Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Hydration of Oxalic Acid –Ammonia Complex: Atmospheric Implication and Rayleigh Scattering Properties

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Table S1. The relative single point energy ΔE_{rel}, the ZPE-corrected binding energies (ΔE_0), intermolecular enthalpy (ΔH), free energy changes (ΔG) and Boltzmann averaged Gibbs free energy of $(H_2C_2O_4)(NH_3)(H_2O)_n$ (n=0~3) (in kcal mol^{-1}) based on PW91PW91/6-311++G(3df,3pd) calculations.

m, n	isomer	ΔE_{rel}	ΔE_0	ΔH	ΔG	Boltzmann averaged Gibbs free energy
m=1,n=0	1.0 -a	0	-11.9	-12.4	-4.4	-4.4
m=1,n=1	1.1 -a	0	-17.7	-18.5	-3.4	-2.8
	1.1 -b	0.3	-17.3	-18.3	-2.7	
	1.1 -c	0.6	-17.0	-18.0	-2.5	
	1.1 -d	0.7	-16.9	-17.8	-2.5	
m=1,n=2	1.2 -a	0	-25.9	-27.8	-3.4	-0.9
	1.2 -b	0.9	-25.0	-26.9	-2.2	
	1.2 -c	1.2	-24.7	-26.3	-2.8	
	1.2 -d	1.7	-24.2	-25.5	-2.8	
	1.2 -e	3.1	-22.8	-24.6	-0.9	
	1.2 -f	3.2	-22.7	-24.5	-0.7	
	1.2 -g	3.2	-22.7	-24.3	-0.8	
	1.2 -h	3.9	-22.0	-23.4	-0.8	
	1.2 -i	4.0	-21.9	-23.3	-0.3	
	1.2 -j	6.0	-19.9	-20.9	0.3	
	1.2 -k	8.3	-17.6	-18.6	4.0	
m=1,n=3	1.3 -a	0	-34.1	-36.5	-4.5	-0.9
	1.3 -b	0.5	-33.6	-36.1	-3.8	

	1.3 -c	0.6	-33.5	-36.1	-3.04	
	1.3 -d	1.0	-33.0	-35.6	-2.7	
	1.3 -e	1.1	-33.0	-35.4	-3.3	
	1.3 -f	1.3	-32.9	-35.3	-2.5	
	1.3 -g	1.3	-32.8	-35.3	-2.8	
	1.3 -h	2.5	-31.7	-34.0	-1.5	
	1.3 -i	2.6	-31.5	-34.0	-0.9	
	1.3 -j	3.2	-30.9	-33.1	-1.2	
	1.3 -k	3.4	-30.8	-33.2	-1.2	
	1.3 -l	4.0	-30.1	-32.6	-0.1	
	1.3 -m	4.4	-29.7	-32.3	0.4	
	1.3 -n	5.1	-29.0	-31.6	1.0	
	1.3 -o	5.3	-28.8	-31.5	1.2	
	1.3 -p	5.9	-28.3	-31.1	1.5	
	1.3 -q	6.8	-27.3	-30.1	2.8	
	1.3 -r	7.2	-27.0	-28.5	0.4	
	1.3 -s	7.8	-26.3	-28.4	3.5	

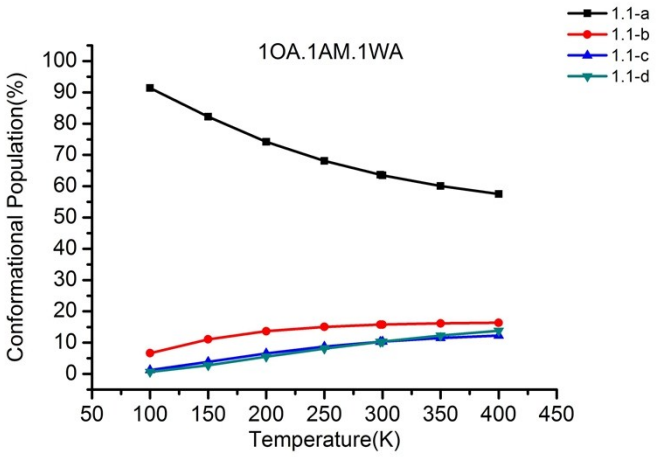
Table S2. The relative single point energy ΔE_{rel}, the ZPE-corrected binding energies (ΔE_0), intermolecular enthalpy (ΔH), free energy changes (ΔG) and Boltzmann averaged Gibbs free energy of $(H_2C_2O_4)(NH_3)_2(H_2O)_n$ (n=0~3) (in kcal mol^{-1}) based on PW91PW91/6-311++G(3df,3pd) calculations.

m, n	isomer	ΔE_{rel}	ΔE_0	ΔH	ΔG	Boltzmann averaged Gibbs free energy
m=2,n=0	2.0 -a	0	-17.4	-18.3	-2.0	-0.7
	2.0 -b	4.1	-13.3	-13.5	0.7	
m=2,n=1	2.1 -a	0	-25.7	-27.4	-2.9	-1.8
	2.1 -b	0.4	-25.4	-26.9	-2.7	
	2.1 -c	0.4	-25.3	-26.9	-2.2	
	2.1 -d	0.7	-25.0	-26.4	-2.3	
	2.1 -e	1.2	-24.5	-25.7	-2.3	
	2.1 -f	1.3	-24.5	-25.9	-1.8	
	2.1 -g	1.4	-24.3	-25.9	-1.6	
	2.1 -h	2.2	-23.6	-25.1	-0.8	
	2.1 -i	3.2	-22.5	-24.1	0.1	
m=2,n=2	2.2 -a	0	-34.4	-36.6	-4.3	-1.6
	2.2 -b	0.3	-34.1	-36.4	-3.7	
	2.2 -c	0.9	-33.4	-35.6	-3.4	
	2.2 -d	1.2	-33.1	-35.3	-2.8	
	2.2 -e	1.3	-33.1	-35.6	-2.2	
	2.2 -f	1.3	-33.1	-34.6	-3.9	
	2.2 -g	1.5	-32.8	-35.1	-2.5	

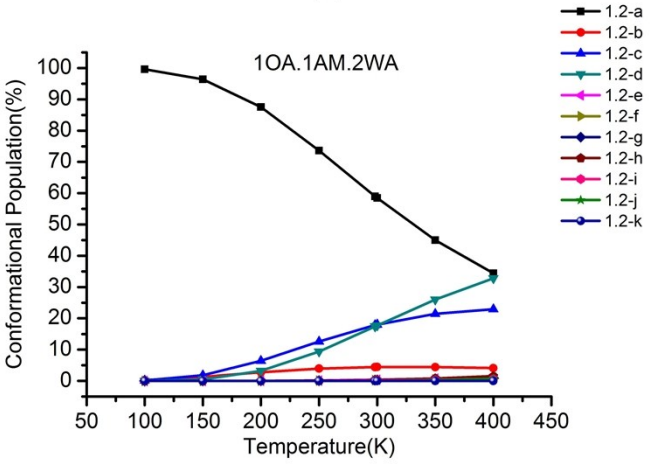
	2.2 -h	1.8	-32.6	-34.9	-1.8	
	2.2 -i	1.8	-32.6	-34.7	-2.6	
	2.2 -j	1.8	-32.5	-34.7	-2.0	
	2.2 -k	1.9	-32.4	-34.7	-2.5	
	2.2 -l	2.3	-32.1	-34.4	-1.1	
	2.2 -m	2.7	-31.7	-33.8	-1.7	
	2.2 -n	4.5	-29.9	-32.2	0.1	
	2.2 -o	4.8	-29.6	-31.6	0.8	
	2.2 -p	5.3	-29.0	-31.0	-0.3	
	2.2 -q	6.6	-27.8	-30.4	3.1	
	2.2 -r	7.0	-27.4	-29.4	2.1	
m=2,n=3	2.3 -a	0	-41.7	-44.4	-4.5	-1.8
	2.3 -b	0.1	-41.6	-44.3	-4.4	
	2.3 -c	0.1	-41.6	-44.3	-4.7	
	2.3 -d	0.8	-40.9	-43.8	-2.9	
	2.3 -e	0.9	-40.8	-43.8	-2.1	
	2.3 -f	1.0	-40.6	-43.7	-2.5	
	2.3 -g	1.1	-40.5	-43.2	-3.4	
	2.3 -h	1.8	-39.8	-42.9	-1.6	
	2.3 -i	2.2	-39.5	-42.6	-1.6	
	2.3 -j	2.4	-39.3	-42.4	-1.0	
	2.3 -k	3.8	-37.9	-40.8	-0.1	

	2.3 -l	5.4	-36.3	-39.0	1.3	
	2.3 -m	8.1	-33.6	-36.3	4.7	

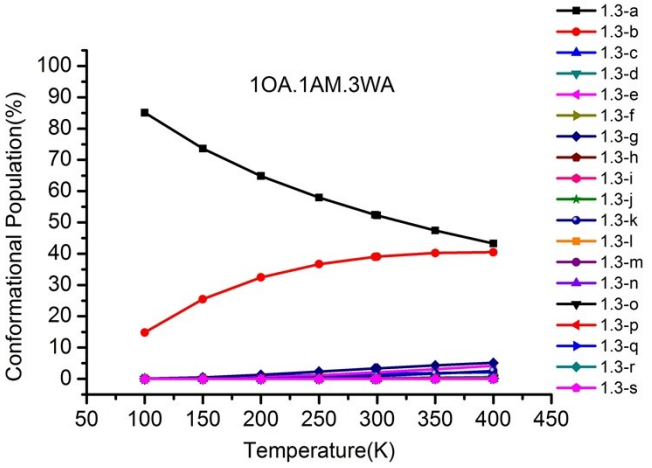
Figure. S1. The conformational population changes in the low isomers of $(H_2C_2O_4)(NH_3)$ $(H_2O)_n$ (n=1~3) as a function of temperature (OA stands for oxalic acid, AM stands for ammonia, WA stands for water).



(a)

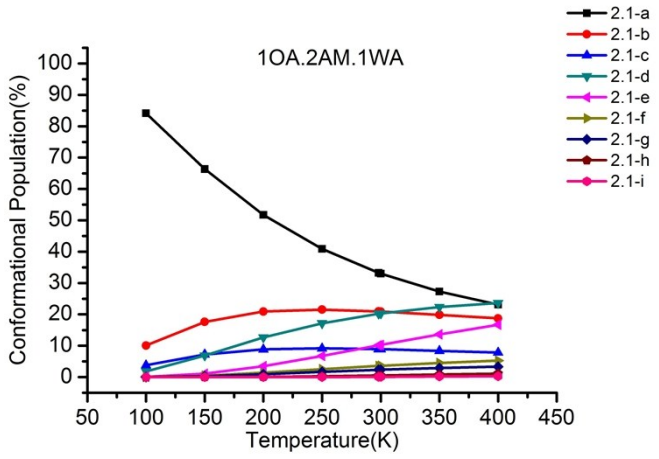


(b)

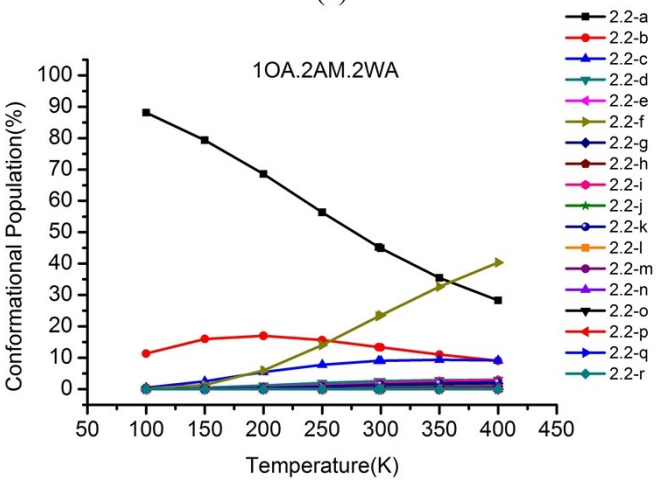


(c)

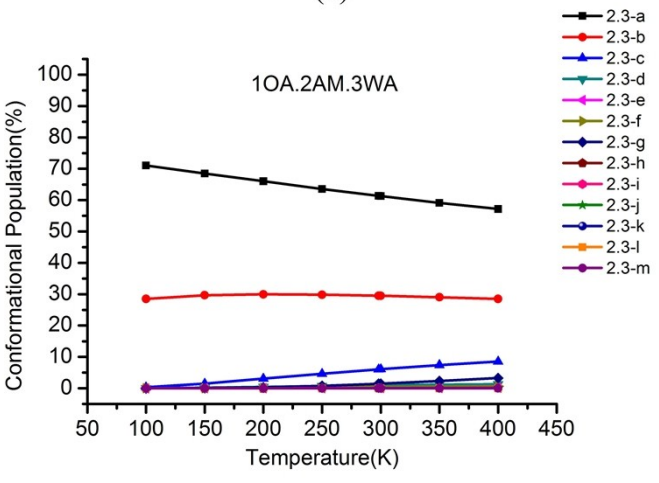
Figure. S2. The conformational population changes in the low isomers of $(H_2C_2O_4)(NH_3)_2(H_2O)_n$ (n=1~3) as a function of temperature (OA stands for oxalic acid, AM stands for ammonia, WA stands for water).



(a)



(b)



(c)

Data S1: The coordinates of $(H_2C_2O_4)(NH_3)_m(H_2O)_n$ (m=1~2, n=1~3) isomers

$(H_2C_2O_4)(NH_3)$ (H_2O)

Isomer 1.1 -a

C	0.791880	-0.799831	0.151041
C	1.339050	0.643604	-0.101105
O	1.783562	-1.680937	0.115448
O	-0.370788	-1.092298	0.353629
O	2.558169	0.711012	-0.274911
O	0.510831	1.628087	-0.115080
H	2.578184	-1.097842	-0.062468
H	-0.627272	1.468643	0.064074
N	-1.972268	1.549067	0.252381
H	-2.182289	1.649147	1.246173
H	-2.460097	0.698594	-0.082122
H	-2.358011	2.363139	-0.227054
O	-3.043376	-1.075347	-0.301953
H	-2.128487	-1.372259	-0.113938
H	-3.308906	-1.539653	-1.108021

$(H_2C_2O_4)(NH_3)$ (H_2O)

Isomer 1.1 -b

C	0.031068	0.819313	-0.024801
C	0.029483	-0.750944	-0.025700
O	1.205728	1.417262	0.019847
O	-1.012518	1.444093	-0.071836
O	1.073819	-1.394063	-0.051627
O	-1.139643	-1.329017	-0.008818
H	2.014064	0.805413	0.054175
H	-2.007764	-0.721773	0.016652
N	-3.417400	-0.051752	0.055685
H	-4.031672	-0.258476	-0.731194
H	-3.952122	-0.184071	0.913501
H	-3.127700	0.926367	-0.001625
O	3.372388	-0.098098	0.146938
H	3.924237	-0.085422	-0.648883
H	2.741271	-0.851398	0.034559

$(H_2C_2O_4)(NH_3)$ (H_2O)

Isomer 1.1 -c

C	1.397608	0.628534	0.046337
C	0.857877	-0.829195	-0.059642
O	0.544385	1.612044	0.043609
O	2.612705	0.759558	0.133803

O	-0.310968	-1.137559	-0.129470
O	1.866629	-1.699019	-0.054784
H	-0.464098	1.373912	-0.053229
H	2.671790	-1.119335	0.020057
N	-3.255482	-0.880175	0.165628
H	-3.688622	-1.123587	1.055740
H	-2.402464	-1.437022	0.069840
H	-3.898515	-1.161291	-0.573902
O	-1.972004	1.466446	-0.224298
H	-2.520097	0.631062	-0.030795
H	-2.368500	2.189683	0.281854

$(H_2C_2O_4)(NH_3)$ (H_2O)

Isomer 1.1 -d

C	-1.398284	0.539624	-0.155646
C	-0.665476	-0.773550	0.297657
O	-2.668236	0.279682	-0.453324
O	-0.894730	1.644287	-0.243141
O	-1.361290	-1.794468	0.254035
O	0.562200	-0.677505	0.656907
H	-2.723886	-0.705951	-0.290765
H	1.175464	0.514742	0.604894
N	1.834884	1.475625	0.404616
H	2.586683	1.158508	-0.219373
H	1.186757	2.118247	-0.060900
H	2.222323	1.900082	1.246111
O	3.051213	-0.851109	-0.641587
H	3.361479	-1.511471	-1.275988
H	2.216293	-1.207064	-0.271478

$(H_2C_2O_4)(NH_3)$ $(H_2O)_2$

Isomer 1.2 -a

C	1.125605	0.744549	0.230463
C	1.924979	-0.547691	-0.161646
O	-0.089959	0.585052	0.597295
O	1.764838	1.800006	0.132567
O	1.477469	-1.679135	-0.190587
O	3.179781	-0.238962	-0.480783
H	-0.699419	-0.763275	0.642005
H	3.184827	0.754879	-0.368872
N	-1.257705	-1.720435	0.549703
H	-1.424215	-2.147149	1.460915
H	-0.632945	-2.317660	0.000193
H	-2.169699	-1.504578	0.068606

O	-3.547313	-0.597113	-0.445588
H	-3.203487	0.344054	-0.384320
H	-3.946227	-0.676728	-1.323290
O	-2.347543	1.775572	-0.217860
H	-2.664787	2.478451	0.366189
H	-1.441803	1.530554	0.117396

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -b

C	-1.703789	0.199826	-0.249290
C	-0.663384	-0.565393	0.640595
O	-2.467706	-0.648892	-0.938337
O	-1.787077	1.409506	-0.345381
O	-0.603609	-1.799851	0.397018
O	0.034256	0.092582	1.455136
H	-2.083743	-1.534891	-0.691813
H	0.424878	1.442854	1.004889
N	0.813395	2.288003	0.399453
H	1.525591	1.840680	-0.235992
H	-0.006198	2.609126	-0.127082
H	1.219466	3.039876	0.954400
O	2.088692	-1.883551	-0.162762
H	2.590906	-2.094784	0.637888
H	1.137802	-1.991922	0.105700
O	2.552627	0.651524	-0.939870
H	2.380330	-0.292907	-0.641363
H	2.782787	0.588800	-1.877066

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -c

C	1.013712	-1.009004	0.114396
C	1.571667	0.457487	0.064606
O	-0.219610	-1.155309	0.375545
O	1.872201	-1.875422	-0.123931
O	0.921506	1.478671	0.218242
O	2.873957	0.447624	-0.183132
H	-1.249627	-0.048034	0.582328
H	3.048269	-0.540656	-0.261184
N	-2.212531	0.479391	0.568953
H	-2.087331	1.403371	0.090744
H	-2.565465	0.619860	1.515609
H	-2.829946	-0.170250	0.055105
O	-2.654909	-2.088145	-0.425369
H	-2.800722	-2.716294	-1.145371

H	-1.685551	-2.100051	-0.242756
O	-1.311943	2.897547	-0.381543
H	-0.401216	2.545482	-0.238156
H	-1.302573	3.320224	-1.251510

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -d

C	0.377880	-0.581601	0.002894
C	0.679672	0.951081	-0.074973
O	1.399099	-1.392315	0.074948
O	-0.782280	-0.968914	-0.013754
O	1.818642	1.370943	-0.187965
O	-0.367059	1.744225	-0.023674
H	2.371261	-0.972260	0.079712
H	-1.278674	1.297188	0.077589
N	3.876796	-0.557602	0.085493
H	4.445119	-0.925077	-0.676743
H	3.742074	0.445958	-0.056847
H	4.387942	-0.700155	0.955752
O	-2.892494	1.178626	0.284714
H	-3.387849	1.757764	-0.312069
H	-3.218328	0.255393	0.104683
O	-3.455368	-1.427335	-0.218577
H	-2.484117	-1.565518	-0.172185
H	-3.824635	-1.948798	0.508596

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -e

C	-1.903440	-0.522733	-0.209524
C	-1.167987	0.763669	0.290347
O	-3.122193	-0.215334	-0.648823
O	-1.444893	-1.645046	-0.217869
O	-1.771827	1.823777	0.167934
O	0.028655	0.641417	0.789174
H	-3.177178	0.769105	-0.523627
H	0.447923	-0.362417	0.813884
N	2.774283	1.734203	-0.297811
H	1.833462	1.730092	0.108819
H	3.370915	2.270505	0.332271
H	2.721630	2.256805	-1.172494
O	3.214142	-0.952475	-0.636510
H	4.086326	-1.227806	-0.320272
H	3.172676	0.052575	-0.525654
O	1.116483	-1.588563	0.833204

H 1.934788 -1.477684 0.254339
H 0.455092 -2.106423 0.335597

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$
Isomer 1.2 -f
C 0.329296 -0.555846 0.285544
C 0.704379 0.952822 0.034849
O 1.262551 -1.472699 0.154585
O -0.818246 -0.853878 0.595078
O 1.895911 1.290862 -0.022309
O -0.287757 1.748417 -0.085366
H 2.197938 -1.122148 -0.064100
H -1.512446 1.390156 -0.031129
N -2.739598 1.263506 -0.008090
H -3.017238 0.302221 -0.295487
H -3.069076 1.407712 0.947284
H -3.192230 1.952008 -0.610126
O -3.246929 -1.514910 -0.345153
H -2.328604 -1.614166 -0.003501
H -3.305240 -2.094864 -1.117301
O 3.657274 -0.579929 -0.394307
H 4.286983 -0.694515 0.332488
H 3.212618 0.304300 -0.244078

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$
Isomer 1.2 -g
C -1.121719 0.731523 0.263488
C -1.834396 -0.588563 -0.184092
O 0.068025 0.646444 0.773857
O -1.748600 1.772386 0.082624
O -1.355354 -1.703811 -0.154537
O -3.057992 -0.321702 -0.633382
H 0.552863 -0.392201 0.834941
H -3.125106 0.667494 -0.547582
N 3.291935 -0.892268 -0.633976
H 3.350939 -1.230653 -1.593965
H 3.178135 0.131715 -0.663013
H 4.186026 -1.093652 -0.186620
O 1.192692 -1.515856 0.864853
H 2.012444 -1.394152 0.239746
H 0.521137 -2.068621 0.416788
O 2.417512 1.904867 -0.199904
H 2.351543 2.786186 -0.592592
H 1.534903 1.723379 0.185659

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -h

C	-1.942275	0.482738	0.078479
C	-1.058925	-0.788607	-0.065938
O	-1.361831	1.643565	0.043488
O	-3.145075	0.294971	0.225852
O	0.147925	-0.775826	-0.193155
O	-1.802611	-1.888509	-0.023657
H	-0.321782	1.664092	-0.120701
H	-2.726438	-1.534929	0.096097
N	3.278836	0.786865	0.345622
H	3.160720	-0.222705	0.163135
H	4.090558	1.098383	-0.188459
H	3.522841	0.880974	1.332035
O	2.577762	-2.081220	0.016316
H	1.636669	-1.835419	-0.118668
H	2.782186	-2.710417	-0.689268
O	1.061597	2.103615	-0.409335
H	1.892764	1.586652	-0.090088
H	1.195690	3.027761	-0.154757

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -i

C	-1.212209	-0.898002	-0.091392
C	-1.581172	0.614898	-0.009380
O	0.021493	-1.212342	-0.344221
O	-2.123939	-1.696646	0.100966
O	-0.797780	1.531414	-0.122440
O	-2.885467	0.764716	0.219933
H	0.770924	-0.416628	-0.517076
H	-3.219557	-0.170479	0.274978
N	1.939038	2.675939	0.325821
H	2.235063	2.859829	1.283825
H	2.325020	3.415178	-0.260618
H	0.918762	2.747568	0.292872
O	1.974711	0.197162	-0.732435
H	2.576954	-0.436736	-0.285678
H	2.060116	1.110542	-0.288962
O	2.650413	-2.191904	0.543961
H	3.102985	-2.934574	0.118353
H	1.701293	-2.346853	0.380071

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -j

C	-0.744511	0.854887	-0.127239
C	-0.690423	-0.711807	-0.203631
O	0.393497	1.502182	-0.317172
O	-1.788274	1.438112	0.090477
O	0.356421	-1.303682	-0.455200
O	-1.809413	-1.340595	0.005128
H	1.193258	0.918974	-0.487934
H	-2.690365	-0.776439	0.226295
N	-4.068098	-0.189366	0.560552
H	-4.432133	-0.423078	1.483818
H	-3.848847	0.808124	0.537494
H	-4.801132	-0.378998	-0.122259
O	4.952080	-0.226397	0.976531
H	4.114003	-0.133098	0.482331
H	4.940192	0.500537	1.614755
O	2.607285	0.013042	-0.720759
H	1.941517	-0.725146	-0.688523
H	2.977025	0.014902	-1.616653

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$

Isomer 1.2 -k

C	0.068851	0.049105	-0.810649
C	-0.803461	1.082990	-0.042261
O	-0.379319	-1.158349	-1.011102
O	1.144830	0.453562	-1.249578
O	-1.928424	0.901958	0.385199
O	-0.180969	2.253136	0.037314
H	-1.284109	-1.360217	-0.573444
H	0.684991	2.097469	-0.420774
N	0.925747	-0.249954	1.894719
H	1.038556	0.529952	2.542939
H	0.621757	-1.049798	2.450100
H	1.854674	-0.478664	1.520440
O	3.261456	-0.941782	0.043713
H	4.148711	-0.607434	-0.148242
H	2.684216	-0.539458	-0.636810
O	-2.714864	-1.609468	0.037024
H	-2.704553	-0.667513	0.345749
H	-2.738492	-2.159686	0.833901

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -a

C	0.991523	-1.183031	0.139753

C 2.058876 -0.040051 0.025961
O -0.186647 -0.850193 0.477336
O 1.433892 -2.312733 -0.133100
O 1.855708 1.150319 0.193852
O 3.243141 -0.544153 -0.296228
H -0.796376 0.608382 0.658686
H 3.028839 -1.523544 -0.365192
N -1.439138 1.472712 0.693182
H -1.589669 1.749550 1.663646
H -0.965793 2.254918 0.182829
H -2.352979 1.182949 0.255201
O -3.602075 0.263118 -0.508672
H -3.270670 -0.681337 -0.408291
H -4.521357 0.254457 -0.207970
O -2.477122 -2.106869 -0.059679
H -1.546774 -1.810304 0.159095
H -2.377407 -2.772475 -0.755109
O 0.320510 3.329897 -0.364465
H 1.026713 2.652852 -0.242767
H 0.437786 3.678968 -1.259045

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -b

C -1.404774 0.734392 0.188030
C -2.298177 -0.496842 -0.204220
O -0.299008 0.502377 0.780122
O -1.877472 1.834449 -0.141976
O -2.013452 -1.671520 -0.050796
O -3.433205 -0.083279 -0.759459
H 0.253954 -0.914585 0.950363
H -3.317355 0.911475 -0.750190
N 0.603268 -1.948302 0.906179
H -0.208242 -2.424071 0.488098
H 1.469055 -1.996318 0.295590
H 0.794735 -2.324718 1.834326
O 1.649853 2.308875 0.448761
H 0.858530 1.724858 0.628273
H 1.298184 3.044366 -0.073819
O 2.902879 -1.805863 -0.545217
H 2.977548 -2.132287 -1.452952
H 3.153813 -0.828813 -0.586856
O 3.516463 0.762440 -0.626837
H 4.333167 0.993238 -0.162065
H 2.812981 1.379832 -0.253676

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -c

C	-0.945271	0.489268	-0.492510
C	-2.068925	-0.376818	0.173407
O	-0.036019	-0.115145	-1.129664
O	-1.062995	1.721063	-0.287854
O	-2.067693	-1.590968	0.237224
O	-3.021255	0.389478	0.704340
H	0.244252	-1.607686	-0.811923
H	-2.685881	1.310900	0.532097
N	0.554466	-2.550031	-0.365070
H	0.794815	-3.249222	-1.067459
H	1.394196	-2.321250	0.252072
H	-0.264642	-2.849858	0.173247
O	2.737248	-1.593826	0.889939
H	2.875469	-1.480260	1.840404
H	2.740491	-0.660702	0.486030
O	1.297727	2.966050	0.482527
H	1.482406	3.767716	-0.027448
H	0.425198	2.642018	0.145756
O	2.548856	0.674798	-0.417869
H	2.320501	1.537175	0.011751
H	1.710158	0.475079	-0.893561

$(H_2C_2O_4)(NH_3)$ $(H_2O)_3$

Isomer 1.3 -d

C	-0.712424	-0.846484	-0.374954
C	-2.018440	-0.073089	0.027806
O	0.029485	-0.327575	-1.265120
O	-0.525960	-1.903040	0.265605
O	-2.312715	1.053103	-0.325484
O	-2.763632	-0.804116	0.855651
H	0.115504	1.241889	-1.232930
H	-2.206008	-1.621965	0.981165
N	0.149297	2.273584	-0.908700
H	-0.837484	2.506199	-0.746033
H	0.576194	2.892211	-1.597260
H	0.690970	2.269605	0.009659
O	1.588981	1.874997	1.329668
H	1.764969	0.878918	1.412029
H	1.459747	2.206111	2.228687
O	2.057996	-0.721377	1.408977
H	2.447952	-0.909113	0.512152
H	1.239387	-1.252465	1.390903
O	2.630774	-1.121903	-1.225892
H	2.790160	-2.040058	-1.488280

H 1.659276 -0.969693 -1.373539

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -e

C -1.985608 -0.513731 -0.141649
C -0.619764 -0.854682 0.542064
O -2.533857 -1.583330 -0.718818
O -2.490806 0.593792 -0.190631
O -0.173901 -1.992692 0.209198
O -0.114535 -0.002384 1.299668
H -1.840439 -2.283337 -0.578291
H -1.555798 2.067497 -0.127689
N 1.432008 1.978548 0.551620
H 2.110361 1.542242 -0.131848
H 1.920235 2.560210 1.231689
H 0.921601 1.173013 1.024106
O -1.011868 2.889283 -0.267354
H -1.403077 3.324863 -1.037036
H 0.659286 2.512820 0.083297
O 2.503349 -1.856334 0.124321
H 2.832611 -2.697989 -0.219901
H 1.512717 -1.974347 0.232134
O 3.127632 0.474073 -0.977974
H 2.925995 -0.448673 -0.626128
H 3.076562 0.405078 -1.941428

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -f

C -0.937133 -0.017966 -0.681232
C -1.388790 -1.166455 0.282313
O 0.207641 -0.055005 -1.170840
O -1.823993 0.878601 -0.803531
O -0.641731 -1.978839 0.810247
O -2.694443 -1.128642 0.518323
H 0.947428 -1.405724 1.002195
H -2.966135 -0.292684 0.042465
N 1.886657 -0.932052 1.113533
H 2.386522 -1.054387 0.193945
H 1.723380 0.099752 1.288568
H 2.413061 -1.353296 1.878982
O 1.439968 1.763097 1.433333
H 1.280923 2.201708 2.280688
H 0.818260 2.216020 0.782032
O -0.245364 3.010507 -0.230712
H 0.216816 3.290388 -1.034416
H -0.896689 2.324828 -0.547593

O 2.523285 -1.324621 -1.509410
H 1.614978 -0.924913 -1.580184
H 3.087490 -0.791582 -2.087171

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -g

C -1.064708 0.580484 0.479404
C -2.125529 -0.286272 -0.284273
O -0.231649 0.008435 1.225575
O -1.150180 1.812998 0.229363
O -2.162165 -1.502042 -0.300172
O -2.985414 0.483739 -0.951900
H 0.048946 -1.431230 1.043972
H -2.643502 1.401237 -0.763136
N 0.315419 -2.454692 0.713070
H 0.495751 -3.086801 1.492007
H 1.166541 -2.361573 0.091584
H -0.514319 -2.751601 0.187234
O 3.134091 0.700168 -0.391123
H 3.820200 0.825743 0.279599
H 2.445899 1.403002 -0.188530
O 2.563049 -1.865413 -0.706413
H 2.747374 -0.881248 -0.586369
H 2.726986 -2.048375 -1.641790
O 1.427049 2.682340 0.163634
H 0.473470 2.422321 0.294330
H 1.407895 3.364301 -0.522882

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -h

C 2.187683 0.570906 -0.000081
C 1.389975 -0.780792 -0.000959
O 1.533822 1.647248 -0.000643
O 3.423321 0.379582 0.000737
O 0.168311 -0.874234 -0.002011
O 2.218774 -1.807590 -0.000279
H 0.036492 1.699741 -0.000761
H 3.105103 -1.301563 0.000431
N -1.057499 1.870792 -0.000379
H -1.497127 1.422670 -0.833828
H -1.496351 1.423022 0.833691
H -1.258398 2.871294 -0.000497
O -2.299365 -1.669170 0.001136
H -2.569136 -2.598172 0.001606
H -1.302590 -1.645221 0.000143
O -2.506369 0.353617 1.931236

H -2.545430 -0.467692 1.387118
H -2.107751 0.083349 2.771135
O -2.509498 0.353218 -1.929445
H -2.547193 -0.468268 -1.385534
H -2.113049 0.083248 -2.770464

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -i

C 1.484260 -0.106141 0.580594
C 0.533422 -1.303008 0.219642
O 1.237243 0.569020 1.605809
O 2.382735 0.066404 -0.288545
O -0.526710 -1.559003 0.772651
O 0.982627 -1.966627 -0.839193
H -0.244004 0.752596 1.949854
H 1.804942 -1.435542 -1.069153
N -1.310944 0.982935 1.948615
H -1.535926 1.260364 0.923339
H -1.817300 0.128713 2.185653
H -1.544272 1.730878 2.601383
O -1.694388 1.518185 -0.635230
H -0.817300 1.676701 -1.069776
H -2.027797 0.654959 -0.984563
O -2.579265 -1.072769 -1.051526
H -2.565435 -1.555314 -1.890569
H -1.912053 -1.518606 -0.482608
O 0.827903 1.905610 -1.755696
H 1.160465 2.814410 -1.767665
H 1.528048 1.378632 -1.303775

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -j

C 1.234334 0.633705 0.362931
C 1.925888 -0.535128 -0.434321
O 0.099896 0.625322 0.844291
O 2.040629 1.670397 0.425639
O 1.260882 -1.567483 -0.698455
O 3.106703 -0.240190 -0.726920
H -0.246157 -1.689265 -0.615670
H 2.853521 1.265816 -0.055810
N -1.323489 -1.884948 -0.531365
H -1.528927 -1.922437 0.489155
H -1.886677 -1.104444 -0.956100
H -1.552948 -2.771193 -0.980974
O -2.750003 0.289518 -1.549687
H -3.717173 0.293270 -1.517194

H -2.467995 1.094928 -1.030509
O -1.889764 2.321538 0.005951
H -1.533572 3.126768 -0.396809
H -1.120787 1.887271 0.445703
O -1.449754 -1.263016 2.190115
H -1.023878 -1.701702 2.940255
H -0.821031 -0.564510 1.898368

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -k

C 2.265838 0.399777 -0.234035
C 1.308492 -0.776254 0.174129
O 1.917922 1.583920 0.037871
O 3.290483 -0.011345 -0.813646
O 0.247744 -0.664205 0.780812
O 1.797083 -1.929516 -0.245112
H 0.639415 1.860457 0.595440
H 2.661010 -1.604029 -0.674491
N -0.371188 2.110218 1.051937
H -0.370179 3.030087 1.493344
H -1.139912 2.054115 0.326982
H -0.546248 1.386221 1.751274
O -1.903772 -2.286617 0.572824
H -1.040096 -1.809772 0.689941
H -1.684769 -3.097898 0.092137
O -3.514837 -0.536970 -0.654575
H -4.374710 -0.598585 -0.215383
H -2.935442 -1.225940 -0.214544
O -2.448445 1.898543 -0.736325
H -2.282974 2.078649 -1.672739
H -2.863172 0.983566 -0.710870

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -l

C -2.220504 0.489183 0.067040
C -1.419574 -0.862941 -0.046402
O -1.580853 1.564632 0.225494
O -3.451598 0.305304 -0.025498
O -0.202941 -1.008746 0.053500
O -2.249909 -1.857515 -0.283083
H -0.150096 1.730810 0.055348
H -3.132769 -1.345970 -0.277460
N 0.943605 1.953641 -0.052498
H 1.356858 1.355303 -0.822702
H 1.097637 2.944863 -0.236640
H 1.405065 1.673273 0.821872

O 3.837299 -0.653211 0.026644
H 4.218819 -1.542582 0.026825
H 3.188552 -0.632959 0.771842
O 2.000744 0.134341 -1.843885
H 1.313718 -0.549574 -1.771787
H 2.750982 -0.222641 -1.299273
O 1.726916 -0.207819 1.736359
H 1.595055 -0.507369 2.646952
H 0.954132 -0.551983 1.212426

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -m

C 1.230471 1.066789 -0.048007
C 0.615382 -0.333116 -0.432461
O 0.388660 2.008996 0.042733
O 2.460235 1.159195 0.128406
O -0.513706 -0.390003 -0.920261
O 1.304348 -1.429748 -0.209085
H -0.990672 1.847872 -0.161594
H 2.260311 -1.285747 0.143717
N -2.124593 1.840767 -0.326694
H -2.283757 1.559039 -1.295074
H -2.531076 2.763999 -0.171435
H -2.591638 1.128597 0.294741
O -2.428561 -2.167756 -0.351365
H -1.610036 -1.689972 -0.652743
H -2.125625 -3.023203 -0.015765
O 3.710753 -1.025666 0.658403
H 4.396344 -1.259569 0.015619
H 3.460207 -0.067211 0.470358
O -3.405348 -0.153594 1.125911
H -3.093062 -0.991684 0.675840
H -3.225016 -0.280922 2.068060

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -n

C 1.516090 0.651655 0.198487
C 2.279094 -0.681648 -0.108130
O 0.242415 0.608689 0.114439
O 2.235137 1.619626 0.490101
O 1.765478 -1.731724 -0.434300
O 3.596270 -0.506032 0.031831
H -0.494524 -0.750389 -0.264206
H 3.653825 0.456363 0.289796
N -3.092061 0.456791 -0.755648
H -3.880868 0.667342 -1.366675

H -3.390694 -0.087112 0.095064
H -2.557219 1.353339 -0.467057
O -1.129914 -1.493909 -0.548313
H -0.510193 -2.190081 -0.820670
H -2.421256 -0.185712 -1.220301
O -1.498061 2.482681 -0.151106
H -0.685361 1.893227 0.027606
H -1.551210 3.109797 0.583456
O -3.203503 -1.492333 1.137940
H -2.342740 -1.707769 0.680066
H -3.009007 -1.472579 2.085572

$(H_2C_2O_4)(NH_3)$ $(H_2O)_3$

Isomer 1.3 -o

C 1.099135 -1.039659 0.103868
C 2.113817 0.152811 -0.018708
O -0.130267 -0.759097 0.244414
O 1.635487 -2.160860 0.037085
O 1.846981 1.341197 -0.054478
O 3.355697 -0.313036 -0.093026
H -0.938665 0.600223 0.687228
H 3.196482 -1.304558 -0.063551
N -3.577720 0.022607 -0.221223
H -3.173776 -0.965878 -0.238363
H -4.413072 0.054159 0.363616
H -3.827780 0.302620 -1.170250
O -0.172349 3.122467 -0.461155
H 0.109948 3.942488 -0.031242
H 0.597539 2.505422 -0.365786
O -1.644997 1.306897 0.817274
H -2.744458 0.703017 0.208436
H -1.243953 2.110876 0.378321
O -2.175648 -2.266752 -0.338386
H -1.288637 -1.847841 -0.087004
H -2.226535 -3.104216 0.142375

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -p

C	-2.144778	0.485523	0.243416
C	-1.278978	-0.734002	-0.245094
O	-3.234763	0.047355	0.868398
O	-1.879153	1.667685	0.113923
O	-1.724660	-1.841517	0.109535
O	-0.226703	-0.492581	-0.916692
H	-3.108816	-0.946462	0.819862
H	0.297334	0.982608	-1.146386
N	2.645234	1.810034	0.424230
H	2.795815	0.787407	0.701828
H	3.455410	2.130341	-0.108897
H	2.570759	2.382289	1.266536
O	0.573280	1.961389	-1.070066
H	1.693084	1.917453	-0.212464
H	-0.250471	2.287600	-0.640079
O	3.091554	-0.793035	1.020604
H	2.918459	-1.127060	1.912047
H	2.584465	-1.413416	0.394073
O	1.743154	-2.225780	-0.703363
H	0.920456	-1.665422	-0.857268
H	1.407733	-3.102827	-0.467498

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -q

C	0.419145	-1.133104	0.515036
C	1.777466	-0.688550	-0.135373
O	-0.215869	-0.326704	1.249408
O	0.092128	-2.306729	0.222682
O	2.261646	0.429316	-0.112469
O	2.359998	-1.714877	-0.744526
H	-0.444009	1.004482	1.006372
H	1.687891	-2.444725	-0.608587
N	-2.861159	-1.485947	-0.257158
H	-3.424866	-1.641342	0.579452
H	-3.255391	-2.072169	-0.993621
H	-1.924000	-1.857185	-0.042769
O	-2.637186	1.124868	-0.848734
H	-2.763254	0.120924	-0.630987
H	-3.512435	1.533703	-0.790770
O	-0.834892	1.977411	0.724659
H	-1.592117	1.731668	0.051414
H	-0.066809	2.464547	0.259032
O	1.294494	2.924168	-0.383928

H 1.807019 3.571751 0.121531
H 1.773870 2.060288 -0.285684

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -r

C 0.190094 -0.467902 -0.239063
C 0.018581 1.086390 -0.149644
O -0.877903 -1.181294 -0.512471
O 1.289215 -0.963845 -0.057304
O -1.057316 1.635505 -0.344146
O 1.101730 1.760102 0.143414
H -1.759910 -0.660241 -0.650624
H 1.967215 1.225021 0.301168
N 4.156226 -1.604347 0.011907
H 4.635238 -1.848735 -0.853934
H 4.553887 -2.179141 0.753885
H 3.169629 -1.858869 -0.091655
O -3.127068 0.019469 -0.892646
H -2.698469 0.881124 -0.693277
H -3.781077 -0.150634 -0.177699
O -5.026108 -0.625336 1.073033
H -4.744637 -1.381101 1.610765
H -5.854703 -0.907977 0.657095
O 3.478381 0.949924 0.674919
H 3.828111 0.039827 0.403581
H 4.091635 1.604032 0.311198

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$

Isomer 1.3 -s

C 1.030132 -1.203544 -0.109921
C 0.498246 -0.090338 0.843128
O 0.159249 -2.086477 -0.497608
O 2.214671 -1.235882 -0.438534
O -0.365206 -0.313526 1.667041
O 1.025381 1.128247 0.698967
H -0.852765 -1.911306 -0.194542
H 1.848251 1.180012 0.088799
N -3.116058 0.520988 -1.070442
H -3.008098 0.508770 -2.085066
H -4.101701 0.707954 -0.884580
H -2.575650 1.323320 -0.714258
O -2.240441 -1.739079 0.151853
H -2.601803 -0.909153 -0.325903
H -2.108642 -1.445610 1.071143
O -1.309021 2.732306 -0.006282
H -1.627766 3.315280 0.697742

H	-0.506741	2.314363	0.365279
O	3.236668	1.183484	-0.657433
H	3.156704	0.193822	-0.691307
H	3.249948	1.486331	-1.577477

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -a

C	-1.892994	-0.535837	-0.222680
C	-1.144827	0.733239	0.333100
O	-3.107180	-0.199699	-0.649597
O	-1.446519	-1.668082	-0.281338
O	-1.793788	1.787215	0.218666
O	0.021580	0.575129	0.819213
H	-3.112844	0.788248	-0.470152
H	0.663706	-0.743059	0.817075
N	1.193126	-1.716225	0.673726
H	2.076397	-1.523542	0.131223
H	1.404899	-2.175210	1.558952
H	0.504044	-2.264529	0.145615
N	2.495850	1.815704	-0.268581
H	1.580076	1.643161	0.173680
H	2.319910	2.361639	-1.112446
H	3.030410	2.414762	0.360849
O	3.444133	-0.715166	-0.509794
H	3.167134	0.267858	-0.497992
H	3.824544	-0.885264	-1.382537

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -b

C	1.856144	-0.586454	0.169008
C	1.122687	0.741101	-0.245411
O	3.067900	-0.312050	0.645454
O	1.399610	-1.713438	0.094974
O	1.765293	1.774021	0.003000
O	-0.034470	0.636935	-0.769910
H	3.085710	0.688715	0.584979
H	-0.729587	-0.692756	-0.879273
N	-3.372566	-0.706713	0.831068
H	-4.350372	-0.829220	0.567165
H	-3.313824	-0.893871	1.832370
H	-3.135259	0.290117	0.687176
N	-1.278080	-1.644124	-0.787617
H	-1.560835	-2.011587	-1.695669

H	-2.127186	-1.461476	-0.158507
H	-0.582175	-2.262609	-0.354511
O	-2.320202	1.899542	-0.029000
H	-1.413213	1.634721	-0.329231
H	-2.216771	2.785857	0.343617

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -c

C	-1.708515	0.317580	-0.275588
C	-0.793071	-0.603493	0.611679
O	-2.566900	-0.418158	-0.981300
O	-1.640226	1.530774	-0.352759
O	-0.938147	-1.826437	0.374175
O	0.004839	-0.062449	1.427061
H	-2.299540	-1.346902	-0.718692
H	0.514177	1.264115	1.072503
N	0.953716	2.148479	0.554797
H	1.369928	2.832334	1.184769
H	1.665175	1.743720	-0.113875
H	0.150993	2.540161	0.048444
N	2.153871	-1.881997	-0.139603
H	1.154040	-2.035864	0.047974
H	2.625090	-1.980775	0.760582
H	2.474968	-2.653679	-0.724960
O	2.684401	0.664764	-0.949927
H	2.767218	0.686614	-1.913418
H	2.482633	-0.307567	-0.704234

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -d

C	1.207482	-0.869797	0.075423
C	1.488981	0.673123	0.105534
O	0.025083	-1.240201	0.354162
O	2.196206	-1.557955	-0.230850
O	0.663727	1.537962	0.341019
O	2.764787	0.918904	-0.180119
H	-1.129871	-0.256429	0.667124
H	3.113688	-0.012117	-0.324538
N	-1.948717	2.616957	-0.562465
H	-0.935253	2.601277	-0.399464
H	-2.095472	2.641964	-1.571691
H	-2.309454	3.494445	-0.188391
N	-2.149660	0.127308	0.760672
H	-2.229290	1.060662	0.252684

H	-2.396108	0.238641	1.744045
H	-2.727040	-0.615198	0.335434
O	-2.275115	-2.359824	-0.550064
H	-1.318248	-2.265888	-0.323862
H	-2.460596	-3.308258	-0.537706

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -e

C	0.283392	-0.471325	-0.387656
C	0.695741	1.016808	-0.154980
O	1.181711	-1.394004	-0.143945
O	-0.842304	-0.734358	-0.793153
O	1.870141	1.354981	-0.227744
O	-0.280375	1.846959	0.096829
H	2.140749	-1.065919	0.146050
H	-1.287258	1.462426	0.156265
N	-2.783185	1.242557	0.319098
H	-3.240195	1.483463	-0.561103
H	-3.008567	0.254027	0.507141
H	-3.208168	1.816854	1.047315
N	3.632632	-0.724457	0.513604
H	4.342882	-1.159492	-0.073847
H	3.927191	-0.816362	1.484813
H	3.571382	0.270675	0.279672
O	-3.146137	-1.708296	0.278866
H	-2.272459	-1.643515	-0.168736
H	-3.050779	-2.424015	0.922498

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -f

C	1.077228	-0.754780	0.077420
C	1.581391	0.732486	-0.075524
O	2.104516	-1.552405	0.301898
O	-0.084599	-1.145866	0.016031
O	2.824784	0.810424	0.027888
O	0.736524	1.646938	-0.269327
H	2.858031	-0.864073	0.278112
H	-0.730984	1.481511	-0.284430
N	-1.840259	1.417024	-0.295099
H	-2.261731	2.336373	-0.423061
H	-2.110623	0.770237	-1.062163
H	-2.151136	0.973487	0.612664
N	-2.324202	-0.194635	2.019194
H	-2.040536	0.107014	2.951553

H	-1.613007	-0.851488	1.684244
H	-3.192455	-0.719290	2.126472
O	-2.121763	-0.923955	-1.821341
H	-1.895173	-1.169331	-2.729317
H	-1.338574	-1.168486	-1.275304

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -g

C	1.798805	-0.546036	-0.278133
C	1.099591	0.706535	0.365159
O	1.194721	-1.659707	-0.239057
O	2.905143	-0.275131	-0.781862
O	0.019451	0.714067	0.937368
O	1.847511	1.786952	0.182364
H	-0.075461	-1.762304	0.309770
H	2.634279	1.379516	-0.307865
N	-1.121729	-1.901295	0.777321
H	-1.873678	-1.508149	0.149584
H	-1.316815	-2.878822	0.994675
H	-1.118439	-1.348041	1.635856
N	-2.475482	1.904781	-0.208580
H	-1.587975	1.777554	0.294471
H	-3.115973	2.398042	0.413414
H	-2.289073	2.527950	-0.994453
O	-3.127909	-0.694121	-0.694234
H	-3.234688	-0.850621	-1.643181
H	-2.943415	0.301001	-0.592250

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -h

C	1.029413	0.740191	-0.250742
C	1.810446	-0.551341	0.183916
O	1.727158	1.822203	0.053960
O	-0.073976	0.762309	-0.781006
O	2.927898	-0.291343	0.671233
O	1.248911	-1.673449	0.020709
H	2.554953	1.391044	0.451920
H	-0.084165	-1.758461	-0.459864
N	-1.148041	-1.882412	-0.847340
H	-1.342211	-2.851830	-1.100043
H	-1.226447	-1.286348	-1.672928
H	-1.854174	-1.530486	-0.121549
N	-2.933936	-0.747182	1.031851
H	-2.599705	-0.819152	1.993527

H	-3.918276	-1.015151	1.043139
H	-2.888404	0.250285	0.766337
O	-2.470259	1.924123	-0.158319
H	-1.547729	1.719622	-0.438925
H	-2.437006	2.823786	0.195161

$(H_2C_2O_4)(NH_3)_2(H_2O)$

Isomer 2.1 -i

C	-0.358590	-0.540132	-0.381984
C	-0.688780	0.930087	0.092012
O	-1.330727	-1.432043	-0.402222
O	0.779970	-0.839579	-0.717137
O	-1.865183	1.247463	0.338171
O	0.316132	1.705733	0.186796
H	-2.245643	-1.088711	-0.117380
H	1.571965	1.353114	-0.108291
N	2.721829	1.199673	-0.351570
H	2.812815	1.090329	-1.362117
H	3.282520	1.997652	-0.051194
H	3.063292	0.308528	0.102945
N	3.292351	-1.395011	0.735794
H	2.414304	-1.697370	0.299430
H	4.031648	-2.016285	0.407928
H	3.199684	-1.548689	1.740033
O	-3.701758	-0.578209	0.357872
H	-4.336740	-0.485469	-0.367162
H	-3.196367	0.287623	0.398235

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-a

C	2.063389	0.012230	0.096062
C	1.059823	-1.190791	0.091904
O	3.286160	-0.400645	-0.231124
O	1.779192	1.169427	0.344836
O	1.564745	-2.277393	-0.241306
O	-0.142907	-0.931982	0.409310
H	3.131806	-1.380971	-0.377442
H	-0.749830	0.535765	0.663858
N	0.057830	3.419876	-0.572779
H	0.924712	2.897052	-0.404542
H	0.187991	4.361531	-0.203470
H	-0.053669	3.510675	-1.582701
N	-1.407187	1.380670	0.766321
H	-2.337420	1.084148	0.377487

H	-0.989203	2.211415	0.252344
H	-1.503711	1.608364	1.756190
O	-3.624273	0.151652	-0.369899
H	-4.516768	0.085303	-0.003037
H	-3.251568	-0.782418	-0.347050
O	-2.406152	-2.205671	-0.136560
H	-2.314686	-2.811683	-0.885359
H	-1.475560	-1.894744	0.069077

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-b

C	1.276956	0.799227	0.223089
C	2.060318	-0.527419	-0.074071
O	0.055810	0.666393	0.509710
O	1.985329	1.822200	0.122081
O	1.572835	-1.649470	-0.127696
O	3.343938	-0.279394	-0.289240
H	-2.010591	0.009215	-2.833143
H	3.356417	0.724402	-0.200794
N	-2.177447	-0.473948	2.076505
H	-2.792808	0.240784	1.681047
H	-1.283425	-0.001259	2.234127
H	-2.560237	-0.754170	2.978473
N	-1.187003	-1.897334	-0.139824
H	-0.139217	-1.762171	-0.098821
H	-1.415914	-2.885345	-0.251422
H	-1.616635	-1.500561	0.756394
O	-2.139166	1.807578	-0.231804
H	-1.209776	1.561497	0.079891
H	-2.112631	2.749982	-0.448053
O	-2.412032	-0.206379	-1.979426
H	-2.358365	0.635364	-1.438322
H	-1.583027	-1.337056	-0.939243

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-c

C	1.028663	-1.199300	0.153735
C	2.115420	-0.073554	0.005437
O	-0.156482	-0.850760	0.427435
O	1.483723	-2.345544	-0.032756
O	1.931080	1.128049	0.106254
O	3.298794	-0.612772	-0.257030
H	-0.748203	0.588495	0.622264
H	3.059184	-1.592301	-0.271813

N	-1.368723	1.473366	0.697873
H	-0.894977	2.253244	0.189039
H	-2.311847	1.227392	0.291343
H	-1.477453	1.735298	1.678033
N	-2.728395	-2.080300	-0.290449
H	-2.699769	-2.582386	-1.178045
H	-3.118575	-2.724832	0.397345
H	-1.749790	-1.889814	-0.017147
O	-3.737464	0.421857	-0.195255
H	-4.235710	0.645852	-0.993283
H	-3.445945	-0.555188	-0.297295
O	0.406397	3.318254	-0.383622
H	1.092512	2.616170	-0.281332
H	0.537528	3.691064	-1.266322

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-d

C	-1.113092	-1.512894	-0.058477
C	0.280532	-1.149632	0.562697
O	-1.025535	-2.591550	-0.841387
O	-2.141499	-0.887492	0.108911
O	1.225462	-1.850308	0.092940
O	0.348232	-0.224240	1.400191
H	-0.050257	-2.801338	-0.799208
H	-0.230314	1.213903	1.095909
N	-2.927127	1.914405	-0.491970
H	-3.068359	2.072820	-1.489762
H	-3.756248	2.272638	-0.017751
H	-2.905965	0.896843	-0.344075
N	-0.372913	2.205484	0.708045
H	-0.329248	2.888884	1.463900
H	-1.319144	2.246857	0.221472
H	0.432013	2.355586	0.046022
O	1.947335	2.241978	-0.779752
H	2.423078	1.369945	-0.607806
H	2.110757	2.447063	-1.710386
O	3.207307	-0.067568	-0.324729
H	2.544476	-0.788497	-0.117157
H	3.754434	-0.005337	0.471615

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-e

C	2.088323	-0.298779	-0.221376
C	0.981443	0.506007	0.548917

O 3.010636 0.524869 -0.718305
O 2.105801 -1.504843 -0.378952
O 1.098630 1.747202 0.454158
O 0.087254 -0.154783 1.157608
H 2.660329 1.419382 -0.444231
H -0.149224 -1.617273 0.788955
N -1.583095 2.971486 -0.485007
H -1.499523 3.209492 -1.472977
H -0.634901 2.797395 -0.127855
H -1.944922 3.796344 -0.006978
N -0.426989 -2.575812 0.335916
H -0.538087 -3.309909 1.034509
H -1.331249 -2.408862 -0.201166
H 0.365304 -2.788793 -0.279500
O -2.637457 -1.673836 -0.923453
H -3.536565 -2.029059 -0.898295
H -2.678716 -0.762962 -0.461586
O -2.540944 0.545038 0.438159
H -1.695887 0.382933 0.915307
H -2.355936 1.429056 -0.001522

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$
Isomer 2.2-f
C 1.478461 0.842476 -0.024442
C 1.545961 -0.730370 0.016715
O 0.342586 1.371959 -0.176396
O 2.597464 1.375292 0.109760
O 0.600834 -1.502448 -0.091508
O 2.793941 -1.125425 0.206496
H -1.037419 0.593888 -0.193833
H 3.262368 -0.227896 0.247664
N -2.068335 0.280778 -0.183182
H -2.215594 -0.309384 0.678596
H -2.626422 1.140734 -0.190937
H -2.220334 -0.318167 -1.011450
N -1.907060 -1.606800 1.959923
H -1.776460 -1.322076 2.930752
H -0.995344 -1.913461 1.608706
H -2.514898 -2.426048 1.967774
O -1.754513 3.124756 0.019969
H -0.825239 2.807311 -0.043913
H -1.728833 4.062120 -0.213545
O -1.537380 -1.926781 -1.830221
H -1.294763 -2.142661 -2.741214

H -0.689284 -1.873653 -1.334218

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$
Isomer 2.2-g
C -1.250524 0.781893 0.199905
C -1.933676 -0.545814 -0.285659
O -0.047212 0.696833 0.582689
O -1.995581 1.776212 0.114495
O -1.390739 -1.637426 -0.396514
O -3.202365 -0.333156 -0.600142
H 0.772793 -0.045178 1.905400
H -3.277983 0.655744 -0.427173
N 2.699136 -0.235399 -1.791645
H 2.542460 0.688000 -1.348067
H 2.304816 -0.186748 -2.731864
H 3.706972 -0.348793 -1.904978
N 1.320191 -1.940750 -0.027902
H 1.872647 -1.354155 -0.743889
H 0.281330 -1.797875 -0.175627
H 1.552142 -2.930943 -0.108983
O 2.067573 2.138314 -0.186443
H 1.200319 1.774689 0.139969
H 1.882351 3.055104 -0.432951
O 1.381415 -0.645514 2.411932
H 2.090564 -0.070551 2.734452
H 1.536763 -1.584822 0.936930

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$
Isomer 2.2-h
C 1.014932 0.241756 0.684334
C 1.659237 -0.752285 -0.346330
O -0.090636 -0.044445 1.191753
O 1.714849 1.280105 0.839412
O 1.100437 -1.707773 -0.869819
O 2.904676 -0.398861 -0.633225
H -1.188562 -1.230325 1.645274
H 2.982111 0.458576 -0.112670
N -1.619491 -1.420726 -1.027247
H -0.577486 -1.598354 -0.960913
H -1.769790 -0.396079 -1.267437
H -2.041641 -2.025401 -1.731794
N -0.821076 2.877749 0.276663
H 0.108199 2.523382 0.545577
H -1.396933 2.815758 1.116886

H	-0.723945	3.868617	0.054231
O	-1.971455	1.241864	-1.542604
H	-1.517154	1.881593	-0.878313
H	-1.793577	1.606741	-2.420774
O	-1.961233	-1.861940	1.644951
H	-2.603856	-1.488085	2.263875
H	-2.011510	-1.624011	-0.071611

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-i

C	-1.458771	0.730429	0.178495
C	-2.296399	-0.528400	-0.254378
O	-0.355376	0.533174	0.782178
O	-1.978740	1.815207	-0.135592
O	-1.975686	-1.695392	-0.110541
O	-3.431929	-0.145128	-0.830378
H	0.233887	-0.862356	0.982631
H	-3.347477	0.854045	-0.795076
N	3.595054	0.735864	-0.820833
H	2.908575	1.365666	-0.364256
H	4.510059	0.955154	-0.425529
H	3.633031	1.000037	-1.805821
N	0.597723	-1.892471	0.979108
H	0.749977	-2.240484	1.925339
H	1.492658	-1.955435	0.408720
H	-0.191619	-2.386241	0.539524
O	1.634737	2.366789	0.608052
H	1.282399	3.221528	0.322484
H	0.831902	1.791003	0.716249
O	2.950949	-1.832217	-0.364637
H	3.209611	-0.857145	-0.579222
H	3.116947	-2.341147	-1.170319

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-j

C	1.031488	0.394280	0.531868
C	2.022733	-0.586526	-0.192317
O	0.048677	-0.094227	1.150620
O	1.335604	1.605001	0.385889
O	1.871136	-1.788165	-0.309048
O	3.059566	0.076543	-0.703202
H	-0.406731	-1.524316	0.841013
H	2.838479	1.022385	-0.470663
N	-2.694365	0.936992	0.291472

H -2.302442 1.742377 -0.216033
H -1.981121 0.728870 0.999119
H -3.527428 1.264705 0.780602
N -0.782080 -2.454719 0.406181
H 0.021144 -2.795934 -0.134172
H -1.614405 -2.191964 -0.209609
H -1.049309 -3.136002 1.115947
O -2.920450 -1.446148 -0.874887
H -2.887609 -0.473925 -0.509261
H -3.036242 -1.379218 -1.832965
O -0.833083 3.166511 -0.409395
H -0.044553 2.699410 -0.040137
H -0.491594 3.665052 -1.164537

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$
Isomer 2.2-k
C 1.488541 0.734598 0.238984
C 2.349965 -0.497429 -0.231654
O 0.366517 0.510854 0.793893
O 2.018646 1.834352 -0.004761
O 2.037227 -1.673406 -0.155597
O 3.498255 -0.076763 -0.752855
H -0.191358 -0.877227 0.917906
H 3.399782 0.919460 -0.667532
N -1.806681 2.419256 0.179840
H -0.976419 1.877755 0.471713
H -1.511434 3.004622 -0.602573
H -2.033073 3.055211 0.945016
N -0.542385 -1.921637 0.880821
H -0.677576 -2.307903 1.814689
H 0.254523 -2.383422 0.419658
H -1.438270 -1.987575 0.320486
O -3.684697 0.634880 -0.562953
H -4.511379 0.844284 -0.106385
H -3.002504 1.340379 -0.260377
O -2.938025 -1.884386 -0.431621
H -3.043428 -2.235693 -1.326863
H -3.239814 -0.920485 -0.483206
$(H_2C_2O_4)(NH_3)_2(H_2O)_2$
Isomer 2.2-l
C 1.519352 -0.076874 0.330577
C 0.593410 -1.345613 0.245721
O 1.480966 0.631077 1.362834
O 2.175564 0.111346 -0.732266

O -0.270794 -1.654625 1.046601
O 0.821193 -2.017779 -0.884855
H 0.091354 0.757948 2.002145
H 1.524027 -1.442410 -1.314411
N -2.533234 -1.064977 -1.141845
H -2.040439 -1.678939 -0.486845
H -3.519178 -1.325546 -1.129644
H -2.178321 -1.288778 -2.072089
N -0.973469 0.898691 2.185551
H -1.386806 1.178310 1.212844
H -1.158680 1.604541 2.897337
H -1.344683 -0.010473 2.466160
O 0.476519 2.083260 -1.750426
H 0.833425 2.979889 -1.677287
H 1.212996 1.490915 -1.462568
O -1.810248 1.480571 -0.259729
H -2.122829 0.610904 -0.653870
H -1.026116 1.751759 -0.802773

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-m

C 0.645178 -0.923437 0.557523
C 1.962373 -0.460853 -0.159362
O 0.055930 -0.120762 1.310102
O 0.323186 -2.109519 0.259068
O 2.390339 0.679630 -0.207992
O 2.568608 -1.483474 -0.759628
H -0.815963 1.166052 1.044104
H 1.926577 -2.230480 -0.588990
N -1.363379 1.994786 0.654725
H -1.777727 2.539419 1.410616
H -2.121464 1.586380 0.011445
H -0.646148 2.563674 0.146097
N -3.225561 0.590397 -0.915116
H -4.217357 0.704370 -0.702880
H -2.972806 -0.384372 -0.664631
H -3.136331 0.672479 -1.928518
O -2.411391 -2.088801 -0.021717
H -2.623183 -2.918493 -0.471485
H -1.441144 -2.156523 0.185357
O 1.001146 3.007060 -0.295975
H 1.530062 2.171795 -0.181642
H 1.350203 3.422083 -1.096562

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-n

C	-1.224781	-1.069528	0.031755
C	-0.649664	0.286166	-0.535423
O	-0.371457	-1.996685	0.167996
O	-2.440628	-1.150188	0.292900
O	0.448298	0.317396	-1.082390
O	-1.359553	1.390767	-0.393160
H	0.984873	-1.852584	-0.142283
H	-2.284027	1.263406	0.023823
N	2.378378	2.307126	-0.025723
H	1.624517	1.865905	-0.571370
H	1.938011	2.980198	0.601792
H	2.960355	2.840966	-0.671076
N	2.101994	-1.843211	-0.402503
H	2.631008	-1.157712	0.202767
H	2.162649	-1.516306	-1.367743
H	2.515480	-2.773011	-0.327241
O	-3.731057	1.051452	0.654263
H	-3.456629	0.087011	0.558460
H	-4.448395	1.191877	0.019143
O	3.527090	0.069876	0.991419
H	3.536704	0.100031	1.958528
H	3.137978	0.962029	0.686559

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-o

C	1.101144	-1.260559	0.119350
C	0.308256	-0.072278	0.726975
O	0.383460	-2.182012	-0.452772
O	2.324670	-1.290762	0.217473
O	-0.699065	-0.262690	1.388370
O	0.780372	1.146594	0.482069
H	-0.716918	-2.005387	-0.527552
H	1.735983	1.190227	-0.004381
N	-2.136309	-1.927358	-0.753731
H	-2.611804	-2.543783	-0.093628
H	-2.507761	-0.968527	-0.596333
H	-2.399835	-2.227214	-1.692697
N	3.135316	1.287895	-0.595628
H	3.216094	1.463832	-1.596326
H	3.772539	1.918160	-0.110205
H	3.414664	0.318661	-0.405925
O	-3.041923	0.698167	0.101904
H	-2.474110	0.517209	0.875951
H	-2.596997	1.484057	-0.289496

O	-1.281696	2.811232	-0.608113
H	-0.538521	2.364158	-0.148066
H	-1.469329	3.597645	-0.075216

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-p

C	1.783127	0.641616	0.257526
C	2.440289	-0.688924	-0.252082
O	2.556201	1.676004	-0.032973
O	0.702859	0.730426	0.827492
O	3.566634	-0.501412	-0.754430
O	1.786522	-1.762917	-0.123291
H	3.334295	1.192200	-0.471018
H	0.434537	-1.746302	0.346456
N	-0.622435	-1.848438	0.744001
H	-0.910716	-2.827511	0.733051
H	-0.613106	-1.511496	1.707529
H	-1.321259	-1.251291	0.196564
N	-5.184048	-0.276166	-0.284062
H	-5.606245	-0.260635	-1.212930
H	-5.455910	0.591671	0.179251
H	-5.626893	-1.037698	0.230443
O	-2.358199	-0.264846	-0.603201
H	-2.097518	0.671632	-0.410427
H	-3.340189	-0.305685	-0.460589
O	-1.462119	2.230633	0.174589
H	-1.234024	2.897716	-0.488776
H	-0.593261	1.880364	0.492724

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-q

C	-1.674684	0.621022	0.165786
C	-1.384673	-0.925480	0.090378
O	-2.833747	0.895646	-0.423002
O	-0.937922	1.472738	0.639370
O	-2.249186	-1.547035	-0.561545
O	-0.330525	-1.362961	0.635402
H	-3.111890	-0.028268	-0.721273
H	0.603071	-0.468094	1.549038
N	1.349545	2.277153	-1.168943
H	0.488786	2.248399	-0.605927
H	1.072454	2.234592	-2.149997
H	1.785122	3.188263	-1.023218
N	1.939417	-2.041379	-0.966035
H	2.528699	-2.811910	-0.650064
H	1.763119	-2.182958	-1.960672

H 1.032306 -2.103168 -0.468128
O 2.706177 0.269216 -0.096359
H 2.227300 1.043872 -0.609926
H 2.442973 -0.683811 -0.546598
O 1.325320 0.092664 2.006303
H 2.201316 0.244529 0.840598
H 0.859213 0.932749 2.152678

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2-r

C -0.699611 -1.737776 0.006577
C -1.630957 -0.485895 -0.081554
O 0.540984 -1.554655 -0.187947
O -1.301352 -2.791669 0.278070
O -1.248896 0.647292 -0.316582
O -2.894182 -0.820715 0.151667
H 1.095030 -0.309813 -0.486094
H -2.802118 -1.811409 0.305393
N 3.592806 -1.373236 0.231113
H 2.790876 -2.011739 0.265367
H 4.033466 -1.382603 1.150448
H 4.264455 -1.759842 -0.431771
N 1.439783 2.770106 0.424951
H 0.442601 3.038939 0.332057
H 1.679319 2.826214 1.415235
H 1.989468 3.483712 -0.055050
O -1.382709 3.333623 -0.058128
H -1.582664 2.375652 -0.182719
H -2.075860 3.668928 0.526899
O 1.857148 0.448256 -0.677783
H 2.678188 -0.031315 -0.309995
H 1.674575 1.380157 -0.186741

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-a

C -1.346993 -1.491511 0.277390
C 0.130703 -1.866276 -0.077769
O -2.145857 -2.544321 0.125265
O -1.727100 -0.390177 0.635878
O 0.288734 -3.057908 -0.399046
O 0.980794 -0.927983 -0.006229
H -1.486643 -3.246065 -0.163759
H 0.612588 0.609322 0.446575
N 0.697918 1.636340 0.728862
H 1.698707 1.913284 0.563925

H 0.022165 2.237867 0.186380
H 0.478686 1.718425 1.722121
N -3.472647 1.794001 -0.335723
H -3.977869 1.554086 -1.188639
H -4.160341 2.160923 0.322093
H -3.101911 0.918547 0.057022
O 3.556163 -0.622520 -0.568060
H 4.113968 -1.281466 -0.131534
H 2.612688 -0.916765 -0.403538
O 3.431707 1.885658 0.317391
H 3.871339 2.463397 -0.321772
H 3.588720 0.948323 -0.011562
O -1.184437 3.243212 -0.497500
H -2.077849 2.752941 -0.504532
H -1.073434 3.613823 -1.384071

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-b

C 2.534920 -0.384156 0.234518
C 1.080364 -0.738930 -0.216575
O 3.225769 -1.484695 0.567489
O 2.981900 0.738077 0.294771
O 0.788627 -1.960818 -0.130172
O 0.352627 0.213501 -0.601166
H 2.568169 -2.214329 0.430526
H 0.865526 1.871351 -0.496174
N -3.575954 -1.177861 0.968489
H -3.416210 -1.200383 1.975705
H -4.561600 -1.394319 0.820636
H -3.015944 -1.937110 0.542993
N -2.276241 0.800477 -0.552554
H -2.707582 0.874218 -1.474537
H -2.852632 0.140226 0.064802
H -1.295002 0.408502 -0.654939
O -1.744836 -2.773123 -0.608735
H -1.691402 -3.716748 -0.812620
H -0.799483 -2.485958 -0.460314
O 0.876061 2.862928 -0.411144
H -0.625836 3.262620 0.156349
H 1.717419 3.037646 0.035895
O -1.612269 3.320699 0.353936
H -2.171753 1.762624 -0.131603
H -1.683042 3.639307 1.264246

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-c

C	-2.416348	-0.392241	-0.036277
C	-1.161733	-1.320289	0.084062
O	-3.481469	-1.095064	-0.417116
O	-2.431448	0.805549	0.175224
O	-1.374343	-2.510848	-0.214027
O	-0.073773	-0.780437	0.456259
H	-3.093652	-2.015749	-0.501398
H	0.205805	0.807412	0.656854
N	0.600820	1.793508	0.791235
H	0.695251	1.973106	1.791676
H	1.555550	1.843835	0.344196
H	-0.064565	2.506933	0.373384
N	-1.392136	3.522690	-0.321901
H	-2.084230	2.766593	-0.277766
H	-1.322127	3.816743	-1.296082
H	-1.767389	4.315154	0.199091
O	2.081723	-2.343473	0.316653
H	1.834984	-3.114794	-0.214060
H	1.233097	-1.813251	0.395659
O	3.991221	-0.710954	-0.487252
H	4.747048	-0.916831	0.080884
H	3.274248	-1.370736	-0.223021
O	3.154980	1.786935	-0.260962
H	3.489516	0.838448	-0.348178
H	3.369043	2.211267	-1.103510

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-d

C	1.479322	-1.600590	0.006315
C	0.013709	-1.250349	-0.433513
O	1.550211	-2.852432	0.446969
O	2.436673	-0.848276	-0.024426
O	-0.803458	-2.173032	-0.201757
O	-0.197523	-0.119261	-0.947360
H	0.596328	-3.149448	0.360251
H	0.605657	1.279352	-0.781450
N	-3.647920	-1.236992	0.597111
H	-4.419391	-1.632581	0.060099
H	-2.791537	-1.734157	0.318676
H	-3.824549	-1.453339	1.577701
N	0.897947	2.285582	-0.569105
H	0.106965	2.719488	-0.005756
H	1.805669	2.253676	-0.049986
H	1.021222	2.801145	-1.441103
O	3.374681	1.654355	0.482897

H 3.791494 1.710538 1.353798
H 3.170858 0.699122 0.340803
O -2.634898 1.132816 -0.439920
H -1.847661 0.635147 -0.766718
H -3.144099 0.414436 0.035266
O -1.383885 3.155079 0.620025
H -1.974512 2.385133 0.303781
H -1.539217 3.243012 1.570356

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-e

C -2.311921 0.283153 0.254218
C -1.284935 -0.442439 -0.681643
O -3.210404 -0.579860 0.731872
O -2.288518 1.464117 0.537791
O -1.405565 -1.684070 -0.722114
O -0.431594 0.287921 -1.275065
H -2.903879 -1.444397 0.340974
H -0.125380 1.741352 -0.670222
N 1.396255 -2.457724 0.387209
H 1.937209 -2.159349 -0.429824
H 1.660815 -3.417770 0.605427
H 0.416353 -2.467258 0.080923
N 0.317017 2.545356 -0.107920
H -0.297551 2.676939 0.699441
H 1.310187 2.189662 0.165750
H 0.358756 3.407420 -0.650830
O 2.122619 -0.364447 -1.780765
H 2.352449 -0.358446 -2.720291
H 1.133781 -0.228415 -1.736190
O 1.858909 -0.427798 2.137795
H 2.427084 -0.720503 2.863958
H 1.687348 -1.251876 1.561474
O 2.663005 1.403140 0.353775
H 2.692179 0.837547 -0.453597
H 2.471269 0.745367 1.086224

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-f

C -2.101593 -0.620294 -0.063254
C -1.635895 0.875402 -0.057703
O -3.204946 -0.768053 0.668492
O -1.529761 -1.536514 -0.623423
O -2.315570 1.621512 0.670429
O -0.615336 1.166961 -0.757798
H -3.358970 0.167132 0.992838

H 0.413109 0.102182 -1.431001
N 2.217232 -1.491558 1.826296
H 2.570311 -0.608968 1.437602
H 3.010153 -1.985695 2.235717
H 1.589758 -1.254659 2.595157
N 1.296335 -0.435257 -1.711246
H 1.388744 -0.481339 -2.725298
H 1.236800 -1.418155 -1.277827
H 2.096830 0.073288 -1.283060
O 1.140484 2.929745 0.126016
H 0.830466 3.358278 0.936685
H 0.354515 2.398168 -0.207271
O 1.056596 -2.755090 -0.371159
H 1.423562 -2.401656 0.494745
H 0.085045 -2.692231 -0.290672
O 2.969748 1.026052 0.074926
H 2.333702 1.804209 0.182904
H 3.846215 1.419598 -0.039988

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-g

C -0.092314 -1.861603 0.019570
C 1.396107 -1.399384 0.153218
O -0.978810 -0.991700 0.258943
O -0.212967 -3.052043 -0.328608
O 1.750924 -0.276800 0.482200
O 2.225834 -2.385324 -0.153424
H -0.667134 0.602809 0.541514
H 1.570706 -3.122289 -0.364719
N -0.780074 1.649698 0.718462
H -1.762335 1.920824 0.393056
H -0.036739 2.204895 0.227583
H -0.693191 1.817574 1.721600
N -3.440672 2.017440 -0.193775
H -3.571820 2.453619 -1.106727
H -4.136816 2.429489 0.428007
H -3.673943 1.013336 -0.293301
O -3.643499 -0.893835 -0.148274
H -3.987541 -1.597841 -0.714533
H -2.680291 -1.106486 -0.020649
O 1.267156 3.223389 -0.366639
H 1.228306 3.613989 -1.250887
H 2.125196 2.708481 -0.343087
O 3.448138 1.661555 -0.283628
H 3.006792 0.830890 0.028066

H 4.147053 1.844737 0.359979

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-h

C 0.608005 -1.395064 -0.436982
C -0.857698 -1.758161 -0.016303
O 0.794801 -0.761857 -1.497896
O 1.471478 -1.761123 0.416817
O -1.861449 -1.382192 -0.586756
O -0.871568 -2.495816 1.099781
H -0.075265 0.550806 -1.814069
H 0.100172 -2.567736 1.315585
N -0.439434 1.556103 -1.759456
H 0.256281 2.068081 -1.177368
H -0.523743 1.972184 -2.685979
H -1.385136 1.543216 -1.242418
N -1.134807 1.718812 2.020611
H -0.204797 1.949671 1.650271
H -1.039440 0.863615 2.569705
H -1.402154 2.458021 2.670446
O 3.162029 0.325716 0.400301
H 3.647310 0.256602 -0.435526
H 2.623361 -0.520944 0.425679
O -2.668206 1.362301 -0.268428
H -2.221618 1.494857 0.624433
H -2.776953 0.393406 -0.338992
O 1.412864 2.317708 0.256648
H 2.095891 1.569678 0.304307
H 1.904343 3.125596 0.461818

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-i

C 1.574297 -0.643090 -0.365652
C 2.647761 0.426577 0.033264
O 0.418996 -0.217166 -0.690839
O 1.962128 -1.825221 -0.301575
O 2.460360 1.621278 0.128788
O 3.819890 -0.165434 0.286704
H 0.034278 1.385619 -0.582688
H 3.602766 -1.129303 0.144717
N -2.528749 1.416613 0.815690
H -3.126906 2.086820 1.298148
H -3.029743 1.000819 -0.035352
H -2.295372 0.606544 1.446903
N -3.525335 0.024031 -1.428549
H -2.959995 -0.824869 -1.286592

H -3.241425 0.426958 -2.322298
H -4.498035 -0.266211 -1.528028
O -1.484056 -1.945594 -0.386201
H -1.159687 -2.847175 -0.528125
H -0.683120 -1.343008 -0.584121
O -0.316564 2.305461 -0.373124
H 0.481205 2.722816 -0.006129
H -1.625073 1.884872 0.467428
O -2.031406 -1.003259 2.073989
H -1.286264 -1.163213 2.670912
H -1.801182 -1.486607 1.227643

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-j

C -1.533010 0.847819 -0.034792
C -2.233319 -0.556089 0.033797
O -0.357327 0.903019 -0.494565
O -2.246281 1.771599 0.409892
O -1.728773 -1.641968 -0.207793
O -3.492386 -0.420419 0.429014
H 0.693336 0.003541 -1.599519
H -3.538367 0.573938 0.581612
N 2.412431 -1.234580 1.880803
H 1.795250 -0.924489 2.632494
H 1.848322 -1.834890 1.261280
H 3.122625 -1.825767 2.313288
N 2.987189 0.782795 -0.043424
H 2.897050 0.105520 0.772960
H 2.447212 1.672251 0.147554
H 3.964685 0.992647 -0.243631
O 1.264578 2.892034 0.084317
H 0.929935 3.469999 0.784081
H 0.500807 2.276378 -0.147688
O 1.511862 -0.447761 -1.932276
H 1.390577 -1.358523 -1.580033
H 2.514736 0.296932 -0.881224
O 0.767273 -2.593815 -0.303082
H 0.636730 -3.530806 -0.507874
H -0.153836 -2.206133 -0.273045

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-k

C 1.576983 1.038508 0.044477
C 0.972486 -0.398306 -0.223108
O 0.721406 1.925528 0.294491
O 2.819039 1.184500 -0.015376

O -0.234293 -0.506479 -0.447713
O 1.743203 -1.461045 -0.187550
H -0.804038 1.724174 0.360339
H 2.747683 -1.271830 -0.053936
N -1.893685 1.716145 0.441450
H -2.313180 1.406836 -0.480222
H -2.197076 1.016826 1.154463
H -2.235211 2.643116 0.696032
N -2.940455 0.504644 -1.945368
H -3.014837 -0.454126 -1.589906
H -2.191540 0.496474 -2.638842
H -3.806737 0.720853 -2.437944
O -2.900987 -0.441403 2.002159
H -2.470554 -0.758933 2.808602
H -2.738783 -1.146630 1.321672
O -2.325440 -2.037151 -0.143329
H -2.241308 -3.000437 -0.167329
H -1.410301 -1.665400 -0.303736
O 4.259541 -0.923538 0.004983
H 3.886905 0.021933 -0.004353
H 4.671392 -1.042879 0.873065

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-l

C -0.336848 0.016625 -0.001111
C -0.573128 -1.503948 -0.255089
O 0.581384 0.318456 0.830146
O -1.041729 0.803211 -0.660600
O 0.361762 -2.284693 -0.423335
O -1.821933 -1.915515 -0.315500
H 1.824871 -0.657703 1.039907
H -2.518331 -1.187373 -0.151528
N 2.621814 -1.338541 0.792175
H 2.100102 -1.999142 0.182827
H 3.366899 -0.779628 0.254979
H 3.007758 -1.812178 1.607732
N 4.271847 0.447026 -0.594949
H 5.188195 0.721405 -0.240453
H 3.635037 1.255062 -0.470414
H 4.378785 0.291564 -1.597667
O 2.207635 2.391906 0.144588
H 1.489890 1.762079 0.421027
H 1.755709 3.057241 -0.393055
O -3.115964 2.247307 0.133315
H -2.226845 1.918232 -0.168067

H	-3.474365	2.735941	-0.621812
O	-3.846817	-0.340786	0.176058
H	-4.241992	-0.545604	1.035446
H	-3.676191	0.645566	0.180319

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$

Isomer 2.3-m

C	0.167531	-0.578455	-0.817636
C	0.427812	-1.296256	0.563802
O	1.181767	-0.374764	-1.615675
O	-0.963659	-0.176120	-1.122920
O	1.468113	-1.957098	0.686447
O	-0.475834	-1.115275	1.445449
H	2.108384	-0.513102	-1.157361
H	-1.452461	-0.165211	1.335628
N	-3.931705	-0.576908	-0.657780
H	-4.579049	-0.134416	-1.309575
H	-3.040326	-0.711531	-1.146638
H	-4.305689	-1.502666	-0.448620
N	-2.297440	0.640172	1.347493
H	-2.654683	0.794407	2.290117
H	-3.061775	0.295073	0.706927
H	-1.912072	1.515087	0.971481
O	-0.501456	2.406408	-0.358862
H	-0.670156	1.612574	-0.924389
H	-0.519755	3.168697	-0.956119
O	3.405463	-0.395765	-0.354748
H	3.045691	-1.090655	0.245190
H	3.178278	0.453042	0.090858
O	2.199253	1.979575	0.696705
H	2.083750	2.006414	1.657598
H	1.302658	2.142014	0.328746

Data S2: Harmonic frequencies (in cm^{-1}) and IR intensities for $(H_2C_2O_4)(NH_3)_m(H_2O)_n$ (m=1~2, n=1~3) isomers

$(H_2C_2O_4)(NH_3)$ (H_2O)

Isomer 1.1 -a

#	**Frequency**	**Infrared**
1	20.6046	2.2731
2	50.5227	5.3033
3	79.5122	52.8219
4	118.4299	25.0683
5	153.3719	205.0578
6	171.6078	63.6237

7	189.5602	81.3178
8	263.0015	54.4717
9	267.0184	143.6603
10	350.0765	436.364
11	384.1838	87.4936
12	403.8517	27.4412
13	450.3192	13.3877
14	473.0479	45.5347
15	503.2944	282.5148
16	571.3061	53.2217
17	599.9861	593.694
18	650.2708	27.6945
19	759.0525	358.4579
20	810.8537	0.0324
21	878.4891	68.0847
22	1013.4499	1660.3405
23	1171.6516	38.8234
24	1268.2907	843.1861
25	1328.5373	179.8393
26	1398.7265	138.8765
27	1409.2377	52.876
28	1551.1957	202.0903
29	1596.1981	29.7237
30	1634.8083	17.4915
31	1659.4483	34.4752
32	1702.9178	34.9464
33	1778.2755	698.2716
34	3198.3165	351.0248
35	3225.0776	287.4707
36	3449.6179	44.1541
37	3516.0747	22.7266
38	3551.3226	460.6117
39	3791.713	92.9358

Isomer 1.1 -b

#	**Frequency**	**Infrared**
1	23.1218	8.4788
2	79.8153	2.8371
3	89.3973	1.6368
4	108.7615	0.3436
5	151.4147	25.3832
6	168.197	8.2557
7	198.2126	57.5657
8	268.4661	1.4371

9	320.3191	79.6824
10	354.8165	8.1374
11	358.3842	102.9298
12	379.5689	52.9778
13	414.0073	40.6841
14	451.453	41.0803
15	466.8666	31.7855
16	544.0387	41.4771
17	674.1525	266.7591
18	735.9893	40.9844
19	805.0924	1.0259
20	829.6182	39.3182
21	1003.9841	76.4895
22	1089.2665	113.3196
23	1224.6508	60.6394
24	1228.4395	68.6929
25	1278.7305	225.0296
26	1309.8243	1301.9309
27	1379.7422	11.9474
28	1587.8149	149.8901
29	1601.036	24.6216
30	1626.6006	14.4316
31	1697.1689	177.6736
32	1739.8479	381.8313
33	2263.7937	2518.8411
34	2926.5995	1292.044
35	3395.1549	16.5039
36	3400.6567	702.2089
37	3514.2593	52.5895
38	3531.1491	17.1276
39	3772.4074	76.1267

Isomer 1.1 -c

#	**Frequency**	**Infrared**
1	32.5337	1.0011
2	50.5354	4.4424
3	103.3281	1.5505
4	124.3747	1.3028
5	132.2472	10.233
6	138.5806	0.2269
7	209.867	79.4485
8	276.3088	25.6737
9	280.1722	76.3432
10	306.0181	0.7686

11	356.0718	13.5275
12	402.5705	36.5272
13	425.0844	111.5909
14	451.0498	39.1484
15	556.732	2.1201
16	650.058	43.6016
17	682.4402	7.2609
18	802.7416	2.0127
19	816.6103	26.8367
20	826.1072	68.9065
21	989.948	11.813
22	1070.064	94.5582
23	1097.5987	138.8525
24	1161.6938	11.7334
25	1292.2265	103.4576
26	1325.0482	1041.6526
27	1406.7783	4.6738
28	1595.9384	28.2395
29	1630.791	14.2401
30	1653.2038	31.5395
31	1718.3958	134.0553
32	1790.4122	369.2491
33	2522.0692	2557.1114
34	2867.8263	1187.1725
35	3330.2945	202.3965
36	3388.4227	56.837
37	3502.8422	82.7367
38	3529.5931	12.0692
39	3777.0201	49.8487

Isomer 1.1 -d

#	**Frequency**	**Infrared**
1	30.7959	0.4764
2	56.5148	0.8658
3	103.3567	16.9111
4	105.4749	86.2482
5	125.5892	17.1995
6	154.1379	25.6264
7	164.7067	54.7957
8	215.856	1.2552
9	265.3478	32.6882
10	369.1564	182.1902
11	411.495	115.8289
12	428.5903	41.9

13	459.1331	49.306
14	461.0468	104.1176
15	515.54	65.3747
16	532.8025	109.2574
17	569.6441	1.4079
18	704.7006	30.5824
19	815.1479	0.0488
20	842.5462	19.8218
21	870.0589	67.6363
22	1021.1027	1202.7453
23	1165.077	17.9174
24	1253.9303	1302.9828
25	1387.5485	946.7156
26	1391.4926	232.1125
27	1518.3284	104.3418
28	1568.9695	160.5548
29	1598.972	36.5657
30	1655.1881	95.4728
31	1678.2988	33.944
32	1727.683	39.8356
33	1771.7202	616.2287
34	3237.9678	220.3107
35	3335.1684	38.9122
36	3444.5057	151.33
37	3519.5467	64.086
38	3539.6753	376.3221
39	3798.4611	82.7788

$(H_2C_2O_4)(NH_3)\ (H_2O)_2$
Isomer 1.2 -a

#	Frequency	Infrared
1	26.8568	0.5509
2	44.8266	0.1221
3	59.9921	3.0848
4	90.9901	12.4219
5	114.9439	1.0347
6	137.6795	2.5576
7	183.6642	9.5217
8	252.1944	103.24
9	261.64	20.7836
10	272.2575	53.7723
11	285.214	106.1489
12	303.3056	38.3136
13	338.6652	137.93

14	356.807	28.1015
15	404.7787	16.0234
16	441.1902	26.366
17	460.1326	46.0891
18	470.4673	22.6719
19	512.4787	87.8144
20	561.0382	29.9245
21	619.0499	37.1805
22	696.0653	29.1438
23	786.2887	45.9512
24	817.502	1.4103
25	853.0744	40.2146
26	869.9265	67.3891
27	973.4584	118.9343
28	1164.284	12.4028
29	1266.1565	278.345
30	1318.1006	415.8095
31	1391.1228	253.6271
32	1503.3059	76.917
33	1533.1684	228.5074
34	1599.0758	39.7119
35	1629.4453	149.6236
36	1649.3698	377.1634
37	1671.9189	53.1571
38	1705.9134	112.7969
39	1766.3418	331.3953
40	2131.6647	1730.7274
41	2917.9369	683.5782
42	3106.3771	1390.9946
43	3242.8114	466.5643
44	3249.6081	818.1995
45	3418.7384	101.0052
46	3508.1588	64.6081
47	3783.1609	55.5486
48	3785.603	67.8324

Isomer 1.2 -b

#	**Frequency**	**Infrared**
1	43.0276	0.4968
2	49.227	2.1954
3	81.5546	5.0478
4	91.3038	6.1121
5	119.8111	2.3303
6	135.6326	10.7652
7	178.0509	0.5871

8	228.5498	48.4188
9	233.9079	51.4289
10	262.634	24.3719
11	292.2435	131.4735
12	302.5372	90.46
13	325.0408	4.9278
14	366.2623	70.3804
15	418.012	17.5513
16	436.745	96.054
17	446.258	29.7172
18	454.6293	27.864
19	520.6096	74.7037
20	577.8516	12.1189
21	613.0652	17.2429
22	689.908	61.9138
23	758.9791	60.3556
24	826.9713	4.1492
25	839.9152	55.593
26	847.9701	45.2254
27	979.6521	94.9209
28	1160.4764	8.6076
29	1251.2355	110.6195
30	1325.0486	363.648
31	1376.869	331.9027
32	1458.916	107.9352
33	1525.6964	709.2574
34	1595.6076	53.9907
35	1622.4138	95.0274
36	1642.6209	24.6585
37	1664.3366	45.1448
38	1688.1726	31.51
39	1762.691	313.6019
40	2194.6532	1360.3388
41	2918.8047	881.8178
42	3083.1435	1030.8796
43	3282.4262	900.8598
44	3305.7005	107.7128
45	3396.0732	105.2534
46	3514.9905	67.3408
47	3771.8913	62.0836
48	3787.3883	51.2747

Isomer 1.2 -c

#	**Frequency**	**Infrared**

1	31.447	1.0804
2	41.9114	2.1008
3	53.8186	1.9166
4	59.6315	1.0232
5	110.2619	5.1448
6	132.1175	94.7863
7	154.7188	28.6815
8	167.6326	18.7752
9	194.1664	8.4455
10	257.8312	89.458
11	271.3049	21.9446
12	283.3182	36.5568
13	323.4451	144.6717
14	346.5017	60.0828
15	415.8566	41.6807
16	431.0701	10.2764
17	446.6373	43.7418
18	465.911	44.0433
19	477.0882	149.2501
20	552.151	71.2538
21	593.6157	73.1942
22	654.027	97.683
23	700.5579	24.6707
24	708.8457	69.1365
25	815.971	0.2371
26	841.6493	24.7556
27	908.9117	65.8237
28	1173.7032	3.9079
29	1302.2203	251.9613
30	1334.9553	292.2047
31	1398.421	345.756
32	1494.3191	150.7741
33	1526.5563	139.1035
34	1598.4671	39.3902
35	1604.5597	22.4093
36	1649.5033	367.4563
37	1681.5787	2.388
38	1711.5989	90.1073
39	1760.6839	639.7025
40	2313.5839	1665.2358
41	3007.5663	625.2012
42	3143.4743	302.8208
43	3282.0259	237.1172
44	3421.075	366.7939

45	3432.3773	1081.5149
46	3495.7045	60.3121
47	3790.3747	83.2171
48	3798.6684	74.3054

Isomer 1.2 -d

#	**Frequency**	**Infrared**
1	11.3746	6.6732
2	29.7935	1.0927
3	80.4546	1.1972
4	90.2157	3.7928
5	92.8128	3.2564
6	118.7862	0.1467
7	156.5919	20.8405
8	163.7116	29.7801
9	196.6561	32.0685
10	235.8967	21.2743
11	266.6738	82.035
12	282.8349	103.0074
13	307.6107	21.6169
14	332.2042	136.265
15	342.2013	2.0534
16	351.9211	6.3371
17	395.5459	37.1815
18	445.5819	37.4302
19	470.968	39.194
20	487.7282	111.9497
21	564.2775	8.8709
22	648.6225	111.96
23	708.264	72.3625
24	804.9783	0.3039
25	828.7561	6.3083
26	905.2972	46.4917
27	1020.3965	97.2597
28	1084.551	134.5951
29	1219.9446	160.048
30	1224.2473	51.6075
31	1265.0302	460.6669
32	1304.1774	1010.6212
33	1377.078	136.8541
34	1598.3374	56.8307
35	1599.5715	56.9286
36	1627.0485	24.5601
37	1627.5015	64.9215

38	1712.2052	79.5906
39	1739.6806	572.3102
40	2270.6149	2587.8872
41	2855.6001	1642.2981
42	3250.2342	705.1537
43	3389.0393	29.9602
44	3508.4048	67.2214
45	3522.8529	641.2822
46	3532.6727	16.605
47	3777.4819	58.9238
48	3782.5179	93.073

Isomer 1.2 -e

#	**Frequency**	**Infrared**
1	27.8775	2.2463
2	30.1852	0.3355
3	56.0849	0.9581
4	85.6015	0.146
5	103.9667	10.4076
6	131.7416	1.2922
7	151.4154	0.537
8	153.0796	0.5459
9	238.1265	80.1886
10	256.882	20.9839
11	278.5262	41.6744
12	303.8931	34.4979
13	311.0932	105.2185
14	375.9979	57.5718
15	404.6981	29.5659
16	430.7087	80.3045
17	453.4038	35.3472
18	542.3139	23.7572
19	577.5352	75.175
20	594.7071	11.7166
21	645.2039	195.4645
22	681.8729	18.9916
23	803.6885	14.5552
24	808.604	54.5819
25	820.9317	60.5956
26	923.2779	72.2844
27	1032.7595	94.8024
28	1125.8242	90.7768
29	1163.5865	6.6255
30	1268.2008	97.7264

31	1294.8777	536.2173
32	1376.7334	408.1273
33	1474.6982	721.3297
34	1590.7886	51.951
35	1608.8501	35.1295
36	1628.7407	20.5528
37	1649.6485	1.4486
38	1705.7911	193.5624
39	1773.7693	168.8527
40	1946.6039	1862.9777
41	2917.2102	1475.5964
42	3066.7047	1109.308
43	3346.8288	184.0305
44	3369.0832	76.6684
45	3482.5308	72.7107
46	3520.0043	12.0374
47	3639.2125	217.9984
48	3777.5789	48.8193

Isomer 1.2 -f

#	**Frequency**	**Infrared**
1	22.7957	10.7224
2	28.0023	2.0624
3	69.8376	6.3265
4	79.2866	0.4307
5	105.0416	26.1794
6	150.1904	122.8877
7	187.7877	71.5124
8	197.0564	66.1154
9	211.8872	148.0224
10	264.0213	69.8561
11	295.7493	190.5355
12	307.4699	20.6698
13	389.0004	650.177
14	404.4148	17.0087
15	412.1563	186.3969
16	425.3537	123.1631
17	432.5654	41.3478
18	453.9467	250.5963
19	488.5541	36.5038
20	539.9324	234.6672
21	584.6101	37.1605
22	647.788	1372.4723
23	710.8739	200.3525

24	778.3053	525.8845
25	809.747	142.2121
26	818.547	94.7176
27	907.6382	653.9191
28	1054.0707	70.4605
29	1259.7139	71.9382
30	1311.3919	598.0024
31	1365.984	207.0395
32	1393.9149	518.0838
33	1488.2019	51.3753
34	1524.7271	85.9201
35	1594.9538	122.957
36	1597.9415	32.0504
37	1652.824	16.9565
38	1667.4825	14.8977
39	1682.9197	42.4077
40	1716.1835	626.181
41	2775.3777	1313.9798
42	3117.528	488.703
43	3198.5951	1285.2733
44	3444.8504	97.5796
45	3459.7283	537.6946
46	3516.7579	30.0137
47	3770.4757	62.4996
48	3787.8078	78.3208

Isomer 1.2 -g

#	Frequency	Infrared
1	31.6244	0.9896
2	37.8599	2.2666
3	57.4075	1.8663
4	85.0753	6.5343
5	109.1642	25.4938
6	128.6293	61.1774
7	138.6194	36.408
8	153.625	13.9745
9	175.5388	26.3652
10	204.7212	3.7099
11	257.9201	140.2338
12	294.0075	138.7771
13	358.8109	15.2463
14	381.4871	106.5129
15	400.3732	17.5802
16	449.685	34.9789

17	473.3317	136.8561
18	520.0537	54.7989
19	546.0058	17.9746
20	573.0676	58.3973
21	643.3778	58.5645
22	663.0876	249.5364
23	735.2244	46.2243
24	788.5916	348.7775
25	807.8197	5.3026
26	831.7856	69.1843
27	1065.3787	32.3943
28	1158.1975	749.4258
29	1161.8677	407.6572
30	1176.9488	1940.5885
31	1317.7429	303.6972
32	1362.2906	163.1664
33	1389.6193	109.5848
34	1596.2355	1.2182
35	1602.2238	128.746
36	1625.6348	28.2636
37	1642.7337	29.262
38	1682.0465	81.213
39	1719.126	44.55
40	1780.8257	634.5747
41	2558.7914	1809.1866
42	3288.4157	231.478
43	3325.9133	197.113
44	3466.2198	54.2887
45	3525.3933	12.6345
46	3535.6627	464.3703
47	3603.9182	244.6555
48	3794.5059	82.0999

Isomer 1.2 -h

#	**Frequency**	**Infrared**
1	18.8398	1.8287
2	29.8164	0.4464
3	44.7188	3.4046
4	59.407	1.2058
5	118.9218	2.1999
6	127.2362	3.4743
7	158.849	42.1309
8	161.1979	31.4148
9	174.3389	18.1892

10	217.3656	39.1243
11	242.4896	63.2407
12	282.6791	42.8772
13	311.6016	52.294
14	347.6266	34.4818
15	378.8852	14.1358
16	398.7334	51.2444
17	417.8481	13.2624
18	454.3878	31.7562
19	486.3094	119.7268
20	565.7615	11.0832
21	643.5183	62.0008
22	671.0248	25.1488
23	712.1501	21.7779
24	804.0017	0.5666
25	821.3579	40.7033
26	833.3649	69.8873
27	1043.4575	8.8848
28	1096.4649	93.6828
29	1171.6711	4.2852
30	1179.5642	95.2661
31	1303.0784	243.2663
32	1343.882	1073.4427
33	1415.9635	37.6923
34	1598.5697	13.0165
35	1610.6253	53.9262
36	1646.5338	12.0389
37	1661.2177	20.4797
38	1718.4875	120.8394
39	1782.857	418.8958
40	2340.5023	3095.9605
41	2689.5826	1207.7748
42	3254.5617	335.2614
43	3310.2788	227.9466
44	3452.1305	46.036
45	3505.1825	689.7393
46	3514.8476	8.4706
47	3772.6434	42.5685
48	3791.3131	83.875

Isomer 1.2 -i

#	**Frequency**	**Infrared**
1	26.7689	0.2334
2	43.5759	3.6098

3	59.8451	8.9643
4	74.7061	3.6849
5	109.0589	3.257
6	124.2349	3.4816
7	127.7113	3.5055
8	136.9118	0.8215
9	165.6065	35.742
10	212.5819	101.3922
11	236.9743	127.0389
12	279.1091	54.3149
13	288.4237	40.8908
14	315.8667	31.1585
15	387.9359	48.0864
16	401.4902	41.5168
17	414.179	71.5534
18	452.9801	25.0147
19	508.7865	203.1261
20	562.6111	6.5838
21	666.1554	48.2342
22	697.1006	131.1145
23	792.3282	72.5412
24	804.9793	22.7523
25	808.2473	333.0215
26	824.228	67.8251
27	1000.5696	43.5917
28	1096.3458	137.5467
29	1160.215	7.9286
30	1235.7451	84.6186
31	1290.1373	1500.0314
32	1340.5506	954.9991
33	1397.6547	56.4319
34	1589.9188	30.0563
35	1598.1447	91.907
36	1628.9831	12.6122
37	1635.9092	12.4941
38	1707.7932	185.4273
39	1776.3537	35.1811
40	1848.0802	1639.9402
41	2835.2245	1506.2231
42	3335.184	192.7812
43	3386.6605	49.5636
44	3501.7023	72.4132
45	3518.0437	376.1583
46	3529.6678	12.3506

47	3633.4822	187.6718
48	3787.5771	103.7672

Isomer 1.2 -j

#	**Frequency**	**Infrared**
1	14.4894	1.1242
2	20.2787	3.3345
3	36.3971	9.5687
4	76.6515	2.053
5	89.5347	29.8112
6	94.15	56.7053
7	97.1375	2.7102
8	124.2314	2.5851
9	150.6788	44.4649
10	182.7708	21.3515
11	208.6227	72.6261
12	263.4597	6.9116
13	307.1171	117.4631
14	327.1398	61.949
15	365.9598	4.8442
16	382.2012	24.4319
17	405.477	10.2505
18	429.3241	73.457
19	455.0979	49.0855
20	467.4782	25.4379
21	544.9932	35.9366
22	631.5028	193.3521
23	698.4784	120.957
24	770.3007	103.489
25	803.6137	4.043
26	830.1505	102.8539
27	952.55	86.0063
28	1099.8712	95.9118
29	1216.2414	42.5292
30	1252.0637	64.3883
31	1285.0335	48.5904
32	1298.5613	1591.202
33	1377.4593	76.4953
34	1588.4668	184.0272
35	1601.6908	26.5462
36	1616.161	18.1128
37	1625.0249	14.4848
38	1693.4649	263.5577
39	1745.7522	324.4154

40	2148.1014	2633.9816
41	3079.7385	842.8352
42	3309.3822	1303.458
43	3396.6941	12.1033
44	3515.2033	52.649
45	3529.7044	19.0883
46	3583.0916	310.6116
47	3764.588	83.3385
48	3792.006	71.2727

Isomer 1.2 -k

#	**Frequency**	**Infrared**
1	26.0509	0.83
2	48.5771	2.8297
3	68.6184	6.1468
4	94.3959	4.5539
5	111.1348	49.0385
6	112.804	2.4493
7	129.6541	22.6541
8	151.0823	6.3707
9	170.9706	7.8689
10	179.2126	7.8674
11	186.127	1.3443
12	240.0874	24.0829
13	264.4856	54.9534
14	319.2284	132.2931
15	331.9202	42.0147
16	358.7685	94.232
17	410.1245	34.9711
18	417.71	106.3586
19	431.5212	23.2314
20	476.158	105.3583
21	547.7397	23.3746
22	552.1879	36.0852
23	679.6559	49.7608
24	744.9791	200.4638
25	776.384	10.2879
26	791.8175	68.1664
27	824.3376	5.8267
28	1048.843	104.1297
29	1076.2134	53.1963
30	1177.9303	7.763
31	1291.7334	189.6888
32	1362.0319	535.2701

33	1435.8203	95.7513
34	1591.0469	109.5079
35	1603.7903	26.8368
36	1614.0568	57.7675
37	1633.6031	7.9707
38	1700.664	118.511
39	1761.9216	358.7334
40	2744.3673	1502.3326
41	3329.4403	92.1127
42	3356.8438	673.7482
43	3379.9537	195.665
44	3469.1307	39.193
45	3518.1001	4.3968
46	3558.9537	283.0634
47	3770.1899	71.0207
48	3791.6957	78.2668

$(H_2C_2O_4)(NH_3)\ (H_2O)_3$
Isomer 1.3 -a

1	23.582	0.5797
2	40.2768	1.8807
3	45.9428	0.0472
4	50.9852	3.0132
5	66.9367	8.5598
6	83.1876	0.5481
7	117.7833	2.8877
8	179.2231	11.3478
9	192.5338	5.8655
10	217.5772	37.3883
11	256.3782	74.3894
12	263.5136	97.7813
13	272.2717	50.5542
14	281.2037	76.5532
15	300.2521	99.8651
16	313.021	5.7983
17	318.434	85.8623
18	390.7544	67.3942
19	422.0277	31.198
20	449.7359	19.158
21	461.8561	40.4478
22	467.3793	25.2215
23	505.772	48.5169
24	535.9182	64.9929
25	565.3715	35.5599

26	630.3518	154.418
27	700.4877	5.486
28	722.3007	57.8599
29	815.4315	7.238
30	821.7632	52.2813
31	846.663	63.3855
32	900.7991	68.4281
33	976.0508	80.4995
34	1173.0647	5.4593
35	1317.5429	448.0866
36	1392.8985	195.6269
37	1398.1092	202.1516
38	1489.1823	96.1852
39	1536.5666	59.6245
40	1602.8211	24.7872
41	1611.4136	21.747
42	1640.5362	110.1359
43	1669.4787	259.5541
44	1701.278	8.9679
45	1727.1373	73.7879
46	1763.5493	541.6477
47	2558.1512	1344.5536
48	2909.1428	722.6389
49	3023.461	618.8495
50	3067.9893	1819.9183
51	3168.3806	366.8627
52	3184.6151	988.1027
53	3447.8714	724.4135
54	3487.2171	49.148
55	3778.7656	54.3726
56	3784.4044	50.6432
57	3788.2285	85.1821
Isomer 1.3 -b		
1	24.1945	0.5686
2	39.4633	0.658
3	49.9177	4.3962
4	54.3798	0.6084
5	74.1504	1.0153
6	89.2497	9.1875
7	116.0218	1.6222
8	141.6128	3.9678
9	189.2969	5.6736
10	239.3548	73.8764
11	257.7149	41.1271

12	267.6584	63.8099
13	297.6416	30.7228
14	299.8969	78.0903
15	329.5234	225.2926
16	335.125	67.2738
17	350.2564	35.7048
18	369.8241	9.8643
19	424.7258	11.0523
20	452.0448	31.6063
21	462.16	14.9642
22	493.9077	47.4595
23	512.913	34.614
24	530.0177	24.8368
25	564.6401	19.7025
26	607.5274	29.3045
27	701.9589	40.0395
28	806.0349	74.6787
29	819.722	23.3658
30	839.7443	26.6572
31	878.4069	68.6748
32	934.9144	62.4434
33	1051.9189	76.0515
34	1167.5217	9.4673
35	1298.0735	386.7207
36	1336.8352	238.5245
37	1393.38	289.2113
38	1480.9219	78.6929
39	1535.2193	265.8776
40	1603.3351	59.5173
41	1627.8376	51.4535
42	1645.1299	204.895
43	1672.1806	129.6026
44	1680.0427	50.8097
45	1699.1691	101.2062
46	1760.3808	309.5541
47	2384.6976	1504.6484
48	2797.6611	1005.7852
49	2970.2244	2088.6875
50	3077.972	1205.1536
51	3192.7695	915.7542
52	3220.3832	231.3894
53	3345.5434	195.8804
54	3500.3403	66.2483
55	3772.5755	50.9903

56	3779.8906	52.146
57	3781.2674	48.769
Isomer 1.3 -c		
1	36.0643	3.4614
2	44.0456	0.654
3	53.014	5.685
4	79.6382	5.8624
5	88.7703	7.1027
6	115.8028	1.7101
7	130.8109	3.9142
8	161.3869	5.2214
9	179.8703	9.5659
10	194.8398	12.1529
11	260.6484	56.1153
12	261.0835	97.8876
13	262.5767	49.1415
14	284.7523	107.2445
15	332.8159	74.9001
16	336.4769	44.5989
17	357.6305	9.0118
18	408.067	66.1754
19	416.9767	29.4775
20	446.0103	21.0442
21	462.2172	19.2893
22	531.9904	27.6791
23	545.5989	99.3557
24	571.8622	14.7442
25	616.0775	30.7748
26	691.0606	38.1675
27	706.5905	28.4674
28	764.8281	79.4149
29	819.7023	10.5537
30	829.7362	72.015
31	834.4762	118.6959
32	847.3437	11.5235
33	979.3328	153.8606
34	1162.2711	8.7664
35	1298.657	217.1414
36	1330.8323	315.9907
37	1381.1965	218.4575
38	1475.4503	86.4772
39	1545.2878	314.6199
40	1613.9384	211.2052
41	1631.8072	165.3586

42	1651.1711	27.9769
43	1673.1401	22.7367
44	1686.1553	57.2075
45	1706.3854	139.701
46	1767.0353	313.366
47	2426.0647	1283.6549
48	2718.5987	1228.5955
49	2906.0832	1526.4585
50	3312.7489	378.2989
51	3334.7568	175.9053
52	3396.7452	695.2645
53	3407.0061	77.3562
54	3464.7533	663.693
55	3507.6189	73.9905
56	3779.224	68.4589
57	3785.0018	48.3307
Isomer 1.3 -d		
1	30.1414	2.3866
2	46.4077	1.4246
3	58.0713	4.6156
4	78.2477	3.7335
5	89.3192	9.2215
6	100.5246	1.0291
7	120.3103	0.1561
8	130.8835	8.4478
9	181.1904	17.3297
10	213.395	12.3749
11	231.8761	94.5536
12	254.8186	25.1935
13	276.2345	51.9588
14	313.2962	26.4916
15	315.5656	141.3034
16	336.1428	66.8499
17	353.3381	32.9906
18	421.3911	32.9518
19	427.3989	30.8075
20	452.0905	13.7348
21	457.7283	28.5486
22	466.9053	53.8216
23	529.4854	58.7437
24	568.163	46.626
25	573.7265	6.9605
26	644.7904	61.5162
27	691.7976	50.2127

28	780.9921	129.7572
29	822.5373	0.5578
30	841.0783	72.9865
31	851.8534	59.6572
32	948.7687	101.6931
33	994.3745	39.7877
34	1161.8887	11.0519
35	1303.1937	333.8494
36	1334.6432	152.0561
37	1382.4483	276.4213
38	1446.6925	66.522
39	1539.1468	335.766
40	1601.0087	54.4572
41	1628.6215	91.7991
42	1637.9185	176.4341
43	1662.1427	4.0617
44	1677.5352	77.4804
45	1698.8198	22.0856
46	1764.0644	300.2808
47	2511.8137	1034.023
48	2736.7229	1327.3653
49	2927.6804	1314.0093
50	3226.6873	447.7786
51	3279.4628	241.5575
52	3311.8583	1002.8214
53	3381.3199	98.7436
54	3509.2989	75.1245
55	3638.9915	151.6546
56	3776.0785	59.8768
57	3790.8629	51.5622
Isomer 1.3 -e		
1	28.3676	7.0854
2	32.8268	0.5233
3	53.9567	0.6356
4	65.0151	1.3027
5	69.5351	5.6473
6	86.2765	2.154
7	107.9521	6.5265
8	178.0226	4.9064
9	189.2557	1.3777
10	215.0352	78.9606
11	230.8418	81.2158
12	246.5657	45.8237
13	271.7336	85.3614

14	284.0172	77.351
15	290.3825	69.0587
16	316.4314	29.8879
17	324.7299	59.3293
18	392.1934	70.7615
19	420.822	47.428
20	444.0616	9.493
21	452.1125	28.4162
22	473.2569	19.5765
23	509.8422	31.7606
24	545.7833	73.0394
25	581.7354	19.5051
26	622.5834	48.5973
27	694.4176	25.0717
28	782.8151	94.9952
29	795.5151	54.704
30	824.169	13.0943
31	827.8865	43.106
32	837.4515	45.5216
33	993.6215	94.2799
34	1169.7839	9.839
35	1322.9236	335.5388
36	1361.3047	36.8978
37	1374.5797	376.2819
38	1454.3951	56.8447
39	1536.3335	260.5769
40	1611.8048	0.9697
41	1617.6294	40.9794
42	1650.3357	63.0931
43	1652.8314	243.983
44	1691.3704	32.138
45	1701.8709	3.5468
46	1751.3002	486.6045
47	2759.6793	635.399
48	2864.981	1033.6633
49	2996.2787	360.4527
50	3031.8157	2010.0699
51	3135.2871	1131.7336
52	3266.76	1082.4733
53	3323.6914	140.6432
54	3498.645	61.9024
55	3783.7639	43.1098
56	3786.1307	58.8755
57	3789.2369	62.7014

Isomer 1.3 -f

1	38.8627	0.1903
2	46.4744	1.1558
3	50.0854	3.2451
4	74.6675	4.2393
5	81.1715	1.2224
6	100.5125	7.2674
7	124.5414	0.3765
8	188.8657	3.789
9	202.0827	22.7235
10	208.8304	25.4509
11	224.2136	53.8558
12	237.1214	76.5584
13	277.292	67.2311
14	292.9912	72.9268
15	300.1246	23.7333
16	318.6115	163.4677
17	325.8401	32.2812
18	399.9519	49.8501
19	423.801	40.4308
20	431.1616	34.8229
21	443.9766	89.5988
22	459.4908	31.5661
23	483.2062	5.4875
24	588.1026	17.5918
25	591.8508	15.9791
26	633.5793	27.4681
27	694.5723	46.2963
28	786.2	69.1393
29	809.2961	103.5884
30	826.4847	53.7856
31	853.0355	79.0613
32	863.6951	29.7378
33	1002.6854	95.6589
34	1178.3569	3.7488
35	1325.2314	228.0371
36	1377.933	435.1681
37	1409.3212	62.2424
38	1443.8321	40.4277
39	1552.5024	144.0616
40	1601.7625	30.3418
41	1611.7978	35.3771
42	1645.2213	26.8239
43	1664.7835	174.3124

44	1700.4291	54.4892
45	1718.9188	17.77
46	1735.4097	469.4497
47	2817.801	964.7835
48	2861.453	961.3977
49	2928.2683	530.7961
50	3037.2079	1181.4982
51	3226.7328	1113.3392
52	3259.0723	107.6832
53	3290.7454	1072.2801
54	3488.6246	42.4809
55	3771.3991	51.4535
56	3782.0926	74.263
57	3783.0256	43.6404
Isomer 1.3 -g		
1	32.2626	0.2334
2	45.0925	0.5562
3	53.3099	1.2127
4	64.4828	1.7799
5	72.6946	3.4153
6	91.2137	7.7011
7	122.5321	3.6618
8	144.7551	5.1132
9	170.9612	0.399
10	221.3052	38.6946
11	230.077	27.2018
12	260.3413	37.2863
13	275.5657	34.6628
14	290.7558	183.6945
15	321.3507	151.0904
16	345.7338	46.4957
17	353.337	82.9665
18	365.7982	41.3854
19	422.2952	19.8029
20	452.1145	7.4676
21	456.9656	21.8672
22	460.4323	64.3495
23	503.6567	39.906
24	526.9772	37.8295
25	569.2254	9.3464
26	622.3059	21.8571
27	699.5408	45.8874
28	773.1056	90.159
29	821.722	2.8375

30	841.1969	22.9759
31	848.5428	65.174
32	916.0212	57.4247
33	1016.9164	86.564
34	1161.7223	10.2305
35	1283.4225	126.4993
36	1331.8036	338.9914
37	1380.7942	328.024
38	1474.0197	56.7935
39	1534.6952	586.2839
40	1597.9208	77.3523
41	1624.43	79.4801
42	1627.9908	214.5167
43	1664.1198	68.5586
44	1678.1311	47.047
45	1692.4545	30.9505
46	1763.0402	302.9196
47	2199.2281	1608.8141
48	2842.5286	1114.3565
49	3008.5921	1796.1277
50	3120.7509	948.6002
51	3236.588	1011.9646
52	3291.6511	75.7739
53	3388.2055	121.2509
54	3509.7237	64.9007
55	3777.7995	54.9103
56	3779.018	50.5193
57	3786.7412	49.2759
Isomer 1.3 -h		
1	26.7908	0.1293
2	41.3129	0.0015
3	59.1853	2.5692
4	73.0986	0.0483
5	74.7347	10.0271
6	123.126	6.0794
7	129.1839	0.2781
8	173.4679	0.8942
9	193.7187	6.637
10	210.3235	12.849
11	215.3398	63.4637
12	236.8499	30.1251
13	277.1023	41.2124
14	277.7068	5.7057
15	304.957	59.4774

16	319.8303	310.8854
17	327.987	5.5336
18	398.3782	87.9392
19	412.4268	24.3231
20	421.9917	8.6547
21	439.5323	0.6534
22	459.0825	22.3259
23	467.0449	164.9555
24	522.1437	5.2926
25	582.3149	6.652
26	637.1937	67.9207
27	700.8204	18.3314
28	704.8029	142.1091
29	784.2925	250.6532
30	815.2886	0.1569
31	836.4657	40.2856
32	898.8969	5.6096
33	978.0829	60.8416
34	1172.6691	1.3343
35	1310.4966	257.6265
36	1393.8288	32.0627
37	1408.0125	542.0609
38	1462.6176	34.3626
39	1548.749	136.6429
40	1580.5086	50.3397
41	1608.8801	9.0007
42	1630.3024	15.1221
43	1652.4339	336.0853
44	1690.5112	0.3754
45	1723.5989	55.6252
46	1751.1407	821.0622
47	2177.2218	2170.2276
48	2941.5124	364.784
49	3088.5051	452.08
50	3090.6669	485.4837
51	3221.225	1274.1821
52	3414.6498	577.6664
53	3460.1438	526.151
54	3485.3438	23.9116
55	3777.5151	119.8668
56	3778.5829	27.2417
57	3786.5166	68.7699
Isomer 1.3 -i		
1	38.7495	4.4666

2	46.7949	6.055
3	61.0525	1.3742
4	75.1926	1.4283
5	99.1071	10.3474
6	112.0314	2.5935
7	131.2887	9.1812
8	165.8368	4.8217
9	180.7098	3.9553
10	194.5149	17.7772
11	220.5633	67.8132
12	224.2041	63.3368
13	260.9633	5.4915
14	269.9787	92.9186
15	298.5015	113.2893
16	334.5096	23.855
17	365.5479	95.6749
18	390.4882	23.569
19	407.9677	71.6562
20	423.6685	5.3601
21	448.0053	53.5
22	481.7201	20.3271
23	573.8218	19.1744
24	597.7989	44.7077
25	621.9966	93.5329
26	671.3651	37.0941
27	694.805	69.3029
28	722.7653	83.8788
29	823.7366	14.6391
30	832.79	15.6739
31	876.6059	148.5438
32	880.4461	30.65
33	906.8798	79.5363
34	1165.444	1.7881
35	1308.4757	172.4598
36	1327.3228	67.4997
37	1381.0925	440.7139
38	1455.7733	109.1759
39	1559.6844	175.0508
40	1596.4946	82.1234
41	1601.1207	80.3919
42	1634.1484	156.8435
43	1640.5236	78.1031
44	1679.3269	11.7713
45	1714.4309	8.6102

46	1740.7883	413.034
47	2337.7431	1341.9862
48	2509.9664	1546.2623
49	3159.2822	239.561
50	3320.4902	543.2468
51	3368.6467	444.5857
52	3434.4363	619.3129
53	3443.6226	31.56
54	3476.0898	582.7822
55	3524.7682	46.4063
56	3782.1631	72.8795
57	3782.864	74.8125
Isomer 1.3 -j		
1	29.4154	1.4266
2	41.9328	2.8414
3	43.9594	3.1721
4	54.6298	3.0646
5	63.0231	2.4651
6	100.6191	5.1346
7	126.603	0.3829
8	158.8442	4.3093
9	184.2408	1.8982
10	221.797	22.4323
11	232.5571	30.4538
12	240.8691	17.5607
13	249.9815	170.6088
14	275.9786	40.6716
15	289.2059	7.4726
16	301.5318	116.7717
17	314.2557	166.1918
18	373.7698	77.3919
19	402.2645	60.1765
20	417.6443	2.7478
21	462.2664	69.0265
22	466.1883	82.5444
23	481.1806	9.2468
24	533.6102	27.589
25	572.4127	7.4094
26	627.4575	17.3145
27	666.9486	13.1278
28	690.6572	224.5146
29	706.2994	8.0884
30	817.087	7.9312
31	834.6297	31.4061

32	912.7804	74.5765
33	1008.6432	57.6591
34	1171.6535	5.8657
35	1312.3984	210.0683
36	1377.769	4.6105
37	1412.1516	592.6732
38	1464.8588	47.0792
39	1558.8076	111.7188
40	1603.4704	19.2918
41	1610.246	52.312
42	1639.6298	66.3239
43	1650.8237	75.4131
44	1701.8947	40.3805
45	1706.6473	104.9226
46	1731.6874	818.0215
47	2292.848	1967.5658
48	2845.1267	381.8994
49	2943.1642	875.5199
50	3117.153	359.2403
51	3197.3755	1034.9321
52	3417.6687	698.3937
53	3475.7173	562.175
54	3491.9767	48.9099
55	3777.1193	78.9942
56	3779.5665	54.5628
57	3784.8225	74.1706
Isomer 1.3 -k		
1	27.2497	0.8688
2	35.6004	0.6203
3	42.6411	6.8813
4	52.9794	1.0134
5	71.983	2.4643
6	78.262	6.6191
7	124.3359	4.2556
8	137.8836	3.4231
9	169.6368	3.4081
10	213.8955	35.6127
11	250.19	45.5786
12	276.6411	47.8737
13	285.2506	6.2063
14	293.3743	187.3795
15	314.098	82.5909
16	328.4608	95.5959
17	337.5523	16.0928

18	348.4543	216.7462
19	433.4124	44.0278
20	456.0093	4.1027
21	477.6299	53.9766
22	483.6947	36.4699
23	509.2133	13.3296
24	546.2131	28.649
25	580.5127	4.7195
26	629.5347	8.8287
27	708.9284	47.4886
28	767.5347	93.6637
29	816.8968	0.701
30	839.5596	34.2888
31	889.7358	61.0452
32	964.1505	59.7728
33	1019.5529	73.7762
34	1171.7287	2.6794
35	1277.9929	502.3049
36	1341.6623	49.8459
37	1403.1101	551.2875
38	1461.8332	54.6758
39	1548.5806	518.9582
40	1603.5637	33.9408
41	1612.311	573.0744
42	1627.66	12.4168
43	1653.2747	24.5285
44	1668.977	20.7659
45	1709.7567	98.1722
46	1741.8378	658.3867
47	1897.7164	1654.1671
48	2842.6481	1049.3872
49	2975.5912	378.5287
50	3059.0332	1487.3114
51	3161.7418	1046.1167
52	3298.4518	963.0846
53	3435.9382	34.719
54	3515.4419	44.8591
55	3776.5646	65.9662
56	3777.3796	47.6064
57	3782.1875	54.2388
Isomer 1.3 -l		
1	27.6499	3.0122
2	45.1262	1.7508
3	47.0009	7.6027

4	56.1073	4.9877
5	78.7369	3.4813
6	88.2591	7.3128
7	131.3329	3.0306
8	149.2734	17.1393
9	200.2157	4.4463
10	230.1718	56.192
11	240.2762	18.887
12	263.9356	32.0098
13	268.7245	13.4434
14	290.7053	99.018
15	299.9151	93.1171
16	329.5033	144.8333
17	357.4502	54.1162
18	401.1199	84.9502
19	421.6027	16.5242
20	437.1023	79.2142
21	455.6125	44.7758
22	486.4303	61.4483
23	505.6536	21.4366
24	532.5237	22.3246
25	566.5112	10.3969
26	660.8481	33.7339
27	704.4831	21.4409
28	713.74	199.2079
29	816.8666	8.1781
30	828.4871	104.5906
31	836.6007	28.7707
32	935.0287	72.7406
33	987.1796	60.6229
34	1177.4109	1.3092
35	1302.525	347.9187
36	1367.9873	2.2874
37	1411.2799	593.9154
38	1454.4927	41.6854
39	1549.2525	155.6173
40	1595.8068	56.8616
41	1619.8566	46.1625
42	1630.8968	244.0199
43	1642.7689	104.0816
44	1683.4009	7.3059
45	1702.7107	120.9863
46	1733.4435	901.8353
47	2024.5712	2095.8811

48	2836.1488	821.0629
49	2944.0584	405.7779
50	3246.69	561.6355
51	3296.9117	905.9049
52	3357.9912	410.7923
53	3402.9063	520.8626
54	3499.8439	65.7305
55	3716.6357	104.5704
56	3782.8428	72.4683
57	3784.8911	74.9544
Isomer 1.3 -m		
1	25.3063	2.9584
2	41.4577	3.4384
3	44.3852	6.3991
4	65.5336	2.0637
5	77.1598	8.0576
6	99.7342	2.2072
7	127.9476	11.4885
8	175.8591	1.4517
9	201.4423	1.8259
10	235.4423	79.2612
11	251.0141	19.2437
12	281.3185	30.9886
13	289.4852	25.1047
14	300.008	38.9397
15	313.716	172.3024
16	341.0087	60.4055
17	372.855	244.1695
18	411.9002	76.3
19	420.8552	30.9253
20	442.6	125.7473
21	459.1942	113.8243
22	462.9491	22.8009
23	514.1907	21.5565
24	549.5363	50.9491
25	583.8351	3.2089
26	613.9296	19.7032
27	725.4541	120.9108
28	745.5104	46.3874
29	816.2054	10.0755
30	841.1608	177.4393
31	871.6846	148.5684
32	945.4059	134.7182
33	1083.0125	69.0179

34	1245.6558	418.8754
35	1292.0465	140.8914
36	1343.5644	131.1468
37	1408.3965	395.3701
38	1473.7445	79.3033
39	1533.5657	1229.0684
40	1563.25	887.6626
41	1607.287	30.6929
42	1615.2763	10.8037
43	1634.8175	17.3089
44	1671.6719	3.1607
45	1692.4829	538.2074
46	1701.736	113.0367
47	1818.0392	1251.6158
48	2660.2963	1384.9281
49	2904.9714	826.1819
50	3083.6414	1615.7161
51	3147.0346	903.3784
52	3283.8203	1020.7867
53	3441.2416	34.9083
54	3516.7747	35.2288
55	3769.2953	57.0763
56	3779.8429	49.2285
57	3783.5664	64.021
Isomer 1.3 -n		
1	22.4821	0.7396
2	42.2841	1.3829
3	58.7477	2.3777
4	65.2676	3.1404
5	72.879	1.1201
6	91.0149	9.6504
7	112.2316	2.0861
8	128.4937	13.6168
9	193.7035	19.0287
10	236.1441	59.5406
11	259.5277	85.7556
12	273.9008	32.8505
13	291.655	43.0382
14	308.1167	95.4477
15	332.3372	9.7086
16	338.0138	124.1214
17	366.0243	7.1631
18	437.2333	15.9378
19	462.0024	36.661

20	465.9365	33.4844
21	478.396	43.0628
22	512.0276	47.8816
23	530.5047	53.1612
24	551.6678	65.6823
25	582.4694	71.2587
26	641.7912	36.8565
27	693.8913	36.0799
28	814.1127	0.4395
29	831.4691	9.6611
30	852.8268	63.5589
31	899.3261	224.7645
32	979.9286	53.2548
33	986.8528	35.5966
34	1155.8113	22.7106
35	1312.8674	598.7334
36	1390.2724	230.3561
37	1408.5813	49.3562
38	1424.1805	46.6663
39	1545.7984	231.8745
40	1598.123	78.6197
41	1611.767	93.8239
42	1651.401	12.4259
43	1672.4279	477.1899
44	1687.6416	44.8729
45	1726.2962	23.2658
46	1777.9449	315.3913
47	2468.9972	1130.2136
48	2798.354	1800.702
49	2911.7725	1945.6918
50	2954.3172	617.4565
51	3183.3846	245.8969
52	3238.6231	857.9673
53	3274.0235	243.3782
54	3497.3999	73.6218
55	3735.2904	72.8339
56	3782.6497	44.3695
57	3783.4651	70.9219
Isomer 1.3 -o		
1	29.2027	4.091
2	41.6336	2.1107
3	47.5409	1.633
4	60.5431	8.2959
5	63.5715	4.2518

6	82.8919	4.4659
7	115.2155	0.9743
8	161.5407	15.2538
9	194.9913	20.04
10	225.4471	113.7521
11	244.2512	82.9133
12	255.1679	25.6191
13	293.5757	43.4677
14	310.4301	74.1593
15	321.0088	33.5353
16	337.7432	40.6844
17	417.6111	36.3587
18	439.3633	31.7726
19	461.7793	25.446
20	465.5364	38.9606
21	471.4549	95.9788
22	555.0401	62.589
23	569.6261	84.0019
24	658.9954	44.6872
25	693.5551	69.9392
26	704.0352	11.2801
27	807.639	72.6608
28	815.6393	2.3551
29	831.4623	22.4732
30	901.983	30.1389
31	906.5813	84.5909
32	944.4313	52.257
33	983.9038	76.7868
34	1171.8067	11.7758
35	1277.6534	346.4235
36	1328.2185	504.6338
37	1400.3682	369.7149
38	1505.0135	217.8049
39	1549.8495	273.7329
40	1578.0539	1290.0222
41	1611.8789	484.7807
42	1620.7138	280.8045
43	1657.6534	21.2943
44	1673.0314	139.0859
45	1702.5816	129.8909
46	1756.8188	341.6025
47	1777.6104	481.3919
48	2698.1843	1147.7963
49	2951.4806	1765.7472

50	3060.4692	1079.5087
51	3169.2477	221.4245
52	3180.1126	1032.454
53	3358.774	1125.3943
54	3445.613	37.3417
55	3521.1084	39.7736
56	3778.9881	71.1707
57	3788.1209	54.6928
Isomer 1.3 -p		
1	23.9872	2.2384
2	27.892	10.6375
3	41.3727	2.6359
4	47.8836	0.8668
5	75.4802	3.5591
6	98.8574	4.4478
7	115.8944	3.2987
8	133.4211	14.2314
9	199.3586	4.0436
10	244.1589	62.1664
11	258.503	86.5824
12	262.4153	131.9458
13	312.4397	78.8961
14	333.1751	24.5601
15	353.0191	27.6018
16	359.6644	64.9878
17	416.099	42.9107
18	460.5452	18.1261
19	473.5811	92.0216
20	477.5172	46.3441
21	491.3406	18.2209
22	519.4537	38.8258
23	568.7507	11.0363
24	609.1564	50.7389
25	635.5395	36.9741
26	702.4509	42.1975
27	775.4035	15.8009
28	813.0064	25.4642
29	821.4652	39.533
30	851.6082	35.1962
31	888.7003	64.8164
32	1010.3944	103.9555
33	1037.9514	124.9328
34	1163.9405	14.1243
35	1317.3056	554.6896

36	1332.4807	60.7555
37	1393.1786	380.6296
38	1486.1159	119.1821
39	1576.1674	130.2698
40	1610.5636	348.693
41	1636.8656	1327.6928
42	1657.7234	299.0769
43	1665.7963	218.6011
44	1680.9825	859.8584
45	1715.825	117.7346
46	1730.7636	83.248
47	1764.5737	275.3702
48	2653.4138	1192.603
49	2854.3191	1475.962
50	2899.2465	1718.7088
51	3071.2316	1082.1893
52	3195.8892	265.4639
53	3437.8492	39.4758
54	3501.5151	324.3949
55	3510.2877	44.2967
56	3774.2037	44.2498
57	3779.2026	48.6353
Isomer 1.3 -q		
1	28.9859	0.4662
2	38.5969	2.9088
3	60.281	3.9037
4	64.651	2.1538
5	79.6375	3.9056
6	90.7517	2.7301
7	124.8863	4.0523
8	132.4929	4.6263
9	169.0945	0.7744
10	207.8216	8.8349
11	246.2302	62.2644
12	275.2492	27.9407
13	303.0533	54.762
14	316.1464	18.2718
15	346.249	186.9651
16	358.1702	106.6794
17	372.8943	32.0548
18	395.8638	38.1317
19	420.8777	35.4514
20	452.4679	96.732
21	459.3762	57.2486

22	480.3574	25.7731
23	562.2726	10.7351
24	666.7171	60.2181
25	699.55	65.7616
26	727.6457	83.3912
27	821.1056	3.8026
28	837.7361	37.133
29	857.5144	32.9133
30	880.5277	70.2353
31	985.2094	17.5181
32	1022.9679	43.6482
33	1106.3776	63.2558
34	1172.8749	7.4986
35	1184.9892	83.2619
36	1311.6162	889.5044
37	1369.0383	374.5213
38	1395.1584	92.3656
39	1587.1997	264.7188
40	1597.2164	37.8222
41	1606.3694	124.8037
42	1626.9362	9.2351
43	1641.0647	210.8359
44	1667.0468	48.0734
45	1709.6438	29.4501
46	1760.1855	449.4817
47	1946.6053	1366.2876
48	2447.9648	3282.403
49	2658.6886	1317.8707
50	2841.0937	827.7352
51	3220.4213	379.4815
52	3296.4509	227.2659
53	3326.6024	996.8511
54	3454.1096	49.4281
55	3513.8674	11.072
56	3775.1699	39.2542
57	3775.901	91.02
Isomer 1.3 -r		
1	10.8846	5.4078
2	21.4603	3.723
3	32.8594	2.8041
4	45.6034	1.5611
5	49.7082	39.9
6	89.5453	0.46
7	96.7168	9.1877

8	99.3269	3.7159
9	133.9355	12.1139
10	146.5839	0.1979
11	150.8219	16.1369
12	190.3422	127.9046
13	219.6687	1.7644
14	244.1751	101.2595
15	263.8322	49.6414
16	266.1582	42.0237
17	274.5986	141.4247
18	294.3162	4.6069
19	314.8356	19.3444
20	345.8672	16.7146
21	403.5208	143.7208
22	440.2169	14.6403
23	452.085	41.3368
24	535.7078	32.2208
25	544.3874	50.5336
26	628.4333	52.2917
27	659.014	307.7974
28	724.4263	21.5913
29	788.3562	46.6748
30	807.5832	8.6497
31	834.6587	2.423
32	956.0382	14.4837
33	1055.8111	85.9469
34	1088.9586	134.85
35	1112.0672	78.1992
36	1231.0979	167.6933
37	1256.6378	502.8867
38	1327.8138	609.4801
39	1397.693	181.4446
40	1587.0917	66.6567
41	1595.5391	24.6468
42	1604.2481	95.4551
43	1632.4888	13.6154
44	1649.1028	49.3316
45	1710.3292	42.0057
46	1739.5646	552.0976
47	2625.5372	1903.4764
48	2698.2956	2441.6173
49	2959.2079	1048.8306
50	3377.4628	103.695
51	3459.1848	331.009

52	3496.1832	95.7963
53	3525.7135	814.6446
54	3531.2247	9.954
55	3712.0615	6.9456
56	3778.0375	45.234
57	3810.8435	77.2895
Isomer 1.3 -s		
1	30.7307	3.4361
2	40.6064	1.3914
3	48.1293	0.7864
4	63.9995	4.1141
5	87.2022	1.8398
6	104.2248	0.5184
7	133.4819	3.8193
8	149.2014	15.6132
9	166.5264	25.6764
10	184.5414	47.0754
11	190.1357	11.0576
12	220.1317	63.9965
13	239.0398	40.4238
14	272.164	39.6528
15	298.8909	33.1572
16	331.8669	18.7879
17	351.5696	10.6476
18	367.5834	38.9046
19	371.564	108.0581
20	377.8689	44.7009
21	416.9711	72.5023
22	438.0877	10.5248
23	442.8408	139.9064
24	528.7132	82.0267
25	575.3411	91.2834
26	635.1897	27.4728
27	684.1607	114.1627
28	697.8356	110.8334
29	756.4175	156.6149
30	809.2734	0.8032
31	830.2255	49.648
32	1030.2503	65.1555
33	1045.3337	84.5687
34	1156.9183	109.2564
35	1198.5597	158.0919
36	1311.6655	49.1839
37	1321.4286	22.4131

38	1395.0242	771.3995
39	1437.1577	202.2252
40	1593.6556	100.9273
41	1610.3275	24.3295
42	1613.9124	27.4909
43	1642.8377	28.6165
44	1674.2679	127.2574
45	1691.2092	235.8246
46	1739.7832	284.1162
47	2098.5625	2511.4629
48	2731.4171	1535.5963
49	2785.0483	1356.9245
50	3284.1563	223.2191
51	3323.4335	712.8969
52	3458.6378	48.5733
53	3516.0032	10.3519
54	3579.3489	327.456
55	3684.271	84.1163
56	3769.6692	71.0055
57	3784.8186	91.5003

$(H_2C_2O_4)(NH_3)_2(H_2O)$
Isomer 2.1 -a

#	**Frequency**	**Infrared**
1	25.6227	1.0258
2	36.8249	1.3845
3	50.7703	2.6116
4	93.3009	7.9661
5	113.5454	4.6172
6	141.6023	7.1021
7	159.6635	4.886
8	210.7611	4.1045
9	241.0138	114.2679
10	245.179	31.412
11	266.2272	45.6682
12	304.3327	40.3783
13	323.3526	13.5274
14	343.1894	180.3427
15	365.8361	2.7426
16	417.2377	9.0375
17	449.2227	20.0685
18	458.7485	22.0375
19	463.5307	62.007
20	557.1044	26.3171

21	599.1403	80.8721
22	655.9605	37.7566
23	700.1552	30.6515
24	817.0787	0.2321
25	834.8088	21.0815
26	898.5189	64.9543
27	1021.6171	90.5907
28	1159.0485	66.4363
29	1163.1706	15.8175
30	1262.3677	240.1407
31	1321.1881	371.5923
32	1394.041	382.0459
33	1497.345	101.2719
34	1529.8638	364.1247
35	1602.0342	18.9322
36	1626.1491	409.4526
37	1641.0689	104.997
38	1655.3251	12.3623
39	1671.9861	25.0887
40	1698.9212	92.497
41	1759.9228	311.0123
42	2090.071	1514.0948
43	2765.604	1582.6277
44	2934.7758	978.5244
45	3178.0562	261.8008
46	3276.1278	330.0412
47	3379.6428	155.1846
48	3457.7902	53.1547
49	3506.3038	60.4311
50	3516.9484	10.2682
51	3783.5977	42.4247

Isomer 2.1 -b

#	**Frequency**	**Infrared**
1	26.0351	0.8732
2	37.0509	0.6877
3	49.8335	2.7366
4	83.1566	7.7651
5	114.2843	1.467
6	138.5153	6.9375
7	178.3153	0.1266
8	197.3201	19.0836
9	204.1692	92.2343
10	211.7706	7.4433
11	263.9538	51.006

12	280.3213	113.6428
13	313.0918	14.1091
14	337.7189	131.4729
15	380.1435	4.2205
16	429.6702	3.0383
17	450.6321	55.6768
18	467.2598	73.5746
19	502.3754	28.9887
20	540.9809	95.3681
21	565.6099	14.2013
22	655.308	11.827
23	697.9593	42.0223
24	727.7878	67.5003
25	816.954	0.578
26	837.0483	17.6856
27	889.8147	66.1731
28	1162.8764	13.8142
29	1170.8717	122.1879
30	1279.2152	280.2728
31	1326.0814	307.8653
32	1393.4778	331.3702
33	1482.7593	48.1663
34	1549.6121	363.3597
35	1606.1896	7.5518
36	1613.0452	9.0821
37	1641.6801	10.6463
38	1652.6957	351.5647
39	1681.8767	10.2037
40	1700.3062	192.1949
41	1761.84	330.7075
42	2251.7054	1793.6221
43	2633.9167	1277.3876
44	3200.3555	223.8955
45	3222.4902	446.8726
46	3325.5058	880.3491
47	3379.5721	139.2317
48	3454.2688	35.8995
49	3504.039	60.1666
50	3516.7281	9.0125
51	3789.996	57.0444

Isomer 2.1 -c

#	**Frequency**	**Infrared**
1	37.279	0.8478
2	44.0555	4.0413

3	65.774	2.0662
4	90.8484	6.8787
5	109.4723	3.1759
6	123.6415	2.8837
7	140.412	4.5361
8	164.014	5.8918
9	223.307	112.7754
10	231.9914	13.1443
11	261.1061	41.2171
12	311.0688	59.311
13	333.3883	27.3739
14	358.3247	24.7392
15	369.8873	106.4132
16	430.9629	30.3022
17	444.5095	79.4595
18	462.0044	3.8325
19	469.9186	12.4824
20	569.9914	7.6707
21	578.7239	83.232
22	665.235	22.5114
23	697.3537	35.5373
24	822.9599	2.0994
25	832.0751	22.5913
26	879.6557	67.3364
27	1020.5272	73.4857
28	1159.966	10.1256
29	1173.5391	93.5993
30	1250.3644	143.1689
31	1325.6473	310.07
32	1384.6612	418.2147
33	1460.0376	64.9688
34	1524.1643	742.7749
35	1607.6929	42.4837
36	1611.4374	10.355
37	1625.6343	100.7439
38	1653.0049	16.1726
39	1672.1139	39.9649
40	1688.8431	27.4191
41	1759.4078	314.8402
42	2138.904	1284.3792
43	2738.6524	1807.8472
44	2907.023	791.6568
45	3217.9713	265.9192
46	3318.8469	168.5558

47	3379.1755	122.0194
48	3458.1268	47.7369
49	3513.5442	8.1366
50	3514.3145	64.0265
51	3781.5687	40.1462

Isomer 2.1 -d

#	**Frequency**	**Infrared**
1	26.4668	0.8147
2	39.3882	0.9243
3	49.9367	3.8612
4	76.7621	2.7821
5	109.4038	4.067
6	142.1638	21.8729
7	149.4333	83.0543
8	159.8238	44.0731
9	171.7296	4.17
10	172.7392	10.3492
11	269.1131	45.6682
12	281.6969	57.6372
13	300.0033	42.0337
14	317.3197	105.9651
15	388.4268	69.2891
16	415.4524	43.5033
17	434.4398	46.2834
18	461.4828	27.2743
19	466.8893	110.9189
20	516.7448	23.7597
21	562.9456	21.3947
22	637.1811	13.2138
23	682.7444	57.4377
24	703.8575	55.7077
25	818.1882	0.2745
26	839.4705	21.9465
27	901.6014	64.7151
28	1112.9587	127.7817
29	1163.5737	10.7837
30	1306.3685	388.3736
31	1350.9725	111.8972
32	1395.0551	340.1129
33	1472.6967	107.8874
34	1546.872	160.8244
35	1600.9032	46.4927
36	1605.5533	17.3837
37	1634.074	9.7835

38	1654.5578	364.6699
39	1687.9575	16.3531
40	1710.9142	62.8565
41	1763.7031	583.4997
42	2364.5967	1759.2624
43	2726.0173	1180.7785
44	3171.1536	267.1962
45	3292.6199	171.7742
46	3350.8484	115.7799
47	3400.1472	785.1071
48	3478.0201	76.0814
49	3495.6137	53.3551
50	3521.9534	10.674
51	3798.8609	70.2564

Isomer 2.1 -e

#	**Frequency**	**Infrared**
1	20.4542	5.0997
2	31.0252	3.688
3	69.6765	6.1115
4	78.2923	1.9089
5	104.173	5.1172
6	134.1051	0.5781
7	159.1973	36.3233
8	170.7929	15.0481
9	186.5762	14.5358
10	197.6482	18.4759
11	228.7592	65.8153
12	263.0227	93.3574
13	279.6528	14.1378
14	313.0654	90.4034
15	352.8549	9.2387
16	376.8976	53.9537
17	388.8484	2.4063
18	417.0394	7.1758
19	431.8359	90.4047
20	478.1497	75.6001
21	525.8132	105.1689
22	615.2378	17.5463
23	665.7959	80.3884
24	698.4021	133.6909
25	812.6884	0.2284
26	828.927	7.5737
27	1079.3285	184.9471
28	1183.5922	16.6295

29	1210.693	49.2142
30	1246.9899	175.2265
31	1262.0607	272.66
32	1316.6074	55.8878
33	1344.3314	1766.1547
34	1393.6275	56.7719
35	1597.6173	60.535
36	1599.8454	31.7438
37	1612.9988	36.0792
38	1627.7455	14.584
39	1644.6303	8.6919
40	1692.3741	37.2458
41	1718.696	602.2287
42	2022.9163	2397.4401
43	2322.5695	2537.0741
44	3273.7551	228.0269
45	3374.0767	61.1826
46	3453.2766	69.5346
47	3473.5144	563.1072
48	3498.2009	60.7471
49	3517.3552	13.4245
50	3534.6122	15.1985
51	3789.6506	68.1381

Isomer 2.1 -f

#	**Frequency**	**Infrared**
1	32.9785	3.578
2	39.1742	1.2686
3	50.256	3.1004
4	84.2921	5.3718
5	95.5627	10.3727
6	127.4162	1.3201
7	140.6515	0.2879
8	185.4585	5.2102
9	220.3549	34.7503
10	242.3511	13.9324
11	255.2886	76.3657
12	266.0247	35.7798
13	309.9964	94.6295
14	327.0705	136.4691
15	354.3953	117.1896
16	413.103	44.4131
17	433.9447	48.6637
18	462.1635	51.2336
19	489.7295	39.36

20	548.3102	22.0274
21	576.4135	2.2965
22	660.6683	31.9882
23	688.7813	86.9137
24	702.0399	4.6299
25	818.8035	1.045
26	832.5282	34.3009
27	986.8928	58.9711
28	1102.0265	125.9728
29	1169.22	0.9038
30	1307.9453	271.0775
31	1364.0177	0.7493
32	1409.6729	604.6108
33	1452.0642	26.342
34	1566.332	159.3212
35	1604.8423	8.1333
36	1615.7825	14.494
37	1631.9779	20.4225
38	1639.7693	263.3588
39	1693.4155	16.1345
40	1709.924	71.477
41	1736.8979	785.2794
42	2136.653	2104.484
43	2863.6265	925.8543
44	2935.016	377.5853
45	3158.329	392.4849
46	3374.1767	36.8747
47	3446.1237	621.3106
48	3487.9989	57.4046
49	3496.649	45.3181
50	3521.1227	10.8021
51	3787.4951	76.6714

Isomer 2.1 -g

#	**Frequency**	**Infrared**
1	30.6677	0.1728
2	34.5789	1.0489
3	48.3155	4.1952
4	84.3994	4.7814
5	119.0957	4.1964
6	124.2597	8.9309
7	155.762	8.084
8	195.6899	1.8845
9	231.8505	94.1397
10	242.7687	13.6871

11	279.0276	74.0985
12	291.949	34.1162
13	316.308	11.6342
14	337.5684	39.5253
15	353.2141	233.1419
16	431.2959	13.9509
17	440.37	113.1381
18	461.272	40.9632
19	522.499	9.1482
20	573.933	13.8209
21	595.077	10.1396
22	641.3298	44.3157
23	704.344	34.8032
24	817.4661	0.3805
25	839.0325	29.6431
26	943.3554	61.3425
27	1001.85	92.9601
28	1132.4496	80.087
29	1163.2104	1.2007
30	1230.2988	897.4666
31	1330.7129	132.532
32	1399.2497	547.2977
33	1461.4312	113.0841
34	1520.4167	1245.388
35	1585.6856	284.7061
36	1605.8747	26.7806
37	1635.4334	24.4592
38	1648.7414	17.3484
39	1664.8882	5.4161
40	1707.6517	38.2689
41	1749.6093	469.646
42	1794.7595	980.3693
43	2813.914	1503.7602
44	2937.1621	940.2588
45	3052.0496	331.8461
46	3325.8036	203.4117
47	3438.0105	31.2913
48	3468.5102	69.488
49	3517.4183	36.5859
50	3520.2537	10.5273
51	3777.1116	42.3198

Isomer 2.1 -h

#	**Frequency**	**Infrared**
1	36.0978	1.6225

2	37.8158	1.5052
3	43.3856	3.9912
4	76.3718	4.9702
5	121.1639	4.5892
6	132.8144	4.8043
7	173.7359	9.2509
8	183.4415	9.5796
9	218.6006	21.189
10	233.0055	57.9346
11	257.5824	29.7208
12	275.8098	121.2163
13	320.1248	34.3848
14	335.7219	128.8353
15	371.7945	102.4087
16	412.3388	69.3984
17	432.0873	39.8116
18	463.3439	43.2177
19	504.5774	16.6544
20	570.2255	30.8816
21	598.8454	46.6427
22	661.1352	8.7139
23	687.5269	87.4151
24	708.3695	11.9605
25	817.6982	0.5665
26	839.1075	33.8479
27	952.3992	60.0164
28	1164.819	103.776
29	1170.5173	2.0382
30	1278.9087	618.5185
31	1350.6587	15.1964
32	1402.517	523.8338
33	1452.8751	41.4647
34	1553.3642	457.2828
35	1595.2459	702.0686
36	1607.603	10.4432
37	1618.5516	121.2313
38	1641.9957	11.7043
39	1675.3942	16.908
40	1706.2888	27.3676
41	1747.32	648.2383
42	1869.2334	1604.1645
43	2633.0463	1333.0826
44	3024.0785	336.1066
45	3245.8252	307.4844

46	3430.3416	649.4166
47	3435.2159	60.0901
48	3454.6883	83.9258
49	3515.2553	8.4378
50	3516.4087	34.0621
51	3790.4844	70.0136

Isomer 2.1 -i

#	**Frequency**	**Infrared**
1	18.3476	6.2752
2	30.1094	2.1586
3	73.9417	4.0784
4	78.6559	1.6305
5	108.7534	10.2208
6	132.7858	6.5013
7	160.9042	0.083
8	176.1998	3.379
9	231.3246	145.8914
10	245.3059	19.3999
11	269.7521	121.5829
12	304.4313	30.3553
13	337.8037	38.0384
14	383.7973	399.5944
15	395.328	18.7779
16	421.1816	234.5051
17	436.4578	45.5738
18	456.0821	50.166
19	458.323	27.5919
20	527.0881	69.1953
21	548.9829	2.0466
22	650.6357	89.6006
23	734.2325	79.0213
24	813.1996	10.6974
25	828.5888	269.3388
26	859.9802	146.6911
27	1034.4114	140.2046
28	1085.9816	1979.7004
29	1099.3791	326.7969
30	1246.948	62.8798
31	1324.4869	350.8475
32	1375.9637	136.9107
33	1426.1245	1547.7379
34	1472.203	75.879
35	1545.8975	89.1789
36	1599.7882	59.861

37	1605.717	3.2396
38	1633.8925	23.4457
39	1660.6057	7.6282
40	1681.4515	26.1795
41	1700.6547	33.5873
42	1716.5727	662.0683
43	2842.0391	926.5206
44	2855.9674	1109.5815
45	3165.4942	1488.6356
46	3355.2804	89.3609
47	3441.7261	29.6757
48	3479.8105	57.154
49	3519.6807	26.7564
50	3521.9981	9.5291
51	3772.4584	55.4691

$(H_2C_2O_4)(NH_3)_2(H_2O)_2$

Isomer 2.2 -a

#	Frequency	Infrared
1	23.1854	0.313
2	35.9236	1.8768
3	44.4608	0.1497
4	67.1645	1.8242
5	70.2903	6.3015
6	85.4377	2.4327
7	114.6665	2.4871
8	143.1107	13.1148
9	165.0003	0.2759
10	184.1971	11.9213
11	225.3825	46.9115
12	256.2665	56.0284
13	270.0192	72.6469
14	270.742	86.1138
15	292.5577	71.6633
16	307.0835	7.7361
17	315.1398	32.593
18	320.005	85.5602
19	409.9657	98.5826
20	426.7323	29.3247
21	460.7049	21.8958
22	467.8264	11.4548
23	508.749	46.3303
24	525.2446	9.6064
25	544.3456	75.5003
26	567.3179	26.1841

27	685.5441	39.6063
28	705.1469	26.3728
29	816.7454	0.5456
30	827.1036	34.3971
31	849.8832	83.2585
32	889.183	68.7706
33	981.8175	83.5545
34	1107.2551	127.3313
35	1163.4364	13.2075
36	1316.9221	446.7963
37	1394.0239	342.0825
38	1404.6603	17.6222
39	1477.882	74.0237
40	1553.0102	53.194
41	1606.9042	9.1778
42	1613.5157	18.8882
43	1634.6671	9.9999
44	1642.3092	138.3439
45	1669.318	265.7077
46	1704.4125	11.4092
47	1728.2431	57.9747
48	1766.9149	496.3703
49	2587.8982	1442.0605
50	2774.1501	1177.2761
51	2949.0174	592.7051
52	3064.256	1960.1401
53	3161.2447	1005.5895
54	3195.1706	251.3166
55	3354.5434	120.5294
56	3479.5522	71.6833
57	3485.6532	41.647
58	3521.9751	9.934
59	3780.6479	51.7199
60	3784.4561	47.6611

Isomer 2.2 -b

#	**Frequency**	**Infrared**
1	26.4683	3.6441
2	36.2347	2.5262
3	48.4146	1.3134
4	64.191	4.3248
5	82.7333	2.7379
6	109.5129	3.2926
7	119.2744	9.6853
8	128.1402	4.456

9	130.6869	2.0623
10	194.9805	6.0817
11	231.3218	40.8795
12	254.9182	78.7914
13	273.6338	54.6116
14	288.6698	17.8953
15	305.0159	116.5916
16	312.0907	28.1916
17	332.5085	19.4484
18	380.4626	85.2416
19	402.8082	71.9237
20	425.2017	24.6576
21	459.0366	18.5009
22	466.9882	10.7661
23	505.6697	113.544
24	549.2715	32.8113
25	561.4644	22.6338
26	571.397	32.6922
27	696.8911	27.2952
28	703.3134	9.1823
29	819.263	38.4894
30	821.4878	24.9934
31	840.5051	67.9652
32	918.5204	63.7137
33	1003.2592	87.9827
34	1122.4853	120.6565
35	1179.7221	1.5745
36	1323.1341	286.1529
37	1398.3567	452.4634
38	1422.0051	46.0316
39	1455.0423	60.7578
40	1539.383	97.7721
41	1590.4929	17.4586
42	1606.0468	30.3433
43	1624.6088	36.5263
44	1636.0026	35.4208
45	1673.0311	124.8539
46	1709.4404	17.2181
47	1724.5517	37.2037
48	1739.4482	689.0556
49	2658.5393	1289.4677
50	2862.9445	580.7649
51	2914.0551	570.2697
52	2978.7261	2228.3362

53	3126.5728	245.4484
54	3162.9645	920.7928
55	3378.0565	32.7222
56	3475.0616	48.6109
57	3483.2046	35.9242
58	3522.9113	20.7888
59	3779.3168	49.1645
60	3784.9171	53.2428

Isomer 2.2 -c

#	**Frequency**	**Infrared**
1	24.2607	0.1507
2	35.5126	1.2776
3	40.7428	1.6119
4	49.1669	1.8048
5	66.0684	2.9638
6	86.0859	4.7768
7	118.6097	3.2602
8	148.1057	18.0412
9	194.7452	4.3734
10	212.5445	29.393
11	221.6837	5.0811
12	237.6612	112.398
13	261.6769	49.7856
14	274.1135	90.2908
15	283.7691	48.9443
16	307.2037	116.545
17	320.3538	24.522
18	333.2275	15.6191
19	398.0093	43.5861
20	417.722	29.8173
21	453.7886	15.7246
22	464.917	55.5777
23	474.9359	33.6946
24	487.8362	14.5248
25	559.935	42.0983
26	625.9956	100.079
27	661.2919	161.4431
28	702.1486	0.4015
29	747.1911	29.822
30	816.7078	0.2214
31	838.7076	24.4339
32	924.7363	63.6551
33	1040.2402	80.6515
34	1167.1479	52.7557

35	1170.5342	12.402
36	1319.2725	372.696
37	1394.9548	106.1004
38	1399.5393	381.5475
39	1496.8791	81.635
40	1533.2174	51.0718
41	1601.0676	18.8756
42	1604.2466	31.5214
43	1639.3679	27.3224
44	1655.4693	113.3076
45	1659.0913	227.649
46	1708.3094	23.1222
47	1721.6744	43.7532
48	1760.7415	560.5118
49	2475.3417	1211.0257
50	2715.843	2044.2321
51	2910.1641	979.7915
52	3059.5019	638.3448
53	3112.4287	383.4414
54	3239.3105	481.5733
55	3426.887	789.2148
56	3455.6619	51.5578
57	3486.5119	47.1815
58	3517.9819	9.18
59	3783.4392	38.211
60	3790.5154	80.3043

Isomer 2.2 -d

#	**Frequency**	**Infrared**
1	28.1239	1.3764
2	36.1792	2.9718
3	47.1173	4.9521
4	58.3455	2.4756
5	70.8495	2.4368
6	94.1403	3.0811
7	116.4808	2.1071
8	159.2455	15.2578
9	179.8916	0.237
10	186.4832	3.2882
11	202.669	64.651
12	235.1641	25.5717
13	265.5266	58.3537
14	281.4294	14.1105
15	294.9079	176.8887
16	302.9338	96.0453

17	323.5647	12.2652
18	334.7625	40.2453
19	414.6786	46.8442
20	434.2046	48.0921
21	454.723	81.8231
22	463.9911	12.2976
23	472.742	31.7138
24	531.3193	18.121
25	565.6205	20.5532
26	576.6079	32.488
27	685.6313	53.1714
28	694.3287	16.9746
29	793.7864	37.1278
30	825.3729	1.3075
31	859.7926	63.4491
32	866.7157	51.2503
33	1010.6664	86.2999
34	1130.9988	119.3372
35	1155.0471	17.5714
36	1326.5109	282.6766
37	1374.0231	385.7151
38	1392.3309	57.9661
39	1464.8107	65.1384
40	1553.3141	165.75
41	1605.6725	28.3105
42	1608.2634	27.2093
43	1634.4773	43.6301
44	1643.1965	215.4539
45	1649.4403	53.2075
46	1704.5668	16.1858
47	1716.5219	4.3086
48	1765.2569	425.8383
49	2604.3369	1289.0398
50	2740.6927	1177.2456
51	2921.3871	951.4255
52	3035.8276	1352.2347
53	3170.0986	1112.4991
54	3267.8973	158.8736
55	3327.746	205.8687
56	3468.4423	68.5622
57	3489.6372	46.4739
58	3519.2574	9.3626
59	3773.627	53.8284
60	3788.5509	44.8412

Isomer 2.2 -e

#	Frequency	Infrared
1	36.3807	1.7156
2	38.6022	0.2309
3	54.4831	8.0368
4	76.0937	1.16
5	88.8367	2.2833
6	107.9213	8.9369
7	133.036	8.7684
8	138.5716	7.9438
9	166.45	9.6865
10	186.0478	1.6086
11	210.8129	23.4952
12	260.7865	43.3012
13	280.0314	6.1032
14	287.9558	112.7306
15	297.0859	66.6376
16	339.145	97.122
17	349.5273	34.7916
18	356.6908	6.4321
19	408.4514	35.8063
20	427.5726	60.1832
21	445.3433	5.9974
22	465.3926	16.6913
23	524.9444	127.5
24	567.0797	8.6511
25	620.7004	10.7976
26	648.4831	56.3257
27	696.2626	27.9537
28	729.6311	46.8173
29	820.2756	0.1
30	835.2659	21.3913
31	860.4193	67.6762
32	919.676	85.0927
33	1088.6869	55.9571
34	1109.8031	123.1233
35	1162.0278	11.6973
36	1292.0048	227.4703
37	1330.6663	273.7123
38	1385.7266	298.6919
39	1475.1974	71.2905
40	1552.242	312.0441
41	1603.4658	39.0992
42	1617.5071	130.6206

43	1632.0686	78.1597
44	1639.8372	189.1211
45	1677.7128	23.1976
46	1688.0766	6.8573
47	1715.3589	130.9947
48	1766.0477	306.4185
49	2325.4288	1325.6022
50	2707.6309	1701.2338
51	2841.9305	1593.9444
52	3100.3892	698.4819
53	3258.6464	264.4604
54	3326.1999	149.5315
55	3398.9873	96.1807
56	3470.2654	22.9332
57	3478.2162	514.2544
58	3508.7876	65.1792
59	3525.3636	7.9382
60	3785.3446	44.3889

Isomer 2.2 -f

#	**Frequency**	**Infrared**
1	29.7002	0.7235
2	36.5272	0.8396
3	38.8615	2.9045
4	48.2847	2.0219
5	73.8316	3.8576
6	82.7451	5.1478
7	89.9571	104.2972
8	111.7328	14.7394
9	124.0655	2.1419
10	138.6285	1.0956
11	150.9867	13.5205
12	176.3682	7.7761
13	211.4395	49.9783
14	218.3106	29.7025
15	259.9895	103.56
16	264.6803	2.4718
17	299.7502	79.7994
18	310.645	125.1955
19	347.2721	75.4306
20	410.2611	40.1974
21	429.4754	26.8074
22	446.8056	161.1204
23	464.6988	60.5288
24	475.7756	24.7996

25	537.7206	25.8771
26	569.7409	5.8705
27	602.9443	26.6489
28	629.9773	68.2546
29	654.5192	88.351
30	697.5507	15.9424
31	817.9196	0.6557
32	833.3461	23.6983
33	952.5691	61.7244
34	1100.5352	127.7084
35	1172.9948	1.8438
36	1319.8023	253.4415
37	1357.6059	93.2726
38	1402.8627	501.5568
39	1466.2865	23.9135
40	1548.8751	167.2536
41	1605.4767	13.5498
42	1609.7011	27.3766
43	1614.7025	30.4298
44	1629.5473	8.4499
45	1667.3718	208.3758
46	1688.2123	28.2287
47	1720.3284	51.8693
48	1742.786	766.084
49	2560.5502	1536.7927
50	2899.7025	865.677
51	3042.7369	332.215
52	3255.4092	215.213
53	3378.5074	24.466
54	3418.8621	106.6272
55	3465.5767	508.1269
56	3474.8342	727.2371
57	3491.3899	90.2595
58	3521.9195	10.6584
59	3792.0839	78.2321
60	3801.4558	71.755

Isomer 2.2 -g

#	**Frequency**	**Infrared**
1	26.8189	1.5896
2	33.2531	1.9805
3	43.3854	0.0922
4	59.7382	0.8621
5	64.6627	2.4147
6	99.2744	5.7606

7	121.4773	3.0141
8	180.0851	0.5434
9	190.9325	10.8132
10	213.4141	7.9727
11	220.2686	16.0074
12	239.3196	76.1244
13	253.3972	39.7933
14	275.2771	66.4684
15	281.0128	30.3742
16	297.2253	52.7594
17	312.9966	121.5045
18	373.1236	24.9756
19	401.0634	15.3525
20	436.0792	87.1845
21	442.336	48.8738
22	448.996	23.7432
23	479.1472	127.8012
24	511.0248	16.7993
25	565.9276	18.391
26	612.3595	34.5713
27	697.8326	27.0071
28	705.3352	16.717
29	786.2473	150.3884
30	792.5268	14.665
31	821.4891	5.7995
32	836.3311	19.294
33	912.3829	65.219
34	1181.1772	1.318
35	1186.3245	99.6186
36	1319.4905	352.8992
37	1397.5475	411.462
38	1431.1939	24.8109
39	1444.8182	54.1199
40	1548.6745	121.8254
41	1602.5831	14.6564
42	1615.9491	14.3464
43	1621.5627	8.7061
44	1644.8431	24.0405
45	1667.8996	133.8591
46	1711.6449	7.6647
47	1723.7455	105.8153
48	1740.1587	642.6913
49	2539.2231	1604.482
50	2844.4987	1002.3751

51	2963.774	595.8119
52	3141.2244	267.0849
53	3186.2093	599.3575
54	3248.4395	771.6392
55	3308.5216	1124.7595
56	3447.7215	31.4345
57	3484.6965	38.9492
58	3512.1711	7.5882
59	3775.3018	67.7103
60	3785.8087	53.812

Isomer 2.2 -h

#	**Frequency**	**Infrared**
1	39.5007	1.9441
2	44.1569	0.1159
3	53.3547	2.0434
4	65.653	1.2536
5	74.678	5.9176
6	97.3847	5.8919
7	122.3477	0.6952
8	131.6688	5.434
9	177.6177	5.2129
10	212.4893	5.2024
11	220.5304	15.3183
12	236.5352	82.6827
13	251.8498	51.8418
14	282.9309	97.1758
15	293.825	98.9947
16	300.2185	43.5443
17	336.7576	46.2037
18	368.6344	21.6583
19	404.3163	21.7274
20	432.9697	50.1553
21	442.7204	58.2636
22	461.4305	9.5468
23	478.5971	84.6358
24	502.149	21.4139
25	579.8522	17.6977
26	632.0652	6.448
27	677.4253	42.2488
28	699.221	23.7811
29	816.1989	29.1221
30	828.8619	35.3926
31	844.8278	91.798
32	904.6194	70.4719

33	1038.7759	69.092
34	1174.5171	91.8074
35	1175.5228	4.9021
36	1325.6587	199.1818
37	1387.4907	458.3664
38	1410.4749	82.0755
39	1445.8978	37.2931
40	1553.0902	122.3432
41	1602.6344	60.9068
42	1613.3844	9.9256
43	1615.6573	13.8637
44	1658.4082	56.3238
45	1669.4808	68.2152
46	1704.2586	66.1966
47	1716.3185	25.9933
48	1734.2889	488.8767
49	2636.2749	1742.567
50	2814.519	1106.581
51	2841.5663	767.8461
52	2939.1413	741.2493
53	3149.111	312.7962
54	3232.4959	1270.7039
55	3294.7334	244.0202
56	3456.8811	39.4507
57	3489.324	41.4637
58	3517.2029	9.1377
59	3778.2693	36.3831
60	3784.0592	61.2967

Isomer 2.2 -i

#	**Frequency**	**Infrared**
1	21.691	1.8673
2	34.0873	2.7132
3	39.8003	1.3648
4	47.0151	2.9602
5	68.5976	3.3082
6	92.338	6.7211
7	116.4024	1.6345
8	138.2297	4.0818
9	173.9144	1.351
10	217.182	26.7093
11	224.2915	31.6014
12	246.3964	104.4771
13	259.9713	45.2743
14	263.8662	70.4979

15	271.5877	55.2685
16	321.6236	92.777
17	346.461	82.9986
18	364.3481	21.7703
19	372.4198	9.8931
20	430.1057	7.2075
21	448.1213	4.153
22	456.6229	39.9917
23	465.3923	43.8399
24	523.3098	36.7693
25	561.1186	21.953
26	592.1096	53.2773
27	685.2303	53.7159
28	701.5966	41.4472
29	770.4294	57.9467
30	816.6385	1.3217
31	839.2035	23.3267
32	891.7862	66.265
33	1065.6651	61.9903
34	1166.1516	10.6745
35	1204.9859	86.5642
36	1303.1513	398.626
37	1344.17	182.9902
38	1394.9628	342.1428
39	1478.2324	85.5316
40	1534.0317	228.7996
41	1604.8395	32.2922
42	1619.3474	47.0119
43	1643.174	41.8944
44	1653.2608	284.265
45	1670.028	69.8928
46	1682.2947	37.2982
47	1699.9435	81.8428
48	1758.9511	318.1427
49	2375.4534	1339.3466
50	2599.1013	2503.2517
51	2805.8629	937.7519
52	3174.4507	726.8519
53	3191.0557	260.2072
54	3282.7915	936.8842
55	3341.3282	209.2818
56	3446.894	28.9482
57	3500.6331	63.2293
58	3512.775	8.3372

59	3780.4753	40.3001
60	3781.7233	45.7286

Isomer 2.2 -j

#	**Frequency**	**Infrared**
1	34.2881	0.629
2	38.551	0.3475
3	52.8828	0.3313
4	65.6169	5.2906
5	87.7221	8.5369
6	100.283	4.4009
7	126.6918	6.8762
8	144.9833	2.8994
9	157.0964	3.8798
10	168.4198	65.6613
11	185.4506	15.4773
12	239.3515	40.3619
13	247.7376	49.9764
14	278.8466	87.1516
15	280.6534	91.2393
16	333.9532	130.5474
17	339.6198	30.1609
18	369.0027	5.8059
19	399.1364	29.0113
20	426.1597	30.0967
21	432.5321	16.3597
22	447.0264	22.6854
23	456.8262	35.9829
24	479.3242	46.1919
25	567.2827	13.2121
26	593.3622	79.0609
27	685.6825	102.4126
28	688.7836	72.4322
29	707.2156	17.7697
30	819.7137	1.3937
31	835.5038	11.7325
32	858.2152	67.8168
33	1104.1627	84.9339
34	1161.5106	10.5671
35	1216.6634	66.0575
36	1298.6145	183.3679
37	1333.6847	252.3462
38	1381.5995	344.328
39	1475.6176	58.4576
40	1540.0413	388.9987

41	1586.8335	32.0858
42	1621.3638	45.5249
43	1632.2351	403.8081
44	1648.2586	17.2244
45	1660.9187	8.6512
46	1682.0633	16.9547
47	1699.8129	71.3464
48	1763.8469	315.5411
49	2346.4611	696.357
50	2496.9984	2850.3695
51	2740.474	1082.0175
52	3262.2838	298.0009
53	3313.4696	166.0967
54	3378.3469	195.6663
55	3385.5816	124.7693
56	3403.145	531.7558
57	3498.0633	31.328
58	3506.3749	66.9332
59	3779.0434	37.0791
60	3787.6782	53.0344

Isomer 2.2 -k

#	**Frequency**	**Infrared**
1	21.6193	0.6523
2	30.5807	1.8177
3	42.6329	2.8287
4	47.6679	1.4924
5	71.3686	1.442
6	88.8942	8.5817
7	114.3508	3.4294
8	139.82	6.0019
9	171.6185	9.8783
10	217.0099	3.8209
11	230.6574	76.0493
12	239.6569	63.1806
13	258.6266	34.8858
14	293.1762	100.639
15	297.31	20.3565
16	335.2021	192.9577
17	338.5407	55.8362
18	358.2585	7.8659
19	378.3389	14.6299
20	427.2724	5.7154
21	453.8544	37.3928
22	463.5089	45.0392

23	469.2413	27.4786
24	532.5184	33.2124
25	561.2904	15.9109
26	598.23	4.2615
27	644.3675	55.9562
28	701.0559	32.4599
29	817.071	0.1278
30	834.5612	26.5549
31	903.2193	63.8762
32	968.5571	75.6874
33	1078.2761	62.9166
34	1164.1592	7.4716
35	1182.117	37.3463
36	1294.376	342.8301
37	1335.9039	218.9594
38	1394.5715	408.1872
39	1484.4534	136.8363
40	1535.129	255.6889
41	1603.7437	54.7813
42	1618.3359	31.3232
43	1640.7982	412.5056
44	1642.418	20.3933
45	1673.4733	3.5731
46	1680.2965	46.0798
47	1695.0983	45.9528
48	1756.5382	305.1525
49	2260.3456	1424.8891
50	2666.7033	2059.443
51	2832.8951	1789.4181
52	3008.6621	835.1856
53	3169.7315	281.061
54	3245.0647	455.5055
55	3334.3682	219.9503
56	3450.714	47.6072
57	3500.1255	58.2901
58	3512.2194	9.0804
59	3780.7288	39.8361
60	3781.1128	46.7475

Isomer 2.2 -l

#	**Frequency**	**Infrared**
1	35.873	0.9626
2	52.1725	4.0962
3	56.3078	1.9369
4	81.0535	0.15

5	87.7504	7.1905
6	107.8304	10.2373
7	113.4628	6.0344
8	141.8552	8.3159
9	148.5922	2.6133
10	172.202	3.2704
11	208.6686	25.3741
12	232.35	38.2291
13	251.4368	76.4262
14	256.7611	27.8334
15	299.6386	58.4736
16	320.6016	58.2767
17	333.4612	26.1974
18	368.3236	55.488
19	384.3868	42.4189
20	419.4337	77.5495
21	428.6349	13.6598
22	454.221	49.1049
23	496.8665	6.0595
24	570.5753	12.2412
25	624.5698	60.9124
26	678.4384	64.2739
27	702.4272	12.5586
28	791.7293	45.7079
29	823.9612	17.0413
30	829.4357	9.3547
31	879.0819	80.2557
32	900.3096	70.5142
33	964.6949	85.4503
34	1109.3363	115.9949
35	1147.8355	10.7977
36	1304.4559	132.5285
37	1325.7379	93.7462
38	1378.455	442.3025
39	1449.4422	91.0787
40	1562.1915	237.4122
41	1602.3466	84.4314
42	1610.5742	39.3618
43	1624.69	20.6067
44	1636.8433	216.4228
45	1656.1473	5.0215
46	1683.1384	19.1947
47	1717.2352	11.2882
48	1753.9931	338.4483

49	2296.4867	1458.2067
50	2472.037	1588.9163
51	3077.526	964.9058
52	3165.5585	304.5214
53	3318.9902	618.622
54	3375.5516	45.3185
55	3401.5536	622.2713
56	3440.3126	24.4936
57	3487.4342	41.0569
58	3520.9262	11.1337
59	3525.6041	46.3367
60	3781.6263	64.5701

Isomer 2.2 -m

#	**Frequency**	**Infrared**
1	27.0761	1.5394
2	29.3805	3.1313
3	47.3711	1.3962
4	60.3057	1.9684
5	66.888	1.5684
6	82.5189	3.8533
7	108.5665	3.408
8	162.324	3.6951
9	188.3702	5.7968
10	203.533	59.5886
11	214.6573	49.4013
12	223.765	60.3558
13	233.3486	19.6075
14	250.888	31.193
15	280.2244	40.9236
16	293.3203	103.8742
17	312.8681	81.7058
18	357.7822	26.4398
19	406.7117	56.5569
20	417.9944	44.0086
21	442.3258	45.7374
22	456.7535	21.5438
23	481.2572	17.9083
24	522.7498	55.0398
25	567.5103	53.5238
26	572.692	12.3507
27	663.2717	27.9666
28	696.6037	36.2756
29	750.0199	70.5814
30	785.7731	91.6967

31	824.1568	6.0317
32	831.5518	15.2433
33	864.107	71.1434
34	1168.5677	8.6466
35	1193.2711	90.0674
36	1326.4401	288.3806
37	1368.2458	47.0575
38	1381.3485	414.9049
39	1455.9391	40.0075
40	1553.8501	212.3569
41	1609.3014	11.7303
42	1620.0225	21.5003
43	1627.0637	5.6279
44	1649.656	5.7229
45	1657.8981	288.9667
46	1699.8751	0.4478
47	1705.9594	34.8142
48	1750.5602	527.3573
49	2577.2217	1487.0082
50	2742.8568	1121.1782
51	3032.5586	604.067
52	3174.6156	570.8954
53	3238.7005	898.7085
54	3270.9319	785.6601
55	3283.1058	665.7249
56	3446.4629	28.3565
57	3493.5331	50.7546
58	3511.4162	7.5159
59	3785.5101	50.1009
60	3790.2941	61.6622

Isomer 2.2 -n

#	**Frequency**	**Infrared**
1	16.0288	1.9762
2	29.7498	1.2955
3	38.573	4.2109
4	58.3384	3.0099
5	75.1082	6.7779
6	95.7141	1.0788
7	126.6159	13.2391
8	151.8015	11.4602
9	182.0795	1.6348
10	199.4293	3.5882
11	229.9119	71.4025
12	237.5438	64.1985

13	271.6082	20.2696
14	287.3665	32.7111
15	306.4646	132.0731
16	322.5005	6.4146
17	343.2369	17.4169
18	374.8053	266.3698
19	400.8926	60.3456
20	424.0316	43.0751
21	437.4471	138.744
22	446.5105	63.7823
23	454.6938	59.7548
24	523.4231	6.2608
25	574.5039	26.4645
26	597.9917	11.7283
27	643.8691	47.1984
28	736.3448	48.4166
29	815.732	10.9129
30	837.5758	176.3483
31	868.625	138.7108
32	1009.2218	96.8647
33	1052.0117	71.1641
34	1138.5499	68.5839
35	1232.9896	383.3653
36	1276.8306	262.7765
37	1337.9233	193.5477
38	1390.4392	320.7263
39	1466.5651	143.1197
40	1525.1479	1495.9066
41	1570.1469	609.7461
42	1601.8045	14.7234
43	1610.8129	45.5546
44	1636.1302	10.8223
45	1650.4979	23.647
46	1669.2929	5.6308
47	1697.4002	199.3429
48	1703.9111	290.1712
49	1817.0834	1198.1441
50	2763.616	1163.4795
51	2777.0616	1541.299
52	2914.6125	922.3382
53	3103.2166	1575.521
54	3296.081	274.0727
55	3441.2821	30.1314
56	3463.4374	57.1072

57	3519.4938	33.5096
58	3520.8473	10.0528
59	3770.4588	54.4975
60	3777.2804	39.7031

Isomer 2.2 -o

#	**Frequency**	**Infrared**
1	32.6398	6.4276
2	40.196	4.4745
3	50.0579	8.6875
4	77.7531	0.6763
5	79.435	6.8054
6	108.8654	13.0524
7	136.0555	8.6942
8	149.164	21.1435
9	153.3961	0.4914
10	169.5691	14.1331
11	187.974	22.5389
12	225.7871	33.9019
13	236.629	33.1977
14	251.5239	78.6898
15	271.3505	62.8594
16	306.9004	20.0587
17	322.9311	37.9347
18	334.5082	224.3774
19	351.5895	21.8193
20	376.208	4.1552
21	409.194	69.0188
22	421.4044	14.4684
23	445.9208	9.2144
24	498.7185	97.874
25	558.6713	171.2023
26	630.3479	13.9875
27	653.5023	200.9203
28	679.4427	132.9274
29	685.5772	11.1787
30	781.5877	109.1869
31	813.6155	3.337
32	824.1946	35.0297
33	1105.1235	245.2891
34	1197.6578	512.2421
35	1212.758	75.014
36	1253.0849	28.3124
37	1313.7484	1048.2361
38	1330.1723	15.6722

39	1391.4501	1371.4145
40	1441.6811	450.5051
41	1592.6881	401.3011
42	1600.7188	28.1249
43	1607.827	43.9377
44	1626.4396	12.0448
45	1638.6291	23.1294
46	1664.7341	409.9398
47	1674.1131	70.1061
48	1711.1776	27.0986
49	1728.0535	899.567
50	2064.0733	2569.401
51	3128.5165	511.6646
52	3350.0163	85.2366
53	3445.2469	60.1998
54	3465.1402	249.9522
55	3485.2717	52.7327
56	3515.8336	22.961
57	3517.6501	472.6002
58	3533.1841	18.2836
59	3622.1299	225.8902
60	3778.009	85.3026

Isomer 2.2 -p

#	**Frequency**	**Infrared**
1	16.9729	0.4228
2	31.3071	0.7365
3	33.7043	0.1027
4	40.747	2.034
5	46.6196	1.4311
6	60.3376	14.1286
7	82.0418	3.6711
8	107.4103	7.6496
9	130.4049	1.5489
10	184.8018	15.9565
11	190.8002	30.854
12	227.4255	8.661
13	239.8052	17.9089
14	270.7445	22.2571
15	274.3773	4.7866
16	286.4051	71.27
17	320.0113	166.2987
18	334.8565	172.5133
19	344.5	20.848
20	418.3162	34.6626

21	431.0212	20.3854
22	467.8883	58.0669
23	518.0712	2.3886
24	569.1196	3.7304
25	618.0155	13.1111
26	672.8782	129.5288
27	705.8788	36.2591
28	744.0007	67.9909
29	817.6108	0.787
30	838.9335	32.7938
31	856.3864	99.5809
32	891.4019	41.7267
33	955.3229	60.0084
34	1081.2515	150.39
35	1168.1745	0.5646
36	1292.1939	527.9086
37	1362.3006	0.6013
38	1403.6345	522.1329
39	1456.3954	54.765
40	1550.7928	122.9671
41	1609.4791	724.092
42	1613.4844	186.018
43	1618.712	16.3943
44	1620.6176	112.0922
45	1661.3103	30.3444
46	1676.8854	6.3445
47	1705.4642	8.5114
48	1745.776	754.7992
49	1906.0725	1935.1836
50	2676.2261	1442.5621
51	3011.8807	359.043
52	3273.4354	955.1939
53	3310.6948	1091.8616
54	3389.2351	686.2979
55	3401.1308	7.5423
56	3439.3862	23.0706
57	3517.2675	28.6892
58	3517.8074	13.9037
59	3520.6789	11.0085
60	3778.0889	59.4502

Isomer 2.2 -q

#	**Frequency**	**Infrared**
1	26.376	3.2711
2	34.6403	3.2693

3	57.3804	2.5037
4	72.7506	8.1396
5	79.4486	4.8869
6	101.2889	1.395
7	115.0895	0.4518
8	150.7319	12.024
9	157.4319	5.9667
10	201.936	0.6247
11	234.9937	29.5896
12	238.9257	33.8853
13	269.0287	75.9816
14	290.8232	126.8418
15	319.0118	29.2274
16	363.0406	41.7511
17	396.5481	34.4565
18	400.3784	34.4661
19	428.6639	28.9539
20	448.1322	29.9915
21	470.9607	81.2113
22	472.8183	41.9685
23	532.2477	97.0127
24	559.4082	4.3925
25	643.6764	46.1221
26	695.2334	26.9641
27	822.2131	0.8434
28	829.134	21.7361
29	904.2567	40.9934
30	935.5879	64.4536
31	1031.3572	55.1775
32	1085.8456	38.7392
33	1152.4136	65.3515
34	1155.3648	37.703
35	1163.0893	36.9427
36	1184.9593	54.6696
37	1317.0373	270.0496
38	1394.2711	547.259
39	1438.2823	233.4859
40	1600.2935	17.3662
41	1609.3923	11.0956
42	1628.68	60.7471
43	1637.4246	14.3127
44	1652.1566	48.753
45	1667.3814	357.4239
46	1682.1085	223.0035

47	1742.3237	299.567
48	1770.4793	346.5295
49	1828.4111	2098.9546
50	2167.4584	2442.7929
51	2528.9511	1095.3635
52	2831.1694	1377.1134
53	3089.973	330.4337
54	3194.9415	471.6034
55	3318.6284	188.6898
56	3454.7742	42.5502
57	3465.1912	66.7422
58	3517.7386	14.2614
59	3520.6308	16.7989
60	3723.3973	46.4276

Isomer 2.2 -r

#	**Frequency**	**Infrared**
1	20.4824	0.4196
2	30.5243	0.886
3	35.3092	5.1236
4	53.6021	5.5555
5	68.8251	5.2458
6	80.5919	2.933
7	107.1333	6.0407
8	124.1707	1.3075
9	146.4488	0.2308
10	168.0634	15.2767
11	190.3651	40.1891
12	203.9177	64.8797
13	233.7612	150.24
14	250.4093	52.2781
15	289.8938	15.7725
16	311.1405	26.0444
17	324.3849	225.6067
18	336.2183	48.3069
19	407.5425	55.0577
20	419.2277	52.7935
21	430.8519	28.5557
22	454.6569	133.5782
23	463.7781	38.6392
24	555.8826	62.5794
25	570.4347	41.4001
26	698.9409	33.1659
27	710.83	74.5372
28	814.7107	0.0927

29	835.0313	34.9658
30	893.4905	71.3694
31	905.85	64.1329
32	954.3446	103.6339
33	1114.6734	203.8262
34	1124.5368	28.5798
35	1170.6346	5.7189
36	1220.805	90.8273
37	1283.8037	992.8128
38	1341.0659	166.3939
39	1399.5131	311.2168
40	1522.5193	712.5176
41	1596.7222	111.167
42	1605.0646	2.876
43	1615.1458	263.4354
44	1628.7652	16.1331
45	1644.6987	7.9453
46	1671.6817	254.1318
47	1714.1396	73.8577
48	1767.5523	765.3636
49	1888.8597	2120.3148
50	2163.6572	2073.6593
51	2868.988	1210.8584
52	3141.8993	297.5216
53	3187.7558	459.1358
54	3366.6002	59.5112
55	3421.5149	834.7215
56	3448.4625	66.3821
57	3486.4423	50.5005
58	3514.168	11.6133
59	3527.4055	12.8458
60	3791.4491	70.9289

$(H_2C_2O_4)(NH_3)_2(H_2O)_3$
Isomer 2.3 –a

1	23.8013	0.7729
2	26.5705	1.0414
3	29.8495	1.7737
4	43.7118	0.0882
5	58.8803	0.0227
6	67.8136	0.2821
7	87.2531	4.8846
8	95.219	6.0263
9	114.1852	2.5237

10	149.7878	11.1085
11	185.9379	19.2598
12	195.7754	4.053
13	212.5558	42.9971
14	230.2678	51.5119
15	243.1274	95.9066
16	263.9479	115.0885
17	276.767	88.1368
18	290.9886	65.6853
19	306.7478	76.0075
20	313.6578	16.0543
21	319.07	14.9178
22	324.4221	43.7425
23	413.3125	15.7977
24	436.4303	3.7119
25	448.1683	36.9642
26	462.0278	31.9308
27	480.1809	17.2738
28	500.1029	61.8234
29	516.1778	52.0083
30	571.2783	26.671
31	629.8264	50.3442
32	674.2641	59.7488
33	697.1185	14.3252
34	815.5104	9.787
35	820.0319	22.7008
36	861.1195	64.8839
37	900.4962	65.2243
38	993.6274	98.2135
39	1006.4814	86.8426
40	1137.2417	75.461
41	1166.6313	15.5626
42	1318.8242	401.5642
43	1394.6178	390.6196
44	1413.07	13.2583
45	1484.5462	84.982
46	1532.0925	55.8462
47	1604.6602	13.7033
48	1609.2475	35.3244
49	1636.9532	15.547
50	1641.1801	60.2739
51	1656.7743	11.648
52	1667.0501	292.4393
53	1706.4983	22.4052

54	1728.7586	45.8233
55	1761.1992	554.6842
56	2687.9369	1011.0985
57	2794.2498	1934.0767
58	2932.3425	707.5417
59	2945.0165	815.5703
60	3068.7625	1997.9998
61	3162.66	404.7339
62	3170.332	980.1915
63	3318.207	265.5627
64	3468.1493	76.2875
65	3485.7894	43.271
66	3521.6529	9.7374
67	3780.9317	38.1858
68	3783.4376	56.5589
69	3784.5673	48.9136
Isomer 2.3 -b		
1	19.4636	0.1531
2	23.9973	1.8306
3	38.4318	0.5224
4	54.6855	1.0079
5	59.7258	2.7007
6	73.5885	1.6173
7	81.1349	1.9886
8	89.1432	1.7085
9	110.0721	0.3935
10	156.5812	1.8344
11	179.8262	17.7242
12	195.2088	76.4356
13	222.68	74.9509
14	227.5345	40.7636
15	236.2176	27.4688
16	249.0946	37.9386
17	256.3362	32.3399
18	277.5418	143.0128
19	309.4116	31.1761
20	320.4566	8.4332
21	341.2169	35.7433
22	351.6925	61.1882
23	420.2299	18.333
24	427.5146	19.2635
25	456.6876	91.0474
26	466.1659	28.7344
27	488.9048	41.0031

28	541.0425	32.6258
29	558.0398	42.42
30	572.3669	17.148
31	583.2151	91.0174
32	689.4922	37.1154
33	719.94	59.5237
34	771.1085	51.46
35	797.7937	82.2356
36	801.8	18.2656
37	818.9822	15.7861
38	847.6167	26.3717
39	956.446	121.0352
40	1146.6084	26.052
41	1149.965	111.7289
42	1323.8065	523.8927
43	1381.1633	165.8049
44	1422.8988	25.5861
45	1477.3133	45.9243
46	1544.5202	79.1353
47	1605.087	19.3902
48	1613.633	48.4572
49	1632.64	26.4951
50	1642.3709	46.0898
51	1646.3979	466.1457
52	1655.2974	48.8799
53	1715.8995	4.0944
54	1731.2248	44.3165
55	1786.9077	309.1147
56	2618.3186	1645.8589
57	2789.7607	815.6827
58	2892.5634	839.1817
59	3051.5099	1426.736
60	3166.7143	1877.6285
61	3230.4904	435.6998
62	3273.4652	755.8433
63	3375.4759	156.9128
64	3456.7745	35.8791
65	3483.274	48.8386
66	3520.2746	8.202
67	3771.3306	52.5323
68	3787.0527	48.5181
69	3789.5646	48.861
Isomer 2.3 -c		
1	11.721	0.8921

2	25.5797	1.0454
3	37.1305	1.3633
4	53.0217	1.2052
5	56.2116	1.1615
6	65.037	3.7796
7	76.6396	0.6817
8	85.4682	4.0432
9	116.8421	1.3712
10	146.9749	11.593
11	158.4945	0.3224
12	178.1248	19.5444
13	217.7736	35.3382
14	242.3082	66.8536
15	246.5643	76.6775
16	259.3314	63.3658
17	286.5255	33.0412
18	298.7052	116.9549
19	316.0957	53.8321
20	319.4137	91.5559
21	344.1379	52.641
22	350.7836	16.5879
23	415.1314	75.9907
24	433.9189	18.9709
25	461.8807	13.6893
26	473.2456	34.752
27	499.5177	35.9434
28	512.4311	39.5234
29	517.0386	12.1752
30	553.3523	31.0993
31	568.18	28.1007
32	693.7829	38.0621
33	718.8784	29.1158
34	814.9184	3.489
35	837.4942	32.1408
36	856.7873	78.9082
37	886.1922	70.696
38	938.1364	60.6385
39	1061.363	61.7957
40	1106.7822	134.9516
41	1162.9473	13.6078
42	1320.4875	475.6083
43	1394.3262	310.7172
44	1434.2699	32.8923
45	1479.4249	47.9183

46	1539.0617	38.5491
47	1605.6715	44.5681
48	1608.0628	17.2422
49	1628.2525	83.7486
50	1635.5311	19.6864
51	1653.0127	144.6231
52	1678.2444	145.4173
53	1716.9801	44.9245
54	1727.7691	4.2213
55	1769.5929	455.0603
56	2647.4596	1378.2592
57	2789.911	1438.3984
58	2865.0076	694.2945
59	2962.301	2693.4108
60	3062.1825	1362.0784
61	3131.4038	666.0083
62	3204.1926	271.0084
63	3359.3339	127.5434
64	3479.5158	40.7951
65	3481.26	81.1832
66	3521.513	9.1696
67	3772.1504	45.8348
68	3778.0366	47.6991
69	3782.6363	43.0269
Isomer 2.3 -d		
1	26.3338	1.8032
2	35.7772	3.2635
3	40.3288	0.7841
4	55.2017	2.8324
5	65.1935	3.0159
6	74.0179	1.3532
7	82.4843	1.7543
8	111.4263	10.6227
9	129.9304	4.9509
10	163.303	8.9723
11	190.2711	4.0569
12	194.8134	4.2851
13	206.5318	16.4634
14	230.7403	39.9131
15	247.4708	107.7515
16	265.6211	70.2971
17	277.8321	11.3714
18	290.5549	47.0805
19	293.5359	89.7644

20	313.7407	82.6026
21	352.8988	23.8214
22	410.4229	61.9552
23	417.7271	39.5502
24	436.6534	44.3553
25	448.3639	23.7947
26	467.1314	20.802
27	477.1903	8.0675
28	560.9724	29.0888
29	575.7476	55.2418
30	647.2174	89.604
31	659.9441	116.5055
32	699.0971	1.0401
33	731.068	70.0556
34	765.7259	19.3842
35	818.6544	0.3713
36	839.1767	29.9289
37	888.1779	64.6348
38	916.524	85.3205
39	1016.6727	140.6864
40	1108.0327	113.5339
41	1168.9926	6.0769
42	1325.5824	365.3471
43	1388.8869	349.3148
44	1401.5261	60.4648
45	1484.4361	92.3037
46	1540.2803	72.655
47	1602.7005	21.1519
48	1605.4246	23.2423
49	1636.0359	46.9986
50	1645.7183	216.5201
51	1651.0173	18.8878
52	1694.0586	73.8295
53	1713.8311	13.6903
54	1724.964	87.1438
55	1763.9911	510.4116
56	2655.0079	499.6257
57	2754.8941	2171.9385
58	2864.527	1606.3943
59	3039.7639	656.0252
60	3163.622	642.8145
61	3198.3949	384.59
62	3318.2159	192.4906
63	3410.0321	677.7595

64	3426.214	806.893
65	3470.469	76.4927
66	3485.9291	52.5987
67	3524.9723	6.9633
68	3786.6267	37.8325
69	3790.8589	84.53
Isomer 2.3 -e		
1	28.5392	0.7817
2	39.9692	4.2337
3	46.8425	0.9435
4	69.507	7.5153
5	81.1817	2.2806
6	89.8899	2.1904
7	109.7857	4.2847
8	121.4592	4.0317
9	134.161	8.0841
10	144.7834	6.0991
11	168.6258	4.7794
12	183.2274	9.2468
13	216.2467	16.6774
14	230.5566	69.6071
15	272.331	16.0724
16	279.2133	88.6678
17	283.1852	43.2794
18	298.8846	52.8072
19	311.5952	68.9211
20	348.6961	22.3318
21	364.9375	50.0448
22	391.8624	62.0082
23	414.6972	14.6413
24	439.9527	16.0212
25	444.1018	25.8285
26	454.8991	67.532
27	475.7992	47.5206
28	556.0248	58.0764
29	577.2491	18.0042
30	613.9245	60.9426
31	689.2607	38.5083
32	697.5081	24.6483
33	781.5689	42.4592
34	820.6248	0.6362
35	831.1705	8.8348
36	854.7255	68.0438
37	902.0099	49.9619

38	951.1459	143.2066
39	1024.0878	50.614
40	1157.4466	82.5422
41	1160.8993	19.5005
42	1288.1391	154.2188
43	1330.4951	368.0925
44	1386.6978	222.328
45	1472.055	115.3098
46	1569.8376	235.8126
47	1600.1474	70.5528
48	1605.3925	67.9709
49	1632.5837	82.5795
50	1642.9427	174.3719
51	1652.824	5.0937
52	1677.4573	26.0259
53	1692.4469	89.2416
54	1697.663	62.5561
55	1772.0957	307.447
56	2379.9732	1389.719
57	2617.2001	1198.8195
58	2796.2619	1471.1776
59	3142.9338	721.6116
60	3180.8352	1211.8461
61	3290.0908	216.3201
62	3339.6179	109.8337
63	3427.0345	115.5914
64	3429.8217	104.9864
65	3447.1855	405.2631
66	3509.7345	30.7004
67	3513.8432	60.4104
68	3780.7545	38.0499
69	3785.21	58.2489
Isomer 2.3 -f		
1	20.8375	0.8329
2	29.1537	1.6507
3	51.0355	1.6872
4	58.4205	1.2453
5	65.0912	1.2913
6	80.3332	4.4938
7	97.1915	3.02
8	114.7013	1.6199
9	117.8979	3.3135
10	144.3342	6.0527
11	186.3738	3.7866

12	195.9569	2.6756
13	216.805	61.4462
14	239.736	50.4191
15	269.7421	58.8168
16	295.3126	13.1648
17	302.5259	48.0665
18	310.132	24.5537
19	316.3781	20.7663
20	328.3702	141.793
21	344.9149	21.4761
22	421.9511	25.3801
23	428.7533	46.3203
24	442.3082	44.821
25	462.197	22.4333
26	498.5901	73.4111
27	511.3341	36.0862
28	532.723	50.8006
29	549.9061	92.3667
30	572.0345	22.1106
31	642.8482	43.8874
32	694.9813	22.5438
33	733.8851	103.3338
34	819.1535	1.734
35	839.7733	34.8134
36	863.5238	94.1144
37	879.369	73.0884
38	969.6522	86.2698
39	992.653	52.2928
40	1118.3206	115.6576
41	1159.8393	12.1374
42	1315.5178	449.3771
43	1390.2561	269.5764
44	1401.5311	58.3457
45	1440.8456	32.4807
46	1570.4309	123.256
47	1610.7783	24.2229
48	1615.2967	52.6495
49	1630.7381	7.3336
50	1643.3391	189.9349
51	1654.6852	1.8534
52	1667.244	135.2936
53	1704.0042	104.5385
54	1722.5646	20.1256
55	1766.555	425.2292

56	2559.7412	1417.3592
57	2675.2674	892.5617
58	2949.1675	1449.8509
59	3084.8064	440.8357
60	3102.7495	1446.6124
61	3150.7018	861.8266
62	3216.0346	251.4077
63	3340.8465	103.8833
64	3472.2812	54.8848
65	3499.1675	55.4749
66	3519.2318	8.7823
67	3623.5818	265.9424
68	3776.5939	47.8542
69	3778.8134	49.2419
Isomer 2.3 -g		
1	19.9467	0.6715
2	31.1901	0.5527
3	32.6287	0.337
4	47.1809	0.4448
5	59.9629	0.8487
6	61.2264	1.9204
7	88.1179	4.0022
8	92.1021	4.7126
9	119.7321	0.6191
10	159.3911	9.9723
11	191.5857	59.6459
12	195.4852	16.8318
13	208.1914	22.682
14	212.1786	41.0962
15	224.628	7.7055
16	244.4776	150.0124
17	256.705	45.1848
18	267.5714	48.1723
19	298.137	175.9383
20	300.5382	8.8879
21	315.1599	32.2625
22	348.7503	31.3285
23	422.1418	31.3406
24	430.1104	46.3138
25	451.3561	24.5207
26	464.84	13.3474
27	473.8856	71.1471
28	501.3647	37.138
29	535.0595	29.8104

30	567.8887	79.1638
31	575.2531	24.6261
32	686.9296	48.3554
33	710.6131	7.0328
34	739.1603	65.0438
35	777.1607	57.7059
36	816.8794	0.5437
37	842.5894	32.1241
38	919.454	64.0182
39	953.3204	99.4656
40	1172.8631	122.0952
41	1175.655	1.4131
42	1320.2766	360.0085
43	1399.0598	439.7092
44	1414.3761	5.7538
45	1486.5418	86.9948
46	1540.938	32.04
47	1603.6186	45.9931
48	1609.2869	3.9654
49	1621.5287	10.0024
50	1639.1484	25.1408
51	1643.5789	37.3332
52	1669.3163	255.0035
53	1714.3466	38.3212
54	1727.0731	37.9522
55	1753.9523	641.7542
56	2642.623	1617.3698
57	2732.3386	1167.5274
58	2974.4839	883.6815
59	3116.933	367.0155
60	3156.0959	870.4469
61	3202.5836	784.1838
62	3272.2904	1172.7387
63	3348.3808	925.1781
64	3452.5945	33.3051
65	3480.4123	39.957
66	3516.2189	7.3408
67	3782.3384	51.2064
68	3783.5219	74.9082
69	3792.5502	49.7384
Isomer 2.3 -h		
1	22.4531	2.2722
2	33.4114	1.135
3	47.2668	1.8072

4	52.7215	7.7584
5	68.1494	6.8513
6	84.4307	1.9824
7	102.0913	0.7627
8	119.0462	1.5119
9	120.6781	3.7477
10	150.8116	5.7978
11	180.2486	6.9659
12	195.9468	5.1959
13	222.7669	48.1924
14	243.5984	37.1347
15	276.6187	15.8447
16	288.8436	6.4318
17	298.4212	128.1918
18	309.0355	23.5996
19	320.1047	27.636
20	332.3611	19.4904
21	341.7129	122.2043
22	420.0677	27.8842
23	431.2469	57.7973
24	443.1009	28.9464
25	461.1119	45.5594
26	487.0062	18.6817
27	496.9304	77.9528
28	534.3618	16.2166
29	567.3721	22.0482
30	574.6992	107.0497
31	630.4844	42.5087
32	688.1186	35.6389
33	730.1928	66.857
34	812.2952	51.0523
35	827.5286	11.3633
36	860.5289	66.4324
37	918.4414	80.6703
38	982.7862	85.0727
39	1000.2198	36.1933
40	1116.5136	104.0852
41	1149.8362	15.7308
42	1324.9386	259.4685
43	1371.5841	376.6518
44	1397.4693	32.3938
45	1428.9745	41.1317
46	1568.719	244.6
47	1612.6881	62.445

48	1620.1703	25.1791
49	1631.9448	31.486
50	1639.5286	168.2993
51	1661.3973	13.1598
52	1665.9164	69.9782
53	1692.0044	26.1217
54	1722.4794	23.3126
55	1767.4426	323.2683
56	2537.8356	1334.4426
57	2684.9163	829.7255
58	2906.4982	1534.7112
59	3047.2244	698.4432
60	3125.7243	1176.0912
61	3135.9492	677.9042
62	3273.6511	166.5936
63	3333.9657	110.6592
64	3468.7668	53.5133
65	3500.2685	56.5911
66	3517.6783	9.5921
67	3613.2659	218.019
68	3763.4372	45.7528
69	3778.6114	44.1547
Isomer 2.3 -i		
1	15.2044	0.2926
2	38.1045	0.5765
3	40.1846	3.2542
4	50.8984	1.0357
5	62.2191	6.0354
6	69.5155	3.6652
7	100.1666	0.9862
8	109.3101	5.3185
9	116.9029	3.898
10	151.4691	4.5761
11	193.5287	6.1078
12	205.3115	4.1482
13	233.4545	75.9177
14	245.6804	52.5918
15	266.7223	59.163
16	285.4423	21.4719
17	311.1163	82.9388
18	311.7388	6.7685
19	337.8435	13.897
20	365.203	65.533
21	382.3178	35.6618

22	421.9368	38.9913
23	443.571	35.6635
24	463.2798	69.8627
25	466.7858	88.519
26	478.792	35.9121
27	518.1894	7.2349
28	524.6664	93.3623
29	557.6859	42.1694
30	570.3688	13.039
31	614.4403	19.6217
32	695.947	46.931
33	737.7257	17.0803
34	815.5671	1.6146
35	832.6751	37.4853
36	855.4419	62.5616
37	888.8333	132.2823
38	908.6631	99.8028
39	1044.0942	61.3643
40	1144.0054	116.1843
41	1151.347	22.0572
42	1318.942	531.8613
43	1388.2024	242.5545
44	1414.9132	12.0333
45	1446.7386	32.4724
46	1576.438	199.7736
47	1601.8661	78.2984
48	1611.3757	38.8275
49	1630.3084	4.3561
50	1640.8318	83.3683
51	1656.5204	24.0559
52	1678.8726	323.3722
53	1709.4958	27.718
54	1740.5741	28.9621
55	1777.0354	276.4507
56	2560.3581	1152.1881
57	2661.4028	1015.2795
58	2777.5037	2243.7018
59	2933.6943	792.066
60	3083.7374	1088.8133
61	3163.8463	900.7369
62	3269.4084	235.3007
63	3306.6896	195.8794
64	3462.0634	50.5724
65	3491.924	44.1479

66	3518.4963	10.8595
67	3715.8289	75.3277
68	3767.5984	47.8196
69	3775.7949	48.1445
Isomer 2.3 -j		
1	23.7165	2.8097
2	33.6566	2.0304
3	42.699	0.3257
4	60.3688	1.2885
5	69.0535	0.1648
6	77.7876	3.3753
7	90.0749	3.448
8	114.3616	2.3389
9	142.3083	1.4963
10	173.5432	0.7825
11	180.5435	1.3092
12	206.337	18.348
13	213.8788	29.938
14	246.0063	50.9423
15	252.4301	15.2661
16	267.8381	19.3025
17	287.4448	148.9099
18	309.7008	35.9616
19	314.3845	22.9896
20	333.3932	27.8931
21	344.1722	37.0832
22	422.96	34.0003
23	452.5685	59.8728
24	459.0849	44.7013
25	484.3114	37.1132
26	491.6317	63.3683
27	528.0894	21.7473
28	549.745	63.0636
29	568.8675	28.1263
30	576.9295	50.531
31	675.1151	23.4965
32	703.7166	25.9428
33	798.5692	26.4522
34	816.6802	0.4157
35	834.0849	19.2726
36	859.46	37.3658
37	866.2336	129.5268
38	881.2856	119.0714
39	913.223	87.0416

40	1151.2247	91.8465
41	1176.2109	3.8001
42	1329.9643	378.9811
43	1394.5103	18.0604
44	1399.368	428.413
45	1470.206	33.3342
46	1571.7076	134.6275
47	1608.382	35.4699
48	1618.2321	88.2665
49	1628.8739	50.5537
50	1646.8533	13.6815
51	1669.622	26.101
52	1678.9247	214.38
53	1706.7485	15.237
54	1743.143	36.5428
55	1748.1052	604.7616
56	2556.3398	1122.9218
57	2750.1755	1100.7745
58	2846.7851	817.7408
59	3045.4012	1516.2554
60	3129.6664	361.9703
61	3176.3537	937.5206
62	3291.7978	182.5748
63	3344.5219	999.0999
64	3456.2922	48.5785
65	3485.9125	408.2356
66	3492.1491	36.688
67	3513.9479	7.9559
68	3776.9861	60.8597
69	3784.0718	46.1263
Isomer 2.3 -k		
1	17.9943	1.1624
2	35.0151	1.7893
3	41.701	3.6693
4	55.7581	6.3717
5	65.1787	1.7247
6	75.2582	3.2381
7	93.2389	0.5285
8	104.9538	6.5292
9	118.4374	3.0395
10	155.6358	0.4808
11	180.4694	4.1772
12	205.5677	1.0604
13	213.8618	42.1877

14	242.4109	29.3995
15	258.916	44.2763
16	268.3451	1.1372
17	291.6891	102.8481
18	312.24	129.9262
19	314.3284	15.3699
20	349.94	103.1724
21	350.2892	79.0686
22	404.3207	42.0453
23	409.8314	112.809
24	430.357	71.4261
25	441.9676	28.623
26	465.2087	38.0933
27	472.4075	119.2375
28	480.8004	60.7538
29	515.2375	17.2369
30	555.3052	22.4635
31	579.6131	13.2839
32	688.1155	9.1513
33	737.1695	52.925
34	777.0049	143.9347
35	815.5878	1.834
36	841.082	61.3857
37	917.7244	308.0957
38	936.9287	44.9793
39	1093.299	84.6397
40	1116.3285	122.1238
41	1265.1177	101.9473
42	1333.3189	69.7926
43	1412.7853	25.6235
44	1414.1028	538.2971
45	1454.1164	24.2791
46	1547.4969	79.8687
47	1595.1073	89.9492
48	1599.043	407.1623
49	1608.3667	20.559
50	1623.2461	14.3608
51	1632.5024	34.197
52	1641.4915	275.2581
53	1691.1118	751.7992
54	1701.6304	1.7095
55	1722.9958	14.9297
56	2354.268	2182.893
57	2610.4261	1281.7063

58	2835.0888	952.621
59	2969.8027	2007.5511
60	3073.4689	328.5279
61	3151.3814	1420.5936
62	3307.5795	717.241
63	3365.6985	73.9597
64	3479.2415	51.6298
65	3486.1847	36.5736
66	3521.5184	9.0408
67	3770.2395	47.6648
68	3781.1844	56.2744
69	3787.0018	63.1391
Isomer 2.3 -l		
1	20.3537	0.2108
2	25.5197	3.4017
3	34.8429	1.052
4	46.7651	4.4378
5	51.4042	3.5191
6	88.509	2.3356
7	95.3096	5.4867
8	112.0401	0.0222
9	149.2815	8.4065
10	172.7784	4.8441
11	197.225	17.1916
12	212.6231	46.4186
13	219.273	31.218
14	232.1485	31.4974
15	255.5947	44.5517
16	265.8308	11.726
17	273.7906	40.4866
18	286.5367	220.0809
19	296.2355	32.8235
20	328.1373	15.0618
21	339.7623	115.8098
22	348.9171	56.6959
23	358.2708	40.7579
24	374.1135	24.4461
25	420.0416	38.4516
26	431.318	10.4593
27	458.2281	74.6681
28	518.5065	98.1818
29	529.5837	36.8226
30	541.4145	76.2851
31	649.7711	13.5519

32	675.1807	22.3021
33	725.4894	41.5809
34	733.3731	83.7738
35	773.1295	88.8126
36	824.9876	5.3713
37	850.8775	9.7954
38	960.8563	83.2149
39	1052.662	70.6176
40	1175.2965	122.9234
41	1247.1294	164.6807
42	1304.5634	109.7471
43	1328.0986	521.0105
44	1388.8607	125.8202
45	1458.2092	94.9679
46	1531.2537	720.1593
47	1600.0983	105.6555
48	1606.9425	6.9544
49	1616.1113	64.8583
50	1630.4892	76.6132
51	1641.3936	31.8001
52	1648.7642	123.7397
53	1665.5823	239.7287
54	1689.3444	259.4946
55	1711.8491	69.1793
56	2549.2872	1637.7917
57	2637.4375	940.8508
58	2822.0461	1578.8444
59	3142.5714	969.7195
60	3187.3652	184.8541
61	3199.5931	730.187
62	3273.4592	722.9424
63	3296.4072	1216.779
64	3452.7419	31.7985
65	3501.1807	54.6728
66	3517.5898	8.9655
67	3774.6733	68.3921
68	3778.2861	48.8263
69	3784.391	48.5504
Isomer 2.3 -m		
1	27.5336	2.5311
2	41.017	5.5132
3	45.9226	3.4135
4	69.4533	0.4408
5	85.5799	0.5909

6	90.5799	4.598
7	102.2227	5.403
8	112.4215	11.1134
9	133.6284	3.8941
10	152.1451	13.4047
11	157.579	3.5095
12	172.2796	3.215
13	194.5176	6.439
14	202.8562	37.5104
15	219.1448	109.1582
16	238.3271	40.0348
17	252.1931	95.6808
18	286.5332	64.8441
19	307.498	3.9185
20	320.9985	111.6283
21	351.4106	66.9298
22	368.1538	76.2938
23	399.8697	282.8059
24	422.4447	68.4446
25	427.7549	13.2205
26	435.9974	45.6266
27	477.7872	15.4037
28	532.7261	72.8094
29	565.0807	63.7873
30	593.7248	47.7703
31	650.998	51.3634
32	661.257	64.2378
33	675.0823	3.1068
34	727.8849	221.5663
35	752.4537	242.4552
36	802.3752	81.3591
37	831.937	1.8601
38	848.9301	8.5479
39	1096.0815	145.7985
40	1152.5845	891.3957
41	1179.8782	387.7724
42	1284.2807	56.1606
43	1329.9199	127.9471
44	1427.1825	490.561
45	1473.0232	112.1175
46	1481.8251	1495.9888
47	1570.5367	69.1888
48	1580.7393	220.7832
49	1610.7702	17.8905

50	1617.4987	109.8882
51	1633.3264	13.53
52	1638.2866	24.8385
53	1666.072	272.3388
54	1673.7775	360.1377
55	1699.2047	66.4091
56	1730.7581	214.0369
57	2495.7195	1573.6283
58	2881.6464	960.2563
59	3341.7818	64.9671
60	3362.1155	185.8284
61	3371.2577	400.1004
62	3449.7887	388.3026
63	3475.1416	458.2091
64	3483.6704	69.3669
65	3497.8065	81.0067
66	3506.6702	312.3584
67	3523.7271	9.9017
68	3772.4147	83.9932
69	3779.6791	58.8509