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Supporting information for:

A Theoretical Approach to Investigating the Mechanism of Action and Efficiency of N-Heterocyclic Olefins as Organic Catalysts for Transesterification Reactions

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		Zwitterionic pathway M062X, 6-311++G(2d,p)				Anionic pathway M062X, 6-311++G(2d,p)			
NHO		G	H	S	E	G	H	S	E
1a	Step1-reacs	-882.479608	-882.405	156.369	-882.7845614	-577.478374	-577.415	133.786	-577.7255468
	TS1	-882.457917	-882.387	149.582	-882.7650465	-577.458907	-577.399	125.304	-577.7050773
	Step1-prods	-882.469401	-882.398	149.755	-882.7790282	-577.474896	-577.417	122.074	-577.7282887
	Step2-reacs	-1037.436205	-1037.35	178.005	-1037.8202813	-1037.43265	-1037.35	172.832	-1037.8184586
	TS2	-1037.415590	-1037.33	174.609	-1037.7996631	-1037.41204	-1037.33	173.942	-1037.7954445
	Step2-int	-1037.420701	-1037.33	182.487	-1037.800301	-1037.42815	-1037.35	174.126	-1037.8131341
	TS3	-1037.412756	-1037.33	176.349	-1037.7957223	-1037.41965	-1037.34	170.789	-1037.8044201
	step2-prods	-1037.439219	-1037.36	177.024	-1037.8235164	-1037.43427	-1037.35	173.585	-1037.8195957
	Step3-reacs	-921.751573	-921.677	156.34	-922.0877693	-538.190454	-538.137	111.597	-538.4194329
	TS4	-921.738203	-921.667	150.799	-922.0749957	-538.175798	-538.119	118.988	-538.3953386
	Step3-prods	-921.763925	-921.689	157.728	-922.0974105	-538.195942	-538.136	127.096	-538.4165544
2a	Step1-reacs	-961.020024	-960.94	169.38	-961.3786828	-656.017273	-655.946	150.481	-656.3163914
	TS1	-960.992847	-960.92	152.327	-961.3591118	-656.003172	-655.936	141.088	-656.3014136
	Step1-prods	-961.007418	-960.935	153.209	-961.3750253	-656.027282	-655.964	133.577	-656.3350678
	Step2-reacs	-1115.976025	-1115.89	182.777	-1116.4172644	-1115.985791	-1115.9	182.829	-1116.4262769
	TS2	-1115.954181	-1115.87	181.215	-1116.3950032	-1115.958436	-1115.87	179.781	-1116.3992575
	Step2-int	-1115.955517	-1115.87	185.858	-1116.3927637	-1115.977653	-1115.89	180.905	-1116.4201766
	TS3	-1115.950831	-1115.86	183.787	-1116.3894223	-1115.969161	-1115.88	181.396	-1116.4091294
	step2-prods	-1115.976659	-1115.89	179.642	-1116.4198132	-1115.987161	-1115.9	182.6	-1116.4277641
	Step3-reacs	-1000.288816	-1000.21	158.707	-1000.6838982	-616.744352	-616.685	125.904	-617.0261194
	TS4	-1000.275350	-1000.2	157.871	-1000.6686025	-616.719928	-616.657	132.377	-616.9927813
	Step3-prods	-1000.302547	-1000.22	178.327	-1000.6867782	-616.735441	-616.67	137.887	-617.0111037
1b	Step1-reacs	-805.097226	-805.031	140.435	-805.3754355	-500.096208	-500.039	119.554	-500.3159922
	TS1	-805.065295	-805	137.643	-805.3432465	-500.063447	-500.008	116.435	-500.2798884
	Step1-prods	-805.070997	-805.006	137.053	-805.3515908	-500.098200	-500.048	105.662	-500.3249779
	Step2-reacs	-960.038038	-959.96	164.998	-960.3932032	-960.057722	-959.983	156.317	-960.416697
	TS2	-960.020285	-959.942	164.304	-960.3743703	-960.019919	-959.945	157.645	-960.3760157
	Step2-int	-960.026619	-959.942	177.177	-960.3727061	-960.028344	-959.953	159.346	-960.3857855
	TS3	-960.015848	-959.938	164.102	-960.3695802	-960.022001	-959.945	161.073	-960.3766156
	step2-prods	-960.041383	-959.964	162.112	-960.397868	-960.059177	-959.983	160.174	-960.4159109
	Step3-reacs	-844.354802	-844.285	145.925	-844.6606073	-460.815541	-460.769	98.972	-461.0159996
	TS4	-844.346768	-844.279	141.941	-844.6521286	-460.781613	-460.729	111.091	-460.9709983
	Step3-prods	-844.379501	-844.309	148.306	-844.6838359	-460.812703	-460.759	112.073	-461.0062365
2b	Step1-reacs	-883.642492	-883.566	160.532	-883.9700699	-578.639386	-578.577	131.329	-578.9130007
	TS1	-883.599398	-883.532	142.277	-883.935238	-578.608705	-578.547	129.22	-578.8779359
	Step1-prods	-883.608593	-883.54	144.049	-883.9453824	-578.651705	-578.596	117.402	-578.9324638
	Step2-reacs	-1038.576016	-1038.49	171.531	-1038.9875476	-1038.610537	-1038.53	168.524	-1039.0234448
	TS2	-1038.554802	-1038.47	169.689	-1038.9656346	-1038.566953	-1038.49	171.303	-1038.9772306
	Step2-int	-1038.560105	-1038.47	180.6	-1038.9645297	-1038.579598	-1038.5	172.623	-1038.9906371
	TS3	-1038.553141	-1038.47	172.526	-1038.962699	-1038.572116	-1038.49	172.774	-1038.9808793
	step2-prods	-1038.578077	-1038.5	167.689	-1038.9915479	-1038.611923	-1038.53	169.673	-1039.0242429
	Step3-reacs	-922.891737	-922.82	151.944	-923.2543041	-539.369452	-539.316	111.601	-539.6233835
	TS4	-922.879750	-922.811	145.726	-923.2442541	-539.325997	-539.268	121.558	-539.5691587
	Step3-prods	-922.923098	-922.846	162.588	-923.2798137	-539.357944	-539.299	124.436	-539.6051539
1c	Step1-reacs	-844.370780	-844.304	140.913	-844.6793004	-539.369012	-539.312	119.384	-539.6202172
	TS1	-844.338902	-844.272	140.565	-844.6466209	-539.341765	-539.283	124.442	-539.5854683
	Step1-prods	-844.346032	-844.279	141.069	-844.6558202	-539.376287	-539.324	109.687	-539.6318695
	Step2-reacs	-999.312561	-999.235	162.743	-999.6996051	-999.336031	-999.26	159.927	-999.723689
	TS2	-999.294866	-999.216	166.501	-999.6781108	-999.295639	-999.219	160.957	-999.6815609
	Step2-int	-999.300577	-999.217	175.807	-999.6793844	-999.305299	-999.228	162.306	-999.6921085
	TS3	-999.294621	-999.214	168.816	-999.6765908	-999.297974	-999.218	167.633	-999.6800432
	step2-prods	-999.317565	-999.237	170.081	-999.7008465	-999.340401	-999.262	165.695	-999.724835
	Step3-reacs	-883.630047	-883.558	151.533	-883.9643079	-500.094548	-500.045	103.564	-500.3230401
	TS4	-883.619913	-883.552	143.798	-883.9563133	-500.058378	-500.003	116.053	-500.2763233
	Step3-prods	-883.654870	-883.584	148.586	-883.98984	-500.087432	-500.033	115.011	-500.3104084
2c	Step1-reacs	-922.914378	-922.838	161.152	-923.2718057	-617.915470	-617.85	137.27	-618.2161763
	TS1	-922.861586	-922.793	143.379	-923.227849	-617.880084	-617.818	131.573	-618.1787023
	Step1-prods	-922.873218	-922.803	147.02	-923.2394745	-617.919636	-617.862	121.528	-618.2288836
	Step2-reacs	-1077.843669	-1077.76	173.815	-1078.284709	-1077.879237	-1077.8	176.226	-1078.3187057

	TS2	-1077.818694	-1077.74	174.68	-1078.2579474	-1077.841474	-1077.76	174.715	-1078.2806158
	Step2-int	-1077.827006	-1077.74	178.485	-1078.2624666	-1077.850110	-1077.77	174.138	-1078.2910802
	TS3	-1077.819219	-1077.74	176.749	-1078.2570899	-1077.843143	-1077.76	174.626	-1078.2824686
	step2-prods	-1077.845303	-1077.76	178.029	-1078.2843571	-1077.880563	-1077.8	174.929	-1078.3203991
	Step3-reacs	-962.154939	-962.082	152.959	-962.5482646	-578.636670	-578.582	114.046	-578.9197306
	TS4	-962.144314	-962.072	151.407	-962.5363382	-578.597077	-578.538	123.763	-578.8696912
	Step3-prods	-962.198305	-962.119	166.782	-962.5825558	-578.632256	-578.571	128.778	-578.9071995
	Step1-reacs	-803.910817	-803.843	141.947	-804.1632416	-498.909042	-498.852	119.169	-499.1038243
	TS1	-803.887177	-803.824	133.042	-804.1430029	-498.889067	-498.836	111.931	-499.0823153
	Step1-prods	-803.898700	-803.834	136.677	-804.155436	-498.904670	-498.854	106.002	-499.1067171
	Step2-reacs	-958.864639	-958.788	161.937	-959.1970655	-958.860393	-958.784	161.674	-959.1921954
	TS2	-958.845530	-958.768	162.852	-959.1757937	-958.841422	-958.767	156.09	-959.1745589
1d	Step2-int	-958.848727	-958.77	165.418	-959.1774943	-958.857470	-958.782	159.763	-959.1900244
	TS3	-958.841321	-958.764	162.441	-959.1716737	-958.846056	-958.772	156.711	-959.1788347
	step2-prods	-958.868194	-958.79	164.305	-959.1992016	-958.859300	-958.783	160.283	-959.191818
	Step3-reacs	-843.180197	-843.113	141.91	-843.464104	-459.622652	-459.575	100.021	-459.7977926
	TS4	-843.169102	-843.104	137.479	-843.4526261	-459.606405	-459.556	106.216	-459.7727389
	Step3-prods	-843.194044	-843.124	146.398	-843.4738212	-459.626114	-459.573	111.412	-459.7949576
	Step1-reacs	-882.471986	-882.399	154.029	-882.7781861	-577.468262	-577.408	127.107	-577.7189012
	TS1	-882.450343	-882.381	146.772	-882.7586745	-577.450918	-577.392	124.379	-577.6976291
	Step1-prods	-882.461040	-882.391	147.179	-882.7716486	-577.463381	-577.407	119.218	-577.7185336
	Step2-reacs	-1037.428704	-1037.34	176.632	-1037.8131748	-1037.421399	-1037.34	171.682	-1037.8075876
	TS2	-1037.407497	-1037.33	170.891	-1037.7932195	-1037.404267	-1037.33	166.367	-1037.7917475
1e	Step2-int	-1037.412598	-1037.33	180.087	-1037.7930962	-1037.415010	-1037.34	165.544	-1037.8050859
	TS3	-1037.407859	-1037.33	173.505	-1037.7917536	-1037.406589	-1037.33	166.391	-1037.7941769
	step2-prods	-1037.427709	-1037.35	170.542	-1037.8155202	-1037.425445	-1037.34	180.445	-1037.8070727
	Step3-reacs	-921.742348	-921.67	152.789	-922.0803704	-538.180760	-538.128	111.404	-538.4096305
	TS4	-921.731550	-921.661	149.325	-922.0684405	-538.167397	-538.111	117.863	-538.3874603
	Step3-prods	-921.755314	-921.68	158.929	-922.0881931	-538.185774	-538.128	121.831	-538.4093557

Cartesian coordinate of the optimized species and imaginary frequency of TSs computed at M06-2X/6-311++G (2d, p) level of Density Functional Theory:

Methyl benzoate

0 1

C	-0.74776300	-1.17483100	-0.00030900
C	-2.12189300	-1.36920800	0.00004800
C	-2.98021500	-0.27570700	0.00041900
C	-2.46582000	1.01642800	0.00043200
C	-1.09368400	1.21438500	0.00007700
C	-0.23321900	0.11961700	-0.00030800
H	-0.07457300	-2.02129400	-0.00060400
H	-2.52326600	-2.37441800	0.00003700
H	-4.05187900	-0.43084500	0.00070000
H	-3.13434700	1.86767700	0.00071900
H	-0.67482300	2.21235000	0.00007500
C	1.23279200	0.38354600	-0.00073900
O	1.71986200	1.48796500	-0.00002000
O	1.96232100	-0.73385900	-0.00021800
C	3.38020900	-0.54188300	0.00031800
H	3.68295200	0.00865700	0.88941800
H	3.81238500	-1.53746400	0.00063200
H	3.68364600	0.00840100	-0.88870300

Ethyl benzoate

0 1

C	2.29856700	-1.57439000	0.00013200
C	0.97757200	-1.14908100	0.00012300
C	0.69090300	0.21435800	-0.00003500
C	1.72509000	1.14650400	-0.00018100
C	3.04351700	0.71821400	-0.00017200
C	3.33022500	-0.64282800	-0.00001600
H	2.52332000	-2.63335300	0.00025200
H	0.16946900	-1.86816800	0.00023700
H	1.48148900	2.20114300	-0.00030200
H	3.84798100	1.44250800	-0.00028900
H	4.35998800	-0.97825600	-0.00001100
C	-0.70940500	0.72517700	-0.00006000
O	-0.99668100	1.89846800	-0.00020700
O	-1.61852500	-0.24984500	0.00006900
C	-2.99510700	0.17154200	0.00002200
H	-3.16836000	0.78673600	0.88364800
H	-3.16839300	0.78641700	-0.88382100
C	-3.84831600	-1.07321000	0.00025900
H	-4.90170400	-0.79237500	0.00020400
H	-3.65020700	-1.67584500	-0.88629200
H	-3.65021200	-1.67550600	0.88704100

Ethanol

0 1

C	-1.20678800	-0.24275100	-0.02169000
H	-1.25290800	-0.96931800	0.79273000
H	-1.27089500	-0.77957000	-0.96903200
H	-2.07209100	0.41668100	0.06452500
C	0.07831600	0.55930000	0.04737100
H	0.12064900	1.28368400	-0.76650900
H	0.13288800	1.11437800	0.98918300
O	1.23404200	-0.25721900	-0.10829300
H	1.24085200	-0.90739600	0.60136300

Methanol

0 1

C	-0.04718700	0.66492200	0.00000000
H	0.44199600	1.06647500	0.89058800
H	0.44199600	1.06647500	-0.89058800
H	-1.08810100	0.98311500	0.00000000
O	-0.04718700	-0.75571100	0.00000000
H	0.86472100	-1.05990900	0.00000000

Ethoxide ion

-1 1

C	1.17225100	-0.20955000	-0.00002400
H	1.25884200	-0.84840200	-0.88393900
H	1.25807000	-0.84905900	0.88351000
H	2.00869500	0.49884200	0.00067600
C	-0.19442600	0.49732400	-0.00006800
H	-0.18704200	1.18535900	0.87954100
H	-0.18669200	1.18624000	-0.87893600
O	-1.25235300	-0.36245400	-0.00003700

Methoxide ion

-1 1

C	-0.56217900	0.00001700	0.00002100
H	-1.02093900	0.84892300	-0.55934400

H	-1.02086300	0.05983400	1.01478000
H	-1.02059100	-0.90900500	-0.45557600
O	0.80443300	0.00001800	0.00000200

The hemiacetal anion (anionic mechanism)

-1 1

C	3.01284200	-0.28040200	1.06480800
C	1.69299400	0.14704800	1.18736800
C	0.79538100	-0.01056600	0.14078600
C	1.23832800	-0.60159200	-1.04124300
C	2.55250000	-1.03148100	-1.17080400
C	3.44630400	-0.87165400	-0.11477900
H	3.70394300	-0.15046600	1.88967200
H	1.33413200	0.61283300	2.09698400
H	0.53942200	-0.71798200	-1.86066700
H	2.88478000	-1.48992800	-2.09519200
H	4.47240200	-1.20503100	-0.21417900
C	-0.66329300	0.47477500	0.29954200
O	-0.93281600	1.08168800	1.39763500
O	-1.43969000	-0.72641700	0.03274800
C	-2.82267500	-0.56299100	0.26233200
H	-3.21116500	0.25514000	-0.35417500
H	-3.00006100	-0.30114900	1.30931700
C	-0.42574700	2.56827900	-0.84694900
H	-0.84891300	3.13244400	-0.01191500
H	-0.66488900	3.07558300	-1.78329600
O	-0.95941400	1.27231400	-0.91652900
H	0.66681600	2.54945100	-0.73104700
C	-3.51705400	-1.86460800	-0.08680600
H	-3.13255800	-2.68024100	0.52847900
H	-3.35405700	-2.12064500	-1.13528500
H	-4.59196300	-1.78153900	0.08495000

Catalysts:

NHO 1a

0 1

C	-0.00005300	-1.21242800	-0.05407700
C	-0.67338700	0.96158700	-0.00215300
C	0.67348900	0.96153100	-0.00228200
N	1.09337900	-0.37714400	-0.07226200
N	-1.09340300	-0.37704100	-0.07199200
C	-0.00011400	-2.57461600	0.00160900
C	2.43662800	-0.87904300	0.05512500
C	-2.43672900	-0.87882500	0.05492700
C	-1.64793300	2.08468100	0.00847300
C	1.64812400	2.08454000	0.00833700
H	-2.30152800	2.04358200	0.88335800
H	-1.11906700	3.03552200	0.03038400
H	-2.28298600	2.07119800	-0.88117200
H	1.11933300	3.03543300	0.02985100
H	2.30149900	2.04361600	0.88339700
H	2.28341100	2.07080200	-0.88113800
H	2.56956300	-1.40038700	1.00857300
H	2.65484500	-1.57980900	-0.75401700
H	3.14111800	-0.05304100	-0.00034700
H	-0.93024900	-3.11980300	0.00907100
H	0.92997500	-3.11988700	0.00880000
H	-3.14112500	-0.05275400	-0.00069700
H	-2.65474200	-1.57952600	-0.75433000
H	-2.57002600	-1.40021800	1.00829600

NHO 1b

0 1

C	0.00000000	0.67859200	0.00000000
C	0.74955000	-1.50599700	0.12065600
C	-0.74954900	-1.50599700	-0.12065600
N	-1.09258800	-0.14455300	0.27458400
N	1.09258800	-0.14455200	-0.27458400
C	-0.00000100	2.02527400	0.00000000
C	-2.42393900	0.32518900	-0.03837600
C	2.42393900	0.32519000	0.03837700
H	-3.14321200	-0.43729900	0.25946500
H	-2.64605900	1.23333600	0.52066600
H	-2.54472400	0.53110200	-1.11004200
H	3.14321200	-0.43729600	-0.25946800
H	2.64605800	1.23334000	-0.52066100
H	2.54472500	0.53109800	1.11004400
H	-0.91073100	2.57606100	0.17355700
H	0.91072900	2.57606200	-0.17355800
H	0.97304200	-1.68329800	1.18173200
H	-0.97304200	-1.68329900	-1.18173200
H	1.28676700	-2.23479000	-0.48493900
H	-1.28676600	-2.23479100	0.48493900

NHO 1c

0 1

C	1.23330400	1.27642300	0.25670700
C	-0.00020500	2.06363300	-0.13195000
C	-1.23354400	1.27618400	0.25676100
H	-0.00028800	3.03134100	0.37174300
H	1.31660500	1.22315800	1.35438400
H	2.13494500	1.76208900	-0.11813100
H	-1.31679100	1.22289800	1.35444200

H	-2.13529600	1.76167800	-0.11803700
C	0.00008300	-0.79210500	-0.06769900
C	0.00032000	-2.09392300	0.28637200
H	0.91948500	-2.64017900	0.41277700
H	-0.91861400	-2.64052900	0.41288100
N	-1.18176600	-0.07029900	-0.31526000
N	1.18175400	-0.07007100	-0.31531000
C	2.42198200	-0.79241700	-0.10631000
H	2.55957900	-1.10066800	0.93979400
H	2.45327300	-1.67910400	-0.73807200
H	3.24900000	-0.14184000	-0.38722900
C	-2.42192600	-0.79278800	-0.10633000
H	-2.45314900	-1.67940800	-0.73818300
H	-2.55950300	-1.10114600	0.93974500
H	-3.24899900	-0.14225300	-0.38719100
H	-0.00024500	2.23650900	-1.21024800

NHO 1d

0 1

C	0.00000000	0.62313100	-0.00013700
C	0.67157700	-1.54245900	0.00004300
C	-0.67157600	-1.54245900	0.00006000
N	-1.09323400	-0.21585500	-0.00013800
N	1.09323400	-0.21585500	-0.00013900
C	0.00000000	1.98580900	0.00018400
C	-2.44916900	0.26648700	0.00004800
C	2.44916900	0.26648800	0.00005400
H	-2.63970400	0.87561400	0.88756100
H	-2.63959200	0.87637400	-0.88695900
H	-3.12684300	-0.58399100	-0.00038100
H	0.93067600	2.53017900	-0.00014500
H	-0.93067800	2.53017800	-0.00016700
H	3.12684300	-0.58399000	-0.00049200
H	2.63955500	0.87646600	-0.88689800
H	2.63974200	0.87552400	0.88762100
H	1.37274700	-2.35818200	0.00011600
H	-1.37274600	-2.35818300	0.00017000

NHO 1e

0 1

C	0.70668600	0.58632100	-0.21039600
C	1.29669600	-1.55030500	0.26487000
C	-0.04259500	-1.51969800	0.17469700
N	-0.41814200	-0.21444200	-0.14417000
N	1.76661200	-0.26556500	0.01619500
C	0.77936500	1.92815700	-0.44138500
C	3.13353500	0.18223400	0.06181500
C	-1.77246700	0.31436300	-0.23934300
H	3.43220800	0.60614700	-0.90018400
H	1.74022000	2.41392800	-0.49959700
H	-0.11426400	2.51629500	-0.57065900
H	-1.73830500	1.07495900	-1.02534800
H	-0.75810900	-2.31379400	0.28504400
H	1.96666900	-2.36752300	0.46662600
H	3.77527200	-0.66517600	0.29159500
C	-2.19247800	0.96972300	1.07397600
H	-3.16879700	1.44474000	0.96544600
H	-2.26023600	0.21331900	1.85957500
H	-1.46794000	1.72556100	1.37873300
H	3.25969500	0.94809000	0.83198900
C	-2.75400700	-0.76762900	-0.66442400
H	-2.88444500	-1.51502500	0.12082200
H	-3.72674200	-0.31289100	-0.85159800
H	-2.42292500	-1.26757500	-1.57549100

NHO 2a

0 1

C	-0.65758600	0.00001100	0.00000100
C	1.52131500	-0.65684100	0.11503000
C	1.52131000	0.65684700	-0.11492700
N	0.17752000	1.12381100	-0.22235500
N	0.17750700	-1.12384000	0.22229400
C	-2.00442900	-0.00002100	0.00007700
C	-0.11394900	2.33764400	0.53831800
C	-0.11388000	-2.33744800	-0.53879400
C	2.65765000	-1.60845700	0.25557300
C	2.65767500	1.60844000	-0.25538300
H	2.71177800	-2.30808400	-0.58204900
H	3.60219500	-1.07024000	0.30513900
H	2.54989800	-2.19705400	1.17018200
H	3.60224800	1.07020200	-0.30415400
H	2.55041400	2.19655300	-1.17036300
H	2.71133800	2.30850300	0.58189800
H	0.56272400	3.12968400	0.22157400
H	-1.12872500	2.67255000	0.35395200
H	0.01219000	2.16867600	1.61517800
H	0.56320100	-3.12937400	-0.22263900
H	-1.12846800	-2.67279300	-0.35415000
H	0.01179400	-2.16798900	-1.61562400
C	-2.80837500	1.14222000	-0.56027100
H	-3.22515900	1.79689300	0.21407400
H	-2.22362000	1.75641100	-1.24644100
H	-3.65919900	0.74146600	-1.11975400
C	-2.80816800	-1.14237300	0.56050100
H	-3.22500900	-1.79703900	-0.21382100

H	-2.22321800	-1.75654200	1.24652300
H	-3.65894700	-0.74174700	1.12014300

NHO2b

0 1

C	0.19769000	0.05193500	-0.18296700
C	-1.98321300	-0.74861500	-0.41522200
C	-1.86348000	0.69602100	-0.89577700
N	-0.66054800	1.20434000	-0.22353200
N	-0.58131100	-1.14445400	-0.24169600
C	1.53248700	0.11841600	-0.17337800
C	-0.95354900	1.70079900	1.12687100
C	-0.40845300	-2.10511300	0.84284400
H	-1.63148900	2.55220000	1.05305100
H	-1.41054800	0.94208200	1.77602300
H	-0.02668100	2.03506900	1.59264600
H	-0.99382300	-2.99882300	0.62115600
H	0.63175600	-2.40001400	0.94566500
H	-0.75236700	-1.69458400	1.80262900
H	-2.52004300	-0.80354100	0.54085200
H	-1.70077700	0.72354500	-1.97520900
H	-2.49352200	-1.39446000	-1.13084500
H	-2.73252900	1.30563600	-0.65457900
C	2.25134600	1.43490600	-0.07942900
H	3.00682900	1.51229100	-0.86686600
H	1.56680500	2.27621700	-0.17138500
H	2.78193100	1.52592200	0.87447900
C	2.40135400	-1.10568000	-0.26602500
H	2.74929400	-1.45180700	0.71294900
H	1.88026800	-1.93148200	-0.75185000
H	3.29281000	-0.87346300	-0.85362700

NHO 2c

0 1

C	-1.61138300	-1.22880100	-0.75078000
C	-2.45518900	-0.00000100	-0.42327300
C	-1.61138200	1.22879900	-0.75077900
H	-3.37420000	0.00000000	-1.01350600
H	-1.41046700	-1.23898200	-1.82777200
H	-2.13472200	-2.15566200	-0.50848600
H	-1.41047300	1.23898500	-1.82777100
H	-2.13471700	2.15566100	-0.50847800
C	0.39505200	-0.00000400	-0.16104500
C	1.72739100	-0.00000500	-0.29208400
N	-0.32653200	1.23809000	-0.05097300
N	-0.32653500	-1.23809800	-0.05096900
C	-0.43003400	-1.73078200	1.32182600
H	-0.80732100	-2.75565500	1.30414600
H	0.56234900	-1.73846500	1.77404500
H	-1.09390200	-1.13361200	1.96083900
C	-0.43001400	1.73080400	1.32181200
H	0.56236500	1.73844400	1.77403700
H	-0.80725000	2.75569500	1.30411200
H	-1.09391800	1.13367800	1.96083100
H	-2.74115200	-0.00000100	0.63245900
C	2.53354200	1.26628600	-0.32623400
H	1.90043600	2.14691800	-0.40473900
H	3.14329000	1.35310200	0.57948400
H	3.22913000	1.24615300	-1.16984400
C	2.53354300	-1.26629600	-0.32622500
H	3.14333000	-1.35307800	0.57947000
H	1.90043700	-2.14693300	-0.40467600
H	3.22909600	-1.24619000	-1.16986500

Protonated catalysts (anionic mechanism):

NHO1a-H^+

1 1

C	-4.25663400	-0.40401300	-1.23414100
C	-4.90103200	1.69088900	-0.85218000
C	-5.80042600	0.86451900	-0.25566800
N	-5.38007200	-0.43229000	-0.51605300
N	-3.95560300	0.87553500	-1.45928600
C	-3.48277800	-1.58324700	-1.69196000
C	-6.05219900	-1.64224400	-0.05394900
C	-2.79508200	1.34728900	-2.20788600
C	-4.83338000	3.17441500	-0.91873900
C	-7.02324300	1.15904300	0.53677300
H	-4.96557300	3.53225700	-1.94139500
H	-5.62268900	3.60508900	-0.30707100
H	-3.87576900	3.54236100	-0.54728100
H	-7.10998500	2.23167600	0.69383200
H	-7.92275100	0.81902400	0.02019100
H	-6.98400800	0.67373000	1.51320400
H	-7.11387600	-1.43426700	0.04201600
H	-5.91536400	-2.43294500	-0.78613000
H	-5.65004400	-1.95019000	0.91012000
H	-2.42854100	-1.33071600	-1.78284500
H	-3.57855900	-2.39464500	-0.97334300
H	-2.57854800	0.65208900	-3.01387500
H	-3.02909200	2.31737200	-2.63644100
H	-1.93404600	1.43673300	-1.54721300
H	-3.84562800	-1.93005200	-2.66186700

NHO 1b-H^+

1 1

C	0.01386700	0.58958500	0.00332100
C	-0.81810000	-1.54839500	0.05405900
C	0.71007700	-1.59938900	-0.05952400
N	1.08012000	-0.18701200	0.08529200
N	-1.10141500	-0.11203800	-0.07348700
C	0.10453700	2.07120900	-0.00396200
C	2.46659500	0.22907900	-0.00291000
C	-2.47439300	0.35020400	0.00169000
H	2.84415300	0.07749100	-1.01591300
H	2.56180400	1.27654000	0.26879200
H	3.05486300	-0.36819400	0.69195100
H	-0.86908800	2.53581100	-0.10747700
H	0.55994300	2.40772500	0.92812600
H	-2.53360200	1.41637200	-0.18718200
H	-3.05840000	-0.17302900	-0.75407300
H	-2.88517300	0.13166900	0.98869200
H	0.73971700	2.38942200	-0.83071700
H	-1.32463900	-2.10080300	-0.73472400
H	1.04559300	-1.96167600	-1.03304300
H	-1.17774000	-1.89769300	1.02357500
H	1.17613700	-2.19404300	0.72330500

NHO 1c-H$^+$

1 1

C	1.23631600	1.40118600	0.18975900
C	0.00181300	2.04983900	-0.39520900
C	-1.23338500	1.40335400	0.19072200
H	0.00293100	3.11510100	-0.17101400
H	1.35023200	1.64116500	1.25003200
H	2.12885300	1.73739400	-0.33336400
H	-1.34544300	1.64265800	1.25135700
H	-2.12590900	1.74181300	-0.33096800
C	-0.00052800	-0.69677500	-0.00254600
C	-0.00290100	-2.19037500	-0.11581900
H	0.87994700	-2.61909900	0.34544000
H	-0.87851200	-2.61630100	0.36197500
N	-1.16003700	-0.05647200	0.03933800
N	1.16015200	-0.05876100	0.04000400
C	2.43409100	-0.78532100	0.03076700
H	2.59924100	-1.29823700	0.97838900
H	2.46871400	-1.49955400	-0.78863700
H	3.22822600	-0.05927400	-0.11280800
C	-2.43497300	-0.78104000	0.03062500
H	-2.46860900	-1.49962700	-0.78497600
H	-2.60317200	-1.28886700	0.98052600
H	-3.22772000	-0.05465200	-0.11893900
H	0.00123000	1.92860600	-1.47985900
H	-0.01341400	-2.46970300	-1.17234400

NHO 1d-H$^+$

1 1

C	0.00319000	0.53781700	0.00587500
C	-0.69042800	-1.56177400	-0.00236500
C	0.66239700	-1.57337400	-0.00505100
N	1.07372800	-0.26005700	-0.00154500
N	-1.08114100	-0.24140900	0.00357600
C	0.02814100	2.01801500	-0.00612800
C	2.45937900	0.20205800	0.00605400
C	-2.46333600	0.23361200	0.00318900
H	3.10115100	-0.65374800	-0.17951100
H	2.60166200	0.93928200	-0.78065600
H	2.69801700	0.63662600	0.97486300
H	-0.91341300	2.41620400	0.36516500
H	0.83624400	2.38457400	0.62527500
H	-2.63197900	0.87549900	-0.85835800
H	-3.11412500	-0.63322200	-0.05710100
H	-2.66683900	0.77614000	0.92377900
H	0.18688800	2.38513400	-1.02226900
H	-1.40506900	-2.36536600	-0.00494900
H	1.36329100	-2.38899000	-0.00990100

NHO 1e-H$^+$

1 1

C	0.69813100	0.50277600	-0.17582800
C	-0.08198500	-1.53701200	0.16030900
C	1.26607400	-1.58841100	0.26004600
N	1.73198700	-0.31268600	0.04800800
N	-0.41936400	-0.22911000	-0.11711200
C	0.81899800	1.95980800	-0.41814400
C	3.13216200	0.10151000	0.05580300
C	-1.79588800	0.30881800	-0.24575300
H	3.42344200	0.43690300	-0.93752300
H	3.27187500	0.90343600	0.77749100
H	3.73505200	-0.75468700	0.34213800
H	-0.11428700	2.37456600	-0.78859500
H	-1.74703200	1.04802300	-1.04525200
H	1.08495200	2.47283000	0.50839500
H	1.60157400	2.15035200	-1.15273800
H	-0.81629500	-2.31498900	0.25793700
H	1.92989900	-2.41108800	0.45800900
C	-2.76117900	-0.78729200	-0.66219700
H	-2.91612000	-1.51051100	0.13982200
H	-3.72365500	-0.32721100	-0.88188400

H	-2.41633600	-1.30719400	-1.55610400
C	-2.20336800	0.97553600	1.06059300
H	-3.19980400	1.40354900	0.95196500
H	-2.22605400	0.23998000	1.86662600
H	-1.51323400	1.77421300	1.33446500

NHO2a-H$^+$

1 1

C	0.54473300	-0.19338300	-0.03487000
C	-1.66442100	-0.50367000	-0.01757600
C	-1.43167400	0.83387700	0.02632800
N	-0.05368300	1.00027700	0.02261600
N	-0.42091400	-1.11849000	-0.05124300
C	2.01125600	-0.49894700	-0.07548200
C	0.59723800	2.30676100	0.05284400
C	-0.19921200	-2.56255300	-0.09588000
C	-2.94245200	-1.26434100	-0.03058700
C	-2.37024600	1.98627800	0.07364700
H	-3.03217100	-1.90421000	0.84884000
H	-3.78034300	-0.57136300	-0.02835500
H	-3.02184100	-1.88929400	-0.92137900
H	-3.39255300	1.63112200	-0.03051700
H	-2.29357700	2.52254900	1.02130500
H	-2.17061700	2.69019600	-0.73566900
H	-0.01001400	2.97992100	0.65148800
H	1.57455500	2.21898600	0.51299700
H	0.69432000	2.70019900	-0.95785600
H	2.07267400	-1.56176900	-0.31332700
H	0.45183700	-2.86334400	0.72156900
H	-1.15708300	-3.05919900	0.01697500
H	0.23983000	-2.84431700	-1.05079800
C	2.74653700	0.24532400	-1.19651500
H	2.87106300	1.30522100	-0.98016600
H	3.74158300	-0.18624600	-1.30516200
H	2.22467100	0.14351600	-2.14853200
C	2.67031300	-0.30149800	1.29618400
H	2.15808300	-0.87938100	2.06603600
H	3.70600000	-0.63777400	1.24401300
H	2.67332800	0.74559600	1.60036900

NHO 2b-H$^+$

1 1

C	0.01631800	-0.12238200	-0.03531900
C	2.30546200	0.04113500	0.08349200
C	1.69845900	1.43977700	-0.03003500
N	0.26102100	1.17012400	0.11262600
N	1.13622200	-0.82016000	-0.13816800
C	-1.33963600	-0.76388800	-0.06164200
C	-0.66920900	2.28438400	0.05999100
C	1.27318900	-2.26999500	-0.10480900
H	-0.75532500	2.66311000	-0.96036500
H	-1.64578000	1.98989800	0.42554200
H	-0.28307000	3.07341500	0.70308200
H	-1.15962700	-1.82308000	-0.23868700
H	0.62489300	-2.73530300	-0.84285800
H	2.30337300	-2.50607800	-0.36008900
H	1.05403000	-2.66361300	0.88864100
H	3.06915900	-0.15530700	-0.66525100
H	1.88022100	1.89549700	-1.00588100
H	2.71313300	-0.15731900	1.07691800
H	2.03381200	2.11812300	0.75129200
C	-2.20884700	-0.25874500	-1.21959500
H	-3.08000200	-0.90874900	-1.30072800
H	-2.56746700	0.75700100	-1.06458700
H	-1.66749300	-0.29661900	-2.16549300
C	-2.02366100	-0.65020700	1.30736700
H	-2.26885500	0.37948900	1.56396900
H	-2.95180600	-1.22077400	1.28016500
H	-1.39235300	-1.05991400	2.09641700

NHO 2c-H$^+$

1 1

C	1.26369500	1.45414200	0.10581100
C	-0.02733600	2.06358100	-0.38399800
C	-1.17669100	1.38543000	0.32362700
H	-0.03790700	3.13189200	-0.17568500
H	1.45661000	1.71098200	1.15073700
H	2.11086800	1.79428600	-0.48952900
H	-1.18812900	1.62522700	1.39007200
H	-2.13093100	1.68965400	-0.10432100
C	0.07967100	-0.68672300	-0.04822200
C	0.04351200	-2.17740000	-0.34589600
H	-0.97169500	-2.36141700	-0.68779600
N	-1.07934100	-0.07217100	0.16408700
N	1.21921800	-0.01012700	-0.01724100
C	2.54703600	-0.62352200	-0.03902700
H	3.18707200	-0.02505000	0.60748000
H	2.52535900	-1.63137000	0.35287400
H	2.95918600	-0.62054500	-1.04845900
C	-2.36193500	-0.77544700	0.27326800
H	-2.81396000	-0.92147500	-0.70875400
H	-2.25618100	-1.72816500	0.78175000
H	-3.01862600	-0.15086000	0.87426700
H	-0.12110000	1.92331600	-1.46263500
C	0.93568600	-2.62276300	-1.51429700

H	1.95108000	-2.86598600	-1.21128200
H	0.50043200	-3.52644900	-1.94057900
H	0.97635400	-1.86789500	-2.30091400
C	0.25368500	-3.01737200	0.92066800
H	1.26412000	-2.91956600	1.31650500
H	-0.44264800	-2.73647100	1.71176000
H	0.08907900	-4.06703800	0.67668400

NHO-Alcohol adducts (anionic mechanism):

NHO 1a-EtOH adduct

0 1

C	-0.49598300	-0.00005000	0.93694600
C	1.42842400	-0.66844800	-0.16888600
C	1.42845500	0.66854200	-0.16873600
N	0.39567200	1.12285600	0.69956200
N	0.39583300	-1.12289000	0.69962100
C	-0.19849900	2.43468700	0.53150800
C	-0.19826500	-2.43474900	0.53138100
H	-0.79873800	2.53890900	-0.37972500
H	-0.83858300	2.65202700	1.38622100
H	0.59174900	3.18458600	0.51322700
H	-0.79824000	-2.53896900	-0.38001900
H	0.59203300	-3.18460400	0.51333000
H	-0.83856500	-2.65210500	1.38592600
C	-1.09282500	-0.00011100	2.33271300
H	-1.71889600	-0.88081600	2.47378300
O	-1.64012700	-0.00017600	0.07104300
C	-1.40110800	0.00006000	-1.33051100
H	-0.81577100	-0.87732100	-1.61987100
H	-0.81594900	0.87764700	-1.61960400
C	-2.74750400	0.00004900	-2.02196600
H	-3.32014600	0.88553400	-1.74218800
H	-2.61540600	0.00027200	-3.10463300
H	-3.31996900	-0.88565600	-1.74252800
H	-0.29255300	0.00023100	3.06930200
H	-1.71955400	0.88014700	2.47364000
C	2.35979700	-1.63945600	-0.80281100
H	3.12361300	-1.11617000	-1.37544100
H	2.86075200	-2.25570300	-0.04999000
H	1.83333600	-2.31718300	-1.48088700
C	2.35978200	1.63965600	-0.80258900
H	1.83330700	2.31744300	-1.48058500
H	2.86072300	2.25581600	-0.04968500
H	3.12369200	1.11647200	-1.37519800

NHO 1a-MeOH adduct

0 1

C	-1.00215600	0.00015000	-0.35151800
C	1.21401300	-0.66861200	-0.20053000
C	1.21418500	0.66837200	-0.20051500
N	-0.09541500	1.12181200	-0.52295800
N	-0.09565300	-1.12171700	-0.52310000
C	-0.55413700	2.43729600	-0.12238200
C	-0.55469800	-2.43710900	-0.12256900
H	0.15457400	3.18598700	-0.47515800
H	-1.51278300	2.64261200	-0.59777200
H	-0.67786800	2.55726900	0.96002500
H	-1.51345200	-2.64209800	-0.59787100
C	-2.14993900	0.00031600	-1.34499800
H	-2.77518200	-0.87964700	-1.19630900
H	-2.77472100	0.88065600	-1.19662200
H	-1.75467200	0.00002400	-2.35822800
O	-1.65674000	0.00006700	0.92844700
C	-0.81642700	-0.00001700	2.06843600
H	-0.17458400	-0.88290200	2.10126100
H	-0.17364500	0.88216700	2.10083600
C	2.32933400	1.64066600	-0.04757700
H	2.45044500	2.24709200	-0.95040200
H	3.26664400	1.11957800	0.13934500
H	2.15229200	2.32763200	0.78475700
C	2.32889500	-1.64119700	-0.04751300
H	3.26640500	-1.12036100	0.13911000
H	2.44967500	-2.24789000	-0.95020100
H	2.15177400	-2.32789800	0.78502400
H	0.15374200	-3.18598000	-0.47551100
H	-0.67830700	-2.55713800	0.95984300
H	-1.47335600	0.00051300	2.93770300

NHO 1b-EtOH adduct

0 1

O	1.05690800	-0.61188300	0.54778900
C	1.68428000	-0.69612300	-0.72531100
H	1.41904400	0.16867400	-1.33804000
C	-0.26796400	-0.09990200	0.56785000
C	-1.92124500	0.31348100	-1.06491800
C	-1.00363800	1.52154600	-1.02262400
N	-0.35738600	1.33050600	0.26514600
N	-1.07586100	-0.71106200	-0.47715300
C	-0.74188300	-0.34832100	1.99469200
C	0.80519500	2.14405900	0.54118900
C	-1.73526700	-1.95791500	-0.15579400
H	1.62419500	1.99553900	-0.17623100
H	1.18539600	1.92315700	1.53892900

H	0.51616800	3.19641100	0.51363700
H	-0.62059400	-1.39395300	2.27699800
H	-1.79037900	-0.06348300	2.08528100
H	-1.00868000	-2.66719400	0.24332800
H	-2.15375800	-2.38222500	-1.06977300
H	-2.54999100	-1.84085100	0.57292000
H	-0.15352300	0.26687300	2.67644900
H	-2.22140100	0.03244100	-2.07554700
H	-0.29657000	1.50446900	-1.86529000
H	-2.82734200	0.49822800	-0.46643500
H	-1.54617400	2.46834700	-1.04670500
H	1.33340900	-1.58796700	-1.25127600
C	3.18020100	-0.75272300	-0.49948700
H	3.44037500	-1.61125500	0.12141400
H	3.70273300	-0.84602700	-1.45254500
H	3.52648200	0.15316300	0.00105600

NHO 1b-MeOH adduct

0 1

O	0.42718200	-1.56882400	-0.16269700
C	0.60035600	-1.54892900	-1.56843700
H	1.12842600	-0.65321100	-1.90146200
H	1.19720400	-2.42563900	-1.81782500
C	-0.03290200	-0.35593100	0.42422600
C	-0.94180600	1.64717400	-0.43620500
C	0.57035600	1.75536300	-0.50804400
N	0.96238400	0.71591500	0.42894200
N	-1.12387400	0.20851800	-0.35264300
C	-0.37687700	-0.74350000	1.85671000
C	2.35633100	0.33375200	0.44507200
C	-2.46370900	-0.23722200	-0.04001700
H	2.71474300	-0.06403700	-0.51390100
H	2.52326500	-0.42568800	1.20928500
H	2.95960200	1.20741800	0.69842200
H	-1.06440800	-1.58852100	1.88380600
H	-0.82447500	0.11005600	2.36619500
H	-2.50109200	-1.32743700	-0.04462100
H	-3.14562900	0.12567400	-0.81075600
H	-2.82445500	0.12387700	0.93367100
H	0.53699100	-1.02260800	2.38224000
H	-1.44802400	2.05025600	-1.31473100
H	0.92749400	1.56956500	-1.53167100
H	-1.32142400	2.16486100	0.45871100
H	0.94300400	2.72834600	-0.18299600
H	-0.35874300	-1.59760100	-2.08671100

NHO 1c-EtOH adduct

0 1

C	-1.83194200	1.33473600	-0.38292900
C	-2.39654800	0.13942500	-1.12488700
C	-1.98155000	-1.13064100	-0.40888800
H	-3.48505600	0.20610800	-1.17299100
H	-2.34054800	1.44755900	0.59000400
H	-2.01381500	2.25616000	-0.94062000
H	-2.49963500	-1.20056000	0.56282700
H	-2.27307000	-2.01149200	-0.98524000
C	0.02621100	-0.02580700	0.48147000
N	-0.53314400	-1.17381700	-0.24395800
N	-0.38945900	1.19822200	-0.21842200
C	0.17370900	2.40968900	0.36144300
H	1.23786300	2.27448800	0.54772600
H	0.04670000	3.22617800	-0.35116100
H	-0.31524700	2.70308800	1.30160000
C	-0.12426800	-2.45632300	0.31221800
H	0.94376900	-2.44951100	0.52396800
H	-0.66290900	-2.71480500	1.23509000
H	-0.32803300	-3.23550100	-0.42422400
H	-2.00704100	0.12657700	-2.14521200
O	1.43308300	-0.11061300	0.45013300
C	2.04121300	-0.19590800	-0.83481900
H	1.84925300	-1.18053000	-1.27084400
H	1.60996200	0.55657300	-1.49793700
C	-0.31531700	-0.01850000	1.97474100
H	0.17845000	0.81921500	2.46518600
H	0.03809100	-0.93632700	2.44234900
H	-1.39010100	0.06642700	2.13548300
C	3.52595200	0.02808100	-0.64334400
H	4.04391500	-0.04970500	-1.60017300
H	3.71368600	1.01883600	-0.22632800
H	3.94257500	-0.71721800	0.03606100

NHO 1c-MeOH adduct

0 1

C	2.02518100	-0.31253200	-0.14488800
C	1.97948100	1.07758200	-0.74787600
C	0.84550200	1.85607000	-0.11130100
H	2.92871200	1.59067300	-0.58336200
H	2.35288700	-0.25524300	0.90765200
H	2.75515100	-0.93502600	-0.66724600
H	1.08295300	2.06988600	0.94509000
H	0.71318000	2.82123700	-0.60538700
C	-0.38523800	-0.22408100	0.34498000
N	-0.40877100	1.12313700	-0.23715700
N	0.72700300	-0.96462500	-0.26547200
C	0.80926800	-2.34776500	0.18219900

H	-0.17666400	-2.80833300	0.15496800
H	1.46602100	-2.89404700	-0.49676900
H	1.21808300	-2.44686200	1.19813200
C	-1.52117300	1.93372300	0.23921500
H	-2.43868400	1.34758900	0.23997000
H	-1.35958100	2.33231900	1.25091800
H	-1.64889400	2.77979500	-0.43811000
H	1.81030200	1.00207600	-1.82430600
O	-1.59329800	-0.87744100	0.01874300
C	-1.91498200	-0.93548400	-1.36231500
H	-2.71285600	-1.67060200	-1.45688200
H	-2.26691700	0.03209000	-1.72642600
H	-1.05381000	-1.24779500	-1.95363100
C	-0.35364200	-0.23077300	1.87577500
H	-0.40264300	-1.25351200	2.24639700
H	-1.21232000	0.31070300	2.27002500
H	0.55746700	0.23455900	2.25270000

NHO 1d-EtOH adduct

0 1

C	0.45101300	0.00056100	0.62058000
C	1.26486400	-0.66479000	-1.44026200
C	1.26224800	0.66939400	-1.44018700
N	0.98541300	1.12486800	-0.13491900
N	0.98994200	-1.12146300	-0.13497300
C	0.44646900	2.44783800	0.10146200
C	0.45582400	-2.44650500	0.10100500
H	-0.61240300	2.54602100	-0.16208700
H	0.56364800	2.70921700	1.15316100
H	1.01947300	3.16483400	-0.48623900
H	-0.60266100	-2.54842500	-0.16263800
H	1.03151300	-3.16114200	-0.48693800
H	0.57386100	-2.70775000	1.15264900
C	0.88139400	0.00133800	2.07597500
H	0.48925700	-0.88083100	2.58160900
O	-0.97988100	-0.00225500	0.68229200
C	-1.68297700	-0.00300500	-0.55412600
H	-1.41094000	-0.88041600	-1.14724800
H	-1.41279500	0.87499900	-1.14719200
C	-3.16305900	-0.00457500	-0.23837100
H	-3.43057200	0.88091600	0.33992500
H	-3.74528500	-0.00522500	-1.16062400
H	-3.42879900	-0.89050600	0.34005800
H	1.96738700	0.00400300	2.13510500
H	0.48480600	0.88127600	2.58203400
H	1.51790200	-1.35437800	-2.22863100
H	1.51251700	1.36007600	-2.22849200

NHO 1d-MeOH adduct

0 1

C	0.00000400	-0.51339600	-0.32805300
C	-0.66711200	1.70262700	-0.28783900
C	0.66716400	1.70261600	-0.28800600
N	1.12228300	0.39050100	-0.52951200
N	-1.12229000	0.39050100	-0.52935100
C	2.44833700	-0.03337300	-0.13160900
C	-2.44837200	-0.03332700	-0.13155300
H	3.16545500	0.71897900	-0.45981800
H	2.56026000	-0.17596600	0.94866100
H	2.69761800	-0.97076400	-0.62868800
H	-2.56000200	-0.17738500	0.94853400
H	-3.16527800	0.71978800	-0.45849600
H	-2.69830300	-0.96990000	-0.62988000
C	-0.00012000	-1.69147500	-1.28485200
H	-0.88093300	-2.31011300	-1.11430800
O	0.00015100	-1.12372200	0.96968900
C	0.00001500	-0.24303400	2.07952600
H	-0.88271000	0.39951100	2.08783700
H	0.88283700	0.39939700	2.08812900
H	-0.00056900	-1.32916400	-2.31030100
H	0.88108600	-2.30975200	-1.11500500
H	-1.35833600	2.52639400	-0.21957900
H	1.35837300	2.52638700	-0.21959600
H	-0.00015500	-0.86847500	2.97136100

NHO 1e-EtOH adduct

0 1

C	-0.36340400	-0.55246900	0.54771000
C	0.55030300	-0.79234400	-1.57146800
C	-0.68082900	-1.30395900	-1.62621900
N	-1.21110100	-1.36336900	-0.31915700
N	0.85681700	-0.47622200	-0.23911600
C	-2.64437200	-1.32739200	-0.10904000
C	1.96512900	0.37220100	0.19690500
H	-3.10696100	-2.08060200	-0.74701000
H	-2.87064900	-1.58018900	0.92684500
H	-3.09599800	-0.35410700	-0.33203800
H	1.54468000	1.10687900	0.89280400
C	-0.17145200	-1.16691700	1.92412000
H	0.45647300	-0.51889700	2.53648000
H	-1.13684600	-1.26901600	2.42049800
H	0.29356100	-2.14597100	1.82833000
O	-0.93379500	0.73094800	0.83522200
C	-1.12189900	1.60406200	-0.26995900
H	-0.15045800	1.90501800	-0.67421800

H	-1.66412300	1.09526000	-1.07091400
H	1.27443200	-0.68802600	-2.36062800
H	-1.21763000	-1.71819100	-2.46335000
C	-1.89423500	2.80939400	0.22101600
H	-1.35201000	3.30943200	1.02479100
H	-2.04192400	3.52144400	-0.59186100
H	-2.87211700	2.50683300	0.59884100
C	2.60607300	1.12791800	-0.96359800
H	3.33981600	1.83315600	-0.57240300
H	3.13104000	0.44122200	-1.63160400
H	1.87177100	1.68288400	-1.54824300
C	3.02959700	-0.44696700	0.92936300
H	3.82707700	0.20301000	1.29580700
H	2.60514000	-0.98399100	1.77694500
H	3.46561300	-1.17775400	0.24408600

NHO 1e-MeOH adduct

0 1

C	-0.58161000	0.59295400	-0.08416400
C	0.21166600	-1.19971600	1.15531600
C	-1.10939100	-1.16027100	1.34089300
N	-1.61495800	0.02778800	0.77207500
N	0.60601300	-0.05893700	0.43880700
C	-2.99666500	0.11340600	0.34608500
C	1.90170800	0.12910900	-0.21277200
H	-3.63406900	-0.21144700	1.16867500
H	-3.24626800	1.14962800	0.11871300
H	-3.22423500	-0.49670900	-0.53481500
H	1.69369600	0.47762600	-1.23041800
C	-0.52945800	2.11007000	-0.02965900
H	0.25620900	2.47867600	-0.69003600
H	-1.47821700	2.52522300	-0.37048300
H	-0.33449600	2.43523700	0.99011400
O	-0.80656900	0.32021900	-1.47687100
C	-0.79968700	-1.04526300	-1.84798700
H	-1.02364700	-1.08112000	-2.91334100
H	0.17768800	-1.50081300	-1.67254800
H	-1.55042900	-1.61883100	-1.30035500
H	0.92654600	-1.90993700	1.53302500
H	-1.74667500	-1.82450100	1.90051100
C	2.73069200	1.18929000	0.51431500
H	3.67724200	1.35786400	-0.00354300
H	2.19723000	2.13717600	0.57675200
H	2.94749100	0.85089300	1.53035300
C	2.69676000	-1.16961800	-0.30927500
H	3.59730400	-0.99509300	-0.89863700
H	3.01071000	-1.50866900	0.68039600
H	2.12501600	-1.96867300	-0.78208200

NHO 2a-EtOH adduct

0 1

C	-0.56548800	-0.18048800	-0.21102700
C	1.75341500	-0.30714600	-0.43111900
C	1.48071600	-0.50280600	0.86307100
N	0.07172400	-0.60306100	1.03083200
N	0.53623500	-0.28971700	-1.15491300
C	-0.53947500	-0.24343100	2.30387100
C	0.41409400	0.38538100	-2.42945200
C	3.05587000	-0.25164800	-1.14869700
C	2.39539900	-0.75466200	2.01079500
H	3.19249000	0.70443100	-1.66189500
H	3.88091600	-0.37604800	-0.44961900
H	3.12477700	-1.03996800	-1.90459400
H	3.42625600	-0.81881400	1.66638900
H	2.34633400	0.03561000	2.76412400
H	2.14288100	-1.69530900	2.50924400
H	0.14637400	0.34341100	2.91742600
H	-1.42653000	0.36475800	2.13141300
H	-0.83403400	-1.12878100	2.87203400
H	0.37844500	1.47882400	-2.35209700
H	1.25861300	0.10941800	-3.05983100
H	-0.49437400	0.05168700	-2.93205600
C	-1.76991400	-1.04451300	-0.63678000
H	-2.13559200	-0.59869500	-1.56722300
O	-1.09202800	1.14841400	-0.14660700
C	-0.18647700	2.16663700	0.25775400
H	0.71464400	2.14473900	-0.36093100
H	0.12949000	2.00219900	1.29284100
C	-2.91739300	-1.01383100	0.37198200
H	-3.20476600	0.00508500	0.63083900
H	-3.78777000	-1.51740200	-0.05244100
H	-2.64488000	-1.54504500	1.28640800
C	-1.34928800	-2.48330400	-0.91145300
H	-2.21824100	-3.07740700	-1.20124100
H	-0.60655600	-2.53930900	-1.70673400
H	-0.91770200	-2.92488900	-0.00986000
C	-0.89833300	3.49554100	0.12195400
H	-1.79556400	3.51333700	0.74234600
H	-0.24329400	4.30887200	0.43682900
H	-1.19015300	3.66704900	-0.91534500

NHO 2a-MeOH adduct

0 1

C	0.61544400	-0.22534500	0.18788600
C	-1.64398400	-0.34829500	-0.38207200

C	-1.32243100	0.94917900	-0.37312200
N	0.08351800	1.07777800	-0.19215100
N	-0.46161800	-1.10943700	-0.22311300
C	0.62913400	2.27961200	0.42678600
C	-0.47726100	-2.46468600	0.28241100
C	-2.94186800	-1.02356700	-0.65293800
C	-2.15717500	2.14947800	-0.65563300
H	-3.25383700	-1.64693800	0.18972000
H	-3.72364100	-0.28765000	-0.83203000
H	-2.87401000	-1.67293200	-1.53115400
H	-3.16474100	1.85172600	-0.94127800
H	-2.24037600	2.81274300	0.20896900
H	-1.72875900	2.73486900	-1.47470000
H	-0.14592400	2.83399100	0.95898800
H	1.39457900	2.00851800	1.15218700
H	1.07681300	2.94507600	-0.31482100
H	-0.65596700	-2.53622000	1.36194300
H	-1.25303800	-3.02829000	-0.23471300
H	0.47768600	-2.94446400	0.06521200
C	1.95104800	-0.59458000	-0.48921100
H	2.22833500	-1.57105000	-0.07979500
O	0.89438700	-0.32809500	1.58966000
C	-0.18400000	-0.01696600	2.45276100
H	-1.06165900	-0.63251200	2.24428100
H	0.16136700	-0.21328000	3.46714600
H	-0.47653300	1.03303200	2.37180200
C	3.08029300	0.38105800	-0.16034200
H	3.19182800	0.52889100	0.91367700
H	4.02197300	-0.00897100	-0.55085500
H	2.90641000	1.35060100	-0.63230300
C	1.78793000	-0.72075900	-1.99933900
H	2.74912000	-0.95517400	-2.46087300
H	1.07486100	-1.50169200	-2.26203400
H	1.42880500	0.22322800	-2.41668300

NHO 2b-EtOH adduct

0 1

O	1.10224000	0.43098500	-0.69323000
C	2.12760900	-0.54264900	-0.54290000
H	2.04346600	-1.03759400	0.42717900
C	-0.16573700	0.09912900	-0.14750300
C	-1.14214700	-1.90725300	0.66741500
C	-0.41108900	-1.23883100	1.82053600
N	-0.19794000	0.11256400	1.31981100
N	-0.50476300	-1.27448100	-0.46753600
C	-1.12296700	1.15986100	-0.73928200
C	0.83310700	0.85602300	2.01658100
C	-0.97050800	-1.59817900	-1.79402800
H	1.78643800	0.31179500	2.07929700
H	1.01961700	1.80494200	1.51967000
H	0.49803500	1.06116400	3.03587700
H	-1.05710000	1.05040200	-1.82677000
H	-0.32588900	-1.11490800	-2.53064100
H	-0.89370100	-2.67769900	-1.94021200
H	-2.00880400	-1.30215400	-1.99490100
H	-0.98595200	-2.98781400	0.64236100
H	0.54020600	-1.75491000	2.02112200
H	-2.22333500	-1.71488200	0.72004900
H	-0.99451600	-1.22601800	2.74346300
H	2.01785200	-1.31505100	-1.30955200
C	-0.71026000	2.58688000	-0.38004700
H	-1.33906600	3.29869500	-0.91875800
H	-0.85282500	2.76487900	0.68849700
H	0.33044800	2.78627600	-0.63384900
C	-2.56814300	0.92931900	-0.30434700
H	-3.21133100	1.69653800	-0.74024600
H	-2.95352200	-0.04131400	-0.61429800
H	-2.64679100	0.99514800	0.78267200
C	3.45917200	0.16551600	-0.67220700
H	4.27784000	-0.55107600	-0.59122600
H	3.53381300	0.66586400	-1.63895100
H	3.57190200	0.91434900	0.11382300

NHO 2b-MeOH adduct

0 1

O	-0.05525000	-0.83343600	-1.43243800
C	-1.37676600	-1.22965700	-1.75423200
H	-1.93513300	-1.54318900	-0.87093400
H	-1.28929200	-2.07143300	-2.44081200
C	0.08394400	-0.04526300	-0.25724800
C	-1.44666700	1.10034900	1.15200600
C	-1.32585400	-0.32911900	1.65404400
N	-0.12084200	-0.79811100	0.98414700
N	-0.95934400	0.95892100	-0.20378800
C	1.52206000	0.51537600	-0.34496100
C	0.02863900	-2.23940700	0.94870200
C	-0.85577600	2.13549500	-1.03194500
H	-0.87139700	-2.75360200	0.58279400
H	0.86069900	-2.51988900	0.30772100
H	0.23318500	-2.60417600	1.95802700
H	1.56674200	1.08421900	-1.27935000
H	-0.55977800	1.84154800	-2.04056300
H	-1.83795800	2.60849700	-1.09729300
H	-0.14209100	2.88539400	-0.66586100
H	-2.47749300	1.46061900	1.15406900
H	-2.21039000	-0.91432800	1.36064900

H	-0.83865600	1.78510400	1.76021100
H	-1.21892100	-0.39101300	2.73910200
H	-1.92650400	-0.41932500	-2.23759800
C	2.57815400	-0.58702400	-0.40981000
H	3.56031700	-0.14546700	-0.59082500
H	2.62927300	-1.12097000	0.54213100
H	2.37152200	-1.30399400	-1.20378400
C	1.84042000	1.44932400	0.82032600
H	2.86378300	1.81860900	0.72732800
H	1.17994400	2.31480000	0.86481800
H	1.75653200	0.90996600	1.76586600

NHO 2c-EtOH adduct

0 1

C	-0.72185000	-1.22640300	1.72822700
C	-2.05299900	-1.44454100	1.04238300
C	-1.82910400	-1.53505200	-0.46210900
H	-2.53321600	-2.35455400	1.40383500
H	-0.05018100	-2.08042100	1.54384300
H	-0.86079800	-1.15306900	2.80952600
H	-1.73914200	-2.58666500	-0.75774100
H	-2.70003000	-1.13856200	-1.00282200
C	0.00206800	0.23766700	-0.16273200
N	-0.59315500	-0.88387300	-0.88707600
N	-0.15743600	0.03896900	1.28139500
C	0.96081100	0.44945600	2.11950000
H	1.45116000	1.32821200	1.71515900
H	0.58207000	0.69056000	3.11561700
H	1.72102800	-0.33651200	2.23217300
C	-0.54005700	-0.76893900	-2.33108500
H	0.41682100	-0.35413200	-2.64468300
H	-0.64313500	-1.76638800	-2.76605500
H	-1.34582200	-0.14117200	-2.74107400
H	-2.70371500	-0.60304000	1.28513100
C	-0.54897100	1.62122400	-0.60217500
H	-0.30694500	1.70585500	-1.66570500
C	-2.06262400	1.70943300	-0.44135200
H	-2.41176600	2.69083100	-0.76851100
H	-2.59035700	0.95893000	-1.03005200
H	-2.34067200	1.58647000	0.60732300
C	0.10750500	2.80065400	0.11308600
H	-0.25320400	3.73537400	-0.32154300
H	-0.15718100	2.80564400	1.17304800
H	1.19332900	2.77951200	0.02036600
O	1.37482200	0.29916300	-0.53698000
C	2.10749300	-0.91597800	-0.45168700
H	1.78543500	-1.49657200	0.41508200
H	1.91639600	-1.52661300	-1.33958600
C	3.57591200	-0.56159400	-0.34815500
H	4.18347000	-1.46728800	-0.32064500
H	3.88481700	0.03394900	-1.20871700
H	3.76809600	0.01512000	0.55823300

NHO 2c-MeOH adduct

0 1

C	-1.12053100	1.37461700	-1.24557800
C	-2.07857200	0.21335800	-1.40269600
C	-2.19518800	-0.51939400	-0.07279300
H	-3.06125400	0.55863600	-1.72573200
H	-1.50541600	2.09251800	-0.50314500
H	-1.02007900	1.91234500	-2.19134700
H	-3.05608600	-0.13372000	0.48549500
H	-2.39202600	-1.58749100	-0.24132900
C	0.30209900	-0.02585200	0.25854800
N	-1.02810600	-0.32196700	0.78262300
N	0.19734400	0.86024900	-0.90346800
C	1.22184800	1.88812200	-1.02864900
H	2.18512300	1.52533300	-0.68684100
H	1.31018300	2.16640900	-2.08139700
H	0.98462700	2.79812600	-0.46048300
C	-1.04931300	-1.23773600	1.90613900
H	-0.22058500	-1.03030700	2.58149200
H	-1.98482000	-1.09744600	2.45363700
H	-0.99669200	-2.29334400	1.59926200
H	-1.68615900	-0.45105100	-2.17426700
C	1.13066900	-1.29426400	-0.07662300
H	1.21123500	-1.84522700	0.86491700
C	0.42272100	-2.17796400	-1.09771900
H	1.01813200	-3.07299300	-1.28902600
H	-0.56157900	-2.50154900	-0.75846500
H	0.30549600	-1.64370900	-2.04279300
C	2.55002100	-0.99858300	-0.55755700
H	3.09996700	-1.93626000	-0.66271000
H	2.53422300	-0.51456600	-1.53681600
H	3.09316300	-0.36293500	0.14171400
O	1.04306100	0.58068100	1.31542700
C	0.39730900	1.64628900	1.98877600
H	1.18232200	2.24367800	2.45284600
H	-0.17459500	2.27378000	1.30505100
H	-0.28071900	1.27478800	2.76135000

Anionic mechanism, transition states:

NHO 1a, TS1 (v = -952.24i (cm^{-1}))

0 1

C	2.29905000	0.88525600	1.60649500
H	1.58959400	1.42984400	0.97754000
H	3.23902800	1.44224800	1.61273000
H	1.90431500	0.86057600	2.62686600
C	2.52572400	-0.52486800	1.05515600
H	3.19501600	-1.05763000	1.75565800
H	1.55487300	-1.06754800	1.12423700
O	3.01084000	-0.53401700	-0.23587100
C	-0.09762000	-0.67169600	-0.90899300
C	-1.15863800	1.10545100	-0.05546900
C	-1.71267000	-0.00354000	0.49186700
N	-1.05241800	-1.09817500	-0.06621400
N	-0.16017300	0.66777600	-0.92202600
C	0.92661500	-1.45266100	-1.57286800
C	-1.25506600	-2.49027100	0.29443400
C	0.74808500	1.49872800	-1.69884800
C	-1.45805200	2.54798200	0.14656800
C	-2.81673700	-0.15580800	1.47687900
H	-1.69608600	3.03960000	-0.79842500
H	-2.31222200	2.65837000	0.81110800
H	-0.61063000	3.06983900	0.59694300
H	-3.16291500	0.82542800	1.79422000
H	-3.66581200	-0.69066500	1.04616300
H	-2.48674300	-0.69975100	2.36397600
H	-2.20912800	-2.58814000	0.80398800
H	-1.27145700	-3.10273800	-0.60433400
H	-0.45466800	-2.82967600	0.95365200
H	1.04908500	-1.14212500	-2.61116800
H	0.73219200	-2.51988700	-1.51552400
H	0.68971200	2.51990800	-1.33194200
H	1.76100000	1.11907800	-1.55910800
H	0.47150700	1.47850500	-2.75319600
H	1.98301100	-1.10879700	-0.98503300

NHO1a, TS2 (v = -230.57i (cm^{-1}))

0 1

C	0.14618400	1.35675900	1.98345300
C	-0.93954600	1.06724000	1.16450400
C	-1.14125300	-0.22665800	0.69556500
C	-0.24028500	-1.22583700	1.06028100
C	0.85044900	-0.93654300	1.87337600
C	1.04825200	0.35883300	2.33579200
H	0.28420300	2.36559900	2.35533300
H	-1.65099900	1.83281500	0.88685000
H	-0.40128200	-2.23856000	0.70491400
H	1.54189800	-1.72361200	2.15321900
H	1.89662300	0.58870200	2.96991500
C	-2.22428700	-0.56808500	-0.31476300
O	-1.97560100	-0.35759500	-1.51725000
O	-3.53352400	0.63471700	0.27009200
C	-4.62446600	0.48027700	-0.56937800
H	-5.22905200	-0.40559300	-0.29697300
H	-4.29483400	0.31752600	-1.60844000
C	-3.39592100	-2.00304700	1.22442400
H	-2.64603800	-1.85314200	2.00459300
H	-3.72884100	-3.03991300	1.24835100
O	-2.86033800	-1.78505500	-0.06937400
C	1.90293700	-0.55082900	-1.26552800
C	2.78362600	1.28091000	-0.36746900
C	3.58118000	0.23402900	-0.03130400
N	3.01694700	-0.89243700	-0.61246900
N	1.74418800	0.76513500	-1.12766900
C	1.03914400	-1.47283400	-2.03788600
C	3.51207900	-2.25755600	-0.49205200
C	0.67703100	1.55906700	-1.72952900
C	2.86857800	2.72419100	-0.02763000
C	4.79764800	0.17401900	0.82123400
H	2.87277900	3.34163200	-0.92752900
H	3.78302200	2.92316700	0.52669300
H	2.01969000	3.02622200	0.58965100
H	5.03202100	1.16882800	1.19350400
H	5.66309900	-0.19230300	0.26621500
H	4.63844700	-0.48008000	1.68121200
H	4.50702400	-2.23016300	-0.05895700
H	3.56581600	-2.71761300	-1.47617500
H	2.85328800	-2.83812300	0.15318400
H	-0.00074600	-1.14268500	-1.99473300
H	1.10309800	-2.47712900	-1.62175500
H	1.00836800	1.94793200	-2.69209400
H	0.44388400	2.38257700	-1.05901200
H	-0.21400700	0.94115500	-1.83860700
H	1.36535800	-1.50798100	-3.08040500
H	-4.23425200	-1.33169800	1.40721300
C	-5.52500000	1.71047700	-0.52768000
H	-4.96887800	2.59656400	-0.84211400
H	-5.89304000	1.88351000	0.48623200
H	-6.38699600	1.59045800	-1.18953200

NHO1a, TS3 (v = -194.66i (cm^{-1}))

0 1

C	-1.66462800	1.29028700	0.24994900
C	-2.91723700	-0.37376900	1.02274600
C	-3.53077700	0.12416300	-0.08242200
N	-2.73656800	1.16834000	-0.53740500
N	-1.75832000	0.36508200	1.20396400
C	-0.57412700	2.28149400	0.11130300

C	-2.97307800	1.95052800	-1.74417500
C	-0.80484800	0.19310100	2.29680300
C	-3.27501600	-1.51091300	1.90917900
C	-4.76942700	-0.30449500	-0.78425200
H	-3.32127100	-1.20047200	2.95427900
H	-4.24679200	-1.91087300	1.62761500
H	-2.53585500	-2.31107600	1.82107800
H	-5.21144300	-1.15086700	-0.26341300
H	-5.51065800	0.49605000	-0.81803000
H	-4.55221000	-0.61358000	-1.80902400
H	-4.00898100	1.82599400	-2.04396200
H	-2.78985200	3.00267000	-1.54262900
H	-2.31924600	1.60604700	-2.54547000
H	0.19883900	0.45409600	1.94804800
H	-1.10604000	0.80863000	3.14463500
H	-0.80632400	-0.85484600	2.58736000
C	-0.92203900	-1.27927900	-1.74521300
C	0.19024200	-0.44989700	-1.62711800
C	1.15098100	-0.69328500	-0.65256200
C	0.99122500	-1.77943500	0.20388800
C	-0.11986000	-2.60392700	0.09412300
C	-1.08095000	-2.35606000	-0.88299200
H	-1.66473300	-1.08572800	-2.51185500
H	0.33039400	0.39539300	-2.29184800
H	1.74149100	-1.96017300	0.96277200
H	-0.23778600	-3.44427900	0.76870900
H	-1.95076500	-2.99770200	-0.96706000
C	2.36490400	0.20931300	-0.56188900
O	2.42750100	1.25469500	-1.22478800
O	3.48716400	-0.60582200	-0.43571000
C	4.71012600	0.09994000	-0.29852400
H	4.63645200	0.77172600	0.56130200
H	4.89097100	0.70641800	-1.18925100
C	2.47388700	1.97229700	1.50972500
H	3.43294000	2.06689900	2.04594900
H	1.70603200	2.45860100	2.13739500
O	2.14311600	0.65771200	1.23289900
H	2.55951500	2.56822100	0.58612100
C	5.81300500	-0.91774400	-0.09970500
H	5.87117100	-1.59232500	-0.95537200
H	5.62973700	-1.51216400	0.79666100
H	6.77535800	-0.41555600	0.00920800
H	0.39105400	1.78592700	0.23126500
H	-0.60185700	2.74174300	-0.87364900
H	-0.67247000	3.06067400	0.87086400

NHO 1a, TS4 (v = -1008.07i (cm^{-1}))

0 1

C	2.50149500	-0.27017500	0.90053300
H	3.20919200	-0.41896300	1.73234500
H	1.60661500	-0.87679300	1.15834800
O	3.03323500	-0.60613100	-0.32915300
C	-0.10612500	-0.72994700	-0.88998100
C	-1.11381700	1.05777200	0.00348300
C	-1.71529400	-0.04599500	0.50995200
N	-1.08567400	-1.14657100	-0.07096200
N	-0.12119000	0.61086600	-0.86418500
C	0.89506800	-1.52985000	-1.56780700
C	-1.35410800	-2.54071400	0.23653000
C	0.83581900	1.43415600	-1.59002900
C	-1.36771100	2.50321400	0.24314700
C	-2.83927600	-0.18806900	1.47368500
H	-1.58465800	3.02710500	-0.68952500
H	-2.22199000	2.62319600	0.90590200
H	-0.50683100	2.98544800	0.71107000
H	-3.15787700	0.79500600	1.81342100
H	-3.69867600	-0.68163200	1.01520300
H	-2.54193300	-0.76781800	2.34956500
H	-2.32655300	-2.61586000	0.71448200
H	-1.36805100	-3.12163600	-0.68289800
H	-0.58984600	-2.93539800	0.90700500
H	1.01464000	-1.21263100	-2.60491700
H	0.67528700	-2.59240000	-1.51905600
H	0.80166700	2.44389300	-1.19086300
H	1.83205400	1.01167100	-1.44458000
H	0.58397100	1.45919900	-2.65052400
H	1.97472600	-1.20398000	-1.00327300
H	2.16976300	0.78639800	0.95940600

NHO 1b, TS1 (v = -387.28i (cm^{-1}))

0 1

C	0.80934500	-0.01116200	0.63906700
C	1.43369200	1.26963100	-1.16600600
C	2.23982400	-0.03164400	-1.16267500
N	1.56347100	-0.80776300	-0.12179800
N	0.76492900	1.21778500	0.13470300
C	0.05435100	-0.40620800	1.81382300
C	2.02793900	-2.13256200	0.23196600
C	-0.14550900	2.26367000	0.57436800
H	2.92713800	-2.08787900	0.85176600
H	1.24744000	-2.67527500	0.75830800
H	2.25694500	-2.67081100	-0.68638000
H	-0.41674100	2.86158700	-0.29507900
H	-1.05087700	1.81424900	0.98618200
H	0.33473600	2.91116400	1.30947300
C	-3.39533500	-0.89702000	-1.18928800

H	-4.31064100	-0.31318500	-1.06558300
H	-3.56687800	-1.88717500	-0.76009200
H	-3.19976400	-1.01124000	-2.25994700
C	-2.23210300	-0.21071800	-0.46993700
H	-1.31922600	-0.81427500	-0.67988500
H	-2.04986300	0.75995700	-0.98153600
O	-2.44084600	-0.05797300	0.88092800
H	-1.10241200	-0.35791500	1.47043200
H	0.35571300	-1.37331500	2.20152500
H	0.14196800	0.35662100	2.58787900
H	2.20713500	-0.55543400	-2.11628900
H	2.05803300	2.15688400	-1.24953900
H	3.28352100	0.13202000	-0.87941500
H	0.67852100	1.28373800	-1.95748900

NHO 1b, TS2 (v = -206.59i (cm^{-1}))

0 1

C	0.13930900	-2.90658300	0.43398700
C	-1.02264000	-2.18805900	0.18864500
C	-1.11390400	-1.35378900	-0.92224500
C	-0.03301000	-1.25787800	-1.79054100
C	1.12922200	-1.98747300	-1.55558100
C	1.21912400	-2.81125000	-0.44044500
H	0.20394600	-3.54809400	1.30542400
H	-1.86709800	-2.25180500	0.86261900
H	-0.11910600	-0.60996200	-2.65529000
H	1.96062600	-1.92050700	-2.24869200
H	2.12245500	-3.38114300	-0.25429600
C	-2.38462100	-0.59059700	-1.24594300
O	-2.38327800	0.29928100	-2.10709000
O	-2.60976700	0.20733100	0.43200500
C	-3.15028000	1.48160500	0.34597400
H	-4.25254500	1.46184600	0.28141800
H	-2.80992700	1.98835800	-0.57326600
C	-4.69712700	-0.97061000	-1.51737300
H	-4.99165400	-0.21596100	-0.78572200
H	-5.40396200	-1.79816700	-1.49247300
O	-3.43175200	-1.50885300	-1.18815900
H	-4.68895700	-0.52288800	-2.51203300
C	-2.77341800	2.33344800	1.55818100
H	-1.69237800	2.47676700	1.62253300
H	-3.10308600	1.84900000	2.48042600
H	-3.24339400	3.31901700	1.50184300
C	1.32244700	0.87840600	0.14076000
C	3.38665000	-0.10629600	0.35048500
C	2.55433200	-0.37867100	1.60907100
N	1.24324500	0.16902200	1.24755000
N	2.54117500	0.84060200	-0.38250900
C	0.20291000	1.66611400	-0.42651000
C	0.13915100	0.13217300	2.19128700
C	2.92653800	1.30830400	-1.69887200
H	0.26171000	0.91299500	2.94618200
H	-0.81253100	0.23983000	1.66657200
H	0.15646900	-0.84210600	2.67890700
H	0.25851600	1.68322800	-1.51217600
H	-0.75102800	1.22525100	-0.13777300
H	2.35676600	2.19422400	-1.96523300
H	3.98268900	1.57171000	-1.67262900
H	2.77057100	0.52971600	-2.44983900
H	0.26900100	2.69017100	-0.04910100
H	4.35592300	0.33976200	0.56560200
H	2.93653400	0.14893500	2.48580300
H	3.52928000	-1.00594400	-0.25263500
H	2.46178100	-1.43922600	1.83820400

NHO 1b, TS3 (v = -201.60i (cm^{-1}))

0 1

C	-0.80480800	-0.82663400	-2.17979600
C	0.38150900	-0.14027000	-1.93607600
C	1.14710000	-0.43021500	-0.81411400
C	0.71919600	-1.42281200	0.06466100
C	-0.46983400	-2.10084000	-0.16707500
C	-1.23543000	-1.80504100	-1.29315400
H	-1.38827500	-0.60268600	-3.06592000
H	0.72982100	0.62876400	-2.61522500
H	1.32039700	-1.64175300	0.93774100
H	-0.79869000	-2.86803600	0.52487400
H	-2.15526800	-2.34669800	-1.48254600
C	2.44645300	0.32192000	-0.60531400
O	2.68264700	1.35630200	-1.24447300
O	3.45264100	-0.62253500	-0.40978600
C	4.73693600	-0.06092800	-0.18716800
H	4.68693300	0.60100100	0.68235600
H	5.03171100	0.53788700	-1.05182900
C	2.59163400	2.05102300	1.48662600
H	3.50433600	2.04956500	2.10487200
H	1.82682300	2.61841200	2.04748800
O	2.15434700	0.77502200	1.17819100
H	2.81754800	2.62718600	0.57484800
C	5.71066500	-1.19537000	0.04662300
H	5.73999400	-1.85949700	-0.81867700
H	5.42127500	-1.77982700	0.92124300
H	6.71428900	-0.80040600	0.21121200
C	-1.75570500	0.79606900	1.01296900
C	-3.59198200	0.56822500	-0.35372900
C	-2.69122900	1.69176500	-0.88228700

N	-1.52949800	1.61193200	0.00490200
N	-2.94567300	0.21517700	0.91433200
C	-0.82118400	0.62349000	2.15017600
C	-0.40373200	2.51275300	-0.15820300
C	-3.45220300	-0.89172100	1.69819900
H	-0.63832800	3.49544700	0.25715700
H	0.48138900	2.09000700	0.31157000
H	-0.20115600	2.60793100	-1.22415000
H	-0.98331400	-0.33107200	2.64345900
H	0.22043900	0.67643500	1.80986400
H	-3.01039100	-0.88990100	2.69007600
H	-4.53065300	-0.77677400	1.80115500
H	-3.23864000	-1.84119700	1.20074100
H	-1.00765000	1.42698400	2.86809900
H	-4.61618100	0.89167000	-0.17512600
H	-3.15239700	2.67701000	-0.78795500
H	-3.60106100	-0.30320800	-1.01152800
H	-2.37872600	1.53915300	-1.91440100

NHO 1b, TS4 (v = -318.21i (cm^{-1}))

0 1

C	-0.33620600	-0.18729300	-0.57563300
C	-2.08414700	0.65420800	0.66133400
C	-0.98306500	1.71186800	0.54903000
N	-0.07773900	1.10808700	-0.42906700
N	-1.42797400	-0.53268800	0.10987000
C	0.53342700	-1.07769200	-1.32501300
C	1.16033000	1.75677900	-0.83439700
C	-2.14456100	-1.78601800	0.00611200
H	1.98377300	1.04170600	-0.77979000
H	1.35492400	2.57157300	-0.13816600
H	1.06970100	2.16929700	-1.84023800
H	-2.66585800	-1.96213000	0.94590900
H	-1.44814200	-2.60390500	-0.15530400
H	-2.87512700	-1.75814600	-0.80652100
C	2.16654100	-0.58201600	1.39213500
H	2.03366500	0.50855100	1.55986200
H	1.14991300	-1.02050700	1.50138000
O	2.75354400	-0.88553000	0.18384500
H	1.55468000	-1.12469800	-0.68940900
H	2.73575200	-0.95171600	2.26314000
H	0.08707400	-2.04957600	-1.50584200
H	0.81892700	-0.61048400	-2.26797100
H	-2.95908200	0.90501700	0.05501700
H	-0.44955100	1.85171500	1.49356500
H	-2.40126700	0.47672900	1.68749100
H	-1.35166400	2.67399000	0.19909200

NHO 1c, TS1 (v = -208.88i (cm^{-1}))

0 1

C	3.45706000	0.48066400	-0.01591700
O	2.35801400	1.07694500	-0.58840700
H	4.29437700	1.19082800	0.13437200
C	-1.61764700	-1.83033900	-0.33101000
C	-2.93526500	-1.08641400	-0.32688700
C	-2.70828200	0.32359400	-0.82702500
H	-3.65436500	-1.59784000	-0.96483100
H	-1.27521800	-2.01922900	-1.35292300
H	-1.71516700	-2.79100900	0.17466900
H	-2.44193500	0.32635200	-1.88835500
H	-3.60853200	0.92465500	-0.70265800
C	-0.66693000	0.26474100	0.52859000
C	0.39471100	0.95598100	1.26413600
H	0.75878100	0.34859000	2.08884700
N	-1.64156100	0.96353300	-0.05589300
N	-0.60062100	-1.05861500	0.38344300
C	0.56151600	-1.80309000	0.86266800
H	1.47559800	-1.25174500	0.65043700
H	0.48953600	-2.00767600	1.93274800
H	0.59350700	-2.74836300	0.32518700
C	-1.62228100	2.42462400	-0.05638800
H	-0.62707900	2.79728300	-0.29078600
H	-2.30652200	2.76453600	-0.82987800
H	-1.94819200	2.82839100	0.90357000
H	-3.33818700	-1.05496200	0.68752200
H	0.06959400	1.92091900	1.63800200
H	3.23187900	0.09681400	1.00691000
H	1.28246400	1.08605600	0.46750200
C	3.99829100	-0.69542600	-0.83451100
H	4.29817000	-0.35156200	-1.82757400
H	4.86361600	-1.16349500	-0.35461900
H	3.22180500	-1.45454200	-0.96566600

NHO 1c, TS2 (v = -199.71i (cm^{-1}))

0 1

C	-0.50579600	-1.87115500	-1.94473900
C	0.69324400	-1.34106800	-1.49131100
C	0.97373100	-1.30885500	-0.12703400
C	0.04604100	-1.81844200	0.77195200
C	-1.15659700	-2.35448600	0.31974100
C	-1.43465900	-2.38264000	-1.03994500
H	-0.72079600	-1.88954600	-3.00705200
H	1.41911600	-0.93608500	-2.18456500
H	0.28476100	-1.79381300	1.82907900
H	-1.87194200	-2.75413700	1.03070800

H	-2.36782700	-2.80239700	-1.39849700
C	2.28147200	-0.77178300	0.41055700
O	2.42717900	-0.53859000	1.61523800
O	2.18143700	0.89971700	-0.50319600
C	2.64291600	1.97219200	0.23408500
H	2.96465600	1.64262500	1.23713500
H	1.83805400	2.71385000	0.40774700
C	4.60186400	-1.01217800	0.15943100
H	4.72390700	0.07084700	0.20928200
H	5.31423500	-1.43096600	-0.54894100
O	3.31216400	-1.34227900	-0.32081600
H	4.77284800	-1.43537500	1.15035400
C	3.79157600	2.71495100	-0.45170700
H	3.46682500	3.09011800	-1.42521800
H	4.64407100	2.05287600	-0.61719100
H	4.12705500	3.56537700	0.14901400
C	-3.92313600	-0.09765000	0.52459200
C	-4.20047400	0.78380800	-0.67355200
C	-2.96900600	0.83244300	-1.55183000
H	-5.04478800	0.38982900	-1.23698500
H	-3.80927800	-1.14519300	0.22899200
H	-4.73470800	-0.03299200	1.24879900
H	-2.79108000	-0.12452000	-2.04842600
H	-3.07038400	1.60093600	-2.31818300
C	-1.72877100	0.97116700	0.54975600
C	-0.55747000	1.51771500	1.30284000
H	-0.73520700	1.51554600	2.37208400
H	0.34945300	0.95008600	1.07590500
N	-1.78820300	1.17437400	-0.75501400
N	-2.70097200	0.34284200	1.20105700
C	-2.56074300	-0.06576300	2.59869300
H	-1.55789500	-0.43683600	2.79522100
H	-2.79572200	0.75429000	3.27867600
H	-3.26178400	-0.87883300	2.77331800
C	-0.68660900	1.79654200	-1.49324500
H	-0.83248800	2.87832600	-1.54810400
H	0.28065600	1.54322000	-1.05338700
H	-0.70838400	1.38614500	-2.50240600
H	-4.45507800	1.79083300	-0.33706000
H	-0.39149600	2.54557700	0.98178800

NHO 1c, TS3 (v = -199.35i (cm^{-1}))

0 1

C	-0.68050000	-2.35497900	-0.95924300
C	0.43335900	-1.56824300	-1.23431400
C	1.16184000	-0.99198800	-0.20130000
C	0.76293300	-1.20466100	1.11546300
C	-0.35870200	-1.97452300	1.39346900
C	-1.08129300	-2.55710400	0.35565500
H	-1.23417900	-2.81060600	-1.77273600
H	0.75364800	-1.39180100	-2.25435000
H	1.32878400	-0.74164300	1.91366400
H	-0.66869800	-2.12754300	2.42089800
H	-1.95037600	-3.16670100	0.57570400
C	2.38363600	-0.16323800	-0.54278200
O	2.58865500	0.20399900	-1.70752800
O	3.43825300	-0.61271600	0.24547600
C	4.64797600	0.10503800	0.05597600
H	4.45473500	1.16888900	0.21984000
H	4.99679000	-0.02247800	-0.97155100
C	2.18214500	2.52829000	-0.16839900
H	3.06208200	3.05016900	0.24461700
H	1.33094300	3.22894200	-0.09522200
O	1.91587600	1.33578900	0.47848900
H	2.37727600	2.36722700	-1.24136900
C	5.66423500	-0.42296400	1.04529200
H	5.83727100	-1.48857800	0.88655500
H	5.31626600	-0.27817200	2.06909000
H	6.61378100	0.10064200	0.92524600
C	-2.90102300	0.36824900	-1.83050600
C	-3.81660300	-0.63270700	-1.15999900
C	-4.35703200	-0.05527700	0.12784300
H	-4.64031500	-0.88185900	-1.82746900
H	-3.46483500	1.20951400	-2.24501000
H	-2.35442300	-0.10642500	-2.64507900
H	-5.08635700	0.73718000	-0.06225400
H	-4.84647200	-0.83035800	0.71661900
C	-2.12956600	0.92990300	0.41580100
C	-1.10704000	1.53439500	1.32421600
H	-1.36050900	2.58821800	1.47674100
H	-1.12119800	1.03581200	2.28996200
N	-3.26986600	0.49518000	0.94293900
N	-1.90559900	0.88671600	-0.88797700
C	-0.75572600	1.56428100	-1.49845100
H	-0.92105400	2.64341000	-1.51938200
H	0.16753000	1.33504200	-0.97335600
H	-0.66496100	1.20109600	-2.51915600
C	-3.54530200	0.60789800	2.37561200
H	-3.03919500	-0.18118100	2.93453100
H	-3.24497000	1.57981800	2.75849700
H	-4.61847700	0.50482800	2.51415000
H	-3.26230900	-1.54539700	-0.94418500
H	-0.09481100	1.45788100	0.92278500

NHO 1c, TS4 (v = -264.95i (cm^{-1}))

0 1

C	3.87613700	-0.02400200	-0.32764500
H	4.13777700	-1.01399500	-0.74866300
O	2.80456600	0.57281400	-0.95586900
H	4.80446100	0.57499000	-0.36912500
C	-1.47755600	-1.73799800	-0.34784800
C	-2.71202600	-0.89635400	-0.11183500
C	-2.44751500	0.51549500	-0.58839300
H	-3.56011900	-1.31969300	-0.64790800
H	-1.31582800	-1.90926900	-1.41633600
H	-1.57526500	-2.70938200	0.13720200
H	-2.34386700	0.55054000	-1.67728600
H	-3.26735300	1.17475500	-0.30561600
C	-0.23378600	0.23541100	0.42499600
C	0.98388400	0.79557500	1.01417000
H	1.36699500	0.14197700	1.79540200
N	-1.22947600	1.03477200	0.03538500
N	-0.30034000	-1.07995100	0.21789200
C	0.85514600	-1.93539600	0.48349600
H	1.76862600	-1.44630800	0.14995500
H	0.92625400	-2.18580400	1.54412900
H	0.72279700	-2.85370900	-0.08458300
C	-1.09889600	2.48855200	0.10552900
H	-0.14302700	2.81263500	-0.30167000
H	-1.89235500	2.92181300	-0.49796800
H	-1.20006200	2.84923800	1.13013700
H	-2.95184700	-0.88368300	0.95346300
H	0.83055600	1.79049000	1.41601600
H	3.69200700	-0.20362500	0.75531000
H	1.80010000	0.79506700	0.12673400

NHO 1d, TS1 (v = -861.18i (cm^{-1}))

0 1

C	-2.24791800	-0.00829100	-1.62177200
H	-1.52579700	0.79000100	-1.42919000
H	-3.24736900	0.43356200	-1.62061200
H	-2.05087100	-0.41532400	-2.61841700
C	-2.14974600	-1.08813100	-0.54056300
H	-2.83486200	-1.91002500	-0.81912000
H	-1.13047800	-1.53498000	-0.61150300
O	-2.39731900	-0.61110200	0.72856800
C	0.73384500	-0.01064300	0.69208800
C	1.25675400	1.51041600	-0.84810200
C	1.95146300	0.38801200	-1.13044000
N	1.62546300	-0.54316000	-0.16199800
N	0.50638200	1.24706800	0.28098100
C	0.02955600	-0.66803200	1.77431000
C	2.09856700	-1.91659400	-0.10490500
C	-0.45961100	2.13873000	0.90925400
H	2.84808600	-2.05301200	-0.87917500
H	2.54348600	-2.11452200	0.86842000
H	1.26860100	-2.60221400	-0.27622700
H	0.01653400	-0.04315800	2.66840400
H	0.45393800	-1.64266800	2.00030300
H	-0.58381400	3.00900900	0.27013300
H	-1.40627400	1.60415000	1.00534200
H	-0.09686800	2.45419100	1.88693700
H	-1.14966200	-0.71929100	1.37509900
H	1.22495300	2.46521900	-1.34203300
H	2.64857900	0.16771100	-1.91900000

NHO 1d, TS2 (v = -218.41i (cm^{-1}))

0 1

C	1.63206200	1.15324200	-0.56955100
C	3.50283600	0.67835600	0.51494200
C	2.75535600	1.47856000	1.30877800
N	1.59934500	1.76029700	0.61974600
N	2.78949600	0.48727600	-0.64706200
C	0.58893700	1.26355000	-1.61104700
C	0.48222200	2.56934500	1.10385400
C	3.24995800	-0.28759700	-1.79356600
H	0.46907500	3.52431000	0.57919900
H	-0.45006800	2.02537900	0.92749400
H	0.63002700	2.74054700	2.16694200
H	2.42968500	-0.88732500	-2.17808300
H	3.62652900	0.37934000	-2.56711000
H	4.04314500	-0.94872000	-1.45489000
C	1.06090100	-1.45524800	1.72338100
C	-0.15559100	-0.97939900	1.24855100
C	-0.62451400	-1.36524400	-0.00670200
C	0.14794400	-2.23752800	-0.77072300
C	1.36079900	-2.72303900	-0.29285000
C	1.82337400	-2.32908700	0.95606500
H	1.41915700	-1.13622100	2.69521300
H	-0.74188100	-0.28819200	1.83818600
H	-0.21083400	-2.52335900	-1.75221700
H	1.94778700	-3.40216100	-0.90044300
H	2.77261100	-2.69620700	1.32855000
C	-1.93905200	-0.90111400	-0.62470600
O	-1.99120800	-0.74662100	-1.85062800
O	-2.01135800	0.77064200	0.21368100
C	-3.13351400	1.42879400	-0.26394900
H	-4.03837200	1.14827100	0.30564900
H	-3.32705000	1.14908700	-1.31237400
C	-3.21283100	-1.58608200	1.32245700
H	-2.46514300	-2.25614100	1.75518700
H	-4.20376900	-1.99606900	1.51332900

O	-3.08379300	-1.49709100	-0.08291400
H	-3.12288700	-0.59837000	1.77717700
C	-2.95135800	2.94215800	-0.18524100
H	-2.09001000	3.24937400	-0.78461700
H	-2.77391900	3.25659500	0.84666100
H	-3.83467400	3.46821900	-0.55644700
H	-0.39999900	1.20623100	-1.14406000
H	0.67257000	0.44860600	-2.32636700
H	0.69676900	2.21500700	-2.13859000
H	4.46226000	0.21883000	0.67370400
H	2.93279700	1.85652200	2.29985900

NHO 1d, TS3 (v = -198.92i (cm^{-1}))

0 1

C	2.17764900	-1.06161700	0.06570800
C	3.26876100	0.38625100	1.32894500
C	3.96040200	0.24568800	0.17509500
N	3.26865400	-0.66169200	-0.59621900
N	2.16514600	-0.42933100	1.24045000
C	1.18047300	-2.05208500	-0.39442200
C	3.63109500	-1.07226700	-1.94831100
C	1.16261700	-0.62354000	2.28769400
H	4.58412100	-0.61342100	-2.19428200
H	3.72725500	-2.15460700	-1.99561900
H	2.87266300	-0.73281300	-2.65229400
H	0.17631300	-0.75621000	1.83065500
H	1.43687100	-1.48854900	2.89105400
H	1.15508700	0.27051600	2.90648300
C	1.24847300	1.86958600	-1.20722600
C	0.20435800	0.96087400	-1.35940400
C	-0.80493800	0.88141500	-0.40819200
C	-0.76788500	1.72898800	0.69640200
C	0.27433300	2.63101800	0.85513300
C	1.28689700	2.70424600	-0.09798100
H	2.03154700	1.92730100	-1.95546100
H	0.15830600	0.29936600	-2.21760400
H	-1.55711600	1.65918200	1.43372100
H	0.29943800	3.28083200	1.72210200
H	2.10067200	3.40874300	0.02536100
C	-1.93076500	-0.11377600	-0.59855200
O	-1.87640500	-0.96641700	-1.49693700
O	-3.12811500	0.54400100	-0.33068300
C	-4.27828300	-0.28441500	-0.39481100
H	-4.15805200	-1.10701300	0.31574500
H	-4.37459000	-0.70959000	-1.39639500
C	-1.90708700	-2.33495400	0.97385900
H	-2.84825900	-2.65085300	1.45413100
H	-1.09133500	-2.88996300	1.47046800
O	-1.70644100	-0.96788800	1.04208400
H	-1.94522500	-2.68237600	-0.07162900
C	-5.48212600	0.56326900	-0.04383100
H	-5.59456500	1.38422200	-0.75370600
H	-5.37676400	0.98434200	0.95716500
H	-6.38967000	-0.04165900	-0.07029200
H	0.17104100	-1.67466200	-0.21985200
H	1.30046000	-2.24282100	-1.45871700
H	1.30835200	-2.99097000	0.14918800
H	4.86640000	0.71078400	-0.17024900
H	3.45428300	0.99773200	2.19405600

NHO 1d, TS4 (v = -916.53i (cm^{-1}))

0 1

C	-2.01716500	-0.76682700	-1.39639500
H	-2.54611500	-1.29774300	-2.20478500
H	-0.96974000	-1.13898700	-1.43428400
O	-2.59861900	-0.94511700	-0.15726300
C	0.37660100	-0.09236100	0.61286400
C	0.99636300	1.68155400	-0.58074400
C	1.91625600	0.71422800	-0.78035200
N	1.52631600	-0.37559000	-0.02420100
N	0.05114700	1.16889000	0.28505400
C	-0.45821400	-0.98675100	1.38970700
C	2.19548900	-1.66560700	0.01926000
C	-1.17128200	1.82926700	0.72527800
H	3.14184100	-1.57815900	-0.50698900
H	2.38259200	-1.94947900	1.05301900
H	1.57870900	-2.42285100	-0.46414500
H	-0.77535000	-0.51486900	2.32103100
H	0.03750600	-1.93183600	1.59364100
H	-1.28168300	2.75062800	0.15996000
H	-2.01171000	1.15825400	0.53397500
H	-1.10649700	2.06170100	1.78786200
H	-1.50450700	-1.09036900	0.70871300
H	-1.96580900	0.29609600	-1.70733000
H	2.81068100	0.70229800	-1.37727800
H	0.92849900	2.68213200	-0.96896000

NHO 1e, TS1 (v = -871.35i (cm^{-1}))

0 1

C	-1.54861400	1.90059100	-1.42572600
H	-0.83501300	1.07907100	-1.53944000
H	-1.06271300	2.81791600	-1.76856000
H	-2.40826200	1.70087500	-2.07322900
C	-1.96336100	2.03853200	0.04143700
H	-2.74812000	2.81389900	0.10528200

H	-2.47766100	1.09109500	0.32491900
O	-0.90616900	2.30110300	0.88677800
C	-0.22335000	-0.76966500	0.61237900
C	0.77231200	-1.23490200	-1.32440600
C	-0.39251700	-1.91621100	-1.28909600
N	-0.99732400	-1.62169100	-0.08266900
N	0.85777600	-0.51838900	-0.14552200
C	-0.53775900	-0.12167200	1.87232400
C	-2.29416700	-2.10881700	0.35961900
C	1.93762000	0.40163300	0.25394200
H	-2.19558700	-2.60126600	1.32513600
H	-2.99475700	-1.27788100	0.44039200
H	-2.65950900	-2.82157900	-0.37416600
H	0.31453500	-0.13547800	2.55144300
H	-1.40418400	-0.57255500	2.34890400
H	1.45095400	1.13405100	0.89978000
H	-0.72608500	1.06263500	1.53481500
H	1.53235600	-1.19290500	-2.08313000
H	-0.84273900	-2.58221400	-2.00345600
C	2.49160700	1.12948000	-0.95991400
H	3.18861400	1.89443700	-0.61822300
H	3.03888500	0.45455700	-1.62058500
H	1.69202700	1.61457800	-1.52102600
C	3.01101200	-0.36205500	1.01844100
H	3.78016000	0.32890200	1.36451900
H	2.58791900	-0.87147600	1.88524700
H	3.47867100	-1.10642400	0.37049100

NHO 1e, TS2 (v = -217.99i (cm^{-1}))

0 1

C	1.69137800	0.44302600	-0.86332500
C	3.55258700	-0.06315400	0.22120700
C	2.93420200	0.93172700	0.89857200
N	1.77824400	1.23062900	0.21344300
N	2.76786000	-0.35152700	-0.87021000
C	0.63266900	0.46814100	-1.89695400
C	0.77548000	2.26067700	0.57477300
C	3.06093700	-1.35424200	-1.88764600
H	-0.19257600	1.82936300	0.30156800
H	2.24963500	-2.07792100	-1.92822400
H	3.18497300	-0.87315800	-2.85581800
H	3.98214000	-1.85766100	-1.60877200
C	0.77951400	-1.54249200	1.86145300
C	-0.37635100	-0.99999300	1.31181100
C	-0.93599900	-1.54717300	0.15834200
C	-0.32018200	-2.65263800	-0.42482900
C	0.82896300	-3.20492400	0.13013700
C	1.38740900	-2.64573300	1.27296700
H	1.21126000	-1.09935900	2.75185700
H	-0.84354500	-0.13216000	1.75730000
H	-0.74751400	-3.06664800	-1.33022000
H	1.29275200	-4.06720800	-0.33487300
H	2.28957800	-3.06531500	1.70213300
C	-2.18604400	-1.01869500	-0.53728700
O	-2.24732200	-1.08962300	-1.77050000
O	-1.98693700	0.77047600	-0.02531900
C	-3.00368100	1.50261000	-0.61557400
H	-3.92291300	1.48693800	-0.00177700
H	-3.27494500	1.07144300	-1.59337600
C	-3.49152700	-1.13211700	1.50300300
H	-2.83124300	-1.80673300	2.05461200
H	-4.52381700	-1.35578100	1.76915400
O	-3.39024400	-1.32623600	0.10604500
H	-3.25398200	-0.09919900	1.76186700
C	-2.57269500	2.95257800	-0.82053900
H	-1.69760600	2.99612200	-1.47533400
H	-2.30171600	3.41110600	0.13489100
H	-3.37075600	3.54714000	-1.27286300
H	-0.33176000	0.71775000	-1.44532200
H	0.53493400	-0.51570200	-2.35257300
H	0.88679400	1.19375800	-2.67411700
H	4.46651400	-0.59348800	0.42149100
H	3.21217600	1.43132500	1.80829300
C	1.04184100	3.53061900	-0.22191800
H	1.00658400	3.33985000	-1.29547200
H	0.27909000	4.27297300	0.01582500
H	2.02122000	3.94343700	0.02994100
C	0.78858100	2.50974400	2.07368600
H	-0.06509500	3.14066700	2.32170700
H	0.69814400	1.57735600	2.63307500
H	1.69246800	3.03268200	2.39331100

NHO 1e, TS3 (v = -198.73i (cm^{-1}))

0 1

C	-2.13254200	-0.20938700	-0.80027500
C	-3.79128200	0.13939900	0.62318300
C	-3.02776500	-0.86688600	1.11121500
N	-2.00306000	-1.06928800	0.21580400
N	-3.22398400	0.52950600	-0.56586500
C	-1.26791000	-0.10846700	-1.99687800
C	-0.93024200	-2.09121500	0.30776200
C	-3.71675200	1.58773800	-1.43859500
H	-0.01202500	-1.57590900	0.01764100
H	-2.97667600	2.38384600	-1.50508600
H	-3.91836300	1.18351600	-2.42859000
H	-4.63517300	1.97935000	-1.01109800

C	-1.02151800	1.88125800	1.67290600
C	0.04419900	0.99026900	1.59840900
C	0.95262100	1.05914600	0.55003700
C	0.79694400	2.03974800	-0.42689600
C	-0.27116600	2.92352600	-0.36212600
C	-1.18371200	2.84675500	0.68877700
H	-1.72163000	1.82052300	2.49747700
H	0.19126500	0.23533600	2.36026400
H	1.50617200	2.08301200	-1.24302100
H	-0.39495400	3.67827000	-1.13044500
H	-2.01354500	3.54238500	0.74048200
C	2.10171000	0.08497400	0.53319900
O	2.10269800	-0.92455900	1.23214100
O	3.26080800	0.74980200	0.22652100
C	4.40862900	-0.08358700	0.11649800
H	4.20544300	-0.85326100	-0.63218300
H	4.59648700	-0.57606700	1.07292000
C	1.92396700	-1.90689000	-1.48808900
H	2.85157400	-2.15333100	-2.03801400
H	1.09963800	-2.40793600	-2.03243800
O	1.71465100	-0.55432600	-1.35095500
H	2.00266300	-2.41557700	-0.50695600
C	5.57659600	0.78723700	-0.28984900
H	5.75077500	1.56711600	0.45302100
H	5.38756100	1.26225100	-1.25342200
H	6.48145000	0.18365600	-0.37313400
H	-1.30575500	0.90800300	-2.38653400
H	-0.22066400	-0.34027500	-1.74678500
H	-1.62838800	-0.78840800	-2.77338200
H	-3.12345500	-1.43571000	2.01758900
H	-4.67417400	0.61105600	1.01634000
C	-1.24152000	-3.23288300	-0.65162200
H	-0.43334800	-3.96360100	-0.61019700
H	-2.17384500	-3.72401800	-0.36393400
H	-1.32885500	-2.88343700	-1.68016200
C	-0.78210400	-2.59323400	1.73250800
H	-1.63996800	-3.19751700	2.03595600
H	0.10737000	-3.22084300	1.77260700
H	-0.64441700	-1.77628800	2.43887900

NHO 1e, TS4 (v = -882.03i (cm^{-1}))

0 1

C	-0.01673500	2.49184900	-1.16016500
H	-0.23494600	3.39546400	-1.75368900
H	-0.98118000	1.94044500	-1.09835500
O	0.51154300	2.77151500	0.08368800
C	-0.72026500	-0.14948000	0.54224600
C	-0.06319300	-1.57733000	-1.03480000
C	-1.41266900	-1.58700000	-1.01162900
N	-1.80646000	-0.70659500	-0.02290100
N	0.35339000	-0.67723800	-0.07183800
C	-0.69364400	0.91784400	1.52578800
C	-3.17935300	-0.36192400	0.31022400
C	1.74447900	-0.32011700	0.26642200
H	-3.84070400	-0.99895000	-0.27015100
H	-3.35614600	-0.52713700	1.37126500
H	-3.37236900	0.68185000	0.06385900
H	-0.01349500	0.68826200	2.34649100
H	-1.68698500	1.12607300	1.91420800
H	1.69832900	0.73606300	0.54166400
H	-0.17263000	1.88348700	0.92602500
H	0.64381300	1.86088700	-1.78593000
H	-2.12489400	-2.13987600	-1.59764300
H	0.62551400	-2.12805600	-1.64873900
C	2.22611300	-1.17033300	1.43560800
H	3.23272900	-0.86439100	1.72204500
H	1.57324500	-1.06283400	2.30228000
H	2.25250200	-2.22408600	1.14902300
C	2.64528000	-0.46868100	-0.94937500
H	2.24644200	0.07245300	-1.80764800
H	3.62461100	-0.05659900	-0.70741300
H	2.78523400	-1.51730600	-1.21953900

NHO 2a, TS1 (v = -1244.77i (cm^{-1}))

0 1

C	-0.23663300	0.35885900	0.51671500
C	-2.23666700	0.29808900	-0.52583500
C	-1.99967400	-0.93673200	-0.02911500
N	-0.76445400	-0.88537100	0.60613800
N	-1.14940900	1.09237300	-0.16149600
C	1.08816900	0.71239100	1.00288800
C	-0.11022000	-2.04160100	1.20074000
C	-1.11155800	2.53132200	-0.38492800
C	-3.38741900	0.82653900	-1.30716500
C	-2.80904000	-2.18323600	-0.08792800
H	-3.96907500	1.55257700	-0.73488500
H	-4.04948200	0.00842400	-1.58292600
H	-3.05038500	1.31173300	-2.22505700
H	-3.77611200	-1.97739800	-0.54166500
H	-2.98133700	-2.58516700	0.91244500
H	-2.31424600	-2.95645600	-0.67936700
H	-0.42071800	-2.16796400	2.23846600
H	0.96785400	-1.90707500	1.13429000
H	-0.39003500	-2.92808000	0.63568000
H	-2.13322600	2.89384100	-0.45894000
H	-0.57878500	2.77534100	-1.30312100

H	-0.63348800	3.01663800	0.45814300
C	1.22669400	0.63391200	2.52337800
H	0.75430600	1.48753000	3.02556200
H	2.28688200	0.64206900	2.79109600
H	0.79362600	-0.27565300	2.94253400
C	1.73234700	1.97839400	0.45245500
H	1.42916400	2.90205000	0.95847800
H	1.56161400	2.09650400	-0.61962700
H	2.81393500	1.88646500	0.58639700
C	3.46829800	-0.36791800	-2.19669300
H	3.59363600	0.67083000	-1.88110500
H	4.43192000	-0.87184700	-2.09273300
H	3.18435500	-0.37882500	-3.25305300
C	2.41815800	-1.05218500	-1.32393100
H	2.27041700	-2.08122200	-1.69307900
H	1.44972000	-0.53559600	-1.49267900
O	2.74846000	-1.04348100	0.02357800
H	1.91408500	-0.22688400	0.53055000

NHO 2a, TS2 (v = -199.72i (cm^{-1}))

0 1

C	1.32113000	1.10056500	-0.01805400
C	3.27914900	0.03007000	0.07117400
C	2.59647900	-0.26001700	1.20660700
N	1.38515000	0.40494700	1.12401500
N	2.47358100	0.88658200	-0.67056600
C	0.16665500	1.99796500	-0.35978600
C	0.36695700	0.38810800	2.17272000
C	2.87862800	1.46028700	-1.95129300
C	4.60286800	-0.45498800	-0.40407400
C	2.95209900	-1.11958100	2.36524700
H	5.31731400	0.36091300	-0.52672000
H	5.01280300	-1.15449900	0.32102800
H	4.51113800	-0.97755100	-1.35841900
H	3.96595800	-1.49678300	2.25219100
H	2.89843400	-0.55996100	3.30071400
H	2.27574300	-1.97390800	2.43951800
H	0.58030000	1.17009600	2.90251600
H	-0.62636500	0.51189200	1.73042400
H	0.40565200	-0.58112900	2.66382100
H	2.24301800	1.09079700	-2.75164200
H	2.83388200	2.54459600	-1.90540900
H	3.90387300	1.16282400	-2.14446500
C	0.24968900	3.27864300	0.48500200
H	0.30768900	3.06554000	1.55274800
H	1.12419700	3.87042700	0.20408300
H	-0.64392900	3.87927900	0.30715900
C	-0.00019800	2.34906600	-1.83712300
H	0.74080600	3.07190300	-2.17899600
H	0.01619500	1.46423400	-2.46934300
H	-0.98727700	2.79606500	-1.95286800
C	0.10990700	-2.83056400	0.79426500
C	-1.03094600	-2.07783200	0.54646000
C	-1.17537200	-1.38772900	-0.65587900
C	-0.13955900	-1.44679800	-1.58778000
C	1.01153200	-2.18365600	-1.33367700
C	1.13501400	-2.88811800	-0.14333800
H	0.20436500	-3.36271100	1.73420700
H	-1.79251800	-1.98441800	1.30613200
H	-0.24710300	-0.89936700	-2.51617900
H	1.80937500	-2.20947900	-2.06728700
H	2.03108500	-3.46279600	0.06176200
C	-2.37634100	-0.54219400	-1.03621400
O	-2.23300700	0.37254600	-1.83638700
O	-2.49826900	0.29492700	0.83941800
C	-3.23705300	1.44497800	0.68120500
H	-4.31011700	1.23023600	0.50447600
H	-2.90414500	2.01750800	-0.20811300
C	-4.00421100	-2.06808000	-0.06423200
H	-3.40444900	-2.97999500	-0.10286600
H	-5.04164200	-2.31996800	-0.27826100
O	-3.61562000	-1.14352900	-1.06363000
H	-3.92416400	-1.60530500	0.91900600
C	-3.12782000	2.36031800	1.90183000
H	-2.08009600	2.61210800	2.08829700
H	-3.51570600	1.85993100	2.79265000
H	-3.68488100	3.29103100	1.75877400
H	-0.72702500	1.43357700	-0.06664900

NHO 2a, TS3 (v = -187.23i (cm^{-1}))

0 1

C	1.75880900	1.00245200	0.14273900
C	3.50976300	-0.37276700	-0.00176800
C	2.72650300	-0.80445300	1.01940100
N	1.64600300	0.05998400	1.08542700
N	2.89521800	0.75959400	-0.52262200
C	0.78951400	2.13099800	-0.01723500
C	0.58503800	-0.01465800	2.08877400
C	3.45252600	1.56612200	-1.60396800
H	0.48941300	-1.04830000	2.40937300
H	0.84330100	0.61058400	2.94354000
H	-0.35873100	0.29863600	1.64400900
H	2.89415400	1.41154900	-2.52478500
H	3.43531800	2.61630700	-1.32671200
H	4.48406000	1.26476700	-1.75577800
C	0.34582700	-2.87409100	-0.38512200

C	-0.80561200	-2.34937400	0.19202100
C	-1.39725300	-1.20318800	-0.32528600
C	-0.82609800	-0.58449400	-1.43335400
C	0.33390900	-1.09658700	-2.00287100
C	0.92427600	-2.24381200	-1.47993700
H	0.78912600	-3.77786700	0.01660800
H	-1.26337700	-2.82211600	1.05285300
H	-1.29341100	0.30748000	-1.83125000
H	0.77699100	-0.60746500	-2.86384100
H	1.82581200	-2.64527000	-1.92769600
C	-2.66408500	-0.68621500	0.32708800
O	-3.01639400	-1.11446700	1.43428800
O	-3.60623000	-0.47778300	-0.67557100
C	-4.84289900	0.03841400	-0.20764500
H	-4.65425400	0.98141300	0.31394000
H	-5.28768400	-0.66036600	0.50443500
C	-2.44482300	1.61851600	1.76288400
H	-3.28608500	2.33003300	1.70921300
H	-1.59535200	2.16312600	2.21508800
O	-2.11065500	1.09027400	0.52899100
H	-2.73714000	0.82747200	2.47249800
C	-5.74745800	0.24606700	-1.40262000
H	-5.91611300	-0.69715100	-1.92461400
H	-5.30621600	0.95544100	-2.10430100
H	-6.71318600	0.63653100	-1.07809600
C	1.14798000	3.27101000	0.94730900
H	1.18844700	2.92497600	1.98125500
H	2.11444700	3.71315500	0.69363600
H	0.38740800	4.05031300	0.87901300
C	0.61164600	2.64910200	-1.44719700
H	0.56209800	1.83768200	-2.17344100
H	-0.33490700	3.18933400	-1.49000700
H	1.39889300	3.34139900	-1.74568700
H	-0.18303400	1.71531100	0.27191200
C	2.88329300	-1.95422800	1.94716700
H	2.05794900	-2.66065800	1.83955200
H	3.81132100	-2.47929900	1.73268400
H	2.91304200	-1.61927200	2.98560800
C	4.77103000	-0.93283400	-0.55675500
H	4.66189300	-1.17500900	-1.61564100
H	5.60487600	-0.23683300	-0.44839400
H	5.02653100	-1.84768500	-0.02698100

NHO 2a, TS4 (v = -1221.52i (cm^{-1}))

0 1

C	0.17255500	0.35548300	-0.34573500
C	-2.02375600	0.39533200	0.16841000
C	-1.72100300	-0.86295700	-0.22159100
N	-0.36622300	-0.87398900	-0.53281200
N	-0.84970600	1.14137700	0.06452700
C	1.59388300	0.64123600	-0.47459900
C	0.36199200	-2.07224200	-0.92466800
C	-0.81141000	2.58335400	0.26588400
C	-3.31048600	0.98837500	0.62294400
C	-2.56863600	-2.08043500	-0.33045800
H	-3.69730900	1.71828900	-0.09160000
H	-4.05548800	0.20374500	0.73727600
H	-3.19553200	1.48740900	1.58697500
H	-3.60852700	-1.82795100	-0.13460800
H	-2.50525600	-2.51319400	-1.33070400
H	-2.26439000	-2.84598200	0.38660900
H	0.32057900	-2.21128700	-2.00542600
H	1.39353500	-1.98541500	-0.58717000
H	-0.09733400	-2.93008300	-0.43880000
H	-1.79953300	2.98474100	0.05745200
H	-0.53429100	2.83187700	1.28973300
H	-0.10486700	3.02688900	-0.42566200
C	2.13371200	0.47524800	-1.89532300
H	1.87248800	1.32842300	-2.53380200
H	3.22470300	0.41088800	-1.86525800
H	1.76887800	-0.42703500	-2.38740600
C	2.12685200	1.91465400	0.16949300
H	1.99875300	2.81927000	-0.43600800
H	1.69424500	2.09266300	1.15582600
H	3.20270800	1.78786500	0.31743000
C	1.78892300	-1.33258100	2.04360900
H	1.13584500	-2.21301600	1.89931200
H	1.11184500	-0.45906300	2.12270100
O	2.71968500	-1.17806300	1.02563600
H	2.17646900	-0.31243200	0.25804100
H	2.26074800	-1.44662100	3.03021000

NHO 2b, TS1 (v = -1019.62i (cm^{-1}))

0 1

C	-0.80272200	0.16072700	0.20112400
C	-2.12190900	-1.27690200	-1.04265800
C	-1.75825600	-1.95122700	0.27629700
N	-0.75883200	-1.03337900	0.81467300
N	-1.68562400	0.09975600	-0.80904000
C	0.06824600	1.25783200	0.58948800
C	0.09648300	-1.43796600	1.91138300
C	-2.11124100	1.14189200	-1.72101000
H	-0.41965500	-1.35230300	2.87125100
H	1.00554900	-0.83902500	1.90692800
H	0.37093600	-2.48209400	1.75692100
H	-3.14093900	0.93137300	-2.00871300

H	-1.49457600	1.16659400	-2.62266000
H	-2.08440000	2.10894300	-1.23347400
C	3.49463800	-0.75240500	-1.53443000
H	3.67680500	0.24179500	-1.94930100
H	4.38770300	-1.05857300	-0.98485100
H	3.34191800	-1.45149700	-2.36179000
C	2.28743000	-0.71787000	-0.59984100
H	2.08479600	-1.75336800	-0.25851800
H	1.40049300	-0.43855500	-1.21128700
O	2.45312000	0.15009400	0.46238400
H	1.21599100	0.70944300	0.57595100
H	-1.32614300	-2.94119800	0.13988200
H	-3.18861100	-1.30472700	-1.25603100
H	-2.61278200	-2.02616000	0.95503300
H	-1.57599400	-1.70354700	-1.88984500
C	0.24076300	2.43434600	-0.36289000
H	1.17540400	2.93460200	-0.09794500
H	-0.55181800	3.18573400	-0.29106200
H	0.33530700	2.11892800	-1.40266800
C	-0.14827900	1.74577200	2.02415000
H	0.72743400	2.31473400	2.34550500
H	-0.29565600	0.93789700	2.73933300
H	-1.01645000	2.41042300	2.08916000

NHO 2b, TS2 (v = -201.76i (cm^{-1}))

0 1

C	0.27987200	-2.77373500	1.20979500
C	-0.85090900	-2.02418800	0.91949100
C	-1.00941000	-1.45734200	-0.34201100
C	-0.03459800	-1.66183900	-1.31110800
C	1.10026800	-2.41464700	-1.02382900
C	1.25894200	-2.97225600	0.23831300
H	0.40142500	-3.20966000	2.19491300
H	-1.61604300	-1.85431500	1.66576500
H	-0.19018800	-1.24731900	-2.29908200
H	1.85023100	-2.57670700	-1.79009100
H	2.13718900	-3.56585600	0.46638500
C	-2.25481900	-0.70028100	-0.72299600
O	-2.29883100	0.02924400	-1.70554600
O	-2.18668300	0.57417900	0.89092700
C	-2.57303900	1.84314700	0.52451300
H	-3.66063600	1.92410900	0.32962100
H	-2.10166800	2.15869500	-0.42876900
C	-4.59656000	-0.81315500	-0.59131200
H	-4.68804100	0.13624100	-0.06327900
H	-5.35913200	-1.50677200	-0.24342000
O	-3.34629500	-1.41044000	-0.29435200
H	-4.70657400	-0.64660200	-1.66323600
C	-2.23057700	2.87724200	1.60069600
H	-1.16180100	2.86103100	1.82487700
H	-2.76742100	2.64928300	2.52487400
H	-2.50055000	3.89009200	1.28608300
C	1.78968600	0.77870100	0.01141300
C	3.72431400	-0.44371100	0.24228200
C	2.99487800	-0.38737900	1.58333200
N	1.72509500	0.24535300	1.22079800
N	2.94451000	0.49166300	-0.57841400
C	0.69540900	1.66654100	-0.50360600
C	0.73021700	0.50138900	2.24996300
C	3.36127900	0.74761100	-1.94682000
H	1.01718300	1.37373200	2.84434700
H	-0.26260400	0.63132600	1.80968800
H	0.70401100	-0.37323000	2.89901000
H	2.90045900	0.04311100	-2.64173100
H	3.12680600	1.76573900	-2.23872100
H	4.44179300	0.62337400	-1.98402900
C	0.93535600	3.07876200	0.05607400
H	1.03949200	3.08090100	1.14148200
H	1.83824800	3.51291500	-0.37911300
H	0.08513000	3.70950100	-0.20734900
C	0.49227300	1.72117900	-2.01997000
H	1.16282500	2.43573900	-2.49724100
H	0.60987100	0.74920100	-2.49337200
H	-0.53318400	2.04182900	-2.20048300
H	-0.22180500	1.25918300	-0.06596400
H	3.68595000	-1.43752800	-0.20934000
H	2.81374900	-1.37054000	2.01456500
H	3.51285800	0.23782600	2.31519000
H	4.75975300	-0.11444400	0.30252100

NHO 2b, TS3 (v = -202.32i (cm^{-1}))

0 1

C	2.11218400	-0.66216300	0.03907300
C	3.75880900	0.83662700	-0.53940400
C	2.90254600	0.52193600	-1.76587100
N	1.81487400	-0.27212200	-1.19046600
N	3.25420600	-0.12531500	0.44833400
C	1.26104300	-1.65222200	0.77355300
C	0.78151100	-0.81255200	-2.05810700
C	3.88811600	-0.21673200	1.75090900
H	0.55017300	-0.05471000	-2.80468900
H	1.13880200	-1.71377300	-2.56318500
H	-0.12401500	-1.01505400	-1.49003800
H	3.45577100	0.49550200	2.45621900
H	3.80985300	-1.22422300	2.14568600
H	4.94305800	0.01551500	1.61707200

C	0.48120300	2.83745100	-0.91073000
C	-0.60602400	2.02496400	-1.21841100
C	-1.15957600	1.19069700	-0.25515500
C	-0.61205100	1.17204300	1.02447500
C	0.47974400	1.97298600	1.33291300
C	1.02722500	2.81310500	0.36649600
H	0.89528200	3.49668600	-1.66508700
H	-1.04225300	2.03179600	-2.21020400
H	-1.04528100	0.51308900	1.76655600
H	0.89876600	1.95779800	2.33305300
H	1.86381900	3.45538400	0.61564800
C	-2.37319000	0.35678700	-0.61787100
O	-2.68571400	0.18446300	-1.80357000
O	-3.35448900	0.61032300	0.33640200
C	-4.55124500	-0.12876900	0.14796600
H	-4.30555800	-1.19415200	0.11969200
H	-5.00582600	0.14117700	-0.80809100
C	-2.03664300	-2.34326900	-0.75059800
H	-2.83407800	-2.99178100	-0.35033800
H	-1.14837900	-2.98513200	-0.89950800
O	-1.75675400	-1.26918000	0.07437200
H	-2.36339600	-2.00824900	-1.74841800
C	-5.47971600	0.18634200	1.30080200
H	-5.70464600	1.25362900	1.33221700
H	-5.02468300	-0.09878500	2.25051600
H	-6.41787200	-0.35921600	1.18932800
C	1.71966800	-3.06794600	0.38836600
H	1.70109000	-3.22209100	-0.69134700
H	2.73160100	-3.26324000	0.75080900
H	1.04548900	-3.79234800	0.84689900
C	1.18139000	-1.48937800	2.29518500
H	1.17134500	-0.44398500	2.60148600
H	0.24414600	-1.93906400	2.62542500
H	1.99082100	-2.00106500	2.81539300
H	0.24427300	-1.49279600	0.39708400
H	2.50044900	1.41176400	-2.24650400
H	3.59840300	1.85178600	-0.17032800
H	4.82223100	0.67710300	-0.70687000
H	3.43662100	-0.07976500	-2.50573700

NHO 2b, TS4 (v = -960.78i (cm^{-1}))

0 1

C	-0.39643600	0.14956100	0.28645900
C	-2.42872400	-0.56368700	-0.55837200
C	-1.81623200	-1.68365400	0.27598300
N	-0.47220700	-1.17058700	0.52147700
N	-1.56610100	0.56983700	-0.22257800
C	0.82901100	0.89967200	0.51191200
C	0.57148000	-2.04708100	1.01170000
C	-1.97251600	1.90618700	-0.60793600
H	0.48853000	-2.19976300	2.09103400
H	1.54642800	-1.63560400	0.75420200
H	0.46112500	-3.01218000	0.51597800
H	-3.05324600	1.97175500	-0.48636300
H	-1.72517000	2.11978300	-1.65054700
H	-1.51278900	2.64589500	0.03645800
C	1.83568100	-0.89747400	-1.92579400
H	1.47818700	-1.93818500	-1.80487600
H	0.92061200	-0.28047400	-2.06024900
O	2.61102900	-0.46278300	-0.86688000
H	1.69346500	0.21692200	-0.11396600
H	-1.76708200	-2.63082800	-0.25864400
H	-3.46081000	-0.34640100	-0.29026900
H	-2.34463300	-1.83588500	1.22159900
H	-2.37310000	-0.76952000	-1.63173000
C	0.97093900	2.28547300	-0.10566500
H	2.03816200	2.51705600	-0.14185100
H	0.49279600	3.08234500	0.47220700
H	0.60449200	2.32529700	-1.13209700
C	1.28640300	0.90992500	1.97335100
H	2.34172700	1.18967300	2.01623100
H	1.18231500	-0.05485800	2.46786700
H	0.72484200	1.64629100	2.55820000
H	2.36642800	-0.85733000	-2.89025500

NHO 2c, TS1 (v = -983.46i (cm^{-1}))

0 1

C	-3.51776900	-0.07573200	-0.08874400
H	-3.32256300	-0.60889800	0.86559900
O	-2.43084600	-0.13741400	-0.94391800
C	2.85236500	-0.12975700	-1.14118000
C	3.28990800	-1.15221100	-0.10852900
C	2.05802800	-1.96828600	0.22592300
H	4.07292000	-1.80910000	-0.48560000
H	2.40051000	-0.62680100	-2.00323800
H	3.66977500	0.49283600	-1.49700300
H	1.90552400	-2.73908100	-0.53414800
H	2.15755400	-2.47204100	1.19031800
C	0.79233700	0.16708600	0.08744200
C	-0.41630600	0.92496400	0.40813700
N	0.82889500	-1.16088400	0.27189200
N	1.85781400	0.73826800	-0.51446600
C	2.35356000	2.04458500	-0.08118000
H	2.31257100	2.77274800	-0.89199300
H	1.78173800	2.40664800	0.76552900
H	3.39054600	1.92951500	0.24085300

C	-0.33824600	-1.96260300	0.62854400
H	-1.25660300	-1.44791800	0.36244700
H	-0.28598700	-2.89420900	0.06227700
H	-0.32034800	-2.20791600	1.69261200
H	3.67417900	-0.63157400	0.77148800
H	-1.32402800	0.34127100	-0.24404500
C	-0.55863000	2.32784800	-0.17583900
H	-1.62774700	2.53402300	-0.27043700
H	-0.13182400	3.12122800	0.44407900
C	-0.82366500	0.89473100	1.88248400
H	-0.78409800	-0.10150000	2.32219300
H	-0.18283500	1.54941300	2.48425200
H	-1.84884800	1.25698400	1.98168000
H	-3.75185900	0.96580900	0.20819600
H	-0.12711900	2.40122400	-1.17576900
C	-4.77498600	-0.68171100	-0.70809100
H	-5.62809100	-0.62717000	-0.02552400
H	-5.03281600	-0.15106300	-1.62760100
H	-4.60032500	-1.73029600	-0.96061500

NHO 2c, TS2 (v = -200.15i (cm^{-1}))

0 1

C	-0.21578100	2.80696600	0.89909400
C	0.97100600	2.09720800	0.77799600
C	1.29420900	1.46516300	-0.42064700
C	0.42133300	1.56424000	-1.49598600
C	-0.77616300	2.26250900	-1.37501900
C	-1.09505300	2.88958700	-0.17702600
H	-0.45668800	3.30044700	1.83393700
H	1.65597900	2.02437200	1.61321600
H	0.70167700	1.09347500	-2.42919300
H	-1.45094400	2.32959300	-2.22139600
H	-2.01764600	3.45136100	-0.08230200
C	2.59318100	0.71400300	-0.60396500
O	2.88822300	0.19567400	-1.68498700
O	2.14704800	-0.68429100	0.61447700
C	2.64495300	-1.91304100	0.22199700
H	3.28662500	-1.80548200	-0.66816500
H	1.83592100	-2.60460600	-0.08768200
C	4.85259500	0.75473500	0.04368800
H	4.82398800	-0.28199100	0.38384700
H	5.51585900	1.33251500	0.68491900
O	3.57129400	1.34422300	0.15362400
H	5.21437400	0.78452000	-0.98479400
C	3.42762900	-2.60778300	1.33718000
H	2.78206900	-2.77739700	2.20263300
H	4.26819400	-1.99121600	1.66368400
H	3.81676500	-3.57472200	1.00523400
C	-3.87067600	0.48246300	-0.39568200
C	-4.20975200	0.32597200	1.07164000
C	-2.93551400	0.51631000	1.86097000
H	-4.94683200	1.06513900	1.38195600
H	-3.47128800	1.47860200	-0.59978700
H	-4.73813400	0.32341200	-1.03165300
H	-2.66612300	1.57371500	1.92514700
H	-3.04471000	0.13361400	2.87652600
C	-1.83447400	-0.75451800	0.05548600
C	-0.72062900	-1.70033900	-0.33528100
H	0.13638600	-1.40705800	0.26441800
N	-1.79623300	-0.19470100	1.25894500
N	-2.86231500	-0.51760400	-0.75670400
C	-3.18420600	-1.30897400	-1.94200200
H	-4.20147800	-1.68676000	-1.83262600
H	-3.13183600	-0.68227300	-2.83371500
H	-2.51696800	-2.15112100	-2.05633600
C	-0.67734100	-0.34428500	2.19902800
H	-0.81065500	-1.25221100	2.79262300
H	0.28792600	-0.35305000	1.69779900
H	-0.70701800	0.51645100	2.86575800
H	-4.62729200	-0.66819000	1.24243000
C	-1.11334100	-3.12645700	0.08720200
H	-1.98089600	-3.49537000	-0.46304600
H	-0.27634800	-3.79656800	-0.11035500
H	-1.34212300	-3.17268300	1.15351500
C	-0.22603000	-1.59932000	-1.79276200
H	-0.39273700	-2.53248300	-2.33444900
H	-0.70822700	-0.79589400	-2.34647500
H	0.84382700	-1.38349500	-1.78172900

NHO 2c, TS3 (v = -190.87i (cm^{-1}))

0 1

C	0.25865200	2.99648200	0.05616400
C	-0.79474900	2.28783800	-0.51352200
C	-1.34642200	1.19500200	0.14427400
C	-0.82528100	0.80544800	1.37454800
C	0.23096100	1.50492000	1.94279800
C	0.76959300	2.60984400	1.28883300
H	0.67326200	3.85664400	-0.45681800
H	-1.20549300	2.57679200	-1.47366500
H	-1.25176000	-0.05853800	1.86789500
H	0.63131400	1.19768600	2.90259900
H	1.57700100	3.17104600	1.74462500
C	-2.52843900	0.47941300	-0.48085800
O	-2.79790300	0.63940000	-1.67891000
O	-3.54648700	0.44765600	0.46869400
C	-4.71827500	-0.22830600	0.03932100

H	-4.44506500	-1.24159700	-0.26878000
H	-5.14758600	0.28565800	-0.82394000
C	-2.12728100	-2.07180900	-1.34317800
H	-2.91837400	-2.82044100	-1.16977300
H	-1.21748600	-2.62992300	-1.63252700
O	-1.90227000	-1.26787000	-0.24028000
H	-2.43134600	-1.47616900	-2.21909900
C	-5.69201700	-0.25485900	1.19759000
H	-5.95286700	0.75927100	1.50442500
H	-5.25706700	-0.77332500	2.05334400
H	-6.60749300	-0.77296700	0.90827900
C	3.81592200	0.89964900	0.39386100
C	4.07583600	0.96257100	-1.09702500
C	2.73009600	0.96639600	-1.78386200
H	4.62468300	1.86522500	-1.36143100
H	3.21005200	1.75083000	0.71138900
H	4.73462200	0.89346600	0.97378200
H	2.26200500	1.95202500	-1.72256700
H	2.82489000	0.70205100	-2.83801700
C	2.04467800	-0.67721400	-0.07033400
C	1.13284000	-1.83161700	0.28847300
H	0.14825700	-1.54492400	-0.08394500
N	1.79175900	0.00055200	-1.18445600
N	3.08539800	-0.33526700	0.68762200
C	3.68433000	-1.21408200	1.69000500
H	4.76595700	-1.16411000	1.57277100
H	3.42023700	-0.89749700	2.69971600
H	3.38191200	-2.24156600	1.53608500
C	0.63733800	-0.25008700	-2.05593300
H	0.87504400	-1.03828500	-2.77367700
H	-0.25671000	-0.49603000	-1.49296700
H	0.44147800	0.67257400	-2.59972100
H	4.66848700	0.09734700	-1.40007300
C	1.56753800	-3.10106100	-0.45806700
H	2.53653000	-3.46607700	-0.10994900
H	0.82841600	-3.88341500	-0.28047900
H	1.63182800	-2.93417900	-1.53411900
C	0.89597100	-2.09059800	1.78362400
H	1.55080700	-2.85763200	2.19561200
H	1.00204700	-1.18441200	2.37955600
H	-0.13215100	-2.43760900	1.89299900

NHO 2c, TS4 (v = -1005.85i (cm^{-1}))

0 1

C	-3.82248000	-0.59879700	-0.45316200
H	-3.62729700	-1.19540700	0.46060300
H	-4.64548100	-1.11007800	-0.97791300
O	-2.70068500	-0.45225400	-1.25424800
C	2.59274500	0.18764300	-0.95394700
C	3.03999700	-0.85079400	0.05856300
C	1.89056900	-1.82668800	0.19748400
H	3.93456700	-1.38189200	-0.26474700
H	2.30232700	-0.29290000	-1.89158400
H	3.36048100	0.92559700	-1.17365800
H	1.91137000	-2.54399400	-0.62736100
H	1.95236900	-2.39402900	1.12907300
C	0.39458900	0.15381800	0.05472200
C	-0.92246600	0.74463700	0.29669800
N	0.57435700	-1.17057700	0.16480700
N	1.43668600	0.88583000	-0.39429100
C	1.71440900	2.21290500	0.15578800
H	1.64632300	2.98348700	-0.61294700
H	1.02826300	2.44119200	0.96320400
H	2.72576300	2.20979400	0.56680800
C	-0.51519000	-2.12370300	0.35642400
H	-1.45683700	-1.70871000	0.00937100
H	-0.28612800	-3.01055400	-0.23697200
H	-0.57942800	-2.42254800	1.40492200
H	3.25966100	-0.35587600	1.00716900
H	-1.70756600	0.10108200	-0.45698100
C	-1.17944100	2.15455000	-0.22806500
H	-2.25275000	2.24182800	-0.41528100
H	-0.90876200	2.95391000	0.46742300
C	-1.43856300	0.58154400	1.72816600
H	-1.33958600	-0.43471800	2.10888900
H	-0.91185700	1.24984800	2.41941800
H	-2.49780700	0.84333400	1.76113400
H	-4.23291200	0.36514300	-0.09911000
H	-0.67154100	2.33605500	-1.17711400

Cationic ketone-type intermediates (zwitterionic mechanism): NHO1a Ketone-type cation

1 1

C	1.20523900	0.21806100	-0.48145100
C	3.17839700	-0.71943200	-0.07200800
C	3.28715000	0.60983500	0.19068300
N	2.04550600	1.17060300	-0.07037900
N	1.87595600	-0.93433300	-0.48997600
C	-0.23098400	0.36973100	-0.81982000
C	1.75392200	2.58545800	0.13353300
C	1.32188000	-2.24866200	-0.79001100
C	4.16779200	-1.82406100	0.02458500
C	4.43775900	1.42632100	0.65741800
H	4.36135000	-2.26649800	-0.95417600

H	5.10821300	-1.44432300	0.41703100
H	3.81071200	-2.61119300	0.69083800
H	4.75091100	2.14118200	-0.10578200
H	4.18452200	1.98130700	1.56204600
H	5.28166600	0.77824900	0.88200600
H	1.78880100	2.81088600	1.19775300
H	2.49540600	3.18026600	-0.39466700
H	0.76856400	2.82198700	-0.25118300
H	2.01975100	-2.79178500	-1.42243000
H	1.15495300	-2.79091900	0.13896900
H	0.37912600	-2.13678800	-1.31644400
C	-1.12483200	-0.21037000	0.28273500
C	-2.59608800	-0.06380000	0.13664200
C	-3.17432400	0.53192700	-0.98407900
C	-3.40962500	-0.54452100	1.16452500
C	-4.55450600	0.64567100	-1.07449400
H	-2.56240700	0.90725300	-1.79437200
C	-4.78551800	-0.42679000	1.07307100
H	-2.94632200	-1.00464300	2.02768800
C	-5.35833500	0.16866200	-0.04725900
H	-5.00125900	1.10653900	-1.94571400
H	-5.41510300	-0.79678300	1.87188300
H	-6.43502500	0.26046700	-0.11845000
O	-0.62160900	-0.77281500	1.22725000
H	-0.47957400	1.41649000	-0.98371600
H	-0.44920800	-0.14126600	-1.76121500

NHO1b Ketone-type cation

1 1

C	0.96485100	-0.73379200	0.07862400
C	2.67190700	-2.15895600	-0.45677600
C	2.89866100	-1.59103500	0.94777000
N	1.63879600	-0.87686100	1.20207900
N	1.53201800	-1.36348700	-0.93241300
C	-0.30579300	0.02821900	-0.04962100
C	1.42230300	-0.19650200	2.46725600
C	0.93499200	-1.64760000	-2.22397800
H	0.36634200	0.01162100	2.61277000
H	1.75211300	-0.85937800	3.26474600
H	1.99720300	0.72987600	2.50798400
H	0.14650400	-0.93253800	-2.44247600
H	1.70463700	-1.56762500	-2.98976900
H	0.51679200	-2.65564400	-2.22449800
C	-1.49644100	-0.93531500	-0.10872700
C	-2.85616500	-0.34979300	-0.21672600
C	-3.06450800	1.02692500	-0.29586300
C	-3.94719000	-1.22093000	-0.24341700
C	-4.35431700	1.52746600	-0.40279100
H	-2.23257700	1.71934000	-0.27799500
C	-5.23246700	-0.71830500	-0.34796500
H	-3.76900000	-2.28665600	-0.18128200
C	-5.43589400	0.65650100	-0.42818300
H	-4.51445300	2.59579800	-0.46562700
H	-6.07793000	-1.39364000	-0.36756300
H	-6.44151900	1.04928400	-0.51123200
O	-1.30142000	-2.12786700	-0.07204900
H	-0.42720900	0.72260300	0.77973300
H	-0.27655000	0.63069900	-0.96006800
H	3.05380500	-2.35903900	1.70173300
H	3.52707800	-2.02951900	-1.11591500
H	2.38345500	-3.21215600	-0.43838700
H	3.72449900	-0.87772700	0.98185000

NHO1c Ketone-type cation

1 1

C	-0.75570800	0.00004400	0.35758200
O	-0.24307300	0.00023500	1.45296400
C	3.58192800	1.23540100	0.13033800
C	3.94261700	0.00012900	0.92547800
C	3.58195900	-1.23534500	0.13063800
H	5.00885800	0.00016700	1.14449800
H	4.21870700	1.34572400	-0.75082900
H	3.68645100	2.12877400	0.74203000
H	4.21877400	-1.34589800	-0.75047300
H	3.68645300	-2.12856100	0.74256400
C	1.57414800	-0.00006100	-0.49060700
C	0.12948700	-0.00013200	-0.89308900
N	2.17933600	-1.16097200	-0.30296800
N	2.17928800	1.16091100	-0.30318500
C	1.48326400	2.43286700	-0.52704200
H	1.26382800	2.58019200	-1.58399200
H	0.56596200	2.48257200	0.05808100
H	2.14029300	3.23206600	-0.19958500
C	1.48337900	-2.43299600	-0.52664900
H	1.26392700	-2.58046400	-1.58357500
H	2.14046300	-3.23212000	-0.19911200
H	0.56609400	-2.48268400	0.05850400
H	3.39665700	0.00023900	1.87057200
H	-0.10419800	-0.87112900	-1.50233800
H	-0.10421500	0.87068300	-1.50258800
C	-2.22872900	0.00001100	0.16816800
C	-2.81336500	-0.00018600	-1.09803100
C	-3.03719000	0.00018500	1.30693900
C	-4.19537700	-0.00020400	-1.22297400
H	-2.20500200	-0.00032900	-1.99381100
C	-4.41504100	0.00016500	1.17891300

H	-2.56867300	0.00033100	2.28261900
C	-4.99463200	-0.00002900	-0.08674100
H	-4.64724100	-0.00035100	-2.20625300
H	-5.04054600	0.00030400	2.06223900
H	-6.07282600	-0.00004300	-0.18672200

NHO1d Ketone-type cation

1 1

C	-1.84447900	0.09112200	0.39240200
C	-3.80182500	-0.74465300	-0.18872500
C	-3.84248000	0.59290400	-0.39766200
N	-2.61470400	1.09321900	-0.03334100
N	-2.55090300	-1.03597100	0.30074600
C	-0.42896600	0.19419600	0.81387600
C	-2.20880600	2.49540200	-0.11459900
C	-2.05032200	-2.36876600	0.62902800
H	-1.29700100	2.57699400	-0.70227600
H	-3.00471900	3.04532000	-0.60700800
H	-2.05432600	2.89446300	0.88550000
H	-2.83981200	-3.08414400	0.42128300
H	-1.18355400	-2.59329200	0.01056300
H	-1.78867800	-2.41484200	1.68396900
C	0.50490800	-0.12261700	-0.36310700
C	1.96916200	-0.03410300	-0.13687800
C	2.50672600	0.31164700	1.10252500
C	2.81857700	-0.31297800	-1.20963400
C	3.88318400	0.37654500	1.26691600
H	1.86549700	0.53183300	1.94652500
C	4.19070200	-0.24595600	-1.04281700
H	2.38659300	-0.58012700	-2.16539700
C	4.72326000	0.09866900	0.19624800
H	4.29880400	0.64424600	2.22953800
H	4.84821200	-0.46217300	-1.87489300
H	5.79699300	0.15006800	0.32669700
O	0.02940700	-0.43900700	-1.42875400
H	-0.22134600	1.19523800	1.19536500
H	-0.22820200	-0.50179400	1.63185000
H	-4.54487000	-1.50707900	-0.34155800
H	-4.62744700	1.22813000	-0.76739100

NHO1e Ketone-type cation

1 1

C	1.42990100	0.55102400	-0.38237600
C	3.50379900	0.40495200	0.35263400
C	3.22839000	1.71397500	0.14427800
N	1.93383700	1.78430100	-0.30947600
N	2.36832000	-0.30393000	0.02989900
C	0.04470000	0.22738000	-0.79928800
C	1.20042900	3.00896100	-0.62101100
C	2.22522300	-1.77873400	0.08373400
H	0.28439000	3.03879600	-0.03474000
H	1.82727300	3.85392900	-0.35366800
H	0.97462000	3.04546700	-1.68472800
H	1.16097900	-1.96212900	0.23106200
C	-0.92867700	0.38263900	0.37682000
C	-2.35672000	0.04709900	0.14874400
C	-2.82598800	-0.38262700	-1.09257200
C	-3.24301200	0.17671500	1.21990300
C	-4.17118400	-0.67974000	-1.25991100
H	-2.15559400	-0.48676800	-1.93614000
C	-4.58374800	-0.12182300	1.05009900
H	-2.86430000	0.51285400	2.17653700
C	-5.04794300	-0.55012200	-0.19060800
H	-4.53378800	-1.01251300	-2.22366500
H	-5.27047100	-0.02204000	1.88062800
H	-6.09710900	-0.78295800	-0.32307300
O	-0.51572400	0.77907200	1.44192000
H	-0.26322300	0.89703600	-1.60630700
H	-0.01000200	-0.78356200	-1.20324300
H	4.40174500	-0.07032900	0.70311600
H	3.83244900	2.59332100	0.28088100
C	2.97635900	-2.33707500	1.28157600
H	4.05613300	-2.26653600	1.14482700
H	2.69486700	-1.82217500	2.19992100
H	2.72480600	-3.39196400	1.38374900
C	2.68713300	-2.38242600	-1.23480000
H	2.54868600	-3.46295000	-1.20586000
H	2.12102600	-1.98152400	-2.07640400
H	3.74622500	-2.17231300	-1.39455200

NHO2a Ketone-type cation

1 1

C	1.27021300	-0.34216100	0.09103400
C	2.80496100	1.27481200	0.19393600
C	3.45344800	0.10578100	-0.03453900
N	2.48254600	-0.88815200	-0.08603600
N	1.45765600	0.97008100	0.28431300
C	-0.08310300	-1.02212500	0.16449000
C	2.82257300	-2.30789100	-0.20909300
C	0.44471600	1.99469300	0.52195200
C	3.31471400	2.66469400	0.33264700
C	4.90565900	-0.16485300	-0.21020800
H	3.15889400	3.04603900	1.34332400
H	4.38138600	2.68878500	0.12409200
H	2.81579600	3.33675700	-0.36728300

H	5.29746000	-0.78948500	0.59424100
H	5.10530200	-0.65899000	-1.16191200
H	5.45135200	0.77546800	-0.19794700
H	2.47260900	-2.70837400	-1.15545000
H	3.90247300	-2.39391800	-0.16736800
H	2.40143500	-2.86388500	0.62355300
H	-0.45140300	1.55513300	0.94896000
H	0.84484600	2.71020700	1.23507200
H	0.19755900	2.49408500	-0.41357400
C	-1.05864700	-0.16966300	-0.68776700
C	-2.49558400	0.00039900	-0.31074500
C	-3.28703300	-0.99451100	0.26446300
C	-3.06564700	1.23943800	-0.61268000
C	-4.62562400	-0.74775900	0.53427900
H	-2.88939200	-1.97775000	0.47159600
C	-4.39589800	1.49110200	-0.31787400
H	-2.45210800	2.00171900	-1.07694800
C	-5.17837800	0.49551400	0.25489500
H	-5.23768400	-1.53121400	0.96190400
H	-4.82390600	2.46018600	-0.53977800
H	-6.22045900	0.68659900	0.47837000
O	-0.63102900	0.35717000	-1.68851200
C	-0.13278600	-2.39235700	-0.54770400
H	0.29829600	-2.33251200	-1.54607600
H	0.36187200	-3.16778400	0.03144000
H	-1.17492200	-2.69125100	-0.65891200
C	-0.43457100	-1.18448700	1.65500900
H	-0.62822600	-0.23011000	2.14460400
H	-1.30300000	-1.82290400	1.79128500
H	0.40456300	-1.66142000	2.16439300

NHO2b Ketone-type cation

1 1

C	-1.74064400	0.01389000	0.09491000
C	-3.06453000	-1.86202000	0.21776500
C	-3.94483500	-0.62988400	0.05357500
N	-2.96107500	0.43837600	-0.19941600
N	-1.74418600	-1.26508900	0.44598100
C	-0.46839300	0.84625000	0.13240800
C	-3.47459400	1.80219100	-0.32707500
C	-0.62634500	-2.16173700	0.68041500
H	-3.12081500	2.27788200	-1.23596600
H	-4.55725800	1.72292000	-0.38274300
H	-3.21878300	2.40370100	0.54363500
H	0.25076500	-1.62475500	1.03003300
H	-0.92345300	-2.86713900	1.45490500
H	-0.37893400	-2.70451600	-0.23410800
C	0.58423000	0.06335400	-0.69053000
C	2.03010400	0.05010500	-0.31748300
C	2.71045000	1.13269300	0.24049500
C	2.72516900	-1.13005700	-0.59218500
C	4.06629900	1.03131100	0.51820100
H	2.21072300	2.07194600	0.42887400
C	4.07282200	-1.23648700	-0.28930700
H	2.19376300	-1.96138400	-1.03912500
C	4.74539500	-0.15358200	0.26501600
H	4.59169300	1.88161200	0.93318400
H	4.59957300	-2.16025400	-0.49081500
H	5.80051500	-0.23126400	0.49507800
O	0.19967600	-0.54030700	-1.66555900
C	-0.56381900	2.19091900	-0.61676100
H	-0.97055700	2.05845300	-1.61814100
H	-1.15137200	2.91858700	-0.06278600
H	0.44020200	2.60130900	-0.72292200
C	-0.15736500	1.08935600	1.62181800
H	0.16239400	0.18568900	2.13903100
H	0.61369500	1.84573600	1.73834700
H	-1.05688000	1.46198200	2.11547700
H	-3.34900100	-2.48547700	1.06243800
H	-4.63834300	-0.70339800	-0.78049900
H	-4.49679500	-0.38690700	0.96369800
H	-3.02538100	-2.47308800	-0.68666400

NHO2c Ketone-type cation

1 1

C	0.75881500	-0.00957200	-0.65159300
O	0.33688700	-0.68262300	-1.56218400
C	-3.98866200	0.02841600	-0.26022500
C	-3.72378800	-1.42551900	-0.55042300
C	-2.79973700	-1.94000900	0.52737300
H	-4.65884000	-1.98249300	-0.54596100
H	-4.59988900	0.14220400	0.63884100
H	-4.50460000	0.51912400	-1.08652600
H	-3.26917700	-1.89731000	1.51350700
H	-2.49887000	-2.96836800	0.33488600
C	-1.57326200	0.14512000	0.19643400
C	-0.23442800	0.90563100	0.11053100
N	-1.56860200	-1.13281500	0.54815500
N	-2.72612400	0.75919100	-0.06317700
C	-2.94407900	2.20636800	0.03671500
H	-2.24012200	2.66593300	0.72027500
H	-2.90277000	2.68869100	-0.93846100
H	-3.94081500	2.34210700	0.45349400
C	-0.40370200	-1.91232900	0.96462500
H	0.42884700	-1.29032300	1.27138000
H	-0.70741400	-2.50358500	1.82773700

H	-0.09021300	-2.57832500	0.16042200
H	-3.25452100	-1.54485700	-1.52890600
C	2.21802600	-0.02864800	-0.31889500
C	2.94465100	1.08192800	0.11028400
C	2.87364000	-1.24809000	-0.50185200
C	4.30664000	0.96881800	0.35221300
H	2.47626700	2.04924800	0.22377100
C	4.22827700	-1.36378200	-0.23480900
H	2.30703400	-2.10303500	-0.85000200
C	4.94723500	-0.25306900	0.19116800
H	4.86810000	1.83987300	0.66446300
H	4.72366500	-2.31734000	-0.36486000
H	6.00770600	-0.33821600	0.39213300
C	-0.25190900	2.11816700	-0.86180700
H	-0.86539000	1.90768000	-1.73675100
H	-0.57941200	3.03456800	-0.38195600
H	0.76464900	2.29483200	-1.21597300
C	0.16546900	1.34489000	1.53343900
H	0.64298900	0.55090000	2.10586800
H	0.84308600	2.19375800	1.50191200
H	-0.72144600	1.66136000	2.08425500

Zwitterionic NHO-ester adducts (zwitterionic mechanism): NHO1a-Ethyl benzoate adduct

0 1

C	-0.46224100	0.22961000	0.83508700
C	-2.27849700	0.90768300	1.93400200
C	-2.40071200	-0.42711500	1.71564800
N	-1.26230200	-0.82415500	1.02874200
N	-1.06422700	1.28899800	1.38307300
C	0.86245500	0.23832200	0.18295600
C	-0.98560600	-2.20416300	0.65710500
C	-0.51893000	2.64308500	1.38887300
C	-3.18507500	1.87053900	2.61404000
C	-3.47236900	-1.39003200	2.08386900
H	-3.44020700	2.70398600	1.95749700
H	-4.10735300	1.36888200	2.89887300
H	-2.72685400	2.27726100	3.51758500
H	-4.23988200	-0.88580500	2.66680700
H	-3.94422300	-1.81804600	1.19732300
H	-3.07305700	-2.21040600	2.68328500
H	-1.87177500	-2.62976400	0.19074400
H	-0.15234800	-2.23101500	-0.03561500
H	-0.71261200	-2.77150400	1.54493200
H	1.02972100	1.20569000	-0.29036700
H	-0.93544800	3.17724600	2.23869700
H	0.55917800	2.56483700	1.50893600
H	-0.78984000	3.15945500	0.46803300
H	0.90517500	-0.52867200	-0.58947200
C	1.99575600	0.02842200	1.26558800
C	3.32997100	-0.06932300	0.48872800
C	3.63185400	-1.16102700	-0.32471200
C	4.24642400	0.97113800	0.57677100
C	4.82624500	-1.21163700	-1.03247100
H	2.92900200	-1.98489300	-0.38609200
C	5.44337200	0.92842500	-0.13233500
H	4.00449800	1.80743800	1.22089400
C	5.73655000	-0.16311900	-0.93990300
H	5.05181700	-2.07022100	-1.65416100
H	6.14969400	1.74648000	-0.05175300
H	6.66815900	-0.20041100	-1.49138700
O	1.97470800	0.93405000	2.20353400
O	1.66799800	-1.33662600	1.72663800
C	2.45408100	-1.76033300	2.81801500
H	2.36168900	-1.04532800	3.63993500
H	3.51332200	-1.79755100	2.52831300
C	1.97892900	-3.13509800	3.24350100
H	2.57574700	-3.50376300	4.07964100
H	0.93424700	-3.09682100	3.55916900
H	2.06362300	-3.84609200	2.41921900

NHO1a-methyl benzoate adduct

0 1

C	-1.30038500	0.11068700	-0.61097800
C	-3.36411500	0.77003700	-0.08849400
C	-3.37558400	-0.58395400	-0.19219300
N	-2.08266400	-0.96944300	-0.51700900
N	-2.06367900	1.17511900	-0.34781700
C	0.14532300	0.14644900	-0.90879100
C	-1.67483800	-2.35699900	-0.68205200
C	-1.58976800	2.55566900	-0.34246700
C	-4.44960100	1.73203400	0.23931600
C	-4.47031100	-1.57496600	-0.02005400
H	-4.56145300	2.48442400	-0.54315300
H	-5.39440000	1.20189500	0.33760000
H	-4.25102200	2.24765100	1.18089800
H	-5.38700300	-1.06738600	0.27188900
H	-4.66218000	-2.11847300	-0.94722200
H	-4.22355400	-2.30396800	0.75409200
H	-2.30510600	-2.82943900	-1.43366300
H	-0.63468500	-2.39194500	-0.98388800
H	-1.77522000	-2.87729900	0.26903900
H	0.38398300	1.07402900	-1.42895800
H	-2.22799800	3.13655300	0.31806600

H	-0.57620900	2.55561900	0.05066700
H	-1.63707400	2.97108200	-1.34908700
H	0.41688900	-0.68433700	-1.55887400
C	0.97272900	0.11977800	0.43695200
C	2.46607000	0.12382800	0.03168300
C	3.06352400	-0.96979800	-0.59387900
C	3.23206300	1.25829400	0.26849600
C	4.40001900	-0.92933700	-0.97168000
H	2.47681900	-1.86488600	-0.76977900
C	4.57039800	1.30687400	-0.11075800
H	2.75820600	2.09612000	0.76467600
C	5.15855500	0.21240600	-0.73221000
H	4.85358200	-1.78952200	-1.45000100
H	5.15534400	2.19825800	0.08392600
H	6.20087200	0.24518200	-1.02574700
O	0.62797800	1.06594100	1.26437900
O	0.66512300	-1.24658600	0.91203200
C	1.18475400	-1.49849100	2.19566000
H	0.79665400	-0.78476400	2.92517900
H	2.28054200	-1.44315300	2.20155600
H	0.88446100	-2.50812900	2.47834100

NHO1b-Ethyl benzoate adduct

0 1

C	1.79288800	-0.53518400	-0.58937000
C	3.96711100	-0.84273200	0.07484600
C	3.80259400	0.56649300	-0.49634100
N	2.45774600	0.50934200	-1.07651100
N	2.58044000	-1.30770500	0.13992100
C	0.36100500	-0.79877100	-0.81694000
C	1.89482700	1.70976900	-1.66121000
C	2.26086600	-2.62377800	0.66054100
H	2.56897000	2.06360500	-2.44095000
H	0.92130600	1.50150700	-2.09323500
H	1.77405200	2.47763400	-0.89503400
H	2.78995100	-2.75259600	1.60422300
H	1.19449900	-2.67266600	0.85981700
H	2.58326300	-3.39990400	-0.03827400
C	-0.47922500	-0.31130700	0.44850000
C	-1.96288200	-0.34900600	0.00765000
C	-2.47930400	0.55565900	-0.91948000
C	-2.80251900	-1.32461400	0.52936100
C	-3.80953100	0.48756900	-1.31320700
H	-1.83236000	1.32887000	-1.32017700
C	-4.13497300	-1.40251200	0.13398400
H	-2.39213400	-2.01189000	1.25876300
C	-4.64249500	-0.49611200	-0.78841800
H	-4.20032300	1.20271700	-2.02764800
H	-4.77915300	-2.16857000	0.54949900
H	-5.67993400	-0.55174600	-1.09517600
O	-0.21356700	-0.97787100	1.53042300
O	-0.07736900	1.10889000	0.48787300
C	-0.59229200	1.80093900	1.60450400
H	-0.26344400	1.31389800	2.52648100
H	-1.69041600	1.77493600	1.59013100
C	-0.10123000	3.23322300	1.54249600
H	-0.48105100	3.80556600	2.39058300
H	0.99002500	3.26389300	1.56908700
H	-0.43632800	3.71622500	0.62244800
H	0.18646200	-1.86749800	-0.92803200
H	0.03406200	-0.29344800	-1.72244100
H	4.42119900	-0.85543000	1.06365500
H	4.53991600	0.81017200	-1.25865000
H	3.82444400	1.33356100	0.28324600
H	4.53814200	-1.49625000	-0.59005000

NHO1b-methyl benzoate adduct

0 1

C	-1.79940900	0.16580100	-0.55489500
C	-3.81236000	0.98445200	0.17198800
C	-3.98060000	-0.47615600	-0.24856400
N	-2.59131900	-0.89341100	-0.45381900
N	-2.45872500	1.28635700	-0.30074900
C	-0.36359600	0.10255000	-0.88359300
C	-2.28133300	-2.24577700	-0.87660500
C	-1.90319300	2.60314800	-0.05990800
H	-2.53238900	-2.38972900	-1.93038200
H	-1.22997900	-2.44917400	-0.69552600
H	-2.87476800	-2.93204500	-0.27384500
H	-1.88613000	2.80297400	1.01196600
H	-0.88452600	2.65488200	-0.42732500
H	-2.52427600	3.34191200	-0.56743100
C	0.46798800	-0.00906200	0.46847400
C	1.95618200	0.07947700	0.05413200
C	2.58800900	-0.94142800	-0.65425200
C	2.67672100	1.22708500	0.36152600
C	3.91542800	-0.81683000	-1.04561300
H	2.03560200	-1.84511600	-0.88618600
C	4.00549400	1.35906300	-0.03031800
H	2.17449200	2.00741900	0.92019800
C	4.62860400	0.33719400	-0.73606900
H	4.39738800	-1.62100800	-1.58928300
H	4.55647000	2.25868200	0.21799200
H	5.66336800	0.43575600	-1.04085100
O	0.09383400	0.85265600	1.36532500
O	0.21061300	-1.41993600	0.82826600

C	0.73463100	-1.75195200	2.09228500
H	0.30377000	-1.12469100	2.87539800
H	1.82567700	-1.63887900	2.11461000
H	0.48749000	-2.79648500	2.28487700
H	-0.06261200	1.02013100	-1.38449700
H	-0.15794700	-0.73852400	-1.54337800
H	-4.53822600	1.65270000	-0.28682100
H	-4.53105200	-0.57549500	-1.18807100
H	-4.45770900	-1.08990200	0.51254900
H	-3.84531400	1.10880600	1.25773900

NHO1c-Ethyl benzoate adduct

0 1

C	-0.21990400	-0.51980700	0.84582200
C	0.63008100	-0.02225500	-0.41601000
C	2.10319100	-0.31952100	-0.03863500
C	2.78714600	0.42226800	0.92285400
C	2.75217400	-1.38862900	-0.64532700
C	4.09541100	0.10314000	1.26748900
H	2.29180200	1.26597200	1.39062100
C	4.06058600	-1.71490800	-0.30225700
H	2.21383600	-1.95109200	-1.39866800
C	4.73651700	-0.96968400	0.65606400
H	4.61835200	0.69290000	2.01122700
H	4.55489000	-2.54924800	-0.78627300
H	5.75645200	-1.21904500	0.92289600
O	0.24855000	-0.52690600	-1.55090300
O	0.45125100	1.43691600	-0.31303800
C	1.00147300	2.13920800	-1.40659700
H	0.49777600	1.84515800	-2.33123800
H	2.06541200	1.88924100	-1.51739700
C	0.83554800	3.62277100	-1.14586900
H	1.23291900	4.20517900	-1.97892300
H	-0.22048200	3.87220100	-1.02447600
H	1.36426900	3.91515700	-0.23661500
H	0.07378700	-1.54443600	1.05709100
H	0.02793700	0.08288000	1.71500900
C	-3.81609600	0.72546900	0.60626700
C	-4.17794500	-0.11405100	-0.59689400
C	-3.67129300	-1.52290000	-0.38784800
H	-5.25799600	-0.12094300	-0.73517200
H	-4.38561700	0.41854800	1.48896100
H	-4.03015100	1.77627500	0.41686600
H	-4.21859400	-2.02719600	0.41411100
H	-3.78921200	-2.10927000	-1.29716600
C	-1.67903800	-0.46608300	0.55379000
N	-2.24364200	-1.49939200	-0.05958400
N	-2.38377600	0.61252900	0.89203600
C	-1.82183600	1.66021600	1.75035700
H	-1.67774200	1.28847100	2.76640200
H	-0.88435900	2.02344900	1.33978600
H	-2.53647400	2.47834600	1.78164500
C	-1.48774700	-2.72331000	-0.35035500
H	-0.55400800	-2.46355200	-0.84274700
H	-1.31079100	-3.29149900	0.56502000
H	-2.08910800	-3.33078600	-1.02143200
H	-3.71897500	0.30971400	-1.49226500

NHO1c-methyl benzoate adduct

0 1

C	0.69198500	0.25262400	0.52202700
C	2.17173800	0.14553800	0.07051000
C	2.69373200	-1.03094400	-0.46567000
C	2.99916100	1.25637000	0.17544100
C	4.01535600	-1.09518700	-0.88788200
H	2.05928400	-1.90820200	-0.53541800
C	4.32332300	1.20047200	-0.25042400
H	2.58531700	2.15992600	0.60596800
C	4.83542900	0.02443200	-0.78366800
H	4.40940600	-2.01894400	-1.29528500
H	4.95709500	2.07541200	-0.16410500
H	5.86610800	-0.02268100	-1.11373100
O	0.42727800	1.28099800	1.26969100
O	0.34594200	-1.04393200	1.13717500
C	0.89273200	-1.18956900	2.42671200
H	0.50255300	-0.43441000	3.11221500
H	1.98685000	-1.11289500	2.40819700
H	0.61765200	-2.18209400	2.78515300
C	-3.64598400	-1.25581400	-0.27823500
C	-4.17572400	-0.08497300	0.51627600
C	-3.76435400	1.19848000	-0.16896300
H	-5.26078000	-0.14529900	0.58608800
H	-4.18740400	-1.37175100	-1.22180400
H	-3.75439700	-2.18057300	0.28708500
H	-4.24880200	1.29850700	-1.14546500
H	-4.03831000	2.06276000	0.43259900
C	-1.62304700	0.10766200	-0.56720100
C	-0.15708500	0.18847400	-0.82863700
H	0.15900800	-0.66127300	-1.42538600
H	0.07349500	1.09014800	-1.39117700
N	-2.31129700	1.22242000	-0.34394900
N	-2.21844800	-1.08304800	-0.56719100
C	-1.50628300	-2.30225100	-0.96293000
H	-1.26339100	-2.28062900	-2.02620300
H	-0.60476000	-2.42334900	-0.36878700
H	-2.16910300	-3.14364300	-0.78049600

C	-1.70094400	2.54935100	-0.46827900
H	-0.69945800	2.52693700	-0.05036500
H	-1.70257600	2.87257900	-1.51233700
H	-2.30095400	3.24464600	0.11446400
H	-3.76458700	-0.10531100	1.52737800

NHO1d-Ethyl benzoate adduct

0 1

C	1.86359000	-0.55279500	-0.56936400
C	3.90319000	-0.93437800	0.20713400
C	3.90723300	0.28336000	-0.38110200
N	2.63448600	0.50317100	-0.85999600
N	2.62869600	-1.43574200	0.08148900
C	0.42458700	-0.71598800	-0.84700700
C	2.21310000	1.73658400	-1.51428700
C	2.17089400	-2.73202900	0.57824800
H	3.00569700	2.05515800	-2.18720600
H	1.30159600	1.55512900	-2.07373200
H	2.01471600	2.49606700	-0.76219100
H	0.19689100	-1.77421000	-0.97466900
H	2.90591800	-3.09548500	1.29118700
H	1.21222500	-2.57872500	1.06974500
H	2.08848500	-3.43536200	-0.24940500
H	0.15415400	-0.19208200	-1.76297500
C	-0.40900000	-0.18864000	0.39005000
C	-1.90007200	-0.32882600	0.00228300
C	-2.47777100	0.45367100	-0.99670700
C	-2.68512900	-1.27586200	0.64755000
C	-3.81374100	0.29234900	-1.34176000
H	-1.87602900	1.20791400	-1.49204800
C	-4.02355300	-1.44449800	0.30481200
H	-2.22636300	-1.86666300	1.43044600
C	-4.59172400	-0.66113500	-0.69152500
H	-4.25184500	0.91278300	-2.11473500
H	-4.62423000	-2.18569900	0.81888800
H	-5.63379700	-0.78806900	-0.95860700
O	-0.07372200	-0.76956900	1.50778700
O	-0.08413400	1.25042200	0.33085600
C	-0.61950300	1.98369300	1.41093100
H	-0.29301600	1.54137100	2.35606800
H	-1.71704300	1.94135800	1.38617600
C	-0.14932800	3.41967200	1.29473000
H	-0.56908000	4.02547100	2.09964300
H	0.93937800	3.47306200	1.35920400
H	-0.46018200	3.85098600	0.34106500
H	4.68506900	-1.48224000	0.70233100
H	4.69138700	1.00933900	-0.50269900

NHO1d-methyl benzoate adduct

0 1

C	-1.85238500	0.18515600	-0.57632100
C	-3.87826400	0.82475200	0.05266500
C	-3.91177500	-0.51212700	-0.14767000
N	-2.64734500	-0.89197700	-0.54023800
N	-2.59474300	1.23831200	-0.21685500
C	-0.41130000	0.22741800	-0.88518200
C	-2.25790400	-2.27240900	-0.80384900
C	-2.10609800	2.61267800	-0.12316300
H	-3.07865000	-2.76567400	-1.31911200
H	-1.37042200	-2.28538100	-1.42789300
H	-2.03502600	-2.77213700	0.13534900
H	-0.16255300	1.19455900	-1.32211600
H	-2.84988300	3.19422300	0.41453300
H	-1.16752900	2.59417300	0.42690600
H	-1.97464300	3.02592400	-1.12231100
H	-0.15152700	-0.55218400	-1.60027600
C	0.41377500	0.07519100	0.45632200
C	1.90699800	0.10613200	0.05555100
C	2.50767800	-0.94399400	-0.63751200
C	2.66889700	1.22676800	0.36326200
C	3.84376600	-0.87448400	-1.01273200
H	1.92367200	-1.82795300	-0.86885600
C	4.00614700	1.30471600	-0.01414700
H	2.19209700	2.02977700	0.91167900
C	4.59764300	0.25360800	-0.70374000
H	4.30102600	-1.70158300	-1.54314400
H	4.58797800	2.18478300	0.23407900
H	5.63924100	0.30906600	-0.99621800
O	0.07106900	0.94651600	1.36240000
O	0.09032700	-1.32434200	0.80459100
C	0.59441800	-1.69598800	2.06549400
H	0.21756000	-1.03648500	2.84991800
H	1.69105100	-1.66816500	2.08163600
H	0.26738300	-2.71805600	2.26057100
H	-4.64438100	1.51303900	0.36231800
H	-4.71152900	-1.22416300	-0.04720800

NHO1e-Ethyl benzoate adduct

0 1

C	1.54110000	0.24673200	-0.75111100
C	3.65614000	0.31914900	-0.10049500
C	3.34297800	1.52931500	-0.61635200
N	2.02776400	1.46781300	-1.01425800
N	2.52466500	-0.46268000	-0.18747500
C	0.15610500	-0.19365100	-1.00190100

C	1.27980900	2.55836500	-1.63267900
C	2.44312200	-1.87044600	0.25572200
H	1.89288100	3.45390400	-1.58355900
H	1.07260300	2.31946400	-2.67476600
H	0.35302000	2.70477600	-1.08242400
H	0.14248300	-1.23762700	-1.31445200
H	1.39055900	-2.12892800	0.17707700
H	-0.27468000	0.40993900	-1.80087800
C	-0.69625800	-0.07301300	0.32917900
C	-2.14143300	-0.47445900	-0.04960800
C	-2.93505800	0.32026800	-0.87648200
C	-2.65662300	-1.67820000	0.41509200
C	-4.21645500	-0.08227300	-1.23160700
H	-2.54586000	1.26906300	-1.23010700
C	-3.93832600	-2.08881300	0.06016400
H	-2.03478400	-2.28004600	1.06633100
C	-4.72178000	-1.29241600	-0.76563100
H	-4.82491000	0.54815100	-1.86958900
H	-4.32690300	-3.03027100	0.43089500
H	-5.72021600	-1.60813800	-1.04272400
O	-0.18172700	-0.73500300	1.32401700
O	-0.69356900	1.39547000	0.50678600
C	-1.29089400	1.81285600	1.71436900
H	-0.79686800	1.32603900	2.55929600
H	-2.34876400	1.51675800	1.73348400
H	4.57689300	-0.04523600	0.31875700
H	3.93071000	2.42250100	-0.73218500
C	2.83800700	-1.96992500	1.71994200
H	2.70641900	-2.99996700	2.05239600
H	3.88485500	-1.69986600	1.87314700
H	2.19500200	-1.32255500	2.31435700
C	3.29525700	-2.74109400	-0.65675600
H	4.35024500	-2.46753600	-0.58691100
H	3.19508000	-3.78409200	-0.35572600
H	2.97748900	-2.64696900	-1.69589600
C	-1.16603700	3.32033000	1.80752100
H	-1.61134500	3.68656400	2.73413500
H	-0.11494000	3.61581600	1.79056100
H	-1.67152300	3.80224100	0.96827500

NHO1e-methyl benzoate adduct

0 1

C	1.49772500	0.53345600	-0.54866600
C	3.62088400	0.32551900	0.04177000
C	3.37077500	1.64260200	-0.13589300
N	2.04916300	1.75380200	-0.50046400
N	2.44561900	-0.34770300	-0.21344300
C	0.08819800	0.24543300	-0.87297100
C	1.35578800	3.00255000	-0.80021600
C	2.28958200	-1.81650600	-0.15668300
H	1.99131100	3.82357700	-0.48069200
H	1.17609800	3.07827500	-1.87155700
H	0.41748000	3.02022000	-0.25172000
H	0.01690300	-0.67484000	-1.45229800
H	1.22018200	-1.98951400	-0.24969900
H	-0.31730900	1.05978800	-1.47311700
C	-0.74206200	0.04213400	0.45940000
C	-2.20846000	-0.19268500	0.02563700
C	-2.95165100	0.80121800	-0.61026300
C	-2.80004300	-1.42959900	0.24839400
C	-4.25730200	0.56197700	-1.01806300
H	-2.50406500	1.77610600	-0.77057300
C	-4.10799900	-1.67678900	-0.15929400
H	-2.21638800	-2.18792100	0.75529700
C	-4.84021300	-0.68232800	-0.79519900
H	-4.82376800	1.34570700	-1.50728200
H	-4.55714500	-2.64653700	0.02138900
H	-5.85844000	-0.87177700	-1.11262500
O	-0.24009200	-0.87286300	1.23489500
O	-0.68645300	1.41427900	1.02092700
C	-1.27155000	1.49432500	2.29910700
H	-0.79946100	0.79464400	2.99217000
H	-2.34636000	1.27750200	2.26009200
H	-1.13326100	2.51361900	2.66103800
H	4.52475700	-0.18132100	0.32857100
H	4.00729000	2.50355800	-0.03469400
C	2.72058500	-2.32641700	1.20865300
H	2.52794500	-3.39825100	1.26189200
H	3.78743700	-2.16939800	1.38011100
H	2.14205200	-1.82552800	1.98341800
C	3.05924700	-2.45226800	-1.30563900
H	4.13025600	-2.25923400	-1.21374300
H	2.90618800	-3.53149500	-1.28893700
H	2.71617600	-2.06693700	-2.26670400

NHO2a-Ethyl benzoate adduct

0 1

C	1.37473100	-0.39738600	-0.44824900
C	3.47029900	-0.76186900	0.25912500
C	3.45369500	0.44147300	-0.36048700
N	2.14889500	0.65620900	-0.78255800
N	2.17719600	-1.25803000	0.20534700
C	-0.08996500	-0.60812700	-0.79503200
C	1.74849000	1.92286200	-1.39890000
C	1.80457100	-2.49357200	0.89950900
C	4.59235200	-1.49764100	0.90335100

C	4.55742900	1.41197500	-0.59585700
H	4.67338900	-2.51413200	0.51571000
H	5.52977000	-0.98382800	0.70342800
H	4.46606800	-1.55546100	1.98619800
H	5.49896900	0.97542300	-0.27061700
H	4.64813700	1.66362600	-1.65359900
H	4.40809100	2.33715700	-0.03608800
H	1.64044600	1.81063600	-2.47505500
H	0.82321400	2.25918300	-0.94333500
H	2.52929000	2.64849000	-1.19544500
H	2.54319200	-2.66753400	1.67609500
H	0.83285200	-2.33359400	1.35557600
H	1.80533400	-3.33499300	0.20932000
C	-0.92480400	-0.11824000	0.48277200
C	-2.43624700	-0.21724400	0.16146700
C	-3.13929400	0.78905600	-0.49987900
C	-3.13015400	-1.35883000	0.55483800
C	-4.49724300	0.65477100	-0.76845100
H	-2.61651900	1.69275300	-0.78940400
C	-4.48489300	-1.50522700	0.27925000
H	-2.58750600	-2.12563400	1.09398600
C	-5.17435200	-0.49733400	-0.38570000
H	-5.02829400	1.45282500	-1.27430600
H	-5.00660800	-2.40307800	0.58956000
H	-6.23158700	-0.60500200	-0.59593800
O	-0.58064300	-0.75976600	1.56965500
O	-0.58496300	1.31553100	0.50393600
C	-0.98682900	1.97614400	1.68358900
H	-0.51153700	1.51110300	2.55063500
H	-2.07329400	1.88749900	1.81676200
C	-0.59010500	3.43391900	1.56130900
H	-0.88050700	3.98805200	2.45550400
H	0.49111000	3.52531000	1.43678200
H	-1.07471400	3.89430700	0.69773200
C	-0.37669900	-2.09983800	-1.05097300
H	-0.46142000	-2.66763900	-0.13044500
H	-1.32859200	-2.18541300	-1.57353800
H	0.39193600	-2.54737500	-1.68601200
C	-0.45926500	0.12266600	-2.09941400
H	-1.42045700	-0.25490000	-2.44473400
H	-0.56293500	1.19505900	-1.97627700
H	0.27408000	-0.08157500	-2.88435400

NHO2a-methyl benzoate adduct

0 1

C	-1.35132600	0.10327500	-0.41632100
C	-3.43464400	0.74605600	0.10484300
C	-3.46183600	-0.59087100	-0.10489800
N	-2.16391800	-0.97317000	-0.41343500
N	-2.12265300	1.15380600	-0.07832900
C	0.11721300	0.14370800	-0.80878700
C	-1.80918400	-2.38296300	-0.58656400
C	-1.70060000	2.52649400	0.21153400
C	-4.52996100	1.68771600	0.46328700
C	-4.59894400	-1.54958800	-0.04842300
H	-4.55458900	2.54159100	-0.21519900
H	-5.48776800	1.17645400	0.39908600
H	-4.41917800	2.06601400	1.48126000
H	-5.53078900	-1.00221000	0.07396800
H	-4.66842200	-2.13624800	-0.96564500
H	-4.50428300	-2.24008600	0.79182400
H	-1.74010200	-2.63701700	-1.64192400
H	-0.87363400	-2.57374400	-0.07371800
H	-2.59282100	-2.97711800	-0.12725800
H	-2.42536500	2.95290900	0.89879000
H	-0.73145800	2.47331100	0.69753900
H	-1.67660000	3.12076900	-0.69991900
C	0.95037500	0.04983200	0.55389500
C	2.46316200	0.07318300	0.22402100
C	3.17305100	-1.06151900	-0.16626300
C	3.15070400	1.27908400	0.33087600
C	4.53292000	-0.99067900	-0.44937900
H	2.65524300	-2.01093000	-0.23035000
C	4.50748000	1.35991000	0.03888700
H	2.59934600	2.15067700	0.66175400
C	5.20432600	0.22269400	-0.35352400
H	5.07109200	-1.88542500	-0.73985900
H	5.02402600	2.30876200	0.12518300
H	6.26329200	0.27912400	-0.57475600
O	0.59004400	0.97109900	1.40918500
O	0.63405900	-1.32426700	0.99403400
C	1.05899000	-1.58488800	2.31066000
H	0.60617200	-0.88612100	3.01636600
H	2.14972000	-1.51366400	2.40130000
H	0.75363400	-2.60321100	2.55526300
C	0.44876600	1.47390200	-1.51308500
H	0.56977800	2.29367200	-0.81288700
H	1.39453000	1.35877300	-2.04084500
H	-0.31517000	1.73337600	-2.25007000
C	0.44667600	-0.96392500	-1.82754300
H	1.41365500	-0.74154600	-2.27579500
H	0.52099200	-1.94979500	-1.38266000
H	-0.29114200	-0.98594600	-2.63414000

NHO2b-Ethyl benzoate adduct

0 1

C	-1.80319600	-0.43783000	0.37401000
C	-3.97839600	-0.72545500	-0.34041900
C	-3.86593300	0.60087700	0.38841600
N	-2.51633300	0.53318000	0.96154200
N	-2.57654600	-1.13084100	-0.45778700
C	-0.34812300	-0.75353900	0.67050500
C	-2.06268100	1.72963100	1.66955800
C	-2.28092200	-2.28491600	-1.29628800
H	-2.86586400	2.46020200	1.59130800
H	-1.88857600	1.52530700	2.72361300
H	-1.17043800	2.13423000	1.19956200
H	-3.00336900	-2.27222000	-2.11162800
H	-1.28287100	-2.17526700	-1.70521400
H	-2.39933800	-3.21586900	-0.73885000
C	0.50488800	-0.12585700	-0.55064600
C	2.00599400	-0.19602100	-0.17642300
C	2.66180500	0.80665700	0.53671200
C	2.73929900	-1.30977800	-0.57793600
C	4.01319200	0.69661600	0.84516000
H	2.10697000	1.68763200	0.83790400
C	4.08718100	-1.43339200	-0.26010500
H	2.23466900	-2.07320800	-1.15742100
C	4.72981700	-0.42859000	0.45418700
H	4.50905000	1.49235200	1.38889000
H	4.63976700	-2.31050200	-0.57626000
H	5.78191000	-0.51722800	0.69652800
O	0.23012300	-0.68094600	-1.69703500
O	0.09830700	1.28752300	-0.45515400
C	0.51700200	2.07558300	-1.54854100
H	0.06692900	1.70388800	-2.47262700
H	1.60637300	2.01275700	-1.66701700
C	0.09954800	3.50721300	-1.27780900
H	0.39624100	4.15645400	-2.10323100
H	-0.98442100	3.57253200	-1.16115200
H	0.56529400	3.87750500	-0.36196000
H	-4.43080800	-0.63678000	-1.32595600
H	-4.60750000	0.72726800	1.17435200
H	-3.91880200	1.45329600	-0.29423100
H	-4.52341300	-1.47797600	0.23583300
C	0.06703800	-0.20663700	2.04760400
H	1.01067800	-0.67005700	2.32893900
H	0.22387800	0.86644900	2.04894900
H	-0.66938700	-0.46552400	2.81269400
C	-0.12411600	-2.27557800	0.72189100
H	-0.91793800	-2.77795900	1.28022100
H	-0.04664400	-2.71075500	-0.26812500
H	0.81595000	-2.46941700	1.23685800

NHO2b-methyl benzoate adduct

0 1

C	-1.81267600	0.13117100	-0.35261700
C	-3.96257800	0.79098100	0.17307900
C	-3.92901800	-0.72015700	0.02228300
N	-2.57717100	-0.95738000	-0.49675200
N	-2.54127200	1.13946800	0.11972500
C	-0.35117600	0.23213100	-0.76129700
C	-2.20314900	-2.35309100	-0.71003300
C	-2.16219400	2.49775100	0.48380000
H	-2.08661100	-2.57520600	-1.76897800
H	-1.29695400	-2.59026900	-0.16187900
H	-3.02053300	-2.95762500	-0.32076300
H	-2.87612100	2.83205200	1.23572200
H	-1.16995700	2.47523700	0.92133000
H	-2.22031200	3.16825100	-0.37525100
C	0.50957000	0.06559800	0.58829500
C	2.01300400	0.06312000	0.21308600
C	2.69324600	-1.08004000	-0.20380100
C	2.72219800	1.25748900	0.30754100
C	4.04584900	-1.02866700	-0.52369600
H	2.15861500	-2.02047800	-0.26167100
C	4.07115400	1.31918100	-0.02282000
H	2.19619200	2.13560200	0.66138100
C	4.73857600	0.17355200	-0.44066100
H	4.56137700	-1.92995600	-0.83427000
H	4.60449600	2.25954200	0.05323100
H	5.79158800	0.21479400	-0.69194100
O	0.20240800	0.95672500	1.48955200
O	0.16024100	-1.31557000	0.97329300
C	0.59858500	-1.64601600	2.27009000
H	0.16166900	-0.97932300	3.01566500
H	1.69081400	-1.59032200	2.35103500
H	0.28468200	-2.67213200	2.46650000
H	-4.48617700	1.28509200	-0.64925900
H	-4.67303100	-1.10069000	-0.67454700
H	-4.03964800	-1.23609200	0.97952900
H	-4.39655100	1.11788500	1.11583700
C	-0.01019300	-0.80598800	-1.84544800
H	0.94853100	-0.53726800	-2.28502400
H	0.08496500	-1.81366100	-1.45709000
H	-0.75459400	-0.79580100	-2.64590300
C	-0.06316200	1.61306600	-1.38018100
H	-0.85652200	1.91454000	-2.06835700
H	0.07036500	2.38046600	-0.62541400
H	0.86341000	1.55100600	-1.94916100

NHO2c-Ethyl benzoate adduct

0 1

C	-0.75974300	-0.11055600	0.63454100
C	-2.21341700	-0.27611500	0.11581500
C	-2.87845700	0.70633400	-0.61607400
C	-2.89507000	-1.45499400	0.40852800
C	-4.18469300	0.51332200	-1.05159300
H	-2.36787300	1.63700700	-0.83474000
C	-4.19554500	-1.66180300	-0.03708500
H	-2.39129800	-2.20504800	1.00565300
C	-4.84626700	-0.67651400	-0.77094300
H	-4.68845500	1.29450700	-1.60892800
H	-4.70597700	-2.58898500	0.19593300
H	-5.86250700	-0.83043900	-1.11299600
O	-0.58634100	-0.64646500	1.81330400
O	-0.45062900	1.32283900	0.59162100
C	-1.02266200	2.06501900	1.64794400
H	-2.09951200	1.86645700	1.71243400
H	-0.57846900	1.76457200	2.60019400
C	3.75163900	0.93506200	-0.89798400
C	4.47128300	-0.36627800	-0.67479900
C	3.94516400	-0.93194100	0.61684800
H	3.97646500	1.35241700	-1.88026400
H	4.03971000	1.67548700	-0.14536600
H	4.32503300	-1.93784100	0.79732200
H	4.23443700	-0.30704600	1.46719200
C	1.71407000	-0.28031600	-0.20916500
C	0.23985100	-0.68310300	-0.50138300
N	2.48152200	-1.04303900	0.57604300
N	2.29497200	0.74491000	-0.85164800
C	1.62338800	1.90810000	-1.44140400
H	1.58772600	1.82806800	-2.52830900
H	0.64213300	2.04534100	-1.01363200
H	2.22978400	2.77559700	-1.17726900
C	2.00740500	-1.98156300	1.59976900
H	0.97371000	-1.76235500	1.85170100
H	2.16156800	-3.01052700	1.27083100
H	2.62432500	-1.80257800	2.48241700
C	0.12588000	-2.22577800	-0.53696800
H	-0.01840300	-2.65669900	0.44667000
H	-0.74338900	-2.49656100	-1.13320600
H	1.00238500	-2.67822000	-1.00639300
C	-0.16261400	-0.23238200	-1.92538700
H	-0.46614200	0.80536000	-1.98925600
H	0.64460600	-0.41400600	-2.63899800
H	-1.02016700	-0.82338600	-2.23932000
H	4.27559600	-1.05627700	-1.49834100
H	5.54544500	-0.20021800	-0.61052400
C	-0.77474800	3.53426100	1.36963200
H	0.29627300	3.73431200	1.29769300
H	-1.24227100	3.83085600	0.42821800
H	-1.18721000	4.15159200	2.16936400

NHO2c-methyl benzoate adduct

0 1

C	-0.78002600	0.04758400	0.65868200
C	-2.24581200	-0.07445300	0.15876700
C	-2.92916200	0.97886600	-0.44715300
C	-2.91816200	-1.27999000	0.33844200
C	-4.24284800	0.82635800	-0.87723900
H	-2.43077900	1.93317900	-0.56484600
C	-4.22871300	-1.44304800	-0.09593500
H	-2.39615700	-2.08534100	0.84036800
C	-4.89621300	-0.38902600	-0.70935800
H	-4.75912700	1.65974500	-1.33934600
H	-4.73259200	-2.39131800	0.05074000
H	-5.91894900	-0.51019700	-1.04517300
O	-0.50434900	-0.77017200	1.63909100
O	-0.58449200	1.46337100	1.01009200
C	-1.19047600	1.81511900	2.23192700
H	-0.79553700	1.21804700	3.05555300
H	-2.27802000	1.68119400	2.19271400
H	-0.97372600	2.86971500	2.40711200
C	3.88137000	1.05147200	-0.24612700
C	4.44221100	-0.28936000	-0.63337100
C	3.79572900	-1.30261300	0.27094400
H	4.20250500	1.83226600	-0.93633000
H	4.20560800	1.33782900	0.75900400
H	4.05007700	-2.32159400	-0.02263000
H	4.11522400	-1.16366600	1.30826900
C	1.69244900	-0.08798300	-0.16337700
C	0.19794000	-0.13746400	-0.60598600
N	2.33230800	-1.20460900	0.20111000
N	2.41205200	1.03563800	-0.29115300
C	1.89790100	2.40815400	-0.34136400
H	1.93718300	2.79920300	-1.35869400
H	0.90264200	2.46219300	0.07397200
H	2.56211600	3.00533300	0.28480900
C	1.71473000	-2.42345700	0.73749400
H	0.71790500	-2.19859000	1.09976300
H	1.73568000	-3.22128200	-0.00635800
H	2.32950400	-2.72466100	1.58737800
C	-0.09607900	-1.51199600	-1.25688400
H	-0.34240200	-2.27984200	-0.53268300
H	-0.95962800	-1.40744600	-1.91036200
H	0.74440400	-1.84949000	-1.86723600
C	-0.05390500	0.88449100	-1.74055900
H	-0.22512900	1.89527100	-1.39246900

H	0.77530800	0.88748700	-2.45262300
H	-0.94788500	0.58372900	-2.28209600
H	4.21275000	-0.51025500	-1.67806600
H	5.52364100	-0.30021600	-0.50734400

Zwitterionic mechanism, transition states:

NHO 1a, TS1 (v = -388.93i (cm^{-1}))

0 1

C	-0.29766400	-0.09972300	0.09503700
C	1.01132600	-0.21128400	-0.35622000
C	1.77777500	0.92877100	-0.57321000
C	-0.08041300	2.29314000	0.12497200
C	1.22709500	2.18193300	-0.33094200
C	-0.85217400	1.15530500	0.33764500
H	1.43621800	-1.19145200	-0.53699300
H	2.79742800	0.84034500	-0.92716900
H	1.81854700	3.07476100	-0.49473200
H	-7.34179500	3.19957600	1.26875500
H	-0.52007500	3.26286100	0.32367000
C	-2.27249700	1.33575900	0.82046900
O	-2.63352500	2.39741200	1.35700900
O	-2.75986800	0.12354100	1.31768900
C	-3.85095400	0.24177600	2.21635900
H	-4.25833100	-0.76230700	2.33313900
H	-3.51725300	0.61825100	3.18500500
H	-4.62502200	0.90878300	1.83446600
C	-4.44860200	1.21924900	-0.79333100
C	-6.44799600	0.39120500	-0.18178000
C	-6.50836100	1.73889700	-0.05952900
N	-5.26135200	2.23865100	-0.43478000
N	-5.16891100	0.08286000	-0.64383800
C	-3.07404800	1.29886500	-1.07981600
C	-4.63615000	-1.23924500	-0.91699700
C	-4.88223300	3.63910000	-0.52777800
C	-7.61731500	2.62756500	0.38007600
C	-7.46306600	-0.65780000	0.10269500
H	-0.89514900	-0.98716900	0.26178100
H	-7.89404000	3.33577400	-0.40372800
H	-8.49511600	2.03220300	0.62227500
H	-8.38042800	-0.19670500	0.46245900
H	-7.70392200	-1.23664000	-0.79145400
H	-7.11101200	-1.35160400	0.86973500
H	-3.75476500	-1.41580500	-0.30037500
H	-5.39585700	-1.98101300	-0.68699300
H	-4.36654300	-1.32308300	-1.97088200
H	-2.64879200	0.43019700	-1.56667500
H	-2.71795600	2.24910100	-1.45773400
H	-3.89301700	3.76575700	-0.09473900
H	-4.88926100	3.96587600	-1.56949500
H	-5.59362100	4.23470800	0.03811400

NHO 1a, TS2 (v = -181.22i (cm^{-1}))

0 1

C	-1.18023000	-0.85862900	-0.00280100
C	-3.07292200	-0.26683900	-1.01789500
C	-3.40273200	-0.95625000	0.10513800
N	-2.21062900	-1.30394700	0.72165800
N	-1.68683600	-0.22117600	-1.06433800
C	0.25025300	-0.98434800	0.36836700
C	-2.10333400	-2.06688400	1.96260600
C	-0.93251400	0.47793800	-2.09863500
C	-3.92054900	0.36488000	-2.06331000
C	-4.72741300	-1.33028100	0.66708400
H	-3.77817000	-0.11311100	-3.03428300
H	-4.96969400	0.27399300	-1.79133000
H	-3.68702200	1.42577300	-2.16890500
H	-5.51767700	-1.01138900	-0.00868800
H	-4.80701300	-2.41059500	0.79939400
H	-4.89579000	-0.85551400	1.63547800
H	-2.08007200	-3.13357500	1.74236200
H	-1.20572800	-1.75154900	2.48686400
H	-2.96893300	-1.84099500	2.57959100
H	-0.89232100	1.54436800	-1.87265100
H	0.07796400	0.08362300	-2.14132500
H	-1.42111900	0.31534700	-3.05616900
C	0.63232700	0.19113300	1.30332400
C	0.79842200	1.50952000	0.56623300
C	1.71942900	1.70504200	-0.46237400
C	-0.08991500	2.53347100	0.88196800
C	1.74805500	2.90455900	-1.15967800
H	2.41565800	0.91492700	-0.71504700
C	-0.07128500	3.73230100	0.17546400
H	-0.80073300	2.37434500	1.68392700
C	0.84833700	3.91975500	-0.84826600
H	2.47465100	3.04914200	-1.95011800
H	-0.77335200	4.51848700	0.42563000
H	0.86871700	4.85248000	-1.39851000
O	0.14258400	0.20269500	2.44490300
O	2.44457700	-0.41067100	1.39162000
C	3.14842600	0.43341300	2.24393700
H	4.04713900	-0.06507800	2.62799000
H	2.53330800	0.71550400	3.11106700
H	3.47092600	1.36180500	1.74651300
H	0.88174100	-1.00100900	-0.51867800
H	0.40918400	-1.91042000	0.91815300
O	3.35634300	-1.27120300	-0.87021200

H	3.07739600	-0.92008500	0.02813900
C	3.34959000	-2.68172700	-0.81035300
H	2.37802100	-3.04504700	-0.44917200
H	4.10957700	-3.04225300	-0.10550400
C	3.62391400	-3.24112100	-2.19145400
H	4.59380400	-2.89559200	-2.55367000
H	3.62895900	-4.33215700	-2.17493000
H	2.85766200	-2.90774000	-2.89398200

NHO 1a, TS3 (v = -142.41i (cm^{-1}))

0 1

C	1.34497500	-0.64279600	0.45566200
C	3.31541700	0.34096100	0.78511200
C	3.53728100	-0.81861800	0.11209200
N	2.29714400	-1.40516200	-0.08830800
N	1.94523400	0.42710300	0.98810700
C	-0.11538900	-0.90057500	0.38028100
C	2.07616500	-2.68108800	-0.76390300
C	1.28095000	1.55586700	1.63206900
C	4.25553500	1.38815000	1.26475800
C	4.79924300	-1.44359700	-0.36451500
H	4.25878700	1.45057300	2.35451600
H	5.26561200	1.15402800	0.93640600
H	3.98645100	2.36862400	0.86816400
H	4.92450800	-2.44427400	0.05242800
H	4.81587300	-1.52339100	-1.45296600
H	5.64903500	-0.83853800	-0.05681300
H	1.09948400	-2.66099700	-1.23837200
H	2.83578500	-2.80091100	-1.53176700
H	2.14898200	-3.49795500	-0.04688100
H	1.09149300	2.34324700	0.90197700
H	0.33761300	1.22710100	2.05763700
H	1.92160200	1.92759100	2.42752200
C	-0.64417000	-0.28701800	-0.93735000
C	-0.97999000	1.18130400	-0.87299400
C	-1.76280800	1.73179500	0.14123000
C	-0.40390000	2.02006400	-1.82186200
C	-1.96526600	3.10275900	0.19953300
H	-2.21793700	1.08011100	0.87798200
C	-0.60044200	3.39589100	-1.75943500
H	0.20421200	1.58170800	-2.60369600
C	-1.38070600	3.93952900	-0.74774700
H	-2.58171100	3.52304800	0.98499700
H	-0.14323800	4.04168200	-2.49922400
H	-1.53643800	5.01018400	-0.69659800
O	-0.25459800	-0.79192300	-1.99040700
C	-3.06427800	-3.30750800	-0.19956000
H	-3.98244900	-3.07454200	0.34517300
H	-2.26860600	-3.44551100	0.53673900
H	-3.20902500	-4.25115500	-0.73194300
C	-2.71737000	-2.18009700	-1.17217600
H	-1.80110100	-2.45447400	-1.72542000
H	-3.51361100	-2.12015700	-1.93202000
O	-2.54615300	-0.95356500	-0.54516600
O	-2.92226700	-0.87831100	1.98267200
H	-2.77874400	-0.96894300	0.98022900
C	-4.24949600	-0.44967400	2.17133000
H	-4.43940700	-0.34397200	3.24104800
H	-4.43730900	0.52158400	1.69539900
H	-4.97299000	-1.16758300	1.76676500
H	-0.29695700	-1.97333200	0.34628600
H	-0.62692400	-0.49904500	1.25189800

NHO 1a, TS4 (v = -395.73i (cm^{-1}))

0 1

C	-3.03444900	1.09261200	-0.24310100
C	-4.34477800	1.19139300	-0.69197400
C	-5.18451000	0.08282000	-0.65461200
C	-4.70482400	-1.12425800	-0.15967100
C	-3.39482200	-1.22155800	0.29339500
C	-2.54987700	-0.11699900	0.25140100
H	-2.38078200	1.95530500	-0.27395400
H	-4.71390200	2.13702500	-1.07082700
H	-6.20560300	0.16107700	-1.00680500
H	-5.35380600	-1.99104500	-0.12312500
H	-3.01066100	-2.15394200	0.68889300
C	-1.12864000	-0.28272200	0.74126400
O	-0.81868600	-1.23936700	1.47473300
O	-0.56853600	0.97409100	0.98991700
C	0.53935100	0.97383900	1.88425000
H	0.20580600	0.65996200	2.87593500
H	1.29653700	0.25861300	1.55417800
C	1.01221600	-0.52035500	-0.91731400
C	3.01182700	0.46594500	-0.61747600
C	3.11477700	-0.81201300	-0.17947200
N	1.86858600	-1.40915000	-0.36413700
N	1.70439800	0.63243200	-1.07343600
C	-0.37047400	-0.68413800	-1.12445300
C	1.53710900	-2.80040300	-0.10527800
C	1.13429000	1.82367100	-1.67507800
C	4.01562400	1.56284500	-0.65926600
C	4.26317000	-1.54862300	0.41288400
H	3.70250800	2.41599400	-0.05292600
H	4.96690600	1.20594200	-0.27011300
H	4.17885100	1.91583300	-1.67972700
H	5.14243100	-0.90812900	0.43550100

H	4.04812200	-1.86421300	1.43630800
H	4.50817400	-2.43924400	-0.16946300
H	2.23728000	-3.20020000	0.62372800
H	0.53401000	-2.84979800	0.30886000
H	1.60156300	-3.38491700	-1.02511800
H	-0.81963300	0.02850000	-1.80528700
H	-0.72068400	-1.70124000	-1.24690800
H	0.89301100	1.63790600	-2.72300300
H	0.23180600	2.10671500	-1.13459500
H	1.85815900	2.63220400	-1.61487800
C	1.10565900	2.37597300	1.91728000
H	0.35583300	3.09039100	2.26056500
H	1.95856700	2.41683800	2.59674800
H	1.44250100	2.68148300	0.92516200

NHO 1b, TS1 (v = -414.62i (cm^{-1}))

0 1

C	2.59300900	-1.14016600	-0.17829400
C	3.89600000	-1.18758700	-0.65628500
C	4.66228900	-0.02805200	-0.71745700
C	2.81384800	1.22343100	0.18697200
C	4.11728300	1.17788700	-0.29390400
C	2.04381500	0.06746600	0.24650000
H	4.31606500	-2.13174600	-0.98181800
H	5.67830600	-0.06633000	-1.09046700
H	4.70974900	2.08415900	-0.33264600
H	2.37855000	2.15392500	0.53025500
C	0.61858800	0.17589300	0.76677000
O	0.27843100	1.17726300	1.43114900
O	0.21373900	-1.10109200	1.21624000
C	-0.82642000	-1.07318100	2.17443300
H	-1.11929000	-2.10903100	2.34278000
H	-0.48690300	-0.63279200	3.11341500
H	-1.68466000	-0.49750000	1.82221500
C	-1.61580000	0.16323000	-0.73614400
C	-3.66783900	-0.73855300	-0.19350500
C	-3.77852400	0.78337900	-0.23966000
N	-2.37281200	1.17910100	-0.28242200
N	-2.36234900	-0.96117600	-0.80891900
C	-0.23186100	0.25384800	-0.98824400
C	-1.84384600	-2.30834400	-0.90650100
C	-1.99899800	2.57491500	-0.38400700
H	1.99585100	-2.04250200	-0.13347400
H	-1.63297500	-2.72403700	0.08226000
H	-2.58631100	-2.93011000	-1.40656400
H	-0.93000000	-2.31815700	-1.49469800
H	-0.96277000	2.68986500	-0.07732000
H	-2.14534200	2.95552000	-1.40013800
H	-2.62398600	3.14660300	0.30071100
H	0.11069300	1.22467000	-1.32411500
H	0.18823100	-0.57171400	-1.54651200
H	-4.29416400	1.12549000	-1.14352000
H	-4.45224500	-1.24409300	-0.75409200
H	-4.27303000	1.20377100	0.63427700
H	-3.66625300	-1.11583600	0.83569000

NHO 1b, TS2 (v = -170.84i (cm^{-1}))

0 1

C	-0.95374800	-1.43132600	0.17278900
C	-2.51622400	-1.93204300	-1.43251700
C	-3.13628300	-2.11310800	-0.04461500
N	-2.09214700	-1.57807400	0.83320300
N	-1.10377300	-1.69455100	-1.11657900
C	0.31485200	-0.98258500	0.79743700
C	-2.27399500	-1.58922500	2.27324700
C	-0.15032800	-1.54734200	-2.20059000
H	-1.42796700	-1.10564100	2.75336000
H	-3.17723000	-1.02892700	2.51446400
H	-2.38824000	-2.61817500	2.62222800
H	0.85404800	-1.37463500	-1.82168600
H	-0.15915600	-2.46053300	-2.79600000
H	-0.44164400	-0.70458000	-2.83107900
C	0.20956200	0.49685100	1.29355300
C	-0.34733900	1.45382200	0.24803400
C	0.14502900	1.52416500	-1.05381700
C	-1.42551700	2.25598800	0.60699700
C	-0.43480900	2.38112100	-1.97971000
H	1.00290200	0.92659200	-1.33798400
C	-2.00807300	3.11618000	-0.31822500
H	-1.79601800	2.19562700	1.62284700
C	-1.51490600	3.17954100	-1.61471200
H	-0.03728400	2.43500200	-2.98628300
H	-2.84721800	3.73602600	-0.02599700
H	-1.96360700	3.85053400	-2.33703100
O	-0.10979900	0.68020800	2.48427700
C	2.32284200	2.07576500	1.52829600
H	3.39067600	2.15873000	1.76110600
H	2.08069300	2.84503600	0.77897300
H	1.76284300	2.30905400	2.44434900
O	2.02371400	0.79031900	1.08088700
H	2.69573100	0.23878300	-0.28293800
C	3.71037400	-2.20409300	0.08378800
H	2.95567400	-2.80931400	-0.42415900
H	3.29087000	-1.84767400	1.02686000
H	4.57088600	-2.83868500	0.30578300
C	4.11785500	-1.02659700	-0.78783700

H	4.89368400	-0.44130400	-0.27967700
H	4.54651800	-1.38559500	-1.72643000
O	3.01811200	-0.20074100	-1.12170300
H	1.12507900	-1.09058100	0.08563900
H	0.53437200	-1.59179500	1.67425900
H	-3.30901700	-3.16346400	0.20211400
H	-2.62035500	-2.80884900	-2.06864900
H	-4.06401200	-1.55952900	0.08539600
H	-2.91274300	-1.05870500	-1.95622000

NHO 1b, TS3 (v = -139.98i (cm^{-1}))

0 1

C	1.02824300	-1.38293200	0.01033300
C	3.05368900	-1.48509100	1.08629800
C	3.21819100	-1.97385200	-0.35559300
N	1.90548200	-1.67823300	-0.93567500
N	1.59895200	-1.33539500	1.20419800
C	-0.40332500	-1.08175600	-0.24817900
C	1.63262700	-2.00442600	-2.32288200
C	1.02206300	-0.96917000	2.48409500
H	0.60877200	-1.74121800	-2.57102600
H	2.30288100	-1.42734500	-2.96042800
H	1.81061200	-3.06938900	-2.48698700
H	-0.06193200	-0.90959900	2.42477300
H	1.30115200	-1.72610800	3.21762100
H	1.41515100	-0.00071500	2.80016100
C	-0.54284300	0.24413500	-1.05834700
C	0.18000300	1.42092600	-0.43864600
C	0.05481100	1.75371300	0.90894400
C	1.05075800	2.15072400	-1.24114500
C	0.78966700	2.80380700	1.44160200
H	-0.64065100	1.20743600	1.53521500
C	1.78675400	3.20437700	-0.70913900
H	1.13997700	1.88148500	-2.28651900
C	1.65918000	3.53181700	0.63424000
H	0.67849700	3.06192300	2.48804300
H	2.46014000	3.76807200	-1.34351100
H	2.23051000	4.35165800	1.05214500
O	-0.62153400	0.15898500	-2.29000400
C	-3.96626600	-0.82161000	-1.31504600
H	-4.47552900	-0.98102800	-0.36179100
H	-3.23430500	-1.62236500	-1.44738800
H	-4.70595800	-0.89695500	-2.11665400
C	-3.26552900	0.53466300	-1.33121400
H	-2.79047100	0.67114200	-2.31491700
H	-4.01734300	1.33192500	-1.23292100
O	-2.30806600	0.66098000	-0.33363000
O	-2.49612500	-0.16411700	2.10559900
H	-2.54279300	0.16240500	1.15306400
C	-3.15901000	-1.40487600	2.19219900
H	-2.91199200	-1.86610000	3.15013600
H	-4.24767300	-1.29442600	2.13794800
H	-2.84977900	-2.08946200	1.39223500
H	-0.85027300	-1.87319900	-0.84891100
H	-0.93027000	-1.01016800	0.69481500
H	3.42442200	-2.19321500	1.82475400
H	3.40321100	-3.04886100	-0.41552200
H	4.00094700	-1.44716300	-0.89784800
H	3.52337400	-0.51282400	1.25300000

NHO 1b, TS4 (v = -411.87i (cm^{-1}))

0 1

C	-2.92494300	1.24117600	-0.05565800
C	-4.24855000	1.34638100	-0.46382400
C	-5.10996400	0.26235100	-0.33199800
C	-3.31609300	-1.02768900	0.62713600
C	-4.63950200	-0.92561700	0.21480900
C	-2.45066900	0.05221100	0.49366000
H	-4.61064500	2.27732500	-0.88364400
H	-6.14135600	0.34458200	-0.65206500
H	-5.30631900	-1.77256100	0.32348600
H	-2.93701300	-1.94382100	1.06348800
C	-1.00709500	-0.12361800	0.94378800
O	-0.72546100	-1.02978800	1.76032600
O	-0.44211400	1.15628500	1.13231000
C	0.67382000	1.18643700	2.00916600
H	0.34401400	0.98299200	3.03127900
H	1.38702500	0.40174700	1.74210000
C	1.10182100	-0.46958900	-0.69493900
C	3.18606800	0.50340600	-0.89076600
C	3.29091500	-0.75567100	-0.03161300
N	1.98512600	-1.37774500	-0.23684400
N	1.73973300	0.68348700	-0.97227500
C	-0.29809800	-0.62933200	-0.78872200
C	1.15148500	1.76737200	-1.72952100
C	1.66055700	-2.58757900	0.48959800
H	-2.25350300	2.08459900	-0.15759900
H	0.20111000	2.05170500	-1.27933600
H	1.82476100	2.62189000	-1.67983700
H	1.00073100	1.49583200	-2.77877900
H	0.63015800	-2.87146800	0.29911100
H	2.33053000	-3.38662700	0.16971100
H	1.77268700	-2.42586600	1.56436700
C	1.31124800	2.55398900	1.90218400
H	2.16700200	2.62313200	2.57570800
H	1.65527600	2.73652000	0.88264900

H	0.59792800	3.33477500	2.17075000
H	-0.65141500	-1.65097200	-0.83882300
H	-0.76406100	0.02475100	-1.51555400
H	4.09281000	-1.42294200	-0.34344700
H	3.60707400	0.35094400	-1.88974100
H	3.42318800	-0.51538500	1.02983700
H	3.65976500	1.37094200	-0.43291700

NHO 1c, TS1 (v = -405.45i (cm^{-1}))

0 1

C	2.85130700	-1.10671400	-0.33830000
C	4.16142600	-0.96343500	-0.77820300
C	4.83352200	0.24068800	-0.59812900
C	2.87788200	1.15501000	0.46969600
C	4.18731400	1.30032100	0.02793200
C	2.20114800	-0.04626800	0.28863000
H	4.66043000	-1.79443000	-1.26230200
H	5.85419400	0.35118300	-0.94291500
H	4.70532000	2.24021700	0.17629700
H	2.36343200	1.96877500	0.96626300
C	0.76406300	-0.13906300	0.77275200
O	0.33542500	0.69606800	1.59460400
O	0.44091600	-1.50010900	0.96692900
C	-0.60008700	-1.73199600	1.89684300
H	-0.29352600	-1.46675300	2.90993700
H	-1.49683100	-1.16104300	1.65131500
H	-0.82066400	-2.79784900	1.84874600
H	2.32832400	-2.04422900	-0.48002000
C	-3.55105300	-0.93018100	-0.21330100
C	-3.87176000	0.30211300	0.60795300
C	-3.39439400	1.52706600	-0.14630500
H	-4.94457400	0.35029500	0.79080000
H	-4.30166500	-1.07661900	-0.99530400
H	-3.55496100	-1.82259500	0.41952600
H	-3.91098400	1.61332000	-1.10988500
H	-3.58694200	2.43411600	0.42250700
C	-1.43106300	0.24927300	-0.76561800
C	-0.03672900	0.14832300	-1.01788100
H	0.29165500	-0.73368700	-1.54614700
H	0.44318500	1.05480500	-1.35993900
N	-1.95615600	1.41556700	-0.34726000
N	-2.23505600	-0.83440300	-0.84852100
C	-1.74134200	-2.08301500	-1.41585100
H	-1.27805800	-1.90685500	-2.38572500
H	-1.02039400	-2.56750100	-0.75399700
H	-2.59481800	-2.74251700	-1.56133900
C	-1.15889100	2.63565200	-0.36116400
H	-0.20778400	2.46071800	0.13419100
H	-0.99371700	2.99218100	-1.38245900
H	-1.70001400	3.39993300	0.19160800
H	-3.36190300	0.26608300	1.57271300

NHO 1c, TS2 (v = -181.94i (cm^{-1}))

0 1

C	0.00836000	1.18371500	1.18833200
C	-0.57516200	1.39597000	-0.20117300
C	0.00772800	0.87257800	-1.35491700
C	-1.78759500	2.06919500	-0.30220200
C	-0.62042700	1.01233500	-2.58497100
H	0.96982600	0.37880000	-1.29021200
C	-2.41973300	2.21151300	-1.53407500
H	-2.22590100	2.48118500	0.59859200
C	-1.83970500	1.67859900	-2.67759800
H	-0.15556600	0.60807900	-3.47627400
H	-3.36440200	2.73779300	-1.59916600
H	-2.32847200	1.78689200	-3.63819600
O	-0.40170700	1.88947900	2.11891600
O	1.82807800	1.64933100	0.83330900
C	1.89041400	3.02450000	0.63240800
H	2.90704300	3.39800600	0.80749700
H	1.22193800	3.54976500	1.32973700
H	1.60107200	3.31306100	-0.39074700
O	3.23120200	0.11423300	-0.67696900
H	2.70935200	0.77195300	-0.11676000
C	4.10769000	-0.59030200	0.17571100
H	3.55591800	-1.04032800	1.01395000
H	4.85003500	0.08849300	0.61373800
C	4.80705900	-1.67836100	-0.61377900
H	5.36922700	-1.24165200	-1.44097900
H	5.49845800	-2.23557600	0.02036300
H	4.07777900	-2.37773000	-1.02852300
C	-1.29113600	-2.62270300	-1.01148600
C	-2.61878200	-1.90966300	-0.89486300
C	-2.98963000	-1.83353100	0.57097900
H	-0.87264900	-2.50437200	-2.01290700
H	-1.39221000	-3.69171700	-0.80694400
H	-3.90754300	-1.26659700	0.71919500
H	-3.12738400	-2.82886500	1.00294300
C	-0.66471200	-1.22473200	0.90880600
C	0.37100800	-0.31274800	1.49831500
N	-1.92771500	-1.13120400	1.29597400
N	-0.31629100	-2.04606700	-0.07730000
C	1.07901100	-2.40378800	-0.34968500
H	1.60306300	-1.62733000	-0.90932800
H	1.61135100	-2.60343000	0.57789800
H	1.06455400	-3.32271600	-0.93220900

C	-2.38652900	-0.32133400	2.42129500
H	-3.08177100	-0.92909600	3.00093000
H	-1.56060300	-0.00988800	3.04795400
H	-2.89981600	0.56885900	2.05465700
H	1.33948600	-0.53629100	1.06894600
H	0.43573000	-0.41278200	2.58038000
H	-2.53717500	-0.89656100	-1.29917600
H	-3.38103300	-2.44884800	-1.45470500

NHO 1c, TS3 (v = -149.60i (cm^{-1}))

0 1

C	-0.63421200	0.49741200	-1.22065600
O	-0.76723800	1.07905900	-2.30059000
C	-4.65152800	0.95828000	-0.49234300
H	-4.93335800	0.31082400	0.34142200
H	-4.91871700	0.45242900	-1.42238600
H	-5.22964800	1.88295300	-0.42111300
C	-3.15470900	1.24329900	-0.45932800
H	-2.89441700	1.90639800	-1.29914200
H	-2.91504400	1.79522700	0.46631400
O	-2.41633900	0.06779700	-0.54653300
O	-2.62222600	-1.52486600	1.43048500
H	-2.56965200	-0.84905500	0.67354500
C	-3.21267400	-2.68899000	0.90276500
H	-3.32787100	-3.42269500	1.70260100
H	-4.20265600	-2.48871700	0.47736100
H	-2.59588300	-3.14254700	0.11499500
C	2.66846100	-1.62388400	1.16333300
C	3.40681400	-0.38803100	0.70295800
C	3.52669300	-0.43965600	-0.80523800
H	2.36759500	-1.53106400	2.20863300
H	3.28774500	-2.51937200	1.06492700
H	3.98234800	0.46875000	-1.19685800
H	4.12629900	-1.29413900	-1.13149900
C	1.20403500	-1.14948700	-0.74886400
C	-0.20989200	-1.01270900	-1.23498400
N	2.18616300	-0.53353800	-1.38983700
N	1.43734300	-1.80297700	0.38486000
C	0.46965000	-2.73770300	0.96764700
H	-0.32500700	-2.22516700	1.51198000
H	0.03274000	-3.36509700	0.19412800
H	1.02118100	-3.38066300	1.65033800
C	2.03545100	0.13410500	-2.67976500
H	1.12291800	-0.16785000	-3.17803000
H	2.01545000	1.21588500	-2.54000500
H	2.89620400	-0.13809900	-3.29062100
H	-0.32606800	-1.37128800	-2.25625900
H	-0.87549000	-1.57401000	-0.59050300
C	-0.11750000	1.27683300	-0.02290800
C	-0.19923400	0.79784800	1.28428500
C	0.54062800	2.47814800	-0.26309100
C	0.37759900	1.50582500	2.32925800
H	-0.74164300	-0.11752200	1.48795200
C	1.12120600	3.18951000	0.78282500
H	0.58992200	2.84719300	-1.28038900
C	1.04598600	2.70195200	2.08058300
H	0.30075000	1.12808400	3.34179400
H	1.63221900	4.12348700	0.58269200
H	1.49866200	3.25189200	2.89663600
H	4.39266100	-0.35058500	1.16341100
H	2.85146100	0.50935900	0.99079600

NHO 1c, TS4 (v = -449.81i (cm^{-1}))

0 1

C	2.79009300	-1.26466200	-0.28738500
C	4.07107000	-1.31542000	-0.82277200
C	4.86757900	-0.17541500	-0.84445800
C	3.09608400	1.06348500	0.21740200
C	4.37553900	1.01526500	-0.32228200
C	2.29437500	-0.07307900	0.23645300
H	4.45093900	-2.24829200	-1.22212300
H	5.86589100	-0.21676400	-1.26228400
H	4.99146100	1.90663000	-0.33089700
H	2.70267900	1.98149600	0.63678200
C	0.89806600	0.04199100	0.82563400
O	0.64407100	0.96656400	1.62760400
O	0.42097000	-1.25094000	1.11338300
C	-0.60071200	-1.29900400	2.10118300
H	-0.16244800	-1.12245900	3.08756500
H	-1.32653200	-0.50450000	1.92323800
H	2.17118500	-2.15303600	-0.27042700
C	-3.42841600	-1.10549800	-0.69585700
C	-3.95853600	-0.21515100	0.40512400
C	-3.53501400	1.21164200	0.13365900
H	-5.04547300	-0.27852900	0.44561000
H	-3.93377700	-0.89145300	-1.64493400
H	-3.60563000	-2.15373700	-0.45538700
H	-4.06378600	1.61068500	-0.74026200
H	-3.77513200	1.84784000	0.98520900
C	-1.39090300	0.27654500	-0.63876300
C	0.00107200	0.42623900	-0.88947800
H	0.42022200	-0.27794300	-1.59224300
H	0.34712700	1.43645100	-1.05369500
N	-2.09329100	1.28743400	-0.08461500
N	-1.98771400	-0.92007300	-0.84648500
C	-1.27472400	-1.97603800	-1.55601300

H	-1.07566600	-1.69820900	-2.59464900
H	-0.33811600	-2.20641000	-1.05238200
H	-1.89897100	-2.86684500	-1.54961700
C	-1.50779500	2.62391300	-0.00657100
H	-0.54049200	2.57959500	0.48615400
H	-1.40892300	3.07032600	-1.00059200
H	-2.17237400	3.24571300	0.58900800
H	-3.56241700	-0.54671800	1.36728100
C	-1.25244300	-2.66267600	2.03618800
H	-2.02093500	-2.74873400	2.80639400
H	-1.71918900	-2.81895900	1.06181900
H	-0.51628500	-3.45203600	2.19660600

NHO 1d, TS1 (v = -393.44i (cm^{-1}))

0 1

C	-0.28601500	-0.10017600	0.10234400
C	1.02428600	-0.20828100	-0.34633500
C	1.78417000	0.93414300	-0.57299100
C	-0.08273100	2.29417000	0.11014700
C	1.22589900	2.18639900	-0.34319900
C	-0.84780500	1.15373700	0.33282400
H	1.45518400	-1.18759200	-0.51726900
H	2.80478100	0.84844900	-0.92485700
H	1.81222200	3.08106500	-0.51507500
H	-0.52820100	3.26324200	0.29906300
C	-2.27071900	1.33029900	0.81204400
O	-2.63378900	2.39051400	1.35190100
O	-2.75416100	0.11580700	1.31013000
C	-3.83559400	0.23320900	2.22027600
H	-4.23078300	-0.77338200	2.35300400
H	-3.49510300	0.62467800	3.18041700
H	-4.62142200	0.88779000	1.84027900
C	-4.44514500	1.21959500	-0.79277300
C	-6.44263100	0.40186500	-0.20208700
C	-6.49675200	1.74418200	-0.07364100
N	-5.25806300	2.24209700	-0.43477800
N	-5.17355800	0.08472700	-0.64995300
C	-3.06980500	1.29699300	-1.07408800
C	-4.66213400	-1.24817000	-0.91484300
C	-4.88618600	3.64681900	-0.50944600
H	-0.87818500	-0.98950600	0.27743300
H	-3.78368000	-1.43341300	-0.29700900
H	-5.44065000	-1.96753100	-0.67438100
H	-4.39703400	-1.34404000	-1.96832300
H	-2.64794900	0.43046800	-1.56816300
H	-2.71512500	2.24938000	-1.44850200
H	-3.93082200	3.78765200	-0.00944000
H	-4.82319000	3.96215300	-1.55214100
H	-5.65257700	4.22834900	-0.00323600
H	-7.29749600	2.38888700	0.24222200
H	-7.18560300	-0.35396200	-0.01863000

NHO 1d, TS2 (v = -180.61i (cm^{-1}))

0 1

C	-1.28715900	-1.37255900	-0.25547800
C	-3.20192800	-1.41386900	-1.36813100
C	-3.33148300	-2.22275300	-0.29191600
N	-2.13716400	-2.18059100	0.38743800
N	-1.92747200	-0.89389400	-1.33033900
C	0.07667900	-1.02891900	0.21056300
C	-1.82982900	-2.92189000	1.61082000
C	-1.40856400	0.06985500	-2.29859600
H	-1.17182800	-3.75722100	1.37677600
H	-1.35908600	-2.24240100	2.31691800
H	-2.76507600	-3.29717500	2.01617400
H	-1.62732900	1.08425000	-1.96597500
H	-0.33412100	-0.05739100	-2.39839100
H	-1.88597800	-0.12516700	-3.25526600
C	-0.01976900	0.17209300	1.18677600
C	-0.19203400	1.50469300	0.48095500
C	0.68910500	1.97571100	-0.49205400
C	-1.34426800	2.23223500	0.76167600
C	0.41460100	3.15205200	-1.17495400
H	1.59378400	1.42012700	-0.70910300
C	-1.62613600	3.40701600	0.07127100
H	-2.02007300	1.85843800	1.52114700
C	-0.74825100	3.86736900	-0.90099900
H	1.10816700	3.51424500	-1.92421400
H	-2.53059700	3.96043400	0.29292900
H	-0.96383000	4.78159200	-1.44029900
O	-0.59950400	-0.01370400	2.26942100
O	1.87188400	0.15932700	1.46191800
C	2.19375500	1.17499900	2.35654200
H	3.14533800	0.96164300	2.85910000
H	1.42405900	1.26737800	3.13717700
H	2.29063000	2.15577500	1.86523600
H	0.73282900	-0.80810300	-0.63046100
H	0.49575000	-1.86779900	0.76430500
O	3.24202700	-0.36077600	-0.66701000
H	2.75758000	-0.10655100	0.17477500
C	3.74324700	-1.66886000	-0.48718600
H	2.91922200	-2.37775500	-0.32721000
H	4.38377700	-1.71450700	0.40245900
C	4.53646100	-2.07611500	-1.71218300
H	5.36778800	-1.38702600	-1.87025600
H	4.93886900	-3.08376000	-1.59575300

H	3.90153400	-2.05706700	-2.59990200
H	-3.89276300	-1.16377500	-2.15338100
H	-4.15801600	-2.82191000	0.04625700

NHO 1d, TS3 (v = -146.18i (cm^{-1}))

0 1

C	1.77109000	-0.71593200	0.56413900
C	3.74851200	0.16833700	1.02185400
C	3.95676600	-0.97672400	0.33244000
N	2.71941900	-1.50821400	0.05395500
N	2.38596100	0.31503900	1.15723100
C	0.31102200	-0.91911300	0.39898800
C	2.47341800	-2.75691300	-0.66727300
C	1.74024000	1.45582100	1.80405900
H	1.72976000	-2.57430500	-1.43897900
H	3.41057100	-3.07275600	-1.11625100
H	2.12672400	-3.51920500	0.02846200
H	1.54139600	2.23551600	1.06974400
H	0.80549800	1.13573100	2.25612100
H	2.40849800	1.82623500	2.57685400
C	-0.12485200	-0.21679200	-0.90952300
C	-0.44092100	1.25039100	-0.77858100
C	-1.24914700	1.75923300	0.23763100
C	0.18195900	2.12827200	-1.65993500
C	-1.42774500	3.12877900	0.36564900
H	-1.74142100	1.07897200	0.92322200
C	0.00858700	3.50210800	-1.52737500
H	0.80981200	1.72137900	-2.44302900
C	-0.79501000	4.00472300	-0.51277400
H	-2.06293900	3.51726900	1.15247600
H	0.50300500	4.17810900	-2.21433700
H	-0.93164000	5.07393500	-0.40579000
O	0.32214100	-0.66886400	-1.96367500
C	-2.61105600	-3.22577200	-0.49056000
H	-3.56090400	-3.02340200	0.01009400
H	-1.85879400	-3.39994400	0.28274400
H	-2.71954400	-4.14057700	-1.07907100
C	-2.20969500	-2.04926200	-1.38091700
H	-1.26802400	-2.30144000	-1.90108100
H	-2.96592500	-1.93981700	-2.17484900
O	-2.06093200	-0.86037800	-0.67925200
O	-2.57514900	-0.92173800	1.82639900
H	-2.38088100	-0.95568900	0.82954700
C	-3.90489300	-0.48396400	1.97276900
H	-4.14171900	-0.41959200	3.03637000
H	-4.06002000	0.50787200	1.52901700
H	-4.61731800	-1.17583800	1.50750800
H	0.10726400	-1.98290600	0.28575200
H	-0.23528800	-0.55520600	1.26658400
H	4.86637800	-1.45859300	0.02098000
H	4.43970300	0.88517100	1.42829000

NHO 1d, TS4 (v = -394.66i (cm^{-1}))

0 1

C	2.54775100	-1.05679800	-0.38177500
C	3.86494100	-1.09618300	-0.82008200
C	4.70204600	-0.00283200	-0.62324100
C	4.21289900	1.12875700	0.01845800
C	2.89608600	1.16602400	0.46053500
C	2.05455900	0.07643500	0.26139300
H	1.89523500	-1.90669400	-0.53709900
H	4.24101800	-1.98368900	-1.31469500
H	5.72888600	-0.03448800	-0.96606200
H	4.86047500	1.98214500	0.18006000
H	2.50440300	2.03796800	0.96962900
C	0.62553900	0.17347400	0.75067200
O	0.30589700	1.01350300	1.61297700
O	0.06496700	-1.10794500	0.81060400
C	-1.02854700	-1.24762200	1.71156700
H	-0.67811600	-1.08636800	2.73367400
H	-1.79258100	-0.49326800	1.50720300
C	-1.49424100	0.65193600	-0.85843300
C	-3.48534400	-0.35787400	-0.70198800
C	-3.58669800	0.84284500	-0.09386700
N	-2.35280900	1.45992900	-0.19201300
N	-2.19051400	-0.46783400	-1.17420400
C	-0.11060800	0.83916900	-1.03049600
C	-2.02408700	2.79918600	0.27257800
C	-1.63333700	-1.57725700	-1.92669200
H	-2.84141200	3.15257400	0.89606000
H	-1.10854100	2.75894200	0.85701100
H	-1.90322700	3.47042600	-0.57895300
H	0.34188700	0.23452600	-1.80697500
H	0.23785300	1.86403700	-0.99821100
H	-1.36494800	-1.24931700	-2.93167600
H	-0.75005100	-1.95651800	-1.41381300
H	-2.38447000	-2.36059600	-1.99310700
C	-1.59212600	-2.64138000	1.54408600
H	-0.82129100	-3.39381100	1.71765600
H	-2.39928200	-2.80227500	2.26027800
H	-1.99363200	-2.78339500	0.53947300
H	-4.41801500	1.31295200	0.40093600
H	-4.21083000	-1.13954900	-0.84280800

NHO 1e, TS1 (v = -383.56i (cm^{-1}))

0 1

C	3.05805700	-0.90713000	0.00314100
C	4.36895800	-0.66824200	-0.38811700
C	4.87200500	0.62846900	-0.39981800
C	4.05488700	1.68448000	-0.01297200
C	2.74487400	1.44496500	0.38222600
C	2.23617500	0.14977400	0.38944500
H	2.66591400	-1.91614100	0.00860100
H	5.00117200	-1.49708700	-0.68312200
H	5.89423900	0.81379400	-0.70574000
H	4.44071300	2.69678300	-0.01475500
H	2.10004400	2.25824600	0.69177900
C	0.79966600	-0.05403100	0.81189100
O	0.19436000	0.81587600	1.46017200
O	0.58372900	-1.40193500	1.11520700
C	-0.51673500	-1.64954500	1.97495300
H	-0.65852200	-2.72962500	1.98023500
H	-0.30622700	-1.30058400	2.98746100
H	-1.42830500	-1.16221000	1.62523900
C	-1.26053600	-0.38374200	-0.90765700
N	-1.72938100	-1.65542800	-0.99173800
C	-3.04030300	-1.69580100	-0.55860000
C	-3.38411600	-0.43994200	-0.20630500
N	-2.27588300	0.36574800	-0.41079500
C	0.07267600	0.00969000	-1.11633500
H	-0.61883000	-2.63139600	-2.47296000
H	-1.55073300	-3.67982500	-1.38414800
C	-2.23208500	1.82493500	-0.23698300
H	-0.06127000	-2.89590300	-0.80171900
C	-0.93655400	-2.78492800	-1.44109000
H	0.24305600	1.05335900	-1.34587100
H	0.67103500	-0.68037200	-1.69799700
H	-1.17785700	2.06560100	-0.11706600
H	-4.31410900	-0.05593700	0.17194900
H	-3.60508600	-2.61108400	-0.54086500
C	-2.94844400	2.22871000	1.04198600
H	-2.80671300	3.29723700	1.20525400
H	-4.02265100	2.04343700	0.97990000
H	-2.53525600	1.68762000	1.89328600
C	-2.80219800	2.51013300	-1.47287700
H	-2.73373100	3.59311700	-1.36295100
H	-2.25120800	2.21586100	-2.36759600
H	-3.85291100	2.24304200	-1.60703400

NHO 1e, TS2 (v = -179.42i (cm^{-1}))

0 1

C	-1.38471900	1.03909200	-0.51045800
C	-3.42946700	0.85175700	0.31872300
C	-3.53762200	1.31595600	-0.94651000
N	-2.26186300	1.42264100	-1.44651400
N	-2.08584400	0.68389000	0.57462500
C	0.08496700	0.98099700	-0.70505400
C	-1.91307300	1.93189500	-2.77353600
C	-1.54777100	0.20882700	1.86789200
H	-1.55711000	2.95751700	-2.68704900
H	-1.14709100	1.28927400	-3.19993200
H	-2.80970600	1.90800200	-3.38628900
H	-0.46608600	0.20901500	1.75571700
C	0.47192400	-0.34349400	-1.41050300
C	0.51327000	-1.56334900	-0.50679800
C	1.17670600	-1.57715500	0.72006700
C	-0.16307300	-2.70547900	-0.92245900
C	1.15816600	-2.71408300	1.51534800
H	1.73054100	-0.70244200	1.04194200
C	-0.18448000	-3.84668200	-0.12540500
H	-0.67029500	-2.68440800	-1.87899000
C	0.47567200	-3.85270500	1.09553700
H	1.68401600	-2.71658600	2.46253400
H	-0.71669900	-4.72921400	-0.45935500
H	0.46379600	-4.73966700	1.71729200
O	0.10716300	-0.49218500	-2.58902900
O	2.31930700	0.14585100	-1.36648600
C	3.06146100	-0.86925800	-1.96186600
H	4.02102500	-0.48422400	-2.32848100
H	2.52621600	-1.29050200	-2.82608900
H	3.27769900	-1.69643600	-1.26774200
H	0.60847000	1.10117100	0.24126900
H	0.39209900	1.79083800	-1.36575800
O	3.02176300	1.23952200	0.87022200
H	2.82839200	0.78501500	-0.00501900
C	3.11115200	2.62853300	0.63249600
H	2.27045200	2.96354400	0.01071700
H	4.03152800	2.86878100	0.08513800
C	3.09420500	3.36510300	1.95649200
H	3.93149800	3.04478700	2.57914800
H	3.17092000	4.44274500	1.80233700
H	2.16725700	3.15591600	2.49429400
H	-4.18578900	0.62853100	1.04984200
H	-4.40179700	1.57635200	-1.53165400
C	-1.93954000	1.17926000	2.97302000
H	-3.02082300	1.19242200	3.12069800
H	-1.47590900	0.85921500	3.90602500
H	-1.60172400	2.19002300	2.74354100
C	-2.01746200	-1.21405600	2.13114400
H	-1.72407200	-1.87758200	1.31652300
H	-1.55863500	-1.57445800	3.05212400
H	-3.10199100	-1.24978500	2.25401200

NHO 1e, TS3 (v = -162.16i (cm^{-1}))

0 1

C	1.54147300	-1.14844700	-0.15626000
C	3.66266900	-0.51498400	-0.21109700
C	3.51659700	-1.54517800	-1.07458100
N	2.19571800	-1.92232600	-1.03134300
N	2.42658500	-0.27986200	0.35100100
C	0.08559600	-1.23507900	0.11974700
C	1.60877800	-3.03081500	-1.78591500
C	2.16845200	0.76388600	1.36689300
H	1.47368200	-3.88732100	-1.12712300
H	0.65784100	-2.70495800	-2.19961000
H	2.29682300	-3.29027500	-2.58546300
H	1.11607000	0.67044400	1.62456100
C	-0.69645100	-0.43188000	-0.94840600
C	-0.75358500	1.06697400	-0.72514700
C	-1.05477500	1.64354000	0.50871900
C	-0.46379700	1.89364900	-1.80574300
C	-1.05489100	3.02308500	0.65616500
H	-1.31539000	1.01049400	1.34962100
C	-0.46333800	3.27743000	-1.66004600
H	-0.23932600	1.43465200	-2.76034900
C	-0.75620700	3.84479700	-0.42767400
H	-1.29550300	3.46159900	1.61715200
H	-0.23205800	3.90969000	-2.50874500
H	-0.75703500	4.92143500	-0.30918900
O	-0.68749000	-0.86126800	-2.10981300
O	-2.37741200	-0.93304800	-0.08922600
C	-3.43664900	-0.35649300	-0.78142200
H	-3.21773400	-0.35203700	-1.86148700
H	-3.58348100	0.69648900	-0.48516400
H	-0.14389200	-0.89862500	1.12888000
H	-0.23512400	-2.27210800	0.03074600
O	-2.26507800	-0.84111300	2.47040000
H	-2.37625400	-0.83707700	1.46584500
C	-2.23730100	-2.19052000	2.87336800
H	-1.39832000	-2.73398000	2.42076100
H	-3.16194000	-2.71619000	2.60880400
H	4.53109000	0.06437500	0.04725400
H	4.22805500	-2.03753700	-1.71340300
C	3.01524000	0.49703200	2.60318700
H	4.07889500	0.60417300	2.38332500
H	2.75601600	1.22330100	3.37334900
H	2.83420200	-0.50483100	2.99272800
C	2.40981800	2.14055300	0.76630000
H	1.78612100	2.29526500	-0.11526300
H	2.15567100	2.89953500	1.50658300
H	3.45956900	2.26844500	0.49410600
H	-2.12151900	-2.23213800	3.95769500
C	-4.73222000	-1.12171900	-0.53853400
H	-4.96812900	-1.13735100	0.52819000
H	-5.56789800	-0.65802100	-1.06861500
H	-4.63316100	-2.15369700	-0.88100500

NHO 1e, TS4 (v = -385.70i (cm^{-1}))

0 1

C	3.04426900	-0.95080500	0.04300400
C	4.37079400	-0.76934300	-0.32604700
C	4.91853700	0.50848500	-0.36666800
C	4.13035800	1.60340900	-0.03139600
C	2.80447900	1.42115900	0.34175900
C	2.25136700	0.14500900	0.37808600
H	2.61750500	-1.94527800	0.07347500
H	4.98008700	-1.62794100	-0.58191400
H	5.95264000	0.64935500	-0.65575800
H	4.55085400	2.60154200	-0.05654000
H	2.18203400	2.26499400	0.61314700
C	0.80000300	0.00182800	0.77761800
O	0.21664900	0.90933000	1.39645300
O	0.53208000	-1.33016400	1.10915900
C	-0.58011200	-1.52512600	1.97698000
H	-0.35771000	-1.08989400	2.95457500
H	-1.46384800	-1.01350700	1.58853800
C	-1.22170900	-0.36622000	-0.96652100
N	-1.64337000	-1.65348300	-1.06460500
C	-2.95785100	-1.74462300	-0.65001300
C	-3.35021500	-0.50472900	-0.29185700
N	-2.27052500	0.34281700	-0.48003600
C	0.10370200	0.06459000	-1.15288400
H	-0.54259400	-2.55548300	-2.59944700
H	-1.38642700	-3.66237900	-1.49521800
C	-2.28055700	1.79378200	-0.24503000
H	0.08386500	-2.81978700	-0.95148600
C	-0.81659800	-2.73859000	-1.55970300
H	0.25381100	1.11535800	-1.36243800
H	0.72131400	-0.60007900	-1.74412600
H	-1.23326200	2.08684700	-0.21958800
H	-4.29723300	-0.15662400	0.07960800
H	-3.49067100	-2.67923600	-0.65002100
C	-2.88058500	2.10054200	1.11858800
H	-2.78849200	3.16876600	1.31706500
H	-3.94170200	1.84576800	1.15817800
H	-2.34211300	1.55166000	1.89112000
C	-3.00655500	2.49874700	-1.38422500
H	-2.98461900	3.57761500	-1.22674100

H	-2.53327300	2.27669800	-2.34180700
H	-4.05050000	2.18006000	-1.42921400
C	-0.82382000	-3.01375900	2.08854600
H	0.06794700	-3.52564100	2.45358400
H	-1.64094900	-3.20458200	2.78587800
H	-1.09453500	-3.43806800	1.12017000

NHO 2a, TS1 (v = -325.88i (cm^{-1}))

0 1

C	-2.96042900	1.24310400	0.36416800
C	-4.29361000	1.37649500	-0.00216500
C	-5.08574500	0.24930000	-0.18765500
C	-3.20718700	-1.14690400	0.38218600
C	-4.53846400	-1.01386900	0.01057200
C	-2.40149900	-0.02186500	0.54719100
H	-4.71737700	2.36428800	-0.13907800
H	-6.12477700	0.35444700	-0.47461100
H	-5.15347300	-1.89671000	-0.11659500
H	4.18039900	-1.86068000	1.45367700
H	-2.77397300	-2.12403700	0.55442700
C	-0.96426000	-0.22171600	0.93770800
O	-0.59061200	-1.26798000	1.49612000
O	-0.41172000	1.00224400	1.32589200
C	0.69310100	0.91092200	2.20861200
H	1.14434800	1.90312600	2.23678700
H	0.36589000	0.62914000	3.21148900
H	1.42936400	0.18311400	1.86802900
C	1.15503500	-0.18125800	-0.75011500
C	3.14021500	0.76714800	-0.19787400
C	3.25485500	-0.55876400	0.01861100
N	2.03436400	-1.14016600	-0.32599900
N	1.85166600	0.99521500	-0.67852300
C	-0.22752500	-0.34827100	-1.07432400
C	1.35198200	2.34444100	-0.92066100
C	1.80059900	-2.57538400	-0.16588700
C	4.41614100	-1.34371200	0.52134700
C	4.13332800	1.85782400	0.00338800
H	-2.34737600	2.12197000	0.51442900
H	4.74609100	-2.08925700	-0.20495600
H	5.25144700	-0.67464000	0.71452300
H	5.07268500	1.43694600	0.35411900
H	4.33316400	2.39702900	-0.92471700
H	3.79196800	2.58002400	0.74835800
H	0.51541300	2.55605600	-0.25925500
H	2.15514600	3.04188700	-0.70674400
H	1.05482400	2.47163300	-1.95755300
H	1.00088400	-2.74236900	0.54775500
H	1.56976600	-3.03978900	-1.11994500
H	2.71436700	-3.01856100	0.21574900
C	-0.87606900	0.71238100	-1.95368800
H	-0.96132300	1.68995200	-1.48559500
H	-0.36401100	0.83695200	-2.91609000
H	-1.89656400	0.39574900	-2.17289300
C	-0.67573600	-1.73519300	-1.50809600
H	-0.10056500	-2.12841400	-2.35423200
H	-0.64428300	-2.45925900	-0.69629500
H	-1.71397800	-1.67614300	-1.83514900

NHO 2a, TS2 (v = -172.51i (cm^{-1}))

0 1

C	-1.40155400	-0.83149700	-0.40568900
C	-3.41414200	0.00785300	-0.92568800
C	-3.60430500	-0.99182200	-0.03146700
N	-2.35075200	-1.48754600	0.28742600
N	-2.04631900	0.09812400	-1.14123400
C	0.10256000	-1.08540700	-0.33416300
C	-2.17587100	-2.53021900	1.30373200
C	-1.48221600	1.15333500	-1.98798100
C	-4.40954200	0.88601600	-1.59950200
C	-4.86212200	-1.53628700	0.54862000
H	-4.32013700	0.83205000	-2.68538100
H	-5.41337900	0.56866300	-1.32787900
H	-4.29596200	1.92831500	-1.29582000
H	-4.93020700	-2.61491900	0.40076200
H	-4.93339700	-1.33204100	1.61839900
H	-5.71801700	-1.07434800	0.06253300
H	-1.31595900	-2.28026700	1.91478200
H	-3.06684900	-2.53623300	1.92321600
H	-2.05966900	-3.50300300	0.83068800
H	-0.71560400	1.69760000	-1.44467400
H	-1.08089700	0.73684800	-2.90712600
H	-2.28414400	1.84100500	-2.23169400
C	0.57422300	-0.30741300	0.95591000
C	0.44921900	1.20721700	0.83801900
C	1.36242100	2.04948700	0.20703100
C	-0.72242100	1.76011500	1.35928600
C	1.09558700	3.40904000	0.08238300
H	2.28424700	1.64062700	-0.18418900
C	-0.99737300	3.11477000	1.22222700
H	-1.42473700	1.11046900	1.87054000
C	-0.08760300	3.94454900	0.57720000
H	1.81724100	4.05253000	-0.40629700
H	-1.91787700	3.52259000	1.62260400
H	-0.29436300	5.00226800	0.46969500
O	0.27966600	-0.81080700	2.05645600
C	0.39639600	-2.58849000	-0.16947000

H	0.25815200	-2.92769300	0.85030600
H	-0.22237100	-3.18515900	-0.84369000
H	1.44150800	-2.74913900	-0.42270500
C	0.80443100	-0.65477800	-1.63215800
H	0.90469500	0.41935600	-1.74846600
H	1.80962800	-1.06558000	-1.62025800
H	0.27899900	-1.06096700	-2.49986100
C	3.10224100	-0.26675900	1.82541400
H	4.05746900	-0.80803000	1.86915500
H	3.32675400	0.80912700	1.92007700
H	2.51314800	-0.56381300	2.70334200
O	2.43057100	-0.56606300	0.64434900
H	3.39756200	-0.05567300	-0.54956400
C	5.18867300	-1.87342800	-0.87321500
H	4.86637300	-2.24225000	-1.84914200
H	4.45212100	-2.18432400	-0.12848100
H	6.14949800	-2.33107700	-0.62806300
C	5.29779000	-0.35696200	-0.89278200
H	5.65900000	-0.00079100	0.08096800
H	6.02763400	-0.04037400	-1.64220500
O	4.06859900	0.25990300	-1.21970100

NHO 2a, TS3 (v = -168.00i (cm^{-1}))

0 1

C	1.54255100	-0.65521300	0.53401300
C	3.47380500	0.47663100	0.63596500
C	3.70248100	-0.66483100	-0.05747300
N	2.49622200	-1.34252700	-0.12205600
N	2.13101000	0.47161400	0.98530500
C	0.07897800	-1.07166700	0.69369500
C	2.35815700	-2.58781600	-0.88351300
C	1.51684000	1.62456200	1.65165900
C	4.41057600	1.57345000	1.00375700
C	4.95759200	-1.18721000	-0.66303100
H	4.41024300	1.75412400	2.07940600
H	5.42100600	1.30054700	0.70915400
H	4.15561000	2.50618600	0.49737300
H	5.16975800	-2.20014300	-0.31847700
H	4.90152700	-1.20047600	-1.75299200
H	5.79298700	-0.55200700	-0.37910600
H	1.42823200	-2.55913900	-1.43934800
H	3.18909500	-2.64028100	-1.57918200
H	2.39301400	-3.44567700	-0.21588200
H	0.63553700	1.94434300	1.10316800
H	1.26629900	1.38553100	2.68099200
H	2.24000800	2.43235400	1.63988000
C	-0.58304800	-0.61859100	-0.65561600
C	-0.69912400	0.88268000	-0.84660300
C	-1.65122800	1.70297500	-0.24586200
C	0.29049700	1.46576700	-1.64009200
C	-1.60288100	3.08062600	-0.42598100
H	-2.42200500	1.25166500	0.36281200
C	0.34843400	2.84376900	-1.80777900
H	1.02457900	0.82650100	-2.11882200
C	-0.59914900	3.65621600	-1.19704300
H	-2.35266700	3.70745700	0.04184100
H	1.12960200	3.28158100	-2.41728900
H	-0.56081200	4.73071800	-1.32746500
O	-0.38305000	-1.31086800	-1.65527500
C	-0.04701200	-2.59741500	0.85264400
H	0.04458200	-3.12218300	-0.09114900
H	0.69181800	-2.97836000	1.56120800
H	-1.04229300	-2.80146400	1.23854600
C	-0.54039200	-0.45852500	1.95923600
H	-0.74290100	0.60427000	1.89104600
H	-1.49252800	-0.94981000	2.13439800
H	0.10766800	-0.64390100	2.81951200
C	-4.33289000	-2.20845500	-1.05379100
H	-4.95858200	-2.06482200	-0.16928600
H	-3.84222700	-3.18031800	-0.96407300
H	-4.97946200	-2.22547800	-1.93536900
C	-3.28574400	-1.10142900	-1.15536800
H	-2.66700000	-1.28907400	-2.04744600
H	-3.80173500	-0.13856600	-1.33067400
O	-2.48819000	-1.04622800	-0.02064200
O	-3.92537900	-0.00371900	1.84363800
H	-3.35727900	-0.42975300	1.12120200
C	-4.99152600	0.68410000	1.23359300
H	-5.63159700	1.10008200	2.01407000
H	-4.64421700	1.51503100	0.60559600
H	-5.60544200	0.02622700	0.60738100

NHO 2a, TS4 (v = -317.80i (cm^{-1}))

0 1

C	-2.93170200	1.27902000	-0.03410500
C	-4.25328700	1.39409800	-0.44589100
C	-5.11779900	0.31064900	-0.33767200
C	-3.33488000	-0.99828600	0.61739700
C	-4.65465400	-0.88550200	0.20045900
C	-2.45727900	0.07690000	0.48983500
H	-4.61134200	2.33380900	-0.84946500
H	-6.14743200	0.40057700	-0.66137000
H	-5.32699400	-1.72904100	0.30166200
H	4.23717800	-1.46685200	1.70172900
H	-2.96552000	-1.91918300	1.05110000
C	-1.03137100	-0.10847500	0.93097200

O	-0.73172300	-0.98858900	1.76023500
O	-0.39505600	1.13629500	0.99278900
C	0.69996800	1.21041100	1.89737300
H	0.34607900	1.01598400	2.91263900
H	1.44511500	0.44717600	1.66073500
C	1.06063900	-0.56714900	-0.74486700
C	3.05243700	0.50944800	-0.61707000
C	3.20135400	-0.68585900	-0.00978100
N	1.97665400	-1.34742200	-0.09402100
N	1.73501200	0.57723400	-1.06816900
C	-0.33283900	-0.83323200	-0.94537000
C	1.20146500	1.77028000	-1.71600800
C	1.76288100	-2.64523300	0.54740000
C	4.40265800	-1.28123000	0.63859200
C	4.04645800	1.59384300	-0.84952900
H	-2.26000400	2.12403700	-0.11474000
H	4.68619900	-2.22551300	0.16975500
H	5.24298000	-0.59697700	0.54767700
H	5.01596100	1.28766100	-0.46361600
H	4.16226700	1.80793600	-1.91391600
H	3.76657100	2.52158600	-0.34598900
H	0.35611000	2.15146400	-1.14922500
H	1.98326600	2.52356400	-1.72576200
H	0.90906500	1.56226600	-2.74181400
H	0.98296300	-2.55945100	1.29652800
H	1.51180400	-3.40506900	-0.18676000
H	2.69044700	-2.93135400	1.03176700
C	-1.01176100	-0.12660300	-2.11419800
H	-1.10306200	0.95001100	-2.00033400
H	-0.51709200	-0.32962000	-3.07223300
H	-2.03179400	-0.50515600	-2.19240100
C	-0.76484600	-2.29070300	-0.91034700
H	-0.20415900	-2.92054000	-1.61056900
H	-0.69812900	-2.72279200	0.08547500
H	-1.81233300	-2.34570600	-1.20780500
C	1.29848200	2.59535400	1.78687900
H	2.13825100	2.69352900	2.47670900
H	1.66225500	2.78193400	0.77552100
H	0.55837700	3.35899800	2.03142500

NHO 2b, TS1 (v = -374.44i (cm^{-1}))

0 1

C	-2.62239500	1.21193900	0.21760900
C	-3.95043500	1.27743700	-0.18606000
C	-4.69111500	0.11274800	-0.34934200
C	-2.77362800	-1.18132400	0.32166300
C	-4.09895700	-1.11802600	-0.08834600
C	-2.01760700	-0.01970100	0.46271400
H	-4.40945400	2.24150600	-0.37009300
H	-5.72548100	0.16387900	-0.66671900
H	-4.67344900	-2.03027400	-0.19611800
H	-2.30967400	-2.13319000	0.54576300
C	-0.57333000	-0.14998800	0.89802900
O	-0.22821600	-1.13780300	1.58268300
O	-0.10254700	1.13155500	1.26652800
C	0.93268300	1.13424700	2.23149900
H	1.36515900	2.13560200	2.21723100
H	0.53927000	0.92498900	3.22887200
H	1.70260000	0.39534200	2.00740000
C	1.62900000	-0.14576900	-0.59213100
C	3.62904400	0.91716700	-0.06044500
C	3.82014100	-0.58296400	0.04297100
N	2.44789600	-1.07249800	-0.04192600
N	2.32318300	1.02063700	-0.71209000
C	0.25168300	-0.34464100	-0.93911700
C	1.81616700	2.37779000	-0.89654100
C	2.23905300	-2.49447800	0.18951300
H	-2.05012000	2.12059400	0.34899700
H	2.64536900	3.05122600	-0.68702400
H	1.49478100	2.55134000	-1.91999400
H	1.00293700	2.59712400	-0.20647700
H	1.29196900	-2.65626600	0.68871700
H	2.30357600	-3.07436600	-0.73308900
H	3.03535400	-2.82271200	0.85647400
H	4.41320000	-0.98265500	-0.78642800
H	4.39435100	1.40703500	-0.65978900
H	4.27724500	-0.89022200	0.98265000
H	3.59052000	1.39522400	0.92457400
C	-0.12895600	-1.75504000	-1.38265000
H	0.57263500	-2.16968400	-2.11292800
H	-0.21312200	-2.44850900	-0.54954600
H	-1.10615900	-1.71726700	-1.86324800
C	-0.34762200	0.68467300	-1.89108000
H	-0.46580300	1.67016800	-1.44830200
H	0.23692100	0.78668900	-2.81255500
H	-1.34643400	0.35300800	-2.17367300

NHO 2b, TS2 (v = -162.08i (cm^{-1}))

0 1

C	-1.70248900	-0.97880400	-0.46554100
C	-3.75177100	-0.15164800	-1.12317600
C	-3.96520700	-1.34782200	-0.21508300
N	-2.61052500	-1.59238000	0.28871000
N	-2.30276300	-0.19215600	-1.36494200
C	-0.19278000	-1.15186100	-0.30713300
C	-2.46166300	-2.58081300	1.35063900

C	-1.77013200	0.88407800	-2.20255200
H	-1.62437800	-2.31595700	1.98442700
H	-3.37669500	-2.54663200	1.93927300
H	-2.34720100	-3.58369400	0.93725500
H	-1.11769400	1.54563900	-1.63677000
H	-1.25328100	0.49137100	-3.07339900
H	-2.62793200	1.45965800	-2.54341800
C	0.16799900	-0.26518000	0.95625400
C	-0.06305000	1.22508700	0.73357500
C	0.82572000	2.10145000	0.11528600
C	-1.30856000	1.70873500	1.14094600
C	0.46378000	3.42584600	-0.11026200
H	1.80122500	1.74647600	-0.18817300
C	-1.67756900	3.02594800	0.90046800
H	-1.99227700	1.03391400	1.64517300
C	-0.79048900	3.88918300	0.26760200
H	1.16680400	4.09774600	-0.58776100
H	-2.65312100	3.37934200	1.21218400
H	-1.07065600	4.91837400	0.07945600
O	-0.12841000	-0.72151500	2.07406300
C	2.65360300	-0.01160100	1.90797900
H	3.63093700	-0.50104900	2.02112800
H	2.82250200	1.07763500	1.94931000
H	2.04285800	-0.28838100	2.77771900
O	2.04775400	-0.41013900	0.72064600
H	3.03410800	0.10791700	-0.45947000
C	4.84249100	-1.68858200	-0.65844300
H	4.54694300	-2.09301300	-1.62883500
H	4.08742300	-1.97522200	0.07744800
H	5.79847700	-2.13233900	-0.37221200
C	4.94659000	-0.17318700	-0.72899700
H	5.28150800	0.21829400	0.24071300
H	5.69395800	0.12072900	-1.47031300
O	3.72330400	0.42586600	-1.10835000
H	-4.31125100	-2.23212800	-0.75656500
H	-4.29431700	-0.21779600	-2.06332800
H	-4.64405000	-1.14548000	0.61037500
H	-3.99515800	0.79393300	-0.62958300
C	0.55201600	-0.75787600	-1.59124600
H	1.57208700	-1.12024800	-1.51040900
H	0.08865200	-1.23251200	-2.45919100
H	0.60728100	0.31272600	-1.75809500
C	0.16050700	-2.62492300	-0.03217700
H	-0.41239100	-3.29369300	-0.67879400
H	1.21802200	-2.75554000	-0.24838500
H	0.00548300	-2.90020100	1.00417400

NHO 2b, TS3 (v = -161.63i (cm^{-1}))

0 1			
C	1.75008200	-0.87935400	0.45495800
C	3.79536100	0.09028400	0.90038600
C	4.00371000	-1.13708400	0.03250700
N	2.62900600	-1.49106900	-0.33416500
N	2.37258100	-0.00795800	1.25506800
C	0.24373600	-1.13952100	0.43059500
C	2.45659300	-2.54792000	-1.32479800
C	1.84563800	1.08502700	2.07387300
H	1.57059900	-2.35734100	-1.91815300
H	3.33086000	-2.51340000	-1.97232000
H	2.41195300	-3.52787000	-0.84810300
H	1.39156300	0.71436300	2.98786400
H	2.69799400	1.70470800	2.34307800
H	1.13859200	1.69577500	1.51578100
C	-0.25948900	-0.34756700	-0.84251200
C	-0.12777400	1.16414600	-0.72356800
C	-1.01354000	2.00842900	-0.05791000
C	1.02686100	1.71145500	-1.28765300
C	-0.73625000	3.36636700	0.05726700
H	-1.92014600	1.60030700	0.36689600
C	1.31249300	3.06485300	-1.15871600
H	1.70573500	1.06034000	-1.82819900
C	0.43016200	3.89734500	-0.48052800
H	-1.43636700	4.01227000	0.57316200
H	2.21936100	3.46948400	-1.59186600
H	0.64505600	4.95406500	-0.37988700
O	-0.03600400	-0.85269200	-1.95041500
C	-4.20638900	-1.02990600	-1.62224500
H	-4.82479300	-0.69960500	-0.78494700
H	-4.06206600	-2.10940000	-1.53667400
H	-4.74570500	-0.82468800	-2.55044500
C	-2.85822000	-0.31730300	-1.60726300
H	-2.27398300	-0.63481800	-2.48249500
H	-3.02857300	0.76903600	-1.71881300
O	-2.15426700	-0.59648700	-0.43897300
O	-3.64436800	0.27296000	1.49833800
H	-3.04516700	-0.06807900	0.76708300
C	-4.21500000	-0.84126600	2.14301700
H	-5.00922500	-0.49425000	2.80625200
H	-4.65144300	-1.54765400	1.42780500
H	-3.48206700	-1.38542400	2.75208900
H	4.40869900	0.09467900	1.79843300
H	4.45543000	-1.96933600	0.57803200
H	4.59055800	-0.93533900	-0.86091700
H	3.95437600	1.02192900	0.34997900
C	-0.05011200	-2.64063200	0.26097100
H	0.57718900	-3.24061400	0.92434900
H	-1.09229400	-2.79878800	0.52746600

H	0.07564200	-2.97629700	-0.76111900
C	-0.41912500	-0.71195400	1.74727800
H	-1.41742900	-1.13550800	1.76543300
H	0.13680300	-1.10959700	2.59938000
H	-0.52758100	0.36161200	1.85898400

NHO 2b, TS4 (v = -363.05i (cm^{-1}))

0 1

C	2.63633400	1.05342600	0.47815200
C	3.94340000	0.97334600	0.94442500
C	4.75318400	-0.09606600	0.57965900
C	2.94723400	-0.99279700	-0.73696200
C	4.25123800	-1.07868700	-0.26682700
C	2.12423400	0.06529100	-0.35922400
H	4.33152500	1.74906200	1.59367700
H	5.77049700	-0.15895200	0.94600900
H	4.87980800	-1.90881400	-0.56630400
H	2.54885100	-1.74094900	-1.41071100
C	0.70348100	0.08285500	-0.88726700
O	0.46902600	-0.46646700	-1.99166800
O	0.15259800	1.36569000	-0.64676400
C	-0.86426100	1.74519000	-1.55958400
H	-0.43331700	1.87858100	-2.55507000
H	-1.61333800	0.95274900	-1.64593300
C	-1.52764500	-0.57430500	0.48661900
C	-3.49945100	0.51343200	1.04156600
C	-3.72003700	-0.30091700	-0.21679500
N	-2.51688000	-1.13363800	-0.26464600
N	-2.04517300	0.46607400	1.17249500
C	-0.15659400	-1.01943000	0.53625600
C	-1.41164900	1.37016200	2.11740000
C	-2.35594000	-1.93647100	-1.48051600
H	2.00892400	1.88884200	0.76201500
H	-2.09775300	2.20305000	2.26571000
H	-1.22779000	0.90099400	3.08437100
H	-0.48853800	1.76087500	1.69813600
H	-1.53114200	-1.56420800	-2.08535900
H	-2.20999000	-2.98815000	-1.24606300
H	-3.28376300	-1.84178600	-2.04212100
H	-4.61446200	-0.91971800	-0.18151400
H	-3.96966500	0.05699500	1.91818900
H	-3.76350900	0.33656400	-1.10783400
H	-3.84447100	1.54230800	0.94972000
C	0.06475600	-2.45180900	0.06539200
H	-0.64940800	-3.15184500	0.51186200
H	0.01929200	-2.53798000	-1.01724700
H	1.06185700	-2.76922200	0.37072700
C	0.52403600	-0.82560000	1.89426400
H	0.74590500	0.20628200	2.14625100
H	-0.06871400	-1.25910300	2.70768400
H	1.48208700	-1.34528900	1.87512900
C	-1.48944500	3.03028800	-1.06243000
H	-0.73629800	3.81448300	-0.96971100
H	-2.25454500	3.36937200	-1.76274900
H	-1.95518700	2.88446700	-0.08658800

NHO 2c, TS1 (v = -201.05i (cm^{-1}))

0 1

C	-3.07258300	-1.08196400	0.03008700
C	-4.38765000	-0.80718800	0.39138100
C	-4.87730700	0.49095500	0.32555300
C	-2.73526100	1.23022800	-0.48825800
C	-4.04619900	1.50997600	-0.12638100
C	-2.22268100	-0.06187900	-0.39604200
H	-5.03387600	-1.61409800	0.71604400
H	-5.90136200	0.70452200	0.60668400
H	-4.42351600	2.52257300	-0.20547100
H	-2.09712600	2.01752300	-0.86998500
C	-0.76066900	-0.29213900	-0.79107100
O	-0.27161200	0.50791700	-1.64978800
O	-0.68276200	-1.69459800	-1.11093000
C	0.44699000	-2.11404800	-1.84342100
H	1.17794700	-2.59957300	-1.18889500
H	0.11307600	-2.83424700	-2.59264600
H	0.91726000	-1.26797900	-2.34541200
H	-2.71125800	-2.10081400	0.05521600
C	3.52127200	-0.55610300	-0.61600000
C	4.22380500	0.71356800	-0.17685600
C	3.19069400	1.80988700	-0.30583700
H	4.17020600	-1.42982700	-0.61485400
H	3.10719000	-0.43836700	-1.62059700
H	3.42988600	2.67497300	0.31595800
H	3.14676900	2.15144300	-1.34263700
C	1.48433200	0.17458500	0.45896100
C	0.10842100	-0.18318800	0.86777400
N	1.81756400	1.39335300	0.04775100
N	2.42932000	-0.80569000	0.31790500
C	2.83209200	-1.64116300	1.45289100
H	3.87706300	-1.42473100	1.68934500
H	2.24655600	-1.41829900	2.33590400
H	2.74136500	-2.70079800	1.20881300
C	0.90803000	2.53552000	-0.06131000
H	-0.08200000	2.20350800	-0.32465900
H	0.92075300	3.11211700	0.86527700
H	1.27250000	3.16544200	-0.87190400
C	-0.05490700	-1.56940300	1.49058800

H	0.47874100	-2.35356400	0.96148500
H	0.23830700	-1.57590900	2.54400600
H	-1.11402500	-1.81918300	1.46362300
C	-0.55823700	0.80220200	1.84315800
H	0.10916500	1.01070300	2.68569800
H	-0.87577900	1.74892200	1.42050000
H	-1.45526100	0.32963800	2.24643600
H	4.56637300	0.60391400	0.85412500
H	5.08699100	0.95284100	-0.79719800

NHO 2c, TS2 (v = -131.28i (cm^{-1}))

0 1

C	0.15868000	-0.28833600	1.00103800
C	0.74527600	1.10646200	0.86820600
C	1.80436500	1.44672000	0.02593900
C	0.12970100	2.11037600	1.61330100
C	2.21488100	2.76891300	-0.08419000
H	2.31138900	0.67558700	-0.53829300
C	0.53786400	3.43472800	1.50133500
H	-0.68191100	1.83945400	2.27736700
C	1.57859600	3.76899000	0.64534600
H	3.04088300	3.02028000	-0.73887300
H	0.04285900	4.20385800	2.08192300
H	1.90079200	4.79892000	0.55304100
O	-0.32401700	-0.59277300	2.10645600
O	1.78641500	-1.25165700	0.76100700
C	1.93281900	-2.24517900	1.71994300
H	1.83054800	-3.25461000	1.29131000
H	1.17038300	-2.14195900	2.50573700
H	2.91628300	-2.18587900	2.20705800
O	3.53143100	-1.40818700	-1.13393400
H	2.83164700	-1.38589400	-0.41536800
C	4.73759500	-0.95630000	-0.55422300
H	5.06804800	-1.64485100	0.23438100
H	4.59087700	0.02541300	-0.08376600
C	5.80249400	-0.85680000	-1.62738200
H	5.49114000	-0.15753800	-2.40556200
H	6.74698300	-0.50869200	-1.20582400
H	5.96757000	-1.83208600	-2.08889600
C	-3.75959300	1.05373400	-1.41904600
C	-4.62947100	-0.17189600	-1.35607000
C	-4.45792700	-0.75091600	0.02203600
H	-4.12963200	1.83314000	-0.74664400
H	-3.72225600	1.46888200	-2.42675000
H	-4.86154100	-0.07946200	0.78537200
H	-4.96232500	-1.71244300	0.11909900
C	-2.05103000	-0.33705700	-0.30522900
C	-0.58277300	-0.87998100	-0.26805600
N	-3.03687600	-1.00004200	0.30395400
N	-2.37188700	0.72660800	-1.05463400
C	-1.48260300	1.80941100	-1.48611700
H	-2.01506800	2.74075100	-1.28808200
H	-0.56269800	1.83526300	-0.92268800
H	-1.28420900	1.74024400	-2.55597800
C	-2.89447500	-1.94374000	1.41996400
H	-3.04480100	-2.96774200	1.07738100
H	-1.94126500	-1.81081100	1.91240100
H	-3.68533200	-1.69323600	2.12819900
H	-4.32267300	-0.89626700	-2.11346500
H	-5.67080400	0.09235000	-1.53217800
C	-0.59817500	-2.42528200	-0.15721200
H	-1.44744400	-2.85312200	-0.69270600
H	0.31520200	-2.79931500	-0.61138900
H	-0.60439300	-2.77039000	0.87021700
C	0.10601600	-0.62180300	-1.62418600
H	1.04991400	-1.16068000	-1.61911100
H	-0.51605900	-1.02493700	-2.42763100
H	0.33517100	0.40847200	-1.85613300

NHO 2c, TS3 (v = -164.36i (cm^{-1}))

0 1

C	-0.46370700	-0.56591200	-0.81108100
O	-0.36164000	-1.17776900	-1.88431300
C	-3.91247700	-2.58211800	-0.76304100
H	-4.42062400	-2.51515600	0.20218500
H	-3.25932500	-3.45737400	-0.73998900
H	-4.66697500	-2.73169700	-1.53987600
C	-3.08915600	-1.32406700	-1.02566300
H	-2.57351600	-1.43619100	-1.99062400
H	-3.77195600	-0.46106000	-1.12922600
O	-2.16136900	-1.11073900	-0.01352400
O	-3.47204300	-0.25592000	2.06993700
H	-2.94648300	-0.60518200	1.28998600
C	-4.70161800	0.23878900	1.59132000
H	-5.29333900	0.57904500	2.44277400
H	-4.56878800	1.08925500	0.91056400
H	-5.27723500	-0.52872700	1.06168200
C	3.66102300	0.92523300	1.26404800
C	4.55210200	-0.25679300	0.99839900
C	4.20616900	-0.75395400	-0.37926000
H	3.91479300	1.76296100	0.60789600
H	3.74465800	1.26953600	2.29556500
H	4.46573600	-0.01352000	-1.14207900
H	4.73095400	-1.67923100	-0.61755100
C	1.85778200	-0.45624500	0.29547200
C	0.41129200	-1.04415600	0.41405800

N	2.77098600	-1.05550700	-0.47419900
N	2.24770200	0.57236000	1.05879200
C	1.38741300	1.60934300	1.63788500
H	1.89453800	2.55862800	1.46212700
H	0.42647600	1.65833000	1.15025500
H	1.27005300	1.46687600	2.71185200
C	2.51483200	-1.91331500	-1.63751100
H	1.47399700	-1.88839700	-1.93117600
H	3.11662900	-1.50791500	-2.45321000
H	2.85096400	-2.93058200	-1.43228400
C	-0.64783600	0.94111700	-0.89842600
C	-1.65151000	1.67695600	-0.27539900
C	0.32403400	1.61862100	-1.63838000
C	-1.66788700	3.06472600	-0.37283100
H	-2.40857500	1.15594000	0.29234300
C	0.31696500	3.00445200	-1.72373600
H	1.09428000	1.04784000	-2.14740300
C	-0.68019300	3.73350300	-1.08514000
H	-2.45643100	3.62442100	0.11612800
H	1.08555400	3.51502000	-2.29137900
H	-0.69151200	4.81446700	-1.15057800
H	5.59836900	0.04099700	1.04402100
H	4.38226100	-1.04022000	1.73965100
C	-0.21440200	-0.69565800	1.78406500
H	-0.93683900	-1.47022600	2.02091900
H	0.54645600	-0.68921100	2.56582200
H	-0.75907500	0.24239700	1.80104800
C	0.49083600	-2.58418800	0.42464400
H	1.10910800	-2.91403400	1.26286400
H	-0.52650200	-2.94043200	0.57269500
H	0.86120500	-3.03229200	-0.48594800

NHO 2c, TS4 (v = -198.32i (cm^{-1}))

0 1

C	3.06845000	0.76711400	0.56242300
C	4.38568400	0.37216300	0.77275000
C	4.87882700	-0.77711900	0.16839000
C	2.73531800	-1.11740000	-0.87477800
C	4.04855700	-1.51721900	-0.66612900
C	2.21978900	0.01576500	-0.24969600
H	5.03058600	0.97193500	1.40421500
H	5.90423900	-1.08487200	0.33269000
H	4.42802300	-2.40313600	-1.16131500
H	2.09810700	-1.67594300	-1.54954400
C	0.75724500	0.38830500	-0.51414700
O	0.27280400	0.01872800	-1.63161900
O	0.67069100	1.79305500	-0.21469800
C	-0.44848400	2.49233400	-0.72381500
H	-1.10051400	2.77595600	0.11123300
H	-1.01138500	1.84174200	-1.39361500
H	2.70353400	1.68103500	1.01084300
C	-3.51533300	0.58026500	-0.26263900
C	-4.23423100	-0.75080600	-0.36152900
C	-3.21559000	-1.71278800	-0.93008400
H	-4.15274600	1.38982500	0.08775600
H	-3.10252200	0.86471100	-1.23387000
H	-3.46036500	-2.75277500	-0.70399500
H	-3.18323700	-1.61050900	-2.01729500
C	-1.49024800	-0.54308400	0.42227900
C	-0.11250200	-0.40548700	0.94255100
N	-1.83563200	-1.48284400	-0.45266700
N	-2.42139700	0.42353600	0.68911300
C	-2.81984500	0.74731300	2.06253300
H	-3.86910200	0.47056200	2.19239700
H	-2.24327700	0.18662800	2.78677300
H	-2.71379600	1.81597500	2.25563300
C	-0.93490700	-2.48221000	-1.03136100
H	0.05256600	-2.06862900	-1.15398300
H	-0.93596200	-3.38655800	-0.42058600
H	-1.31684000	-2.72737800	-2.02159900
C	0.06322300	0.58494600	2.09326700
H	-0.45537100	1.52704900	1.94379200
H	-0.23784800	0.14898600	3.04985400
H	1.12555300	0.80688700	2.17586400
C	0.54590300	-1.71692700	1.40376000
H	-0.13313000	-2.27710400	2.05472100
H	0.88446700	-2.37993600	0.61548600
H	1.42975200	-1.46608000	1.99231100
H	-4.56914700	-1.06008100	0.63059800
H	-5.10370100	-0.71147900	-1.01683900
C	0.02584400	3.72900500	-1.46440000
H	-0.82620200	4.31791200	-1.81064300
H	0.63570000	4.35778500	-0.81302900
H	0.62767000	3.44336300	-2.32867700