
H	1.00181500	4.53962800	0.10179900
H	-2.43574500	1.90963800	-0.25878500
C	-3.95547600	-0.03169500	-0.39623200
H	-4.49111600	0.92200900	-0.35234500
O	-4.70543300	-1.13764800	-0.50092100
C	-6.10690700	-0.97272400	-0.21696000
H	-6.58183200	-1.84324600	-0.67019100
H	-6.47453900	-0.07571800	-0.72801600
C	-6.37463300	-0.91227800	1.27501900
H	-7.45186800	-0.83960400	1.44943500
H	-6.00206400	-1.81271600	1.77033000
H	-5.89825100	-0.03851700	1.72990700

In4

0 1			
C	-2.11527800	-2.81876200	-0.51237800
C	-3.40640200	-2.34271000	-0.11867900
C	-3.60318300	-1.02693000	0.17917700
C	-2.51212900	-0.11987900	0.10177800
N	-1.25383500	-0.63831200	-0.27887900
C	-1.06173500	-1.97073400	-0.58895300
N	-2.46220400	1.17809500	0.33955200
C	-1.15032800	1.51923100	0.12796800
C	-0.40178500	0.42303000	-0.24263700
C	-0.50399600	2.80458000	0.21535300
N	0.77633800	2.92271100	-0.01109300
C	1.50978500	1.80088200	-0.31884400
N	0.92032900	0.54194000	-0.58044600
C	-1.30440200	4.01453700	0.57058000
N	2.79676900	1.76069500	-0.39973200
N	3.09848000	0.43932200	-0.80936600
H	-1.96385200	-3.86325700	-0.75346700
H	-4.23188100	-3.04295100	-0.06189000
H	-4.56914900	-0.63734200	0.47722300
H	-0.06599100	-2.26770400	-0.88224600
H	-2.10153600	4.16482500	-0.16403300
H	-1.78662900	3.87252700	1.54254900
H	-0.66422900	4.89615700	0.60253200
C	1.97901600	-0.43599300	-0.49153900
H	1.89979200	-1.23161600	-1.23790900
O	1.95378800	-0.97768500	0.81070800
C	2.78095900	-2.13150600	1.01169500
H	2.94408800	-2.17314500	2.08986000
H	3.75970300	-1.98035100	0.53922100
C	2.13724900	-3.41900100	0.52289300
H	2.77990600	-4.26500900	0.78335300
H	1.16394300	-3.56705900	0.99875500
H	2.00606700	-3.43216600	-0.56353200
H	3.98171400	0.13693800	-0.41480800

TS3 (v = 330.31 i(cm-1))

0 1			
C	-3.00233800	-2.03689900	-0.74688100
C	-4.05937100	-1.17005400	-0.31470200
C	-3.80774800	0.11966100	0.04885800
C	-2.47176200	0.61130100	0.01005100
N	-1.46821700	-0.28575400	-0.40799100
C	-1.72631200	-1.58297900	-0.79136900
N	-1.98922700	1.80120700	0.31369200
C	-0.63170600	1.68659300	0.09180500
C	-0.28805700	0.41430000	-0.34817600

C	0.44004600	2.59950700	0.25961000
N	1.67328300	2.22534100	-0.01948600
C	1.91778300	0.94099600	-0.45678900
N	0.95135400	-0.00932800	-0.61045900
C	0.19619500	3.99102900	0.75352700
N	3.19370000	0.62201600	-0.71055500
N	3.18182800	-0.69609800	-1.25315400
H	-3.21290800	-3.05593700	-1.04542500
H	-5.07337200	-1.55299600	-0.28360800
H	-4.59267000	0.79297200	0.37207000
H	-0.87778300	-2.16491700	-1.12506900
H	-0.45946100	4.52905300	0.06170900
H	-0.31166800	3.96438400	1.72236900
H	1.13985900	4.52850200	0.85080500
H	3.15065900	-0.70602800	-2.26816300
C	2.32180100	-1.55365100	-0.70110400
H	1.86520400	-2.31087600	-1.33626500
O	2.40702200	-1.77715500	0.58240300
C	1.44541200	-2.67480000	1.19093300
H	2.03023700	-3.49624500	1.60735600
H	0.78473000	-3.07277800	0.41632300
C	0.67610600	-1.93727600	2.26536500
H	-0.02300900	-2.63022000	2.74102400
H	1.35618900	-1.55274300	3.02905800
H	0.10846900	-1.10297600	1.84748800

Me:**In3**

0 1			
C	-3.44963500	-3.11093200	0.01349200
C	-4.75188000	-2.51655600	-0.04748300
C	-4.91070500	-1.16241300	-0.08289200
C	-3.75887700	-0.32523900	-0.05903200
N	-2.50782600	-0.95893900	-0.00199600
C	-2.34554500	-2.32373400	0.03497500
N	-3.66347500	0.99392400	-0.08097800
C	-2.30678700	1.23436500	-0.03570200
C	-1.56985500	0.05104500	0.01228000
C	-1.55133200	2.42196200	-0.02719800
N	-0.22748100	2.33487600	0.02994200
C	0.36167900	1.11015900	0.06495800
N	-0.24456800	-0.07436900	0.05573200
C	-2.19272600	3.77142500	-0.08273600
N	1.73593600	1.16915800	0.05935200
N	2.45686900	0.06261200	0.47981000
H	-3.33617100	-4.18703700	0.04366800
H	-5.62338400	-3.16181600	-0.06431600
H	-5.88672700	-0.69480900	-0.12912900

H	-1.32474100	-2.68088700	0.08099800
H	-2.70169400	3.90427800	-1.04282600
H	-2.95060000	3.86678400	0.70017200
H	-1.44175200	4.55313400	0.03546000
H	2.09540300	2.08881100	0.28731000
C	3.71753200	0.09489100	0.24531900
O	4.38615800	-0.94644300	0.78674100
C	5.73607800	-1.24633100	0.40306900
H	6.09231100	-1.90089800	1.19971900
H	6.34721200	-0.33948600	0.42282500
C	5.80688100	-1.95507600	-0.93781900
H	6.84739400	-2.21009700	-1.15845300
H	5.22148100	-2.87798300	-0.91418500
H	5.43146200	-1.32815500	-1.75179300
C	4.44926500	1.19085100	-0.47318600
H	4.80426400	1.94104700	0.24145200
H	5.31137400	0.82364700	-1.02742600
H	3.77416900	1.67767400	-1.17870700

H	0.44903200	-3.15916500	2.25919300
H	2.19473900	-3.49003400	2.20406900
H	3.79034600	-0.90629200	-0.29823400
C	1.51363400	-1.59446400	-2.13403100
H	2.24311400	-2.39777200	-2.26131800
H	1.65713900	-0.85556400	-2.92271600
H	0.51092700	-2.01600100	-2.21869600

TS3 (v = 262.62 i(cm-1))

O 1			
C	-2.68770200	-2.59275200	-0.52729200
C	-3.90305300	-1.94986400	-0.12221500
C	-3.92843200	-0.61819400	0.16779300
C	-2.72843200	0.14317900	0.07841300
N	-1.55468500	-0.54027400	-0.30007500
C	-1.53786700	-1.88125400	-0.61523100
N	-2.51686900	1.42671900	0.29367800
C	-1.16931700	1.59607000	0.04998200
C	-0.55293000	0.40212000	-0.30851900
C	-0.33329200	2.73784300	0.12060700
N	0.94616400	2.63291600	-0.17517900
C	1.46939500	1.40814900	-0.53163500
N	0.75009600	0.24625200	-0.57082200
C	-0.88311100	4.06967900	0.52609800
N	2.77361800	1.37669700	-0.82161600
N	3.06489200	0.05592300	-1.25869800
H	-2.67759800	-3.64692700	-0.77365300
H	-4.81344300	-2.53522600	-0.05675300
H	-4.83737300	-0.10880700	0.46505100
H	-0.59049700	-2.28855100	-0.93778600
H	-1.65247300	4.39151200	-0.18284900
H	-1.36074800	3.99828600	1.50793500
H	-0.08821100	4.81528200	0.55924200
H	3.05018800	-0.03763300	-2.26908900
C	2.44103900	-0.94114700	-0.61629900
O	2.61180100	-0.93726100	0.69231300
C	1.82665900	-1.81377000	1.52721400
H	2.21978300	-2.82988500	1.43806900
H	0.78973000	-1.78802700	1.17984900
C	1.93126100	-1.29711900	2.94330200
H	1.35538400	-1.94900700	3.60508500
H	2.97062100	-1.29129300	3.28075700
H	1.52642300	-0.28451700	3.01447000
C	2.16161100	-2.21507500	-1.34993900
H	3.11431000	-2.73360100	-1.49644600
H	1.51418600	-2.87676300	-0.77812500
H	1.70783900	-2.01156400	-2.31895900

In4

O 1			
C	-2.80471400	-2.27946400	-0.38082600
C	-3.95879400	-1.47135500	-0.13165700
C	-3.83075200	-0.13089700	0.07721200
C	-2.54429400	0.46917400	0.02224100
N	-1.43892600	-0.35548300	-0.29565200
C	-1.56997500	-1.72607300	-0.44995200
N	-2.18672600	1.72042800	0.23818600
C	-0.82775200	1.72834100	0.06146000
C	-0.35628600	0.47770100	-0.28825200
C	0.11307300	2.80200500	0.24760200
N	1.39563800	2.58814700	0.13727000
C	1.84044700	1.33027400	-0.19649000
N	0.97144200	0.28527600	-0.56442000
C	-0.37925800	4.16682300	0.60340700
N	3.08308300	0.98329100	-0.23900600
N	3.09645400	-0.32706600	-0.75737500
H	-2.90079900	-3.35152700	-0.49776100
H	-4.93539300	-1.93950400	-0.08746600
H	-4.67843500	0.50674400	0.29795200
H	-0.65626000	-2.28962100	-0.56322100
H	-1.08996500	4.51927500	-0.14995600
H	-0.91443200	4.13312500	1.55757500
H	0.45540300	4.86398100	0.67740500
C	1.75800600	-0.93021000	-0.78670900
O	1.51725300	-1.90812400	0.19482700
C	1.64516700	-1.50369800	1.56358600
H	0.89146100	-0.74122600	1.79594100
H	2.63593200	-1.06484400	1.73091000
C	1.44091600	-2.73015300	2.42628200
H	1.52590900	-2.45676200	3.48144200

Et:

In3

0 1

C	3.97795500	-2.99419900	0.23853600
C	5.23564200	-2.31244800	0.16199700
C	5.29888600	-0.95502000	0.04492100
C	4.09044400	-0.20284400	-0.00232300
N	2.88665100	-0.92097000	0.07289400
C	2.82065400	-2.28912700	0.19226300
N	3.90197400	1.10199400	-0.10890600
C	2.53054500	1.24556800	-0.10375700
C	1.87941400	0.01724500	0.00584900
C	1.69139200	2.37242800	-0.18620400
N	0.37578200	2.19236900	-0.16131700
C	-0.12397900	0.93251700	-0.05190000
N	0.56650900	-0.20156500	0.03798800
C	2.23853900	3.75946700	-0.29692100
N	-1.49544000	0.89975200	-0.00713300
N	-2.16716100	-0.28612400	-0.12824000
H	3.94064500	-4.07175100	0.33481300
H	6.15128200	-2.89237000	0.19907800
H	6.24082900	-0.42333000	-0.01412600
H	1.82729100	-2.71575800	0.24415000
H	2.76297300	4.02798100	0.62592400
H	2.96759500	3.81788700	-1.10999600
H	1.43432500	4.47475500	-0.47157900
H	-1.94830900	1.78327400	-0.20630100
C	-3.44575300	-0.25025000	-0.17376100
O	-4.02294300	-1.47816500	-0.14712000
C	-5.25306900	-1.71618600	-0.85249800
H	-5.13086200	-2.70661500	-1.29651400
H	-5.36296400	-1.00085800	-1.67277700
C	-6.44871800	-1.69886200	0.08151400
H	-7.35197400	-1.96461900	-0.47556900
H	-6.31337700	-2.42789400	0.88506700
H	-6.60141800	-0.71363800	0.53053000
C	-4.30934800	0.98346700	-0.10705900
H	-3.85258200	1.79102500	-0.68777500
H	-5.27452000	0.79955400	-0.58004000
C	-4.52307900	1.42899000	1.34868600
H	-3.57161800	1.65081600	1.83977300
H	-5.14241500	2.32852300	1.37741500
H	-5.02672100	0.64568500	1.92183400

In4

0 1

C	2.69752900	-2.45568400	0.32297600
C	3.92181500	-1.72234800	0.22059500
C	3.90570200	-0.36962700	0.05580500
C	2.66310200	0.31781200	0.01232000
N	1.48065800	-0.43770300	0.19470800
C	1.50200000	-1.81902800	0.29999300
N	2.41135200	1.59763000	-0.18479700
C	1.04505200	1.69551000	-0.12763300
C	0.46227100	0.46957100	0.12850300
C	0.19680500	2.83515900	-0.36031100
N	-1.10241500	2.70856900	-0.36098700
C	-1.65910800	1.48015200	-0.09092000
N	-0.89258300	0.35845500	0.27020000
C	0.80773900	4.17190200	-0.62762400
N	-2.92663800	1.23240600	-0.10276600
N	-3.06150600	-0.08285800	0.38306900
H	2.70924200	-3.53560000	0.40153100
H	4.86498100	-2.25563300	0.25332500
H	4.81298200	0.21199800	-0.05484100
H	0.54426800	-2.31811200	0.30560900
H	1.41158600	4.48424500	0.23014300
H	1.48114500	4.11396400	-1.48809400
H	0.03103600	4.91280800	-0.81716000
C	-1.77832000	-0.78819700	0.46767000
O	-1.57814800	-1.78981400	-0.49865600
C	-1.63252100	-1.38901100	-1.87322000
H	-0.84647100	-0.65098600	-2.07462800
H	-2.60077500	-0.92098800	-2.08649900
C	-1.42928400	-2.62662200	-2.72020500
H	-1.46614800	-2.35860800	-3.77956600
H	-0.45668300	-3.08141500	-2.51285500
H	-2.21136900	-3.36465000	-2.52294500
H	-3.77944900	-0.59978200	-0.11103800
C	-1.63684900	-1.47285500	1.83122200
H	-0.74386000	-2.10247300	1.84304400
H	-2.49738100	-2.14412300	1.91911200
C	-1.60145600	-0.48969400	2.99499100
H	-1.60767100	-1.03155600	3.94395700
H	-0.69852800	0.12820200	2.96702600
H	-2.47066500	0.17348100	2.97216600

TS3 (v = 190.53 i(cm-1))

0 1

C	-1.58340800	3.28383500	0.39852500
C	-3.01363600	3.17927900	0.43299800
C	-3.63817100	1.97349800	0.30604100
C	-2.85707300	0.79476400	0.13357400
N	-1.45826600	0.95667300	0.09854500
C	-0.82613500	2.17226000	0.23331100
N	-3.22249900	-0.46647400	-0.00342000

C	-2.03148500	-1.15526000	-0.13431400
C	-0.93821100	-0.30007400	-0.07774700
C	-1.73190100	-2.53299100	-0.28322400
N	-0.47579700	-2.92996100	-0.37861000
C	0.53859700	-1.99925200	-0.32656100
N	0.34024500	-0.66453200	-0.16580200
C	-2.82262200	-3.55693400	-0.32773200
N	1.79720000	-2.45271200	-0.40338100
N	2.64700300	-1.31356000	-0.50649900
H	-1.09933800	4.24612600	0.50659600
H	-3.60175400	4.08073600	0.56494600
H	-4.71699000	1.87634400	0.33390000
H	0.25627900	2.15239300	0.20138500
H	-2.40360100	-4.54957200	-0.49490800
H	-3.37987300	-3.55253100	0.61454400
H	-3.53521300	-3.31943900	-1.12326600
H	2.89228800	-1.11869900	-1.47130100
C	2.32170400	-0.24261700	0.24292500
O	2.62668900	0.97574300	-0.14652800
C	2.72785200	1.28699700	-1.55681600
H	1.84617900	0.86754000	-2.05312200
H	3.63683900	0.83058900	-1.95900500
C	2.78460700	2.79149000	-1.68582400
H	2.87575800	3.05211700	-2.74312500
H	1.87707900	3.25624700	-1.29330100
H	3.65010900	3.19441800	-1.15478300
C	2.20387000	-0.36651300	1.73600400
H	1.51218700	0.40365700	2.08280500
H	1.77888500	-1.34218600	1.97297200
C	3.57574300	-0.20759400	2.40282300
H	4.00474600	0.77768200	2.20514300
H	3.46443400	-0.32234500	3.48346600
H	4.27488900	-0.97039400	2.04953400

C	-5.10697300	0.02669600	0.22551000
C	-3.72064300	0.34396400	0.13882200
N	-2.82715900	-0.73008500	-0.00529800
C	-3.21962000	-2.04650200	-0.06629100
N	-3.11232900	1.51657700	0.17333200
C	-1.77305800	1.20619500	0.04719600
C	-1.56833600	-0.17119600	-0.06526600
C	-0.61280700	1.99529400	0.01554100
N	0.57356200	1.40211300	-0.11796600
C	0.62623100	0.05639500	-0.22123200
N	-0.40656000	-0.79769900	-0.19909300
C	-0.66919500	3.48633700	0.11727500
N	1.84809100	-0.54114400	-0.37521600
N	3.01790600	0.16652500	-0.35591400
H	-4.86500700	-3.36743800	-0.02994300
H	-6.55109100	-1.52753700	0.23294300
H	-5.81649800	0.83769900	0.33690900
H	-2.42766900	-2.77567600	-0.17901400
H	-1.11588900	3.90566300	-0.79039300
H	-1.30070600	3.78976900	0.95691500
H	0.33267200	3.89822500	0.24225800
H	1.85459500	-1.55446600	-0.38976200
C	4.08733300	-0.51987600	-0.40295400
H	4.12561500	-1.61390300	-0.42649900
O	5.26361900	0.12197700	-0.46353600
C	6.42698100	-0.68398000	-0.20214100
H	7.25536000	-0.12012400	-0.63196800
H	6.33813800	-1.63129900	-0.74619300
C	6.62756500	-0.91385300	1.28384500
H	7.54650200	-1.48472200	1.44457400
H	6.71538300	0.03921000	1.81206000
H	5.79546300	-1.47878100	1.71472100

In4

O 1

C	-4.86731800	-1.07175200	0.43530000
C	-5.25111800	0.31108500	0.35096600
C	-4.33355600	1.29354000	0.13889200
C	-2.95511200	0.94434600	-0.00381600
N	-2.63641000	-0.42353600	0.08960700
C	-3.56563600	-1.41717400	0.30315600
N	-1.90930900	1.70937100	-0.21370000
C	-0.84039000	0.82384500	-0.26566200
C	-1.26989600	-0.52609300	-0.07989500
C	0.50312000	1.04072200	-0.44479500
N	1.26338800	-0.08932200	-0.46858700
C	0.76642500	-1.39992300	-0.26761800
N	-0.56393400	-1.62534000	-0.06477800
C	1.14205100	2.37383800	-0.61703300

Route 2

H:

In 3

O 1

C	-4.54147600	-2.33549200	0.01738600
C	-5.49773400	-1.27839000	0.16610200

N	1.70012400	-2.29391600	-0.31433200
N	2.88427500	-1.58337000	-0.68601900
H	-5.61134900	-1.83949200	0.60331100
H	-6.29883200	0.56896800	0.46071000
H	-4.60799300	2.33920300	0.07171200
H	-3.17610300	-2.42605800	0.35167000
H	0.37855600	3.15045800	-0.59458000
H	1.86385400	2.55588000	0.18424700
H	1.67439000	2.42522100	-1.57158300
H	3.67572300	-1.96077400	-0.17679800
C	2.71066900	-0.16331300	-0.42301400
O	3.14641100	0.27572100	0.84205200
C	4.38727000	0.99032100	0.84367700
H	4.45113500	1.43694500	1.83732400
H	4.33684200	1.80594900	0.10945300
C	5.58887800	0.09912200	0.57455600
H	6.50836900	0.68525800	0.66063300
H	5.63309900	-0.71856100	1.29979500
H	5.56134100	-0.32521400	-0.43453200
H	3.18041300	0.44784800	-1.20140800

O	-3.55534900	-0.23391600	0.79742000
C	-3.78890600	1.17509600	1.04100100
H	-4.80513800	1.25804700	1.43099100
H	-3.72699600	1.71620400	0.09333300
C	-2.76396900	1.67363600	2.03587700
H	-2.93288900	2.73738100	2.22335800
H	-2.85186100	1.13747200	2.98379500
H	-1.74901600	1.54289700	1.65152400

Me:

In3

O 1

C	-4.84170900	-2.26841800	-0.06610900
C	-5.79042900	-1.19503000	-0.03446800
C	-5.38637300	0.10682500	0.00638500
C	-3.99314600	0.40393700	0.01798400
N	-3.10782000	-0.68511300	-0.01487700
C	-3.51322100	-1.99822100	-0.05586100
N	-3.37189700	1.57035300	0.05538300
C	-2.03214100	1.23970900	0.04794300
C	-1.84011400	-0.14349700	0.00524200
C	-0.86119700	2.01308500	0.07457500
N	0.32219400	1.39843200	0.07104700
C	0.36338300	0.05073200	0.02022200
N	-0.68015400	-0.78676400	-0.02373400
C	-0.90253300	3.50767200	0.10672200
N	1.59335200	-0.57025700	0.07389100
N	2.71985700	0.11923100	-0.35227300
H	-5.17602500	-3.29747700	-0.09873500
H	-6.84934700	-1.42906300	-0.04388700
H	-6.09035700	0.92981300	0.03015600
H	-2.72519300	-2.73980900	-0.07714600
H	-1.32290000	3.89130200	-0.82874700
H	-1.55125300	3.85463700	0.91617300
H	0.10046100	3.91385100	0.24038600
H	1.53799500	-1.55687500	-0.15323500
C	3.84128600	-0.46218400	-0.13055400
O	4.90700400	0.23499600	-0.57807800
C	6.21859800	-0.34872400	-0.61612900
H	6.68133300	0.08276000	-1.50576100
H	6.14987400	-1.42854600	-0.77057700
C	7.02424600	0.00087300	0.62185300
H	8.03434200	-0.40765500	0.52411100
H	7.09968700	1.08547500	0.73541700
H	6.57552600	-0.41098500	1.53014800
C	4.01540900	-1.78887300	0.54937700
H	3.92090100	-2.61018900	-0.16888400
H	4.98252200	-1.87924700	1.04108500

TS3 ($\nu = 336.61 \text{ i}(\text{cm}^{-1})$)

O 1

C	4.58300300	-1.06791000	0.74374600
C	5.02437600	0.25735900	0.41367400
C	4.15668700	1.19615200	-0.05824400
C	2.78167300	0.85595400	-0.22745100
N	2.40332300	-0.45477900	0.11468900
C	3.27907900	-1.40305400	0.58925400
N	1.77324800	1.58334800	-0.66345400
C	0.68804700	0.72477900	-0.60903800
C	1.04604300	-0.54531100	-0.12676700
C	-0.66395400	0.89923300	-0.91259700
N	-1.47146300	-0.14091600	-0.72087500
C	-1.02233200	-1.36812700	-0.27053400
N	0.27592500	-1.60328300	0.05352300
C	-1.23289200	2.19544800	-1.39381900
N	-1.91234800	-2.36162900	-0.13357100
N	-3.15136000	-1.90886300	-0.67845800
H	5.28408100	-1.80435400	1.11507200
H	6.07114100	0.50861800	0.54569900
H	4.47338400	2.20103100	-0.31105000
H	2.85200100	-2.37311300	0.80954700
H	-1.46077000	2.84099000	-0.53806300
H	-0.50956500	2.72347400	-2.01801600
H	-2.15199000	2.02879700	-1.95780400
H	-3.26900300	-2.16929300	-1.65253800
C	-3.45480000	-0.62667500	-0.44882700
H	-3.99419800	-0.07344300	-1.21583900

H 3.23533100 -1.90644300 1.30497500

C 3.54726300 -1.43953400 0.46263900

N 2.06568600 1.66852800 -0.48523100

C 0.97010400 0.81992100 -0.50417500

C 1.31942700 -0.49499700 -0.15515700

C -0.38411000 1.03875400 -0.76754000

N -1.20750100 -0.00405800 -0.66933200

C -0.75556500 -1.28092200 -0.38541200

N 0.54126700 -1.55894700 -0.08681700

C -0.92907300 2.38444300 -1.13140900

N -1.64253600 -2.28298500 -0.39331500

N -2.87594700 -1.76112600 -0.88085600

H 5.55042300 -1.90872800 0.93708700

H 6.36003600 0.43885900 0.57942300

H 4.77545800 2.22079100 -0.10154200

H 3.11100800 -2.42137800 0.59532300

H -0.12936700 3.03044400 -1.49673500

H -1.69980200 2.29366000 -1.89920200

H -1.37234000 2.86845500 -0.25506200

H -2.97695000 -1.88547000 -1.88275100

C -3.19209800 -0.51903200 -0.46987300

O -3.23851200 -0.38780100 0.84502900

C -3.46595600 0.90775900 1.43205600

H -4.47782300 1.24011800 1.18454700

H -2.73924500 1.60959800 1.01398800

C -3.28181200 0.75992500 2.92476900

H -3.44885500 1.72726400 3.40514000

H -3.99581900 0.04118500 3.33466100

H -2.26724400 0.42681000 3.15680900

C -4.01405200 0.37085000 -1.34668800

H -3.78969200 0.18889800 -2.39692600

H -3.82293200 1.41991500 -1.12498900

H -5.07299100 0.17049100 -1.15728700

Et:

In3

0 1

C -4.90786900 -2.38974600 -0.09734800

C -5.91856600 -1.38357000 0.04305000

C -5.59474500 -0.06202300 0.13303200

C -4.22427300 0.32426000 0.08710800

N -3.27536500 -0.70161600 -0.05074100

C -3.60016100 -2.03469400 -0.14196100

N -3.67598100 1.52508300 0.15471900

C -2.32066500 1.28367700 0.05801300

C -2.04490400 -0.08016800 -0.06979300

C -1.20113600 2.12998800 0.06518700

N 0.01578300 1.59747500 -0.04942400

C 0.13824600 0.25872800 -0.16308600

TS3 (v = 258.14 i(cm-1))

0 1

C 4.85556500 -1.13392900 0.63951100

C 5.30969100 0.21201500 0.43258500

C 4.44913700 1.20011900 0.05858000

C 3.06893000 0.89204100 -0.13088300

N 2.67896200 -0.44183800 0.08601700

N	-0.84952000	-0.64558200	-0.17781000
C	-1.33275700	3.61484500	0.18475000
N	1.39572600	-0.27685000	-0.30854100
N	2.51540500	0.47795100	-0.08669300
H	-5.17764300	-3.43560000	-0.16934700
H	-6.95952500	-1.68585500	0.07792000
H	-6.34556900	0.71162200	0.23864700
H	-2.77049400	-2.72222600	-0.24497100
H	-1.79561500	4.02327500	-0.71969000
H	-1.98230900	3.87600900	1.02495800
H	-0.35281300	4.07336300	0.32059500
H	1.42936500	-1.28778600	-0.27162400
C	3.65300300	-0.10281700	-0.15691200
O	4.69291200	0.69052400	0.21053200
C	5.94954000	0.59009000	-0.48209900
H	6.28060600	1.62313600	-0.61069400
H	5.79809000	0.16765100	-1.47995000
C	6.97260400	-0.19561700	0.31664700
H	7.93900500	-0.16039000	-0.19484200
H	7.09438000	0.24185800	1.31134300
H	6.68551600	-1.24428000	0.43187000
C	3.90627200	-1.55793900	-0.45420800
H	3.16681600	-1.91920700	-1.17518800
H	4.87469900	-1.67635800	-0.94317100
C	3.87314200	-2.40742300	0.82736900
H	2.90242100	-2.34409700	1.32770800
H	4.06542500	-3.45588600	0.58841700
H	4.63564100	-2.07018800	1.53470300

H	3.50026100	-2.48126200	0.08611600
H	0.00440200	3.11831300	-0.36022200
H	-1.58337900	2.44045800	-0.80177800
H	-1.18919300	2.76251500	0.89743100
H	-3.33923600	-1.97318300	-0.03578500
C	-2.43940100	-0.13006100	0.16427400
O	-2.72301800	0.15111200	-1.19809100
C	-4.04352300	0.52766600	-1.59963700
H	-3.91895800	0.81619300	-2.64516800
H	-4.37107100	1.41720700	-1.05106100
C	-5.07457200	-0.58595300	-1.49001600
H	-6.00959300	-0.25399800	-1.95047600
H	-4.73547700	-1.48319700	-2.01636900
H	-5.29936900	-0.84556000	-0.45070400
C	-3.20670500	0.75604400	1.15283600
H	-3.23145700	1.78813000	0.79691500
H	-4.24133200	0.39900300	1.15760100
C	-2.65008900	0.69272800	2.57168800
H	-1.64322800	1.11685600	2.63364900
H	-3.29359100	1.26100600	3.24775600
H	-2.60466600	-0.34133600	2.92258700

TS3 ($\nu = 234.35 \text{ i}(\text{cm}^{-1})$)

O 1

C	5.15661900	-1.12600000	0.52037900
C	5.59328400	0.20697200	0.21644600
C	4.70893700	1.17323700	-0.15983500
C	3.32172200	0.85467600	-0.25283400
N	2.94863900	-0.46507400	0.06024000
C	3.84098000	-1.44096200	0.43722900
N	2.29626500	1.60940100	-0.59256500
C	1.20574300	0.76076300	-0.49795700
C	1.57743900	-0.53083700	-0.09923900
C	-0.16234400	0.96765400	-0.70189200
N	-0.98077400	-0.06015900	-0.48941500
C	-0.50449900	-1.32644600	-0.18211500
N	0.80551700	-1.59101800	0.06123200
C	-0.69743800	2.28645600	-1.16230700
N	-1.38873300	-2.32788500	-0.11786000
N	-2.64769100	-1.81128900	-0.54613500
H	5.87008800	-1.88409700	0.81682400
H	6.64946800	0.44199300	0.29074100
H	5.02143100	2.18437400	-0.39208900
H	3.41684000	-2.41511400	0.64476300
H	-0.45578000	3.07241500	-0.44094200
H	-0.21716800	2.55906500	-2.10647200
H	-1.77511200	2.24995500	-1.31615900
H	-2.77261500	-1.90156500	-1.55032500
C	-2.94025800	-0.56727500	-0.10619700

In4

O 1

C	5.19811000	-1.15797700	-0.17397800
C	5.58255800	0.21873100	-0.32818500
C	4.66028700	1.21955100	-0.33780600
C	3.27576600	0.89628200	-0.19236600
N	2.95731800	-0.46690800	-0.04496000
C	3.89079500	-1.47887900	-0.03506200
N	2.22368800	1.68101300	-0.17705000
C	1.14980600	0.81361700	-0.01255900
C	1.58305700	-0.54178500	0.07080900
C	-0.19939700	1.05998200	0.06091900
N	-0.97838500	-0.04355100	0.26082800
C	-0.47163500	-1.36933900	0.27146400
N	0.86819700	-1.62484600	0.20493600
C	-0.78176000	2.42604200	-0.06033600
N	-1.40111900	-2.26255100	0.35079600
N	-2.61477300	-1.54131700	0.52648200
H	5.94597300	-1.94009800	-0.16858900
H	6.63463200	0.45665000	-0.44125700
H	4.93515300	2.26062900	-0.45541300

O	-2.90173300	-0.45894100	1.20764500
C	-3.33631300	0.71701100	1.92377200
H	-3.55761200	0.32384500	2.91586300
H	-4.26712300	1.09456500	1.49515400
C	-2.26676000	1.78630800	1.99447800
H	-2.58060200	2.54466200	2.71662100
H	-1.31561100	1.36193300	2.32531000
H	-2.11982000	2.27845200	1.03275300
C	-3.82856700	0.30853500	-0.94447900
H	-3.45092400	0.28705000	-1.96847900
H	-3.74882300	1.34057200	-0.59939000
C	-5.29079600	-0.15884600	-0.89764700
H	-5.68269600	-0.16554600	0.12278900
H	-5.90425000	0.51927000	-1.49427800
H	-5.39489800	-1.16559200	-1.30913900