Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Mode-specific fragmentation of amino acid-containing clusters

Supporting Information

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Contents

Section I. Computational Details 2
Section II. Spectral Assignment 3
Section III. Cluster Structures & Energetics 5
Section IV. Local Minima Energies 8
Section V. Transition State Energies 12
Section VI. Vibrational Spectra 16
Section VII. Local Minima X,Y,Z Coordinates 23
Section VIII. Transition State X,Y,Z Coordinates 49

Section I. Computational Details

A common choice for search strategy is the basin-hopping algorithm, which can be employed to map complex PESs and identify stationary points (*viz*. local minima and transition states). This method utilizes Monte Carlo with minimization to transform the potential energy landscape into a set of catchment basins that partition all of configuration space. Importantly, random structural perturbations are tested against energetic and geometric convergence acceptance criteria. These acceptance tests ensure that clusters do not dissociate during simulation and that the basin-hopping algorithm seeks low energy structures, in particular the PES global minimum.

A custom-written basin-hopping routine interfaced with the Gaussian 09 suite for computational chemistry was employed for structural sampling of protonated 3-CF_3-Phe•TMA. The protonated dimer was initially modelled using the AMBER force field, which was amended to include partial charges for the TMA and 3-CF_3-Phe moieties that were calculated at the B3LYP/6-31+G(d,p) level using the CHelpG partition scheme. For each random structural perturbation, the charge-carrying proton and the TMA moiety were given random translational steps of size $-0.2\ \text{Å} \leq \eta \leq 0.2\ \text{Å}$ in each of the X, Y, and Z directions. The TMA moiety was also given a random internal rotation of $-5° \leq \theta \leq 5°$ about the TMA−fixed *x*−, *y*−, and *z*−axes. A random rotation of $-5° \leq \varphi \leq 5°$ was also applied to each of the dihedral angles along the saturated carbon chain of 3-CF_3-Phe. In total, *ca*. 40,000 protonated 3-CF_3-Phe•TMA cluster structures were sampled by the basin-hopping routine, resulting in the identification of 226 cluster isomers as determined by unique energies and geometries. Convergence criteria for the search were set to the default criteria of Gaussian 09.[17] Each unique isomer was found more than hundred times using the basin-hopping search algorithm. This entire test set of unique isomer structures was then carried forward for treatment at the PM6 semi-empirical level of theory to refine cluster geometries, from which unique isomers were carried forward for treatment at the B3LYP/6-311++G(d,p) DFT level of theory.[19-22] This method resulted in identification of 25 unique proton-bound 3-CF_3-Phe•TMA cluster isomers within 60 kJ•mol^{-1} of the calculated ground state. While there may have been some isomers missed by the search algorithm (particularly at higher energies), this treatment is sufficient to confidently map

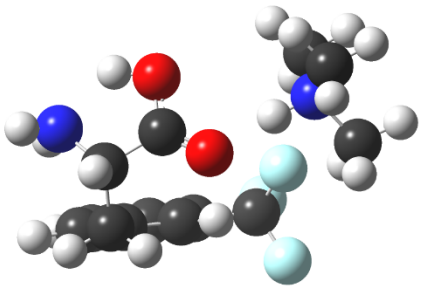
the lower energy regions of the PES. To ensure that each isomer was a local minimum on the PES, normal mode analyses were undertaken. Calculated harmonic frequencies also served to predict the vibrational spectrum for each isomer. Computed IR transitions were broadened by convolution with a $\sigma = 5$ cm^{-1} Gaussian distribution. For selected isomers anharmonically corrected vibrational frequencies were also calculated.

Section II. Spectral Assignment

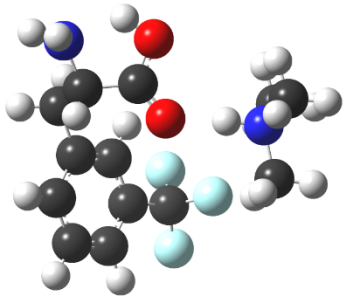
Having assigned the spectral carriers based on the carbonyl stretching modes, it is now possible to assign the rest of the observed spectra. The region from 1300 – 1425 cm^{-1} exhibits vibrational transitions associated with amine and hydroxyl functional groups. Three peaks are observed in the TMA•H$^+$ product channel spectrum (1332 cm^{-1}, 1350 cm^{-1}, and 1418 cm^{-1}) whereas only the 1332 cm^{-1} peak leads to production of 3-CF_3-Phe•H$^+$. Comparison with the calculated vibrational spectra suggest that the peak at 1418 cm^{-1} is associated with the COH bending motion of the charge solvated structures, while the peak at 1332 cm^{-1} is associated with the NH_3 umbrella mode in the zwitterion isomers. Observation of these modes is clear evidence that the hydrogen nuclei associated with the proton transfer coordinates are localized. The peak at 1350 cm^{-1} is somewhat ambiguous; the most likely assignment is to normal modes involving phenyl ring motions and symmetric CF_3 stretching. These modes are predicted to exhibit a relatively large absorption cross-section and they are fairly harmonic (shifting only a few cm^{-1} in the anharmonic calculations; see supporting information). It should also be noted that these normal modes do exhibit small displacements of the proton that is located between the amine and carboxylic acid moieties. There is a possible contribution from the NH_2 twisting mode of the TMA-bridged structures, however, this mode is unlikely to be a major contributor to the spectrum as it is expected to have a relatively small absorption cross section. Furthermore, the TMA-bridged C=O stretch at 1786 cm^{-1} suggests that these isomers are likely only a minor population in the ensemble. Nevertheless, we cannot rule out the possibility that the TMA-bridged NH_2 twist has a minor contribution to either the 1332 cm^{-1} or the 1350 cm^{-1} peak.

Both product mass channels exhibit broad features at 1210 cm^{-1} and 1235 cm^{-1}. In comparing the observed spectra (Figures 2A-B) to calculation (Figures 2C-E), we see that the experimental data appear to be a convolution of all three structural motifs. The peak at 1210 cm^{-1} is in good agreement with the combined phenyl ring vibration and CF_3 umbrella mode that is predicted to occur in the 1206 – 1214 cm^{-1} region for all three structural motifs. However, following anharmonic correction, a combined NH_2 twist / COH bending vibration (observed in canonical and TMA-bridged structures) yields a better match to the observed wavenumber. This treatment also suggests that the transition observed at 1235 cm^{-1} is associated with the TMA•H^+ umbrella mode (observed in TMA-bridged and zwitterion structures). While both of these vibrational modes have relatively small calculated absorption cross sections, they are associated with motions along proton-transfer coordinates, which consistently exhibit intense IRMPD signals across the spectral region studied and in the analogous 3-cyanophenylalanine cluster. It is therefore tempting to conclude that these modes are particularly active in IRMPD owing to efficient coupling with the dissociative threshold leading to TMA•H^+ and/or 3-CF_3-Phe•H^+ production. Parneix *et al.* have, however, shown that such a view may be too simplistic and that dynamic energy flow during the IRMPD process should be considered to properly model observed IRMPD intensities.[25] These same considerations also provide a reasonable explanation for the IRMPD phenomenon whereby predicted (usually weak) transitions are not observed experimentally.

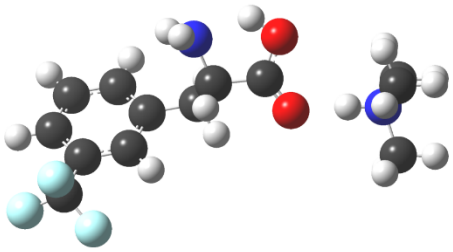
Section III. Cluster Structures & Energetics



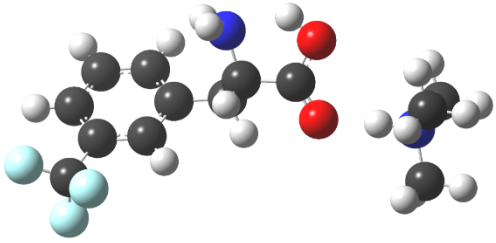
Isomer 1
Charge-Solvated
0.0 kJ•mol^{-1}



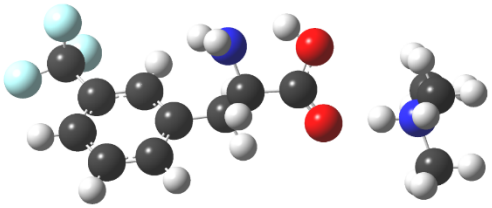
Isomer 2
Charge-Solvated
5.8 kJ•mol^{-1}



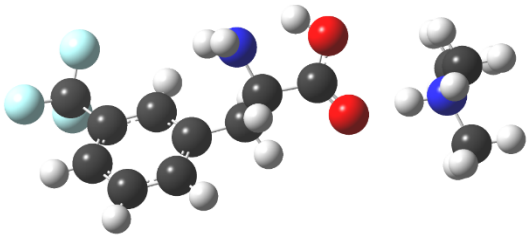
Isomer 3
Charge-Solvated
9.7 kJ•mol^{-1}



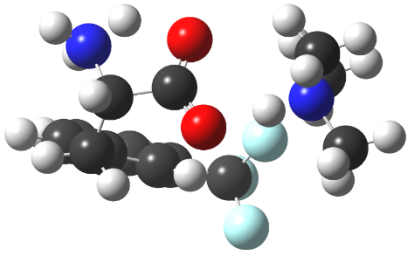
Isomer 4
Charge-Solvated
9.8 kJ•mol^{-1}



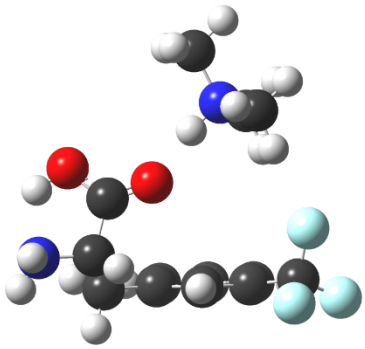
Isomer 5
Charge-Solvated
9.9 kJ•mol^{-1}



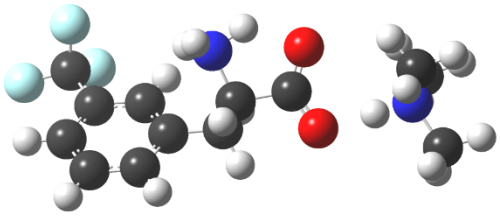
Isomer 6
Charge-Solvated
10.0 kJ•mol^{-1}



Isomer 7
Zwitterion
13.8 kJ•mol^{-1}



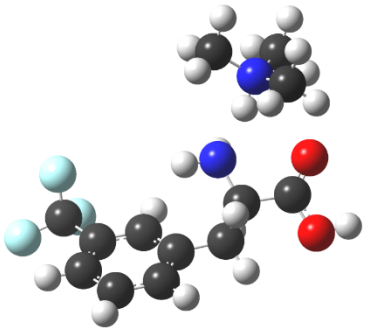
Isomer 8
Charge-Solvated
14.4 kJ•mol^{-1}



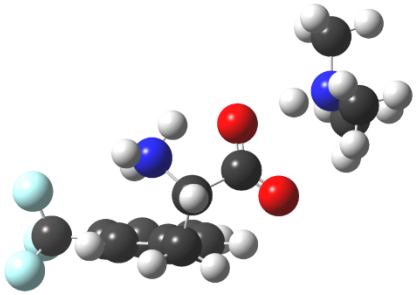
Isomer 9
Zwitterion
17.6 kJ•mol^{-1}

Isomer 10
Zwitterion
18.5 kJ•mol^{-1}

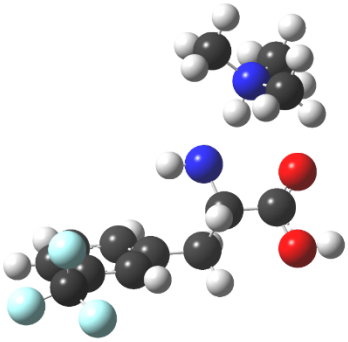
Isomer 11
Zwitterion
19.3 kJ•mol^{-1}



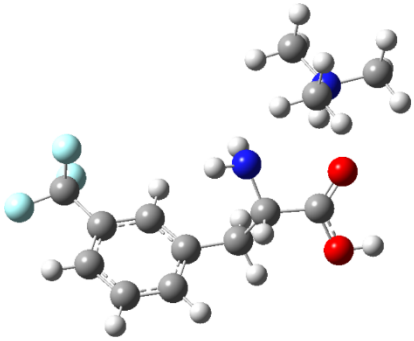
Isomer 12
TMA-bridged
24.4 kJ•mol^{-1}



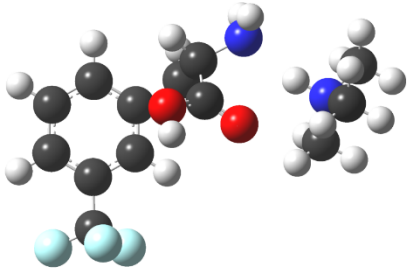
Isomer 13
Zwitterion*
24.4 kJ•mol^{-1}



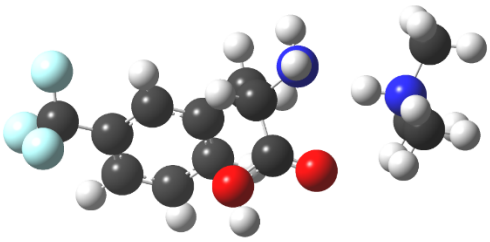
Isomer 14
TMA-bridged
25.5 kJ•mol^{-1}



Isomer 15
TMA-bridged
30.2 kJ•mol^{-1}

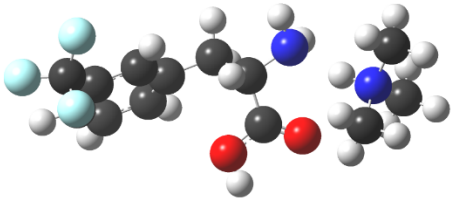


Isomer 16
TMA-bridged
32.4 kJ•mol^{-1}

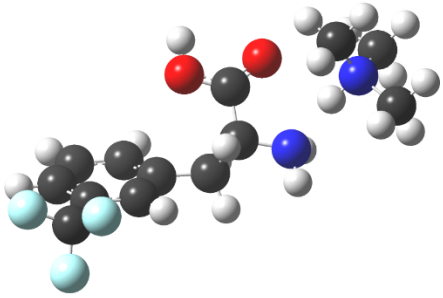


Isomer 17
TMA-bridged
35.2 kJ•mol^{-1}

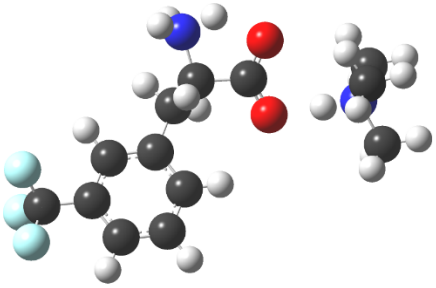
Isomer 18
Charge-solvated*
37.4 kJ•mol^{-1}



Isomer 19
TMA-bridged
38.3 kJ•mol^{-1}

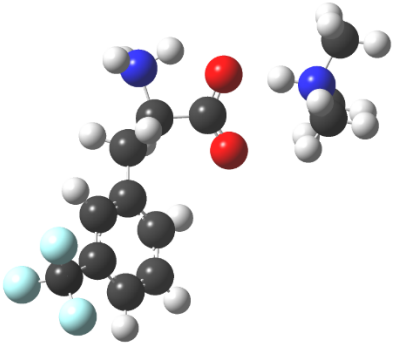


Isomer 20
TMA-bridged
38.5 kJ•mol^{-1}

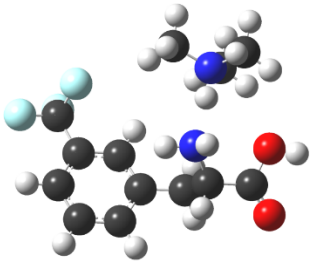


Isomer 21
Zwitterion
39.1 kJ•mol^{-1}

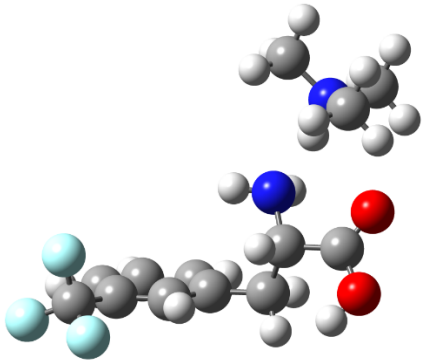
Isomer 22
Charge-solvated*
39.5 kJ•mol^{-1}



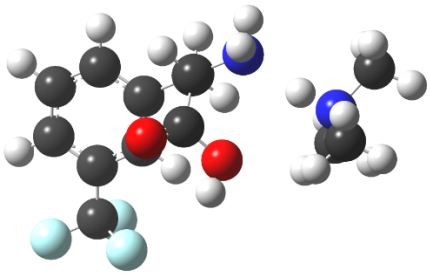
Isomer 23
Zwitterion*
44.4 kJ•mol^{-1}



Isomer 24
TMA-bridged*
45.7 kJ•mol^{-1}



Isomer 25
TMA-bridged
50.3 kJ•mol^{-1}



Isomer 26
TMA-bridged
59.3 kJ•mol^{-1}

Section IV. Local Minima Energies

Iso 1	Eh		Relative Eh	eV	kJ/mol	CS Global Min
Electronic	-1067.057112		0	0	0	
ZPE correction	0.330526	-1066.726586	0	0	0	
Thermal correction	0.35226	-1066.704852	0	0	0	
Gibbs correction	0.275958	-1066.781154	0.0002905	0.007905	0.762721	

Iso 2	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.05491		0.0022023	0.059928	5.782237	
ZPE correction	0.330336	-1066.724574	0.0020123	0.054757	5.283384	
Thermal correction	0.352223	-1066.702687	0.0021653	0.058921	5.685092	
Gibbs correction	0.275932	-1066.778978	0.0024668	0.067125	6.476694	

Iso 3	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.05343		0.0036826	0.100209	9.668831	
ZPE correction	0.329925	-1066.723505	0.0030816	0.083855	8.090879	
Thermal correction	0.352053	-1066.701377	0.0034756	0.094576	9.125343	
Gibbs correction	0.272002	-1066.781428	1.71E-05	0.000465	0.044897	

Iso 4	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.053393		0.0037195	0.101213	9.765714	
ZPE correction	0.329926	-1066.723467	0.0031195	0.084886	8.190387	
Thermal correction	0.352057	-1066.701336	0.0035165	0.095689	9.232728	
Gibbs correction	0.271948	-1066.781445	0	0	0	

Iso 5	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.05334		0.0037724	0.102652	9.904605	

ZPE correction	0.329926	-1066.723414	0.0031724	0.086325	8.329278	
Thermal correction	0.352034	-1066.701306	0.0035464	0.096502	9.311232	
Gibbs correction	0.27228	-1066.78106	0.0003849	0.010474	1.010572	
Iso 6	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.053308		0.0038046	0.103528	9.989148	
ZPE correction	0.329921	-1066.723387	0.0031996	0.087066	8.400693	
Thermal correction	0.352035	-1066.701273	0.0035796	0.097406	9.3984	
Gibbs correction	0.271965	-1066.781343	0.0001021	0.002778	0.268068	
Iso 7	Eh		Relative Eh	eV	kJ/mol	ZW
Electronic	-1067.051851		0.005261	0.143159	13.81299	
ZPE correction	0.330503	-1066.721348	0.005238	0.142533	13.7526	
Thermal correction	0.352074	-1066.699777	0.005075	0.138098	13.32464	
Gibbs correction	0.275968	-1066.775883	0.0055615	0.151336	14.60197	
Iso 8	Eh		Relative Eh	eV	kJ/mol	CS
Electronic	-1067.051638		0.0054747	0.148974	14.37407	
ZPE correction	0.330407	-1066.721231	0.0053557	0.145736	14.06163	
Thermal correction	0.352412	-1066.699226	0.0056267	0.15311	14.77315	
Gibbs correction	0.275455	-1066.776183	0.0052622	0.143192	13.81614	
Iso 9	Eh		Relative Eh	eV	kJ/mol	ZW
Electronic	-1067.050425		0.0066876	0.181979	17.55859	
ZPE correction	0.330275	-1066.72015	0.0064366	0.175149	16.89958	
Thermal correction	0.352084	-1066.698341	0.0065116	0.17719	17.0965	
Gibbs correction	0.274481	-1066.775944	0.0055011	0.149693	14.44338	
Iso 10	Eh		Relative Eh	eV	kJ/mol	ZW
Electronic	-1067.05005		0.0070622	0.192172	18.54212	
ZPE correction	0.330237	-1066.719813	0.0067732	0.184308	17.78334	
Thermal correction	0.352066	-1066.697984	0.0068682	0.186893	18.03277	
Gibbs correction	0.274364	-1066.775686	0.0057587	0.156702	15.11972	
Iso 11	Eh		Relative Eh	eV	kJ/mol	ZW
Electronic	-1067.049752		0.0073605	0.200289	19.32532	
ZPE correction	0.330471	-1066.719281	0.0073055	0.198793	19.18092	
Thermal correction	0.352092	-1066.69766	0.0071925	0.195718	18.88423	
Gibbs correction	0.275131	-1066.774621	0.006824	0.18569	17.91672	
Iso 12	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.047827		0.009285	0.252658	24.37818	
ZPE correction	0.330483	-1066.717344	0.009242	0.251488	24.26528	
Thermal correction	0.352347	-1066.69548	0.009372	0.255025	24.60661	
Gibbs correction	0.275204	-1066.772623	0.0088215	0.240045	23.16124	

Iso 13	Eh		Relative Eh	eV	kJ/mol	ZW Shared O
Electronic	-1067.047803		0.0093094	0.253322	24.44225	
ZPE correction	0.330937	-1066.716866	0.0097204	0.264506	25.52135	
Thermal correction	0.352533	-1066.69527	0.0095824	0.26075	25.15902	
Gibbs correction	0.276159	-1066.771644	0.0098009	0.266696	25.7327	

Iso 14	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.047403		0.009709	0.264195	25.49141	
ZPE correction	0.330444	-1066.716959	0.009627	0.261964	25.27612	
Thermal correction	0.352323	-1066.69508	0.009772	0.26591	25.65682	
Gibbs correction	0.274938	-1066.772465	0.0089795	0.244345	23.57608	

Iso 15	Eh		Relative Eh	eV	kJ/mol	TB O-interaction
Electronic	-1067.045627		0.0114858	0.312545	30.15648	
ZPE correction	0.330198	-1066.715429	0.0111578	0.303619	29.2953	
Thermal correction	0.352428	-1066.693199	0.0116538	0.317116	30.59757	
Gibbs correction	0.272721	-1066.772906	0.0085393	0.232366	22.42031	

Iso 16	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.044759		0.0123535	0.336156	32.43467	
ZPE correction	0.330553	-1066.714206	0.0123805	0.336891	32.50556	
Thermal correction	0.352439	-1066.69232	0.0125325	0.341027	32.90464	
Gibbs correction	0.275493	-1066.769266	0.012179	0.331407	31.97651	

Iso 17	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.043688		0.013424	0.365286	35.24531	
ZPE correction	0.330543	-1066.713145	0.013441	0.365748	35.28995	
Thermal correction	0.35243	-1066.691258	0.013594	0.369912	35.69166	
Gibbs correction	0.275318	-1066.76837	0.0130745	0.355775	34.32769	

Iso 18	Eh		Relative Eh	eV	kJ/mol	CS No H-bond
Electronic	-1067.042856		0.0142566	0.387942	37.43134	
ZPE correction	0.32997	-1066.712886	0.0137006	0.372812	35.97154	
Thermal correction	0.35234	-1066.690516	0.0143366	0.390119	37.64139	
Gibbs correction	0.274751	-1066.768105	0.0133401	0.363003	35.02503	

Iso 19	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.042522		0.0145899	0.397011	38.30644	
ZPE correction	0.330349	-1066.712173	0.0144129	0.392195	37.84171	
Thermal correction	0.352264	-1066.690258	0.0145939	0.39712	38.31694	
Gibbs correction	0.274645	-1066.767877	0.0135674	0.369188	35.62182	

Iso 20	Eh		Relative Eh	eV	kJ/mol	TB
Electronic	-1067.042466		0.0146466	0.398554	38.4553	

ZPE correction	0.330316	-1066.71215	0.0144366	0.39284	37.90394	
Thermal correction	0.352249	-1066.690217	0.0146356	0.398255	38.42642	
Gibbs correction	0.27438	-1066.768086	0.0133591	0.36352	35.07492	
Iso 21	Eh		Relative Eh	eV	kJ/mol	ZW
Electronic	-1067.042203		0.0149093	0.405703	39.14504	
ZPE correction	0.330121	-1066.712082	0.0145043	0.394682	38.08169	
Thermal correction	0.351971	-1066.690232	0.0146203	0.397839	38.38625	
Gibbs correction	0.272973	-1066.76923	0.0122148	0.332382	32.0705	
Iso 22	Eh		Relative Eh	eV	kJ/mol	CS O-interaction
Electronic	-1067.042079		0.0150331	0.409071	39.47008	
ZPE correction	0.329655	-1066.712424	0.0141621	0.38537	37.18323	
Thermal correction	0.351977	-1066.690102	0.0147501	0.401371	38.72705	
Gibbs correction	0.274689	-1066.76739	0.0140546	0.382445	36.90098	
Iso 23	Eh		Relative Eh	eV	kJ/mol	ZW Shared-O
Electronic	-1067.0402		0.0169128	0.460221	44.40531	
ZPE correction	0.330386	-1066.709814	0.0167728	0.456411	44.03774	
Thermal correction	0.352231	-1066.687969	0.0168838	0.459432	44.32917	
Gibbs correction	0.273595	-1066.766605	0.0148403	0.403825	38.96387	
Iso 24	Eh		Relative Eh	eV	kJ/mol	TB OH-interaction
Electronic	-1067.039707		0.0174055	0.473628	45.69892	
ZPE correction	0.330217	-1066.70949	0.0170965	0.465219	44.88763	
Thermal correction	0.352169	-1066.687538	0.0173145	0.471152	45.46	
Gibbs correction	0.274793	-1066.764914	0.016531	0.449831	43.40288	
Iso 25	Eh		Relative Eh	eV	kJ/mol	TB OH-rotation
HF	-1067.037159		0.0199537	0.542968	52.38933	
ZPE	0.330131	-1066.707028	0.0195587	0.532219	51.35224	
Thermal	0.352121	-1066.685038	0.0198147	0.539185	52.02438	
Gibbs	0.274867	-1066.762292	0.0191532	0.521185	50.28758	
Iso 26	Eh		Relative Eh	eV	kJ/mol	TB OH-interaction
Electronic	-1067.034509		0.0226036	0.615075	59.34676	
ZPE correction	0.330118	-1066.704391	0.0221956	0.603973	58.27554	
Thermal correction	0.352141	-1066.682368	0.0224846	0.611837	59.03432	
Gibbs correction	0.274312	-1066.760197	0.0212481	0.57819	55.78784	

Section V. Transition State Energies

TS1	Eh		Relative Eh	eV	kJ/mol	CS TMA/CF3 rotation
HF	-1067.053779		0.0033337	0.09071459	8.752779	
ZPE	0.330171	-1066.723608	0.0029787	0.08105455	7.82071	
Thermal	0.351267	-1066.702512	0.0023407	0.06369369	6.145613	
Gibbs	0.276919	-1066.77686	0.0042947	0.11686473	11.27593	

TS2	Eh		Relative Eh	eV	kJ/mol	CS CF3 rotation
HF	-1067.053309		0.0038035	0.1034985	9.98626	
ZPE	0.329898	-1066.723411	0.0031755	0.08640975	8.337417	
Thermal	0.351111	-1066.702198	0.0026545	0.07223262	6.969509	
Gibbs	0.274714	-1066.778595	0.0025595	0.06964754	6.720082	

TS3	Eh		Relative Eh	eV	kJ/mol	CS TMA rotation
HF	-1067.05323		0.003882	0.10563459	10.19236	
ZPE	0.329961	-1066.723269	0.003317	0.09026016	8.708932	
Thermal	0.351148	-1066.702082	0.00277	0.07537553	7.272759	
Gibbs	0.275309	-1066.777921	0.003233	0.0879744	8.488386	

TS4	Eh		Relative Eh	eV	kJ/mol	CS TMA rotation
HF	-1067.05314		0.0039724	0.1080945	10.42971	
ZPE	0.32988	-1066.72326	0.0033264	0.09051595	8.733612	
Thermal	0.351092	-1066.702048	0.0028044	0.0763116	7.363078	
Gibbs	0.27529	-1066.77785	0.0033044	0.0899173	8.67585	

TS5	Eh		Relative Eh	eV	kJ/mol	CS TMA rotation
HF	-1067.05314		0.0039724	0.1080945	10.42971	
ZPE	0.329882	-1066.723258	0.0033284	0.09057037	8.738863	
Thermal	0.351094	-1066.702046	0.0028064	0.07636603	7.368329	
Gibbs	0.275294	-1066.777846	0.0033084	0.09002614	8.686352	

TS6	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.049298		0.0078144	0.21264064	20.51706	
ZPE	0.327114	-1066.722184	0.0044024	0.1197954	11.5587	
Thermal	0.348279	-1066.701019	0.0038334	0.10431212	10.06476	
Gibbs	0.273446	-1066.775852	0.0053024	0.14428564	13.92169	

TS7	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.047972		0.0091406	0.24872838	23.99905	
ZPE	0.329925	-1066.718047	0.0085396	0.23237433	22.4211	
Thermal	0.351079	-1066.696893	0.0079596	0.21659173	20.89829	

Gibbs	0.275138	-1066.772834	0.0083206	0.22641504	21.84611	
TS8	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.047937		0.0091749	0.24966173	24.08911	
ZPE	0.329865	-1066.718072	0.0085139	0.231675	22.35363	
Thermal	0.351034	-1066.696903	0.0079489	0.21630057	20.87019	
Gibbs	0.275177	-1066.77276	0.0083939	0.22840963	22.03856	
TS9	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.046833		0.0102795	0.27971942	26.98929	
ZPE	0.326699	-1066.720134	0.0064525	0.17558145	16.94133	
Thermal	0.348121	-1066.698712	0.0061405	0.1670915	16.12216	
Gibbs	0.271226	-1066.775607	0.0055475	0.15095515	14.56521	
TS10	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.046832		0.0102801	0.27973575	26.99086	
ZPE	0.326701	-1066.720131	0.0064551	0.1756522	16.94815	
Thermal	0.348122	-1066.69871	0.0061421	0.16713504	16.12636	
Gibbs	0.271241	-1066.775591	0.0055631	0.15137965	14.60617	
TS11	Eh		Relative Eh	eV	kJ/mol	Proton Transfer
HF	-1067.046615		0.0104977	0.28565694	27.56218	
ZPE	0.326566	-1066.720049	0.0065377	0.17789986	17.16502	
Thermal	0.348021	-1066.698594	0.0062587	0.17030789	16.4325	
Gibbs	0.270805	-1066.77581	0.0053447	0.14543668	14.03275	
TS12	Eh		Relative Eh	eV	kJ/mol	CS Dihedral
HF	-1067.046517		0.0105952	0.28831005	27.81817	
ZPE	0.326597	-1066.71992	0.0066662	0.18139653	17.50241	
Thermal	0.348071	-1066.698446	0.0064062	0.17432157	16.81977	
Gibbs	0.270394	-1066.776123	0.0050312	0.13690591	13.20964	
TS13	Eh		Relative Eh	eV	kJ/mol	CS Dihedral
HF	-1067.045851		0.0112611	0.30643011	29.56652	
ZPE	0.330299	-1066.715552	0.0110341	0.30025313	28.97052	
Thermal	0.351164	-1066.694687	0.0101651	0.27660644	26.68893	
Gibbs	0.276828	-1066.769023	0.0121311	0.33010402	31.85075	
TS14	Eh		Relative Eh	eV	kJ/mol	ZW Dihedral
HF	-1067.045111		0.0120013	0.32657198	31.50995	
ZPE	0.326745	-1066.718366	0.0082203	0.22368574	21.58277	
Thermal	0.348095	-1066.697016	0.0078363	0.21323657	20.57456	
Gibbs	0.272696	-1066.772415	0.0087393	0.23780845	22.94542	
TS15	Eh		Relative Eh	eV	kJ/mol	Proton Transfer

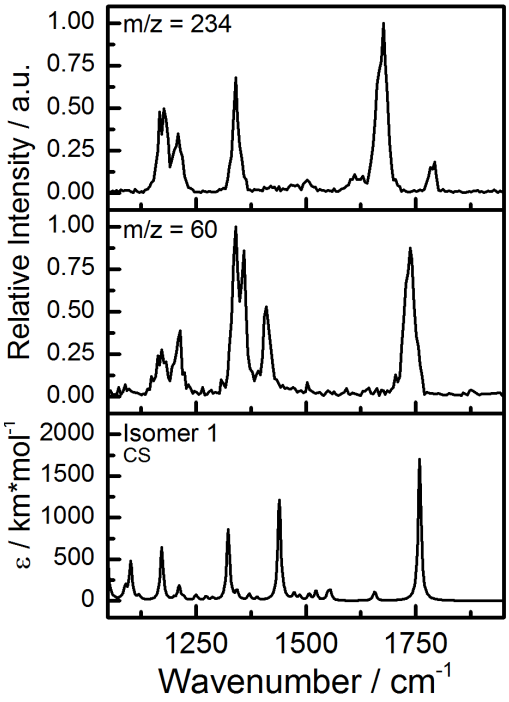
HF	-1067.042715		0.0143977	0.39178134	37.80181	
ZPE	0.329839	-1066.712876	0.0137107	0.37308712	35.99806	
Thermal	0.35071	-1066.692005	0.0128477	0.3496037	33.73221	
Gibbs	0.277004	-1066.765711	0.0154437	0.42024445	40.54813	
TS16	Eh		Relative Eh	eV	kJ/mol	ZW Dihedral
HF	-1067.041691		0.0154213	0.41963491	40.48931	
ZPE	0.326534	-1066.715157	0.0114293	0.31100707	30.00814	
Thermal	0.347982	-1066.693709	0.0111433	0.30322461	29.25723	
Gibbs	0.270477	-1066.771214	0.0099403	0.27048932	26.0987	
TS17	Eh		Relative Eh	eV	kJ/mol	ZW Dihedral
HF	-1067.040882		0.01623	0.44164076	42.61259	
ZPE	0.329815	-1066.711067	0.015519	0.42229347	40.74583	
Thermal	0.350727	-1066.690155	0.014697	0.39992571	38.58763	
Gibbs	0.276536	-1066.764346	0.016808	0.45736894	44.13016	
TS18	Eh		Relative Eh	eV	kJ/mol	TB Dihedral
HF	-1067.040633		0.0164794	0.44842728	43.2674	
ZPE	0.330421	-1066.710212	0.0163744	0.44557008	42.99172	
Thermal	0.351484	-1066.689149	0.0157034	0.42731125	41.22998	
Gibbs	0.27679	-1066.763843	0.0173114	0.47106715	45.45186	
TS19	Eh		Relative Eh	eV	kJ/mol	TB Dihedral
HF	-1067.039518		0.0175941	0.47875981	46.1941	
ZPE	0.33036	-1066.709158	0.0174281	0.47424272	45.75826	
Thermal	0.35146	-1066.688058	0.0167941	0.4569907	44.09366	
Gibbs	0.277404	-1066.762114	0.0190401	0.51810747	49.99064	
TS20	Eh		Relative Eh	eV	kJ/mol	TB Dihedral
HF	-1067.03951		0.0176023	0.47898294	46.21563	
ZPE	0.330369	-1066.709141	0.0174453	0.47471075	45.80342	
Thermal	0.351459	-1066.688051	0.0168013	0.45718662	44.11257	
Gibbs	0.277386	-1066.762124	0.0190303	0.5178408	49.96491	
TS21	Eh		Relative Eh	eV	kJ/mol	TB Dihedral
HF	-1067.038474		0.0186383	0.50717394	48.93569	
ZPE	0.330217	-1066.708257	0.0183293	0.49876562	48.1244	
Thermal	0.351318	-1066.687156	0.0176963	0.48154081	46.46243	
Gibbs	0.276949	-1066.761525	0.0196293	0.53414042	51.53761	
TS22	Eh		Relative Eh	eV	kJ/mol	CS AA rotation
HF	-1067.031601		0.0255116	0.69420594	66.98185	
ZPE	0.330771	-1066.70083	0.0257566	0.70087273	67.62511	
Thermal	0.351919	-1066.679682	0.0251706	0.68492686	66.08654	

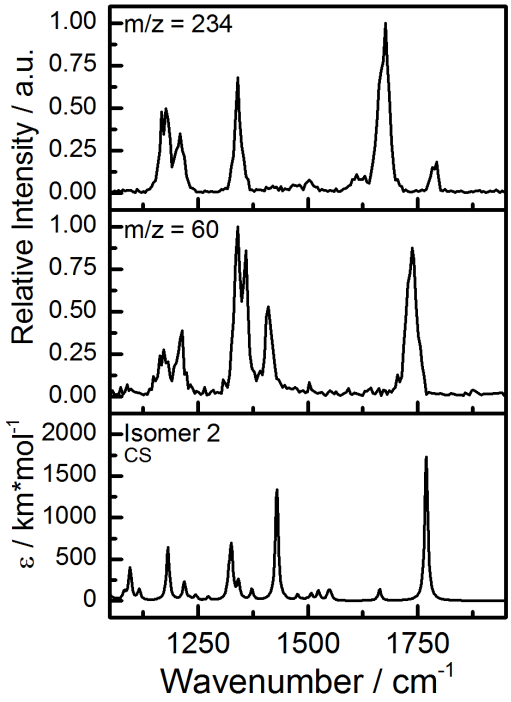
Gibbs	0.27707	-1066.754531	0.0266236	0.724465	69.90145	

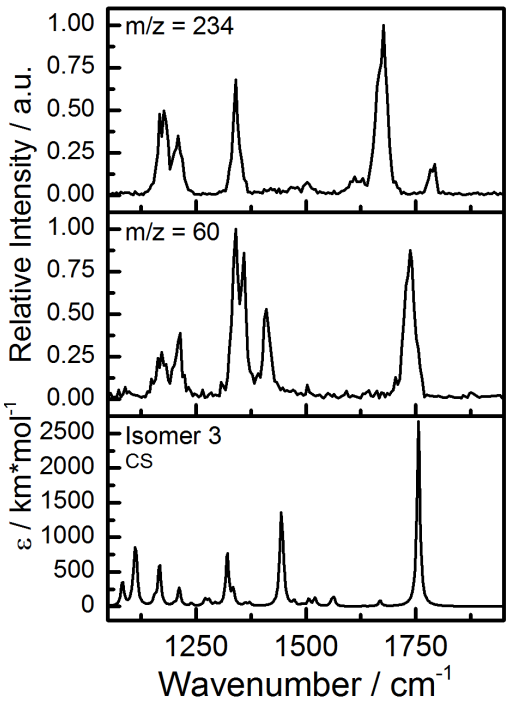
TS23	Eh		Relative Eh	eV	kJ/mol	ZW AA rotation
HF	-1067.030208		0.0269048	0.73211684	70.63976	
ZPE	0.329123	-1066.701085	0.0255018	0.69393927	66.95612	
Thermal	0.350599	-1066.679609	0.0252438	0.68691873	66.27873	
Gibbs	0.273723	-1066.756485	0.0246698	0.6712994	64.77166	

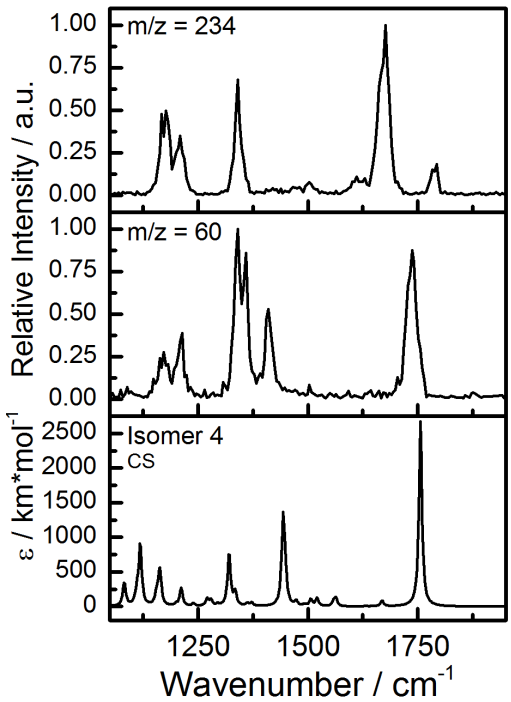
TS24	Eh		Relative Eh	eV	kJ/mol	TB AA rotation
HF	-1067.017279		0.0398331	1.08391377	104.5836	
ZPE	0.329716	-1066.687563	0.0390231	1.06187255	102.4569	
Thermal	0.351097	-1066.666182	0.0386701	1.05226694	101.5301	
Gibbs	0.273045	-1066.744234	0.0369201	1.00464701	96.93538	

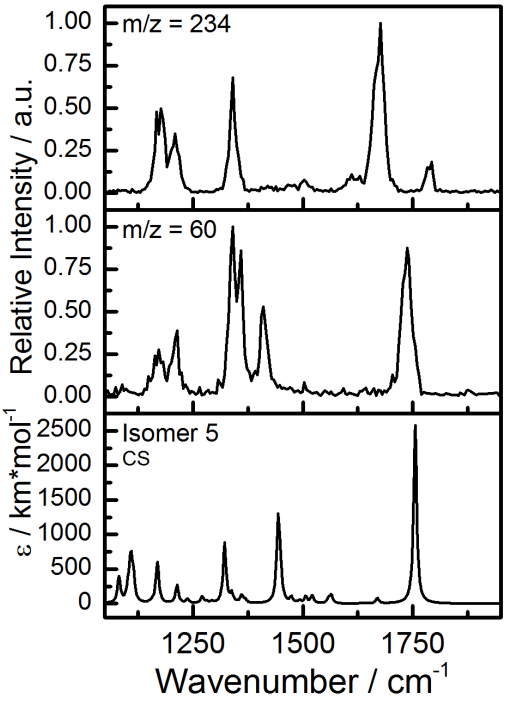
Section VI. Vibrational Spectra







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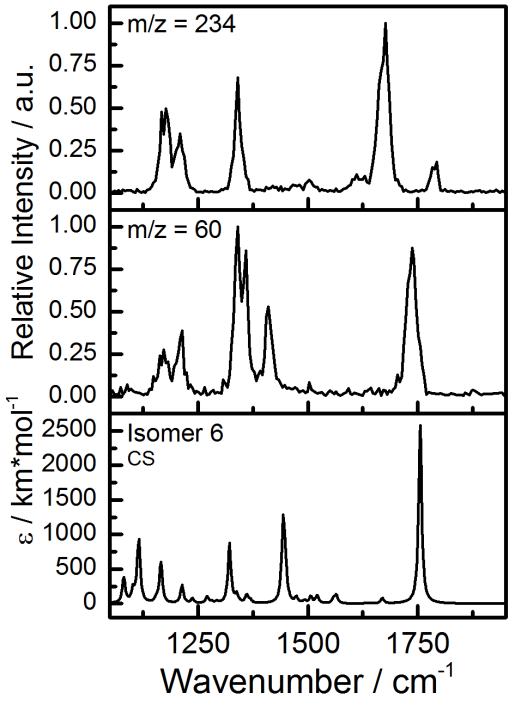
ε / km*mol-1
Wavenumber / cm-1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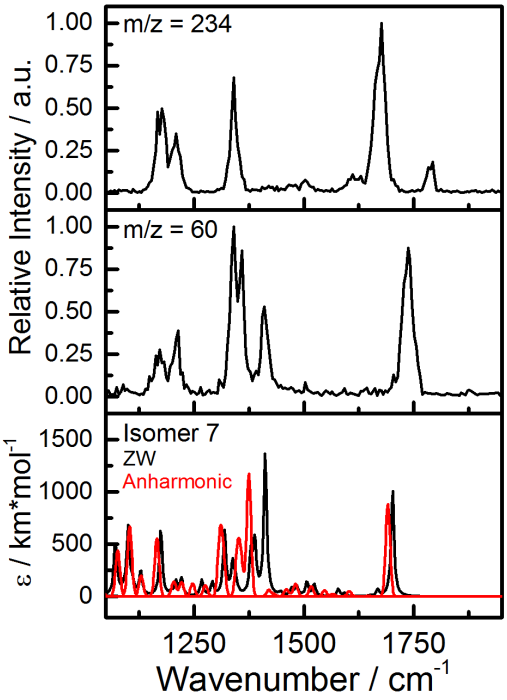
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Anharmonic
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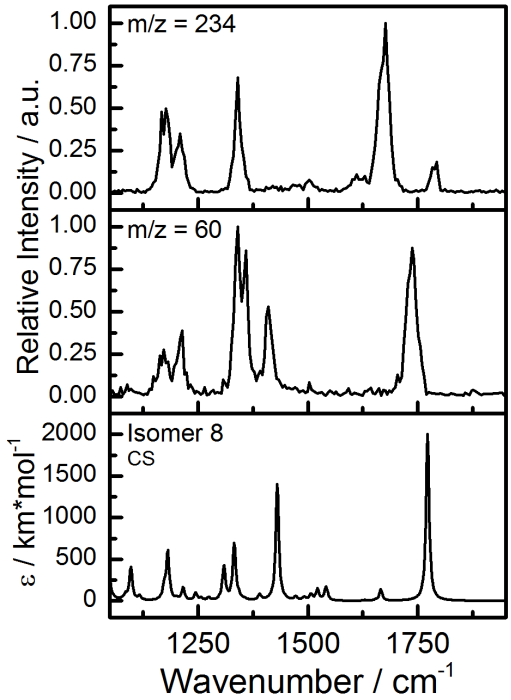
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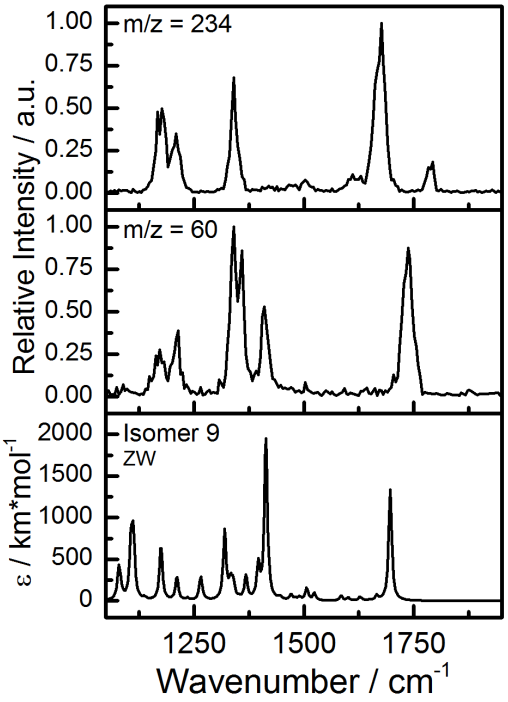
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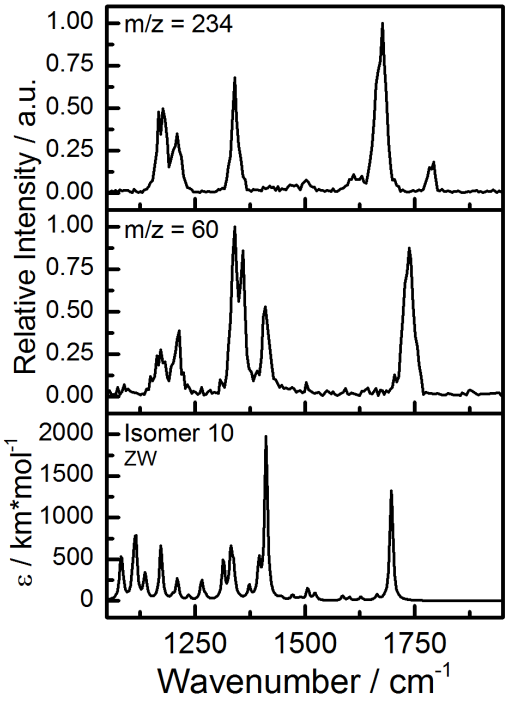
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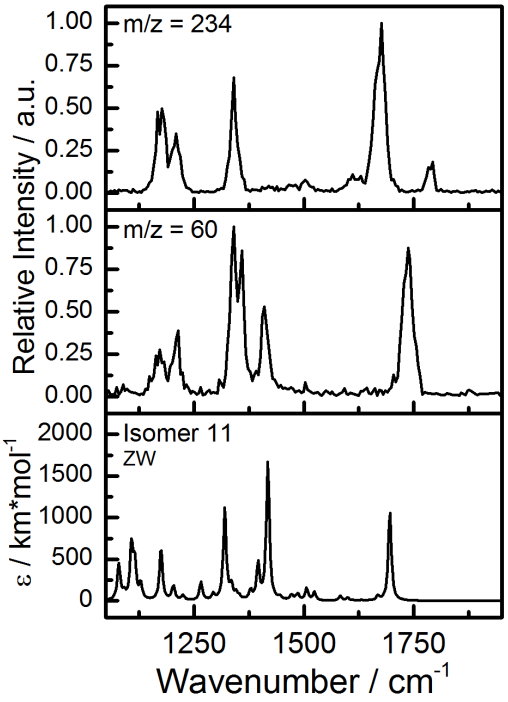
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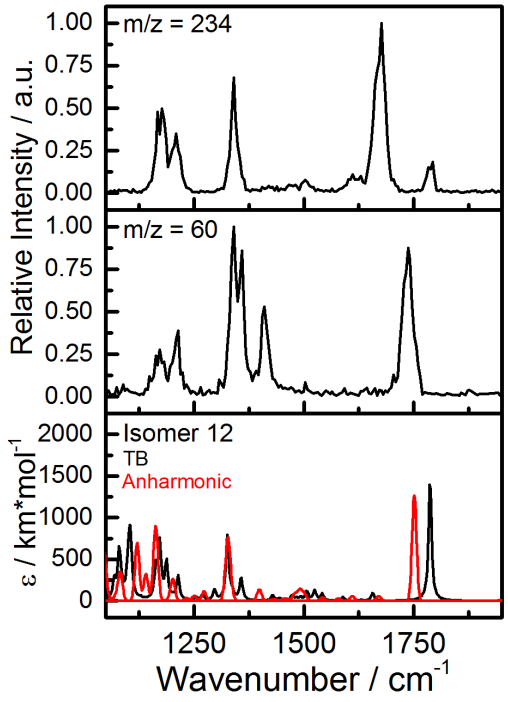
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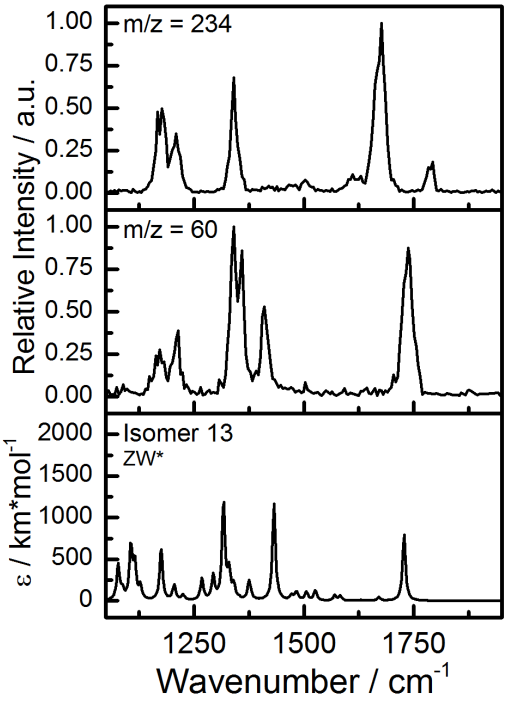
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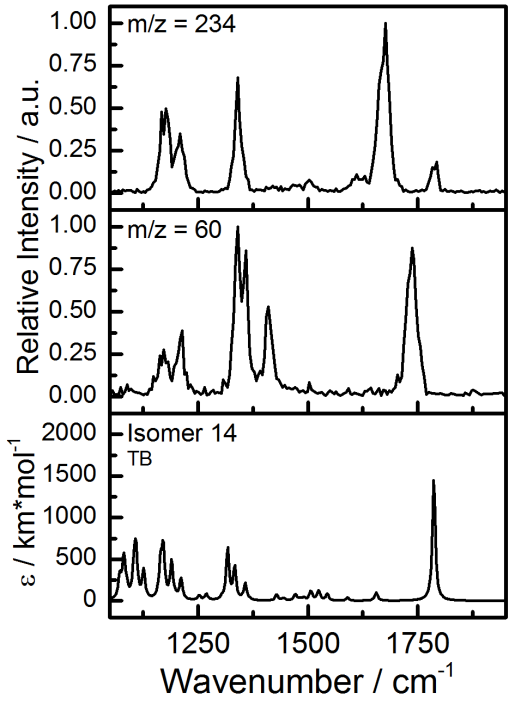
Wavenumber / cm-1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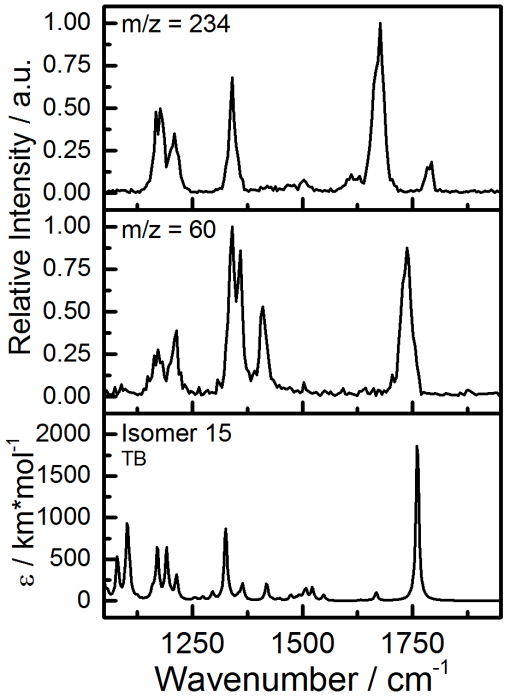
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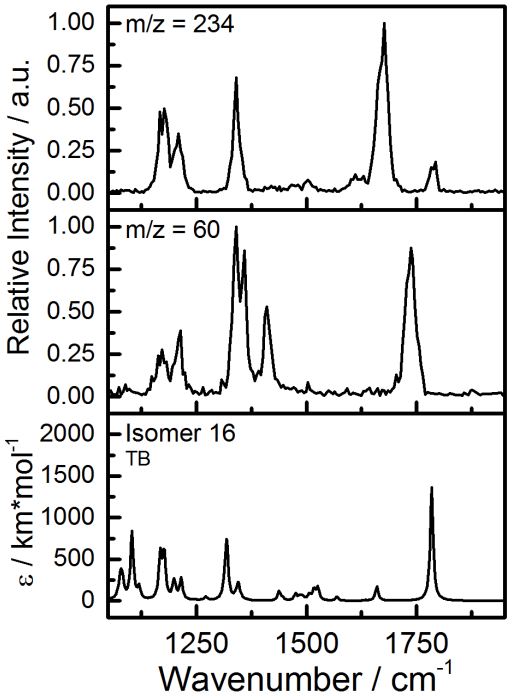
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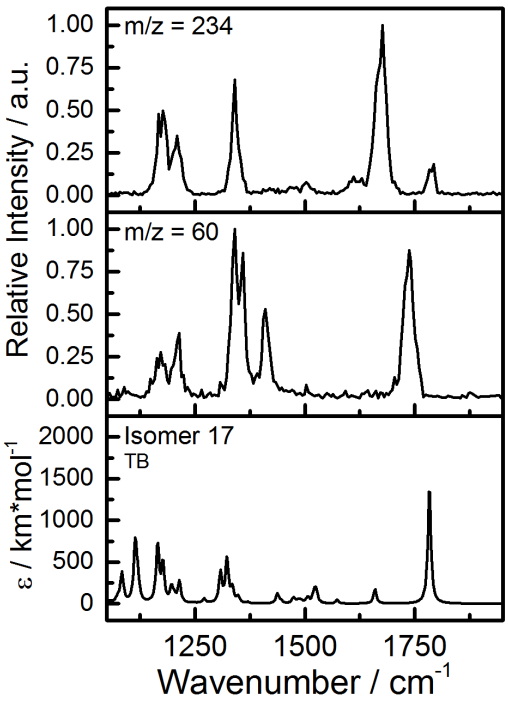
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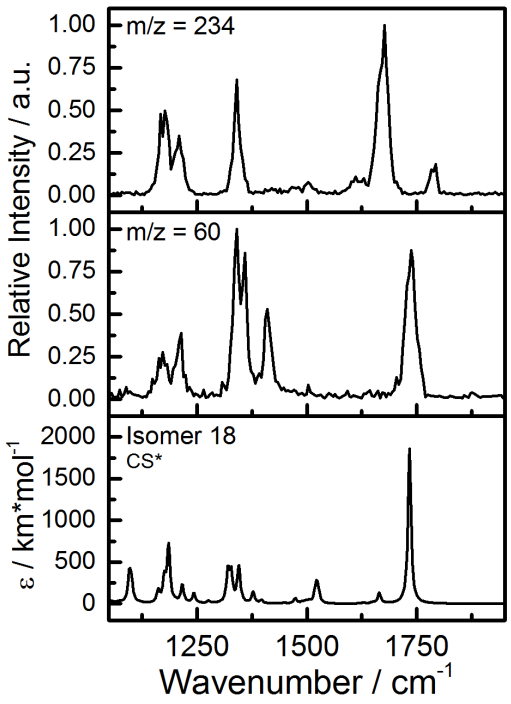
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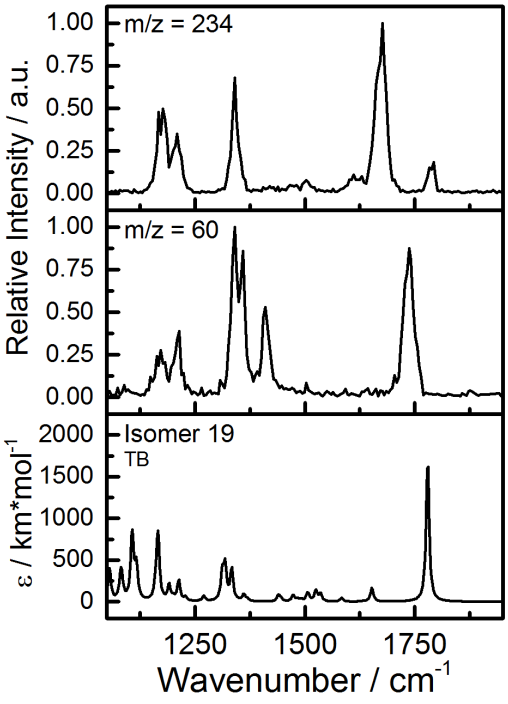
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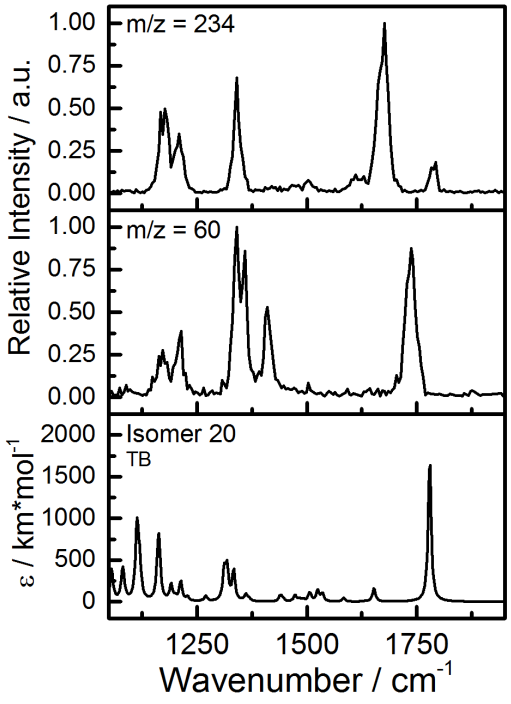
ε / km*mol-1
Wavenumber / cm-1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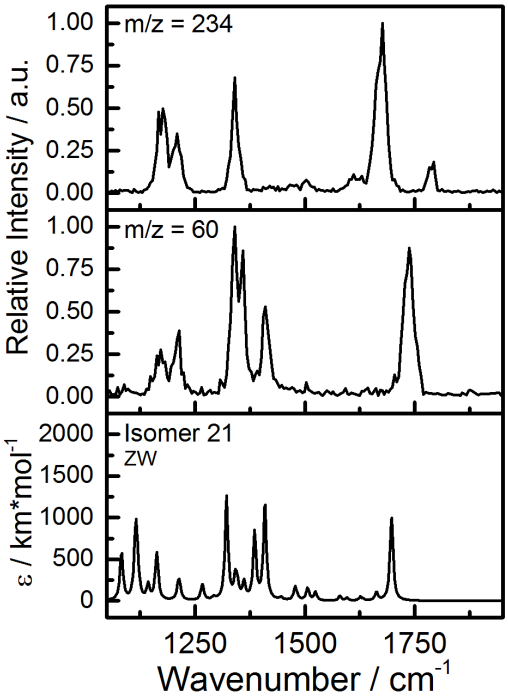
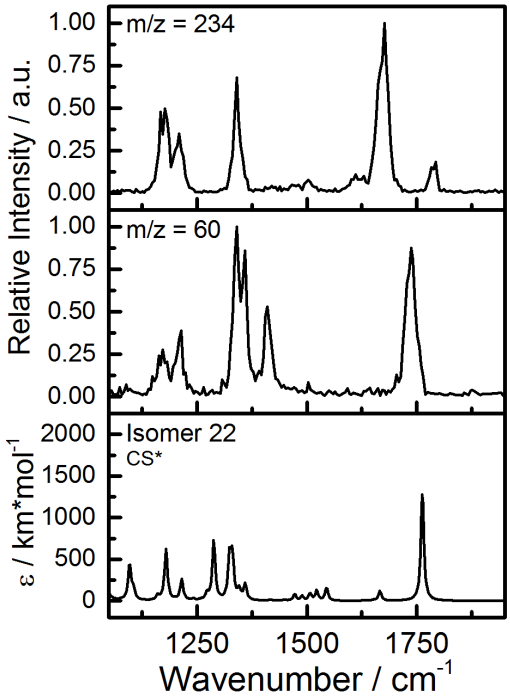
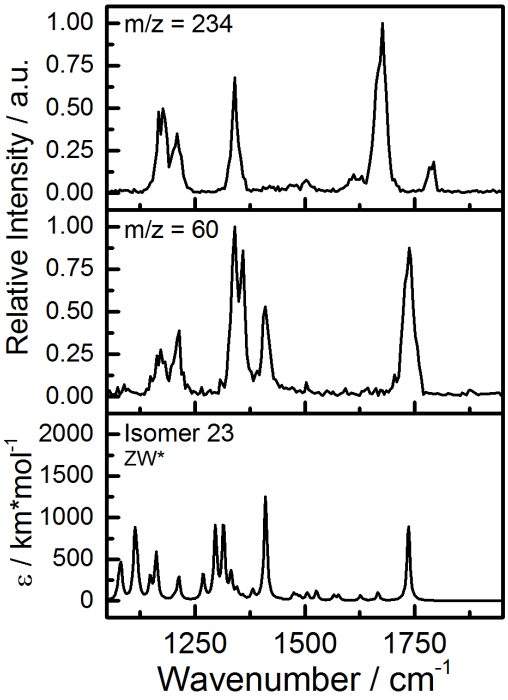
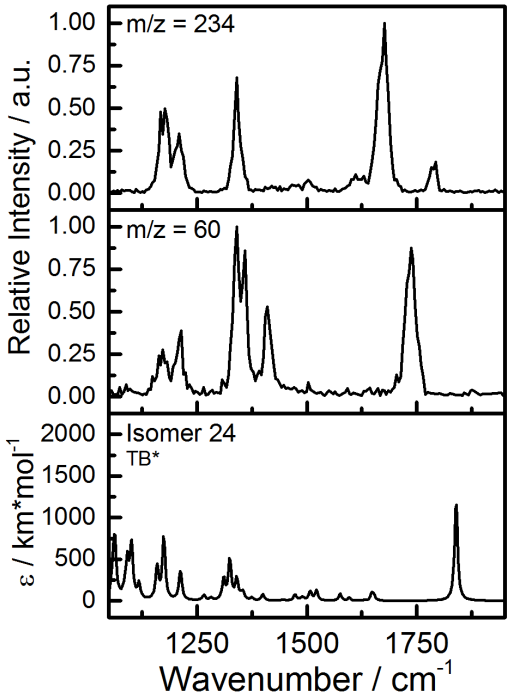
m/z = 60
Isomer 20
TB
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1


m/z = 234
m/z = 60
Isomer 21
ZW
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1


m/z = 234
m/z = 60
Isomer 22
CS*
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1


m/z = 234
m/z = 60
Isomer 23
ZW*
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1


m/z = 234
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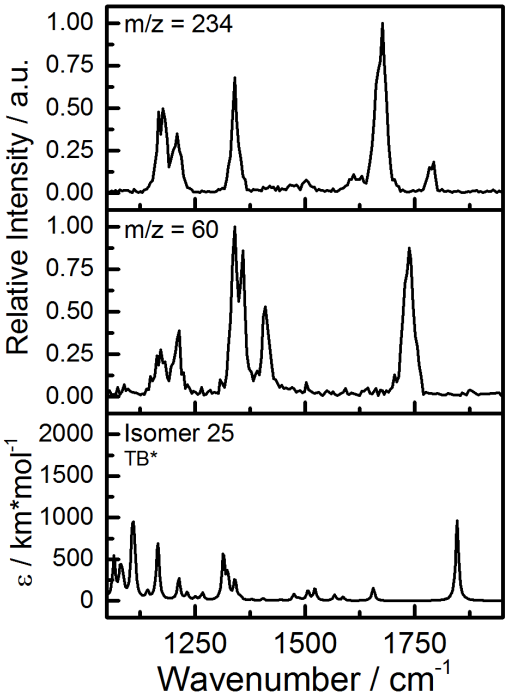
Isomer 24
TB*
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1


m/z = 234
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Isomer 25
TB*
Relative Intensity / a.u.
ε / km*mol-1
Wavenumber / cm-1
1.00
0.75
0.50
0.25
0.00
2000
1500
1000
500
0
1250
1500
1750

Section VII. Local Minima X,Y,Z Coordinates

Isomer 1

C	3.09683700	1.49104500	-0.07814200
C	3.78725600	0.46335800	0.56181500
C	3.25006100	-0.82100000	0.61328900
C	2.02273700	-1.06504000	0.00029000
C	1.41110600	-2.43921100	0.00082900
C	1.33815200	-0.04058300	-0.65175700
C	1.85460200	1.25656900	-0.68311100
H	3.54296300	2.47943600	-0.12904800
H	4.75006700	0.66119700	1.01727000
H	3.78104700	-1.62001700	1.11407400
F	1.41007400	-3.00132100	-1.22694200
F	2.01967600	-3.28864200	0.83797600
F	0.08842000	-2.38758600	0.38230300
H	0.39746900	-0.25014300	-1.14503300
C	1.06751500	2.37130200	-1.33883100
H	1.74272100	3.15954500	-1.68027400
H	0.54228300	1.99412500	-2.21858300
C	0.01823400	3.03166800	-0.40705500
H	-0.48818400	3.81371700	-0.98272300
N	0.54135600	3.63172500	0.82796300
H	0.66844000	4.63399000	0.75500800
H	1.42222000	3.21449400	1.11474100
C	-1.10251800	2.05407600	-0.00668600
O	-1.44672500	2.10731500	1.26608500
O	-1.65525300	1.29741700	-0.79061600
H	-2.73820700	0.05845000	-0.27080900
N	-3.40346700	-0.70650800	-0.00348700
C	-4.78120500	-0.13194400	-0.10492000
H	-4.85994500	0.71510400	0.57464300
H	-4.95092900	0.19971200	-1.12802700
H	-5.50902700	-0.89659500	0.16556300
C	-3.19821900	-1.83416700	-0.96743300
H	-3.37938700	-1.47090600	-1.97779700
H	-2.17411400	-2.19164900	-0.87691400
H	-3.89514300	-2.63750400	-0.72909400
C	-3.07333800	-1.11142500	1.40064300
H	-3.15340200	-0.23710500	2.04408900
H	-2.05546900	-1.49609300	1.42413200
H	-3.77277300	-1.88327000	1.72120300
H	-0.83087600	2.78919900	1.65886700

Isomer 2

C	0.88287300	2.75158300	-1.22342200
C	2.05067600	2.23762300	-1.77869300
C	2.70547900	1.16784500	-1.17165500
C	2.18574100	0.63481600	0.00591900
C	2.82318900	-0.56159100	0.65290000
C	1.02427100	1.16152500	0.57188800
C	0.35174000	2.21493900	-0.04479100
H	0.38724600	3.58779500	-1.70619700
H	2.45688400	2.67319800	-2.68355600
H	3.61512800	0.76607300	-1.59916500
F	4.08055500	-0.77882900	0.24791600
F	2.11596200	-1.71062100	0.34855000
F	2.82422500	-0.48640600	1.99800300
H	0.65008000	0.75101800	1.50317000
C	-0.92526800	2.76247900	0.54945500
H	-0.95327800	2.56549900	1.62592700
H	-0.94883600	3.84928300	0.42419500
C	-2.24239300	2.22477300	-0.08205100
H	-2.22659600	2.42655300	-1.15669400
N	-3.40130600	2.82316200	0.59762400
H	-3.16296900	3.66874100	1.10391900
H	-4.15672100	3.04549700	-0.04215300
C	-2.34582000	0.70193500	0.08513500
O	-1.70724500	-0.09269200	-0.58438700
O	-3.17224300	0.30549600	1.03880500
H	-3.61093200	1.14003800	1.35672800
N	-1.44562500	-2.83527400	-0.43968200
C	-2.79615800	-3.40798000	-0.73267200
H	-3.49324000	-3.07611700	0.03518100
H	-3.12606900	-3.05256200	-1.70756000
H	-2.73134200	-4.49580600	-0.73486500
C	-0.45087600	-3.17904900	-1.50542800
H	-0.82085400	-2.81170000	-2.46125100
H	0.49733200	-2.70240900	-1.26551600
H	-0.32889700	-4.26151400	-1.54231100
C	-0.95974300	-3.23201800	0.92023800
H	0.00913300	-2.76868500	1.09556600
H	-1.67979400	-2.89082300	1.66256600
H	-0.86684100	-4.31713200	0.96202600
H	-1.55394600	-1.79316600	-0.44210100

Isomer 3

C	-2.17174500	2.11636100	-0.97652100
C	-3.56392100	2.17061000	-0.91695700
C	-4.29278000	1.04622000	-0.54420600
C	-3.61680300	-0.13644500	-0.24183100
C	-4.38421700	-1.35482500	0.20786000
C	-2.22652400	-0.19214300	-0.30296900
C	-1.48748700	0.93707100	-0.66634100
H	-1.61731600	2.99584700	-1.28923300
H	-4.08061800	3.08891200	-1.16870200
H	-5.37386700	1.08052300	-0.50252900
F	-5.64099700	-1.37256800	-0.27166500
F	-4.47388200	-1.40481600	1.56093800
F	-3.78239800	-2.50106200	-0.18207300
H	-1.72348200	-1.12768600	-0.08422700
C	0.02392200	0.87465000	-0.71890100
H	0.35189600	0.00937200	-1.29941900
H	0.41438100	1.76521500	-1.22231300
C	0.67052300	0.77021000	0.68573100
H	0.30640000	-0.14084600	1.16966300
N	0.43236300	1.95961400	1.51715000
H	-0.27013900	2.57195400	1.11551000
H	0.12011300	1.71921000	2.45182700
C	2.18789300	0.60453800	0.53290300
O	2.70648700	-0.36331600	-0.00578200
O	2.90345100	1.60085000	1.01787200
H	2.22012900	2.22087800	1.40752400
N	5.38873600	-0.82739600	-0.29327000
C	5.48009800	-2.15792300	-0.97219000
H	6.52891600	-2.41642200	-1.11736800
H	4.99351400	-2.90581600	-0.34836500
H	4.97318700	-2.09831500	-1.93383600
C	5.99792900	-0.85646300	1.07322500
H	5.51238600	-1.63543600	1.65892100
H	7.06412300	-1.06527800	0.98718400
H	5.84241600	0.11138500	1.54713900
C	5.96828200	0.26747300	-1.13249800
H	5.81386700	1.21801400	-0.62440700
H	7.03362500	0.08643200	-1.27414900
H	5.46153400	0.27865800	-2.09617000
H	4.36620800	-0.61236900	-0.16955800

Isomer 4

C	-2.17371100	2.10293200	-0.99306300
C	-3.56493200	2.16318900	-0.91803300
C	-4.29228100	1.05193000	-0.50529300
C	-3.61552500	-0.12192100	-0.17145600
C	-4.38873100	-1.35715700	0.21915400
C	-2.22640400	-0.18399600	-0.24948400
C	-1.48885700	0.93164700	-0.65544800
H	-1.62055100	2.97235600	-1.33482400
H	-4.08189600	3.07691600	-1.18540500
H	-5.37204400	1.09391600	-0.44170500
F	-5.57549300	-1.05718200	0.77989500
F	-3.70286000	-2.11763900	1.10509700
F	-4.64151300	-2.14298100	-0.85356900
H	-1.72208600	-1.10997100	0.00408300
C	0.02199200	0.86480900	-0.71838400
H	0.34354500	-0.01843500	-1.27494100
H	0.40968600	1.73871300	-1.25225600
C	0.68052500	0.80189000	0.68301300
H	0.31659300	-0.09166500	1.19869000
N	0.45484400	2.01743900	1.47948200
H	0.14363500	1.80756500	2.42178600
H	-0.24348600	2.62377300	1.06181900
C	2.19584400	0.62394200	0.52311600
O	2.92042900	1.62897600	0.97563900
O	2.70518300	-0.36108300	0.00722900
H	4.36263800	-0.62240500	-0.16146400
N	5.38345700	-0.84527300	-0.28539600
C	5.99409700	-0.87150100	1.08050200
H	5.84691800	0.10020900	1.54915400
H	5.50317100	-1.64333300	1.67114200
H	7.05852000	-1.08912800	0.99436100
C	5.46465700	-2.17997700	-0.95736400
H	4.97377000	-2.92116700	-0.32892700
H	4.95687100	-2.12194800	-1.91864600
H	6.51145900	-2.44649100	-1.10259500
C	5.96965700	0.24113200	-1.13100500
H	5.46254900	0.25016800	-2.09451300
H	5.82144700	1.19546300	-0.62820900
H	7.03373500	0.05240900	-1.27211800
H	2.24332800	2.26346100	1.35267700

Isomer 5

C	-1.70528900	2.10621700	-0.18139200
C	-3.02934200	2.48465700	-0.37235500
C	-4.05948700	1.56326300	-0.18280000
C	-3.74866800	0.26613400	0.21188100
C	-4.83346300	-0.76664500	0.38843100
C	-2.41853100	-0.11414400	0.40833600
C	-1.38353500	0.79896600	0.20770300
H	-0.91617000	2.83870100	-0.32037400
H	-3.26534100	3.50144600	-0.66253500
H	-5.09144100	1.85600700	-0.32638800
F	-4.60796300	-1.54871900	1.46818300
F	-4.89530200	-1.59738900	-0.68374400
F	-6.05060200	-0.21473000	0.53275600
H	-2.19924400	-1.12159000	0.74604500
C	0.05745800	0.38017500	0.39968800
H	0.60031200	1.12587100	0.98456500
H	0.09802100	-0.55950700	0.96026400
C	0.81490000	0.19487100	-0.94112000
H	0.82599200	1.15263100	-1.46969300
N	0.25731500	-0.88095100	-1.77410700
H	0.13167400	-0.59491600	-2.73910300
H	-0.64560700	-1.19900500	-1.43687200
C	2.27739400	-0.16037900	-0.64357700
O	2.64213800	-1.36538800	-1.03894700
O	3.05139800	0.59379400	-0.07092900
H	4.65833900	0.18930600	0.26138700
N	5.66464900	-0.02240500	0.48492000
C	6.35887100	-0.26843000	-0.81772800
H	5.87140600	-1.10087200	-1.32254300
H	6.28542500	0.62829300	-1.43100900
H	7.40565100	-0.50515200	-0.62803600
C	6.22036300	1.17131100	1.19574700
H	6.13809600	2.03942800	0.54388000
H	5.64453900	1.34019600	2.10416400
H	7.26558600	0.98778300	1.44422900
C	5.67253400	-1.24173500	1.35244400
H	5.11881700	-1.02828700	2.26538000
H	5.19369800	-2.05777200	0.81373400
H	6.70229200	-1.50411000	1.59437800
H	1.82148300	-1.73023000	-1.48445600

Isomer 6

C	1.70623100	2.10366200	0.15514300
C	3.02937800	2.48365400	0.34934100
C	4.05887900	1.55514900	0.19389400
C	3.74790000	0.24683500	-0.16195700
C	4.83781900	-0.77150500	-0.38578700
C	2.41878800	-0.13457800	-0.36313200
C	1.38455800	0.78669800	-0.19966200
H	0.91761700	2.84106400	0.26862300
H	3.26514500	3.50655400	0.61737700
H	5.08963400	1.84723100	0.34713800
F	5.07286600	-0.96367500	-1.70470600
F	4.49830800	-1.97965200	0.12665500
F	6.00290800	-0.40755700	0.17911800
H	2.19864000	-1.15397600	-0.66220000
C	-0.05585200	0.36491600	-0.38893400
H	-0.59410500	1.09678600	-0.99512400
H	-0.09473600	-0.58815500	-0.92658300
C	-0.82149600	0.21351900	0.95141000
H	-0.83333800	1.18372200	1.45675500
N	-0.27153400	-0.84287000	1.81389200
H	0.63041900	-1.17474100	1.48754800
H	-0.14715600	-0.53238100	2.77143000
C	-2.28326700	-0.14532600	0.65424600
O	-3.05146700	0.59565000	0.05709300
O	-2.65410600	-1.33832600	1.07924300
H	-1.83714300	-1.69356200	1.53916500
N	-5.66240100	-0.03078900	-0.49910000
C	-5.66502500	-1.26714700	-1.34222200
H	-5.10639000	-1.07162800	-2.25617300
H	-5.18886800	-2.07206900	-0.78474300
H	-6.69333200	-1.53483200	-1.58451700
C	-6.36329000	-0.25135800	0.80454500
H	-5.87769100	-1.07296100	1.32854300
H	-6.29393300	0.65758200	1.40006400
H	-7.40883100	-0.49290200	0.61409900
C	-6.21509700	1.14813900	-1.23644700
H	-6.13682000	2.02911600	-0.60156600
H	-5.63461700	1.29935300	-2.14501900
H	-7.25888500	0.95894700	-1.48670900
H	-4.65737300	0.18588800	-0.27458500

Isomer 7

C	-2.93027100	1.88804900	0.15196100
C	-3.80770600	0.98245300	-0.44356800
C	-3.47909400	-0.36909500	-0.51348700
C	-2.27163200	-0.80385600	0.03019300
C	-1.87004400	-2.25619900	-0.02021600
C	-1.39486700	0.09818800	0.63045600
C	-1.70836200	1.45822800	0.68916800
H	-3.21952500	2.93216700	0.23426400
H	-4.75406900	1.32773600	-0.84199500
H	-4.15748900	-1.07666700	-0.97183300
F	-1.61045200	-2.74749600	1.21189800
F	-0.72077600	-2.41961800	-0.74056200
F	-2.80174200	-3.03731100	-0.58417800
H	-0.46698800	-0.25343000	1.06481900
C	-0.73414600	2.44414700	1.30054700
H	-1.26382200	3.34814000	1.61436200
H	-0.26586600	2.02236800	2.19177100
C	0.41967400	2.83253100	0.36096200
H	1.00171800	3.64229600	0.80555500
N	-0.06519900	3.32010200	-0.99087900
H	-0.04468800	4.33210900	-1.10692400
H	-1.00807900	2.97164600	-1.19287100
C	1.41873600	1.68448200	0.00279400
O	1.83595700	0.98829400	0.95271000
O	1.71356900	1.60026300	-1.21313800
H	0.62803200	2.82475600	-1.63009300
N	3.50669000	-0.91337800	0.03235500
C	2.76328300	-1.64733800	-1.03725700
H	1.89028800	-2.12766100	-0.59829600
H	2.44349100	-0.92495000	-1.78585600
H	3.41817400	-2.39772800	-1.48099100
C	4.68474900	-0.18444200	-0.52584400
H	4.32808000	0.51161400	-1.28305400
H	5.17325000	0.36441000	0.27812600
H	5.38068600	-0.90061800	-0.96348600
C	3.88603500	-1.80752000	1.16507900
H	4.36467000	-1.21214700	1.94125100
H	2.98619800	-2.27248900	1.56502600
H	4.57271800	-2.57586600	0.80869100
H	2.84518100	-0.16916000	0.41546700

Isomer 8

C	-0.26237600	2.27456200	-1.83391600
C	-1.49442900	1.82408700	-2.30506900
C	-2.36560200	1.15320900	-1.45336900
C	-1.99436800	0.95778500	-0.12215400
C	-2.86512300	0.13465800	0.78534000
C	-0.77725800	1.43724700	0.35746700
C	0.11148600	2.09120000	-0.49872000
H	0.41133600	2.78590300	-2.51347300
H	-1.77299400	1.99491600	-3.33801000
H	-3.32249100	0.79574400	-1.81255000
F	-4.16318800	0.17890400	0.45370500
F	-2.75291300	0.48531100	2.07959300
F	-2.49770100	-1.19503700	0.72170000
H	-0.52689200	1.28334800	1.39921200
C	1.43838500	2.63840100	-0.01265000
H	2.05096200	2.90079400	-0.88092800
H	1.26633500	3.57050800	0.53865000
C	2.29488700	1.74014800	0.91918100
H	1.76877500	1.59090400	1.86602600
N	3.61686900	2.35721400	1.09866000
H	3.98365800	2.22956800	2.03609000
H	3.61411600	3.35122900	0.89856800
C	2.51211200	0.34374000	0.31540300
O	3.68800800	0.15845500	-0.25181000
O	1.66229600	-0.53071400	0.35300200
H	1.24246200	-2.11318500	-0.10823300
N	0.85188400	-3.06173400	-0.30500400
C	1.99997200	-3.94228800	-0.68533900
H	2.48624800	-3.52772800	-1.56694300
H	2.70780900	-3.97627000	0.14126900
H	1.62775100	-4.94384800	-0.89938400
C	0.18267400	-3.52739400	0.95207400
H	0.92105200	-3.55887300	1.75158400
H	-0.61170500	-2.82789600	1.20518900
H	-0.23112900	-4.52204700	0.78690500
C	-0.12981800	-2.91011400	-1.42563700
H	-0.91798900	-2.22980500	-1.10915500
H	0.38776300	-2.50451200	-2.29346900
H	-0.55027900	-3.88687700	-1.66437700
H	4.20246900	0.98380500	-0.05274300

Isomer 9

C	1.82100800	2.24373800	-0.08904900
C	3.16878700	2.50595300	0.12698800
C	4.10689800	1.47313600	0.07526000
C	3.68192900	0.18124800	-0.21223900
C	4.65647800	-0.97027900	-0.24394000
C	2.32773200	-0.08314900	-0.44226000
C	1.38278200	0.94221600	-0.37418900
H	1.10561100	3.05937400	-0.05644900
H	3.49676500	3.51816900	0.33084300
H	5.15666800	1.67624200	0.24233000
F	4.45362600	-1.76455700	-1.31735000
F	4.50446300	-1.75817100	0.85393500
F	5.93493700	-0.56432400	-0.26892800
H	2.02346500	-1.08895900	-0.71626900
C	-0.08648300	0.63713600	-0.56987500
H	-0.57111900	1.39240300	-1.19142600
H	-0.20494100	-0.31994000	-1.08780500
C	-0.87691600	0.59620500	0.75167200
H	-0.87825700	1.57539800	1.22919500
N	-0.27166500	-0.40280200	1.72193500
H	0.64518900	-0.74468200	1.42040300
H	-0.17461200	-0.02719600	2.66499700
C	-2.33668700	0.09931600	0.54072400
O	-3.07929700	0.85088800	-0.12820700
O	-2.60430800	-1.01592600	1.04655600
H	-1.01547900	-1.15716700	1.72551900
N	-5.51261600	-0.21839900	-0.39679000
C	-5.31191900	-1.52858600	-1.08498300
H	-4.90267900	-1.34568600	-2.07762300
H	-4.60738500	-2.11678800	-0.49943800
H	-6.26790000	-2.04652600	-1.16774000
C	-6.03185800	-0.40770400	0.99060500
H	-5.31667200	-1.01543600	1.54227900
H	-6.12977400	0.56745400	1.46574700
H	-7.00376500	-0.90049200	0.95135200
C	-6.36627400	0.70952700	-1.19370900
H	-6.42961700	1.66500200	-0.67506300
H	-5.91065900	0.85713900	-2.17174900
H	-7.36295400	0.28223800	-1.30877400
H	-4.54316800	0.22907500	-0.30207900

Isomer 10

C	-1.96197000	2.13263900	-0.77403800
C	-3.33433000	2.34634600	-0.63839400
C	-4.18398600	1.27969800	-0.36592500
C	-3.65154700	-0.00455700	-0.24180400
C	-4.55081900	-1.16786000	0.10221800
C	-2.28279000	-0.22099200	-0.38052700
C	-1.42031400	0.84830100	-0.64403300
H	-1.31419500	2.96950300	-1.01846700
H	-3.74082400	3.34355200	-0.75650000
H	-5.25025400	1.43767800	-0.26670400
F	-4.59322800	-1.36333300	1.44485000
F	-4.11189800	-2.32087400	-0.44502200
F	-5.81496500	-0.97327200	-0.31007200
H	-1.89492500	-1.23099800	-0.30522000
C	0.07282000	0.62312900	-0.76173000
H	0.29981100	-0.18998900	-1.45440800
H	0.55491400	1.52008400	-1.16333200
C	0.73605500	0.24814500	0.57534700
H	0.36265800	-0.70962500	0.93586300
N	0.45252500	1.29517500	1.63861400
H	0.13894200	0.88887100	2.51979300
H	-0.24376000	1.98295900	1.33993800
C	2.28817000	0.20877000	0.47203200
O	2.76440200	-0.68101100	-0.26603700
O	2.89418100	1.08912400	1.12749400
H	1.41838200	1.71318600	1.76930700
N	5.43136900	-0.59081800	-0.29874900
C	5.79495000	0.76494200	-0.80836300
H	5.43491000	0.86449100	-1.83145800
H	5.31292000	1.50798000	-0.17523100
H	6.87845600	0.88501800	-0.78332200
C	5.86146800	-0.77156100	1.11986100
H	6.94661000	-0.68662100	1.18509600
H	5.38098900	-0.00283700	1.72273800
H	5.54584400	-1.75678800	1.46039900
C	5.94145400	-1.67871300	-1.18269100
H	5.59749200	-2.63752800	-0.79762300
H	5.55002800	-1.53018800	-2.18800200
H	7.03154700	-1.65477000	-1.20095900
H	4.36037300	-0.64179000	-0.30213800

Isomer 11

C	0.53080500	-1.14280800	-0.87926800
C	1.34561700	-2.14022600	-0.35578600
C	2.65158200	-1.85206100	0.04360300
C	3.13822300	-0.55829200	-0.10434300
C	4.53328200	-0.19259300	0.33914900
C	2.32647000	0.44402900	-0.64508100
C	1.01189300	0.16642900	-1.02866200
H	-0.48007200	-1.37699300	-1.19324500
H	0.96946900	-3.15193200	-0.26140000
H	3.28594400	-2.62836700	0.45111400
F	4.49296800	0.60162700	1.44269900
F	5.19093400	0.50510500	-0.61164000
F	5.27542100	-1.26669800	0.64811800
H	2.74335400	1.43416600	-0.80446900
C	0.13082800	1.27258200	-1.56980900
H	0.75149200	2.05179500	-2.02052900
H	-0.53200900	0.89759200	-2.35160800
C	-0.78681900	1.90915300	-0.50969100
H	-1.21454700	2.83293200	-0.90446500
N	-0.05141200	2.26737600	0.76693100
H	0.81084000	1.71817200	0.86195100
H	-0.74901000	1.94200600	1.49651400
C	-1.98229100	1.02955100	-0.02498300
O	-2.15481400	0.99790100	1.21582800
O	-2.66803400	0.48301600	-0.91744300
H	-3.97428200	-0.21019000	-0.28564000
N	-4.84308200	-0.63851600	0.17111800
C	-5.54661200	0.47519500	0.87558200
H	-4.85337500	0.91998200	1.58731000
H	-5.84969500	1.22008500	0.14105700
H	-6.42447400	0.08275100	1.38966000
C	-5.68018600	-1.23312800	-0.91107000
H	-5.95760600	-0.44944000	-1.61448600
H	-5.10056200	-1.99632300	-1.42830700
H	-6.57653200	-1.67794900	-0.47770600
C	-4.35590100	-1.66838700	1.13681700
H	-3.83149800	-2.44768500	0.58551600
H	-3.67158800	-1.18589700	1.83254500
H	-5.20504100	-2.09886400	1.66840200
H	0.16818600	3.25782100	0.86303300

Isomer 12

C	1.67139400	2.10193900	1.18918000
C	2.83568100	1.67744300	1.82140300
C	3.57656100	0.61944900	1.29568700
C	3.14661000	0.00447400	0.12344400
C	3.89270700	-1.17412900	-0.44792200
C	1.98393700	0.43765400	-0.51810500
C	1.22805700	1.48408800	0.01178200
H	1.11262200	2.93539500	1.60337900
H	3.17473200	2.17542700	2.72185500
H	4.48469300	0.28873700	1.78280800
F	3.96519700	-1.11871800	-1.79583300
F	3.25807200	-2.34094600	-0.14582300
F	5.14511400	-1.27349300	0.02578300
H	1.68697900	-0.03084600	-1.45020500
C	-0.05550500	1.92779300	-0.65482500
H	-0.15674800	3.01288600	-0.59778600
H	-0.03920300	1.66408300	-1.71775100
C	-1.31048700	1.28512500	0.00026500
H	-1.33057000	1.58235800	1.05466900
N	-1.33445300	-0.18979400	-0.04332200
H	-1.15124300	-0.49136400	-1.00009100
H	-0.54775100	-0.53708600	0.50192500
C	-2.60562600	1.81179800	-0.60916500
O	-3.50990500	1.11238000	-1.00881000
O	-2.63973300	3.14785600	-0.63248100
H	-3.48021800	3.43672100	-1.02305500
N	-3.80815900	-1.66040100	0.39701900
C	-4.32758500	-2.03322600	-0.95706300
H	-4.58183900	-1.12084800	-1.49080500
H	-3.55119000	-2.57488900	-1.49583900
H	-5.20462100	-2.66960900	-0.83926400
C	-3.33145700	-2.85811000	1.15483600
H	-2.55669300	-3.36000400	0.57701500
H	-2.92538000	-2.53501800	2.11231500
H	-4.16751300	-3.53766300	1.31849500
C	-4.82566800	-0.88740200	1.17541800
H	-4.38706500	-0.58170200	2.12455100
H	-5.11153000	-0.01240300	0.59686900
H	-5.69218500	-1.52285000	1.35847200
H	-2.96704400	-1.03480100	0.25013100

Isomer 13

C	0.66336900	-0.65399100	-1.54270000
C	1.43502400	-1.79286400	-1.34055900
C	2.65093600	-1.71508600	-0.65953400
C	3.09571600	-0.48041900	-0.20071600
C	4.38721400	-0.35170400	0.56798300
C	2.33125200	0.67046600	-0.41790600
C	1.10285700	0.59555800	-1.08003000
H	-0.27760000	-0.72173700	-2.07655800
H	1.09593200	-2.74923800	-1.72057700
H	3.25125500	-2.60178500	-0.50264400
F	4.13951700	-0.08528600	1.87972500
F	5.14299100	0.66765400	0.10688600
F	5.12987300	-1.46794200	0.52256200
H	2.72572600	1.63342300	-0.10648700
C	0.26484400	1.84264400	-1.26786600
H	0.91175400	2.72386000	-1.29949100
H	-0.27893200	1.80766600	-2.21341700
C	-0.80425100	2.03769100	-0.17923200
H	-1.22387200	3.04341500	-0.25255900
N	-0.24016500	1.90222800	1.22468300
H	0.58933400	1.29578000	1.22264000
H	-1.02047200	1.40650900	1.72521700
C	-2.00936500	1.04756900	-0.23519100
O	-2.50765200	0.80225200	-1.32843400
O	-2.38183800	0.62408300	0.91623400
H	-3.77345100	-0.24382700	0.68265700
N	-4.67262200	-0.76845900	0.47026100
C	-5.22394400	-1.26964500	1.76294100
H	-4.49348000	-1.93041500	2.22757500
H	-5.41821100	-0.42147900	2.41784500
H	-6.15027900	-1.81370200	1.57722200
C	-5.59257900	0.20733100	-0.19177500
H	-5.80331600	1.01886200	0.50340900
H	-5.09212700	0.59765700	-1.07584600
H	-6.51930400	-0.29875700	-0.46312200
C	-4.31111100	-1.88417900	-0.45663100
H	-3.83560300	-1.45159800	-1.33470200
H	-3.61582600	-2.55139000	0.05105600
H	-5.21380200	-2.42916900	-0.73365800
H	-0.00351500	2.78881400	1.66917700

Isomer 14

C	1.55487300	-1.14667000	2.10229900
C	2.69227900	-0.44732600	2.50333200
C	3.49297400	0.18903600	1.55973900
C	3.15195600	0.10679000	0.20984600
C	3.97105300	0.83358600	-0.82744600
C	2.02130000	-0.60161900	-0.19290300
C	1.20428400	-1.23150200	0.75080500
H	0.94762900	-1.65010200	2.84775700
H	2.95877900	-0.40442400	3.55259400
H	4.37951900	0.72987800	1.86496400
F	5.23753700	1.04108200	-0.42846400
F	3.43498100	2.05358700	-1.09982800
F	4.01362800	0.16252100	-1.99846800
H	1.79477700	-0.67807300	-1.25098800
C	-0.03273400	-1.98425000	0.30699100
H	0.22184900	-2.71017900	-0.46823500
H	-0.44539600	-2.55079400	1.14818700
C	-1.13040600	-1.03961600	-0.25210700
H	-0.72148300	-0.52692200	-1.12983400
N	-1.57985700	0.00133700	0.69322700
H	-1.83801300	-0.44456900	1.57323800
H	-0.78014000	0.59160400	0.91492800
C	-2.35062900	-1.80624600	-0.75096400
O	-3.49504400	-1.53589500	-0.46102300
O	-2.01228300	-2.80480800	-1.57199900
H	-2.81764400	-3.25761800	-1.87004900
N	-4.01377300	1.49363700	0.13787600
C	-5.09249300	0.89849200	0.98882300
H	-6.00262700	1.48719200	0.87399700
H	-5.25428700	-0.12829200	0.67017800
H	-4.77167300	0.91807700	2.02957400
C	-4.38802200	1.46790300	-1.31068700
H	-4.60731800	0.44106700	-1.59279300
H	-5.26303000	2.09962700	-1.46382500
H	-3.55330700	1.84801400	-1.89846600
C	-3.65413700	2.87397200	0.58612300
H	-2.83938500	3.24823100	-0.03212100
H	-4.52296600	3.52399400	0.48517800
H	-3.33961500	2.83913000	1.62818600
H	-3.14874100	0.89495000	0.26173000

Isomer 15

C	1.86310200	2.20718800	0.93264900
C	3.05954800	1.85950000	1.55150700
C	3.76204700	0.72771900	1.13931600
C	3.25987900	-0.04050700	0.09281900
C	3.96391700	-1.29790900	-0.34842700
C	2.06395700	0.31401500	-0.53539100
C	1.34753700	1.43577000	-0.11761900
H	1.33398800	3.09806800	1.25646200
H	3.45322900	2.47396200	2.35227700
H	4.69498700	0.45554400	1.61562700
F	3.96953100	-1.42629100	-1.69408200
F	3.33473500	-2.40278400	0.13861800
F	5.23831400	-1.35361500	0.07215900
H	1.70805900	-0.27839900	-1.37126600
C	0.03118000	1.80238300	-0.76608300
H	-0.05535400	2.88649200	-0.85602200
H	-0.01492500	1.39314300	-1.78111600
C	-1.18803700	1.26931300	0.04148900
H	-1.13768500	1.70300500	1.04726200
N	-1.25074000	-0.18908500	0.19180000
H	-1.01047800	-0.62944000	-0.69443600
H	-0.52712300	-0.48249300	0.84222100
C	-2.51017300	1.76270800	-0.53597700
O	-3.48291900	1.06072100	-0.74305900
O	-2.50910800	3.07314000	-0.77481800
H	-3.37677800	3.33614400	-1.12207100
N	-4.23487200	-1.44039500	0.30319500
C	-3.63779300	-2.70655900	-0.22306100
H	-3.59387000	-2.65130000	-1.30969200
H	-2.63564400	-2.81564000	0.18555300
H	-4.26106600	-3.54768000	0.07969700
C	-4.25155500	-1.42290600	1.79923900
H	-3.22980400	-1.52880900	2.15725300
H	-4.66509300	-0.47346900	2.13503900
H	-4.86840800	-2.24582100	2.15951600
C	-5.59541600	-1.19050200	-0.27071500
H	-5.95815700	-0.23143900	0.09249900
H	-5.51885200	-1.16058200	-1.35584500
H	-6.26521600	-1.99226200	0.03894400
H	-3.62867900	-0.65062100	-0.00258800

Isomer 16

C	-1.77825400	2.43406700	-0.61829700
C	-3.14184800	2.33936900	-0.35945800
C	-3.73949600	1.09236100	-0.18503200
C	-2.95962400	-0.05678400	-0.28454900
C	-3.56295900	-1.41854100	-0.05459300
C	-1.59281500	0.03745300	-0.54870200
C	-0.98724200	1.28304900	-0.71004700
H	-1.32966500	3.41216100	-0.76065200
H	-3.74459500	3.23744700	-0.29900300
H	-4.80100800	1.01469100	0.01151400
F	-3.04385100	-2.34564300	-0.89311700
F	-4.89673300	-1.42668800	-0.21550200
F	-3.31022800	-1.85889500	1.20642800
H	-1.00595400	-0.86991600	-0.63984700
C	0.49946600	1.37985300	-0.97155000
H	0.86364400	0.44260300	-1.40264300
H	0.69276100	2.16888700	-1.70625600
C	1.36246200	1.70703200	0.27649100
H	1.02442000	2.65854000	0.69714200
N	2.78964100	1.74299300	-0.11591300
H	3.32500700	2.23615400	0.59642200
H	2.88267300	2.30163600	-0.96156000
C	1.18408600	0.63218200	1.34512400
O	1.80757600	-0.40769500	1.37062600
O	0.25108900	0.96186400	2.23587100
H	0.11792100	0.22253800	2.85196700
N	4.23740000	-0.85533500	-0.36981900
C	5.28022500	-0.44279400	-1.35898200
H	4.79388400	-0.15616400	-2.29016900
H	5.83724900	0.40246300	-0.95757900
H	5.95650600	-1.27819800	-1.53792300
C	4.84310900	-1.20441200	0.95506000
H	5.41192000	-0.34973500	1.31888100
H	4.04034100	-1.43910900	1.64903700
H	5.50579000	-2.06013200	0.82682600
C	3.39622600	-1.97775000	-0.89401400
H	2.61980100	-2.19438900	-0.16512000
H	2.94804100	-1.67155300	-1.83829700
H	4.02995000	-2.85000400	-1.05361400
H	3.60998700	-0.02434700	-0.21995700

Isomer 17

C	0.97166100	1.80389200	-0.60423300
C	2.19531800	2.41909900	-0.34671700
C	3.34279000	1.65099900	-0.17747300
C	3.25673800	0.26236600	-0.27775200
C	4.48225200	-0.58814500	-0.05230400
C	2.03478200	-0.35274900	-0.53859200
C	0.87741100	0.41285000	-0.69863700
H	0.08638900	2.41573800	-0.74575400
H	2.25633900	3.49909100	-0.28641100
H	4.29738000	2.12391300	0.01488600
F	4.60897400	-0.92905800	1.25376200
F	5.61447900	0.04879600	-0.40521200
F	4.42934100	-1.74338100	-0.75215200
H	1.99491500	-1.43225900	-0.63190400
C	-0.44855600	-0.26097500	-0.97810000
H	-1.16980800	0.47198200	-1.35105500
H	-0.31616700	-1.01063700	-1.76638500
C	-1.07501000	-0.99612800	0.23619300
H	-0.34294500	-1.70604900	0.63138700
N	-2.32642700	-1.66581800	-0.18678300
H	-2.57414500	-2.37929700	0.49664400
H	-2.14899500	-2.17027200	-1.05283500
C	-1.41020800	-0.00226900	1.34437900
O	-2.44424700	0.62930500	1.39988500
O	-0.42598000	0.10379200	2.23479800
H	-0.65342700	0.78729900	2.88633300
N	-4.81764100	-0.06496700	-0.36793400
C	-5.55466000	-0.87717900	-1.38440600
H	-4.99924100	-0.86451700	-2.32099900
H	-5.64720900	-1.90051400	-1.02366600
H	-6.54522700	-0.44964800	-1.53713300
C	-5.50368500	-0.09534600	0.96322700
H	-5.60250900	-1.13108800	1.28554900
H	-4.89775000	0.45895100	1.67512200
H	-6.49136400	0.35455300	0.86324500
C	-4.60511900	1.34066800	-0.83676600
H	-4.01285800	1.86469700	-0.09125400
H	-4.07489300	1.31864800	-1.78794300
H	-5.57473200	1.82108600	-0.96729500
H	-3.87088900	-0.51065700	-0.24546600

Isomer 18

C	0.02745500	-2.31849500	1.84984900
C	1.31687500	-2.00285700	2.27205100
C	2.21646800	-1.40461200	1.39318300
C	1.81235900	-1.14280000	0.08401300
C	2.73275900	-0.41557900	-0.85510700
C	0.52900500	-1.48274800	-0.34626700
C	-0.38559000	-2.06313300	0.53627400
H	-0.66124300	-2.78966700	2.54329200
H	1.62593500	-2.23353300	3.28462200
H	3.22278100	-1.16497900	1.71336200
F	4.02919600	-0.59780700	-0.57463200
F	2.51194500	0.94951700	-0.77321500
F	2.53231900	-0.73968800	-2.14432900
H	0.25415600	-1.31470200	-1.38145000
C	-1.79207500	-2.40021800	0.09528900
H	-1.79012600	-2.79904700	-0.92337000
H	-2.21443700	-3.17159500	0.74176700
C	-2.78708300	-1.21093900	0.16690500
H	-2.70851600	-0.74678600	1.15259100
N	-4.14491200	-1.70590600	0.00475700
H	-4.29785300	-2.13198500	-0.90308300
H	-4.84682000	-0.98940600	0.15187100
C	-2.41188100	-0.12129800	-0.83864600
O	-1.97747700	0.98640400	-0.55788900
O	-2.62969900	-0.48935600	-2.10301200
H	-2.40921100	0.24316700	-2.69950900
N	-0.43963800	3.04122900	0.54070300
C	-1.46115400	4.00476200	1.06186200
H	-2.14145300	4.26830400	0.25393000
H	-2.01479700	3.52970000	1.86994000
H	-0.95360100	4.89586700	1.42987400
C	0.48459900	2.57066800	1.62313800
H	-0.10553700	2.10693700	2.41179800
H	1.17898000	1.84791200	1.20011400
H	1.02880200	3.42784900	2.01865400
C	0.31778400	3.61067700	-0.62208200
H	1.01105000	2.85788400	-0.99158100
H	-0.39150900	3.88427800	-1.40123500
H	0.86455900	4.49215800	-0.28831700
H	-0.96017700	2.21524300	0.19254700

Isomer 19

C	-1.87471500	2.29043200	0.48744600
C	-3.16451500	2.36949900	-0.03259900
C	-3.90832500	1.21235200	-0.24379400
C	-3.35305600	-0.02389600	0.08424500
C	-4.11927600	-1.29523600	-0.17787100
C	-2.06610400	-0.10195200	0.61222600
C	-1.30939500	1.05451000	0.81065800
H	-1.30746500	3.20102400	0.64920500
H	-3.59312300	3.33563300	-0.27051500
H	-4.91220500	1.26888500	-0.64466500
F	-5.45065200	-1.10416500	-0.16248000
F	-3.83436400	-2.25290600	0.73506900
F	-3.80700000	-1.81636800	-1.39218200
H	-1.66775700	-1.07357100	0.88403700
C	0.08156100	0.95896500	1.40159500
H	0.45976200	1.95956800	1.63461800
H	0.02565100	0.41992200	2.35361500
C	1.14225800	0.20516500	0.54351100
H	0.69002500	-0.71460500	0.16128300
N	2.34380800	-0.17341100	1.31908600
H	2.65356100	0.63369000	1.85945500
H	2.07768900	-0.87627000	2.00495400
C	1.59966600	1.00597100	-0.67167600
O	2.74841900	1.33827200	-0.87331200
O	0.59395800	1.29211900	-1.49825100
H	0.93428400	1.81485200	-2.24248600
N	4.86756100	-0.75966700	-0.05071700
C	5.71510700	0.47057000	0.05676700
H	6.70139500	0.26003000	-0.35660100
H	5.22833500	1.27196900	-0.49329900
H	5.80789000	0.74411700	1.10699300
C	4.68391300	-1.16995600	-1.47845000
H	4.25973500	-0.33247600	-2.02667100
H	5.65188600	-1.44724000	-1.89581000
H	4.00853300	-2.02378500	-1.51709900
C	5.41350100	-1.88063400	0.77483300
H	4.74541400	-2.73728500	0.69834900
H	6.40310800	-2.15030000	0.40686500
H	5.48227100	-1.55777900	1.81263200
H	3.91684500	-0.52172200	0.34404200

Isomer 20

C	-1.87054100	2.27332100	-0.52469400
C	-3.15386600	2.36897100	0.00840200
C	-3.89386500	1.21913100	0.26752600
C	-3.33872100	-0.02748300	-0.01900100
C	-4.14118200	-1.28523700	0.19750000
C	-2.05907500	-0.12220000	-0.56182100
C	-1.30683100	1.02745000	-0.81022200
H	-1.30525700	3.17818300	-0.72156300
H	-3.57901800	3.34213400	0.22269400
H	-4.88885400	1.28809700	0.68813600
F	-5.06586600	-1.14012600	1.16510600
F	-3.35032400	-2.32943800	0.54782600
F	-4.79625100	-1.65827400	-0.92723300
H	-1.65673000	-1.10304700	-0.79129800
C	0.07973700	0.91207300	-1.40800300
H	0.45485100	1.90396200	-1.67993000
H	0.01692900	0.33916200	-2.33958900
C	1.14768300	0.18992100	-0.53185100
H	0.69709600	-0.71252400	-0.10847500
N	2.33998800	-0.22311800	-1.30411400
H	2.06446800	-0.95141800	-1.95903000
H	2.64672400	0.56094600	-1.87903200
C	1.62016200	1.03675000	0.64575000
O	2.77275000	1.36836400	0.82525700
O	0.62294300	1.36474100	1.46725600
H	0.97339100	1.91501000	2.18652800
N	4.87490000	-0.76791800	0.06136200
C	5.40729100	-1.92144200	-0.72735900
H	6.39942200	-2.18205400	-0.35966400
H	4.73619400	-2.77140500	-0.61230900
H	5.46682000	-1.63772600	-1.77710100
C	5.72684400	0.45328700	-0.10038600
H	5.24954100	1.27690200	0.42458100
H	5.80983400	0.68735700	-1.16092200
H	6.71645400	0.25335900	0.31031800
C	4.70400200	-1.12394700	1.50512800
H	4.28920800	-0.26460600	2.02602100
H	4.02518400	-1.97242000	1.58228500
H	5.67491200	-1.39027300	1.92280000
H	3.92121700	-0.54025200	-0.33237800

Isomer 21

C	-0.79412100	-1.28593600	-0.37993100
C	-1.74557700	-2.22403300	0.00983900
C	-3.07261000	-1.84601400	0.20527700
C	-3.43934600	-0.51750300	0.00680600
C	-4.87710400	-0.08920600	0.16040200
C	-2.48924600	0.42486200	-0.38934200
C	-1.15950400	0.05007900	-0.58227500
H	0.23897400	-1.58131400	-0.52043100
H	-1.45511800	-3.25685200	0.16123000
H	-3.81267500	-2.57433200	0.51104400
F	-5.51857900	-0.06801300	-1.03137400
F	-4.97202700	1.16127200	0.67363100
F	-5.57011000	-0.91065100	0.97059100
H	-2.79783700	1.45189000	-0.55108900
C	-0.13222700	1.08873200	-0.99222900
H	0.49081900	0.70030700	-1.80093300
H	-0.66634000	1.95718900	-1.39076400
C	0.78325100	1.54531700	0.17085900
H	0.34889900	1.25413200	1.12820200
N	0.97150600	3.05502300	0.22612200
H	0.45441900	3.50713500	0.97951000
H	0.73139600	3.51240200	-0.65430400
C	2.24678800	1.00147500	0.12676000
O	3.14175000	1.86516000	0.30192600
O	2.38638600	-0.22520900	-0.06193400
H	3.95068000	-0.64285900	0.00012500
N	4.99066200	-0.88010500	0.05806400
C	5.44970800	-0.45713300	1.41561700
H	5.23495700	0.60354000	1.53293100
H	4.90422300	-1.02853800	2.16538300
H	6.51944800	-0.64480000	1.51166100
C	5.13418000	-2.35083400	-0.14860900
H	4.57381100	-2.87304300	0.62547800
H	4.73336600	-2.61152300	-1.12705000
H	6.18782200	-2.62610800	-0.09385000
C	5.67004500	-0.09325600	-1.01494700
H	5.28336900	-0.41043900	-1.98249100
H	5.44768200	0.96056800	-0.85711000
H	6.74497500	-0.26990900	-0.96914500
H	2.02788900	3.10575300	0.37737000

Isomer 22

C	-2.53508200	2.08070500	0.52490900
C	-3.35101200	1.13576200	1.14130300
C	-3.18908000	-0.22248300	0.86779400
C	-2.21570600	-0.61654400	-0.04614900
C	-1.97227500	-2.06781200	-0.35252200
C	-1.41177000	0.33237500	-0.67996400
C	-1.54723000	1.68972400	-0.39023700
H	-2.68025800	3.13455300	0.74104400
H	-4.12072100	1.45519700	1.83360700
H	-3.81838000	-0.95942000	1.34954500
F	-2.83720700	-2.89211000	0.24858000
F	-0.71211200	-2.44631300	0.06895400
F	-1.99936600	-2.32682100	-1.67572200
H	-0.67758600	0.01216800	-1.41109300
C	-0.61144900	2.69694500	-1.01889800
H	-0.22742200	2.30935800	-1.96674800
H	-1.12482400	3.63495300	-1.23811100
C	0.60873000	3.06646900	-0.12913900
H	0.24137700	3.59828600	0.75598800
N	1.47939900	3.96636600	-0.85496500
H	1.89992400	3.51922400	-1.66271900
H	2.21519300	4.35734700	-0.27764200
C	1.30128800	1.77650900	0.34104500
O	2.04992600	1.12577600	-0.36492000
O	1.06648600	1.34179000	1.58914800
H	0.41744800	1.89641600	2.04464600
N	3.06352600	-1.42991400	0.14905400
C	4.54624000	-1.23298000	0.20985800
H	4.87978500	-0.77581800	-0.72024700
H	5.02968000	-2.19997900	0.34611400
H	4.78094600	-0.57759700	1.04700600
C	2.52311400	-1.98623900	1.43127900
H	2.96711300	-2.96591800	1.60635800
H	2.77806300	-1.30749900	2.24315900
H	1.44183200	-2.07466100	1.34715200
C	2.66320000	-2.26709100	-1.02764000
H	1.57914200	-2.36276300	-1.03849200
H	3.00732000	-1.78010300	-1.93863900
H	3.12159000	-3.25139000	-0.93447000
H	2.64235700	-0.48288400	0.01494900

Isomer 23

C	-1.09554700	-0.98835800	-1.66634600
C	-2.04695400	-1.97549400	-1.42457700
C	-3.15067300	-1.70870100	-0.61867700
C	-3.29625900	-0.44102500	-0.05833800
C	-4.50854000	-0.10714700	0.77282400
C	-2.35069500	0.55196100	-0.30975600
C	-1.23884400	0.28451900	-1.10977600
H	-0.23090700	-1.21230300	-2.27915000
H	-1.92743000	-2.95879400	-1.86324500
H	-3.88844500	-2.47662100	-0.42453900
F	-5.05248800	-1.19805600	1.34351700
F	-5.47661600	0.47923700	0.02952400
F	-4.20677100	0.76250500	1.76840800
H	-2.49384600	1.53756700	0.12100400
C	-0.22083400	1.37989700	-1.36507800
H	0.36075900	1.15172100	-2.26245400
H	-0.76455600	2.31218000	-1.55898700
C	0.73568500	1.61649600	-0.18121100
H	0.19582900	1.52871700	0.76349000
N	1.32614400	3.02443400	-0.20346600
H	1.32285700	3.42711100	-1.14226000
H	2.32550900	2.82681000	0.08616600
C	1.97863600	0.67535100	-0.10590500
O	1.82304600	-0.52441400	-0.28943200
O	3.07139100	1.29347100	0.17424000
H	4.23727500	0.10634100	0.36750900
N	4.92167200	-0.69281400	0.49337200
C	6.24027400	-0.10731200	0.87483500
H	6.57306400	0.56277300	0.08345600
H	6.12505800	0.45085200	1.80283100
H	6.96731500	-0.90791200	1.01214400
C	4.36506000	-1.57018400	1.56978100
H	4.30403100	-0.99689700	2.49382300
H	3.37021800	-1.88903900	1.26524300
H	5.02217800	-2.42891200	1.70844900
C	4.98508500	-1.41568600	-0.81431000
H	3.97687800	-1.73331200	-1.07249900
H	5.36547500	-0.73460700	-1.57442100
H	5.65031300	-2.27400400	-0.71837900
H	0.86270600	3.67547200	0.43017500

Isomer 24

C	1.20610200	-2.79301100	-0.28645900
C	2.51843400	-2.69631700	-0.73785700
C	3.23356400	-1.50660100	-0.58942200
C	2.62185100	-0.42202400	0.03041100
C	3.34041000	0.88688000	0.22311200
C	1.31054600	-0.52595600	0.49937900
C	0.58145500	-1.70220600	0.33549700
H	0.66715600	-3.72724000	-0.40646500
H	2.99181700	-3.55053000	-1.20664700
H	4.25170500	-1.42845600	-0.94796400
F	3.55955000	1.15706500	1.52808400
F	2.58305400	1.92653000	-0.25254900
F	4.51871700	0.93785700	-0.40996200
H	0.86161600	0.31736700	1.01248700
C	-0.85935100	-1.77045100	0.79049800
H	-1.06685300	-2.72509300	1.27855200
H	-1.05093000	-0.98412100	1.52666600
C	-1.86319400	-1.62678200	-0.38555200
H	-1.75823000	-2.51053800	-1.02333200
N	-1.61825900	-0.38545600	-1.15592900
H	-2.17948700	-0.41067500	-2.00568200
H	-0.64748800	-0.40532400	-1.46753200
C	-3.27760200	-1.70810800	0.17266900
O	-3.79120500	-2.73441900	0.51601400
O	-3.90009300	-0.49841100	0.28495300
H	-4.77945900	-0.68134500	0.65616600
N	-2.04951300	2.29096500	-0.19381100
C	-0.87558000	3.05055300	-0.73018800
H	-0.97576600	4.10210500	-0.46180400
H	0.04224100	2.64582500	-0.30644100
H	-0.85385700	2.94906500	-1.81435600
C	-2.11443400	2.36038400	1.29851600
H	-2.28346600	3.39324900	1.60292600
H	-2.92934700	1.72675900	1.64221100
H	-1.17067900	2.00863200	1.71221100
C	-3.33044400	2.74911200	-0.81640000
H	-4.14052300	2.12395400	-0.44783400
H	-3.50509000	3.79227800	-0.55333800
H	-3.25330700	2.65147400	-1.89837500
H	-1.91767100	1.27078600	-0.46637900

Isomer 25

C	-1.58054400	1.18020200	2.07718600
C	-2.72490200	0.50248600	2.49475500
C	-3.53189300	-0.14965700	1.56729100
C	-3.18939800	-0.10720300	0.21603700
C	-4.01470400	-0.85265800	-0.80357700
C	-2.05078700	0.57800200	-0.20352000
C	-1.22960900	1.22478600	0.72423900
H	-0.96763700	1.69509000	2.80981200
H	-2.99163300	0.48849100	3.54467400
H	-4.42420400	-0.67291900	1.88630100
F	-5.28681000	-1.02387800	-0.40778500
F	-3.49813000	-2.08850500	-1.03339700
F	-4.03617500	-0.21666300	-1.99528200
H	-1.82267200	0.61920900	-1.26329300
C	0.01611500	1.95530900	0.26541900
H	-0.26241100	2.69086800	-0.49782400
H	0.44349400	2.52287200	1.09781000
C	1.10111000	0.99560300	-0.30007600
H	0.68872400	0.48774800	-1.17986200
N	1.52863300	-0.05326100	0.64173900
H	0.73251200	-0.65570000	0.83989800
H	1.77387800	0.38157600	1.53048200
C	2.35181100	1.74891500	-0.77405700
O	3.46069800	1.47828300	-0.38412000
O	2.17943100	2.72497500	-1.67505100
H	1.25079200	2.86142600	-1.90441700
N	4.12086700	-1.42002600	0.15412300
C	5.13730500	-0.80510500	1.06716300
H	5.28864100	0.22855700	0.76687200
H	4.76297900	-0.84513600	2.08924900
H	6.06654800	-1.36975500	0.99324300
C	3.78406800	-2.81847100	0.56321300
H	4.67680500	-3.43900600	0.49092200
H	3.42187900	-2.81120500	1.59016400
H	3.01011600	-3.20568200	-0.09780900
C	4.56836300	-1.35826600	-1.27400600
H	3.77954600	-1.76014700	-1.90872400
H	4.76353700	-0.31998200	-1.53076200
H	5.47223200	-1.95668100	-1.38716000
H	3.23778200	-0.85491300	0.24054300

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C	-1.67796800	2.34977300	-0.82295800
C	-3.05003400	2.32963600	-0.59502300
C	-3.69714200	1.13015900	-0.30301100
C	-2.95632700	-0.04687600	-0.24270900
C	-3.63234600	-1.36871500	0.01755400
C	-1.58044500	-0.02767100	-0.47349100
C	-0.92693100	1.17018700	-0.75970500
H	-1.19114100	3.29116500	-1.05733800
H	-3.62037400	3.24907500	-0.64724900
H	-4.76414500	1.11188100	-0.12237600
F	-4.81589300	-1.22735000	0.63855000
F	-2.86280400	-2.17750500	0.78933400
F	-3.86159600	-2.04454800	-1.13423400
H	-1.02133200	-0.95531800	-0.42845500
C	0.57107800	1.18594700	-0.97841100
H	0.91604200	0.18187400	-1.23910500
H	0.81469700	1.84160900	-1.82217200
C	1.37825900	1.69033400	0.23992300
H	1.06359400	2.71010300	0.47575400
N	2.83445900	1.63618400	-0.06732800
H	3.34319700	2.14127400	0.65765100
H	2.99157300	2.17161100	-0.92047200
C	1.06728400	0.88697800	1.49940700
O	0.46963500	1.31332300	2.44418300
O	1.52749100	-0.40002600	1.43906200
H	1.20823400	-0.84019300	2.24438700
N	4.24340400	-0.87761300	-0.40558300
C	5.31223200	-0.51441100	-1.38756400
H	4.84666400	-0.20508100	-2.32222400
H	5.90652100	0.30304700	-0.98166500
H	5.94957200	-1.38074800	-1.56317600
C	4.82474600	-1.25016100	0.92226100
H	5.44775700	-2.13666400	0.80488900
H	5.42873000	-0.42183800	1.29015200
H	4.01048900	-1.44894900	1.61481400
C	3.35512100	-1.95858700	-0.93764800
H	2.55217300	-2.13035100	-0.22487900
H	2.94072000	-1.63791700	-1.89239400
H	3.94205800	-2.86615200	-1.07838900
H	3.65040100	-0.00973500	-0.25794400

Section VIII. Transition State X,Y,Z Coordinates

Transition State 1 – CF3 rotation

C	-0.52045200	2.85367000	1.18359700
C	-1.74189200	2.48315400	1.74132600
C	-2.50107100	1.47362500	1.15745300
C	-2.03164900	0.85082000	0.00021000
C	-2.85247900	-0.23379900	-0.64266200
C	-0.82057300	1.23768000	-0.56999400
C	-0.04230500	2.23051300	0.02716400
H	0.06100800	3.64185700	1.65117500
H	-2.10312400	2.98153500	2.63273200
H	-3.44625100	1.17568100	1.59424200
F	-3.84263000	0.24214800	-1.41628600
F	-3.42259300	-1.04541200	0.28088000
F	-2.08853800	-1.04196400	-1.43751900
H	-0.48110100	0.75809500	-1.48026300
C	1.29607100	2.61161200	-0.56192100
H	1.30923000	2.39823300	-1.63557400
H	1.44993100	3.68911500	-0.44946600
C	2.53344600	1.92662900	0.08914000
H	2.53282400	2.14227700	1.16120200
N	3.76121600	2.37146400	-0.58738500
H	3.63314600	3.23840000	-1.09747000
H	4.53582400	2.49973400	0.05528700
C	2.45223900	0.40100200	-0.06132900
O	1.71973200	-0.30299400	0.61383100
O	3.22531200	-0.10269200	-1.00864200
H	3.76394000	0.66863300	-1.33257400
N	1.01712000	-2.96102400	0.43796000
C	-0.11774100	-3.11307000	1.40305300
H	-0.42966000	-4.15710700	1.42497800
H	0.21709700	-2.80121900	2.39091500
H	-0.94467600	-2.48450000	1.07837800
C	2.21130600	-3.76035900	0.85429800
H	2.50621600	-3.45800800	1.85790600
H	1.95506500	-4.81952400	0.84371600
H	3.02505700	-3.56558100	0.15748600
C	0.59868600	-3.27993700	-0.96429200
H	1.43638400	-3.08479000	-1.63211800
H	0.31252700	-4.33007400	-1.02057200
H	-0.24670000	-2.64861000	-1.23124000
H	1.30690900	-1.95392000	0.45578700

Transition State 2 – CF3 rotation

C	2.17634700	-2.11709300	-0.98576900
C	3.56695100	-2.17534900	-0.92236000
C	4.29872800	-1.05744200	-0.53049400
C	3.62458400	0.11926500	-0.20961300
C	4.37456700	1.35863900	0.21150700
C	2.23324700	0.17947000	-0.27624400
C	1.49276600	-0.94033800	-0.65917700
H	1.62054500	-2.99089300	-1.31168300
H	4.08248700	-3.09150200	-1.18417200
H	5.37891600	-1.09609900	-0.48128600
F	4.13632900	2.39145300	-0.63066400
F	5.70423000	1.16986100	0.25254300
F	3.98681800	1.77174300	1.44454500
H	1.73045300	1.11106100	-0.03773300
C	-0.01875600	-0.87493800	-0.71332700
H	-0.34413300	-0.00464900	-1.28787200
H	-0.40983400	-1.76088600	-1.22436300
C	-0.66737300	-0.78058700	0.69094300
H	-0.29934300	0.12385000	1.18408400
N	-0.43672300	-1.97936500	1.51083700
H	-0.12682100	-1.75003100	2.44905400
H	0.26411900	-2.59080300	1.10511300
C	-2.18358400	-0.60651500	0.53608200
O	-2.90471700	-1.60588200	1.00655100
O	-2.69689000	0.36962400	0.00748000
H	-4.35641700	0.61812200	-0.16167100
N	-5.37848200	0.83080800	-0.29363400
C	-6.03736700	0.66179300	1.03930400
H	-5.87192600	-0.35719600	1.38527200
H	-5.59484000	1.36520300	1.74283100
H	-7.10499500	0.85680400	0.93966100
C	-5.47510200	2.23994500	-0.78830500
H	-5.02569000	2.90359800	-0.05148900
H	-4.93511400	2.32070400	-1.73017800
H	-6.52378200	2.49850000	-0.93443400
C	-5.90326100	-0.14812500	-1.29617300
H	-5.35897900	-0.02159100	-2.23068500
H	-5.75128100	-1.15662500	-0.91486500
H	-6.96560000	0.03547900	-1.45592600
H	-2.22534200	-2.23296000	1.39160000

Transition State 3 – TMA rotation

C	2.19551100	2.09769600	1.01671400
C	3.58805300	2.13358600	0.94780700
C	4.29676100	1.01508400	0.52286000
C	3.59997300	-0.14176000	0.17053200
C	4.35359400	-1.38484400	-0.23319300
C	2.20990400	-0.17952500	0.24260800
C	1.49082900	0.94398100	0.66049900
H	1.65686300	2.97238000	1.36811100
H	4.12035700	3.03409000	1.22960100
H	5.37746900	1.03827400	0.46434900
F	4.62468300	-2.16915100	0.83613500
F	5.52999300	-1.09615100	-0.82154600
F	3.64220200	-2.14254200	-1.10097200
H	1.69034200	-1.09270400	-0.02571100
C	-0.02131100	0.90289000	0.71716900
H	-0.35964200	0.01798200	1.26104800
H	-0.39598500	1.77633700	1.26100200
C	-0.67625400	0.87020600	-0.68689300
H	-0.32050100	-0.01840500	-1.21657500
N	-0.43507300	2.09842800	-1.45825600
H	0.28270800	2.67930200	-1.03756200
H	-0.14377000	1.90430200	-2.41028100
C	-2.19384300	0.70652200	-0.53215600
O	-2.71387700	-0.28881500	-0.04698500
O	-2.90594000	1.73393300	-0.95036700
H	-2.22324600	2.37144900	-1.30994700
N	-5.36511300	-0.87884300	0.27901200
C	-5.54960800	-2.18433900	-0.42916400
H	-5.33819100	-2.04392100	-1.48793300
H	-4.85711900	-2.91283300	-0.01082400
H	-6.57668600	-2.52366300	-0.29575500
C	-5.56862500	-1.01738100	1.75500600
H	-4.87440300	-1.76368800	2.13761600
H	-5.37380500	-0.05706900	2.22963800
H	-6.59545400	-1.32729500	1.94867700
C	-6.22905400	0.19614600	-0.30229600
H	-6.01073500	1.13561600	0.20238400
H	-6.00507700	0.29370400	-1.36311000
H	-7.27641100	-0.07112500	-0.16320000
H	-4.36436100	-0.58974100	0.13248500

Transition State 4 – TMA rotation

C	-1.67738500	-2.07975800	0.26008900
C	-2.99547700	-2.47442900	0.45670600
C	-4.04058500	-1.57704400	0.23323800
C	-3.74970600	-0.28826300	-0.20007000
C	-4.84657600	0.72108600	-0.42928600
C	-2.42473400	0.10826700	-0.40241000
C	-1.37566400	-0.77966100	-0.16841700
H	-0.87640800	-2.79343700	0.42654300
H	-3.21587100	-3.48520700	0.77849500
H	-5.06801400	-1.88202400	0.38268400
F	-4.69651500	1.35888600	-1.61260900
F	-6.06992800	0.16519700	-0.41955700
F	-4.83399600	1.68193900	0.52996100
H	-2.21988600	1.10909900	-0.76825300
C	0.05881100	-0.34177900	-0.36611300
H	0.61613100	-1.09310400	-0.92982000
H	0.08579400	0.58357600	-0.95086200
C	0.80787800	-0.10896000	0.97172500
H	0.83307700	-1.05236300	1.52515500
N	0.22929600	0.97685900	1.77658500
H	0.09550100	0.70907500	2.74561900
H	-0.67241900	1.27980900	1.42281500
C	2.26672800	0.26170000	0.67215300
O	2.61450300	1.47615200	1.04826000
O	3.05121800	-0.49393700	0.11478200
H	4.66297100	-0.14166300	-0.24683100
N	5.67611900	-0.02001300	-0.50388500
C	5.81751300	-0.43734700	-1.93401300
H	5.50229400	-1.47489000	-2.03110800
H	5.18365600	0.19765800	-2.55072200
H	6.85884900	-0.33212500	-2.23787900
C	6.01525800	1.42494900	-0.31014100
H	5.38255700	2.02623000	-0.96069400
H	5.82835900	1.69511900	0.72762700
H	7.06470800	1.58266500	-0.55795100
C	6.46654900	-0.90235100	0.41039500
H	6.14146000	-1.93239000	0.27383000
H	6.28779200	-0.59419100	1.43922900
H	7.52612400	-0.80951800	0.17251400
H	1.78795000	1.83938700	1.48307300

Transition State 5 – TMA rotation

C	-1.67768400	2.08009100	-0.25904200
C	-2.99586300	2.47460900	-0.45536900
C	-4.04078400	1.57690900	-0.23228500
C	-3.74963300	0.28796700	0.20035500
C	-4.84631300	-0.72168000	0.42917500
C	-2.42456800	-0.10842600	0.40237800
C	-1.37568400	0.77982300	0.16875900
H	-0.87685700	2.79400900	-0.42519200
H	-3.21647300	3.48551000	-0.77662500
H	-5.06828200	1.88177500	-0.38149800
F	-6.06971700	-0.16589800	0.42037500
F	-4.69572200	-1.36042500	1.61192200
F	-4.83402000	-1.68175100	-0.53086200
H	-2.21949400	-1.10941000	0.76767500
C	0.05888700	0.34207600	0.36605000
H	0.61609100	1.09308600	0.93029400
H	0.08608100	-0.58372000	0.95008300
C	0.80793100	0.11048500	-0.97203000
H	0.83346900	1.05450000	-1.52440200
N	0.22901300	-0.97436600	-1.77794800
H	-0.67338000	-1.27651000	-1.42520800
H	0.09645400	-0.70598000	-2.74699000
C	2.26660200	-0.26100500	-0.67266800
O	3.05146500	0.49398100	-0.11494300
O	2.61376800	-1.47546400	-1.04929200
H	1.78707000	-1.83811200	-1.48428400
N	5.67613600	0.01947700	0.50423700
C	6.46680000	0.90257100	-0.40911300
H	6.28754300	0.59587600	-1.43829500
H	6.14234900	1.93261500	-0.27110000
H	7.52639200	0.80880600	-0.17167300
C	5.81787300	0.43506900	1.93483200
H	5.50343300	1.47273400	2.03313700
H	5.18357000	-0.20018600	2.55082500
H	6.85913900	0.32872300	2.23854700
C	6.01469900	-1.42539300	0.30874300
H	5.38208400	-2.02718700	0.95890600
H	5.82724100	-1.69435600	-0.72923900
H	7.06420500	-1.58374000	0.55590600
H	4.66302100	0.14174300	0.24737100

Transition State 6 – Proton Transfer

C	-3.01267500	1.70986300	0.08537400
C	-3.78397000	0.73335700	-0.54443700
C	-3.34101700	-0.58547400	-0.59686800
C	-2.12485400	-0.91717000	-0.00065300
C	-1.63341400	-2.34107600	0.00596900
C	-1.35835500	0.05504000	0.63798700
C	-1.78429200	1.38525200	0.67524800
H	-3.38829600	2.72741000	0.14373100
H	-4.73579600	0.99914800	-0.98821900
H	-3.93440700	-1.34550800	-1.08847700
F	-1.84643900	-2.94722300	1.19262400
F	-2.20840000	-3.09470400	-0.94344600
F	-0.28033900	-2.39737400	-0.20738300
H	-0.42441400	-0.21929000	1.11195000
C	-0.91526200	2.44437800	1.32161400
H	-1.52569100	3.29906800	1.62483500
H	-0.44659100	2.05148700	2.22643700
C	0.22747300	2.95068900	0.42176600
H	0.76131100	3.75184000	0.93758900
N	-0.20583000	3.45640400	-0.92108900
H	-0.11371800	4.46113800	-1.03948000
H	-1.15456100	3.17009200	-1.16084200
C	1.27878600	1.86780400	0.03385200
O	1.50407300	1.84983900	-1.22418000
O	1.79822200	1.15061900	0.89638600
H	2.78088300	-0.06440600	0.32971900
N	3.42460400	-0.83667900	-0.00293500
C	3.36823300	-1.93194500	1.01281900
H	3.67658500	-1.53445000	1.97860100
H	2.34583800	-2.30109300	1.07501500
H	4.03618400	-2.73893200	0.71092400
C	2.92357900	-1.28994900	-1.33847100
H	1.92501100	-1.70541700	-1.21608500
H	2.88140800	-0.42843100	-2.00220600
H	3.59877000	-2.04868900	-1.73440400
C	4.79026600	-0.23804100	-0.10133800
H	5.08446700	0.13387700	0.87891700
H	4.76045400	0.58544700	-0.81294900
H	5.49475300	-0.99824200	-0.43903900
H	0.63767200	2.76055300	-1.49880600

Transition State 7 – Proton Transfer

C	-1.81589700	2.19223500	0.06642400
C	-3.15466700	2.49374100	-0.15722500
C	-4.12032500	1.48747400	-0.11641500
C	-3.73071900	0.18050700	0.15728300
C	-4.75173700	-0.92555000	0.25760500
C	-2.38648400	-0.12232800	0.39057000
C	-1.41479300	0.87714500	0.33857500
H	-1.07870300	2.98886300	0.04401700
H	-3.45282700	3.51570300	-0.35826000
H	-5.16263800	1.71931500	-0.29293500
F	-4.30372900	-2.06342900	-0.33009200
F	-5.91704100	-0.60173100	-0.32912300
F	-5.02019000	-1.23614100	1.54595700
H	-2.10792800	-1.14279700	0.63341200
C	0.04473200	0.53644500	0.54830700
H	0.52446100	1.25806800	1.21331600
H	0.13435200	-0.44202800	1.03172400
C	0.85681500	0.52801300	-0.75967400
H	0.83875100	1.51747100	-1.21876800
N	0.38531900	-0.49321900	-1.74930600
H	-0.41223500	-1.03314500	-1.41906400
H	0.14531500	-0.09822300	-2.65450500
C	2.33198800	0.10662400	-0.52761800
O	3.06852600	0.74845200	0.22782500
O	2.63940400	-0.94799500	-1.19029600
H	1.50030600	-1.07497000	-1.72521200
N	5.59684200	-0.19795200	0.42828700
C	6.31294900	0.59429400	1.47304700
H	6.31068800	1.64407500	1.18382100
H	5.79348600	0.47686600	2.42276800
H	7.33804200	0.23408000	1.56192700
C	5.48829500	-1.64315300	0.79633700
H	5.01372300	-1.72287200	1.77325900
H	4.87570800	-2.14419000	0.04875300
H	6.48522300	-2.08292300	0.83059500
C	6.21015000	-0.02298800	-0.92375300
H	5.60631100	-0.56355000	-1.65069700
H	6.22218100	1.03760300	-1.17052500
H	7.22764000	-0.41387600	-0.91249500
H	4.60637800	0.17802400	0.36432000

Transition State 8 – Proton Transfer

C	1.81614400	2.19227200	-0.06697700
C	3.15489500	2.49369500	0.15681300
C	4.12048900	1.48733500	0.11627400
C	3.73082300	0.18038700	-0.15734900
C	4.75162400	-0.92591500	-0.25714800
C	2.38658100	-0.12237400	-0.39078100
C	1.41497000	0.87716900	-0.33903500
H	1.07901300	2.98896500	-0.04478400
H	3.45311900	3.51566100	0.35773900
H	5.16279600	1.71912200	0.29289000
F	5.91763200	-0.60132900	0.32773400
F	5.01853000	-1.23857200	-1.54531200
F	4.30413000	-2.06282100	0.33287300
H	2.10797700	-1.14284900	-0.63355200
C	-0.04454900	0.53654000	-0.54892400
H	-0.52405400	1.25781000	-1.21448200
H	-0.13415100	-0.44221300	-1.03177600
C	-0.85691000	0.52892000	0.75889400
H	-0.83891300	1.51863900	1.21742500
N	-0.38562800	-0.49178000	1.74917300
H	-0.14601300	-0.09630500	2.65426700
H	0.41213600	-1.03173300	1.41948000
C	-2.33203000	0.10742500	0.52673400
O	-2.63955400	-0.94693300	1.18984100
O	-3.06844600	0.74886200	-0.22913100
H	-4.60650100	0.17794500	-0.36434800
N	-5.59680800	-0.19842800	-0.42779600
C	-5.48773500	-1.64410300	-0.79391300
H	-5.01411600	-1.72492300	-1.77120500
H	-4.87406000	-2.14368000	-0.04624600
H	-6.48442600	-2.08453100	-0.82654000
C	-6.21019900	-0.02188900	0.92400200
H	-5.60662200	-0.56190400	1.65157100
H	-6.22195100	1.03895800	1.16969500
H	-7.22779900	-0.41249600	0.91301000
C	-6.31316200	0.59221600	-1.47361600
H	-6.31161600	1.64233200	-1.18560200
H	-5.79341900	0.47402200	-2.42308800
H	-7.33800900	0.23126500	-1.56230100
H	-1.50061300	-1.07364000	1.72502900

Transition State 9 – Proton Transfer

C	-2.05923600	2.15712300	-0.80694000
C	-3.43834800	2.32267700	-0.68708800
C	-4.25134400	1.23167200	-0.39601600
C	-3.67316700	-0.02781100	-0.23910700
C	-4.52373400	-1.22047400	0.12339200
C	-2.29545200	-0.19572100	-0.36404500
C	-1.47168800	0.89799500	-0.64285700
H	-1.43987300	3.01336200	-1.05682200
H	-3.88008600	3.30179600	-0.82792300
H	-5.32304700	1.35272500	-0.30614800
F	-5.82046900	-1.03659300	-0.17804600
F	-4.45478100	-1.47751200	1.45483300
F	-4.11064100	-2.34149000	-0.50775700
H	-1.87114600	-1.18886000	-0.26203300
C	0.02828900	0.72089000	-0.75608200
H	0.27693800	-0.08220300	-1.45405100
H	0.48117600	1.63348400	-1.15782500
C	0.70008600	0.37099800	0.58234100
H	0.30918200	-0.57263900	0.96556500
N	0.54467100	1.43465500	1.62635400
H	0.10247000	1.10282300	2.47927900
H	0.02670000	2.24647400	1.29628100
C	2.24220000	0.25459200	0.45619100
O	2.85049000	1.08548700	1.22048000
O	2.75825100	-0.56096000	-0.31451900
H	4.39983200	-0.60532500	-0.32381900
N	5.46118600	-0.62603600	-0.31031400
C	5.90496900	-1.64672900	-1.30692600
H	5.49367100	-2.61537800	-1.02734900
H	5.53415300	-1.36399900	-2.29089700
H	6.99414800	-1.69315400	-1.31812300
C	5.92311400	0.74885500	-0.67250100
H	5.57367000	0.98423000	-1.67669500
H	5.49860800	1.45471200	0.03945200
H	7.01214900	0.78497200	-0.64013500
C	5.86609900	-0.99003800	1.08190500
H	5.44671900	-0.25544500	1.76734500
H	5.47322700	-1.97842100	1.31559000
H	6.95392000	-0.99604700	1.15240200
H	1.78893300	1.57652500	1.71106000

Transition State 10 – Proton Transfer

C	2.07195900	-2.12972800	-0.85207200
C	3.45241800	-2.28804200	-0.72016900
C	4.24983100	-1.20352700	-0.37538600
C	3.65704600	0.04456300	-0.17010100
C	4.52829200	1.23450300	0.15246800
C	2.28139300	0.20452400	-0.30531400
C	1.47127300	-0.88565900	-0.64150900
H	1.46450200	-2.98098300	-1.14468800
H	3.90451400	-3.25748800	-0.89169200
H	5.32094700	-1.32160400	-0.26835700
F	5.12703400	1.72467600	-0.95545400
F	5.50784800	0.91313100	1.02230000
F	3.81900500	2.24709600	0.69998700
H	1.84526100	1.18557100	-0.15533400
C	-0.02867100	-0.71459100	-0.76189100
H	-0.27497500	0.12541800	-1.41589100
H	-0.47064700	-1.60594700	-1.21959300
C	-0.71765400	-0.44449000	0.58639800
H	-0.32420000	0.46933500	1.03375400
N	-0.58577300	-1.57565900	1.56043800
H	-0.05813500	-2.36359400	1.19021500
H	-0.16633800	-1.30139900	2.44476500
C	-2.25671600	-0.30821900	0.44502400
O	-2.75462400	0.56670400	-0.27067700
O	-2.88236800	-1.18929000	1.13527400
H	-1.83068500	-1.72041400	1.60826500
N	-5.45501400	0.67189200	-0.29301400
C	-5.93399200	-0.62088800	-0.87049000
H	-7.02392200	-0.63931200	-0.86140300
H	-5.56959300	-0.70698000	-1.89311000
H	-5.53725800	-1.43703400	-0.26887000
C	-5.86849400	1.84352500	-1.12270800
H	-5.49188700	1.70981000	-2.13557500
H	-6.95638500	1.91329800	-1.13547500
H	-5.44233900	2.74845500	-0.69241000
C	-5.87283600	0.82119900	1.13469200
H	-5.47526000	1.75841200	1.52131600
H	-6.96129300	0.82662100	1.19464200
H	-5.46501900	-0.01329300	1.70271800
H	-4.39392400	0.63504900	-0.29716200

Transition State 11 – Proton Transfer

C	1.37411600	-2.69600900	1.05254300
C	2.47892900	-2.07210800	1.62417900
C	2.95449300	-0.87033700	1.10319800
C	2.32305100	-0.31505000	-0.00730100
C	2.76141800	1.00894300	-0.56776400
C	1.22639300	-0.94900100	-0.59028900
C	0.73039400	-2.13546900	-0.05599000
H	1.01810500	-3.63300900	1.46931800
H	2.97419100	-2.52230500	2.47591000
H	3.81114400	-0.37977600	1.54675300
F	1.84022500	1.99066600	-0.27227400
F	2.85478500	0.99363900	-1.91336500
F	3.93449200	1.43056400	-0.07701400
H	0.75512100	-0.50906100	-1.46153600
C	-0.49209000	-2.79360800	-0.65798400
H	-0.59111800	-2.49742100	-1.70783400
H	-0.36406100	-3.88102800	-0.64112700
C	-1.81314500	-2.46732100	0.07518800
H	-1.75304500	-2.76928200	1.12099200
N	-2.97665500	-3.14975800	-0.59162000
H	-2.71205800	-3.73359700	-1.38222100
H	-3.55013500	-3.69802600	0.04483700
C	-2.23553600	-0.96760800	-0.00612900
O	-1.56330600	-0.10414900	0.56894600
O	-3.29052300	-0.80208300	-0.70224900
H	-3.48772500	-2.09773600	-0.89501100
N	-1.95727600	2.55091500	0.39319600
C	-3.40324400	2.82031900	0.65516200
H	-3.99772200	2.28885200	-0.08639900
H	-3.65433300	2.45719100	1.65060700
H	-3.58956700	3.89258000	0.59230200
C	-1.07465500	3.15149400	1.43982900
H	-1.36830700	2.76113600	2.41298300
H	-0.04331200	2.87519900	1.22811000
H	-1.18361300	4.23622900	1.42453300
C	-1.55523700	2.98133600	-0.98068400
H	-0.50683100	2.73140000	-1.13345600
H	-2.17468300	2.45678900	-1.70678800
H	-1.69880500	4.05772100	-1.07757500
H	-1.82992400	1.49858800	0.44112700

Transition State 12 – Dihedral Rotation

C	2.04705700	2.06606600	-0.39945400
C	3.38103000	2.08593200	-0.80062900
C	4.18110800	0.95708100	-0.64878000
C	3.62605900	-0.19493300	-0.09763300
C	4.45831600	-1.43633500	0.10658200
C	2.29010800	-0.21616900	0.30021700
C	1.48135700	0.91323700	0.15705100
H	1.45611800	2.96486300	-0.52840300
H	3.79969800	2.98682700	-1.23303700
H	5.21702900	0.96914100	-0.96094900
F	5.63934900	-1.37599400	-0.53416300
F	3.81374300	-2.54334500	-0.33433300
F	4.72323500	-1.64247400	1.41905400
H	1.87555200	-1.12705800	0.71788800
C	0.04200000	0.82300700	0.63772200
H	-0.28465200	-0.21347700	0.53819200
H	-0.00883700	1.05481400	1.71086700
C	-0.98619200	1.70925800	-0.09249100
H	-0.77020800	1.68901800	-1.16571500
N	-1.05634400	3.10016100	0.38992600
H	-0.85741200	3.78467800	-0.32990500
H	-0.44108000	3.27472400	1.17649100
C	-2.39642100	1.10476000	0.05114100
O	-3.29984500	1.92219700	0.55109800
O	-2.67002100	-0.04028900	-0.27969500
H	-4.18516200	-0.77960700	-0.19283800
N	-5.09326800	-1.30942500	-0.17216300
C	-4.87682600	-2.57841500	-0.93564900
H	-4.58777500	-2.33059000	-1.95554900
H	-4.07984000	-3.14534900	-0.45754700
H	-5.79941300	-3.15871900	-0.93851800
C	-5.41539800	-1.57332600	1.26507800
H	-4.61181700	-2.16258300	1.70395000
H	-5.50153700	-0.62150200	1.78677900
H	-6.35578800	-2.12067500	1.32796800
C	-6.12470900	-0.43901200	-0.81868000
H	-6.19114300	0.49654200	-0.26568300
H	-5.82274900	-0.23815300	-1.84536600
H	-7.08613500	-0.95208400	-0.80698400
H	-2.79049900	2.76817700	0.72093700

Transition State 13 – Dihedral Rotation

C	2.05582800	2.07552500	-0.37626300
C	3.39324500	2.08527500	-0.76948700
C	4.18583100	0.95503400	-0.60086400
C	3.62351700	-0.18797500	-0.03496400
C	4.44323800	-1.44685900	0.10113500
C	2.28570500	-0.19975100	0.35269100
C	1.48235400	0.93235000	0.18967500
H	1.47056300	2.97645800	-0.51613100
H	3.81952900	2.98091100	-1.20536500
H	5.22620900	0.96188900	-0.89950400
F	5.75576200	-1.18523800	0.24829200
F	4.31653800	-2.23802200	-0.99288200
F	4.05478100	-2.18861800	1.16265300
H	1.86866400	-1.09960900	0.78990300
C	0.04080700	0.85658300	0.66604100
H	-0.28293100	-0.18366900	0.60371200
H	-0.01775100	1.12885300	1.72923100
C	-0.98382700	1.71302900	-0.10462600
H	-0.75382300	1.66027400	-1.17376800
N	-1.06734400	3.11773500	0.33358500
H	-0.45982700	3.32103200	1.11918300
H	-0.86757300	3.78089800	-0.40576600
C	-2.39239100	1.10521500	0.03996500
O	-2.65708300	-0.04904600	-0.26504500
O	-3.30489600	1.93040100	0.51007400
H	-2.80202700	2.78368500	0.66120300
N	-5.08167200	-1.31839400	-0.16662100
C	-4.97240200	-2.42619700	-1.16691900
H	-5.90078600	-2.99713700	-1.17448600
H	-4.79047200	-1.99602800	-2.15031200
H	-4.13939000	-3.06998700	-0.88971300
C	-6.16256100	-0.34724600	-0.52552300
H	-5.97858000	0.02896400	-1.53056600
H	-7.12707600	-0.85323900	-0.48789400
H	-6.14237500	0.47883000	0.18335600
C	-5.24865700	-1.84131900	1.22536000
H	-5.26428500	-1.00095900	1.91752000
H	-6.18433200	-2.39627800	1.29115300
H	-4.41025900	-2.49551100	1.45903100
H	-4.17237200	-0.79068700	-0.18966500

Transition State 14 – Dihedral Rotation

C	-2.46402100	-2.40260800	-0.61536200
C	-3.80089000	-2.10022500	-0.37258200
C	-4.19782200	-0.77994400	-0.16395500
C	-3.24537400	0.23440300	-0.21377400
C	-3.63350500	1.66962700	0.04809100
C	-1.90437200	-0.06519300	-0.46672000
C	-1.49652100	-1.38870500	-0.66589800
H	-2.17183900	-3.43282700	-0.79141500
H	-4.53953200	-2.89252400	-0.35397300
H	-5.23742500	-0.54132100	0.01977400
F	-4.95063900	1.87991000	-0.10051800
F	-2.98367000	2.52007300	-0.77527900
F	-3.30828900	2.03241100	1.31657600
H	-1.18325900	0.74251700	-0.53840000
C	-0.03862100	-1.71120100	-0.91427800
H	0.03729100	-2.64415100	-1.47315700
H	0.41475300	-0.94270000	-1.54131200
C	0.84204100	-1.84785200	0.37206000
H	1.22840000	-2.86356700	0.45174400
N	0.10930800	-1.55275700	1.66467100
H	-0.01848000	-2.36930800	2.26021600
H	-0.80761000	-1.12614600	1.48964900
C	2.06539000	-0.87899300	0.40121200
O	2.80160500	-0.89460200	-0.60890700
O	2.18619400	-0.19186000	1.44293600
H	0.76992500	-0.84976200	2.11097300
N	4.87121200	0.76809100	-0.29491500
C	4.28011100	2.12427200	-0.08988600
H	3.74474700	2.41525200	-0.99268400
H	3.58680800	2.07064900	0.74775100
H	5.07572900	2.84076600	0.11641000
C	5.58420700	0.29585700	0.92970600
H	4.87068000	0.27259000	1.75156600
H	5.96925700	-0.70662800	0.74794000
H	6.40744600	0.97420800	1.15577600
C	5.73990100	0.71124200	-1.50632400
H	6.09208700	-0.31035700	-1.64131100
H	5.15596100	1.01167000	-2.37505900
H	6.58891100	1.38350100	-1.37857600
H	4.05036800	0.09686000	-0.44718500

Transition State 15 – Proton Transfer

C	-0.94310000	-0.36995500	2.18532100
C	-1.77621300	0.72539000	2.40190800
C	-2.72423600	1.08448500	1.44905400
C	-2.83993200	0.32734700	0.28352500
C	-3.82540100	0.73000500	-0.78413500
C	-2.01542600	-0.77517800	0.07218900
C	-1.05125000	-1.12868700	1.01814700
H	-0.21008000	-0.64121700	2.93772800
H	-1.69117900	1.29645900	3.31876500
H	-3.37758600	1.93173300	1.61405100
F	-4.89473800	1.37052000	-0.27717400
F	-4.27990400	-0.33531900	-1.48082800
F	-3.25395800	1.56820800	-1.68743500
H	-2.14488900	-1.36293900	-0.82981100
C	-0.17125600	-2.34238900	0.79792800
H	0.43625100	-2.52205600	1.69079900
H	-0.80746800	-3.22492700	0.66275800
C	0.75392900	-2.25048700	-0.43155400
H	0.17482600	-2.01225100	-1.32435700
N	1.50846400	-3.53168100	-0.65845100
H	1.34026600	-3.95184900	-1.56895200
H	1.34225700	-4.23208200	0.06110100
C	1.91002700	-1.21592900	-0.30198700
O	3.06225000	-1.76850600	-0.37993400
O	1.67053300	-0.01325300	-0.15557500
H	2.95442900	0.98350100	-0.15331800
N	3.79036900	1.64192400	-0.17144200
C	4.46213800	1.44978300	-1.49241800
H	4.75019500	0.40397800	-1.58571300
H	3.76191400	1.71083300	-2.28455300
H	5.34202500	2.09104400	-1.54821800
C	3.26686400	3.03125500	-0.00764700
H	2.57756100	3.24663200	-0.82258200
H	2.73846100	3.09913800	0.94194700
H	4.09726900	3.73753500	-0.02418000
C	4.68102300	1.24043600	0.95910100
H	4.13698700	1.35950900	1.89492600
H	4.95900800	0.19610100	0.82674200
H	5.56948300	1.87224200	0.96315700
H	2.59056800	-2.96616200	-0.56461800

Transition State 16 – Dihedral Rotation

C	2.00249800	2.05907700	-0.21147100
C	3.35263600	2.18868800	-0.53259800
C	4.20480800	1.09446600	-0.43233600
C	3.69015200	-0.12952600	-0.00827500
C	4.58384600	-1.34540400	0.04531700
C	2.33978900	-0.25855400	0.30813000
C	1.47490300	0.83530100	0.21337300
H	1.37535500	2.93983400	-0.30310800
H	3.74094200	3.14587700	-0.85914100
H	5.25500000	1.19062200	-0.67602600
F	4.56577200	-2.01681700	-1.13065500
F	4.19124200	-2.21667600	0.99972000
F	5.86570400	-1.01830200	0.29535300
H	1.96013500	-1.21977300	0.63433100
C	0.02138000	0.63635000	0.61056400
H	-0.23738700	-0.41621600	0.48287600
H	-0.11258100	0.84316300	1.68226100
C	-1.03227900	1.41314800	-0.17897200
H	-0.78012000	1.43698500	-1.24031300
N	-1.20383800	2.85322000	0.28477200
H	-0.68205600	3.06378200	1.13577100
H	-0.97033000	3.54657500	-0.42438800
C	-2.47193600	0.81803900	-0.03230900
O	-2.60781000	-0.38776400	-0.32106200
O	-3.34789500	1.63252800	0.35214100
H	-2.26139000	2.84523200	0.48006400
N	-5.16047500	-1.17270400	-0.12160700
C	-5.57538400	-0.88907300	1.28527100
H	-4.97625200	-1.50034500	1.95875200
H	-5.39598100	0.16527300	1.48850800
H	-6.63194100	-1.12890300	1.40756000
C	-5.91842900	-0.32820800	-1.09293100
H	-5.73911700	0.71770500	-0.84962500
H	-5.55824300	-0.53933500	-2.09881800
H	-6.98179100	-0.55904000	-1.02335700
C	-5.25081400	-2.62514400	-0.45187500
H	-4.88134500	-2.78096900	-1.46435200
H	-4.63543400	-3.18628900	0.24974400
H	-6.28859900	-2.95181000	-0.37996100
H	-4.13449700	-0.88290500	-0.20266100

Transition State 17 – Dihedral Rotation

C	0.73630200	1.51355800	1.19744000
C	1.57729800	0.85136100	2.09116200
C	2.60981800	0.04769700	1.62137500
C	2.78938200	-0.08725100	0.24560600
C	3.85471200	-1.01145200	-0.29216300
C	1.95087500	0.57684300	-0.64618600
C	0.91196400	1.39113500	-0.18540300
H	-0.06678500	2.10758300	1.61825100
H	1.42587400	0.96595900	3.15783300
H	3.26882300	-0.46312600	2.31154600
F	3.35010100	-2.24916900	-0.52884100
F	4.87795300	-1.16117600	0.56878600
F	4.36378700	-0.56854400	-1.46051800
H	2.11147200	0.46029200	-1.71175200
C	0.08061500	2.12606400	-1.22656400
H	0.55902600	3.08169500	-1.47897700
H	0.09863000	1.54149500	-2.14813600
C	-1.40285700	2.38268900	-0.94217100
H	-1.88298700	2.69720900	-1.86965400
N	-1.66525400	3.48591100	0.07699800
H	-2.16390500	4.28394200	-0.31509300
H	-0.82107400	3.82506300	0.53753900
C	-2.19483600	1.16018100	-0.38560000
O	-2.13586100	0.11609800	-1.06604700
O	-2.82039400	1.37020800	0.68194000
H	-2.29323600	2.94908200	0.75952400
N	-3.47994100	-1.91617900	0.01641700
C	-2.88892800	-2.13133800	1.37082600
H	-1.84256500	-2.41131700	1.25785400
H	-2.96129300	-1.19890100	1.92804800
H	-3.43301500	-2.92524400	1.88341500
C	-4.90355900	-1.47456300	0.10688200
H	-4.93953100	-0.55001500	0.68083700
H	-5.28150400	-1.29706800	-0.89900000
H	-5.49535100	-2.24994800	0.59430300
C	-3.31715400	-3.11066400	-0.86259500
H	-3.70989300	-2.87749300	-1.85119800
H	-2.25779200	-3.35068000	-0.94028300
H	-3.85992400	-3.95513400	-0.43662400
H	-2.93693000	-1.10752000	-0.42998800

Transition State 18 – Dihedral Rotation

C	1.57845900	1.99625200	-0.78623500
C	2.93581400	2.28162400	-0.66477700
C	3.83887200	1.27595100	-0.32963400
C	3.37034600	-0.01927300	-0.11856400
C	4.33542500	-1.13784000	0.18339800
C	2.01162900	-0.30697600	-0.24354600
C	1.10114200	0.69915300	-0.57183800
H	0.88612500	2.78898300	-1.04661400
H	3.29309700	3.29022900	-0.83420200
H	4.89451300	1.49452000	-0.23265200
F	3.78802000	-2.06065400	1.01130000
F	5.46445700	-0.69377400	0.76538600
F	4.69872700	-1.79681600	-0.94259500
H	1.67047300	-1.32472900	-0.08815500
C	-0.37572200	0.38088100	-0.66948500
H	-0.84118600	1.01688400	-1.42642500
H	-0.50284200	-0.64816400	-1.01841800
C	-1.14609700	0.51158800	0.69139000
H	-0.41699200	0.72932100	1.47719800
N	-1.91267400	-0.72008600	0.98562800
H	-2.19096800	-0.71163700	1.96591200
H	-1.29043400	-1.51926900	0.88859900
C	-2.11917800	1.68019500	0.63725200
O	-3.31888500	1.57363000	0.50371200
O	-1.48602300	2.85326800	0.72473900
H	-2.13691700	3.57102600	0.66119600
N	-4.55903400	-1.11909700	-0.25693700
C	-4.55690800	-2.60481000	-0.42690500
H	-3.76569400	-2.88228400	-1.12175500
H	-4.38046100	-3.07367000	0.54002200
H	-5.52196100	-2.92337000	-0.82008800
C	-5.59116800	-0.67872600	0.73506300
H	-5.41623100	-1.19389500	1.67868100
H	-5.49718500	0.39506900	0.87513200
H	-6.58029500	-0.93367800	0.35496700
C	-4.73191600	-0.41773500	-1.56801600
H	-4.68754700	0.65429600	-1.39405500
H	-3.92921700	-0.72079100	-2.23907600
H	-5.69470900	-0.69765100	-1.99532900
H	-3.61537700	-0.85260700	0.13117400

Transition State 19 – Dihedral Rotation

C	-1.14560100	1.52519400	0.98076700
C	-2.38856200	2.08038500	1.27353200
C	-3.55068100	1.51322500	0.75827600
C	-3.45321600	0.38367000	-0.05040000
C	-4.70281700	-0.28455200	-0.57008500
C	-2.20875200	-0.17535200	-0.33809300
C	-1.03689800	0.38931800	0.16977000
H	-0.26348600	1.99587500	1.40259600
H	-2.45242400	2.96019500	1.90250500
H	-4.51829900	1.94553300	0.97825100
F	-4.49383100	-0.88105700	-1.76455200
F	-5.71608600	0.58898100	-0.72445000
F	-5.13356400	-1.24800300	0.27857400
H	-2.15601000	-1.05607700	-0.96742500
C	0.29533100	-0.23735000	-0.20532100
H	0.09083000	-1.21011700	-0.65482200
H	0.79103100	0.35756400	-0.98302300
C	1.30586200	-0.42189800	0.96128200
H	0.73964000	-0.53950000	1.89072300
N	2.26080300	0.70709200	1.03231900
H	1.75896300	1.57956800	0.89517200
H	2.65597100	0.76022100	1.96941600
C	2.09589700	-1.71032700	0.75891300
O	3.24071900	-1.76753700	0.36565000
O	1.35835700	-2.78383100	1.05182900
H	1.87828800	-3.58675300	0.88636400
N	4.72965300	0.63424500	-0.63504600
C	4.56857800	-0.06945600	-1.94690900
H	4.38728400	-1.12316000	-1.75241900
H	3.72135200	0.36311300	-2.47736700
H	5.47746700	0.06315700	-2.53361000
C	4.91644500	2.10580300	-0.82310900
H	4.06682400	2.50454100	-1.37539600
H	4.98033500	2.58466000	0.15284200
H	5.83520500	2.28310400	-1.38137100
C	5.84228400	0.03553700	0.16939300
H	5.90598100	0.55457200	1.12482800
H	5.62122400	-1.01590200	0.33293900
H	6.77786200	0.15353600	-0.37704400
H	3.84025900	0.50298400	-0.08814800

Transition State 20 – Dihedral Rotation

C	1.15020700	-1.53603800	0.98377300
C	2.39778700	-2.07203200	1.29191000
C	3.55802600	-1.47881600	0.80197300
C	3.45414000	-0.34015000	0.00706000
C	4.69465200	0.29027300	-0.57753700
C	2.20476200	0.19930800	-0.29644200
C	1.03514400	-0.39133600	0.18611200
H	0.26910700	-2.02633000	1.38522100
H	2.46724500	-2.95531600	1.91539000
H	4.52987700	-1.89056600	1.04204000
F	5.77645800	0.09655900	0.20064900
F	4.54892200	1.62259600	-0.74850100
F	4.98136600	-0.23161300	-1.79432200
H	2.14776100	1.09346700	-0.90601500
C	-0.30234500	0.21958200	-0.19451700
H	-0.10685300	1.18739200	-0.65846700
H	-0.79572600	-0.39035000	-0.96178900
C	-1.31069700	0.41158000	0.97404600
H	-0.74247000	0.52618200	1.90256100
N	-2.27210700	-0.71175300	1.04661500
H	-1.77264800	-1.58799100	0.92482200
H	-2.67728600	-0.75285000	1.98010200
C	-2.09358300	1.70418200	0.77246400
O	-3.23820300	1.76782500	0.37958200
O	-1.34976900	2.77338200	1.06530900
H	-1.86512900	3.57933300	0.90024700
N	-4.72120300	-0.63127800	-0.64883400
C	-4.54687200	0.08580200	-1.95177100
H	-5.44992800	-0.04052100	-2.54878700
H	-4.36729500	1.13737900	-1.74473500
H	-3.69458900	-0.34168700	-2.47823600
C	-5.84061400	-0.03929700	0.15117700
H	-5.61944800	1.01000800	0.32792900
H	-6.77106200	-0.14983800	-0.40548700
H	-5.91439700	-0.56838200	1.10035500
C	-4.90825300	-2.10049600	-0.85439300
H	-4.98430600	-2.58949600	0.11562400
H	-5.82073700	-2.27011400	-1.42521000
H	-4.05295500	-2.49489600	-1.40101500
H	-3.83705800	-0.50710800	-0.09168900

Transition State 21 – Dihedral Rotation

C	1.09934100	-1.53806300	0.19278500
C	2.22670700	-2.28524900	0.52975700
C	3.49340300	-1.71655800	0.45841500
C	3.61698600	-0.38855900	0.05368400
C	4.98559500	0.23486200	-0.07573400
C	2.48882300	0.35839700	-0.27682400
C	1.21027600	-0.20480600	-0.21450600
H	0.13242000	-2.02393500	0.25991100
H	2.11615100	-3.31478300	0.84863300
H	4.37145300	-2.29152300	0.72310000
F	4.95462800	1.56836800	0.13621500
F	5.49476400	0.04610500	-1.31640800
F	5.86550400	-0.29418200	0.79686600
H	2.60817400	1.39345700	-0.57498900
C	0.02981300	0.66513700	-0.61745700
H	0.31956000	1.70501100	-0.46622300
H	-0.15791300	0.55861500	-1.69447200
C	-1.30918200	0.41366400	0.12448600
H	-1.08510800	0.12611200	1.15765600
N	-2.16662000	-0.64211000	-0.45875600
H	-2.14107000	-0.56062900	-1.47427500
H	-1.76542800	-1.55157600	-0.25131200
C	-2.14433100	1.69059700	0.23886900
O	-3.31467800	1.77603300	-0.06210800
O	-1.44181600	2.70549100	0.74914000
H	-2.01481300	3.48570400	0.82004400
N	-5.09588700	-0.64160500	-0.04596500
C	-5.74247400	0.06573100	-1.19692800
H	-6.82269100	-0.06443700	-1.13179400
H	-5.47644200	1.11830900	-1.14726600
H	-5.37560100	-0.36582500	-2.12722800
C	-5.53060600	-0.06014000	1.26324200
H	-5.29765600	1.00148000	1.26387300
H	-6.60265200	-0.21704500	1.38250200
H	-4.99325100	-0.56078600	2.06770400
C	-5.34172500	-2.11553700	-0.09753000
H	-4.82113100	-2.59244200	0.73161700
H	-6.41187400	-2.30508600	-0.01895600
H	-4.96749600	-2.50627200	-1.04265800
H	-4.05495300	-0.50002100	-0.13269400

Transition State 22 – COOH Rotation

C	-2.01775500	2.22896200	-0.85085800
C	-2.90937100	1.57262000	-1.69433900
C	-3.37007000	0.29565900	-1.37941900
C	-2.94981600	-0.30387100	-0.19584800
C	-3.40381500	-1.69681000	0.16151000
C	-2.06456500	0.35997200	0.65498800
C	-1.56186900	1.62260100	0.32928000
H	-1.70253800	3.23712000	-1.09443300
H	-3.25961400	2.06270100	-2.59488500
H	-4.06756600	-0.21447100	-2.03118900
F	-3.57371200	-1.84401400	1.49395100
F	-4.55708800	-2.03286300	-0.43830700
F	-2.47597600	-2.61856600	-0.21270200
H	-1.81737800	-0.10444400	1.60653700
C	-0.57279400	2.31702500	1.24264000
H	-0.87463000	3.35825400	1.38549200
H	-0.61156600	1.86940900	2.24329200
C	0.91271100	2.37929300	0.75558700
H	1.46514600	2.87449000	1.56581500
N	1.17825000	3.13975100	-0.44826000
H	1.05625500	4.13437200	-0.30597100
H	0.61624900	2.84223800	-1.23700300
C	1.64873600	1.02734400	0.64858100
O	1.11205600	-0.06489300	1.20733700
O	2.74327600	0.92348300	0.13289000
H	3.74731000	-0.41604300	-0.10239400
N	4.43985700	-1.17029400	-0.33130200
C	4.62060100	-1.99823700	0.90179400
H	5.00126600	-1.36326200	1.70022600
H	3.65669500	-2.41389300	1.19098400
H	5.32809900	-2.80105400	0.69495800
C	3.85773300	-1.96959800	-1.45464200
H	2.91005100	-2.39572300	-1.12916000
H	3.69279900	-1.31112600	-2.30588200
H	4.55110300	-2.76517900	-1.72674500
C	5.70827000	-0.48523600	-0.73520100
H	6.05794000	0.12523700	0.09554200
H	5.50533700	0.15096200	-1.59486100
H	6.45621100	-1.23594600	-0.98992000
H	0.19244100	0.07208500	1.47379500

Transition State 23 – COO^- Rotation

C	-0.82354000	-0.12130100	1.94872300
C	-1.61368900	1.00852600	2.14675000
C	-2.69225200	1.26991100	1.30574200
C	-2.98068200	0.38436000	0.26865900
C	-4.11102800	0.67231200	-0.68699100
C	-2.19712300	-0.75184300	0.07313600
C	-1.11044700	-1.01229500	0.90992200
H	0.01758800	-0.31798700	2.60323900
H	-1.39467400	1.68394200	2.96521500
H	-3.31290700	2.14300000	1.46169100
F	-4.70877300	-0.46206700	-1.11548300
F	-3.66282900	1.31612500	-1.79502600
F	-5.06081900	1.44992100	-0.13685400
H	-2.45491400	-1.44148600	-0.72337400
C	-0.25865400	-2.24855500	0.68953000
H	0.28247600	-2.49377100	1.60681600
H	-0.91135100	-3.09471700	0.44071600
C	0.75171500	-2.03507800	-0.43504800
H	0.27949700	-1.73090500	-1.36880600
N	1.44815800	-3.36964400	-0.74823800
H	0.78360900	-4.10777900	-0.99589200
H	2.10506200	-3.24237300	-1.52441200
C	1.94363700	-1.07673500	-0.10720900
O	2.42328500	-0.49626200	-1.12495500
O	2.33984100	-1.04666900	1.06272100
H	1.98027100	-3.67499100	0.07377200
N	4.18786200	1.33854900	-0.34533500
C	3.40377600	2.23818100	0.55227700
H	2.60226500	2.69850600	-0.02372400
H	2.98127000	1.63474900	1.35378100
H	4.05980400	3.00874800	0.95862000
C	5.26665800	0.63112800	0.40584700
H	4.80029000	0.04155700	1.19343600
H	5.79960000	-0.02638600	-0.27995300
H	5.95738700	1.36184400	0.82801700
C	4.71260200	2.05966900	-1.53992800
H	5.22069400	1.34738100	-2.18859100
H	3.87842800	2.50844100	-2.07735900
H	5.41107600	2.83498600	-1.22303200
H	3.50333100	0.58287400	-0.68947000

Transition State 24 – COOH Rotation

C	1.59601100	-1.69748300	1.89536700
C	2.69422200	-0.95510500	2.32405000
C	3.32714400	-0.06894900	1.45513600
C	2.85880900	0.04937300	0.14841700
C	3.47541600	1.03083600	-0.81528400
C	1.77573400	-0.71402500	-0.28919200
C	1.12092800	-1.58877800	0.58220700
H	1.11394500	-2.38479200	2.58282100
H	3.05920500	-1.06706900	3.33802200
H	4.17617800	0.51520500	1.78524400
F	4.59209900	1.60064600	-0.33762900
F	2.59987100	2.04205600	-1.09580600
F	3.77884100	0.45632800	-1.99730800
H	1.45955800	-0.63222700	-1.32396000
C	-0.07735900	-2.39373300	0.11856500
H	0.20491500	-3.08354100	-0.68126000
H	-0.45056300	-3.01739300	0.93529700
C	-1.21992700	-1.50761500	-0.40573200
H	-0.87300700	-0.96664400	-1.29360900
N	-1.67234100	-0.46110400	0.56802700
H	-0.82337900	-0.00247300	0.90353300
H	-2.04826800	-0.93602000	1.39014900
C	-2.42301800	-2.35209400	-0.86398800
O	-2.40580500	-3.53809400	-0.98427000
O	-3.53816000	-1.62441300	-1.15157000
H	-3.32612600	-0.69790200	-0.98999100
N	-3.26578200	2.02785100	0.35281900
C	-4.56460300	1.74304100	-0.34120600
H	-4.36773200	1.50085200	-1.38525100
H	-5.05838300	0.90640900	0.15160900
H	-5.19701100	2.62876600	-0.28946200
C	-3.48609500	2.40719700	1.78664800
H	-4.05555200	3.33529400	1.82618700
H	-4.04069600	1.61217500	2.28296900
H	-2.52011000	2.54620400	2.26985700
C	-2.46666000	3.06597900	-0.37651800
H	-1.52192600	3.21846300	0.14315000
H	-2.27785600	2.72249400	-1.39247600
H	-3.03133200	3.99760800	-0.40073800
H	-2.70418400	1.13427100	0.35456800