

Supporting Information

Interaction of Gas Phase Oxalic Acid with Ammonia and Its Atmospheric Implication

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Figure S1. Isomers with ammonia binding to either carboxyl and with the relative single point energy above 6 kcal mol⁻¹.

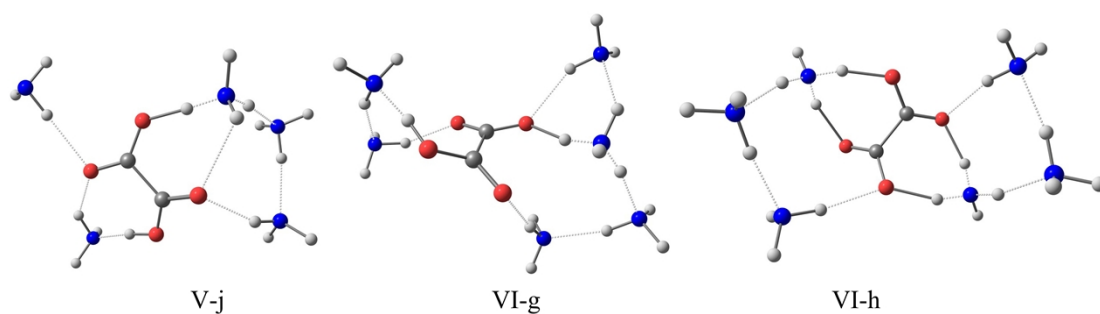


Table S1. Binding energy of isomers with ammonia binding to either carboxyl and with the relative single point energy above 6 kcal mol⁻¹.

n	isomer	E	ΔE_{rel}	H	G	ΔG
5	V -a	-660.430	0	-660.1775255	-660.2521165	0.522
	V -j	-660.413	8.661	-660.1632545	-660.2408555	7.588
6	VI-a	-716.927	0	-716.6358561	-716.7157521	3.495
	VI-g	-716.916	6.103	-716.6256369	-716.7076059	8.607
	VI-h	-716.915	7.573	-716.6246076	-716.7014876	12.446

Data S1: The coordinates of (H₂C₂O₄)(NH₃)_n (n=1~6) isomers

(H₂C₂O₄)(NH₃)₁

Isomer I -a

C	-0.639276	-0.754418	0.000033
C	-0.537555	0.807113	0.000052
O	-1.917020	-1.128235	0.000028
O	0.294250	-1.527973	0.000062
O	-1.599962	1.418935	-0.000325
O	0.639807	1.362387	0.000382
H	-2.410290	-0.263538	0.000047
H	1.486658	0.713407	0.000436
N	2.786220	-0.104510	-0.000208`

H	3.375442	0.007399	-0.824546
H	3.374968	0.006350	0.824625
H	2.394060	-1.049134	-0.000795

(H₂C₂O₄)(NH₃)₂

Isomer II -a

C	0.817538	-0.756859	-0.281213
C	1.296493	0.656309	0.203889
O	1.822969	-1.624668	-0.227260
O	-0.308784	-1.039386	-0.650364
O	2.491472	0.694426	0.535703
O	0.447200	1.607468	0.223139
H	2.565717	-1.039673	0.116485
H	-0.777185	1.430010	-0.187861
N	-2.983417	-0.969069	0.704320
H	-2.155331	-1.459731	0.351731
H	-2.961408	-1.032591	1.722281
H	-3.805451	-1.486074	0.392845
N	-1.929876	1.396792	-0.556541
H	-2.402571	2.287156	-0.397773
H	-1.939430	1.191721	-1.556182
H	-2.438329	0.615704	-0.061775

Isomer II -b

C	-0.127577	0.832002	0.000237
C	-0.093779	-0.730515	0.000238
O	1.098075	1.353123	0.000072
O	-1.135934	1.505352	0.000352
O	1.005043	-1.271242	-0.000075
O	-1.228699	-1.370425	0.000659
H	1.732820	0.589146	-0.000048
H	-2.124010	-0.792893	0.000225
N	4.063418	-0.220193	-0.000379
H	4.005503	0.373746	-0.825597
H	4.002415	0.368658	0.828258
H	3.279268	-0.872727	-0.003770
N	-3.505970	-0.110558	-0.000626
H	-3.216026	0.869791	0.000336
H	-4.079624	-0.281407	-0.825927
H	-4.082227	-0.282437	0.822636

(H₂C₂O₄)(NH₃)₃

Isomers III -a

C	1.624186	0.469353	0.077415
C	1.135100	-1.023775	0.062415
O	2.925484	0.530150	-0.192369
O	0.926063	1.444828	0.293385
O	2.039058	-1.837197	-0.213052
O	-0.086934	-1.238029	0.314046
H	3.134016	-0.448213	-0.316013
H	-1.085537	-0.119157	0.653699
N	-2.046624	0.395231	0.774240
H	-2.256277	0.529993	1.763083
H	-2.018045	1.331384	0.281176
H	-2.720096	-0.283724	0.348266
N	-2.936097	-2.039072	-0.461508
H	-3.421180	-2.799453	0.015230
H	-3.164256	-2.126154	-1.452068
H	-1.928113	-2.217886	-0.368028
N	-1.529174	2.894852	-0.513774
H	-1.734169	3.797799	-0.086191
H	-1.677631	3.003549	-1.517054
H	-0.530526	2.703294	-0.369868

Isomer III -b

C	-1.570061	0.002309	0.738034
C	-1.068843	-0.001214	-0.757295
O	-0.713665	0.004387	1.663134
O	-2.818386	0.002417	0.813054
O	0.096610	-0.002142	-1.132386
O	-2.108807	-0.003489	-1.578132
H	0.762766	0.003314	1.451311
H	-2.862793	-0.001892	-0.894410
N	2.161455	-2.184136	-0.501478
H	2.956081	-2.381925	-1.109310
H	1.456222	-1.694429	-1.062336
H	1.760558	-3.084224	-0.236508
N	1.865852	0.002358	1.355266
H	2.139691	0.853968	0.801000
H	2.311185	0.003893	2.272537
H	2.138492	-0.851838	0.804403
N	2.164456	2.180581	-0.510604
H	1.765540	3.082937	-0.250430
H	1.458044	1.689231	-1.068564

H 2.959279 2.373386 -1.119780

Isomer III -c

C -1.856086 -0.581459 -0.237764
C -1.181468 0.725053 0.332600
O -3.059159 -0.293305 -0.724952
O -1.371563 -1.700339 -0.258233
O -1.875088 1.746474 0.173555
O -0.034021 0.627268 0.869830
H -3.101510 0.698045 -0.555854
H 0.677164 -0.670233 0.928958
N 3.448086 -0.824573 -0.668726
H 3.455582 -1.070354 -1.659370
H 3.233791 0.193138 -0.600629
H 4.400244 -0.963288 -0.328976
N 2.432239 1.997906 -0.251039
H 2.214022 2.549868 -1.081617
H 1.530750 1.767199 0.189395
H 2.916840 2.630250 0.386940
N 1.205579 -1.642279 0.827554
H 1.412703 -2.063522 1.732464
H 0.505068 -2.204625 0.325759
H 2.098005 -1.486204 0.257787

Isomer III -d

C 1.856051 -0.581513 -0.237679
C 1.181445 0.725094 0.332544
O 3.059044 -0.293361 -0.725028
O 1.371578 -1.700420 -0.257903
O 1.875043 1.746484 0.173222
O 0.034073 0.627347 0.869928
H 3.101294 0.698015 -0.556098
H -0.677294 -0.670163 0.929125
N -3.447895 -0.824545 -0.669069
H -3.455140 -1.070288 -1.659723
H -4.400137 -0.963273 -0.329563
H -3.233595 0.193166 -0.600878
N -2.432155 1.997785 -0.250796
H -2.916627 2.629896 0.387511
H -1.530542 1.766982 0.189350
H -2.214180 2.550031 -1.081249
N -1.205727 -1.642146 0.827635
H -1.413005 -2.063364 1.732519
H -2.098074 -1.486028 0.257714

H -0.505140 -2.204516 0.325966

Isomer III -e

C -1.134953 -1.023931 0.062129
C -1.624256 0.469063 0.077512
O 0.087150 -1.238058 0.313541
O -2.038798 -1.837485 -0.213271
O -0.926270 1.444616 0.293503
O -2.925639 0.529753 -0.191980
H 1.085458 -0.119150 0.653467
H -3.134119 -0.448586 -0.315762
N 2.936828 -2.038582 -0.461156
H 1.928848 -2.217623 -0.368091
H 3.165444 -2.125838 -1.451600
H 3.421852 -2.798780 0.015944
N 1.528606 2.895047 -0.513941
H 0.529973 2.703444 -0.369952
H 1.733477 3.798262 -0.086850
H 1.676996 3.003283 -1.517289
N 2.046333 0.395603 0.774351
H 2.255576 0.530484 1.763269
H 2.017636 1.331722 0.281243
H 2.720213 -0.283090 0.348659

Isomer III -f

C 0.709327 1.019785 0.065218
C 0.304665 -0.435546 0.471464
O -0.274474 1.832954 -0.202527
O 1.889244 1.348474 0.026623
O -0.810311 -0.666303 0.915734
O 1.213098 -1.375923 0.320111
H -1.299713 1.466169 -0.141957
H 2.150478 -1.077174 -0.027951
N -2.777221 1.263202 -0.125667
H -3.037490 0.289046 -0.373566
H -3.297062 1.905294 -0.724339
H -3.088572 1.418211 0.833677
N 3.663307 -0.786181 -0.493232
H 4.398659 -1.114659 0.131198
H 3.939527 -1.007390 -1.448737
H 3.578416 0.230102 -0.400343
N -3.206185 -1.698216 -0.538946
H -3.945023 -2.215400 -0.062600
H -2.359252 -1.776418 0.034506

H -3.023685 -2.188471 -1.414593

(H₂C₂O₄)(NH₃)₄

Isomer IV -a

C 1.718357 -0.341253 0.000075
C 1.281676 1.173770 0.001022
O 3.042190 -0.429997 -0.001350
O 0.969727 -1.308808 0.000471
O 2.260810 1.951475 0.000292
O 0.047455 1.428654 0.002361
H 3.281135 0.556060 -0.001081
H -1.057506 0.283421 0.000804
N -1.977761 -0.278629 -0.000298
H -1.976365 -0.885825 0.850116
H -1.974739 -0.885663 -0.850859
H -2.720553 0.443302 -0.001006
N -1.171113 -2.038421 -2.170431
H -0.275663 -2.033616 -1.670392
H -1.433111 -3.013333 -2.316037
H -0.998150 -1.640579 -3.093953
N -2.879036 2.511863 -0.001704
H -3.218344 3.021715 0.814392
H -3.216906 3.021561 -0.818491
H -1.855598 2.597168 -0.000790
N -1.172753 -2.038275 2.170383
H -0.277625 -2.034189 1.669751
H -0.999275 -1.638514 3.092987
H -1.434324 -3.012972 2.318147

Isomer IV -b

C -1.817752 0.526985 0.000140
C -1.350978 -0.974879 0.000723
O -3.147241 0.599070 -0.000346
O -1.081105 1.497194 0.000103
O -2.299483 -1.786178 0.000650
O -0.104262 -1.188550 0.000299
H -3.384099 -0.380108 -0.000178
H 0.965887 0.099293 -0.000058
N 1.302373 3.326190 0.000317
H 0.320653 3.027763 0.000451
H 1.439660 3.919720 -0.817770
H 1.440010 3.919276 0.818670
N 2.141708 -1.385618 -2.199467
H 1.865360 -1.159639 -3.155424
H 2.757168 -2.196914 -2.261518

H	1.291853	-1.688813	-1.708934
N	1.950655	0.511277	-0.000277
H	2.385650	0.100067	-0.850425
H	2.386073	0.099861	0.849562
H	1.915339	1.561146	-0.000139
N	2.143236	-1.386051	2.198355
H	2.759209	-2.197001	2.259845
H	1.293362	-1.689600	1.708079
H	1.867180	-1.160564	3.154512

Isomer IV -c

C	-2.137574	-0.018465	-0.106006
C	-1.115469	-1.210641	-0.056467
O	-3.372713	-0.464147	0.112394
O	-1.861400	1.150962	-0.307449
O	-1.652348	-2.311801	0.183352
O	0.105642	-0.943439	-0.250391
H	-3.194526	-1.448515	0.235745
H	0.687872	0.486181	-0.559238
N	1.287674	1.367213	-0.754911
H	0.881421	2.186634	-0.228480
H	1.249784	1.570955	-1.754128
H	2.290856	1.152865	-0.468998
N	2.691231	-2.315685	0.329596
H	2.699063	-2.774356	1.241369
H	1.712753	-2.045907	0.143444
H	2.930367	-3.038594	-0.350050
N	-0.193509	3.413783	0.636193
H	-0.107842	3.513923	1.647641
H	-1.030627	2.847844	0.454082
H	-0.365365	4.346565	0.261374
N	3.863722	0.450830	0.060038
H	3.595083	-0.549102	0.188615
H	4.222661	0.786382	0.954713
H	4.649487	0.474168	-0.590912

Isomer IV -d

C	-1.313357	0.541328	0.471215
C	-1.942009	-0.453332	-0.576797
O	-2.182173	1.501196	0.754655
O	-0.190920	0.472121	0.955743
O	-3.119197	-0.137367	-0.866427
O	-1.237785	-1.405083	-1.001472
H	-2.960045	1.193356	0.170184

H	0.254547	-1.581097	-0.723852
N	1.319015	-1.807439	-0.600335
H	1.526687	-2.702692	-1.043605
H	1.523047	-1.861132	0.429937
H	1.907059	-1.041335	-1.046603
N	1.926761	2.546288	0.174754
H	1.484035	3.369630	-0.235068
H	2.532550	2.891040	0.919960
H	1.177750	2.004799	0.622299
N	2.800436	0.356065	-1.764912
H	3.815209	0.295946	-1.855816
H	2.442128	0.588184	-2.692502
H	2.592805	1.166868	-1.148892
N	1.505953	-1.637730	2.282900
H	2.314242	-1.321266	2.818001
H	1.029004	-2.337379	2.851631
H	0.868615	-0.840123	2.180977

Isomer IV -e

C	0.283369	-1.017505	0.015581
C	-0.255846	0.334732	-0.521771
O	-0.611048	-1.855158	0.475696
O	1.484018	-1.263757	-0.018734
O	-1.237318	0.349796	-1.256350
O	0.391729	1.415287	-0.158531
H	-1.643503	-1.535946	0.420876
H	1.260516	1.271124	0.474606
N	2.501839	1.250547	1.317896
H	3.264870	0.906704	0.699499
H	2.413401	0.582954	2.084076
H	2.773105	2.149639	1.715465
N	-3.569097	1.664879	0.044382
H	-2.769810	1.596266	-0.597184
H	-4.359508	2.025835	-0.489746
H	-3.334475	2.376767	0.736318
N	4.186584	-0.119100	-0.700308
H	4.963411	-0.757978	-0.533000
H	3.328752	-0.681205	-0.743075
H	4.331774	0.288481	-1.623745
N	-3.134912	-1.303144	0.404878
H	-3.477048	-1.692170	-0.474454
H	-3.643988	-1.761735	1.160767
H	-3.382581	-0.293718	0.402165

Isomer IV -f

C	1.602118	0.709788	0.188859
C	1.517626	-0.863674	0.120635
O	2.646664	1.135482	-0.512345
O	0.822049	1.455829	0.761365
O	2.421177	-1.361305	-0.582855
O	0.572957	-1.443989	0.729850
H	3.015655	0.251731	-0.838960
H	-0.474176	-0.655913	1.531468
N	-3.004688	0.121580	-0.066564
H	-2.722620	-0.720329	-0.600514
H	-4.022700	0.161951	-0.039873
H	-2.657361	0.957193	-0.567456
N	-1.256631	-0.051172	1.996911
H	-1.571284	-0.441940	2.884277
H	-2.080033	0.038077	1.257417
H	-0.819698	0.864085	2.134669
N	-1.444959	2.572423	-1.166660
H	-0.613985	2.443891	-0.579981
H	-1.753809	3.535526	-1.030628
H	-1.126078	2.510889	-2.134432
N	-1.644280	-2.397038	-1.217200
H	-1.309719	-2.384387	-2.181579
H	-0.810252	-2.313334	-0.622083
H	-2.021275	-3.332823	-1.062821

Isomer IV -g

C	1.220505	-1.128232	-0.070981
C	0.619253	0.217597	-0.611966
O	0.362465	-2.027427	0.229126
O	2.451833	-1.226472	0.019070
O	-0.426643	0.232808	-1.259120
O	1.260116	1.338304	-0.340149
H	-0.947575	-1.885578	-0.057614
H	2.173844	1.235964	0.154400
N	-2.085298	-1.823827	-0.356709
H	-2.630816	-1.197752	0.305706
H	-2.519283	-2.744096	-0.423751
H	-2.066872	-1.370771	-1.272845
N	-2.317346	2.404944	-0.298391
H	-1.605535	1.847624	-0.790542
H	-2.891135	2.854620	-1.012410
H	-1.814557	3.154856	0.177504

N	-3.401883	0.078243	1.334435
H	-4.416048	0.100904	1.444861
H	-3.007829	0.107588	2.275736
H	-3.119820	0.957986	0.856128
N	3.632988	1.163384	0.817455
H	3.760543	1.334437	1.813435
H	3.672312	0.150288	0.641878
H	4.392833	1.620833	0.316252

Isomer IV -h

C	-2.378500	-0.501194	-0.222221
C	-1.524832	0.766965	0.169992
O	-3.516320	-0.118047	-0.791856
O	-2.072605	-1.670277	-0.052812
O	-2.070292	1.840549	-0.153753
O	-0.408145	0.594147	0.745767
H	-3.409942	0.884106	-0.769321
H	0.166523	-0.781970	0.987073
N	1.816828	2.598310	0.270198
H	1.532542	3.242174	-0.469594
H	1.990907	3.179198	1.091405
H	0.985409	2.029343	0.485095
N	0.479572	-1.833675	1.054168
H	-0.356059	-2.305010	0.674592
H	0.632546	-2.115096	2.022131
H	1.356935	-2.015301	0.456493
N	2.761148	-2.135206	-0.554425
H	2.500059	-2.342115	-1.519930
H	3.229497	-1.199794	-0.558222
H	3.466243	-2.826768	-0.295979
N	4.003629	0.598163	-0.516538
H	3.288516	1.305578	-0.251906
H	4.367502	0.878297	-1.428730
H	4.779976	0.708613	0.137684

(H₂C₂O₄)(NH₃)₅

Isomer V -a

C	-1.354749	-1.159157	0.078431
C	-2.197446	0.110952	-0.307460
O	-0.128709	-0.984285	0.335589
O	-2.023395	-2.214323	0.079715
O	-1.771989	1.248528	-0.386889
O	-3.464260	-0.229418	-0.542650
H	0.671461	0.520042	0.118300

H	-3.421308	-1.222704	-0.383792
N	-0.021523	3.670647	-0.493409
H	0.106535	4.115318	-1.402297
H	-0.222012	4.416676	0.172506
H	-0.859689	3.082298	-0.555553
N	2.129999	-2.546563	-0.907586
H	1.806010	-3.005120	-1.760301
H	1.286956	-2.189781	-0.432808
H	2.505675	-3.290227	-0.317901
N	1.419205	1.254786	0.266895
H	2.270026	0.981422	-0.297293
H	1.624092	1.179248	1.283384
H	1.046051	2.201407	0.010537
N	3.587094	0.108017	-1.253321
H	4.534805	0.095369	-0.875121
H	3.216511	-0.862767	-1.201578
H	3.674420	0.347672	-2.241511
N	1.284442	0.078604	2.945101
H	1.994336	-0.480694	3.418241
H	0.669778	0.443482	3.673244
H	0.721837	-0.564865	2.376242

Isomer V -b

C	-2.170523	-0.283858	-0.000077
C	-1.095430	-1.440272	-0.000321
O	-1.756943	0.898510	0.000163
O	-3.336418	-0.751567	-0.000139
O	0.124234	-1.297274	-0.000309
O	-1.693385	-2.618570	-0.000567
H	0.787300	0.364765	-0.000260
H	-2.665349	-2.300448	-0.000564
N	-0.347357	2.464454	-2.096237
H	-0.589605	3.452008	-2.175961
H	-0.377778	2.079411	-3.040372
H	-1.093507	2.005190	-1.554021
N	-0.346690	2.463533	2.096864
H	-0.376760	2.078150	3.040872
H	-0.589013	3.451034	2.177019
H	-1.092970	2.004393	1.554723
N	2.998581	-2.413394	0.001099
H	1.984600	-2.249828	0.000015
H	3.200898	-2.994430	-0.813243
H	3.199448	-2.992121	0.817444
N	4.045065	0.477205	-0.000662

H	3.835681	-0.539764	-0.000127
H	4.624935	0.669079	-0.818170
H	4.625735	0.669792	0.816109
N	1.263400	1.297131	-0.000183
H	2.306960	1.154862	-0.000356
H	0.911997	1.810846	-0.846712
H	0.912245	1.810533	0.846639

Isomer V -c

C	1.628778	-0.001231	0.569181
C	2.179680	-0.001597	-0.905741
O	0.368037	-0.000961	0.725968
O	2.521924	-0.001225	1.438649
O	1.510148	-0.001664	-1.920795
O	3.514426	-0.001663	-0.896176
H	-0.631833	-0.000073	-0.557856
H	3.701037	-0.001472	0.089940
N	-1.092129	-2.472811	1.776235
H	-0.432516	-3.243063	1.894122
H	-1.542935	-2.348779	2.683473
H	-0.525590	-1.629836	1.609224
N	-1.086909	2.473672	1.776695
H	-0.425440	3.242289	1.894857
H	-0.522350	1.629339	1.609814
H	-1.538326	2.350703	2.683775
N	-2.723000	-2.455916	-0.808775
H	-2.504467	-3.267624	-1.387513
H	-3.730625	-2.476820	-0.649495
H	-2.256963	-2.595076	0.109782
N	-1.335362	0.000698	-1.365043
H	-0.757604	0.000398	-2.208892
H	-1.922241	0.878241	-1.298751
H	-1.923786	-0.875837	-1.299165
N	-2.717126	2.460631	-0.808777
H	-2.250985	2.598592	0.109914
H	-2.496010	3.271601	-1.387573
H	-3.724733	2.484574	-0.649805

Isomer V -d

C	-1.932391	0.464547	-0.403888
C	-1.595445	-0.955989	0.187535
O	-1.007386	1.315024	-0.444684
O	-3.126610	0.551063	-0.771793
O	-0.516422	-1.312274	0.641727

O	-2.664367	-1.739102	0.119696
H	0.558487	0.996582	-0.001780
H	-3.324122	-1.086124	-0.295270
N	3.225400	-0.453855	-1.446165
H	3.170506	-0.216092	-2.437341
H	2.758493	-1.373345	-1.326034
H	4.215453	-0.584290	-1.235902
N	1.335704	-0.221607	2.843952
H	2.013173	-0.875705	3.235574
H	0.629788	-0.773472	2.343880
H	0.866258	0.222344	3.633418
N	1.570922	-2.981395	-0.912688
H	1.125516	-3.390526	-1.735077
H	0.817249	-2.571447	-0.348711
H	1.946206	-3.764572	-0.376656
N	1.569326	1.171473	0.288045
H	1.676690	0.823136	1.267903
H	2.233489	0.659598	-0.353735
H	1.664897	2.203474	0.219200
N	0.632496	3.892383	-0.272509
H	-0.200475	3.317021	-0.451156
H	0.369852	4.587208	0.426849
H	0.826909	4.408173	-1.131045

Isomer V -e

C	0.146676	-1.850464	0.189249
C	1.510292	-1.310236	-0.374678
O	-0.836463	-1.057930	0.187521
O	0.216370	-3.032679	0.587692
O	1.698555	-0.200636	-0.845224
O	2.455223	-2.240510	-0.258870
H	-0.707488	0.458353	-0.310149
H	1.918369	-2.990760	0.152515
N	-3.807987	-1.047012	0.480362
H	-4.120033	-1.196060	1.440624
H	-2.797183	-1.251766	0.462705
H	-4.262401	-1.770642	-0.077880
N	-3.661276	1.772623	-0.623343
H	-3.854058	0.822915	-0.239839
H	-4.171011	1.853371	-1.503903
H	-4.082167	2.449105	0.014565
N	3.469153	2.083598	0.070811
H	4.168423	1.789462	0.753386
H	3.980735	2.555793	-0.675190

H	3.073074	1.226479	-0.334867
N	-0.800370	1.476386	-0.647710
H	-0.266960	2.127217	0.000785
H	-0.369661	1.523743	-1.571614
H	-1.830371	1.719009	-0.697147
N	0.792265	3.139340	1.070892
H	1.760962	2.883882	0.793336
H	0.718962	4.156155	1.024545
H	0.687023	2.887436	2.054665

Isomer V -f

C	-0.894076	0.260840	0.472601
C	-0.602310	-0.964560	-0.440032
O	-0.117871	0.404695	1.460277
O	-1.834956	1.016601	0.127495
O	0.521411	-1.132500	-0.913059
O	-1.586932	-1.811468	-0.689643
H	1.416254	0.085416	1.333616
H	-2.504169	-1.494622	-0.319891
N	-3.941639	-0.881366	0.119601
H	-4.344618	-1.111546	1.026536
H	-4.683865	-0.926045	-0.576898
H	-3.571836	0.079074	0.156121
N	2.851539	-2.621401	0.096701
H	2.664490	-3.441918	0.673114
H	3.591321	-2.881562	-0.555388
H	2.003679	-2.435958	-0.455303
N	-0.037936	3.491007	-0.185770
H	-0.750878	2.772725	0.005881
H	-0.472169	4.181667	-0.798690
H	0.136708	3.962172	0.702463
N	2.238415	1.664844	-1.145876
H	1.527372	2.376575	-0.885233
H	1.743304	0.939515	-1.671244
H	2.907614	2.102170	-1.778513
N	2.475759	0.061438	1.118898
H	2.755574	-0.915834	0.846458
H	2.586690	0.721882	0.277390
H	3.016648	0.388341	1.918738

Isomer V -g

C	0.449234	-1.342003	0.394866
C	-1.123091	-1.275400	0.477127
O	1.120243	-0.686920	1.218834

O	0.834516	-2.043710	-0.586625
O	-1.783048	-0.570335	1.219809
O	-1.658755	-2.056311	-0.467833
H	0.388889	0.897131	1.914618
H	-0.809156	-2.410880	-0.893420
N	-0.009824	1.851390	2.001036
H	-0.247469	2.172777	0.331566
H	0.611323	2.405892	2.589790
H	-0.889844	1.737101	2.504598
N	3.697444	0.328000	0.041957
H	4.356435	-0.400583	-0.234280
H	2.943521	-0.140981	0.568178
H	4.194056	0.934470	0.694805
N	-0.436923	2.220166	-0.734798
H	-0.385736	3.190680	-1.046717
H	-1.412954	1.849492	-0.912139
H	0.306656	1.630721	-1.271727
N	1.507386	0.667361	-2.005929
H	1.250514	-0.323820	-1.925628
H	2.376460	0.749633	-1.443743
H	1.749404	0.838701	-2.982216
N	-3.086442	1.061958	-0.948493
H	-3.002670	0.467363	-0.113115
H	-3.922812	1.634965	-0.835008
H	-3.268605	0.427845	-1.727423

Isomer V -h

C	-2.520430	-0.199344	-0.055899
C	-1.335854	-1.229858	-0.115729
O	-3.660437	-0.828030	0.221907
O	-2.430609	1.003413	-0.229227
O	-1.695307	-2.405292	0.112656
O	-0.179437	-0.788585	-0.372013
H	-3.331881	-1.778835	0.294735
H	0.184463	0.728794	-0.631237
N	-1.076520	3.390329	0.879894
H	-1.403411	4.325702	0.638623
H	-0.917345	3.383809	1.887367
H	-1.842169	2.734481	0.686925
N	4.061773	-0.702906	0.965278
H	5.020261	-1.046940	0.892468
H	3.441460	-1.456841	0.605482
H	3.868598	-0.620163	1.964610
N	2.104521	-2.766706	-0.130823

H	1.262788	-2.184481	-0.256997
H	1.823777	-3.534606	0.480678
H	2.302366	-3.191563	-1.037705
N	0.547024	1.724155	-0.847231
H	1.609692	1.772067	-0.754547
H	0.276981	1.951914	-1.804965
H	0.069891	2.409251	-0.203818
N	3.388609	1.780214	-0.582148
H	3.890646	1.732818	-1.470266
H	3.766240	2.589905	-0.087565
H	3.663812	0.932249	-0.035392

Isomer V -i

C	-1.372385	-1.085115	0.264230
C	-0.804066	0.131301	-0.535220
O	-0.540685	-1.658865	1.031640
O	-2.566472	-1.383472	0.074776
O	0.288862	0.073962	-1.104352
O	-1.515958	1.244082	-0.572589
H	0.935194	-1.380617	1.072233
H	-2.471105	1.165121	-0.153852
N	2.818623	1.397166	1.695659
H	2.332458	1.775548	2.509987
H	2.498155	1.945799	0.870970
H	3.808409	1.606909	1.830925
N	-3.978669	0.995837	0.345130
H	-4.251250	1.263980	1.289253
H	-3.888319	-0.031400	0.300338
H	-4.711695	1.296983	-0.295051
N	2.037482	-1.316900	1.113653
H	2.387787	-1.969989	1.814696
H	2.355651	-0.332497	1.350692
H	2.386625	-1.593855	0.160116
N	1.709516	2.732387	-0.793955
H	2.309587	3.027252	-1.564669
H	1.022673	3.476061	-0.663854
H	1.179930	1.909962	-1.115519
N	2.412321	-1.931465	-1.668958
H	3.118793	-1.596624	-2.323243
H	2.136483	-2.863464	-1.978060
H	1.588453	-1.321113	-1.755516

Isomer V -j

C	0.041482	0.786197	-0.588925
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C	-1.072488	-0.241657	-0.173269
O	-0.135412	2.056264	-0.286774
O	1.061183	0.411960	-1.165973
O	-2.245064	0.163720	-0.097038
O	-0.666888	-1.428778	0.047888
H	-1.053396	2.310607	0.143672
H	0.627156	-1.845099	-0.254840
N	3.656334	1.465343	-0.018489
H	3.517118	2.299442	0.552951
H	2.784489	1.326450	-0.547756
H	4.381752	1.702420	-0.695898
N	3.590864	-1.267591	1.297017
H	3.212772	-1.182145	2.241474
H	3.727601	-0.302228	0.932261
H	4.513204	-1.693653	1.392179
N	-4.287008	-2.280835	0.132785
H	-3.631571	-1.492866	0.070912
H	-3.750543	-3.052691	0.531099
H	-4.981534	-2.027847	0.836883
N	-2.456606	2.825697	0.713268
H	-2.565763	3.037655	1.703588
H	-2.932470	3.550641	0.178480
H	-2.893069	1.917109	0.513123
N	1.665094	-2.239698	-0.557472
H	1.661072	-3.247973	-0.711085
H	1.871917	-1.746796	-1.428609
H	2.406003	-1.966007	0.160133

(H₂C₂O₄)(NH₃)₆

Isomers VI -a

C	-2.388623	0.465398	-0.009478
C	-1.635553	-0.914249	-0.008119
O	-3.707928	0.268811	-0.002596
O	-1.865726	1.563179	-0.015523
O	-2.405936	-1.898863	-0.000306
O	-0.370645	-0.891634	-0.014427
H	-3.746189	-0.736732	0.001321
H	0.635030	0.522623	-0.001702
N	2.896240	0.305499	-2.363155
H	3.890697	0.084572	-2.303110
H	2.383577	-0.592697	-2.465724
H	2.769250	0.828063	-3.230546
N	2.801437	0.320835	2.445844
H	2.310715	-0.592855	2.512497

H	2.608534	0.831968	3.307895
H	3.803871	0.129897	2.442472
N	1.455718	1.184764	0.011536
H	2.044306	0.982659	-0.839102
H	2.010517	0.988888	0.886097
H	1.104385	2.172073	0.001319
N	0.116443	3.795004	-0.018388
H	-0.773573	3.284893	-0.021318
H	0.112707	4.409494	0.795564
H	0.124887	4.397720	-0.841060
N	1.113378	-2.217570	2.282417
H	1.531319	-3.117798	2.044536
H	0.543091	-1.932110	1.473284
H	0.458761	-2.405663	3.042861
N	1.129592	-2.183168	-2.318004
H	1.507389	-3.107462	-2.106748
H	0.487364	-2.316082	-3.100351
H	0.550642	-1.907832	-1.511539

Isomers VI -b

C	-1.565463	1.445533	0.240681
C	-0.144611	1.975742	-0.182970
O	-1.656649	0.241033	0.572794
O	-2.435068	2.349742	0.166852
O	0.883288	1.309874	-0.245638
O	-0.203927	3.264421	-0.479365
H	0.741865	-0.502211	0.053267
H	-1.199213	3.419651	-0.321367
N	3.799211	-1.701557	0.181549
H	3.986445	-0.705601	-0.045509
H	4.290460	-1.911861	1.051060
H	4.243004	-2.266890	-0.542992
N	-3.311364	-1.685650	-0.980970
H	-4.020835	-2.160880	-0.422057
H	-3.817888	-1.205078	-1.725667
H	-2.903528	-0.949487	-0.383724
N	0.888862	-1.515493	0.251913
H	0.452112	-1.700607	1.188716
H	0.383274	-2.088959	-0.481161
H	1.923566	-1.709947	0.253725
N	3.938106	1.292755	-0.471373
H	4.282631	1.589142	-1.385107
H	2.931616	1.498946	-0.454212
H	4.375463	1.913133	0.210829

N	-0.704524	-1.585391	2.677303
H	-1.351450	-2.334735	2.922367
H	-0.397131	-1.164473	3.553960
H	-1.237709	-0.870571	2.161243
N	-0.661257	-2.988480	-1.698199
H	-0.702629	-4.005955	-1.628283
H	-0.443189	-2.777787	-2.673050
H	-1.620789	-2.627347	-1.517010

Isomers VI -c

C	0.823244	-1.439517	0.129023
C	-0.748098	-1.380570	0.020904
O	1.337251	-1.840916	-1.042878
O	1.496262	-1.123676	1.091491
O	-1.145383	-1.692693	-1.142759
O	-1.402590	-1.007398	1.014104
H	0.472181	-1.978901	-1.558984
H	-0.580085	0.370091	2.055011
N	2.260711	1.351044	-1.570038
H	2.992384	1.171292	-0.856103
H	2.690967	1.893177	-2.320034
H	2.038409	0.432609	-1.961951
N	-0.127483	2.315671	-0.335879
H	-0.988333	1.893624	-0.854211
H	0.776715	1.999418	-0.813434
H	-0.182134	3.334490	-0.366647
N	4.123163	0.335865	0.616154
H	3.378131	-0.319726	0.886405
H	4.904685	-0.227113	0.279464
H	4.444682	0.796498	1.467663
N	-0.128967	1.271622	2.292906
H	-0.122622	1.995344	0.690283
H	-0.643774	1.689293	3.067882
H	0.799226	1.027871	2.639533
N	-2.304586	1.113693	-1.605119
H	-2.685232	1.481142	-2.477298
H	-3.085232	1.023043	-0.929699
H	-2.004074	0.145741	-1.781438
N	-4.148964	0.161985	0.601572
H	-4.852602	-0.500962	0.275000
H	-4.501563	0.548495	1.477306
H	-3.304054	-0.386592	0.824856

Isomers VI -d

C	-1.292374	-1.330158	-0.668426
C	0.230224	-1.227027	-1.058888
O	-1.523928	-2.481171	-0.029852
O	-2.144873	-0.479469	-0.853764
O	0.894123	-2.214920	-0.625223
O	0.615817	-0.222046	-1.688928
H	-0.591977	-2.875107	-0.045822
H	-0.429703	1.319331	-1.912057
N	1.888083	-1.605095	2.197270
H	2.847345	-1.897963	2.386237
H	1.294370	-2.160548	2.814163
H	1.672400	-1.901496	1.235442
N	3.250389	1.019207	-1.034758
H	2.442044	0.484899	-1.390709
H	4.033147	0.366077	-0.986444
H	3.494852	1.703757	-1.750907
N	-0.681340	2.429884	0.960309
H	-1.465718	1.842479	1.353488
H	0.305113	2.032490	1.256967
H	-0.776598	3.383099	1.312821
N	-0.934509	2.221882	-1.824535
H	-0.771715	2.439323	-0.115316
H	-0.550177	2.870560	-2.511200
H	-1.898493	2.025453	-2.094895
N	1.806825	1.448959	1.635204
H	1.781041	0.467592	1.966264
H	2.325410	1.982911	2.334085
H	2.382983	1.437619	0.771292
N	-2.894456	0.721630	1.777197
H	-2.741229	0.037404	2.518856
H	-2.932628	0.193535	0.894647
H	-3.821624	1.117270	1.934312

Isomers VI -e

C	-1.030961	0.071546	-0.505378
C	-1.282868	-1.180706	0.394435
O	-1.981650	0.986157	-0.604667
O	0.038753	0.211934	-1.101744
O	-2.373282	-1.770715	0.265831
O	-0.315530	-1.487228	1.154876
H	-2.887631	0.717341	-0.160465
H	0.956388	-0.619837	1.340788
N	3.903208	-1.228591	-0.077804
H	4.584652	-1.893652	0.288629

H	3.226272	-1.759590	-0.666752
H	4.414275	-0.595101	-0.693244
N	0.746006	3.104080	-1.490852
H	0.451936	2.119546	-1.568145
H	1.379916	3.295836	-2.266721
H	-0.090023	3.666420	-1.652465
N	1.621587	2.758622	1.381244
H	1.367976	2.975691	0.394576
H	2.448292	3.313556	1.606990
H	0.866084	3.124970	1.962708
N	1.562482	-2.443274	-1.463056
H	1.058313	-3.044998	-0.809212
H	1.032324	-1.562185	-1.479930
H	1.475298	-2.870795	-2.384820
N	-4.312068	0.220505	0.379876
H	-5.092862	0.275298	-0.272208
H	-4.650756	0.484235	1.303558
H	-3.964271	-0.751441	0.412807
N	1.880696	-0.109399	1.620423
H	2.074270	-0.327126	2.598959
H	1.788559	0.943606	1.520129
H	2.684254	-0.471602	1.027299

Isomers VI -f

C	-0.308373	-1.762037	0.018262
C	-1.832937	-1.370895	-0.056138
O	0.491376	-0.915939	0.498182
O	-0.083641	-2.902864	-0.451952
O	-2.322314	-0.314877	0.308848
O	-2.531137	-2.363467	-0.604029
H	-0.104538	0.365468	1.779515
H	-1.787089	-3.029550	-0.768456
N	-0.468017	2.885773	0.159413
H	-0.229566	3.868335	0.293065
H	0.264026	2.392846	-0.499623
H	-1.441322	2.797910	-0.244175
N	1.303874	1.399021	-1.310482
H	1.162817	1.292983	-2.315577
H	1.059441	0.499440	-0.872410
H	2.323007	1.518587	-1.152538
N	-3.124148	2.301825	-0.822600
H	-3.298870	2.272161	-1.827463
H	-3.086631	1.326852	-0.494349
H	-3.947583	2.729720	-0.398521

N	-0.395798	1.169800	2.366109
H	-1.328041	0.942337	2.712777
H	0.226349	1.215539	3.172787
H	-0.441120	2.357371	1.096669
N	4.267885	1.262018	-0.616801
H	4.705549	1.817911	0.118747
H	4.121656	0.307871	-0.234488
H	4.959570	1.182461	-1.363124
N	3.470321	-1.521531	0.443000
H	2.444359	-1.428844	0.503763
H	3.792047	-1.822177	1.363970
H	3.640702	-2.310793	-0.182168

Isomers VI -g

C	-0.655717	-0.386255	0.988700
C	-0.631188	0.285850	-0.427316
O	-1.748034	-0.265752	1.706655
O	0.330058	-0.998980	1.403309
O	-1.675795	0.279302	-1.099869
O	0.499318	0.775406	-0.759829
H	-2.546794	0.278732	1.258684
H	1.701473	0.627656	0.176343
N	2.234396	3.324345	-0.666392
H	2.753085	3.606856	-1.498270
H	1.456359	2.732100	-0.983908
H	1.824139	4.174644	-0.279732
N	2.631427	0.801614	0.737054
H	2.431871	0.668830	1.728711
H	2.865563	1.789569	0.518944
H	3.394177	0.127152	0.429439
N	1.868137	-2.649721	-0.651010
H	1.317802	-2.149158	0.061637
H	1.691407	-3.645885	-0.520629
H	1.458167	-2.397244	-1.551464
N	-3.825310	1.006192	0.774574
H	-4.502109	1.323190	1.467961
H	-3.544987	1.806127	0.207592
H	-4.280328	0.333403	0.130193
N	-4.323096	-1.075190	-1.299258
H	-3.331588	-0.811176	-1.382534
H	-4.741056	-0.997370	-2.225948
H	-4.358019	-2.060960	-1.040454
N	4.440287	-1.200773	-0.169923
H	3.665499	-1.856601	-0.406022

H	5.062361	-1.676074	0.484266
H	4.979150	-1.036424	-1.020557

Isomers VI -h

C	-0.404609	-0.849825	-0.800953
C	0.578034	0.346668	-1.033956
O	0.030335	-1.846507	-0.148673
O	-1.588030	-0.754579	-1.246494
O	1.672493	0.117461	-1.607606
O	0.219867	1.485493	-0.578618
H	1.551502	-2.003866	-0.017423
H	-1.333737	1.837595	-0.558019
N	-3.909315	1.128615	1.570619
H	-4.903862	1.340262	1.655759
H	-3.815469	0.094663	1.470869
H	-3.480285	1.388593	2.459450
N	3.699446	-0.314286	1.944965
H	4.687919	-0.310911	2.198550
H	3.478816	0.622400	1.540691
H	3.177265	-0.395226	2.818405
N	2.974067	2.263586	0.529816
H	3.585152	2.354671	-0.283077
H	2.967490	3.174314	0.990328
H	2.031174	2.112456	0.139722
N	-2.382666	1.702674	-0.770941
H	-2.983013	1.650292	0.102202
H	-2.730334	2.387815	-1.439180
H	-2.299025	0.722494	-1.185160
N	2.629926	-1.890364	-0.175308
H	2.577781	-1.189133	-0.960040
H	3.103624	-1.429694	0.656790
H	3.082769	-2.759501	-0.451232
N	-3.389977	-1.781626	0.929310
H	-2.836455	-2.331247	1.587998
H	-2.777866	-1.633576	0.110515
H	-4.151681	-2.388597	0.624205

Data S2: Harmonic frequencies (in cm^{-1}) and IR intensities for $(\text{H}_2\text{C}_2\text{O}_4)(\text{NH}_3)_n$ ($n=1\sim 6$) isomers

$(\text{H}_2\text{C}_2\text{O}_4)(\text{NH}_3)_1$

Isomer I -a

#	Frequency	Infrared
1	60.9994	8.0863
2	117.9171	0.0085
3	132.3868	0.4123
4	160.2857	6.5773
5	226.6888	55.8709
6	322.1229	43.1225
7	369.9357	4.8618
8	404.0486	54.0684
9	454.0701	40.2362
10	466.9056	26.7036
11	563.2971	3.8239
12	676.9683	16.0498
13	804.7402	2.7937
14	805.7403	39.1850
15	830.2722	68.3916
16	1100.7235	126.8496
17	1159.2959	6.7422
18	1243.3951	54.1358
19	1290.2731	281.0922
20	1351.8581	962.2876
21	1417.9748	118.5278
22	1602.1792	51.8365
23	1627.7347	14.2661
24	1709.3027	176.5732
25	1778.4412	286.0028
26	2159.1216	2535.8360
27	3318.7973	191.2303
28	3387.1407	29.0618
29	3505.4038	63.0965
30	3531.4357	19.3314

$(\text{H}_2\text{C}_2\text{O}_4)(\text{NH}_3)_2$

Isomer II -a

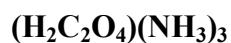
#	Frequency	Infrared
1	34.0819	0.5583
2	48.7033	3.6493
3	102.9048	9.3616

4	118.5109	1.1434
5	136.5841	6.6471
6	153.7197	0.3830
7	218.1095	212.3303
8	247.4513	57.9967
9	277.5922	37.0712
10	331.1091	19.7966
11	365.7070	331.5716
12	432.0672	146.5207
13	453.3256	39.9725
14	459.4173	46.9253
15	529.9556	70.9714
16	566.6357	22.0985
17	649.8279	53.1776
18	710.4576	25.3195
19	815.7582	0.0665
20	830.0247	405.1392
21	905.4763	65.6645
22	926.5383	2395.8764
23	1095.3754	128.8981
24	1162.1261	24.9438
25	1317.1311	274.4419
26	1387.5001	850.3657
27	1398.9225	191.5563
28	1468.8575	54.7261
29	1557.4319	76.7007
30	1606.4451	3.5676
31	1633.2623	22.5701
32	1653.7630	2.3304
33	1686.1579	14.2787
34	1702.8752	40.2984
35	1762.4982	620.4962
36	2883.5507	977.4470

Isomer II -b

#	Frequency	Infrared
1	23.7543	0.9853
2	60.1893	3.7875
3	62.3723	13.9107
4	86.7288	1.4115
5	92.4425	0.6471
6	113.9280	1.2616
7	123.4659	0.1295
8	159.7286	3.9091

9	221.0159	78.6009
10	230.3106	53.4120
11	304.0925	31.9466
12	335.7942	55.2103
13	365.2592	5.1808
14	401.1382	46.2821
15	452.8805	41.3009
16	463.5217	24.0510
17	554.6122	2.7968
18	681.0863	18.6156
19	799.7355	7.1118
20	808.4839	74.3890
21	824.4557	27.8519
22	892.4638	395.2869
23	1100.3411	119.5089
24	1154.4212	10.4309
25	1239.4348	52.8893
26	1265.6899	487.1278
27	1323.1951	694.6013
28	1394.0764	276.1253
29	1602.1715	53.2291
30	1607.6708	21.9863
31	1617.0971	9.0174
32	1626.7860	14.4563
33	1710.4210	223.7897
34	1771.0716	319.9579
35	2180.7979	2621.3160
36	3337.7566	412.1739



Isomers III -a

#	Frequency	Infrared
1	23.6157	0.5384
2	38.1832	2.5363
3	58.6758	1.1846
4	74.3800	1.9637
5	95.2867	15.9394
6	123.7547	6.1198
7	146.9582	15.6465
8	169.1824	0.4667
9	169.5759	2.1406
10	190.7888	32.2758
11	254.7892	33.5930
12	264.0591	4.5928

13	280.1022	81.4291
14	317.6402	66.3626
15	337.2363	96.8838
16	407.9517	54.7801
17	422.0989	82.6110
18	434.6766	72.5817
19	461.3334	42.0473
20	503.4232	55.6462
21	534.9526	14.8941
22	560.9694	15.3299
23	668.2892	21.7170
24	701.7214	22.9661
25	817.7463	0.1175
26	836.1056	19.0621
27	918.4723	62.3292
28	1108.3787	151.1903
29	1116.4079	109.2839
30	1161.5437	10.7813
31	1302.3077	254.3519
32	1341.2822	145.4796
33	1396.7347	419.6148
34	1484.8197	137.2037
35	1556.2864	100.3096
36	1605.7821	5.3874
37	1611.0145	7.0428
38	1635.2842	15.6756
39	1636.2869	12.2767
40	1647.7898	367.4619
41	1690.4177	10.8249
42	1706.2542	96.9136
43	1761.4996	598.0327
44	2329.4522	1761.0912
45	2829.1880	1060.6129
46	3039.9354	692.8696
47	3118.6653	310.5831
48	3334.5130	118.3275
49	3345.9286	162.8398
50	3470.1700	43.2933
51	3476.0821	74.3431
52	3491.0803	41.1614
53	3518.2041	7.5071
54	3521.4804	8.7004

Isomer III -b

#	Frequency	Infrared
1	36.1552	1.1654
2	37.9014	0.8733
3	52.3526	3.0289
4	93.0206	6.8536
5	110.0933	7.4619
6	115.6663	9.3122
7	136.1146	9.9338
8	160.5095	0.0023
9	164.3021	0.3204
10	228.6896	25.9476
11	234.9022	37.3329
12	263.0189	8.5064
13	283.7368	73.5135
14	321.0321	79.8023
15	335.4408	52.6010
16	343.1899	165.9604
17	407.2497	55.3452
18	429.1798	42.5605
19	460.1575	37.6750
20	541.0406	10.5113
21	550.7796	30.0993
22	586.1051	4.2399
23	698.6827	23.4598
24	721.3028	2.8091
25	818.8728	0.0728
26	831.0933	30.2835
27	971.6006	58.6969
28	1092.9563	101.4547
29	1097.3521	137.2847
30	1160.8486	4.6805
31	1310.3881	262.0445
32	1374.4985	8.7597
33	1404.6588	561.8824
34	1459.4864	24.4666
35	1562.9331	103.2517
36	1606.6782	6.8698
37	1617.0924	1.5107
38	1630.8242	0.3630
39	1636.7258	12.4443
40	1644.5220	365.9712
41	1699.8555	19.7955

42	1712.8375	20.6037
43	1742.6873	694.3962
44	2174.1206	2098.0669
45	2927.7398	1187.4281
46	2932.4706	494.3409
47	2974.6728	402.8881
48	3360.8341	67.9945
49	3363.8486	75.7059
50	3481.2171	47.9862
51	3482.7766	60.3465
52	3490.1901	35.7261
53	3521.2812	2.9189
54	3521.3596	15.5016

Isomer III -c

#	Frequency	Infrared
1	26.3797	0.4371
2	29.2068	0.5280
3	48.7525	0.4972
4	86.7782	6.8536
5	110.6076	2.5557
6	139.3215	2.4364
7	160.7986	6.4893
8	183.5757	9.0068
9	193.9680	13.3429
10	235.4777	20.4909
11	254.2368	47.1679
12	278.2122	80.1851
13	284.5840	33.1473
14	338.8545	133.4115
15	368.8162	47.1860
16	393.6457	35.4736
17	411.0955	22.7497
18	439.9070	27.5216
19	461.7016	38.8034
20	512.9281	23.7826
21	548.7023	69.9276
22	566.4323	23.1744
23	664.9168	9.0304
24	700.3995	30.5648
25	817.2880	0.2236
26	832.1459	22.7186
27	913.5943	63.5179
28	1126.3488	67.0602

29	1162.2154	11.5185
30	1177.5882	112.3460
31	1276.2758	281.9155
32	1327.6157	252.4142
33	1396.3852	467.3841
34	1483.9374	76.7732
35	1544.0872	460.3859
36	1601.7397	5.8456
37	1616.3401	26.7089
38	1636.9675	147.9159
39	1643.9800	225.9292
40	1659.0502	24.6949
41	1682.1875	15.5606
42	1693.6765	128.4820
43	1756.5216	319.8691
44	2159.4467	1709.2701
45	2654.2237	1330.1257
46	3091.3292	585.3829
47	3139.4970	292.4570
48	3306.4748	224.4274
49	3346.7521	186.3060
50	3443.7017	22.2300
51	3456.7748	53.3056
52	3501.6051	52.1958
53	3509.7215	4.7959
54	3512.3631	7.0816

Isomer III -d

#	Frequency	Infrared
1	26.3494	0.4353
2	29.1683	0.5299
3	48.7344	0.4961
4	86.7707	6.8536
5	110.6161	2.5512
6	139.3268	2.4346
7	160.7991	6.4969
8	183.5702	9.0272
9	194.0035	13.3469
10	235.4656	20.4669
11	254.2462	47.1526
12	278.2289	79.9033
13	284.5847	33.4770
14	338.8394	133.3446
15	368.8119	47.2362

16	393.6326	35.3556
17	411.1244	22.8217
18	439.8973	27.5347
19	461.6876	38.8108
20	512.9496	23.7521
21	548.7158	69.9188
22	566.4416	23.1908
23	664.9238	9.0277
24	700.3901	30.5605
25	817.2838	0.2237
26	832.1284	22.7222
27	913.5659	63.5108
28	1126.3754	67.0563
29	1162.2484	11.5146
30	1177.6041	112.3338
31	1276.3330	281.9247
32	1327.6332	252.0583
33	1396.4135	467.6498
34	1483.9158	76.6685
35	1544.1032	460.1305
36	1601.7292	5.8400
37	1616.3393	26.6588
38	1636.9863	147.1300
39	1644.0085	226.4954
40	1659.0567	24.7472
41	1682.1991	15.5733
42	1693.6828	128.4626
43	1756.5335	320.0269
44	2159.8740	1709.2355
45	2653.9191	1330.4064
46	3091.2243	585.6150
47	3139.5336	292.5108
48	3306.3851	224.6757
49	3346.7025	186.3619
50	3443.7153	22.2229
51	3456.7639	53.2892
52	3501.6157	52.1923
53	3509.7268	4.7974
54	3512.3816	7.0811

Isomer III -e

#	Frequency	Infrared
1	23.5957	0.5371
2	38.1444	2.5375

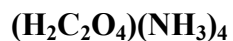
3	58.6936	1.1876
4	74.3720	1.9621
5	95.2825	15.9454
6	123.7104	6.1136
7	146.9691	15.6569
8	169.2429	0.4030
9	169.5347	2.1933
10	190.7583	32.2593
11	254.7846	33.6364
12	264.0951	4.5493
13	280.0918	81.4136
14	317.6563	66.4335
15	337.2590	96.8141
16	407.9730	54.7746
17	422.1086	82.8657
18	434.6675	72.4054
19	461.3329	42.0215
20	503.3988	55.7035
21	534.9656	14.8204
22	560.9673	15.3433
23	668.2856	21.7174
24	701.7322	22.9751
25	817.7456	0.1176
26	836.1458	19.0566
27	918.3766	62.3355
28	1108.4645	151.3555
29	1116.4298	109.0836
30	1161.5257	10.7970
31	1302.3113	254.5115
32	1341.2835	145.8907
33	1396.7019	418.9475
34	1484.8448	137.1268
35	1556.2674	100.3269
36	1605.7998	5.4256
37	1611.0230	7.0353
38	1635.2850	15.6035
39	1636.2939	12.2986
40	1647.8038	367.9307
41	1690.4200	10.8074
42	1706.2512	96.9246
43	1761.5483	597.8143
44	2329.1239	1761.5930
45	2829.2779	1060.5276
46	3040.2706	692.3640

47	3118.9328	310.4401
48	3334.5451	118.1404
49	3345.8832	162.8242
50	3470.1384	43.2710
51	3476.0107	74.3504
52	3491.0381	41.1669
53	3518.1485	7.5026
54	3521.3943	8.6981

Isomer III -f

#	Frequency	Infrared
1	17.7423	6.4869
2	24.7778	0.8956
3	68.6965	7.2596
4	75.3435	1.6088
5	105.9656	9.3604
6	138.1399	20.2005
7	140.2624	0.3143
8	162.0524	11.9927
9	169.3119	16.6579
10	186.5878	28.2657
11	211.8074	40.6778
12	221.4778	73.1895
13	275.1553	19.3784
14	287.7843	46.9856
15	316.7730	87.0738
16	332.5001	8.6836
17	375.7407	50.7636
18	411.6553	11.3513
19	421.3836	48.6585
20	458.5889	73.4909
21	475.4089	49.5589
22	584.6260	18.6825
23	619.5478	17.6691
24	697.1838	152.7362
25	812.2074	0.0999
26	824.4329	25.8846
27	1065.4458	210.5133
28	1073.7495	105.0854
29	1172.7923	54.8125
30	1194.4934	12.8514
31	1237.2297	174.8288
32	1288.8311	482.1148
33	1305.4744	515.7823

34	1330.2716	1323.4037
35	1379.4558	51.1826
36	1597.3839	55.2564
37	1599.5585	23.3405



Isomer IV -a

#	Frequency	Infrared
1	30.0860	2.0029
2	38.0570	0.1052
3	43.3866	0.6940
4	48.3684	4.0551
5	72.0286	8.3420
6	86.5318	11.5681
7	93.5133	13.0057
8	100.4430	17.9648
9	125.2498	4.0463
10	155.0059	1.9942
11	160.8959	0.3208
12	163.5869	0.0009
13	167.5501	0.5696
14	210.6129	7.8864
15	242.3439	54.3848
16	245.2973	1.6217
17	253.3611	0.3073
18	293.5203	33.3450
19	304.2290	59.5707
20	325.1823	132.5570
21	360.9480	133.6781
22	398.8287	27.8711
23	421.6912	5.0030
24	449.7280	223.7948
25	462.3852	40.5778
26	554.8640	17.9118
27	578.2267	0.1572
28	590.2292	4.9660
29	639.1430	2.3061
30	695.8892	20.3205
31	819.4855	0.0375
32	827.3897	20.7952
33	959.3050	58.9276
34	1090.5415	89.8909
35	1095.1663	167.4559
36	1107.9073	111.6461

37	1160.9645	7.3260
38	1315.7301	189.6124
39	1354.2647	59.1227
40	1402.4630	563.3938
41	1504.4580	13.3898
42	1538.2823	115.8216
43	1608.5710	7.8260
44	1614.7602	4.6743
45	1616.4506	5.8898
46	1630.7947	0.5188
47	1636.1136	6.0565
48	1637.1671	21.6604
49	1661.5348	245.5089
50	1697.5319	38.4245
51	1718.9951	71.8865
52	1745.2299	689.4366
53	2551.5664	1495.4535
54	3021.1543	214.9796
55	3036.8513	471.3383
56	3059.1679	852.4991
57	3224.8377	595.8577
58	3347.7219	112.7712
59	3359.6077	66.5718
60	3362.6814	77.8313
61	3472.5310	43.9376
62	3480.1730	39.7371
63	3481.7673	62.4752
64	3515.9189	5.5367
65	3519.8942	3.2118
66	3519.9885	12.0112

Isomer IV -b

#	Frequency	Infrared
1	20.0634	0.0779
2	33.8567	0.1684
3	46.0864	1.5407
4	51.3790	4.9147
5	72.9002	14.1899
6	81.9636	4.5417
7	84.2564	16.0332
8	122.4650	20.9475
9	125.8509	1.7954
10	157.2582	0.1363
11	161.7641	1.2338

12	165.2628	0.0747
13	167.4221	0.0041
14	198.1022	8.3674
15	232.9433	10.1923
16	245.9331	7.9400
17	275.4073	50.8235
18	298.0708	71.9071
19	314.7296	97.0385
20	322.2289	37.3715
21	381.8659	41.4650
22	395.8423	127.0625
23	419.2374	5.3626
24	460.6478	44.5234
25	460.8649	228.3654
26	553.9862	0.4436
27	556.2734	17.3343
28	576.1372	5.7737
29	587.4079	0.6131
30	692.2911	20.9047
31	819.5801	0.0256
32	828.0317	19.5292
33	922.2079	60.7466
34	1100.5662	85.2822
35	1103.3629	261.8435
36	1106.0473	26.0561
37	1159.7073	12.6874
38	1314.4870	268.7628
39	1358.6398	91.7485
40	1396.3980	466.9774
41	1506.0963	142.9232
42	1523.6234	27.1989
43	1608.8451	0.6884
44	1608.8863	4.5633
45	1616.5371	5.7094
46	1631.2858	1.1978
47	1637.5951	25.2704
48	1638.0737	7.1644
49	1653.6646	268.7841
50	1704.2238	103.1601
51	1705.8731	66.9804
52	1763.7416	575.8894
53	2738.5489	1123.4895
54	2945.4856	819.4620
55	3127.5863	203.7781

56	3142.0439	625.3624
57	3176.5581	569.2311
58	3343.2462	84.1008
59	3346.5535	96.1359
60	3359.3976	136.1691
61	3471.7857	28.6452
62	3473.0271	49.4357
63	3480.6063	80.3215
64	3516.7481	3.7659
65	3516.8411	8.9845
66	3520.6934	7.4638

Isomer IV -c

#	Frequency	Infrared
1	17.2338	0.2037
2	28.6218	0.7415
3	36.2085	1.9066
4	58.9847	1.5631
5	68.1731	2.3659
6	84.8266	3.8304
7	115.6961	2.4043
8	138.5151	10.2607
9	148.0275	15.5892
10	169.3817	0.1584
11	195.4317	13.4805
12	199.9046	19.0138
13	221.3291	22.2591
14	242.5993	7.0595
15	256.3226	45.3119
16	271.3183	83.4069
17	278.9396	41.2617
18	310.3084	41.8446
19	319.4183	44.1284
20	391.1781	48.1035
21	412.6104	12.5016
22	430.9980	46.2094
23	440.0846	96.5205
24	463.4689	50.3321
25	513.8833	11.4393
26	536.0070	5.2870
27	564.5684	18.4801
28	588.0472	88.9389
29	693.5172	28.1030
30	746.4401	13.5014

31	817.3705	0.0429
32	835.8482	19.9191
33	918.0988	61.6335
34	1102.3093	128.3685
35	1134.5040	57.7882
36	1158.6762	15.5380
37	1179.9092	103.2521
38	1318.1028	356.0762
39	1396.9915	464.7286
40	1406.1995	12.8163
41	1488.7116	53.8479
42	1555.0254	27.7187
43	1602.3508	12.6667
44	1607.9415	6.8519
45	1619.1153	7.9142
46	1636.6037	10.4266
47	1644.7945	11.1619
48	1655.8193	374.3872
49	1662.1993	19.7608
50	1712.9666	8.6191
51	1722.8311	50.9731
52	1761.9251	520.1342
53	2470.1225	1824.2496
54	2733.8702	1387.5749
55	2882.3171	968.4105
56	3074.0042	658.6470
57	3118.2904	325.9099
58	3269.3340	391.1332
59	3347.6967	147.3372
60	3441.0850	19.5107
61	3451.9427	50.8450
62	3477.0309	69.5837
63	3481.4370	33.4029
64	3509.9771	1.3067
65	3510.1808	7.3757
66	3521.8364	7.8177

Isomer IV -d

#	Frequency	Infrared
1	24.7315	0.2439
2	28.4794	0.9035
3	36.6234	0.9438
4	50.2840	2.5109
5	61.5690	4.0336

6	99.8358	3.7405
7	116.5001	2.3998
8	122.3506	6.9555
9	150.4269	8.8709
10	172.0854	3.7674
11	175.7038	2.4482
12	185.0690	17.9205
13	213.5207	2.9483
14	237.8359	45.7686
15	251.1536	38.2301
16	259.0334	8.4269
17	288.3967	18.6570
18	304.2934	74.0730
19	317.7675	110.7847
20	360.1156	39.3395
21	381.7254	95.5860
22	404.9450	78.8239
23	416.0561	10.3612
24	462.0430	43.6641
25	499.0844	22.0182
26	541.6735	38.5152
27	572.4623	7.6384
28	604.3684	28.0422
29	697.8095	24.3115
30	740.5610	2.6271
31	819.6033	2.4853
32	830.9637	29.4001
33	981.7184	56.7465
34	1089.5424	84.0220
35	1100.5096	114.8841
36	1156.3441	6.9552
37	1170.6220	91.4416
38	1315.4149	210.6436
39	1401.8348	410.9611
40	1413.9353	175.6371
41	1472.9010	28.4218
42	1551.8431	54.7116
43	1605.6990	2.6223
44	1609.7601	8.1343
45	1621.5352	7.1554
46	1632.7703	3.0190
47	1641.8075	16.1477
48	1655.4665	265.1168
49	1657.9838	0.7264

50	1712.4539	20.6890
51	1718.5100	32.1843
52	1742.6802	722.3806
53	2317.8308	2118.9780
54	2746.5087	1290.6776
55	2934.6547	191.5768
56	2940.4692	982.1255
57	3140.8777	523.2682
58	3339.2132	144.0297
59	3354.3627	115.5388
60	3441.0514	24.5773
61	3467.5138	62.1400
62	3480.4364	67.1568
63	3481.7338	28.3895
64	3508.5376	5.2050
65	3512.9055	4.9789
66	3523.3262	7.9528

Isomer IV -e

#	Frequency	Infrared
1	17.8256	3.1918
2	23.8338	2.1860
3	27.5893	3.1478
4	70.6970	3.2494
5	77.6559	1.0284
6	96.9042	11.6174
7	102.1394	11.0958
8	129.5025	16.8624
9	148.8904	16.3942
10	169.9260	1.7548
11	177.0799	1.7801
12	190.3006	10.6255
13	195.8739	52.4544
14	222.4523	54.0256
15	225.9859	17.2518
16	246.8910	76.7820
17	284.2370	54.9460
18	293.0053	50.8092
19	303.8461	12.8024
20	321.1812	61.8861
21	332.6783	12.0859
22	397.5789	11.1130
23	417.9154	130.1515
24	440.8511	16.2803

25	464.1399	49.5618
26	492.5511	34.8689
27	595.8062	38.4489
28	598.8274	5.6984
29	684.5942	89.3797
30	688.0176	110.3450
31	814.8322	2.1153
32	832.3183	9.2677
33	1077.8633	143.8367
34	1083.6730	104.3620
35	1189.3278	32.7419
36	1202.9113	42.8147

Isomer IV -f

#	Frequency	Infrared
1	25.6834	0.2531
2	29.7317	0.9884
3	46.4096	0.9682
4	54.1593	1.2131
5	86.1442	2.4630
6	99.0857	1.0160
7	113.9458	6.0893
8	137.2911	12.5994
9	148.2633	2.4514
10	154.1298	6.7788
11	157.7933	5.7624
12	172.8038	16.3268
13	181.9327	9.8259
14	223.4327	19.8600
15	240.9742	32.9975
16	270.8062	36.7513
17	291.0630	182.1298
18	315.3570	68.8328
19	342.7207	47.2035
20	358.7525	46.5398
21	368.7800	55.3584
22	422.0053	20.3336
23	428.7631	7.5309
24	463.8274	33.4627
25	471.3934	76.5037
26	537.7448	34.6687
27	566.7633	8.5765
28	662.3868	21.5519
29	697.5358	24.8936

30	736.9579	22.5215
31	820.2583	0.0803
32	827.5629	25.8613
33	946.6480	59.7244
34	1092.9013	88.6069
35	1110.0260	79.8560
36	1159.2324	8.7429
37	1184.8730	70.5406
38	1302.9984	304.1439
39	1346.9531	32.6156
40	1397.9684	512.1489
41	1435.3091	38.0953
42	1568.8929	204.1358
43	1600.8018	92.3312
44	1616.5656	16.2000
45	1619.5538	24.1089
46	1635.4623	7.5885
47	1641.2886	15.0215
48	1648.9603	275.3729
49	1658.0782	17.4160
50	1686.3877	183.8214
51	1705.5571	14.3959
52	1748.9420	435.3554
53	2084.7563	2025.9871
54	2391.7890	1465.2254
55	3060.5935	291.6021
56	3171.5378	267.4105
57	3247.8366	481.3321
58	3327.9864	158.1735
59	3362.2139	70.3361
60	3414.8394	41.0702
61	3461.8120	45.7522
62	3476.0535	53.5375
63	3498.2033	16.6186
64	3510.2531	4.0476
65	3511.9812	4.8009
66	3514.1161	47.9087

Isomer IV -g

#	Frequency	Infrared
1	23.2530	4.4965
2	31.0526	0.2139
3	37.4817	2.4710
4	49.7013	2.4948

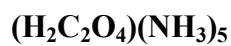
5	74.5781	3.4932
6	84.8831	4.0011
7	131.1492	10.9663
8	154.4471	6.0071
9	180.3623	1.3149
10	180.7348	9.2118
11	182.4868	18.6527
12	187.0732	13.2539
13	219.9010	35.3703
14	235.9502	22.0576
15	247.2107	124.9074
16	271.6140	162.4047
17	294.2061	12.6285
18	318.3077	37.7805
19	337.0562	17.5580
20	358.8526	25.3892
21	374.1863	79.7830
22	381.0088	53.6837
23	417.3431	58.5796
24	431.7676	330.7478
25	502.2065	49.9089
26	527.3479	2.4001
27	604.0256	61.5376
28	634.4093	27.9146
29	652.3445	10.4749
30	742.3324	24.6998
31	818.6019	0.3182
32	850.9863	17.5593
33	1054.8018	876.9907
34	1101.3185	1291.4192
35	1113.8890	260.1542
36	1167.1114	85.5118

Isomer IV -h

#	Frequency	Infrared
1	10.9075	0.4404
2	27.2418	1.2086
3	28.5742	0.3447
4	44.0583	1.1862
5	64.1742	0.8114
6	81.9757	4.7561
7	113.7177	2.6102
8	128.7639	0.8456
9	163.9412	1.8356

10	172.1041	23.0869
11	181.6466	36.7092
12	201.7567	11.3873
13	219.6607	31.2276
14	246.1466	1.3413
15	256.1652	32.7646
16	278.6772	20.6080
17	296.4358	61.5105
18	332.9353	174.4259
19	356.0276	17.1022
20	382.2894	30.5876
21	384.4160	15.3933
22	422.7581	43.0257
23	436.7520	18.1280
24	462.6345	35.9386
25	491.1462	30.6029
26	541.8370	54.4248
27	563.0398	1.8994
28	583.6371	33.4355
29	659.6479	13.1218
30	701.5437	32.7290
31	816.6718	0.0591
32	831.8206	28.1640
33	920.5202	62.0583
34	1132.1345	49.0416
35	1163.0906	33.3983
36	1164.1095	58.2422
37	1204.7089	92.5538
38	1302.5512	376.1960
39	1345.8935	103.8417
40	1397.2796	522.9327
41	1467.2092	94.9037
42	1551.1771	356.3702
43	1603.0368	4.6227
44	1610.4563	47.9961
45	1622.1168	10.0827
46	1639.0086	134.1183
47	1649.3139	220.9401
48	1655.0391	28.3864
49	1669.6060	3.9651
50	1687.7479	98.9038
51	1692.2485	24.6514
52	1753.3367	325.4708
53	2296.7221	1887.8904

54	2553.7268	1489.6731
55	3024.9632	805.6342
56	3116.2900	295.6991
57	3129.3880	566.8046
58	3295.7456	269.6344
59	3305.7880	263.4320
60	3434.8803	14.0959
61	3435.2907	26.8607
62	3451.1541	56.9073
63	3497.0077	48.8272
64	3501.7031	2.1528
65	3504.6702	5.8764
66	3505.8366	3.6204



Isomer V -a

#	Frequency	Infrared
1	19.1243	0.0767
2	26.3206	0.4250
3	30.9918	0.7217
4	44.8118	1.3302
5	51.9964	2.9576
6	69.8007	5.1622
7	72.4017	2.1136
8	83.2442	13.3953
9	110.7938	3.8619
10	130.1991	16.6827
11	149.7477	8.9926
12	162.6032	0.5369
13	168.9254	0.2873
14	172.3427	1.7901
15	179.3810	13.0582
16	191.8943	16.0093
17	207.0913	5.6148
18	229.2559	3.2309
19	242.8935	19.6882
20	254.2026	31.5025
21	260.2990	47.4319
22	293.8511	55.1514
23	302.4731	23.9880
24	321.0442	73.5992
25	382.1257	11.8755
26	386.1622	75.6969
27	412.3114	31.6828

28	420.4660	48.0430
29	433.1900	153.9049
30	464.0177	48.6837
31	551.2280	105.1251
32	556.7826	10.4179
33	573.3745	21.8523
34	622.1657	0.7319
35	677.9500	14.0689
36	692.6525	14.2054
37	820.4501	0.1218
38	828.1736	20.3491
39	914.4015	60.1055
40	1094.8231	142.1652
41	1098.4473	100.1413
42	1130.6979	66.3926
43	1155.6924	22.5649
44	1160.3215	97.7059
45	1317.8568	320.7575
46	1392.9779	450.1416
47	1422.3074	57.3747
48	1513.3091	35.6847
49	1517.6173	81.2105
50	1604.1283	3.5636
51	1608.8157	2.4843
52	1612.3275	9.8884
53	1620.2005	18.7318
54	1632.5010	5.7828
55	1638.3981	8.2413
56	1645.0737	18.5369
57	1654.5888	295.9527
58	1661.1200	34.4376
59	1717.6383	56.5208
60	1723.3706	50.9549
61	1766.3019	517.7944
62	2839.1487	1242.4644
63	2871.2238	809.1901
64	2968.6778	942.2182
65	3120.5792	478.5668
66	3134.1523	315.1803
67	3159.3530	617.5125
68	3279.7872	310.1924
69	3347.0450	88.9497
70	3359.9955	141.9015
71	3444.2215	21.7719

72	3451.4266	48.4270
73	3473.7331	40.3565
74	3481.5836	81.0790
75	3507.3027	3.3918
76	3512.2524	4.4920
77	3518.1972	6.0219
78	3521.8709	6.6499

Isomer V -b

#	Frequency	Infrared
1	16.5031	0.6652
2	30.6610	0.0488
3	39.4851	0.1096
4	48.3300	2.5028
5	56.3432	0.7770
6	63.3576	2.5735
7	82.4456	2.6515
8	112.5533	6.0204
9	116.8575	6.7645
10	136.1074	22.6967
11	155.7483	2.0875
12	164.9190	17.9250
13	183.7988	18.0453
14	192.3314	5.6705
15	195.4707	6.0795
16	196.6481	0.0179
17	208.7383	0.2879
18	208.7499	0.5865
19	225.3522	21.9433
20	261.0579	8.9580
21	277.8807	71.2480
22	288.4054	60.7805
23	291.9153	18.7960
24	335.0704	61.9387
25	366.9270	6.8606
26	377.9081	89.4725
27	413.3730	3.8726
28	422.1760	122.8741
29	461.0860	62.0998
30	462.7241	68.2159
31	541.7673	148.2424
32	565.0827	12.2511
33	619.3716	0.1097
34	643.9252	12.3871

35	672.9947	0.0221
36	695.8277	15.8192
37	816.2009	28.2761
38	820.4051	0.1087
39	993.3682	55.3961
40	1103.4423	81.5647
41	1109.2146	155.3805
42	1112.4105	75.0644
43	1149.6350	112.3759
44	1167.9700	0.7510
45	1311.6574	141.1704
46	1407.4811	633.8049
47	1456.9022	33.1847
48	1492.1809	17.5702
49	1515.5530	88.5348
50	1603.8356	5.3007
51	1606.6804	4.2378
52	1613.1697	2.3334
53	1620.4597	5.8447
54	1636.9934	0.5128
55	1638.2729	12.9628
56	1646.1792	19.4864
57	1657.8402	0.5607
58	1667.1483	98.5145
59	1721.1251	29.4371
60	1730.6107	599.2091
61	1735.7049	254.5895
62	2904.6298	889.8033
63	2905.9445	349.6459
64	2958.3134	898.5501
65	2966.1641	1125.6971
66	3036.1458	591.8952
67	3156.1709	558.3939
68	3288.9251	221.7967
69	3298.2904	283.1622
70	3341.9059	189.9704
71	3446.4318	25.9453
72	3462.7638	31.8871
73	3464.1165	49.6685
74	3466.5877	90.1874
75	3511.3460	3.9035
76	3513.0543	5.1714
77	3519.7956	3.4410
78	3519.9194	8.1569

Isomer V -c

#	Frequency	Infrared
1	16.7736	0.3434
2	24.8215	1.0064
3	27.6171	0.0108
4	31.3261	0.0628
5	45.6593	1.7370
6	67.6710	1.9504
7	78.4907	2.2418
8	104.7546	4.6554
9	119.6141	3.6590
10	135.7643	4.4391
11	164.5259	6.9507
12	172.7769	4.8722
13	179.0371	11.5661
14	186.5025	9.6063
15	188.0771	8.9276
16	220.9175	0.0927
17	224.4225	35.4773
18	235.9292	20.6614
19	245.1404	55.8551
20	252.9759	23.0432
21	275.3079	69.7872
22	306.1699	6.0034
23	308.9523	77.0976
24	365.4483	34.4518
25	385.1325	40.2370
26	387.8286	41.3111
27	397.3640	56.2991
28	423.8191	38.8045
29	464.4103	49.8907
30	473.0268	54.0325
31	517.6647	16.1124
32	558.9464	6.0333
33	584.3013	2.6497
34	586.8507	100.6736
35	693.0692	25.4825
36	720.1232	10.0393
37	820.5524	0.0470
38	827.5733	17.5309
39	901.9050	61.8968
40	1117.3199	3.7223
41	1122.2588	120.5216

42	1151.8469	35.8358
43	1154.8053	157.2159
44	1156.0394	50.1848
45	1312.3290	386.4161
46	1390.2107	452.2395
47	1397.4157	45.8150
48	1504.5751	19.6270
49	1548.7811	67.4443
50	1602.2897	1.0559
51	1606.7340	28.1392
52	1616.5996	13.0712
53	1620.5088	16.6537
54	1636.5247	1.2533
55	1644.2518	19.4231
56	1650.7349	387.1313
57	1657.3615	0.5129
58	1658.7089	1.3807
59	1710.6879	140.3378
60	1723.7166	31.9045
61	1768.3242	318.5341
62	2652.6082	1409.2141
63	2831.9701	1765.0486
64	2844.7207	411.4019
65	3135.5273	32.2809
66	3139.0939	1007.6104
67	3183.1389	287.4657
68	3303.7766	244.1181
69	3313.3224	192.1774
70	3445.8568	0.1644
71	3446.0065	47.7355
72	3455.9327	61.6670
73	3455.9701	68.9136
74	3457.7934	58.1882
75	3509.1845	2.0788
76	3509.2572	5.9960
77	3513.5524	3.0207
78	3513.6136	7.5979

Isomer V -d

#	Frequency	Infrared
1	14.1301	0.1301
2	26.8804	0.9326
3	32.2139	0.8548
4	46.6220	2.0844

5	47.7448	1.8464
6	58.9571	1.7810
7	80.2921	6.3252
8	95.9169	10.4493
9	111.1772	3.9899
10	115.1632	14.3398
11	145.0841	7.8088
12	160.3696	8.0532
13	167.5580	4.3844
14	173.2391	0.7865
15	182.1920	0.7551
16	185.7867	18.8191
17	210.1160	2.9222
18	231.7595	35.3062
19	233.6698	7.9313
20	251.5510	15.3666
21	257.0999	16.9273
22	291.5633	37.3293
23	299.9507	35.4542
24	318.4575	131.8656
25	350.9456	20.7190
26	382.8005	37.6515
27	386.6063	97.1092
28	416.1728	26.4730
29	447.5181	132.7052
30	463.8575	54.8211
31	523.6025	78.2800
32	556.7385	29.6853
33	580.4629	0.4921
34	627.9742	11.5831
35	668.1514	1.9208
36	694.8686	19.9960
37	819.4911	1.0651
38	828.4672	20.6879
39	966.2166	57.6370
40	1090.8110	93.3650
41	1103.7807	108.6882
42	1109.4725	121.7904
43	1154.9697	100.1568
44	1161.8209	7.6080
45	1320.2033	181.6692
46	1402.4077	308.7171
47	1406.3606	318.1681
48	1510.0066	32.0315

49	1522.1248	98.0857
50	1606.1070	4.0612
51	1610.5413	14.6744
52	1613.9507	2.5192
53	1621.8207	8.6618
54	1633.2268	2.2771
55	1638.3262	7.1125
56	1641.8619	20.7537
57	1657.7543	6.6547
58	1663.5073	192.3334
59	1710.5017	36.9430
60	1724.2952	95.8011
61	1744.8991	709.0345
62	2740.7214	1297.4126
63	2862.3093	1046.2869
64	2988.5554	327.9328
65	3035.3309	629.5828
66	3156.2509	606.7991
67	3175.9851	522.4075
68	3333.1833	167.4977
69	3344.3989	124.4339
70	3355.2832	109.6761
71	3444.3766	25.4977
72	3467.3630	65.8289
73	3469.0064	47.6392
74	3479.2425	61.3364
75	3510.5107	3.4184
76	3511.1574	5.6672
77	3516.9058	5.1005
78	3521.3439	6.6215

Isomer V -e

#	Frequency	Infrared
1	19.1330	0.6260
2	23.2383	0.5129
3	26.9322	0.1444
4	30.6168	0.6765
5	53.9073	2.2763
6	58.9808	1.6599
7	68.8353	2.4651
8	107.8826	1.3497
9	112.1599	2.1128
10	137.2110	5.9105
11	145.9204	11.3835

12	175.8409	8.9006
13	180.7703	11.5153
14	189.2544	23.0850
15	196.0808	11.7613
16	216.9639	3.8699
17	227.5566	10.1518
18	238.7712	30.3553
19	250.2554	77.7058
20	271.3403	78.5075
21	283.7988	18.9362
22	288.6437	19.6936
23	307.9585	54.5099
24	360.9832	57.8364
25	385.6054	27.8640
26	406.2897	66.4303
27	412.3263	9.3180
28	433.1120	56.0793
29	463.4047	37.0738
30	500.5989	43.6801
31	515.2146	14.8472
32	566.3962	9.8588
33	576.1044	35.1962
34	598.2767	58.9108
35	693.5706	31.5767
36	745.5721	10.2394
37	818.4718	0.3684
38	831.6689	21.7884
39	930.7740	59.4304
40	1103.0909	81.4062
41	1132.5048	62.5690
42	1156.2376	15.5552
43	1166.5602	107.0684
44	1171.3505	99.4073
45	1318.3930	308.7615
46	1395.6214	491.3640
47	1421.2899	24.9459
48	1486.2009	37.5857
49	1544.5439	48.1440
50	1602.5296	8.0399
51	1605.9729	6.6122
52	1618.5410	2.6849
53	1620.8712	8.2420
54	1640.7694	9.7687
55	1643.4102	11.7334

56	1657.2475	43.3576
57	1660.1640	336.1055
58	1661.0321	2.6351
59	1713.6711	17.8508
60	1726.7688	60.6521
61	1755.9548	521.4277
62	2567.6742	1718.4033
63	2766.8250	1653.2703
64	2818.6343	830.1709
65	3084.7843	222.8238
66	3093.0917	726.4808
67	3134.5715	522.4310
68	3276.3806	404.3666
69	3331.5571	187.6034
70	3441.8958	20.4494
71	3442.1583	24.0459
72	3452.5974	55.6811
73	3465.7883	65.6494
74	3483.7813	33.4823
75	3509.8654	2.5771
76	3509.9156	4.8184
77	3510.6305	5.1140
78	3513.9134	4.4584

Isomer V -f

#	Frequency	Infrared
1	28.4050	7.0983
2	37.0573	3.7225
3	44.5132	1.7507
4	60.6472	4.6665
5	61.1726	1.8399
6	67.3290	5.2207
7	85.8983	6.8453
8	101.2625	4.3000
9	122.5403	1.0220
10	151.7144	14.1809
11	169.4681	3.9868
12	176.1949	8.4416
13	182.8486	1.2552
14	185.0679	3.9262
15	200.4984	9.8467
16	230.7269	20.4819
17	239.3942	27.2610
18	250.0448	85.9991

19	268.3299	65.4809
20	282.2770	56.4122
21	289.9806	14.2701
22	302.6406	57.7578
23	325.4441	45.5585
24	334.5763	24.1692
25	348.7431	21.1788
26	370.1526	21.1123
27	401.6942	135.9513
28	425.3180	32.3794
29	472.6612	112.0159
30	508.6746	69.8614
31	534.9328	13.6722
32	552.2574	42.2612
33	603.5462	22.9787
34	712.0969	21.2519
35	721.7571	20.5037
36	738.9448	8.1870
37	822.4147	2.6908
38	845.0232	17.2458
39	1079.4581	190.0835
40	1103.3256	119.7423
41	1122.8373	104.7341
42	1155.8840	37.6713
43	1168.6279	77.4551
44	1235.0008	238.4739
45	1353.7216	45.9187
46	1373.4976	13.1009
47	1434.4813	519.7409
48	1456.9967	56.8294
49	1560.5323	156.7184
50	1583.4004	431.5494
51	1601.1554	23.4788
52	1605.2574	37.7609
53	1611.3019	24.7037
54	1614.0269	50.7355
55	1629.1728	4.6283
56	1636.3671	55.1977
57	1638.0085	14.9359
58	1662.2864	0.9083
59	1685.2183	359.3003
60	1701.0728	47.6777
61	1710.7688	26.4327
62	2477.9031	1730.2043

63	2519.2245	1773.0343
64	2616.9248	1573.1533
65	2923.1693	862.4357
66	3140.1282	446.4626
67	3294.0616	410.7794
68	3301.8815	99.3403
69	3320.8481	187.8252
70	3421.6203	38.0886
71	3456.2137	41.3472
72	3468.8043	54.3296
73	3476.9811	42.6705
74	3491.3996	29.4464
75	3509.5638	12.2248
76	3513.8465	3.1264
77	3521.3014	6.7873
78	3537.8347	11.2946

Isomer V -g

#	Frequency	Infrared
1	35.6228	0.8581
2	38.4779	2.2120
3	47.4792	0.6297
4	60.3498	0.2521
5	72.9561	1.0384
6	75.5762	4.6965
7	91.3260	3.2567
8	111.3114	1.5710
9	125.4439	0.6721
10	136.8277	14.8317
11	159.7590	8.3801
12	175.9180	6.5164
13	185.1640	5.1286
14	195.6684	30.6306
15	200.5169	20.8180
16	221.3164	3.8260
17	236.2526	21.8288
18	268.9763	19.9388
19	277.9401	51.9071
20	290.5816	38.3519
21	296.0409	35.2717
22	310.2317	24.0025
23	341.5010	49.4502
24	378.5301	51.8470
25	418.3608	24.4328

26	421.8619	25.6458
27	454.9731	74.5419
28	465.8450	42.8316
29	484.0401	72.1341
30	526.6377	97.4569
31	561.4053	29.6761
32	564.6809	4.4448
33	603.5738	28.4762
34	633.8197	9.1164
35	690.5092	22.0472
36	813.7988	0.4740
37	818.6154	28.0712
38	825.3767	1.1473
39	958.0035	57.5335
40	1111.4808	105.0260
41	1129.6125	25.3691
42	1138.9509	92.7554
43	1180.3106	106.6428
44	1227.1892	62.6487
45	1314.5706	114.8040
46	1390.3659	507.8871
47	1438.7520	16.4722
48	1472.6309	17.8815
49	1564.7458	56.2266
50	1587.2277	15.8827
51	1601.0604	7.9567
52	1607.8542	39.3910
53	1614.2532	11.0738
54	1631.8854	13.8260
55	1636.1441	23.2513
56	1644.4999	0.2863
57	1659.8464	37.8084
58	1665.5082	165.3832
59	1728.5186	7.0149
60	1732.9126	28.4340
61	1752.7165	294.6609
62	2334.6968	2008.4978
63	2470.2189	1309.3277
64	2829.5985	909.8472
65	3016.7724	359.5842
66	3162.2654	370.5624
67	3170.9387	498.6859
68	3263.6094	352.8536
69	3315.8316	150.3277

70	3367.0928	98.8061
71	3449.0536	22.7172
72	3454.2404	34.1917
73	3460.8803	37.8424
74	3475.9799	25.4888
75	3489.7978	19.7683
76	3515.3106	2.9881
77	3515.6681	8.3412
78	3521.2940	6.5138

Isomer V -h

#	Frequency	Infrared
1	9.5820	0.8726
2	13.1079	0.0994
3	30.5352	0.8433
4	36.9737	1.8934
5	45.3490	2.3036
6	58.9348	1.0443
7	65.5732	2.2030
8	90.7608	1.3859
9	116.3842	2.0823
10	131.9858	10.3750
11	149.3121	15.7292
12	162.7285	0.1048
13	176.8291	22.3220
14	185.3712	20.0213
15	199.3575	22.9400
16	218.2562	11.1413
17	227.2503	24.9557
18	237.9772	17.7434
19	253.6702	28.3280
20	272.8226	19.3867
21	281.6774	77.4109
22	304.3516	35.7053
23	311.5037	83.1352
24	337.1819	4.2789
25	378.5320	27.7822
26	421.4970	17.6074
27	429.6038	69.6243
28	442.8394	77.2086
29	464.9254	60.5501
30	489.0356	31.2112
31	518.3064	10.2827
32	545.3716	32.8308

33	564.3812	8.0021
34	607.2650	51.9335
35	694.3104	31.4347
36	747.5074	6.3920
37	817.4867	0.0064
38	834.4742	30.2003
39	925.3487	60.3921
40	1096.3498	132.0126
41	1134.7615	56.9346
42	1157.1424	11.9140
43	1160.7195	73.9550
44	1199.5190	93.0708
45	1320.3517	342.3231
46	1397.0104	483.8948
47	1434.3478	28.5580
48	1481.3572	36.0040
49	1543.0016	30.3786
50	1603.8180	9.3007
51	1607.3895	4.4331
52	1609.7539	34.9654
53	1619.2233	9.2949
54	1635.9830	12.1399
55	1644.1442	84.2009
56	1652.8806	168.1573
57	1659.6626	116.7753
58	1668.6509	3.9636
59	1720.3580	4.8430
60	1721.9441	25.7432
61	1759.8920	497.2706
62	2502.2007	2000.1359
63	2686.5715	1502.8731
64	2904.0336	937.7639
65	3030.3046	799.1310
66	3107.6957	345.3457
67	3121.6089	564.1530
68	3279.9659	343.9759
69	3350.3695	132.4997
70	3432.6718	16.3558
71	3436.4132	21.6656
72	3449.4044	53.0871
73	3478.1316	28.2807
74	3478.2556	69.3845
75	3502.4743	3.8933
76	3504.2314	2.0313

77	3506.7556	3.0235
78	3522.2757	7.5895

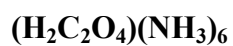
Isomer V -i

#	Frequency	Infrared
1	23.9076	3.2753
2	30.1068	3.4859
3	33.2462	0.6506
4	47.1485	6.1139
5	55.4351	1.5343
6	71.2418	1.7924
7	87.3495	1.0902
8	103.8466	4.1014
9	132.5719	18.2557
10	144.7437	9.3987
11	177.8563	4.2420
12	189.0614	16.0152
13	190.3042	5.7643
14	193.7685	0.7196
15	200.1729	4.6089
16	216.7358	0.8031
17	237.7830	46.5428
18	246.4351	56.8011
19	251.9402	43.4439
20	281.3717	64.8818
21	290.6429	10.5408
22	312.1138	5.2835
23	327.7262	116.6254
24	333.7898	15.2254
25	347.5498	18.3888
26	382.2922	17.8860
27	404.2601	209.3968
28	422.4430	51.2799
29	426.8781	23.6999
30	513.2486	13.8583
31	518.1830	119.3643
32	568.6439	27.7878
33	605.5021	44.2634
34	688.1763	14.1821
35	731.9737	29.0618
36	749.5306	4.4245

Isomer V -j

#	Frequency	Infrared
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1	13.9999	0.6363
2	19.0903	2.1928
3	21.5026	4.9858
4	32.2054	0.5795
5	34.7650	0.8692
6	47.6016	1.3410
7	71.4195	14.7573
8	78.0553	7.9050
9	89.2892	17.2640
10	98.7930	0.9661
11	127.5890	17.3207
12	150.3187	6.8242
13	166.1178	0.2402
14	183.3837	5.2432
15	186.6611	4.8090
16	187.8273	29.0877
17	203.9368	3.2317
18	222.1233	20.2931
19	241.0199	6.2729
20	258.5872	90.8506
21	272.3892	201.4771
22	298.1250	4.1734
23	313.1248	75.1758
24	318.3613	33.6556
25	338.4129	12.6618
26	360.3566	41.0205
27	383.9157	67.5314
28	387.8846	40.9890
29	422.2528	57.0062
30	432.0559	223.1795
31	495.5065	51.6043
32	520.5558	2.3918
33	611.1214	63.5517
34	628.1034	8.8017
35	651.2765	7.9269
36	741.8806	34.4503



Isomers VI -a

#	Frequency	Infrared
1	4.0306	0.6446
2	18.5390	0.0097
3	23.3089	0.5762
4	27.5060	0.0010

5	41.9668	1.5766
6	47.0029	2.4447
7	63.5252	1.1029
8	69.9650	3.9925
9	73.5132	0.6051
10	103.7064	5.1082
11	124.6088	9.9387
12	135.6940	14.4016
13	161.3958	2.8590
14	165.1257	0.0526
15	166.2532	12.5778
16	176.5581	10.9683
17	188.1050	0.9184
18	188.9118	7.6087
19	192.3462	26.5911
20	212.1206	0.7457
21	217.5356	30.1385
22	235.6980	18.4961
23	236.2106	16.0280
24	245.3021	6.7954
25	248.1716	58.5278
26	295.2030	33.6416
27	298.8394	4.7444
28	311.3165	57.1772
29	365.9519	76.1689
30	385.8296	1.6959
31	388.4246	19.5912
32	391.4139	52.0521
33	414.9568	114.5348
34	420.4567	35.8986
35	465.4447	46.8869
36	529.0680	24.7634
37	550.8076	141.2987
38	562.9473	44.3971
39	647.0066	9.9040
40	673.1222	2.2276
41	675.0966	2.0592
42	692.0722	17.3623
43	820.0663	0.1609
44	829.3865	21.0192
45	912.4760	59.9807
46	1093.8123	136.3339
47	1114.8534	13.8386
48	1122.1581	105.8176

49	1151.5475	135.0256
50	1152.6458	69.8119
51	1154.3944	24.2998
52	1320.4779	335.5075
53	1393.5293	453.6792
54	1465.3652	34.9478
55	1508.5570	19.8346
56	1520.7054	44.0924
57	1601.9819	1.0363
58	1606.0570	18.7205
59	1610.1773	15.8837
60	1616.2736	14.9279
61	1621.6669	13.2824
62	1636.2119	1.1733
63	1638.3062	9.7718
64	1647.5430	29.5460
65	1652.8552	308.1594
66	1657.4664	1.6487
67	1659.5758	10.9432
68	1731.8442	49.6404
69	1740.7228	20.4497
70	1769.8757	459.6435
71	2888.2469	946.7082
72	2895.0799	1412.8560
73	2922.0211	536.9021
74	2994.0637	1000.2513
75	3136.9434	57.6206
76	3139.3041	392.9357
77	3143.8006	968.9346
78	3286.8999	251.6429
79	3299.7468	258.9408
80	3360.6426	145.9147
81	3444.5159	2.9372
82	3444.7279	43.1547
83	3453.2305	52.2105
84	3455.1792	48.6212
85	3482.3041	82.2081
86	3508.9474	2.1635
87	3509.0717	4.3846
88	3512.1923	2.6800
89	3512.2721	5.2884
90	3522.2666	5.8675

Isomers VI -b

#	Frequency	Infrared
1	18.1828	0.8817
2	24.1947	0.1908
3	30.8313	0.5862
4	34.7125	0.0492
5	43.8050	1.6164
6	51.9201	2.2940
7	59.5582	0.6803
8	64.1232	3.2599
9	79.4149	1.2855
10	112.4337	3.7431
11	125.1381	6.3515
12	137.1785	12.3436
13	166.8533	2.5607
14	171.8250	12.6426
15	178.5578	4.4688
16	183.0947	24.0004
17	185.5039	16.0232
18	195.2854	16.8672
19	198.8834	12.8388
20	202.4101	2.6138
21	216.8331	4.9453
22	234.8162	21.2954
23	247.4881	30.6986
24	257.6337	29.1539
25	272.5741	14.0230
26	288.5092	34.6868
27	294.7274	28.0188
28	315.0247	50.3807
29	372.7320	49.1249
30	378.5988	60.8188
31	389.7693	48.5619
32	414.9619	28.2809
33	419.0473	19.8285
34	436.9385	90.7168
35	464.2576	60.7309
36	520.9795	45.7368
37	561.8794	120.3750
38	567.2967	23.5583
39	617.3727	6.3905
40	640.0447	3.9822
41	694.8948	20.2249

42	699.4077	0.0907
43	819.6670	14.9560
44	822.7036	10.4274
45	982.0796	56.2567
46	1100.6828	96.4888
47	1110.6423	71.1437
48	1121.1428	88.0238
49	1151.9326	115.3799
50	1167.7849	3.6889
51	1170.5014	94.1271
52	1315.4753	157.1602
53	1405.3778	619.2026
54	1480.2970	28.6479
55	1497.7124	25.3455
56	1502.0979	64.1046
57	1603.3284	6.4182
58	1605.9567	5.5049
59	1606.8851	5.8898
60	1620.1038	5.4540
61	1621.0275	5.7941
62	1637.6369	3.5898
63	1640.2207	13.1869
64	1650.5494	15.9189
65	1658.2897	0.9650
66	1660.4817	7.7445
67	1667.5901	129.9026
68	1730.3965	183.8745
69	1736.3811	77.6061
70	1737.1661	554.4356
71	2814.6590	1300.7971
72	2914.8558	1024.2093
73	2947.8768	253.0558
74	2967.2195	1008.5919
75	3098.7253	226.7544
76	3112.9022	744.4641
77	3153.4183	692.2970
78	3264.8155	349.0902
79	3294.6628	301.6347
80	3335.1578	214.1550
81	3440.0324	20.3813
82	3444.8104	25.1988
83	3451.2912	45.2458
84	3464.5643	39.2882
85	3465.4966	90.0625

86	3508.3915	3.1719
87	3509.4927	3.4887
88	3511.7505	3.2778
89	3512.4811	4.8274
90	3521.5917	5.0499

Isomers VI -c

#	Frequency	Infrared
1	28.0191	1.1305
2	34.5468	0.5368
3	42.5571	0.4960
4	54.8314	3.0460
5	57.9475	1.7833
6	67.1326	1.5319
7	72.2952	3.2245
8	77.9374	1.7963
9	97.2401	0.4546
10	110.6251	1.2740
11	116.6220	0.4805
12	138.9816	11.8383
13	149.9827	17.0179
14	173.7257	1.1564
15	176.1361	30.0584
16	188.3049	7.5908
17	190.2520	30.7361
18	197.9524	9.2860
19	214.2980	6.1055
20	229.1734	25.6267
21	256.6250	30.4731
22	264.7527	6.3398
23	268.7709	48.1709
24	272.3921	5.9963
25	287.6863	92.5883
26	297.5925	32.5290
27	311.5554	18.4250
28	362.8264	7.3274
29	394.7477	34.6422
30	418.1533	43.5434
31	423.8570	31.6955
32	451.7040	76.4790
33	470.8511	75.7588
34	478.7582	80.0887
35	527.5217	117.1272
36	533.4347	15.1315

37	563.1213	8.6996
38	566.9205	11.6271
39	604.3507	24.3484
40	628.0035	12.1798
41	689.6059	20.4206
42	817.3966	27.0245
43	823.2677	1.8234
44	825.3046	0.7909
45	969.4252	57.3303
46	1096.5654	106.8662
47	1105.6945	105.2779
48	1122.8384	15.2566
49	1170.7158	117.2773
50	1194.6393	83.4353
51	1215.8049	68.7239
52	1313.2316	114.3998
53	1393.1392	494.7048
54	1448.3108	10.9571
55	1470.0711	18.5684
56	1566.1033	54.9134
57	1587.4103	13.2069
58	1600.8934	7.2467
59	1605.7543	3.1468
60	1611.0134	33.1194
61	1612.0726	9.7360
62	1633.1284	16.5951
63	1641.4604	7.2264
64	1645.9879	1.2987
65	1655.4736	8.1851
66	1661.9041	41.6533
67	1668.5988	178.3417
68	1732.2523	8.2506
69	1733.1679	3.9805
70	1758.8619	332.1104
71	2351.6036	2001.1553
72	2572.9181	1533.6619
73	2665.0615	871.4951
74	2977.7516	402.9293
75	3164.0924	374.1541
76	3191.5110	330.0129
77	3204.9602	398.2950
78	3267.9874	359.6415
79	3316.0274	231.1099
80	3339.7970	162.8975

81	3423.7046	28.2614
82	3450.3931	22.4997
83	3455.8531	39.8967
84	3464.3341	51.8592
85	3474.5727	23.7377
86	3490.2951	18.7181
87	3499.5914	13.2019
88	3515.6697	2.6908
89	3516.7878	3.6558
90	3520.8291	6.9880

Isomers VI -d

#	Frequency	Infrared
1	23.5144	0.9690
2	33.0035	1.7985
3	36.9028	0.8198
4	42.9092	0.6278
5	55.3341	1.0242
6	60.8083	3.2474
7	67.1104	1.5790
8	81.8014	1.4258
9	98.8261	1.2057
10	100.0231	1.1172
11	141.1209	3.5589
12	148.1158	4.6345
13	160.4885	10.3180
14	167.2630	16.6289
15	168.9817	2.7384
16	184.3420	18.1749
17	187.8428	36.6991
18	194.7001	8.2414
19	202.7345	21.0655
20	226.4063	4.2713
21	235.4758	22.8063
22	252.8572	9.8158
23	275.1463	38.3894
24	285.0227	39.9148
25	300.3105	4.5649
26	308.0735	49.8079
27	325.5218	70.0616
28	342.7033	40.8732
29	375.0985	57.9188
30	413.5916	32.8451
31	417.5336	27.0830

32	447.9826	60.7818
33	457.6776	71.1426
34	468.7280	18.6176
35	479.1943	30.2856
36	522.9314	99.6242
37	563.0096	8.3046
38	581.5938	36.5280
39	629.7431	15.9964
40	664.3049	21.2864
41	689.8002	22.2691
42	820.2231	24.5473
43	822.8274	1.4056
44	825.6221	1.8843
45	947.0766	65.9531
46	1106.0275	75.1776
47	1114.7035	104.2201
48	1123.8555	73.1270
49	1140.9891	35.5158
50	1182.0850	91.7362
51	1249.4056	45.8925
52	1315.8837	119.8197
53	1388.4896	523.0257
54	1437.0420	6.0922
55	1476.7217	18.2409
56	1565.4827	47.1018
57	1594.0635	19.4296
58	1604.0107	5.1473
59	1609.9977	4.9548
60	1614.7276	19.2268
61	1625.2483	11.8353
62	1634.8542	15.2248
63	1638.0445	19.5146
64	1639.4481	7.4260
65	1649.1173	7.0776
66	1666.4659	252.2123
67	1670.2782	13.6131
68	1727.3068	0.9997
69	1734.9241	40.9616
70	1752.9460	356.5793
71	2157.0624	2415.1204
72	2521.4269	1331.3554
73	2875.6209	852.9484
74	3049.9250	327.8387
75	3149.3800	321.6249

76	3171.4936	618.1605
77	3211.6128	298.7068
78	3261.9512	444.5209
79	3306.6152	141.7272
80	3310.7443	257.2301
81	3448.9029	24.8341
82	3451.9691	32.6688
83	3458.0340	38.6734
84	3460.9922	54.2927
85	3472.2714	11.3452
86	3474.3898	24.3033
87	3511.5911	2.5835
88	3512.2233	2.3488
89	3515.2706	6.8116
90	3521.0563	5.5358

Isomers VI -e

#	Frequency	Infrared
1	19.5971	0.3950
2	26.6857	0.8465
3	28.0908	4.3646
4	36.9544	2.0429
5	46.8914	5.0405
6	49.7306	0.6369
7	57.2897	1.1316
8	82.5863	1.2692
9	88.2458	0.4639
10	105.7249	3.6336
11	125.0667	8.5471
12	150.1894	12.4496
13	171.3543	0.3780
14	178.5172	3.7773
15	188.6413	12.2712
16	194.3400	11.3285
17	207.1378	1.1812
18	212.0872	11.6144
19	219.3106	16.4860
20	235.3127	19.6284
21	243.3332	31.2321
22	254.5446	17.5972
23	261.4941	111.8491
24	277.3320	87.3427
25	290.1268	39.2252
26	310.4121	2.2628

27	316.0171	55.1032
28	334.1031	14.8179
29	346.0727	19.0018
30	347.6992	16.8599
31	386.5532	42.1132
32	419.3796	51.0143
33	431.1429	69.9281
34	459.6791	92.3794
35	503.3245	7.8163

Isomers VI -f

#	Frequency	Infrared
1	20.8757	0.9237
2	24.9667	1.9605
3	27.5535	0.3635
4	30.8299	0.3615
5	45.3827	1.8756
6	54.7078	2.6643
7	64.0687	3.7250
8	72.0580	0.2903
9	84.8859	3.6166
10	101.4199	1.0065
11	128.9562	10.0796
12	141.8262	8.3535
13	153.7890	3.9055
14	165.9081	17.5782
15	172.4763	34.0838
16	178.2612	33.2532
17	184.6134	19.6601
18	195.8762	5.1747
19	203.3642	8.0279
20	219.9913	1.8265
21	240.4439	31.8202
22	253.0788	0.9863
23	269.2693	38.0509
24	300.3673	39.9047
25	310.3366	12.4050
26	326.0110	38.8788
27	342.6489	60.0166
28	360.1772	11.0979
29	370.1502	74.7795
30	403.5127	44.5429
31	416.7528	35.1118
32	444.6279	39.0518

33	453.1044	30.7771
34	469.3237	79.0252
35	511.0079	9.4967
36	530.3116	46.1758
37	558.6472	99.4352
38	561.9986	13.3813
39	599.9056	28.1764
40	673.0874	24.5448
41	689.1154	22.3910
42	817.5254	1.7053
43	820.8085	28.7665
44	821.8540	3.4796
45	944.5742	56.3899
46	1126.9134	127.7877
47	1129.1768	68.4750
48	1139.8847	68.7362
49	1152.2057	18.7364
50	1173.7565	76.3530
51	1225.8307	42.7489
52	1319.1657	213.0344
53	1395.9777	567.7777
54	1399.4554	3.5868
55	1472.8579	21.7284
56	1567.7574	72.1641
57	1596.5845	23.1666
58	1604.4209	7.4684
59	1608.5174	8.6838
60	1615.1309	8.1310
61	1628.1691	40.9256
62	1636.9069	1.2872
63	1641.0863	9.8372
64	1643.8281	20.8857
65	1659.6235	137.4182
66	1661.3424	5.8403
67	1668.2470	115.4060
68	1720.2292	10.0801
69	1730.2791	30.4002
70	1752.1699	514.1051
71	2200.6911	2147.5972
72	2571.4693	1375.9987
73	2852.4359	951.5118
74	3053.6921	314.6971
75	3140.6860	316.3295
76	3170.0098	554.8263

77	3180.6860	545.5093
78	3267.7607	310.0791
79	3309.9387	198.0794
80	3319.1116	392.3574
81	3443.0260	23.1672
82	3446.7697	51.7010
83	3450.2587	22.5493
84	3462.3845	61.4494
85	3484.0269	19.1973
86	3485.2480	27.0877
87	3505.4432	2.6552
88	3510.1428	1.9108
89	3515.7410	6.7159
90	3521.0462	5.8638

Isomers VI -g

#	Frequency	Infrared
1	17.2922	1.3316
2	19.1564	0.5646
3	22.5516	1.6670
4	31.0566	2.6238
5	38.1231	3.1362
6	48.9373	3.7829
7	67.4575	0.4574
8	79.1572	3.0004
9	92.6517	3.5368
10	101.1293	8.8093
11	113.2293	22.4177
12	136.5999	5.5681
13	138.4785	13.4362
14	170.6211	21.2432
15	180.2264	42.6659
16	186.8146	8.5292
17	191.8005	27.7215
18	201.0414	6.4162
19	211.7205	18.4759
20	231.7619	29.9257
21	238.0072	12.7251
22	248.7103	59.3446
23	256.8541	17.7561
24	272.0847	43.1846
25	274.2720	52.6367
26	296.8180	102.6697
27	306.1470	33.3808

28	326.5678	28.2942
29	351.1632	11.4399
30	373.2466	44.3123
31	410.4394	23.0842
32	428.6299	89.1865
33	445.1405	24.3604
34	452.3394	190.1928
35	471.8245	33.0345
36	492.7185	28.7595
37	565.5634	46.8225
38	570.7719	23.1965
39	577.3092	18.4013
40	659.7229	19.5676
41	671.7576	36.5931
42	726.2252	37.1824
43	823.9745	0.5483
44	845.0053	28.1297
45	1079.3486	108.3876
46	1104.1589	117.8874
47	1129.7078	74.4087
48	1158.9812	73.3578
49	1160.5532	100.5016
50	1246.5286	75.0063
51	1252.9074	313.1204
52	1322.3505	29.3166
53	1348.9361	282.0621
54	1402.6165	687.8913
55	1482.9997	125.5026
56	1557.4160	70.9359
57	1587.0722	37.1046
58	1599.0719	5.3925
59	1606.4263	4.2886
60	1610.3496	83.8737
61	1612.9887	12.4881
62	1619.8264	479.7463
63	1636.8015	7.8719
64	1641.0078	12.1769
65	1641.4160	30.2655
66	1653.6839	140.2515
67	1659.5454	6.2227
68	1672.3324	679.4287
69	1691.4096	30.1823
70	1711.5871	64.9875
71	2164.7221	2879.9464

72	2273.9310	1613.2594
73	2742.8376	1217.2306
74	3089.1724	684.8038
75	3171.7338	396.7032
76	3174.0409	432.3952
77	3294.9890	239.1646
78	3304.6376	333.2268
79	3331.3157	126.6762
80	3446.1307	20.7861
81	3452.7511	27.8074
82	3454.2225	48.0500
83	3468.3117	89.8668
84	3469.2529	13.7812
85	3489.3779	45.6384
86	3513.3548	4.8947
87	3516.3744	5.2562
88	3517.5814	5.6468
89	3524.6106	3.5119
90	3527.4723	7.2277

Isomers VI -h

#	Frequency	Infrared
1	21.5965	3.3120
2	26.3114	0.2500
3	39.0844	0.6308
4	41.5041	1.4459
5	61.2917	2.9844
6	68.3582	1.8019
7	75.0570	6.2871
8	91.8527	3.3119
9	104.2551	1.2041
10	117.3706	2.5124
11	149.7673	14.3712
12	180.3846	0.8974
13	182.4763	8.1297
14	184.3433	7.5135
15	191.0075	7.1141
16	197.0145	6.6892
17	200.1901	42.4391
18	239.9489	12.8695
19	242.8614	2.9349
20	258.3039	132.2949
21	262.1221	82.9082
22	266.2279	43.7516

23	288.1444	3.5644
24	299.9851	2.9884
25	311.2536	10.4119
26	320.8093	43.8614
27	369.3628	12.6811
28	382.8760	31.2919
29	391.2110	269.5029
30	396.6798	112.7028
31	406.6680	71.8855
32	438.8994	28.8227
33	455.1805	7.5371
34	461.5270	70.6424
35	518.8573	22.5993
36	524.0195	23.0459
37	584.9340	45.9870
38	602.6632	32.2952
39	637.9838	0.7466
40	650.0812	16.4909
41	739.2122	18.4370
42	758.6801	94.4962
43	829.4504	4.0264
44	859.7930	0.6168
45	1141.4535	61.3228
46	1143.2067	66.7374
47	1171.9095	98.1912
48	1179.9590	84.8332
49	1240.9277	164.9746
50	1260.0104	93.7613
51	1313.0037	19.7329
52	1397.7134	40.6439
53	1436.1410	925.9183
54	1449.2830	330.2790
55	1498.6575	1526.2560
56	1543.6917	155.7550
57	1559.5124	20.9987
58	1585.9848	67.8591
59	1599.3864	4.9435
60	1604.0668	12.5129
61	1609.7910	2.4754
62	1618.8393	16.9580
63	1635.7455	34.9693
64	1640.9169	52.2405
65	1650.2461	23.6761
66	1656.1895	9.2454

67	1664.3546	2.6948
68	1669.5668	28.6143
69	1681.3603	49.4496
70	1685.4106	48.2533
71	2366.1228	1253.2705
72	2561.1598	995.5413
73	2758.5635	998.8758
74	2770.4484	1686.4190
75	2808.9132	747.0064
76	2969.7628	486.7661
77	3069.1922	738.1824
78	3079.7736	677.9740
79	3253.2852	415.1438
80	3277.7281	287.5883
81	3440.3525	17.1693
82	3442.7324	18.4435
83	3447.1825	44.9314
84	3447.6027	23.7439
85	3505.0657	39.5325
86	3506.3366	35.2945
87	3509.0053	3.4375
88	3509.7564	3.0278
89	3510.8423	4.3338
90	3512.7721	4.6286