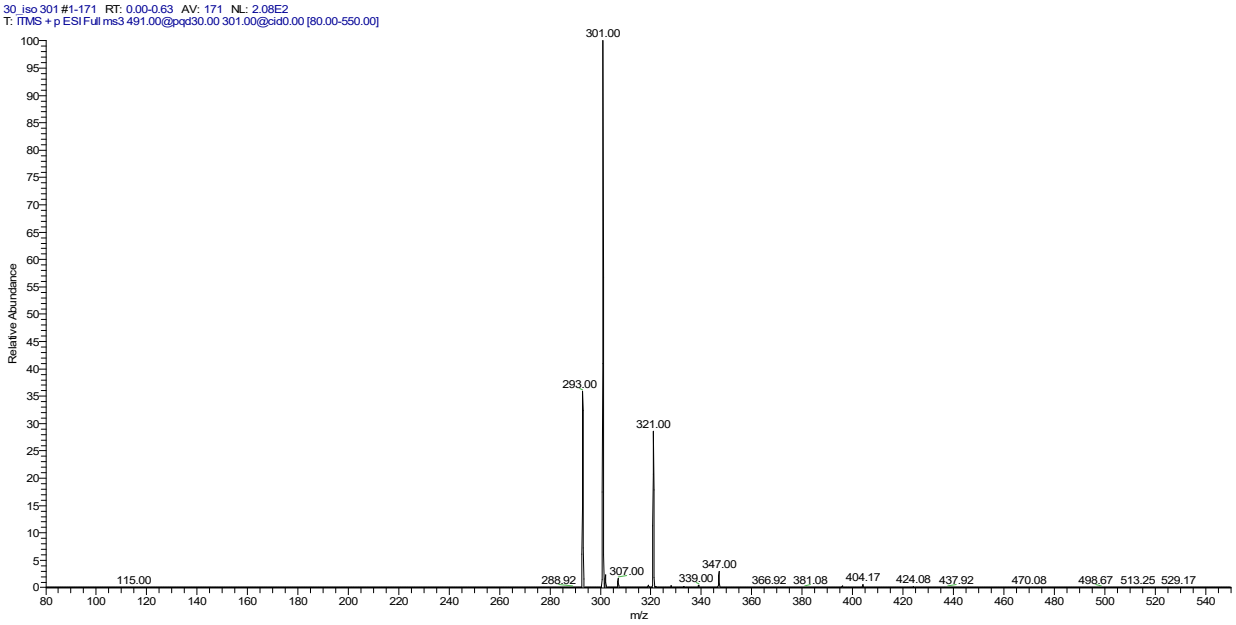
Experimental and Computational Investigation of the Intrinsic Reactions of $[U^{IV}F_2(C{\equiv}CH)]^+$: Formation of $[U^{IV}F_2(O_2CR)]^+$, $[U^{IV}F(O_2CR)_2]^+$, & $[U^{IV}(O_2CR)_3]^+$ by Reactions with Carboxylic Acids

Supporting Information

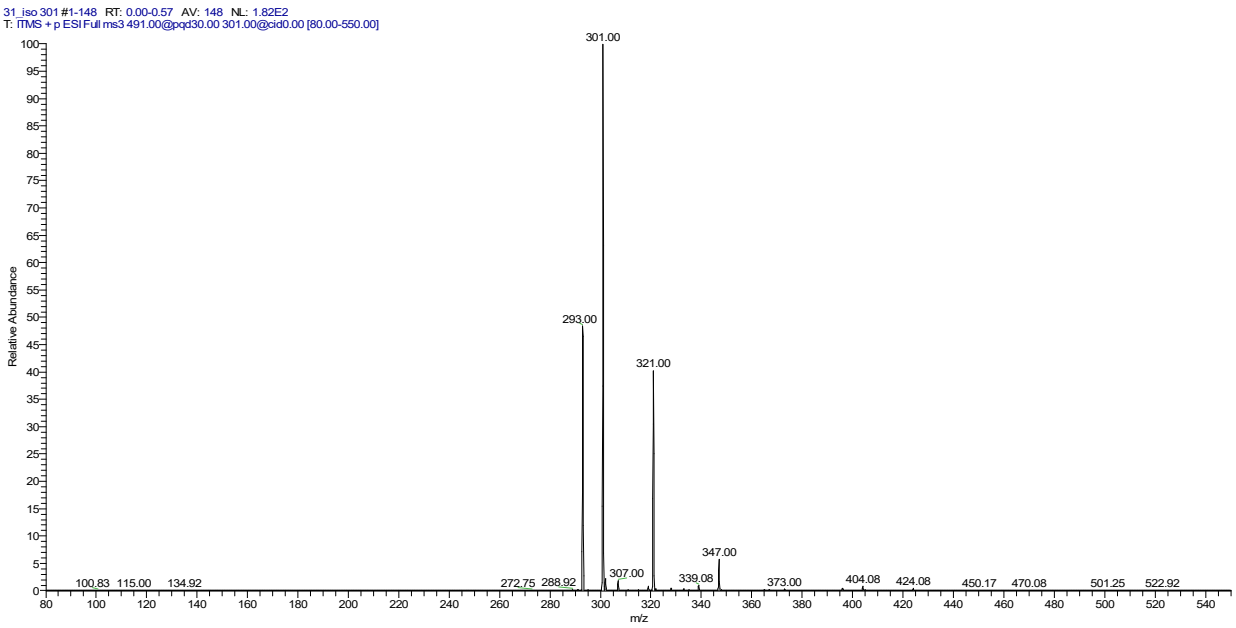
Table of Contents

Isolations of $[UF_2(C{\equiv}CH)]^+$ in the presence of formic acid (1, 10, 100, 1000 ms)

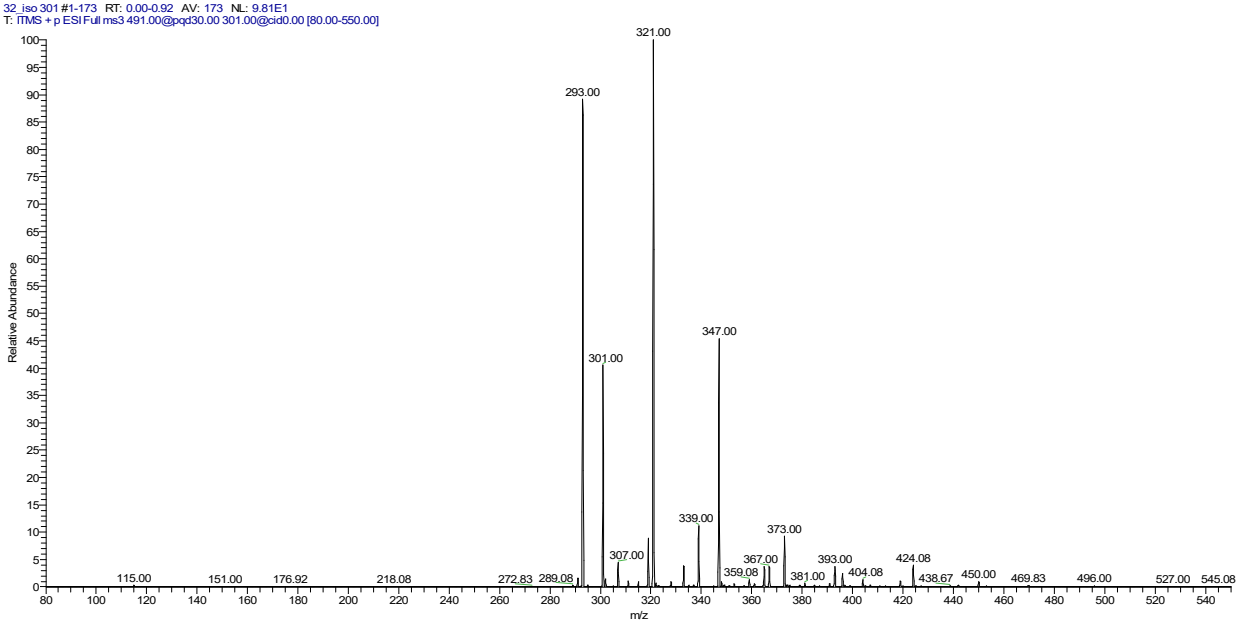
1ms



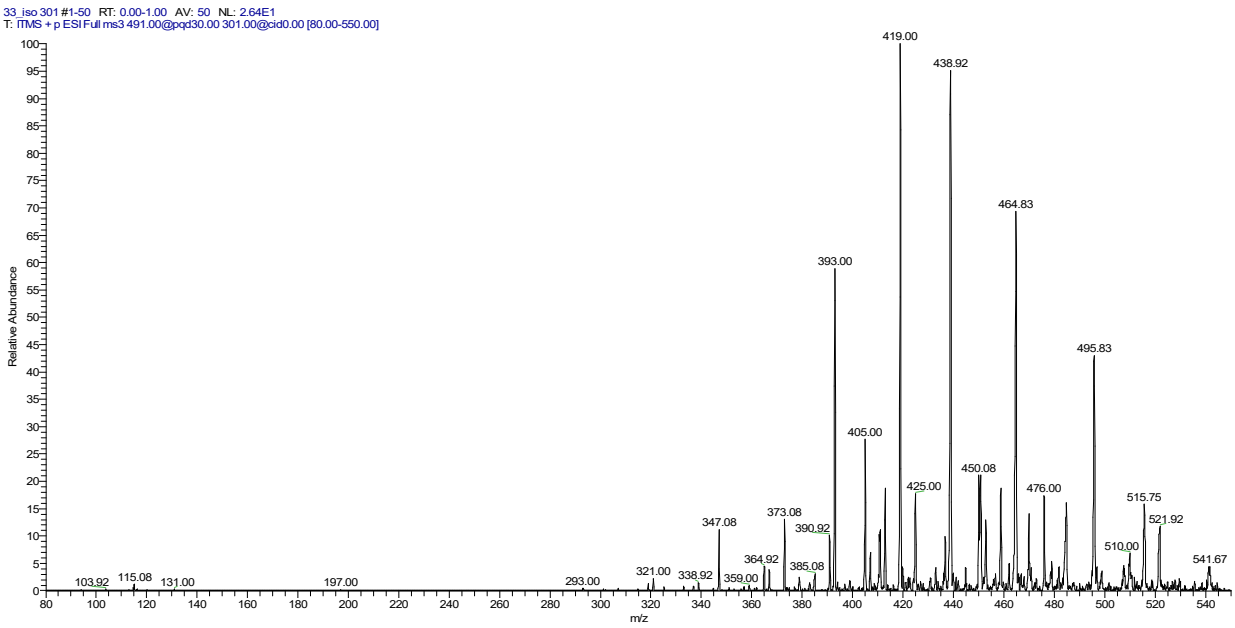
10 ms


31_iso 301 #1-148 RT: 0.00-0.57 AV: 148 NL: 1.82E2
T: ITMS + p ESI Full ms3 491.00@pqd30.00 301.00@cid0.00 [80.00-550.00]
Relative Abundance
m/z
301.00
293.00
321.00
347.00
307.00
100.83
115.00
134.92
272.75
288.92
339.08
373.00
404.08
424.08
450.17
470.08
501.25
522.92

100 ms


32_iso 301 #1-173 RT: 0.00-0.92 AV: 173 NL: 9.81E1
T: ITMS + p ESI Full ms3 491.00@pqd30.00 301.00@cid0.00 [80.00-550.00]
Relative Abundance
m/z
321.00
293.00
347.00
301.00
339.00
373.00
307.00
367.00
393.00
424.08
359.08
381.00
404.08
438.67
450.00
115.00
151.00
176.92
218.08
272.83
289.08
469.83
496.00
527.00
545.08

1000 ms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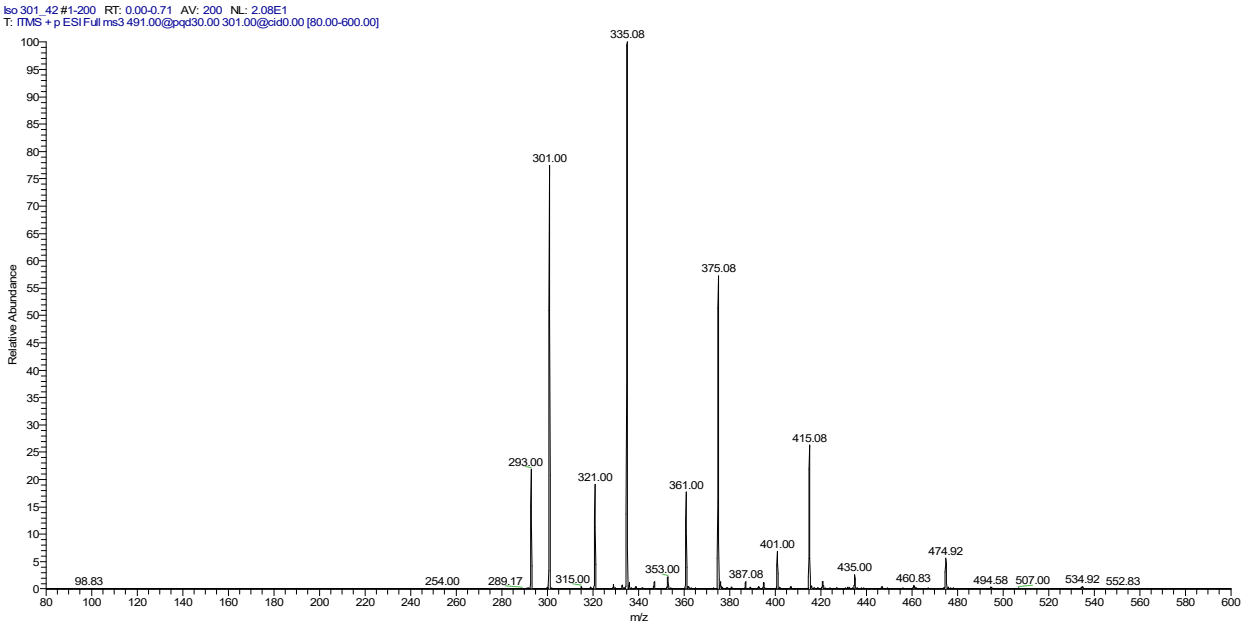
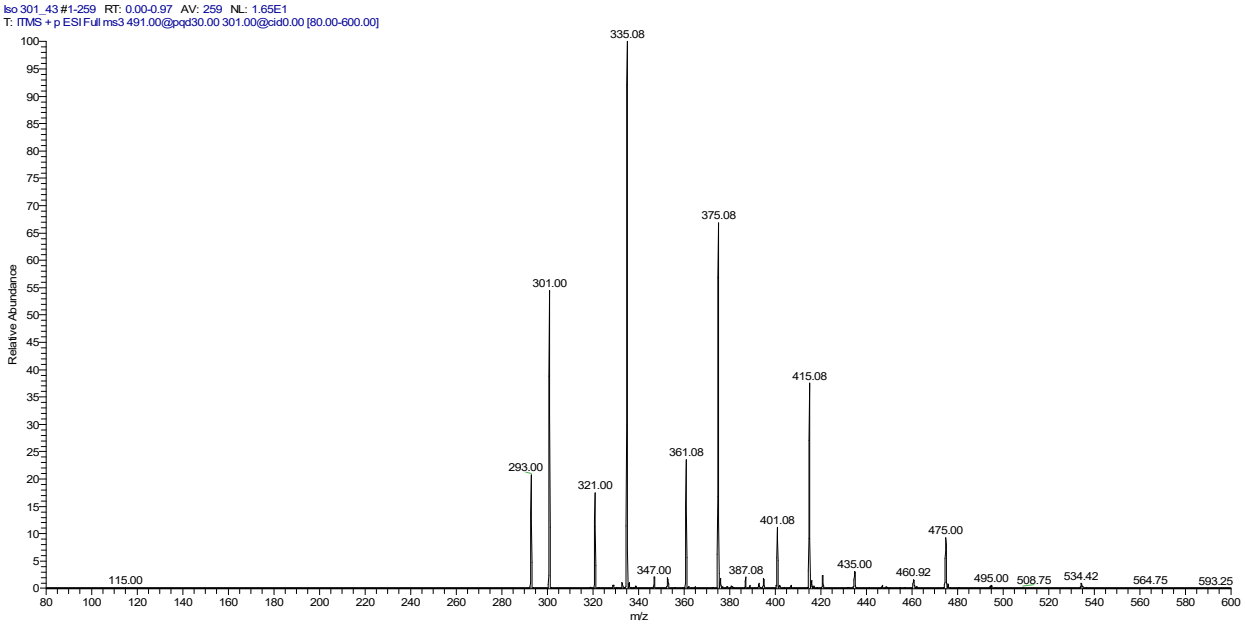
Relative Abundance
m/z
419.00
438.92
464.83
393.00
495.83
405.00
450.08
425.00
476.00
515.75
521.92
347.08
373.08
390.92
364.92
385.08
510.00
541.67
103.92
115.08
131.00
197.00
293.00
321.00
338.92
359.00

Isolations of $[UF_2(C{\equiv}CH)]^+$ in the presence of acetic acid (1, 10, 100, 1000 ms)

1 ms



10 ms


Iso 301_43 #1-259 RT: 0.00-0.97 AV: 259 NL: 1.65E1
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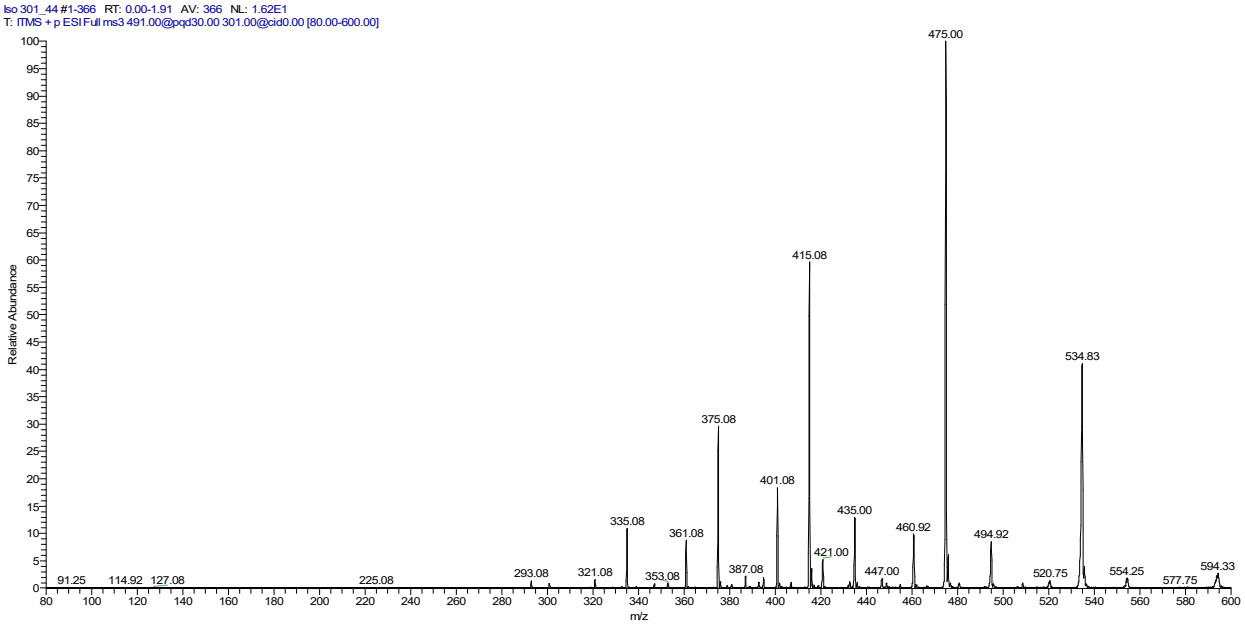
Relative Abundance
m/z
335.08
375.08
301.00
415.08
361.08
293.00
321.00
401.08
475.00
435.00
115.00
347.00
387.08
460.92
495.00
508.75
534.42
564.75
593.25

100 ms


Iso 301_44 #1-366 RT: 0.00-1.91 AV: 366 NL: 1.62E1
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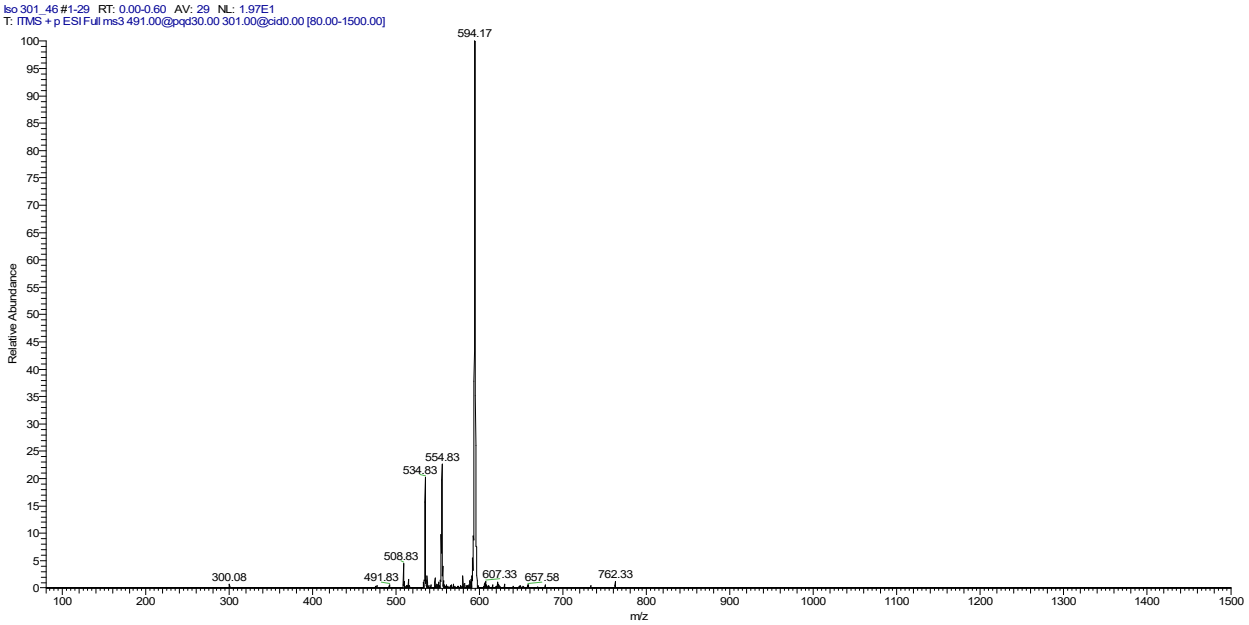
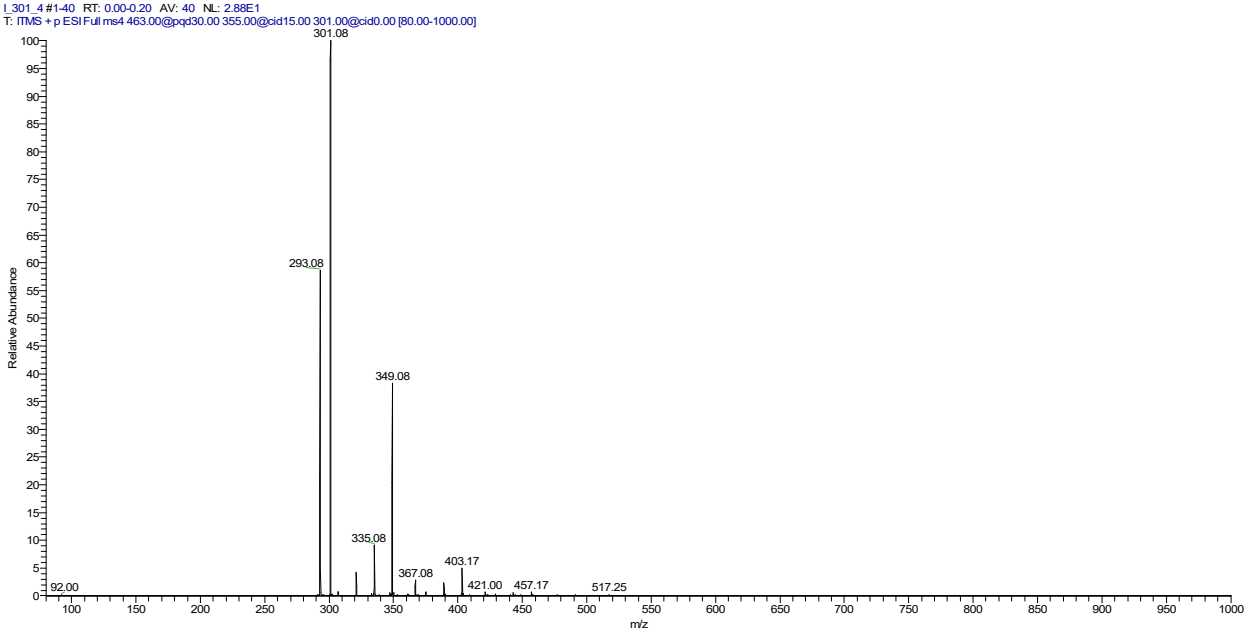
Relative Abundance
m/z
475.00
415.08
534.83
375.08
401.08
435.00
335.08
460.92
361.08
494.92
421.00
387.08
447.00
594.33
91.25
114.92
127.08
225.08
293.08
321.08
353.08
520.75
554.25
577.75

1000 ms

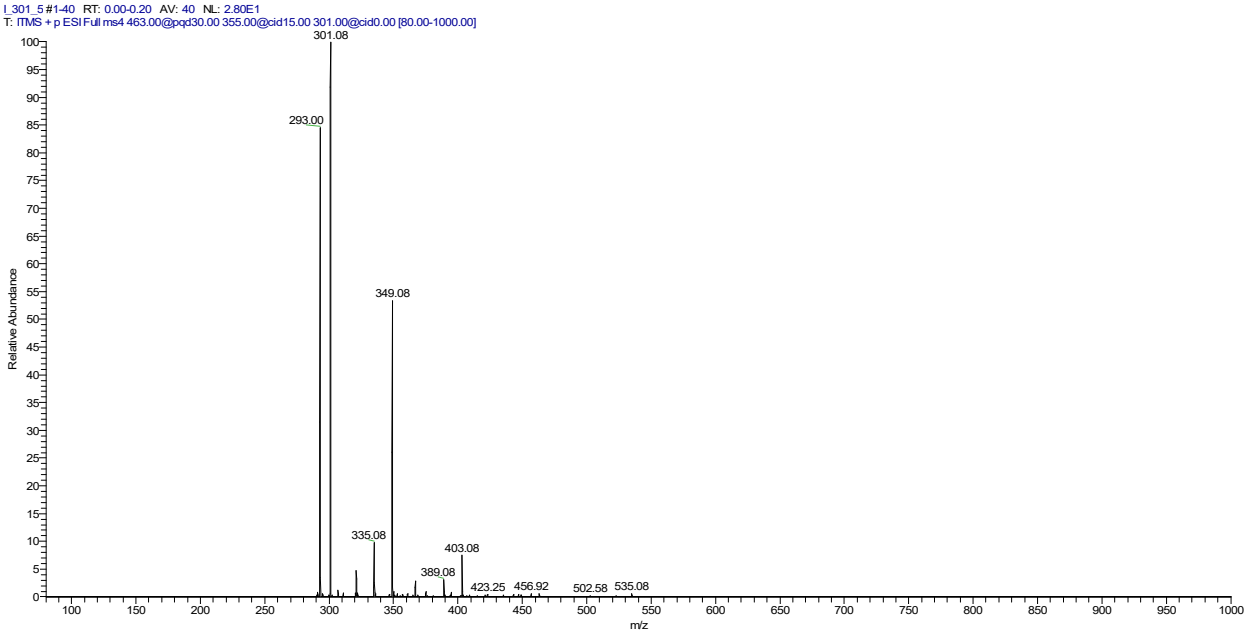


Isolations of $[UF_2(C{\equiv}CH)]^+$ in the presence of propionic acid (1, 10, 100, 1000 ms)

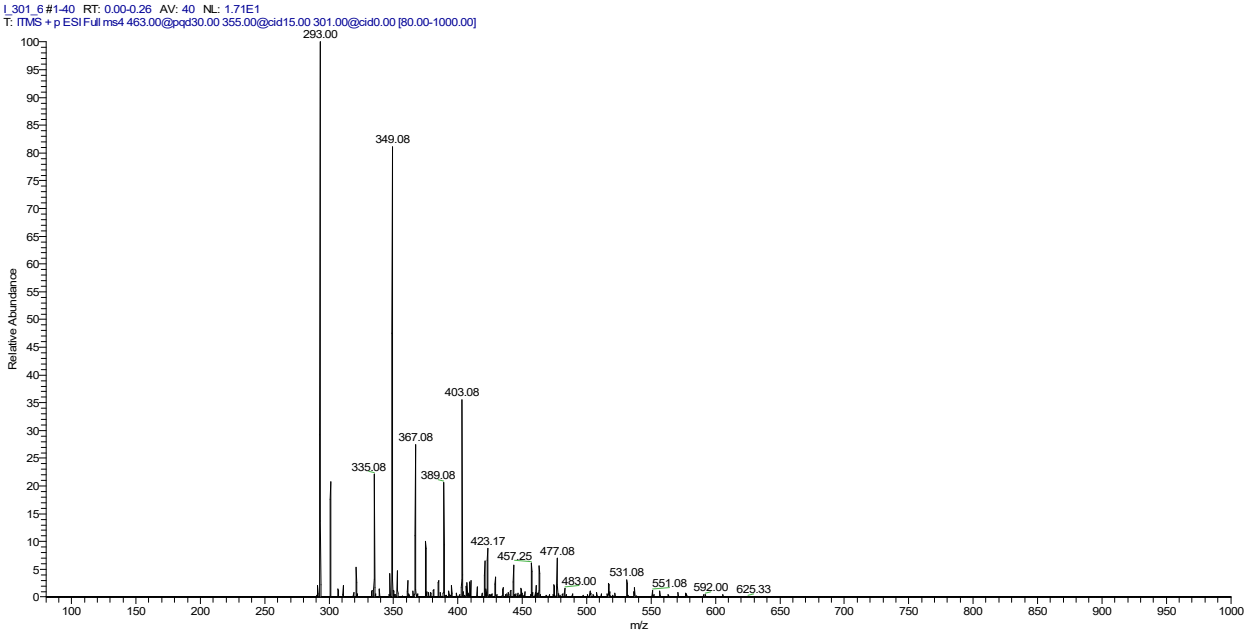
1 ms



10 ms


I_301_5 #1-40 RT: 0.00-0.20 AV: 40 NL: 2.80E1
T: ITMS + p ESI Full ms4 463.00@pqd30.00 355.00@cid15.00 301.00@cid0.00 [80.00-1000.00]
301.08
293.00
349.08
335.08
403.08
389.08
423.25
456.92
502.58
535.08
Relative Abundance
m/z

100 ms


I_301_6 #1-40 RT: 0.00-0.26 AV: 40 NL: 1.71E1
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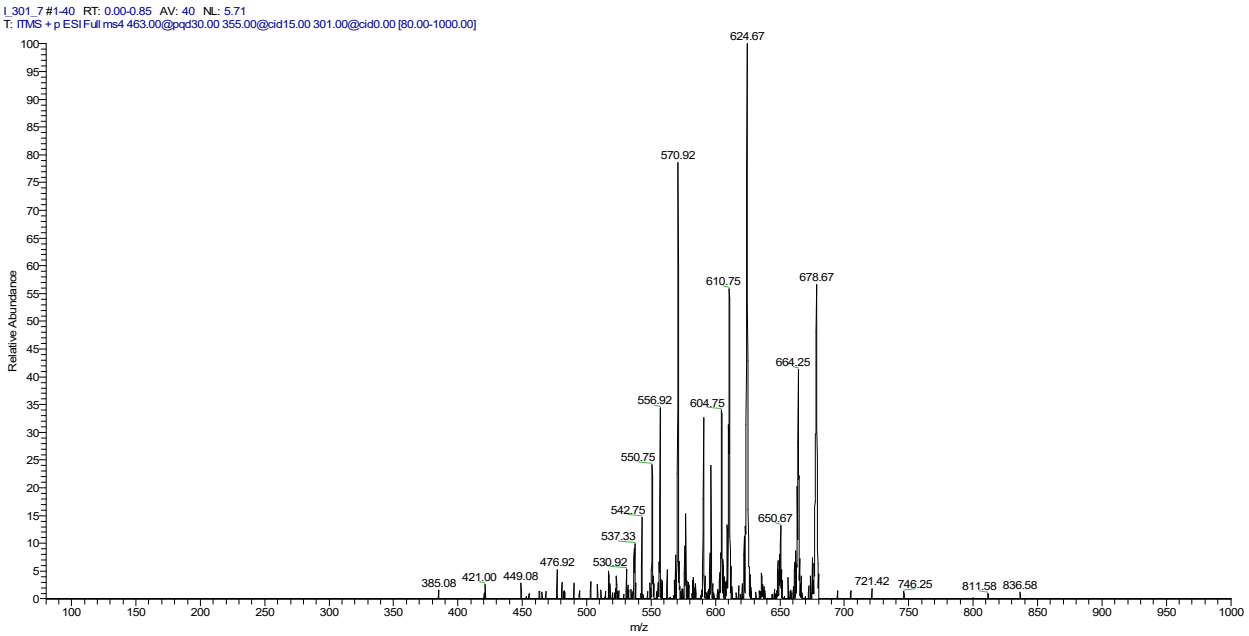
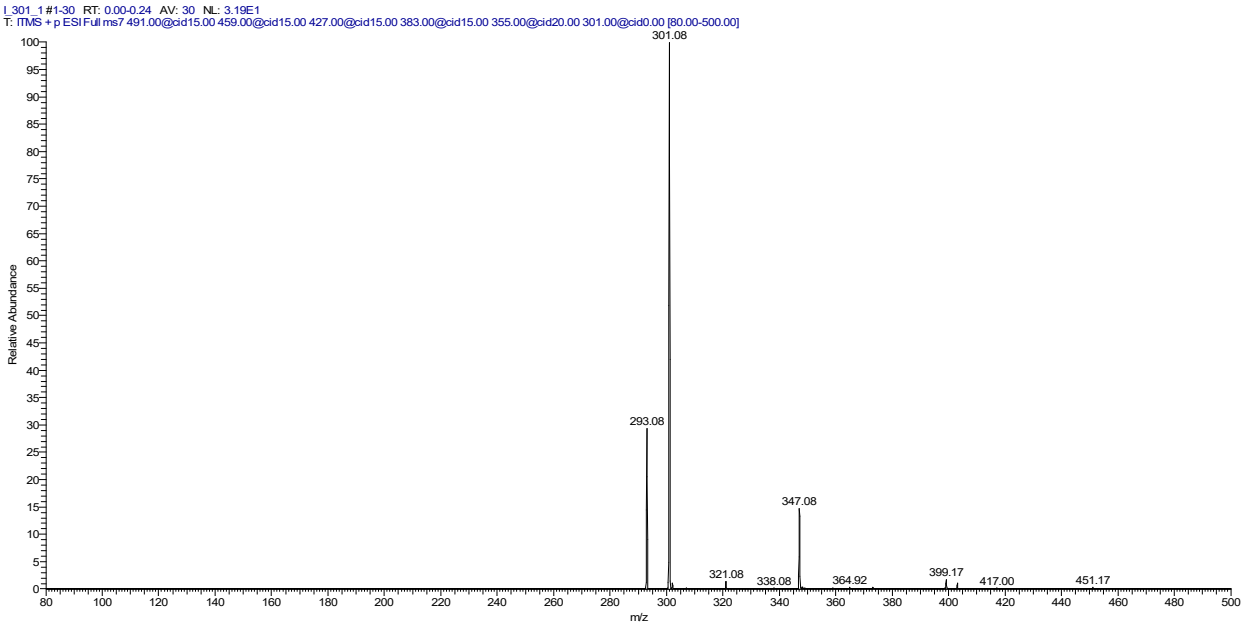
293.00
349.08
403.08
367.08
335.08
389.08
423.17
457.25
477.08
483.00
531.08
551.08
592.00
625.33
Relative Abundance
m/z

1000 ms

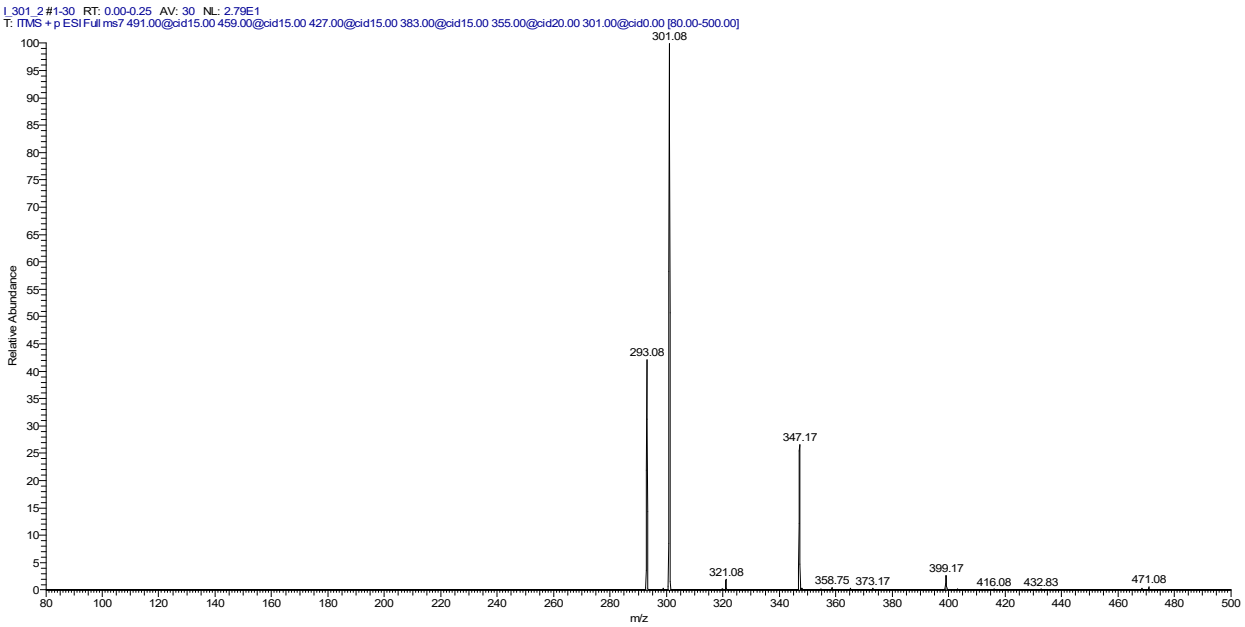


Isolations of $[UF_2(C{\equiv}CH)]^+$ in the presence of acrylic acid (1, 10, 100, 1000 ms)

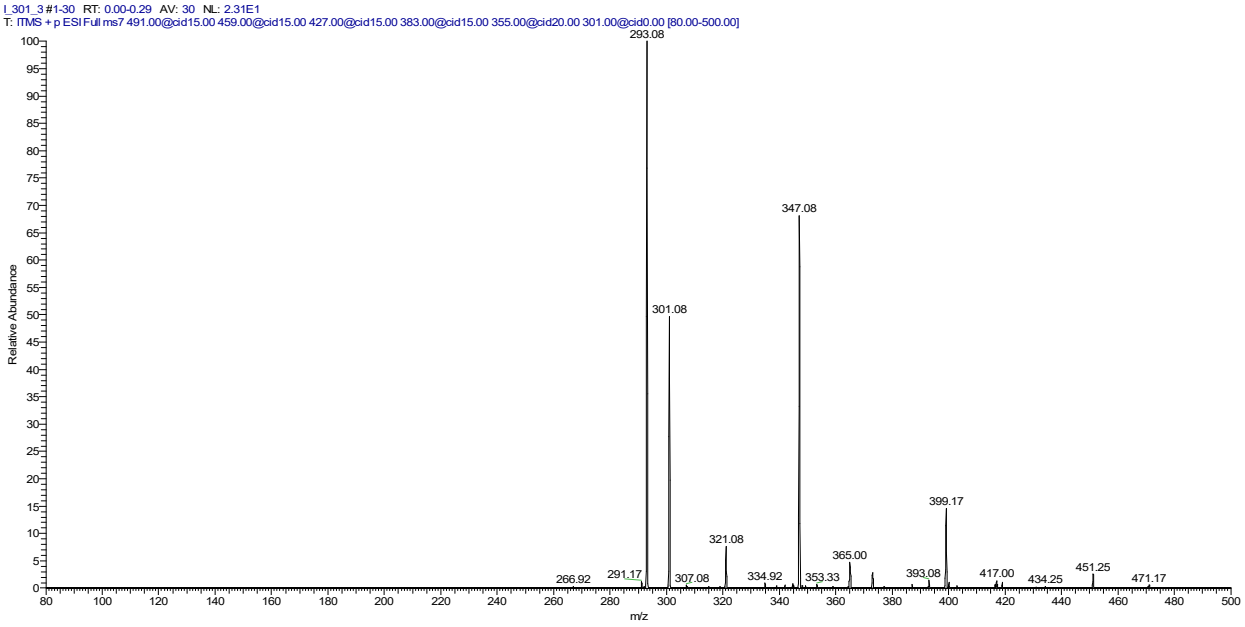
1 ms



10 ms



100 ms



1000 ms

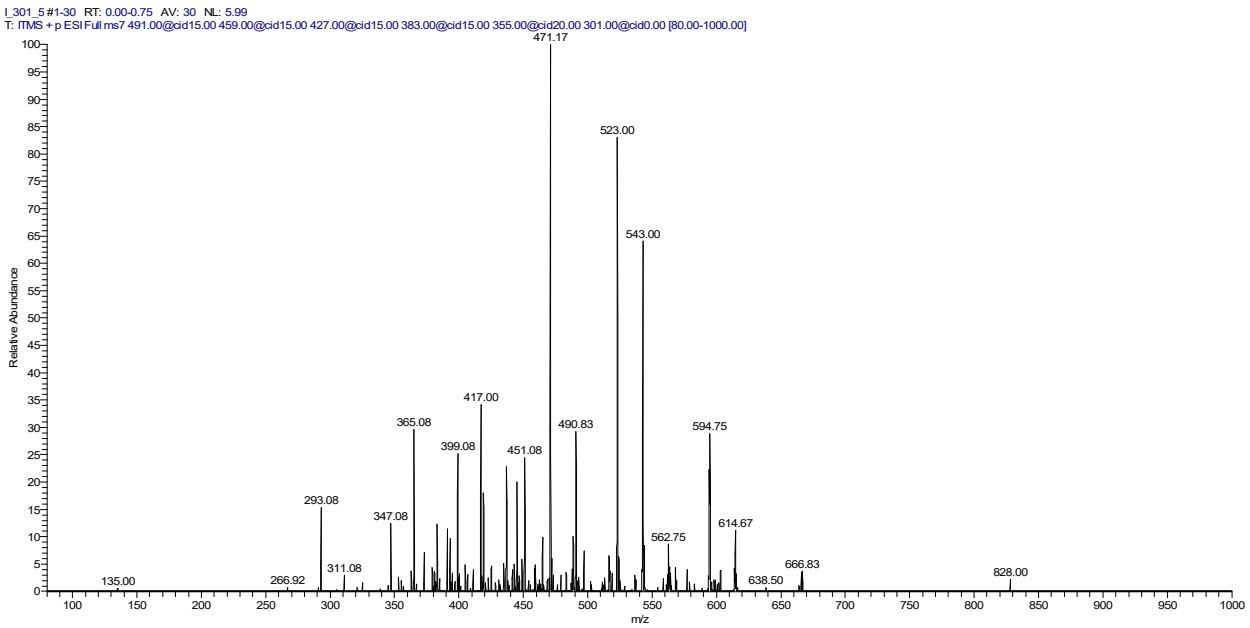


Table S1: Complete List of all Possible U Carboxylate Ions					
Difluoro-MonoCarboxo	***m/z***	**Isobaric ?**	**Monofluoro-Dicarboxo**	***m/z***	**Isobaric ?**
$[UF_2(O_2CH)]^+$	321		$[UF(O_2CH)_2]^+$	347	Yes
$[UF_2(O_2CCH_3)]^+$	335		$[UF(O_2CH)(O_2CCH_3)]^+$	361	
$[UF_2(O_2CCH_2CH_3)]^+$	349		$[UF(O_2CH)(O_2CCH_2CH_3)]^+$	375	Yes
$[UF_2(O_2CCHCH_2)]^+$	347	Yes	$[UF(O_2CH)(O_2CCHCH_2)]^+$	373	
			$[UF(O_2CCH_3)_2]^+$	375	Yes
			$[UF(O_2CCH_3)(O_2CCH_2CH_3)]^+$	389	
			$[UF(O_2CCH_3)(O_2CCHCH_2)]^+$	387	Yes
			$[UF(O_2CCH_2CH_3)_2]^+$	403	
			$[UF(O_2CCH_2CH_3)(O_2CCHCH_2)]^+$	401	Yes
			$[UF(O_2CCHCH_2)_2]^+$	399	Yes

Species	**Mass**
formate	45
acetate	59
propionate	73
acrylate	71
Uranium	238
Fluorine	19

Tricarboxo	***m/z***	**Isobaric ?**
$[U(O_2CH)_3]^+$	373	
$[U(O_2CH)_2(O_2CCH_3)]^+$	387	Yes

Species highlighted in red are not

observed

$[U(O_2CH)_2(O_2CCH_2CH_3)]^+$	401	Yes
$[U(O_2CH)_2(O_2CCHCH_2)]^+$	399	Yes
$[U(O_2CCH_3)_3]^+$	415	Yes
$[U(O_2CCH_3)_2(O_2CH)]^+$	401	Yes
$[U(O_2CCH_3)_2(O_2CCH_2CH_3)]^+$	429	Yes
$[U(O_2CCH_3)_2(O_2CCHCH_2)]^+$	427	Yes
$[U(O_2CCH_2CH_3)_3]^+$	457	
$[U(O_2CCH_2CH_3)_2(O_2CH)]^+$	429	Yes
$[U(O_2CCH_2CH_3)_2(O_2CCH_3)]^+$	443	
$[U(O_2CCH_2CH_3)_2(O_2CCHCH_2)]^+$	455	
$[U(O_2CCHCH_2)_3]^+$	451	
$[U(O_2CCHCH_2)_2(O_2CH)]^+$	425	
$[U(O_2CCHCH_2)_2(O_2CCH_3)]^+$	439	
$[U(O_2CCHCH_2)_2(O_2CCH_2CH_3)]^+$	453	
$[U(O_2CH)(O_2CCH_3)(O_2CCH_2CH_3)]^+$	415	Yes
$[U(O_2CH)(O_2CCH_3)(O_2CCHCH_2)]^+$	413	
$[U(O_2CH)(O_2CCHCH_2)(O_2CCH_2CH_3)]^+$	427	Yes
$[U(O_2CCH_3)(O_2CCH_2CH_3)(O_2CCHCH_2)]^+$	441	

Table S2.1

Reactions 1-3 Free Energy Values (kJ/mol)													
	I	II	TSI	III	IV	V	TSII	VI	VII	VIII	TSIII	IX	X
B3LYP	0.0	-147.5	-132.9	-232.4	-175.2	-313.6	-205.2	-243.6	-208.3	-324.7	-214.1	-240.4	-223.3
PBE0	0.0	-149.1	-149.9	-246.5	-181.0	-322.4	-222.0	-260.1	-223.9	-343.2	-238.2	-266.5	-248.8
M06L	0.0	-155.6	-146.3	-253.2	-181.6	-330.4	-237.8	-269.2	-223.0	-349.0	-246.8	-274.3	-241.4

Table S2.2

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acid → $[U(O_2CR)_3]^+$ + 2 eq. HF + HC≡CH

Free Energy (kJ/mol) All Three Functionals

Reactions 4-6 Free Energy Values (kJ/mol)													
	I	II	TSI	III	IV	V	TSII	VI	VII	VIII	TSIII	IX	X
B3LYP	0.0	-179.0	-162.6	-263.7	-213.1	-374.3	-274.2	-309.7	-285.2	-407.4	-313.5	-338.9	-323.8
PBE0	0.0	-184.7	-180.2	-276.9	-226.7	-383.9	-291.8	-326.5	-299.8	-425.9	-339.1	-363.9	-352.6
M06L	0.0	-151.5	-149.0	-265.8	-206.0	-354.1	-261.5	-295.2	-259.0	-370.4	-269.6	-313.8	-285.2

Table S2.3

Reactions 7-8 Free Energy Values (kJ/mol)													
	I	II	TSI	III	IV	V	TSII	VI	VII	VIII	TSIII	IX	X
B3LYP	0.0	-165.7	-148.3	-248.3	-201.4	-336.7	-245.8	-276.0	-249.5	-360.1	-262.1	-282.1	-276.9
PBE0	0.0	-178.1	-166.6	-261.7	-207.6	-348.0	-264.5	-292.9	-267.8	-381.0	-291.3	-309.3	-301.5
M06L	0.0	-166.9	-157.6	-270.1	-199.8	-362.2	-264.9	-304.2	-262.6	-388.7	-292.7	-318.0	-294.9

Table S2.4

Reactions 9-12 Free Energy Values (kJ/mol)													
	I	II	TSI	III	IV	V	TSII	VI	VII	VIII	TSIII	IX	X
B3LYP	0.0	-168.6	-145.7	-251.6	-208.0	-341.1	-253.3	-281.0	-256.7	-362.8	-266.0	-286.3	-281.0
PBE0	0.0	-177.3	-162.3	-263.6	-212.7	-349.6	-268.9	-295.2	-270.1	-380.6	-289.5	-310.5	-303.7
M06L	0.0	-183.5	-164.8	-273.4	-215.0	-367.3	-270.7	-307.5	-270.2	-393.1	-301.7	-324.6	-301.8

Comparisons of the Free Energies of All Structures at the Singlet and Triplet Spin States

Table S3 Electronic Energy + Free Energy Corrections (in Hartrees)				
		PBE0	B3LYP	M06L
$[UF_2C_2H]^+$	singlet	-750.793627	-751.18128	-751.16616
	triplet	-750.83850	-751.23769	-751.20871
	Diff.	0.04487	0.05641	0.04255
$[UF_2(formate)]^+$	singlet	-863.23366	-863.73314	-863.69200
	triplet	-863.27926	-863.77689	-863.73395
	Diff.	0.04559	0.04375	0.04195
$[UF(formate)_2]^+$	singlet	-952.47096	-953.07911	-953.02515
	triplet	-952.51699	-953.12123	-953.07036
	Diff.	0.04603	0.04211	0.04521
$[U(formate)_3]^+$	singlet	-1041.70196	-1042.41715	-1042.35813
	triplet	-1041.74789	-1042.45869	-1042.39802
	Diff.	0.04593	0.04154	0.03989
$[UF_2(acetate)]^+$	singlet	-902.51474	-903.06682	-903.01480
	triplet	-902.56038	-903.10495	-903.05697
	Diff.	0.04564	0.03814	0.04216
$[UF(acetate)_2]^+$	singlet	-1031.02796	-1031.73628	-1031.66798
	triplet	-1031.07336	-1031.77783	-1031.71148

	Diff.	0.04540	0.04155	0.04350
$[U(acetate)_3]^+$	singlet	-1159.53267	-1160.39805	-1160.31794
	triplet	-1159.57862	-1160.43790	-1160.35579
	Diff.	0.04594	0.03985	0.03785
$[UF_2(propionate)]^+$	singlet	-941.766855	-942.3682	-942.3104
	triplet	-941.8115	-942.4093	-942.3480
	Diff.	0.04466	0.04117	0.03758
$[UF(propionate)_2]^+$	singlet	-1109.5328	-1110.3414	-1110.2571
	triplet	-1109.5780	-1110.381857	-1110.2996
	Diff.	0.04513	0.04048	0.04245
$[U(propionate)_3]^+$	singlet	-1277.2890	-1278.3049	-1278.2000
	triplet	-1277.3344	-1278.3465	-1278.2396
	Diff.	0.04532	0.04158	0.03957
$[UF_2(acrylate)]^+$	singlet	-940.5548	-941.1564	-941.0990
	triplet	-940.6024	-941.1986	-941.1400
	Diff.	0.04759	0.04225	0.04097
$[UF(acrylate)_2]^+$	singlet	-1107.1117	-1107.9170	-1107.8318
	triplet	-1107.1567	-1107.958233	-1107.8750
	Diff.	0.04505	0.04123	0.04313
$[U(acrylate)_3]^+$	singlet	-1273.6564	-1274.6672	-1274.5603
	triplet	-1273.7020	-1274.7085	-1274.6009
	Diff.	0.04566	0.04132	0.04068

Table S4 Bond lengths and Mulliken Charges of U^{IV} Carboxylates

Table S4.1

B3LYP	**Bond Lengths Å**					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**
UF	**2.01**	**2.018/2.018**	**2.020/2.019**	**2.022**	**1.993**	**2.00**
UO	**2.305/2.304**	**2.292/2.266**	**2.275/2.272**	**2.276/2.261**	**NA**	**2.01**
OC	**1.278**	**1.295/1.288**	**1.295/1.293**	**1.302/1.296**	**NA**	**NA**
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
UF	**2.01**	**2.024**	**2.025**	**2.029**		
UO	**2.312**	**2.296**	**2.303/2.283 ***	**2.292/2.289***		
OC	**1.275**	**1.287/1.288**	**1.292/1.284***	**1.294/1.292**		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
UF	**NA**	**NA**	**NA**	**NA**		
UO	**2.333/2.308***	**2.326/2.297***	**2.316/2.305***	**2.312/2.302***		
OC	**1.278/1.270***	**1.290/1.280***	**1.284/1.290***	**1.292/1.289***		
	Mulliken Charges					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**

*** indicates that there are more than two values, so the highest and lowest are reported**

U	**1.61**	**1.591**	**1.587**	**1.584**	**1.426**	**1.683**
F1	**-0.289**	**-0.304**	**-0.308**	**-0.312**	**-0.275**	**-0.284**
F2	**-0.289**	**-0.304**	**-0.308**	**-0.312**	**-0.275**	**-0.284**
O1	**-0.288**	**-0.331**	**-0.347**	**-0.361**	**NA**	**-0.410**
O2	**-0.288**	**-0.328**	**-0.342**	**-0.368**	**NA**	**NA**
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
U	**1.398**	**1.378**	**1.386**	**1.374**		
F1	**-0.291**	**-0.315**	**-0.320**	**-0.326**		
O1	**-0.293**	**-0.343**	**-0.351**	**-0.377**		
O2	**-0.293**	**-0.343**	**-0.361**	**-0.383**		
O3	**-0.293**	**-0.344**	**-0.353**	**-0.377**		
O4	**-0.293**	**-0.345**	**-0.362**	**-0.384**		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
U	**1.283**	**1.231**	**1.223**	**1.209**		
O1	**-0.305**	**-0.362**	**-0.380**	**-0.398**		
O2	**-0.307**	**-0.370**	**-0.383**	**-0.399**		
O3	**-0.306**	**-0.365**	**-0.367**	**-0.398**		
O4	**-0.306**	**-0.366**	**-0.379**	**-0.401**		
O5	**-0.304**	**-0.363**	**-0.386**	**-0.400**		
O6	**-0.307**	**-0.369**	**-0.366**	**-0.402**		

Table S4.2

PBE0	**Bond Lengths Å**					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**
UF	1.993	2.001/2.000	2.003/2.002	2.004	1.974	1.983
UO	2.282/2.281	2.266/2.464	2.252/2.249	2.534/2.240	NA	1.987
OC	1.273	1.289/1.284	1.289/1.288	1.295/1.290	NA	NA
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
UF	1.993	2.006	2.009	2.011		
UO	2.289/2.287	2.273/2.272	2.278/2.263 *	2.270/2.266*		
OC	1.270	1.282	1.287/1.280	1.288/1.286		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
UF	NA	NA	NA	NA		
UO	2.308/2.286*	2.300/2.276*	2.304/2.269*	2.297/2.275*		
OC	1.272/1.266*	1.284/1.276*	1.287/1.275*	1.288/1.281*		
	Mulliken Charges					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**
U	1.543	1.521	1.515	1.512	1.369	1.618

*** indicates that there are more than two values, so the highest and lowest are reported**

F1	-0.272	-0.287	-0.291	-0.294	-0.254	-0.265
F2	-0.272	-0.286	-0.290	-0.293	-0.254	-0.265
O1	-0.259	-0.288	-0.313	-0.337	NA	-0.380
O2	-0.259	-0.296	-0.308	-0.327	NA	NA
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
U	1.305	1.273	1.276	1.266		
F1	-0.274	-0.298	-0.303	-0.307		
O1	-0.262	-0.310	-0.326	-0.351		
O2	-0.263	-0.310	-0.317	-0.341		
O3	-0.262	-0.312	-0.326	-0.351		
O4	-0.263	-0.312	-0.316	-0.341		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
U	1.164	1.097	1.091	1.086		
O1	-0.279	-0.337	-0.353	-0.373		
O2	-0.278	-0.329	-0.330	-0.368		
O3	-0.275	-0.336	-0.351	-0.373		
O4	-0.271	-0.329	-0.333	-0.363		
O5	-0.277	-0.333	-0.353	-0.373		
O6	-0.273	-0.332	-0.331	-0.364		

Table S4.3

M06L	**Bond Lengths Å**					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**
UF	2.009/2.008	2.016	2.018	2.020	1.991	2.000
UO	2.312/2.311	2.301/2.268	2.282/2.277	2.287/2.265	NA	2.005
OC	1.274	1.292/1.284	1.291/1.288	1.298/1.291	NA	NA
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
UF	1.998	2.012	2.014	2.017		
UO	2.345/2.286*	2.327/2.271*	2.309/2.275 *	2.317/2.263*		
OC	1.283/1.261*	1.296/273*	1.292/2.279*	1.301/1.279*		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
UF	NA	NA	NA	NA		
UO	2.352/2.290*	2.345/2.280*	2.330/2.293*	2.336/2.285*		
OC	1.280/1.263*	1.293/1.273*	1.288/1.277*	1.295/1.278*		
	Mulliken Charges					
	$[UF_2(formate)]^+$	**$[UF_2(acetate)]^+$**	**$[UF_2(propionate)]^+$**	**$[UF_2(acrylate)]^+$**	**$[UF_2(C\equiv CH)]^+$**	**$[UF_2(OH)]^+$**

*** indicates that there are more than two values, so the highest and lowest are reported**

U	1.556	1.542	1.543	1.533	1.428	1.627
F1	-0.247	-0.264	-0.267	-0.268	-0.243	-0.250
F2	-0.251	-0.265	-0.268	-0.273	-0.243	-0.254
O1	-0.294	-0.334	-0.328	-0.355	NA	-0.488
O2	-0.294	-0.324	-0.341	-0.355	NA	NA
	$[UF(formate)_2]^+$	**$[UF(acetate)_2]^+$**	**$[UF(propionate)_2]^+$**	**$[UF(acrylate)_2]^+$**		
U	1.321	1.299	1.323	1.297		
F1	-0.221	-0.248	-0.253	-0.258		
O1	-0.284	-0.326	-0.314	-0.352		
O2	-0.291	-0.339	-0.327	-0.369		
O3	-0.285	-0.328	-0.321	-0.347		
O4	-0.294	-0.331	-0.334	-0.357		
	$[U(formate)_3]^+$	**$[U(acetate)_3]^+$**	**$[U(propionate)_3]^+$**	**$[U(acrylate)_3]^+$**		
U	1.187	1.140	1.159	1.120		
O1	-0.293	-0.346	-0.348	-0.362		
O2	-0.294	-0.346	-0.357	-0.382		
O3	-0.296	-0.349	-0.336	-0.381		
O4	-0.296	-0.352	-0.342	-0.383		
O5	-0.296	-0.350	-0.337	-0.366		
O6	-0.297	-0.352	-0.339	-0.379		

Coordinates of Computed Structures and Transition States

Individual Molecular Structures

B3LYP

$[UF_2(C{\equiv}CH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

U 0.16572900 0.74492900 0.65862900

F -1.37687900 1.48853300 -0.36097400

F 1.72568300 1.48787100 -0.33460200

C 0.17616700 -2.66671000 -0.06408100

H 0.18075200 -3.69744000 -0.34587100

C 0.17069800 -1.49005000 0.26051700

$[UF_2(OH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

U 0.15791800 0.91382200 0.71508500

F -1.35544200 1.36686300 -0.51348900

F 1.72252700 1.37755800 -0.44307500

O 0.15804100 -1.08541800 0.87624900

H 0.16027500 -2.05011400 0.81322300

HF cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

F 2.43567300 -0.06465500 0.00000000

H 1.51191300 -0.06465500 0.00000000

HC≡CH cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

C 0.00000000 0.00000000 0.59821300

H 0.00000000 0.00000000 1.65931900

C 0.00000000 0.00000000 -0.59821300

H 0.00000000 0.00000000 -1.65931900

H_2O maug-cc-pVTZ

0 1

O 0.00000000 0.00000000 0.11699300

H 0.00000000 0.76320300 -0.46797000

H 0.00000000 -0.76320300 -0.46797000

Formic Acid maug-cc-pVTZ

0 1

C 2.05647900 -0.04792200 0.00000000

H 0.95663600 -0.12702300 0.00000000

O 2.64978100 0.98491900 0.00000000

O 2.68297700 -1.24573400 0.00000000

H 2.03377300 -1.96003100 0.00000000

Acetic Acid maug-cc-pVTZ

0 1

C 2.38964300 0.03041100 0.00039700

O 3.03272500 1.03976400 -0.00004900

O 3.02470500 -1.17660100 -0.00018900

H 2.38671900 -1.89926600 -0.00024900

C 0.87929000 -0.03454300 0.00008300

H 0.52050000 -0.56698900 -0.88273900

H 0.52015800 -0.56695500 0.88278400

H 0.47452600 0.97235300 -0.00002100

Propionic Acid maug-cc-pVTZ

0 1

C 2.30365300 0.01375200 0.20375500

O 3.00559200 0.96960400 0.41569100

C 0.80689500 0.03766200 0.02710600

H 0.45056300 0.98378800 0.42864100

H 0.37341500 -0.77499000 0.61131800

C 0.40221500 -0.10967200 -1.44667000

H -0.68253800 -0.06968400 -1.54143800

H 0.82225200 0.69550300 -2.04962200

H 0.74393200 -1.05944700 -1.85586200

O 2.80936900 -1.23972900 0.07264200

H 3.77049200 -1.16943900 0.17018800

Acrylic Acid maug-cc-pVTZ

0 1

C 2.49777200 -0.07276300 -0.08911900

O 3.21054200 0.43602300 -0.91911700

C 1.01878000 -0.13265700 -0.12189900

H 0.53290700 -0.62885100 0.70674900

C 0.33412300 0.40117200 -1.12661900

H 0.84763500 0.89178600 -1.94283700

H -0.74564100 0.36084500 -1.15662800

O 2.98873600 -0.67747800 1.02246300

H 3.95352200 -0.60315000 0.98175800

CO_2 maug-cc-pVTZ

0 1

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 1.16051600

O 0.00000000 0.00000000 -1.16051600

$O=C=CH_2$ maug-cc-pVTZ

0 1

C 0.31768500 0.23815100 -0.07993900

O 0.22957600 1.38639300 0.06339600

C 0.41688600 -1.05616600 -0.24143900

H -0.33721300 -1.70437800 0.17496900

H 1.25178900 -1.46225500 -0.78940900

$O=C=CHCH_3$ maug-cc-pVTZ

0 1

C 0.36857600 0.21116700 0.09576200

O 0.36778600 1.27945000 0.56000500

C 0.37402700 -0.98912000 -0.42492100

H -0.57256900 -1.51297400 -0.41039800

C 1.60036400 -1.63993000 -1.01968900

H 2.46740000 -0.98452200 -0.95567700

H 1.84450600 -2.56614600 -0.49637300

H 1.44358800 -1.88198600 -2.07238700

$O=C=C=CH_2$ maug-cc-pVTZ

0 1

C 0.81072300 0.51057500 -0.18264200

O 0.66078500 1.63659700 0.11109900

C 0.97371700 -0.70990500 -0.50094800

C 1.13655200 -1.97039600 -0.83098200

H 2.10107900 -2.46853200 -0.75873200

H 0.31599000 -2.58490400 -1.19539900

$H_2C=CH_2$ maug-cc-pVTZ

0 1

C 0.00000000 0.66247700 0.00000000

H 0.92076500 1.23175800 0.00000000

H -0.92077500 1.23175100 0.00000000

C 0.00000000 -0.66247700 0.00000000

H -0.92076500 -1.23175800 0.00000000

H 0.92077500 -1.23175100 0.00000000

$[UF_2(formate)]^+$ maug-cc-pVTZ

1 3

C 1.19610400 -0.00183900 0.05068100

H 0.10894700 0.02331600 0.14783400

O 1.87237200 1.07941000 -0.02543200

O 1.82478200 -1.11344000 0.00962800

U 3.86647600 -0.06487700 -0.19529600

F 4.74887300 -0.12734800 -2.00056300

F 5.10347300 -0.06650900 1.38965500

$[UF(formate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.25622600 0.38513300 0.26711000

H 0.28122600 0.50869400 0.74280100

C 5.92551400 0.42630800 0.27082700

H 6.89793700 0.56608300 0.74730600

O 1.82959900 1.36366100 -0.31605300

O 1.84878600 -0.74399800 0.27000400

O 5.34866600 -0.71101200 0.27954500

O 5.33979900 1.39316300 -0.31934400

U 3.59508400 0.04779000 -1.02168800

F 3.60142300 -0.51943800 -2.95071200

$[U(formate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.28005200 0.44348700 0.47291300

H 0.33987700 0.59528800 1.00754900

C 5.91660600 0.47125500 0.48187000

H 6.83895300 0.63438200 1.04318300

O 2.00059800 1.43376600 0.12441000

O 1.68435000 -0.72819600 0.18152800

O 5.12784900 -0.48526800 0.79120800

O 5.59713300 1.22644100 -0.48869000

U 3.60478000 0.06856200 -0.85211700

C 3.50823900 -0.68734300 -3.44184000

H 3.44433700 -0.98767700 -4.48975700

O 3.08546600 0.45870400 -3.06691900

O 3.99780800 -1.46592000 -2.56520400

$[UF_2(acetate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.27191400 -0.00221800 0.01091200

O 2.95001900 1.09295900 0.00546900

O 2.97100000 -1.09223100 0.01044500

C 0.79623000 -0.02841500 0.01178100

H 0.45653300 -0.50464100 -0.91157800

H 0.44987500 -0.65812100 0.83312200

H 0.38946300 0.97454500 0.08979500

U 4.96048400 -0.00773400 0.00221300

F 6.01339200 -0.15172700 -1.71337000

F 6.02422700 -0.14158000 1.71189700

$[UF(acetate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.55905900 -0.03568100 0.07348600

O 3.16901600 1.09613000 0.00550800

O 3.21927100 -0.99472300 0.62312100

C 1.17548200 -0.21415500 -0.41826300

H 1.00784400 -1.24650200 -0.71449300

H 0.49311700 0.01624200 0.40580600

H 0.96838900 0.47954900 -1.22917000

U 5.02444100 0.33270900 1.12197900

C 7.24286200 -0.06122500 -0.37365100

O 6.68591600 -1.01466800 0.28831900

O 6.64018200 1.07562700 -0.33058500

F 5.21487200 0.89903100 3.05543300

C 8.48910500 -0.26256400 -1.14463800

H 8.20931200 -0.58043800 -2.15391900

H 9.04183400 0.66969500 -1.22644300

H 9.08895700 -1.05211600 -0.69916600

$[U(acetate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.41598800 -0.10776400 -0.34626300

O 2.83635300 0.99777300 0.16639900

O 3.23295500 -1.09502900 -0.31024300

C 1.05602400 -0.22533400 -0.92184900

H 0.97668300 -1.11140700 -1.54426100

H 0.34328500 -0.30477600 -0.09631900

H 0.80824500 0.67790300 -1.47656200

U 4.88130700 0.13460100 0.76674900

C 7.15403000 -0.09995800 -0.70359200

O 6.82371200 -0.95427600 0.20509500

O 6.33948200 0.86995100 -0.89055000

C 8.41302100 -0.24254600 -1.47158400

H 8.45908700 -1.24287000 -1.90341800

H 8.48452100 0.51694100 -2.24330400

H 9.25536700 -0.15746400 -0.78175500

C 5.08845600 0.63358400 3.43095000

O 4.73134800 -0.51522900 2.98083900

O 5.34579000 1.53196600 2.54977700

C 5.21947200 0.89998000 4.88287100

H 6.24649200 0.66360900 5.17628200

H 5.04301600 1.95153500 5.09392700

H 4.55113400 0.25689000 5.44944500

$[UF_2(propionate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.30705600 0.00203600 -0.03432800

O 2.98598800 1.10098900 0.02744200

O 3.01035600 -1.07670100 -0.16691000

U 4.98960500 0.03807500 -0.14893000

C 0.82884200 -0.02199600 0.00412200

H 0.48360500 0.87017000 0.52318300

H 0.51964100 -0.91210000 0.55183700

C 0.25277600 -0.06705300 -1.43292000

H -0.83248300 -0.08990800 -1.36550500

H 0.53952900 0.81602900 -2.00135600

H 0.58107700 -0.95997300 -1.96147000

F 6.12910100 -0.11951500 1.51139200

F 5.97729000 0.22285700 -1.90152200

$[UF(propionate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.74490100 -0.00872900 0.32750500

O 2.40180100 1.09199800 0.18081700

O 2.40551800 -1.08738600 0.08276700

U 4.37055200 0.03209400 -0.31419000

F 5.77127000 -0.01136600 1.14915600

C 0.31629600 -0.02412200 0.72581100

H 0.16643700 0.75345800 1.47484200

H 0.08918800 -0.99661800 1.15794900

C -0.58986000 0.25011100 -0.49630800

H -1.62722700 0.24113400 -0.16928200

H -0.37803000 1.22458600 -0.93253500

H -0.46821500 -0.51858600 -1.25798200

C 5.18468600 0.10782200 -2.89095200

O 4.93594000 1.17643800 -2.20755600

O 4.95450900 -1.00274800 -2.28740600

C 5.71534700 0.18646800 -4.27709500

H 6.63976400 0.77031500 -4.21189500

H 5.02464200 0.83343700 -4.82758100

C 5.93117800 -1.15253200 -4.97193900

H 6.31801100 -0.98085000 -5.97429300

H 6.64833400 -1.77037800 -4.43464900

H 5.00100700 -1.71111500 -5.06013700

$[U(propionate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.79937000 0.14781300 0.29796700

O 2.13805000 1.24818600 -0.27198500

O 2.74758300 -0.69963400 0.50029000

U 4.37910800 0.67263100 -0.37734100

C 0.39177600 -0.14818200 0.67138500

H -0.11998200 0.79485600 0.85508400

H 0.39974600 -0.74374600 1.58350000

C -0.31523200 -0.92870200 -0.45851900

H -1.33963900 -1.13477000 -0.15587400

H -0.34421900 -0.34832900 -1.37946800

H 0.18071700 -1.87859700 -0.65078900

C 5.15394200 0.63270200 -2.97561900

O 5.17409200 1.70989100 -2.26583100

O 4.74360500 -0.42806100 -2.38067500

C 5.58489200 0.64638300 -4.40052000

H 6.59063700 1.07811900 -4.40755600

H 4.96168900 1.39808700 -4.89574200

C 5.53253500 -0.70000600 -5.11209600

H 5.86502100 -0.57957800 -6.14123100

H 6.18021200 -1.43081700 -4.63102200

H 4.52166900 -1.10349000 -5.12872100

C 6.17119100 1.20901900 1.59405400

O 6.20753000 0.10389900 0.94872900

O 5.25375700 2.04501600 1.23713000

C 7.11514200 1.53771600 2.69760700

H 6.49328800 1.77156700 3.56761800

H 7.57546600 2.49295700 2.42603400

C 8.15413900 0.46713800 3.00761700

H 8.79047500 0.80412500 3.82354200

H 7.68557000 -0.46825800 3.30828400

H 8.78824000 0.26559500 2.14601100

$[UF_2(acrylate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.46752800 0.36046000 -0.36076200

O 3.22442400 1.24830300 0.20433200

O 3.09552000 -0.66625800 -0.85624800

U 5.13306200 0.08621400 -0.22877400

C 1.03594900 0.52446600 -0.42116400

H 0.64810200 1.42640100 0.03060200

C 0.25505800 -0.39199300 -1.00279800

H -0.81735900 -0.26175900 -1.04374100

H 0.66703800 -1.28744200 -1.44828600

F 6.02691400 -0.94199700 1.26517200

F 6.34899000 0.70852300 -1.71963000

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 6.20847800 2.80014800 -1.91561800

O 5.90746400 3.32837500 -0.77299800

C 6.67210700 3.56874700 -3.05222200

H 6.88371900 3.00034600 -3.94671400

C 6.82355000 4.89320900 -2.98173700

H 6.60402000 5.43871400 -2.07392200

H 7.17141300 5.45965800 -3.83412000

O 6.06018900 1.51891000 -1.99238600

C 6.90486600 0.21736800 1.93302600

O 6.53528700 -0.39538900 0.85460900

C 7.75020500 -0.38531500 2.94285800

H 7.97860200 0.23843100 3.79535200

C 8.20984100 -1.63183200 2.81229800

H 7.96570900 -2.23566100 1.94876300

H 8.84168000 -2.07414300 3.56964200

O 6.46033800 1.42312500 2.06779900

U 5.22838900 1.34094400 0.13636400

F 3.22445500 1.08441600 0.32634500

$[U(acrylate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.51898500 0.73589400 0.49760500

O 3.20785800 0.24063500 -0.47655600

C 1.09443700 0.50653600 0.65964700

H 0.63904900 0.98142300 1.51699900

C 0.40699200 -0.24451600 -0.20209200

H 0.88833700 -0.70871900 -1.05215400

H -0.65335700 -0.41072200 -0.07415100

O 3.17199900 1.46142700 1.34030000

C 6.16181300 2.64808200 -1.83479000

O 5.55894600 3.20093800 -0.83776900

C 6.71724700 3.40232100 -2.94544300

H 7.19465500 2.81537100 -3.71716300

C 6.63550300 4.73254900 -2.99439300

H 6.15259200 5.29520600 -2.20698000

H 7.05108600 5.28682500 -3.82407000

O 6.25447300 1.36296400 -1.79797900

C 6.94833400 0.18594700 2.03827200

O 6.37751300 -0.56074000 1.15549800

C 7.91461500 -0.31586300 3.00023600

H 8.31478700 0.41667200 3.68670000

C 8.27380000 -1.60000800 3.02204800

H 7.85759900 -2.31189700 2.32220500

H 8.99297100 -1.96592700 3.74121400

O 6.61605800 1.43161300 2.02601500

U 5.17882500 1.19076800 0.23782900

PBE0

$[UF_2(C{\equiv}CH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

U 0.16540200 0.74014100 0.65274200

F -1.36009300 1.47643000 -0.36160800

F 1.70890000 1.47349900 -0.33594500

C 0.17624200 -2.65511100 -0.06219700

H 0.18192100 -3.68486400 -0.35667000

C 0.16977900 -1.48296200 0.27729600

$[UF_2(OH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

U 0.15758100 0.91343800 0.71712900

F -1.34163600 1.34855800 -0.50566100

F 1.70825800 1.35832700 -0.43570100

O 0.15846100 -1.06778300 0.86742000

H 0.16065600 -2.02982900 0.80480600

HF cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

F 2.43342500 -0.06465500 0.00000000

H 1.51416200 -0.06465500 0.00000000

HC≡CH cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

C 0.00000000 0.00000000 0.59835700

H 0.00000000 0.00000000 1.66189100

C 0.00000000 0.00000000 -0.59835700

H 0.00000000 0.00000000 -1.66189100

H_2O maug-cc-pVTZ

0 1

O 0.00000000 0.00000000 0.11689300

H 0.00000000 0.75964200 -0.46757200

H 0.00000000 -0.75964200 -0.46757200

Formic Acid maug-cc-pVTZ

0 1

C 2.05940400 -0.05248300 0.00000000

H 0.95695400 -0.13099300 0.00000000

O 2.64915200 0.97917400 0.00000000

O 2.68231800 -1.24131200 0.00000000

H 2.03181800 -1.95017800 0.00000000

Acetic Acid maug-cc-pVTZ

0 1

C 2.38912300 0.02767400 0.00022200

O 3.02885900 1.03630600 0.00000100

O 3.01726600 -1.17112800 -0.00011800

H 2.37365300 -1.88510300 -0.00015800

C 0.88545300 -0.03741400 0.00005100

H 0.52729000 -0.57107100 -0.88360000

H 0.52709700 -0.57115400 0.88357100

H 0.47952500 0.97006300 0.00004900

Propionic Acid maug-cc-pVTZ

0 1

C 2.29509600 0.01367100 0.22233700

O 2.98789100 0.93318100 0.56812500

C 0.80806600 0.05954400 0.02332700

H 0.46456900 1.02184600 0.39949400

H 0.36037800 -0.72877200 0.63412300

C 0.41181200 -0.13310300 -1.43754200

H -0.67250000 -0.08231100 -1.54262000

H 0.84637500 0.64510900 -2.06731900

H 0.74544900 -1.10117000 -1.81134100

O 2.80232800 -1.20656700 -0.04505700

H 3.75637700 -1.14408000 0.09221900

Acrylic Acid maug-cc-pVTZ

0 1

C 2.49250500 -0.07448200 -0.08566600

O 3.19625500 0.43502200 -0.91876400

C 1.01689200 -0.13639600 -0.11535800

H 0.52740500 -0.63273100 0.71322300

C 0.34155200 0.39940600 -1.12287600

H 0.86987700 0.88772000 -1.93359800

H -0.73965900 0.36388700 -1.16182300

O 2.98614900 -0.67348700 1.01510800

H 3.94739900 -0.59401100 0.96450600

CO_2 maug-cc-pVTZ

0 1

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 1.15759800

O 0.00000000 0.00000000 -1.15759800

$O=C=CH_2$ maug-cc-pVTZ

0 1

C 0.31778100 0.23707000 -0.08007700

O 0.22988000 1.38225700 0.06288300

C 0.41688000 -1.05599500 -0.24141100

H -0.33969300 -1.70219700 0.17666600

H 1.25387400 -1.45939000 -0.79048300

$O=C=CHCH_3$ maug-cc-pVTZ

0 1

C 0.37560800 0.20679900 0.10115000

O 0.37251200 1.27390100 0.55944200

C 0.38075200 -0.99476600 -0.41451000

H -0.56464600 -1.52227400 -0.37457500

C 1.59549200 -1.63133600 -1.02844000

H 2.45654800 -0.96466300 -0.98550600

H 1.86260100 -2.55268700 -0.50578700

H 1.42063800 -1.88021600 -2.07766500

$O=C=C=CH_2$ maug-cc-pVTZ

0 1

C -0.02013900 -0.44713200 -0.00088500

C 1.25244700 -0.44638700 0.00041000

C -1.33167500 -0.44724900 -0.00108900

H -1.90912600 0.01300300 0.79967300

H -1.90880200 -0.90759700 -0.80201800

O 2.42186800 -0.44596300 0.00114900

$H_2C=CH_2$ maug-cc-pVTZ

0 1

C 0.75708700 3.48584300 0.75901900

H 1.19967800 3.76033100 -0.19178200

H -0.29263100 3.72089700 0.89360100

C 1.46322600 2.89310200 1.70859600

H 1.02032700 2.61868700 2.65927400

H 2.51291600 2.65797100 1.57410100

$[UF_2(formate)]^+$ maug-cc-pVTZ

1 3

C 1.21270600 -0.00237700 0.04976400

H 0.12375800 0.02313700 0.14908000

O 1.88475700 1.07569200 -0.02725300

O 1.83688700 -1.11078100 0.00819800

U 3.85368200 -0.06481400 -0.19625700

F 4.73217600 -0.12602700 -1.98406400

F 5.07705900 -0.06611800 1.37704100

$[UF(formate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.28520900 0.38476300 0.26237900

H 0.30735000 0.50469900 0.73768300

C 5.89719100 0.42504800 0.26640700

H 6.87199700 0.56220400 0.74331800

O 1.85100600 1.36200700 -0.31943900

O 1.87886800 -0.73845000 0.26837600

O 5.31908800 -0.70601800 0.27926000

O 5.31957100 1.39028700 -0.32418300

U 3.59530800 0.05489800 -1.01819400

F 3.59867600 -0.52305300 -2.92581300

$[U(formate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.22108900 0.44540900 0.49574000

H 0.29319100 0.60010400 1.05404800

C 5.89164500 0.45426800 0.37102700

H 6.85047300 0.61779400 0.87205000

O 2.00485800 1.41983300 0.26073300

O 1.54389700 -0.70449800 0.07469600

O 5.18175500 -0.56115600 0.64165100

O 5.46147100 1.27924900 -0.49163600

U 3.52272300 0.08694300 -0.81016600

C 3.61481200 -0.67824200 -3.36689500

H 3.67616700 -0.99458900 -4.41234500

O 3.22599000 0.48731200 -3.06095800

O 3.93797600 -1.47494700 -2.42981000

$[UF_2(acetate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.28012700 -0.01037300 0.02049000

O 2.95894900 1.07724300 -0.04483000

O 2.96878400 -1.09870000 0.07074500

C 0.81082400 -0.02626300 0.02148200

H 0.47824600 -0.38116000 -0.96018900

H 0.45087600 -0.74785600 0.75587300

H 0.41125500 0.96819400 0.20059900

U 4.93979400 -0.02343900 -0.00203700

F 5.97602900 -0.23439300 -1.70053300

F 6.00825500 -0.04241700 1.68908400

$[UF(acetate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.58901100 -0.03406800 0.06861700

O 3.19092900 1.09439100 -0.02393700

O 3.24681700 -0.97586700 0.63807300

C 1.21265700 -0.22695700 -0.41886800

H 1.04700300 -1.26773200 -0.68926900

H 0.53074700 0.02191600 0.40163500

H 1.00366000 0.44934900 -1.24520600

U 5.02208500 0.36355000 1.10638600

C 7.21374300 -0.06242200 -0.36641900

O 6.66226000 -0.99708900 0.31606600

O 6.61252200 1.07021700 -0.35482200

F 5.20700800 0.97091200 3.00946100

C 8.45565200 -0.27904300 -1.12797200

H 8.17244100 -0.59088800 -2.13933300

H 9.01913300 0.64820200 -1.20993000

H 9.04398800 -1.07755700 -0.68115800

$[U(acetate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.53701800 -0.09305100 -0.32229500

O 3.28039800 0.93105500 -0.50995200

O 3.00280100 -0.99827100 0.45200300

C 1.20499700 -0.21126200 -0.94602500

H 0.92611700 -1.25672600 -1.05680900

H 0.48132600 0.26637900 -0.27728800

H 1.18178200 0.31947600 -1.89564200

U 4.95331100 0.13904100 0.83760600

C 7.15671300 -0.16872100 -0.66984400

O 6.34985500 -1.13767800 -0.42779000

O 6.86542600 0.95696200 -0.14358100

C 8.34085000 -0.35307400 -1.53002100

H 8.00135400 -0.37874700 -2.57023200

H 9.04078200 0.46877900 -1.40497600

H 8.80590400 -1.31572500 -1.31958400

C 5.08352500 0.67449100 3.46800900

O 5.48690100 -0.44136900 2.99815600

O 4.62977300 1.52174500 2.61654800

C 5.11105600 0.97768200 4.91144400

H 5.42301900 2.01011700 5.06709900

H 4.08987000 0.88815100 5.29483800

H 5.75299100 0.27883200 5.44097000

$[UF_2(propionate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.30748400 0.00716900 -0.03284800

O 2.98510900 1.09939000 0.04584200

O 3.00122400 -1.06841700 -0.18506700

U 4.96061200 0.03646300 -0.15614300

C 0.83489400 -0.01314500 0.00567400

H 0.49021900 0.88546800 0.51652100

H 0.52469900 -0.89936900 0.56228700

C 0.27479500 -0.07396500 -1.42608000

H -0.81235600 -0.09771400 -1.37041500

H 0.56477900 0.80419600 -2.00313000

H 0.60884200 -0.97285900 -1.94359600

F 6.09431200 -0.14394800 1.48438000

F 5.93777000 0.23964100 -1.89238900

$[UF(propionate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.63509500 -0.13524800 -0.04099200

O 2.02801100 1.02434200 -0.41564600

O 2.54023000 -1.04880700 -0.00372000

U 4.20311900 0.37089700 -0.58646000

F 5.44757600 0.94485200 0.88225000

C 0.23567800 -0.42630200 0.34022300

H 0.28108800 -0.83907900 1.35501200

H -0.07221200 -1.27548900 -0.28117500

C -0.71929000 0.74564100 0.23513300

H -1.71818500 0.42893800 0.53173200

H -0.41844900 1.56596100 0.88627100

H -0.77465500 1.12573100 -0.78467000

C 5.15296000 0.08686900 -3.06897600

O 4.63584900 1.18853100 -2.65101300

O 5.12298300 -0.89130500 -2.24380100

C 5.74996900 -0.01658200 -4.41850500

H 6.49525700 0.78511300 -4.47983700

H 4.96339500 0.29435000 -5.11633600

C 6.32891600 -1.37327700 -4.76589100

H 6.73702800 -1.34732200 -5.77526000

H 7.13263500 -1.65091400 -4.08439600

H 5.56905000 -2.15346700 -4.72889700

$[U(propionate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.86397600 -0.36990200 0.16111900

O 2.05980800 0.67489900 -0.54268600

O 2.91408900 -1.02514500 0.51517100

U 4.34896900 0.41539700 -0.49274300

C 0.51372000 -0.82518400 0.56787500

H 0.53725400 -0.89539200 1.66142900

H 0.43307000 -1.86502500 0.23137300

C -0.63111500 0.03392500 0.07066900

H -1.57684300 -0.37867400 0.41960700

H -0.55176100 1.05641100 0.43905100

H -0.65953000 0.06930500 -1.01817200

C 5.24115700 0.44861100 -3.02708800

O 5.05149700 1.52344900 -2.34500200

O 4.96490600 -0.64976300 -2.44099300

C 5.75768800 0.51262000 -4.41455900

H 6.70075200 1.06834700 -4.35862200

H 5.08051600 1.18239800 -4.95663900

C 5.91905200 -0.82750800 -5.10298700

H 6.30147600 -0.67724500 -6.11173500

H 6.61887100 -1.46910000 -4.56810000

H 4.96812900 -1.35459000 -5.17755400

C 6.00836600 1.22083000 1.46378200

O 6.16902700 0.10031300 0.87272400

O 5.01805400 1.93498000 1.06850700

C 6.90292900 1.69069100 2.54834300

H 6.25111700 1.90924300 3.40179900

H 7.27105400 2.67259200 2.22991800

C 8.02801900 0.74261700 2.91075700

H 8.62631800 1.17322800 3.71266300

H 7.64498600 -0.21836500 3.25334300

H 8.68481700 0.55956300 2.06061500

$[UF_2(acrylate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.47408900 0.36138700 -0.35925100

O 3.23000600 1.24303700 0.20315100

O 3.09036800 -0.66387100 -0.85577900

U 5.11015200 0.07942100 -0.23419900

C 1.04522300 0.52973900 -0.41728500

H 0.65561900 1.43231500 0.03532900

C 0.27268300 -0.38944300 -1.00059100

H -0.80210000 -0.26575100 -1.04551700

H 0.69591600 -1.28286100 -1.44438700

F 5.99697000 -0.93761500 1.24737900

F 6.31629900 0.69856000 -1.71014800

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 6.21573900 2.78022000 -1.89904700

O 5.91888400 3.31216000 -0.76391600

C 6.67347100 3.54665900 -3.03643100

H 6.88535300 2.98070200 -3.93424000

C 6.81811100 4.86916000 -2.95589800

H 6.59576300 5.40307800 -2.03955800

H 7.16201900 5.44612000 -3.80499000

O 6.07117300 1.50452100 -1.97353100

C 6.90355400 0.23806600 1.91605500

O 6.54025600 -0.37699700 0.84407300

C 7.74305000 -0.36401600 2.92767000

H 7.97299700 0.25742600 3.78335300

C 8.19392400 -1.61050500 2.78836800

H 7.94257800 -2.20392000 1.91723400

H 8.82412200 -2.06410200 3.54283100

O 6.46341600 1.43927200 2.04789600

U 5.24594500 1.34326000 0.13473100

F 3.25995900 1.08894700 0.32273900

$[U(acrylate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.42925300 0.78327500 0.40433500

O 3.26941500 -0.14862400 0.11468300

C 1.01073700 0.53630700 0.57212500

H 0.40731900 1.40017700 0.81896500

C 0.50556900 -0.68678300 0.42348400

H 1.14171900 -1.52803300 0.17523700

H -0.55377200 -0.87326400 0.54593000

O 2.91373200 1.96084100 0.54321800

C 6.03415400 2.71264400 -1.90264800

O 6.06203600 3.12844500 -0.68413000

C 6.57429500 3.48224100 -3.00603300

H 6.49528700 3.02494100 -3.98376300

C 7.12529100 4.67745700 -2.80320900

H 7.18569200 5.10382100 -1.80892300

H 7.52673400 5.25534700 -3.62592600

O 5.49967000 1.56553200 -2.09849200

C 6.76411700 0.22764300 1.94147000

O 6.64669400 -0.26411300 0.76078300

C 7.67837700 -0.30918800 2.93117600

H 7.68699700 0.19473900 3.88895500

C 8.44853400 -1.35931100 2.65380100

H 8.41138800 -1.83826800 1.68255100

H 9.13157700 -1.76284800 3.39039700

O 6.02113100 1.23663200 2.21275100

U 5.05917100 1.25716700 0.13429000

M06L

$[UF_2(C{\equiv}CH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

U 0.16376900 0.74708000 0.67360800

F -1.35750600 1.49245200 -0.37270000

F 1.70615300 1.48265300 -0.34844600

C 0.17721900 -2.66844900 -0.06130300

H 0.18437500 -3.69241000 -0.36600600

C 0.16814100 -1.49419300 0.28846600

$[UF_2(OH)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

U 0.20903200 0.91167700 0.71593900

F -1.32623000 1.22674100 -0.52619500

F 1.71636400 1.51377500 -0.45321200

O 0.17199800 -1.08606300 0.88274300

H 0.07215500 -2.04342000 0.82871900

HF cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

F 2.43326500 -0.06465500 0.00000000

H 1.51432200 -0.06465500 0.00000000

HC≡CH cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

0 1

C 0.00000000 0.00000000 0.59875600

H 0.00000000 0.00000000 1.65902400

C 0.00000000 0.00000000 -0.59875600

H 0.00000000 0.00000000 -1.65902400

H_2O maug-cc-pVTZ

0 1

O -0.01452200 -0.01892100 -0.52119600

H 0.94290600 0.02644900 -0.52119600

H -0.29135600 0.89874100 -0.52119600

Formic Acid maug-cc-pVTZ

0 1

C 2.05846900 -0.04957100 0.00000000

H 0.95620200 -0.13506600 0.00000000

O 2.65130600 0.98171400 0.00000000

O 2.68441600 -1.24342000 0.00000000

H 2.02925300 -1.94944900 0.00000000

Acetic Acid maug-cc-pVTZ

0 1

C 2.47409900 -0.07112400 -0.09414600

O 3.18429300 0.43525100 -0.92182800

O 2.96464700 -0.67437000 1.01555600

H 3.92638400 -0.59424500 0.96425300

C 0.98419200 -0.13365800 -0.12392200

H 0.65181200 -1.16944700 -0.09954100

H 0.57098700 0.34724100 0.76033500

H 0.60719700 0.35185900 -1.01571400

Propionic Acid maug-cc-pVTZ

0 1

C 2.27904000 -0.01372000 0.31527300

O 2.86320100 0.57250800 1.18881700

C 0.82148500 0.14219500 -0.00933900

H 0.55828000 1.16973600 0.23478500

H 0.28749400 -0.47067300 0.72138000

C 0.40741400 -0.23320200 -1.41782800

H -0.65865200 -0.07114500 -1.55940500

H 0.93400000 0.36329500 -2.16010200

H 0.61925600 -1.27754900 -1.63162300

O 2.88900200 -0.92881000 -0.47543300

H 3.80532100 -0.97528400 -0.17077700

Acrylic Acid maug-cc-pVTZ

0 1

C 2.49197900 -0.07335200 -0.08916600

O 3.19816500 0.43683700 -0.92279000

C 1.02083600 -0.13590900 -0.11659900

H 0.53351000 -0.63211300 0.71177500

C 0.34050100 0.39862000 -1.12129500

H 0.86372000 0.88733800 -1.93289900

H -0.73810500 0.36496800 -1.16256300

O 2.98302000 -0.67602500 1.01989700

H 3.94474900 -0.59543600 0.96839200

CO_2 maug-cc-pVTZ

0 1

C 0.00000000 0.00000000 0.00000000

O 0.00000000 0.00000000 1.16014300

O 0.00000000 0.00000000 -1.16014300

$O=C=CH_2$ maug-cc-pVTZ

0 1

O 0.00010000 -0.00013600 -0.53924200

C 0.00113000 -0.00061400 0.62086600

C 0.00221500 -0.00110000 1.92692300

H 0.79777300 -0.49392800 2.45761700

H -0.79272100 0.49152200 2.45881600

$O=C=CHCH_3$ maug-cc-pVTZ

0 1

O -0.40352300 -0.33824400 -0.48311000

C -0.13565100 -0.12664800 0.62977000

C 0.16310800 0.11387100 1.87967600

H -0.34343600 0.96254100 2.31708000

C 1.12898700 -0.69826000 2.68768000

H 0.64629600 -1.13892000 3.55997200

H 1.55132500 -1.51186800 2.10453700

H 1.95889800 -0.08917100 3.04589300

$O=C=C=CH_2$ maug-cc-pVTZ

0 1

O -0.39056500 -0.32864500 -0.43050000

C -0.12197100 -0.11366200 0.69080400

C 0.16893900 0.11950500 1.90593500

C 0.46944300 0.35910600 3.15856400

H 0.05892900 1.20594900 3.70639300

H 1.14798300 -0.27397400 3.72828400

$H_2C=CH_2$ maug-cc-pVTZ

0 1

C -0.00106700 0.00056500 -0.66258400

H 0.80971400 -0.42847800 -1.23626600

H -0.81370400 0.43058900 -1.23290200

C 0.00106700 -0.00056500 0.65889600

H -0.80971400 0.42847800 1.23257800

H 0.81370400 -0.43058900 1.22921400

$[UF_2(formate)]^+$ maug-cc-pVTZ

1 3

C 1.19241200 -0.00262800 0.03951900

H 0.10005200 0.02629300 0.10191900

O 1.86381600 1.07791400 -0.03267300

O 1.81045100 -1.11660700 0.03404100

U 3.86461800 -0.07204200 -0.15686000

F 4.71641500 -0.11077700 -1.97607900

F 5.17326100 -0.07344000 1.36664200

$[UF(formate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.58853200 0.44506000 0.21128000

H 0.72329400 0.47906000 0.88078500

C 5.69355500 0.39418300 0.39901200

H 6.47045900 0.45633300 1.16782400

O 1.81035300 1.38476800 -0.60990400

O 2.38832100 -0.54621300 0.24960800

O 5.53041500 -0.65420600 -0.28230600

O 4.93347200 1.40616900 0.18649000

U 3.71109600 0.30541000 -1.40923400

F 3.07476300 -0.95418000 -2.82376000

$[U(formate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.35808400 0.43069700 0.43040200

H 0.41658000 0.58305200 0.96830900

C 5.89653900 0.49784400 0.55635200

H 6.78236200 0.65787600 1.17943400

O 2.04286900 1.42496500 0.03616500

O 1.78085200 -0.74256600 0.19173800

O 5.08311900 -0.44842900 0.84148000

O 5.65887200 1.23417000 -0.44157700

U 3.67390500 0.05660600 -0.89264500

C 3.43148900 -0.69800800 -3.46267800

H 3.30339800 -0.97530300 -4.51395500

O 3.01888400 0.44251300 -3.05298000

O 3.97909500 -1.48593600 -2.64191100

$[UF_2(acetate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.26853400 0.01080200 0.00926900

O 2.93353500 1.10917100 0.00711300

O 2.96551400 -1.07738700 0.00437500

C 0.80157800 -0.02592000 0.01328600

H 0.45936600 -0.53422300 -0.88788100

H 0.45955700 -0.63450500 0.84880700

H 0.38025200 0.97001700 0.06481200

U 4.95542800 0.01005400 -0.00171800

F 6.02673400 -0.17240200 -1.70016800

F 6.03264100 -0.17477000 1.69278800

$[UF(acetate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.89229900 0.15160300 0.11624300

O 3.17733300 1.38191600 0.31987400

O 3.73634900 -0.71560200 0.55338900

C 1.65144900 -0.26212100 -0.55824100

H 1.80468400 -1.18155100 -1.11343200

H 0.90372400 -0.46885500 0.20886200

H 1.27150000 0.53123400 -1.19165100

U 5.13365300 0.84723900 1.42570400

C 7.04892000 0.00380900 -0.27661700

O 6.91442800 -0.54146400 0.86555100

O 6.25220700 0.98867500 -0.55185200

F 4.61167500 0.54936700 3.34593200

C 8.03866000 -0.45478000 -1.26374000

H 7.51365800 -1.02077500 -2.03413700

H 8.49928500 0.39445900 -1.76029100

H 8.77983100 -1.09623800 -0.80227200

$[U(acetate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.61970400 -0.08470400 -0.29009200

O 3.34121700 0.96431800 -0.43485900

O 3.09852500 -1.01885600 0.44372800

C 1.29141900 -0.19944200 -0.91938900

H 1.02012100 -1.23886400 -1.06573300

H 0.55781500 0.24629500 -0.24656400

H 1.25781700 0.35752600 -1.84962100

U 5.04887500 0.14451000 0.89262100

C 7.17532100 -0.15453000 -0.75794400

O 6.33402300 -1.10606900 -0.51576200

O 6.97319900 0.95649800 -0.17089600

C 8.30377300 -0.37235300 -1.67973300

H 7.91434700 -0.61524500 -2.66712500

H 8.93855900 0.50319700 -1.73568600

H 8.87494500 -1.23963700 -1.35515000

C 5.03478800 0.65542200 3.55316400

O 5.53823500 -0.42762600 3.11377200

O 4.55398500 1.47545600 2.67653400

C 4.98177300 0.98230000 4.98876000

H 5.41479100 1.96622000 5.15492100

H 3.93957700 1.05071900 5.29741200

H 5.49296200 0.23295200 5.58027700

$[UF_2(propionate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.30286400 0.03672000 -0.05095100

O 2.99098700 1.11301500 0.11706400

O 2.97927100 -1.03519400 -0.29877800

U 4.98377800 0.03736200 -0.16839000

C 0.83054700 0.02508700 -0.00289800

H 0.49064000 0.93871600 0.47708500

H 0.52629700 -0.82929400 0.60180800

C 0.24903800 -0.11262900 -1.41531100

H -0.83382500 -0.13892300 -1.35103200

H 0.52608900 0.73115300 -2.04223700

H 0.58196300 -1.03050300 -1.89204000

F 6.09624000 -0.27045400 1.48701900

F 6.04849400 0.33785300 -1.85630300

$[UF(propionate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.01542800 -0.01485500 0.09919300

O 2.34264900 1.02840200 -0.58981500

O 2.95950500 -0.61546000 0.71777800

U 4.56849300 0.82267700 -0.10332800

F 6.33352900 0.39536200 0.76674900

C 0.61760500 -0.49490200 0.16394900

H 0.37926900 -0.59177700 1.22630900

H 0.64384800 -1.52998200 -0.18843900

C -0.38925700 0.34660200 -0.58692100

H -1.38153400 -0.08176500 -0.48640100

H -0.42567400 1.36340200 -0.20476000

H -0.15492800 0.39947500 -1.64675500

C 5.09048400 0.37708500 -2.69913300

O 5.05843100 1.56827400 -2.22293300

O 4.83787300 -0.57723900 -1.87645000

C 5.40803500 0.12405900 -4.12156800

H 6.37526900 0.60049300 -4.30301800

H 4.70857700 0.73223700 -4.70109800

C 5.39393800 -1.33116100 -4.53155300

H 5.63943000 -1.42528100 -5.58471500

H 6.11834200 -1.91162300 -3.96653900

H 4.41673600 -1.78059100 -4.37550800

$[U(propionate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 1.90368300 -0.39508900 0.05393700

O 2.18369500 0.74620200 -0.47397800

O 2.88928400 -1.11294700 0.43344700

U 4.45096400 0.46517700 -0.27461800

C 0.50395900 -0.85523400 0.21413300

H 0.37914000 -1.07823500 1.27691200

H 0.45047000 -1.83615500 -0.26465400

C -0.54818500 0.10003400 -0.30208100

H -1.53964700 -0.31349100 -0.14513500

H -0.50177100 1.05875200 0.20771600

H -0.42956300 0.28706000 -1.36617200

C 5.10460600 0.45254400 -2.90433000

O 4.93965300 1.55212000 -2.27536300

O 4.94877200 -0.63282300 -2.22957000

C 5.45839600 0.43047900 -4.34344400

H 6.35101300 1.05246800 -4.44641800

H 4.68150100 1.00540500 -4.85407300

C 5.64132700 -0.94782000 -4.93753100

H 5.89735600 -0.87196000 -5.98982400

H 6.43736000 -1.49483800 -4.43909400

H 4.73419000 -1.54097600 -4.85688500

C 6.12095900 1.22701000 1.71248800

O 6.43491600 0.28397200 0.90181300

O 4.97751400 1.78832000 1.53754000

C 7.02336700 1.66037800 2.80410300

H 6.44237400 1.58069700 3.72663200

H 7.15984700 2.73724600 2.67585900

C 8.33580300 0.91379700 2.87988000

H 8.93269600 1.29018400 3.70483500

H 8.18137300 -0.15031200 3.03772300

H 8.91531600 1.03156000 1.96801700

$[UF_2(acrylate)]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.46307200 0.39503600 -0.38325800

O 3.21126900 1.28395900 0.17943600

O 3.08437800 -0.61418200 -0.91289100

U 5.12846300 0.12182800 -0.27349600

C 1.03100700 0.52540700 -0.40527700

H 0.63023300 1.41074100 0.06688800

C 0.26513000 -0.40588000 -0.97719100

H -0.81113800 -0.31568600 -0.99548000

H 0.69818500 -1.28273700 -1.44005800

F 5.90719600 -0.96772300 1.23877800

F 6.47743000 0.65415400 -1.67874800

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 5.94678100 2.66715400 -1.73140000

O 5.98497600 3.11727600 -0.51185700

C 6.68986300 3.29396100 -2.79905000

H 6.58003500 2.84028900 -3.77369400

C 7.45719100 4.35993700 -2.57593100

H 7.54657600 4.78833700 -1.58655200

H 8.01460200 4.82991900 -3.37277000

O 5.21601500 1.63802500 -1.93945200

C 6.60882500 0.51600200 1.82753600

O 6.36862500 0.07738700 0.63545400

C 7.65952900 -0.03255200 2.65420900

H 7.77364100 0.41787300 3.62972200

C 8.42312400 -1.03533400 2.22418500

H 8.27811700 -1.46676600 1.24272900

H 9.20734700 -1.45141800 2.83927700

O 5.85849000 1.46813800 2.24795700

U 4.62616100 1.48090400 0.29546000

F 3.19041700 0.08091800 0.51151400

$[U(acrylate)_3]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 2.51068700 0.76825100 0.47867300

O 3.35907300 -0.11483000 0.05785100

C 1.11965100 0.44173600 0.71317800

H 0.50099500 1.25432600 1.06644300

C 0.65088700 -0.78569000 0.50065900

H 1.29843900 -1.57606300 0.14531600

H -0.38603000 -1.03256000 0.67459600

O 2.95870300 1.94824100 0.67721200

C 6.03731700 2.84024600 -2.02455700

O 6.27283900 3.15878500 -0.79818300

C 6.51890900 3.62885700 -3.13783700

H 6.25948200 3.26170200 -4.12050800

C 7.23456800 4.73421400 -2.94206900

H 7.47586400 5.07364600 -1.94359800

H 7.59617600 5.32639500 -3.76965900

O 5.34459500 1.77376200 -2.22432000

C 6.67386200 0.19921400 1.93427400

O 6.68310000 -0.24424800 0.73347900

C 7.47588200 -0.37787200 2.99365400

H 7.38216100 0.08800800 3.96413400

C 8.27194600 -1.41950100 2.76438900

H 8.34059000 -1.86166200 1.77938400

H 8.87198100 -1.85592600 3.54916000

O 5.90317900 1.20736300 2.17794100

U 5.12026200 1.34038200 0.03141700

B3PW91

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 6.21960400 2.79308900 -1.90864700

O 5.92600700 3.32186100 -0.76825500

C 6.66566100 3.56292300 -3.04937200

H 6.87414700 2.99662600 -3.94750900

C 6.80588900 4.88744300 -2.97613700

H 6.58885700 5.42727200 -2.06253300

H 7.14149300 5.46076200 -3.83065800

O 6.08113800 1.51390400 -1.98329000

C 6.91149500 0.22615100 1.92457000

O 6.54987500 -0.38570700 0.84703900

C 7.74160900 -0.38132600 2.94178600

H 7.96820200 0.24005100 3.79814500

C 8.19041300 -1.63068000 2.81099200

H 7.94615700 -2.22890000 1.94170000

H 8.81296600 -2.08221300 3.57262000

O 6.47577200 1.43211200 2.05503700

U 5.26132900 1.34447900 0.13271500

F 3.26970100 1.09220000 0.31913700

TPSS

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

1 3

C 6.21573900 2.78022000 -1.89904700

O 5.91888400 3.31216000 -0.76391600

C 6.67347100 3.54665900 -3.03643100

H 6.88535300 2.98070200 -3.93424000

C 6.81811100 4.86916000 -2.95589800

H 6.59576300 5.40307800 -2.03955800

H 7.16201900 5.44612000 -3.80499000

O 6.07117300 1.50452100 -1.97353100

C 6.90355400 0.23806600 1.91605500

O 6.54025600 -0.37699700 0.84407300

C 7.74305000 -0.36401600 2.92767000

H 7.97299700 0.25742600 3.78335300

C 8.19392400 -1.61050500 2.78836800

H 7.94257800 -2.20392000 1.91723400

H 8.82412200 -2.06410200 3.54283100

O 6.46341600 1.43927200 2.04789600

U 5.24594500 1.34326000 0.13473100

F 3.25995900 1.08894700 0.32273900

MP2

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms) (calculation 1, starting from square pyramidal geometry, after 19 steps)

1 3

C 6.15921100 2.68051700 -1.82447200

O 5.81572600 3.23638600 -0.70764600

C 6.75036600 3.42383600 -2.90775500

H 6.99286400 2.86578600 -3.79365600

C 6.97142300 4.73511600 -2.78579000

H 6.71101400 5.25279900 -1.87777200

H 7.41349800 5.29745600 -3.58942900

O 5.95007300 1.41258800 -1.92755700

C 6.80780900 0.31708900 1.85244900

O 6.40751700 -0.34364000 0.81252700

C 7.76131200 -0.22270200 2.78798300

H 8.02445500 0.40635800 3.61865100

C 8.27047000 -1.44355000 2.60482900

H 7.97556600 -2.03888200 1.75692100

H 8.98321900 -1.85424900 3.29823400

O 6.31353000 1.49367500 2.01491700

U 5.05118100 1.30895100 0.14440200

F 3.07107900 1.06251900 0.34050200

$[UF(acrylate)_2]^+$ cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms) (calculation 2, starting from distorted trigonal bipyramidal geometry, after 18 steps)

1 3

C 6.18088900 2.73103300 -1.76639100

O 5.84992200 3.25901200 -0.69813800

C 6.73278900 3.43531700 -2.90194600

H 6.96996600 2.83799600 -3.76820600

C 6.92705000 4.74968300 -2.85987400

H 6.67421200 5.31499300 -1.96943600

H 7.33868200 5.27288600 -3.71065400

O 6.00610500 1.47182500 -1.81050100

C 6.81209000 0.30242500 1.85673100

O 6.46107700 -0.31530700 0.80956800

C 7.74344500 -0.25918100 2.80756900

H 7.98832600 0.34865400 3.66499900

C 8.25793500 -1.48007200 2.60737700

H 7.97938900 -2.05504600 1.73117200

H 8.95290100 -1.91057900 3.31308600

O 6.32922500 1.47742200 2.02721000

U 5.09843900 1.32521500 0.20354100

F 3.12787200 1.08377300 0.28123100

Reaction Intermediates, Transition States

B3LYP

cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Formic Acid

Structure II

1 3

U -0.04091400 0.72607400 0.34126500

F -2.00537200 1.00972000 -0.05594500

F 1.46404600 1.82400900 -0.45155300

C 0.57254200 -2.56189100 -0.76182600

H 0.75522700 -3.55594500 -1.10323500

C 0.36411000 -1.42555200 -0.37466400

C 0.32150200 1.01964300 3.91015600

H 1.16611000 0.70026200 4.52644600

O 0.33662700 0.87815700 2.68965100

O -0.70436200 1.55524600 4.49573600

H -0.60591600 1.61585800 5.46030600

Transition State I

1 3

U 0.11163700 0.86863700 0.47366900

F -1.46009900 1.32444100 -0.70601100

F 1.83982500 1.29437100 -0.46882100

C 0.07319100 -1.37361100 1.56611200

C -0.07698200 -2.16563200 0.65162500

H -0.20750800 -2.89115100 -0.12404400

C 0.23970400 0.96312500 3.75748200

H 0.28307400 1.61940800 4.62766800

O 0.17507400 1.52976500 2.59401500

O 0.25388000 -0.26594400 3.91876600

H 0.18129200 -0.83242000 2.82791900

Structure III

1 3

C 1.50703600 -0.22176500 -0.28905400

H 0.48028700 -0.57459700 -0.40612800

O 1.75608200 1.01705500 -0.14003500

O 2.48102500 -1.04210700 -0.29814900

U 4.03896000 0.63836000 0.01002000

F 4.64928200 0.73320000 -1.91454500

F 4.15107500 0.53585100 2.03020400

C 4.42281400 3.43345600 0.75736600

H 4.34410100 3.45698800 1.82357700

C 4.52087200 3.49303700 -0.44130600

H 4.61990300 3.61836000 -1.49847400

Structure V

1 3

C 1.15067900 0.00169000 -0.21130500

H 0.06629400 -0.08372400 -0.31173100

O 1.69045200 1.10692400 0.09294900

O 1.89415000 -1.01872300 -0.40046600

U 3.84906800 0.14300300 0.02074700

F 4.59741400 0.21036700 -1.86601400

F 4.33630000 -0.67828900 1.81309100

C 5.28169000 3.32160600 0.89163400

H 4.70637700 4.23329600 1.07317900

O 4.72720000 2.26754100 0.59698800

O 6.57435700 3.37531200 0.99481700

H 6.90054500 4.25849800 1.23216800

Transition State II

1 3

U 3.82008100 0.49348400 -0.85029400

F 3.23964200 -0.26516300 -2.60628400

F 3.13988900 2.78239700 -1.01873300

C 6.16397900 0.11987900 0.42944500

H 7.10862400 -0.03645000 0.95415800

O 5.87001900 -0.55724700 -0.60827600

O 5.32501600 0.98909900 0.84301000

C 1.14779600 0.49315100 0.31272600

H 0.21477500 0.16282500 0.77385800

O 2.20344300 -0.22873900 0.50651700

O 1.18187000 1.51808300 -0.39359300

H 2.19873600 2.54327000 -0.77326500

Structure VI

1 3

C 1.45286100 0.32437900 0.47485500

H 0.54725700 0.19039100 1.07054900

C 5.87117600 0.18211200 0.52635300

H 6.73484800 0.02069600 1.17524100

O 1.78079900 1.46402600 0.02613400

O 2.20463800 -0.67420400 0.21341500

O 5.62281200 -0.60761100 -0.43689200

O 5.08879400 1.17232200 0.72800500

U 3.69012900 0.56101900 -1.02983600

F 3.22696000 -0.02552500 -2.89710200

F 3.67541300 3.00792600 -1.69465000

H 3.15171700 3.77051700 -1.54954400

Structure VIII

1 3

C 1.32961100 0.40534900 0.20623900

H 0.42377700 0.46713000 0.81441900

C 5.69593000 0.46187100 0.50589900

H 6.52676000 0.52410300 1.21288600

O 2.10910100 1.41304100 0.11736300

O 1.62037500 -0.66021700 -0.41444500

O 4.91410000 -0.54280300 0.52258100

O 5.49601100 1.38545100 -0.34146800

U 3.62678800 0.26092100 -1.24524700

F 4.22133600 -1.01763900 -2.69165100

C 3.13100200 2.65975100 -3.89567200

H 3.73694100 3.55407100 -4.06501800

O 3.33120600 1.92721800 -2.93463700

O 2.18193200 2.39082900 -4.74321400

H 2.12187000 3.04074500 -5.46167900

Transition State III

1 3

U 3.70198500 0.42727100 -0.63258100

F 3.61374500 2.60475400 -1.71974900

C 1.45620300 0.42440400 0.85152200

H 0.55067900 0.40674700 1.46173300

C 5.97698800 0.24838800 0.80570600

H 6.89585500 0.14609300 1.38685100

O 5.09724900 -0.68038700 0.81546400

O 5.75401900 1.28080900 0.10507100

O 2.34446600 1.31815600 1.03079500

O 1.64440400 -0.45352200 -0.05641900

C 3.42860000 -0.14679800 -3.50741200

H 3.37068800 -0.70477100 -4.44482100

O 4.04738200 -0.71199500 -2.51628400

O 2.90223400 0.97071500 -3.38750900

H 3.30117700 2.23703200 -2.57605100

Structure IX

1 3

C 1.29070400 0.43201900 0.55499600

H 0.31912900 0.40855400 1.05425800

C 6.10128900 0.24905700 0.55420000

H 7.05766900 0.14617200 1.07162800

O 1.91993700 1.51999300 0.39524900

O 1.81623900 -0.64408000 0.11740400

O 5.05443700 -0.32537800 1.01869000

O 6.00162300 0.93129400 -0.50772100

U 3.71386000 0.39454600 -0.70942100

C 3.47514300 -0.36483300 -3.29797300

H 3.35797700 -0.66925100 -4.34036400

O 3.11356400 0.79859300 -2.91899700

O 3.96989300 -1.15680300 -2.43852800

F 3.89869900 2.94305900 -0.80992600

H 3.21542500 3.52487900 -0.54536000

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acetic Acid

Structure II

1 3

U 0.74580500 0.45880000 0.44948800

F -0.48369000 2.02726700 0.09749700

F 2.42543400 0.74016200 -0.64587800

C -0.92805800 -2.52460100 -0.43966800

H -1.43668100 -3.39827700 -0.78026800

C -0.34635600 -1.52564800 -0.05295800

C 1.82748200 -0.38336800 3.72152000

O 1.25695600 0.06417900 2.71343000

O 2.96186000 -1.00694600 3.53020500

H 3.36160700 -1.33671400 4.34972000

C 1.28493800 -0.21220400 5.09697700

H 1.37295700 -1.13670500 5.66839000

H 1.87248800 0.55488300 5.60999700

H 0.24870100 0.10739800 5.05920700

Transition State I

1 3

U 0.70405700 0.57650900 0.74092800

F -0.76679800 1.89813900 0.31781600

F 2.34624300 0.97298300 -0.36507300

C 0.10006200 -1.85693100 0.93916900

C -0.39159600 -2.11426700 -0.14562600

H -0.82892600 -2.38376200 -1.08400800

C 1.29521600 -0.72374300 3.71715900

O 1.24086300 0.25185100 2.83163600

O 0.93051700 -1.87135800 3.40596800

H 0.53347300 -1.90410600 2.22500900

C 1.79954000 -0.39726700 5.07396100

H 1.80602800 -1.28062300 5.70333700

H 2.80407800 0.02111600 4.99166100

H 1.16813000 0.37771700 5.51228900

Structure III

1 3

C 2.41935400 0.48710400 -0.11262400

O 2.81867700 1.45824200 -0.85044300

O 3.34457300 -0.19321100 0.47833400

C 0.98985700 0.13474500 0.03364100

H 0.78095500 -0.70960500 -0.63020600

H 0.78977600 -0.19596900 1.05107600

H 0.35488700 0.96842000 -0.25113500

U 5.07012700 0.92967400 -0.50616100

F 5.57554900 0.10446100 -2.27980400

F 6.73212900 0.82925800 0.65730600

C 4.86982900 3.86845700 -0.51213800

H 3.96421700 4.09031100 -1.03460700

C 5.89767500 3.71947400 0.09623500

H 6.81641100 3.63869900 0.63634500

Structure V

1 3

C 2.17625700 -0.03084900 0.00273000

O 2.76811500 1.05066900 0.33565900

O 2.90811200 -1.09068600 -0.07241700

C 0.72264800 -0.08883500 -0.28797500

H 0.57923700 -0.46088000 -1.30365200

H 0.25544900 -0.81211200 0.38208700

H 0.26408500 0.88782400 -0.17302500

U 4.84930800 -0.02657300 0.51401800

F 5.82235500 -0.11262200 -1.27684000

F 5.12146500 -0.83955600 2.36527900

C 6.62086300 2.91674900 1.45553500

O 5.82556300 2.03203500 1.11723100

O 7.87169300 2.56002800 1.62685900

H 8.44372800 3.29638700 1.89052500

C 6.21518200 4.33449100 1.67041400

H 6.43270100 4.62598200 2.70039200

H 6.79156200 4.98769000 1.01183300

H 5.15602200 4.45967500 1.47313800

Transition State II

1 3

U 5.11647400 0.36347900 1.24474000

F 5.53819300 -0.51886500 2.99944400

F 6.47318300 2.26864600 1.59652200

C 2.78230000 0.42676900 -0.12054900

O 2.98694100 -0.42093400 0.81870800

O 3.75586500 1.24275400 -0.37010700

C 1.52345900 0.46664000 -0.89539800

H 1.27505700 1.49288400 -1.15815800

H 1.68651100 -0.08097800 -1.82879800

H 0.72068000 -0.01629100 -0.34560200

C 7.35394000 -0.00682200 -0.62966200

O 6.50891300 -0.80476700 -0.05063800

O 7.36126100 1.21967800 -0.32870200

C 8.29029400 -0.56056300 -1.63874000

H 7.76279400 -1.23773300 -2.30871000

H 8.78278300 0.23615700 -2.18649900

H 9.04109200 -1.15540500 -1.11118900

H 7.02677700 1.97515900 0.76136100

Structure VI

1 3

C 2.91679700 0.36344400 -0.06207300

O 3.36440500 1.55990300 -0.11878600

O 3.68522700 -0.50615100 0.50050200

C 1.58246100 -0.01538000 -0.58365800

H 1.62531200 -1.00375800 -1.03691100

H 0.89274600 -0.07509800 0.26298700

H 1.21597000 0.72951500 -1.28360300

U 5.34178000 0.97464900 1.00918000

C 7.36008200 -0.10615800 -0.45133600

O 7.16578400 -0.42586200 0.77633000

O 6.55976800 0.77323000 -0.94848100

F 5.07843200 1.22194000 3.00031600

C 8.42815000 -0.73281200 -1.26399900

H 8.00570700 -1.62136800 -1.74281200

H 8.76077800 -0.05534200 -2.04619900

H 9.25000900 -1.05214500 -0.62838300

F 5.39521700 3.49398400 0.60866100

H 4.77770800 4.05685000 0.18763400

Structure VIII

1 3

C 2.70727000 0.10391800 0.05522400

O 3.45971900 0.87117500 -0.65247700

O 3.10725100 -0.17540300 1.23711800

C 1.44509600 -0.45559700 -0.49266700

H 1.68167800 -1.41173800 -0.96765000

H 0.73546400 -0.64576000 0.30831400

H 1.02994500 0.20379200 -1.25017800

U 5.09531200 1.03518200 1.00181600

C 7.05909800 -0.08339800 -0.53299200

O 6.31000700 -0.78596000 0.23702700

O 6.83895000 1.17695800 -0.56323800

F 5.84425000 1.15170700 2.88857000

C 8.14605500 -0.70970200 -1.32878700

H 7.84472000 -1.69995900 -1.66266700

H 8.42546100 -0.07454900 -2.16427400

H 9.01489700 -0.83202800 -0.67664000

C 4.49303300 4.53534400 1.45515400

O 4.78967900 3.39920000 1.07827400

O 3.58759900 4.63878700 2.40373900

H 3.40665200 5.55712700 2.65242900

C 5.11558200 5.76844400 0.89213600

H 4.34501000 6.47376400 0.57689300

H 5.71443500 6.25336300 1.66704800

H 5.75331200 5.51833300 0.05110500

Transition State III

1 3

C 2.71366000 0.45827700 -0.14955800

O 3.47912700 0.90095200 -1.07176200

O 3.18357300 0.50468100 1.05320300

C 1.36684500 -0.09373800 -0.42578400

H 1.40126200 -1.17450100 -0.26637200

H 0.65028900 0.31002300 0.28858200

H 1.06572400 0.11388000 -1.44765300

U 5.18485300 1.41790700 0.42365800

C 7.05815600 -0.06204800 -0.84228900

O 6.27469400 -0.58948200 0.02340200

O 6.90373600 1.20112300 -1.06299900

F 6.69478500 1.58847000 2.33535800

C 8.10276900 -0.84211700 -1.54438900

H 7.92945200 -1.90787300 -1.43231300

H 8.14037700 -0.54995900 -2.59261500

H 9.07001500 -0.58676800 -1.10280600

C 4.80442200 4.08592500 1.59891200

O 4.92369700 3.65671300 0.38043600

O 5.02575200 3.28091100 2.54617500

H 6.14667300 2.36220600 2.66904900

C 4.40135500 5.49526500 1.83683600

H 4.14887900 5.65288100 2.88039800

H 5.24228400 6.13909600 1.56562200

H 3.57304200 5.76489400 1.18326500

Structure IX

1 3

C 2.47467800 0.02751000 -0.40625600

O 3.10221800 1.08694600 -0.74786100

O 3.09600700 -0.77191900 0.38566800

C 1.11086300 -0.28759800 -0.89799300

H 1.18122200 -1.13028100 -1.58996500

H 0.48692900 -0.61164400 -0.06583900

H 0.67278100 0.56497400 -1.40711200

U 5.02148700 0.49037000 0.54235200

C 7.30149800 -0.17681900 -0.78013000

O 6.21613100 -0.87678500 -0.85444300

O 7.24894200 0.88554300 -0.07487500

C 8.53102100 -0.60369200 -1.49026300

H 8.33123600 -0.61422500 -2.56354200

H 9.35721900 0.06412600 -1.26919500

H 8.77277000 -1.62798600 -1.20418000

C 5.08054700 0.86583800 3.23820800

O 5.49154400 -0.22304600 2.70705000

O 4.65156100 1.77168900 2.42947900

C 5.07565200 1.07803400 4.70589700

H 5.39184300 2.09408200 4.93527200

H 4.04812700 0.96941400 5.06284700

H 5.70323700 0.34446800 5.20257000

F 5.05225200 2.84677600 -0.49672200

H 4.25026100 3.08351500 -0.91731500

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Propionic Acid

Structure II

1 3

U 1.20088900 2.86881700 -3.34719300

F 0.00335900 3.87062600 -4.63780200

F 3.16980300 2.99804700 -3.80569200

C 0.14856400 -0.52929400 -2.89899800

H -0.14506800 -1.55498800 -2.85244700

C 0.48835000 0.63959800 -2.97143100

C 0.23412500 2.58953200 -0.07821500

O 0.67311700 3.12998700 -1.13793800

C 0.10511000 3.37266800 1.18023700

H -0.51405300 4.23976400 0.92676400

H 1.09843200 3.79332100 1.36973600

C -0.43549200 2.62066200 2.39069900

H -0.48100500 3.29905000 3.23997300

H -1.43845300 2.23903100 2.20941500

H 0.20573800 1.78390700 2.66102900

O -0.11233500 1.34817300 -0.06014800

H 0.00832300 0.90801800 -0.94303300

Transition State I

1 3

U 0.69943600 0.58051700 0.74191400

F -0.76458100 1.91104400 0.31595900

F 2.35898400 0.99223100 -0.33426900

C 0.09549500 -1.85765900 0.90804100

C -0.40675300 -2.09129600 -0.17729800

H -0.85376000 -2.34165200 -1.11632500

C 1.28821000 -0.75836800 3.70083500

O 1.22634100 0.22820400 2.82330800

O 0.93109600 -1.90328000 3.37219900

C 1.79399200 -0.43212100 5.06412300

H 2.77657700 0.02965600 4.92174500

H 1.16066000 0.37947700 5.43742200

C 1.84865600 -1.60615100 6.03306100

H 0.86184300 -2.03684000 6.19221400

H 2.50691700 -2.39241400 5.66820000

H 2.22857700 -1.26407700 6.99356900

H 0.53432300 -1.92153500 2.19383200

Structure III

1 3

C 2.54263100 -0.69279700 -0.15933800

O 3.32293900 -0.09400400 -0.99125000

O 3.12563400 -1.39989500 0.74856800

U 5.24405200 -0.74973600 0.06549600

C 1.06189300 -0.57463200 -0.21747500

H 0.75162600 -0.20683800 0.76639900

H 0.67860100 -1.59962400 -0.25758200

C 0.51847300 0.28800400 -1.35026200

H -0.56836000 0.30361600 -1.30191900

H 0.87427500 1.31396400 -1.27651800

H 0.80746000 -0.10259800 -2.32432600

F 5.77179800 0.54145700 1.52963000

F 6.78600900 -0.75608000 -1.25901900

C 5.42146500 -3.61187900 0.75042600

H 4.59041300 -3.80026900 1.39531100

C 6.37630900 -3.49930100 0.02640300

H 7.23635000 -3.44803100 -0.60591600

Structure V

1 3

C 2.06015400 0.57204500 -0.56788300

O 2.36635300 1.77771900 -0.22054800

O 3.04008200 -0.19068900 -0.89665200

U 4.62852700 1.44218200 -0.51203600

C 0.64402400 0.11471000 -0.57761100

H 0.10393300 0.82039800 -1.21712000

H 0.25848200 0.30793400 0.42871200

C 0.42755200 -1.33110800 -1.00756000

H -0.63569300 -1.56108000 -0.98102200

H 0.78532900 -1.50395000 -2.02095500

H 0.94023500 -2.02551400 -0.34442300

F 5.48612700 1.02598500 1.35790000

F 5.95248500 1.40880200 -2.05245400

C 5.60248500 4.21166300 1.20149700

O 5.09389500 3.58806700 0.23167900

C 5.68537600 5.69863000 1.20016500

H 4.66346200 6.05153000 1.02839300

H 6.22349800 5.96181600 0.28364600

C 6.31169600 6.34277200 2.43134300

H 6.31406900 7.42362000 2.30659800

H 5.75162300 6.10849900 3.33466900

H 7.34040100 6.01733400 2.57374900

O 6.07504600 3.58535600 2.23399300

H 5.97914400 2.60959900 2.14970000

Transition State II

1 3

U 4.54469200 -0.25261900 -0.34292300

F 5.83848100 0.75734100 0.82600300

F 4.18248000 -2.13968700 0.97830800

C 5.19755400 -0.18551800 -2.96065800

O 4.58780300 0.78865500 -2.36476900

O 5.44111800 -1.21575500 -2.23411200

C 5.58745500 -0.08638200 -4.39077300

H 6.22554600 0.80118900 -4.46402900

H 4.67790500 0.18874800 -4.93444200

C 6.25877000 -1.32457100 -4.97259500

H 6.50284900 -1.14504700 -6.01758900

H 7.18127000 -1.56291300 -4.44650000

H 5.60520800 -2.19372000 -4.92294200

C 1.67991000 -0.58530100 -0.03104400

O 2.37601300 0.46026400 0.13969600

O 2.31904900 -1.68876500 -0.30779800

C 0.19589600 -0.59198300 0.03356100

H -0.14600300 -1.05496300 -0.89796600

H -0.06445300 -1.32437900 0.80638100

C -0.45793500 0.76104500 0.28390800

H -1.53856500 0.63950100 0.31864900

H -0.13565500 1.19060900 1.23063800

H -0.22312000 1.46987600 -0.50827200

H 3.18360800 -2.14936200 0.50462800

Structure VI

1 3

C 1.82326800 -0.47042200 -0.00315600

O 2.40322100 0.60471500 -0.40686700

O 2.59696100 -1.45459000 0.28243100

U 4.52581900 -0.22068300 -0.19355700

F 5.18589000 0.69502100 1.48879300

C 0.34461500 -0.57701100 0.13861400

H 0.16216000 -0.82751100 1.18893400

H 0.04955800 -1.47428800 -0.41367200

C -0.44472800 0.65209000 -0.29587400

H -1.50761700 0.47167600 -0.14805600

H -0.16682200 1.53007700 0.28419500

H -0.28404000 0.87739800 -1.34877800

C 5.34113200 -0.09133500 -2.77903400

O 5.52231900 0.87720200 -1.94812800

O 4.76915500 -1.14340200 -2.31048000

C 5.77125400 0.02785200 -4.19889200

H 6.82016100 0.33863300 -4.17274700

H 5.23947400 0.89834700 -4.59779800

C 5.55721200 -1.21324800 -5.05643600

H 5.89928700 -1.01636700 -6.07048200

H 6.11562300 -2.06516100 -4.67210600

H 4.50561900 -1.49041400 -5.10268800

F 5.21119100 -2.51849600 0.68229200

H 4.64457100 -3.21623200 0.94232500

Structure VIII

1 3

C 1.42828800 -0.19705300 -0.32255300

O 1.47813700 1.04873800 -0.61537800

O 2.55187300 -0.82468800 -0.29078200

U 3.80154500 1.03788800 -0.83251900

F 4.64939600 1.35963800 1.05914000

C 0.15119900 -0.90747300 -0.02587100

H 0.27344800 -1.34588800 0.96942500

H 0.11785000 -1.76644400 -0.70274000

C -1.10744700 -0.05421000 -0.12218600

H -1.97932900 -0.66266500 0.11045600

H -1.07943600 0.77780100 0.57932300

H -1.23671900 0.35323000 -1.12340800

C 4.86145600 0.15512500 -3.17932300

O 3.72938100 0.77218800 -3.12477900

O 5.48499500 0.00226500 -2.07239400

C 5.38707400 -0.35091500 -4.47968100

H 5.38480700 0.50300000 -5.16365000

H 4.61666200 -1.02112600 -4.87409300

C 6.74969700 -1.02935500 -4.41114100

H 7.04010100 -1.36424300 -5.40511600

H 7.51669500 -0.34801800 -4.04673300

H 6.73012400 -1.89668100 -3.75382100

C 4.69372800 4.27801600 -0.14604300

O 4.24544700 3.35139300 -0.86567100

C 4.70826700 5.69026700 -0.62629300

H 3.67394400 5.91903500 -0.90145900

H 5.24848000 5.67418000 -1.57784000

C 5.28152600 6.72607800 0.33372000

H 5.23575400 7.70914400 -0.13056400

H 4.71735300 6.76553500 1.26359700

H 6.32147400 6.51530900 0.57594500

O 5.16403300 4.04889200 1.04349700

H 5.10254600 3.09475000 1.27800000

Transition State III

1 3

U 4.03646900 1.17600800 -0.58375000

F 3.83250300 3.33437200 -1.62656700

C 1.76875700 -0.10128000 0.17662800

O 1.70971000 1.06180200 -0.34032200

O 2.95609400 -0.61107900 0.29780900

C 0.57083800 -0.86118700 0.62713100

H 0.75113500 -1.11687700 1.67607400

H 0.60627100 -1.82065500 0.10127900

C -0.76140500 -0.14798100 0.43134000

H -1.56950100 -0.78269800 0.78958000

H -0.79650300 0.78910700 0.98409000

H -0.94464600 0.07255800 -0.61876800

C 5.72150000 1.47784300 1.52698700

O 5.97102200 0.63645500 0.59744700

O 4.63483300 2.16488900 1.39167400

C 6.60705900 1.67836800 2.70637600

H 5.97914500 1.50247700 3.58594000

H 6.83117400 2.74906200 2.74011400

C 7.86918300 0.82487300 2.72530500

H 8.44133300 1.04236500 3.62505300

H 7.63183900 -0.23743700 2.72349300

H 8.50266200 1.03145500 1.86438300

C 5.25787400 1.00247100 -3.23579600

O 5.54325000 2.12427500 -2.69796100

O 4.40276100 0.24787500 -2.64078500

C 5.92693100 0.57595900 -4.49852600

H 6.99892700 0.72489500 -4.34119000

H 5.65373400 1.32998500 -5.24482400

C 5.60444200 -0.83373500 -4.97807000

H 6.13533000 -1.03184100 -5.90715700

H 5.91071900 -1.58278700 -4.24956800

H 4.53936900 -0.95831900 -5.16502900

H 4.58576100 3.04371400 -2.26126400

Structure IX

1 3

C 1.72712500 -0.14905700 0.07009900

O 1.82850500 0.97676000 -0.52595500

O 2.83553000 -0.70222500 0.43156800

U 4.16633800 1.00074500 -0.33471500

C 0.41992400 -0.80604600 0.35346100

H 0.39136600 -0.96892300 1.43542400

H 0.48751900 -1.81114000 -0.07399100

C -0.80892200 -0.05365800 -0.14222700

H -1.70666700 -0.61342500 0.11291300

H -0.88364900 0.93186600 0.31402200

H -0.78761700 0.07580200 -1.22299500

C 5.03051400 0.72978700 -2.93051100

O 4.79243200 1.88971200 -2.42707200

O 4.83702800 -0.27318300 -2.15884900

C 5.50475900 0.58301800 -4.33653200

H 6.40606100 1.19863900 -4.41697000

H 4.76549300 1.09172700 -4.96298500

C 5.75114800 -0.84922500 -4.79534800

H 6.09522800 -0.84709600 -5.82782200

H 6.51013600 -1.33691200 -4.18632200

H 4.84239400 -1.44622400 -4.74287600

C 5.97001400 1.44832400 1.65982400

O 6.25489300 0.69002100 0.67066800

O 4.81561800 2.02475000 1.62117100

C 6.89294200 1.66753800 2.80923500

H 6.32918300 1.39497500 3.70682900

H 7.02737800 2.75083000 2.88730300

C 8.22367500 0.92990500 2.72493000

H 8.82113100 1.15517300 3.60622300

H 8.07952800 -0.14814600 2.68044000

H 8.79121200 1.23079700 1.84600600

F 3.53577600 3.49007500 -0.71552100

H 3.71405300 3.80039600 -1.57952600

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acrylic Acid

Structure II

1 3

U 1.29232800 2.83877200 -3.26822900

F 0.20977800 3.95385800 -4.56851000

F 3.27754700 2.84333600 -3.67408300

C 0.00427300 -0.49226200 -2.95929800

H -0.35616900 -1.49728900 -2.95771800

C 0.42055300 0.65356400 -2.97945900

C 0.22427400 2.54468700 -0.03497900

O 0.72823100 3.08221200 -1.07167500

C 0.12589300 3.29260000 1.20043300

H 0.50311400 4.30376600 1.15763000

C -0.39455600 2.77029100 2.31487300

H -0.45425700 3.35563500 3.22169600

H -0.77045300 1.75710700 2.35057600

O -0.20754300 1.32231400 -0.06035700

H -0.09278400 0.90294000 -0.95105600

Transition State I

1 3

U -1.68285200 1.04254700 -1.54462200

F -3.45172100 1.84976900 -2.11417700

F 0.20334800 1.26250500 -2.25078600

C -1.99427200 -1.17929900 -0.43133400

C -2.16268200 -1.95167400 -1.35697500

H -2.31528100 -2.66887900 -2.13523600

C -1.53257000 1.20906700 1.71443000

C -1.35417400 2.09169400 2.85594800

C -1.15627400 3.40456800 2.73387600

O -1.49938100 1.71586200 0.48732800

O -1.71545900 -0.01260000 1.87939800

H -1.39466500 1.59928700 3.81701300

H -1.02800300 4.02828700 3.60727200

H -1.11696600 3.89001200 1.76893700

H -1.85128200 -0.61067800 0.76065600

Structure III

1 3

C 2.47392700 -1.11209100 -0.29093900

O 3.26701000 -0.31349600 -0.93799900

O 3.01671300 -1.77996300 0.66990800

U 5.07137800 -0.72776600 0.38109900

C 1.06726300 -1.25048100 -0.60280500

H 0.51521700 -1.94320200 0.01628300

C 0.50284700 -0.55743400 -1.59513200

H -0.54834900 -0.66660400 -1.82222800

H 1.07637500 0.13199200 -2.19983000

F 5.18747600 0.51356500 1.97540100

F 6.76887300 -0.42992000 -0.70017600

C 5.60108800 -3.57158600 0.97549700

H 4.71347300 -3.93013700 1.45005800

C 6.63317200 -3.25871700 0.44137800

H 7.56750300 -3.02928500 -0.02362700

Structure V

1 3

C 2.91038300 0.56334200 0.06635100

O 3.41816900 1.60470700 0.63433600

O 3.69638500 -0.09265400 -0.72516900

U 5.47138300 1.32317800 -0.39705700

C 1.53614400 0.17283300 0.31669400

H 0.98497400 0.80747300 0.99589300

C 1.00247600 -0.90465800 -0.26220900

H -0.02240800 -1.18989200 -0.07083300

H 1.57704100 -1.52342900 -0.93808800

F 7.10222500 0.18561800 0.03012200

F 5.60688500 2.48823200 -2.14020000

C 6.54250200 4.49713800 0.15484500

O 6.22434100 3.32339500 0.49844800

C 6.97761800 5.51553800 1.09326000

H 7.21532800 6.47794800 0.66369000

C 7.07749400 5.26863800 2.40022800

H 6.83815400 4.29937200 2.81527400

H 7.40444200 6.03727500 3.08601700

O 6.50162800 4.87746000 -1.09111200

H 6.20165900 4.15556900 -1.68703200

Transition State II

1 3

U 5.74884200 1.31302100 -0.41735800

F 7.12585900 -0.16218400 -0.45794400

F 6.40882900 2.55418400 -2.28356700

C 3.23459100 0.50506100 0.13356000

O 4.12814000 0.66898200 1.05505300

O 3.61742800 0.78483900 -1.06994200

C 1.90543100 0.03359400 0.45977000

H 1.72228300 -0.16615800 1.50592800

C 0.97867900 -0.14047500 -0.48568500

H -0.01160000 -0.49452600 -0.23574400

H 1.18902900 0.06552000 -1.52647500

C 6.14236700 4.05918100 0.43134700

O 6.58626000 2.97748200 0.94943100

C 6.29617500 5.35764100 1.05385000

H 5.86455600 6.19007600 0.51689200

C 6.94455900 5.50438100 2.21261700

H 7.37215000 4.65724600 2.73163700

H 7.06286400 6.47948000 2.66397500

O 5.49282500 3.96117800 -0.69288300

H 6.04170400 3.42029400 -1.71006000

Structure VI

1 3

C 6.32781200 2.93889000 -1.83396400

O 5.98248100 3.70782700 -0.85770900

C 6.90702100 3.43127700 -3.07125300

H 7.14615000 2.67758100 -3.80791400

C 7.12417300 4.73205300 -3.27015800

H 6.87515900 5.46563500 -2.51547600

H 7.55660500 5.09039100 -4.19367300

O 6.12677900 1.67651100 -1.65847900

C 7.01980600 0.53458200 1.84639100

O 6.00240100 -0.02654400 1.28386900

C 8.02173500 -0.20474700 2.59199300

H 8.82048700 0.38615200 3.01708300

C 7.94816900 -1.52977200 2.73048800

H 7.13847800 -2.09718900 2.29200500

H 8.69898200 -2.07459300 3.28531800

O 7.11159100 1.81624400 1.71143000

U 5.20061200 1.94802800 0.41869300

F 3.22081400 1.64158800 0.05779900

F 4.09162000 3.26660000 2.35139200

H 3.21524000 3.48785000 2.58939300

Structure VIII

1 3

C 6.39995600 2.65579100 -2.05056700

O 5.87400300 2.76791200 -0.87949000

C 6.98235300 3.78196000 -2.76533700

H 7.39773900 3.55429500 -3.73674400

C 6.99306000 5.00922600 -2.24527200

H 6.56748700 5.20946800 -1.27136400

H 7.42670500 5.84013500 -2.78362100

O 6.38481800 1.48107000 -2.57518300

C 6.78276100 -0.21346300 1.38615400

O 7.23952100 -0.27539800 0.18000100

C 7.57689300 -0.58035100 2.54917100

H 7.07547800 -0.48963900 3.50232400

C 8.83917500 -0.99283300 2.43347500

H 9.31816100 -1.07059100 1.46692400

H 9.42115100 -1.25947700 3.30440200

O 5.57229100 0.19828100 1.52276300

U 5.28220000 0.53619600 -0.75752600

F 3.20935400 0.77642000 -0.97446100

C 3.63024800 -2.13533300 -2.12167600

O 4.64561000 -1.52573000 -1.69529600

C 3.68213700 -3.46005500 -2.72109300

H 2.73424100 -3.86838600 -3.04051400

C 4.83199000 -4.11839500 -2.86572200

H 5.77215900 -3.69359500 -2.54180300

H 4.85636400 -5.10093900 -3.31503200

O 2.43573500 -1.61265800 -2.05341800

H 2.45880700 -0.71302600 -1.65704300

Transition State III

1 3

U 5.65311800 0.17500200 -0.87068400

F 3.33953900 1.12840300 -0.12869600

C 6.56350600 2.46409000 -2.04764600

O 5.32315900 2.31696100 -1.74936300

C 7.09272900 3.65323400 -2.69928000

H 8.15543400 3.64495200 -2.89595900

C 6.30590400 4.67880500 -3.02428100

H 5.24516100 4.66007700 -2.81393200

H 6.70623200 5.55914300 -3.50697600

O 7.34582100 1.48680800 -1.73635700

C 6.73646700 -0.36971200 1.57209500

O 7.19471400 -0.89007900 0.48853700

C 7.31760200 -0.62513500 2.88157200

H 6.83579300 -0.13020000 3.71276400

C 8.37903600 -1.41766900 3.03091900

H 8.84384700 -1.89839800 2.18087000

H 8.80623000 -1.60120600 4.00667600

O 5.71757100 0.40848500 1.44507800

C 4.52292200 -1.96251500 -2.13301400

O 5.51517200 -1.29721300 -2.62827000

C 3.94846900 -3.12298900 -2.79529700

H 3.12388700 -3.59475900 -2.28000800

C 4.41899600 -3.56602000 -3.96144500

H 5.24605300 -3.07519800 -4.45613700

H 3.98638800 -4.43006900 -4.44578400

O 4.05937100 -1.54514100 -1.01076900

H 2.74981400 0.76974000 0.49786500

Structure IX

1 3

C 2.33757600 0.80728200 0.40131200

O 3.30608000 0.04636700 0.02381300

C 0.96464700 0.33873800 0.51169900

H 0.24312300 1.07305800 0.84085800

C 0.62980500 -0.91807100 0.21900800

H 1.37078700 -1.63366500 -0.11048300

H -0.39307300 -1.25738800 0.30182100

O 2.64859300 2.02124900 0.67988800

C 5.98801300 2.86144400 -2.02718900

O 6.36490800 3.20321900 -0.84772200

C 6.52712100 3.45425400 -3.24059600

H 6.12667200 3.06953900 -4.16771500

C 7.45501000 4.41068600 -3.19504800

H 7.83677500 4.77790500 -2.25207700

H 7.85195200 4.84661800 -4.10096900

O 5.07980300 1.94172300 -2.09776000

C 6.60630300 0.44510600 1.96637600

O 6.58775900 0.10855800 0.72466100

C 7.46547900 -0.19411000 2.95091400

H 7.38701400 0.18757700 3.95892600

C 8.29174100 -1.18518600 2.61588800

H 8.34954200 -1.54770700 1.59854300

H 8.92788600 -1.65494400 3.35272000

O 5.80942800 1.39808800 2.31187400

U 4.95335000 1.65840300 0.17732500

F 4.32440900 3.92780200 1.23273800

H 3.41356100 3.92107800 1.45221800

PBE0

cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Formic Acid

Structure II

1 3

U 0.13836500 1.11385700 0.10217900

F -1.85478800 1.35429400 0.08882400

F 2.01366500 1.52697500 -0.48517400

C 0.27850000 -2.37961800 -0.09093300

H 0.33391500 -3.44139800 -0.20198400

C 0.21358500 -1.16991900 0.03314800

C 0.23757300 1.22222700 3.58872600

H 0.62184200 1.90298000 4.35523200

O 0.35605600 1.49071300 2.39859700

O -0.34215600 0.13198600 3.96244700

H -0.37295700 0.03348300 4.92527600

Transition State I

1 3

U 0.10927400 0.82542200 0.48504500

F -1.42343000 1.24362900 -0.72888000

F 1.83011000 1.31195500 -0.40031600

C 0.09735000 -1.39220600 1.60140900

C -0.10320700 -2.12144800 0.64471500

H -0.27452000 -2.80547200 -0.16388400

C 0.23961300 0.96141900 3.74374600

H 0.26781500 1.63856000 4.60098900

O 0.13821100 1.50294100 2.57484000

O 0.30409500 -0.25690300 3.92544400

H 0.22777600 -0.83690700 2.83527300

Structure III

1 3

C 1.54441300 -0.17940800 -0.28617200

H 0.51135700 -0.51879000 -0.40661200

O 1.80689300 1.05127400 -0.13534000

O 2.50234300 -1.01081100 -0.29478500

U 4.05923000 0.63965800 0.01570700

F 4.64526600 0.74937100 -1.89732300

F 4.14051700 0.55562100 2.02074600

C 4.39261000 3.38511800 0.75257000

H 4.31929900 3.40486800 1.82199800

C 4.48076300 3.44458400 -0.44801400

H 4.56874400 3.56635200 -1.50929800

Structure V

1 3

C 1.17973800 0.02116300 -0.20409100

H 0.09234100 -0.05461400 -0.30142400

O 1.72652800 1.11858100 0.09708200

O 1.90935200 -1.00266300 -0.39467600

U 3.84991700 0.14166400 0.01927700

F 4.59335200 0.21032800 -1.85046300

F 4.33349400 -0.66786900 1.79808300

C 5.26660300 3.30226200 0.88597500

H 4.68435900 4.21194500 1.06739500

O 4.71885400 2.24894400 0.59079300

O 6.55237500 3.36190200 0.99020100

H 6.86761300 4.24585800 1.22790500

Transition State II

1 3

U 3.81244500 0.50117500 -0.81849500

F 3.21482200 -0.26328900 -2.54554500

F 3.16050900 2.75584700 -0.97585000

C 6.15113600 0.13169500 0.40919900

H 7.10581100 -0.02475000 0.91968700

O 5.85294500 -0.52899500 -0.63199200

O 5.31408500 0.98280800 0.84858400

C 1.16272300 0.50022300 0.29209600

H 0.20712700 0.18016000 0.71711900

O 2.20348200 -0.20449000 0.54656200

O 1.21750000 1.50650300 -0.44061800

H 2.21128700 2.47770400 -0.75147800

Structure VI

1 3

C 1.49227200 0.34626100 0.45752500

H 0.58701700 0.22599500 1.06043700

C 5.84041900 0.19036300 0.51860300

H 6.69530200 0.03184800 1.18308800

O 1.82599800 1.47535600 -0.00044600

O 2.22938100 -0.65842200 0.20304900

O 5.58834400 -0.62380900 -0.41712100

O 5.08047600 1.19833100 0.68038500

U 3.69884900 0.54629400 -1.04723300

F 3.23542000 -0.03475800 -2.89748300

F 3.65993500 2.98262100 -1.67589600

H 3.11399100 3.70596600 -1.45838300

Structure VIII

1 3

C 1.36635000 0.42085800 0.19450900

H 0.46256400 0.47641200 0.80990800

C 5.66351600 0.43886000 0.50641100

H 6.48895700 0.48441000 1.22401400

O 2.13182200 1.43194900 0.09788800

O 1.65978200 -0.64150600 -0.42116500

O 4.88092500 -0.55892600 0.49795300

O 5.47847200 1.37660300 -0.32177800

U 3.63392500 0.28675700 -1.24933700

F 4.22638200 -0.95164600 -2.70791500

C 3.12247600 2.65926500 -3.88496700

H 3.70027500 3.57134700 -4.06978400

O 3.34386500 1.95686300 -2.91062600

O 2.19126800 2.34246700 -4.72557600

H 2.11616300 2.97610700 -5.45317700

Transition State III

1 3

U 3.73113100 0.41075800 -0.63831100

F 3.71166300 2.54336400 -1.72722300

C 1.48941800 0.42081500 0.79741300

H 0.57595600 0.40792500 1.39936900

C 5.95672300 0.26852700 0.82716900

H 6.86684000 0.17495200 1.42706000

O 5.10087800 -0.67775500 0.80508700

O 5.72762000 1.30215700 0.14187100

O 2.35757900 1.33111500 0.95897000

O 1.69968700 -0.47937100 -0.07603800

C 3.37771700 -0.12136100 -3.47655200

H 3.26093800 -0.67432400 -4.41356400

O 4.08382100 -0.66652200 -2.54729000

O 2.82229900 0.97586900 -3.31046900

H 3.32340400 2.15074700 -2.55117300

Structure IX

1 3

C 1.32327400 0.43108700 0.53277400

H 0.34765800 0.41627600 1.02890600

C 6.07848300 0.25935700 0.55876700

H 7.03443300 0.16722700 1.08313300

O 1.95288200 1.51291400 0.36617100

O 1.84393800 -0.64731100 0.11103900

O 5.04356900 -0.33665600 1.00792000

O 5.97731900 0.95041300 -0.49201300

U 3.72468400 0.38170100 -0.70895400

C 3.45773700 -0.34741400 -3.27296200

H 3.32536600 -0.64637800 -4.31721100

O 3.10917000 0.81164800 -2.88627200

O 3.95676300 -1.14581900 -2.42840000

F 3.91354300 2.90979800 -0.82160800

H 3.21677000 3.47097900 -0.56315400

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acetic Acid

Structure II

1 3

U 0.73565100 0.48878700 0.46782000

F -0.50070600 2.01417900 0.06084200

F 2.42367600 0.77518700 -0.57842900

C -0.86194100 -2.52614000 -0.39099500

H -1.35186800 -3.41270600 -0.73343200

C -0.30307600 -1.51547100 -0.00151900

C 1.78708800 -0.38130600 3.69888600

O 1.21665200 0.12277100 2.72201100

O 2.86752000 -1.06696100 3.46223700

H 3.26267600 -1.43497400 4.26429600

C 1.30093000 -0.20301100 5.08672200

H 1.38779000 -1.12927000 5.65703900

H 1.92697700 0.55141500 5.57526800

H 0.27207400 0.14572600 5.08691200

Transition State I

1 3

U 0.69552100 0.53651900 0.74962500

F -0.74484900 1.85472900 0.29919100

F 2.34050700 0.94832100 -0.31126200

C 0.10585400 -1.88886700 0.96579500

C -0.39290900 -2.06719800 -0.13205600

H -0.83946700 -2.28135400 -1.08352800

C 1.29482300 -0.73852600 3.71205000

O 1.21477000 0.22558300 2.82117600

O 0.95633100 -1.89064100 3.41442300

H 0.54827200 -1.92753700 2.22767300

C 1.79630100 -0.38469400 5.05584700

H 1.83052700 -1.26113500 5.69589000

H 2.78888700 0.06138500 4.96107700

H 1.14632200 0.37967700 5.48832400

Structure III

1 3

C 2.44335900 0.51126300 -0.11224400

O 2.83855500 1.48232800 -0.84369900

O 3.36332600 -0.17359700 0.46964100

C 1.01981000 0.16233100 0.03572800

H 0.81001800 -0.67779000 -0.63496600

H 0.82325000 -0.17868800 1.05153600

H 0.38417200 0.99909600 -0.24220200

U 5.06575900 0.93301100 -0.52248400

F 5.57540600 0.10142500 -2.27262600

F 6.71005500 0.87744700 0.64252800

C 4.83439300 3.81226900 -0.51483800

H 3.93004600 4.02506700 -1.04856200

C 5.85591700 3.66823800 0.10743800

H 6.76995000 3.58766200 0.66056900

Structure V

1 3

C 2.19426100 -0.02435400 0.00827900

O 2.78097200 1.05453000 0.34040700

O 2.92207700 -1.08017300 -0.06786700

C 0.74686600 -0.08320500 -0.28100700

H 0.60530300 -0.46017600 -1.29619100

H 0.28180500 -0.80764300 0.39097400

H 0.28645700 0.89394300 -0.16826200

U 4.83826100 -0.01272000 0.51326900

F 5.80779600 -0.08932500 -1.25979200

F 5.12141300 -0.81592000 2.34757200

C 6.59948700 2.90667100 1.44997000

O 5.79596500 2.03463000 1.11152000

O 7.83998500 2.53980000 1.62007500

H 8.41122900 3.27319700 1.88376900

C 6.21093900 4.32183300 1.66575700

H 6.43424800 4.60950600 2.69676500

H 6.79534800 4.96938300 1.00677700

H 5.15193300 4.45943800 1.46977600

Transition State II

1 3

U 5.12121800 0.35162300 1.23714400

F 5.50883500 -0.51986900 2.98433200

F 6.47693400 2.19384400 1.61542200

C 2.81835300 0.43827100 -0.12477000

O 3.00088000 -0.39716800 0.82376700

O 3.80239300 1.22845500 -0.38508300

C 1.56742800 0.48999000 -0.89983700

H 1.34532000 1.51589500 -1.18991400

H 1.72243400 -0.08494000 -1.81935000

H 0.75165700 0.03708400 -0.34156200

C 7.30922400 -0.03373200 -0.61808000

O 6.52420500 -0.85173900 -0.01494000

O 7.26164200 1.20154700 -0.33951000

C 8.25318100 -0.53845500 -1.63445600

H 7.82156500 -1.37724500 -2.17727600

H 8.56613400 0.26146700 -2.30046200

H 9.13547900 -0.91169300 -1.10273400

H 6.99963400 1.88647300 0.73533300

Structure VI

1 3

C 2.95626000 0.37194000 -0.05622300

O 3.40861600 1.56186900 -0.10614100

O 3.70937700 -0.50133900 0.50850800

C 1.62956400 0.00561100 -0.58729500

H 1.65863700 -0.99693600 -1.01120000

H 0.92761400 -0.01543900 0.25265300

H 1.28620100 0.74052100 -1.31080500

U 5.35037400 0.95859400 1.02999900

C 7.33684700 -0.09508700 -0.43995200

O 7.14059100 -0.44183300 0.77529400

O 6.55335200 0.80286000 -0.91565700

F 5.08964100 1.21179600 3.00316000

C 8.39149100 -0.71542100 -1.26295600

H 7.95969100 -1.60138200 -1.74064300

H 8.71808200 -0.03465000 -2.04589600

H 9.21766300 -1.04379500 -0.63570000

F 5.36381000 3.44943800 0.59258500

H 4.70852300 3.92269600 0.12964000

Structure VIII

1 3

C 2.75595300 0.14334700 0.03176000

O 3.49876300 0.89993300 -0.68746900

O 3.15558600 -0.11567700 1.21325400

C 1.50183100 -0.42974100 -0.50315000

H 1.74754200 -1.39259600 -0.96208100

H 0.79420100 -0.61370900 0.30237100

H 1.08264100 0.21387100 -1.27327800

U 5.11925000 1.08117500 0.94839400

C 7.03617900 -0.11810700 -0.52965500

O 6.28440100 -0.77763000 0.26629900

O 6.83689500 1.13893900 -0.60971200

F 5.87123700 1.26633200 2.81051400

C 8.10688800 -0.78693200 -1.30039300

H 7.80036800 -1.79447500 -1.57533500

H 8.38010600 -0.19644900 -2.17133800

H 8.98245400 -0.87403800 -0.64975100

C 4.49894800 4.53019700 1.43930200

O 4.81623200 3.43236800 0.98493600

O 3.65076300 4.54865200 2.43549200

H 3.45617400 5.44538400 2.73664700

C 5.04019300 5.80898800 0.91410200

H 4.22933400 6.50880100 0.70072600

H 5.68087600 6.26304400 1.67589800

H 5.62366100 5.63132300 0.01574500

Transition State III

1 3

C 2.76662600 0.48988700 -0.14156800

O 3.52139200 0.92950900 -1.06803600

O 3.23826500 0.54203100 1.05399600

C 1.42767400 -0.06849000 -0.40882700

H 1.48692000 -1.15495400 -0.29178000

H 0.72024400 0.29363600 0.33715500

H 1.10277600 0.16873100 -1.41810400

U 5.21192300 1.44804200 0.40620000

C 7.02571100 -0.06973200 -0.83644800

O 6.26958000 -0.55770100 0.06935600

O 6.86986400 1.17742400 -1.10707000

F 6.75998700 1.69251900 2.22361000

C 8.04576500 -0.87934100 -1.52749500

H 7.85107500 -1.94044300 -1.39651500

H 8.09120200 -0.60125700 -2.57985900

H 9.01794800 -0.63816800 -1.08555200

C 4.79716100 4.07041300 1.57448200

O 4.95971400 3.68558800 0.35893000

O 5.02133600 3.24503300 2.50646500

H 6.15030900 2.43612300 2.56317400

C 4.34723100 5.44950400 1.85648800

H 3.91446800 5.51650100 2.85133200

H 5.23016000 6.09657500 1.81822900

H 3.65809000 5.79529100 1.08819200

Structure IX

1 3

C 2.50937200 0.02893900 -0.38545500

O 3.14029700 1.08167400 -0.72533800

O 3.12112700 -0.77456600 0.40011600

C 1.15033800 -0.27408100 -0.87905400

H 1.23263700 -1.06490000 -1.63065300

H 0.54133100 -0.66896200 -0.06615400

H 0.69335100 0.60273400 -1.32956300

U 5.03177300 0.47548300 0.55056600

C 7.27833500 -0.18613700 -0.77260000

O 6.20497900 -0.89573800 -0.82620700

O 7.22535200 0.88287800 -0.08600500

C 8.49834400 -0.60763300 -1.48918900

H 8.29580200 -0.58105100 -2.56311400

H 9.33322700 0.04512700 -1.25116500

H 8.72424100 -1.64491600 -1.23681600

C 5.07188900 0.87644800 3.21360600

O 5.48633400 -0.21392200 2.69827900

O 4.65029200 1.77240700 2.39982900

C 5.05322900 1.09468400 4.67387600

H 5.26534700 2.13805200 4.90126900

H 4.04188400 0.87768900 5.03197500

H 5.74863200 0.42287200 5.17080000

F 5.07815700 2.81645800 -0.47251700

H 4.27375400 3.04575400 -0.88283200

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Propionic Acid

Structure II

1 3

U 1.19853000 2.87770000 -3.33146800

F 0.01408400 3.87136000 -4.61154000

F 3.14984700 3.00744600 -3.78380000

C 0.13392000 -0.49774400 -2.81501900

H -0.16704500 -1.52223700 -2.73913600

C 0.48080700 0.66681800 -2.91928800

C 0.23922000 2.58941300 -0.09746400

O 0.67917900 3.14174000 -1.14821600

C 0.10672500 3.35905600 1.16002900

H -0.51289900 4.22847600 0.90958300

H 1.09980000 3.78272900 1.35217900

C -0.43158900 2.59599400 2.35339400

H -0.48315800 3.26262300 3.21289400

H -1.43338600 2.21172600 2.16409100

H 0.21207100 1.75691000 2.61552900

O -0.10191100 1.35524800 -0.09212300

H 0.02520800 0.92966100 -0.98469000

Transition State I

1 3

U 0.69299000 0.53919700 0.75320200

F -0.73527800 1.87968900 0.32435800

F 2.34794800 0.96625200 -0.28866900

C 0.09529600 -1.88975900 0.93496500

C -0.39838700 -2.04636100 -0.16857400

H -0.84063100 -2.24404700 -1.12546500

C 1.27937500 -0.77805600 3.69900900

O 1.20331300 0.19628900 2.81509000

O 0.93563300 -1.92458000 3.38602300

C 1.78526500 -0.43060700 5.04907300

H 2.76219800 0.04246900 4.89487200

H 1.14436100 0.38063500 5.41405900

C 1.85496200 -1.58953300 6.02188200

H 0.87197300 -2.02953900 6.18727600

H 2.51934100 -2.37333100 5.65925400

H 2.23537700 -1.23865800 6.98017600

H 0.53227700 -1.94432400 2.20199600

Structure III

1 3

C 2.56110700 -0.71466100 -0.15930800

O 3.33406500 -0.11182700 -0.98754300

O 3.14124000 -1.42021200 0.74330000

U 5.23373600 -0.74514900 0.07094800

C 1.08707300 -0.59967100 -0.21938600

H 0.77316600 -0.25167200 0.77185800

H 0.70862900 -1.62720800 -0.27643500

C 0.55277200 0.27544400 -1.33540500

H -0.53549200 0.29032900 -1.29638200

H 0.90747200 1.30157000 -1.24274800

H 0.85023400 -0.09886900 -2.31461800

F 5.76107300 0.55260100 1.50570300

F 6.76268900 -0.79734600 -1.24416900

C 5.37110400 -3.55278300 0.74688100

H 4.54192800 -3.72586200 1.40288300

C 6.31841400 -3.45302500 0.00929800

H 7.17236000 -3.41030000 -0.63624500

Structure V

1 3

C 2.11044400 0.60823300 -0.59232500

O 2.41397800 1.83096700 -0.34305100

O 3.08796300 -0.18465100 -0.82911700

U 4.65757000 1.45340000 -0.56485700

C 0.69944200 0.15756700 -0.60138200

H 0.18048000 0.81103200 -1.31212400

H 0.28859800 0.43948200 0.37498300

C 0.49390900 -1.31129200 -0.91194300

H -0.57027900 -1.54257600 -0.89516000

H 0.87966800 -1.56840800 -1.89811600

H 0.98952100 -1.94747500 -0.17910300

F 5.55446500 1.04853200 1.27694900

F 5.84003500 1.48988100 -2.19422800

C 5.57952000 4.18614800 1.18441900

O 5.08769000 3.57749500 0.20091300

C 5.61705500 5.66700900 1.22354600

H 4.58139400 5.99140000 1.06961600

H 6.13510900 5.97139900 0.30671300

C 6.23373000 6.28676500 2.46152300

H 6.20416400 7.37190800 2.37422100

H 5.69055600 6.00603900 3.36339400

H 7.27397900 5.98664100 2.58377500

O 6.07117400 3.54997700 2.19266900

H 5.99812100 2.57684900 2.07246800

Transition State II

1 3

U 4.57479600 -0.27235100 -0.29969500

F 5.91998200 0.71627100 0.79650100

F 4.17974400 -2.10344200 1.05566300

C 5.14997700 -0.18324700 -2.90508000

O 4.55688400 0.78304800 -2.29433900

O 5.40810600 -1.21750600 -2.19731600

C 5.51132300 -0.07602100 -4.33516800

H 6.15109600 0.81165600 -4.41244600

H 4.59167200 0.21006500 -4.85832900

C 6.16194800 -1.30842000 -4.93029900

H 6.39040300 -1.12842700 -5.97981900

H 7.09255000 -1.55465800 -4.41983900

H 5.50402000 -2.17523300 -4.87196800

C 1.73837800 -0.58641000 -0.05387200

O 2.42035300 0.45509600 0.14605600

O 2.38904800 -1.68358400 -0.31502100

C 0.26064800 -0.59994200 -0.04052100

H -0.04566100 -1.05883600 -0.98802700

H -0.02146800 -1.34361100 0.71569100

C -0.39774300 0.74332400 0.19854100

H -1.48024300 0.62440900 0.19657800

H -0.10601600 1.16480300 1.16009200

H -0.13520500 1.46002700 -0.57932500

H 3.20528300 -2.12075100 0.53730500

Structure VI

1 3

C 1.84795300 -0.47263000 -0.02931700

O 2.41465900 0.60741700 -0.42128400

O 2.62488400 -1.45063700 0.24562800

U 4.52142500 -0.19597600 -0.20580800

F 5.18802400 0.69410500 1.46662400

C 0.37693000 -0.58975000 0.10972600

H 0.19723200 -0.88229400 1.15077600

H 0.08747600 -1.47004300 -0.47507000

C -0.40858800 0.64626700 -0.28020700

H -1.47309300 0.46232100 -0.14107800

H -0.13112400 1.50437300 0.33135700

H -0.24537000 0.90959500 -1.32504300

C 5.32490100 -0.08480700 -2.76470600

O 5.46773400 0.90312400 -1.95754100

O 4.80078000 -1.14796200 -2.27973800

C 5.74563700 0.02307400 -4.18093000

H 6.79106600 0.35117400 -4.15909600

H 5.20173000 0.88398200 -4.58722300

C 5.54804500 -1.22768000 -5.01295700

H 5.88351800 -1.04473900 -6.03292400

H 6.11970400 -2.06618700 -4.61563900

H 4.49919400 -1.52104400 -5.05031500

F 5.16471400 -2.49073600 0.64683200

H 4.53785600 -3.14709600 0.85676800

Structure VIII

1 3

C 1.45224200 -0.17341100 -0.33462500

O 1.48721700 1.06594100 -0.63473800

O 2.57651300 -0.78826900 -0.29369000

U 3.78729300 1.07017300 -0.83993000

F 4.61865100 1.39402300 1.04291300

C 0.18640900 -0.88980300 -0.03928900

H 0.31191700 -1.32293900 0.95936200

H 0.16557400 -1.75486700 -0.71104800

C -1.06900200 -0.04818600 -0.14584400

H -1.94143900 -0.65769300 0.08663300

H -1.04725900 0.78972700 0.55067300

H -1.19507400 0.35345300 -1.15108900

C 4.81622100 0.17562600 -3.16174900

O 3.70316400 0.81569200 -3.11062800

O 5.43584900 0.00981900 -2.06037300

C 5.32946600 -0.34280600 -4.45411600

H 5.35035100 0.51230100 -5.13845400

H 4.53921600 -0.99015300 -4.85104500

C 6.66533000 -1.05354800 -4.37552500

H 6.95581100 -1.40039900 -5.36646600

H 7.44844100 -0.39152300 -4.00635500

H 6.61782700 -1.91844000 -3.71442000

C 4.70859500 4.27162000 -0.15570900

O 4.25189900 3.35720200 -0.87997400

C 4.75357500 5.67651900 -0.63270700

H 3.72519200 5.92218900 -0.92064300

H 5.30239600 5.64919900 -1.58060300

C 5.33288300 6.69136400 0.33255600

H 5.31280800 7.67909900 -0.12600400

H 4.75892300 6.73731300 1.25757200

H 6.36655000 6.45825200 0.58642300

O 5.15952800 4.03502900 1.03169000

H 5.07528000 3.08120600 1.25626900

Transition State III

1 3

U 4.04836300 1.20593000 -0.58690600

F 3.90289000 3.33199400 -1.62468500

C 1.83583200 -0.10076100 0.17182600

O 1.75852600 1.05818600 -0.34646900

O 3.02130800 -0.59455000 0.29331400

C 0.64994300 -0.86623800 0.62169500

H 0.83336200 -1.11451900 1.67330900

H 0.69990700 -1.83013900 0.10246600

C -0.67907700 -0.16777800 0.41716100

H -1.48674400 -0.80455900 0.77576400

H -0.72251400 0.77399800 0.96364100

H -0.85907100 0.04560900 -0.63622000

C 5.68955500 1.49586200 1.52140000

O 5.94620200 0.66039800 0.59349500

O 4.60816900 2.17823200 1.38736500

C 6.57023900 1.69167600 2.69659700

H 5.93686300 1.52245800 3.57511000

H 6.79791100 2.76307300 2.72898900

C 7.81903300 0.83371700 2.71384200

H 8.39570400 1.04390400 3.61366900

H 7.57309400 -0.22788000 2.70972000

H 8.45364600 1.03642600 1.85136400

C 5.23159100 0.97480200 -3.20571100

O 5.56868700 2.06661500 -2.62979900

O 4.33517400 0.25879400 -2.65239300

C 5.90456800 0.55602800 -4.45924600

H 6.98012500 0.63276500 -4.26694500

H 5.70281600 1.35613400 -5.18188800

C 5.50512800 -0.80491000 -4.99163800

H 6.04446400 -1.00987100 -5.91550900

H 5.74221800 -1.59653200 -4.28088300

H 4.43782100 -0.85188400 -5.20643700

H 4.66283800 2.98795100 -2.24487100

Structure IX

1 3

C 1.73017700 -0.14614700 0.06093800

O 1.83788100 0.97578400 -0.53072500

O 2.82717400 -0.70207400 0.43415300

U 4.14943900 0.98810000 -0.30711300

C 0.42328600 -0.79525800 0.32685500

H 0.38373300 -0.95976900 1.40958400

H 0.49493200 -1.80220100 -0.09899600

C -0.78636300 -0.03807500 -0.18244600

H -1.69404700 -0.58970600 0.05917600

H -0.85921400 0.94927000 0.27300300

H -0.74847900 0.09233800 -1.26382200

C 5.00872000 0.72775200 -2.87399700

O 4.72374900 1.87791400 -2.38451600

O 4.86630500 -0.27141100 -2.09613300

C 5.47860900 0.58729700 -4.27469200

H 6.35476800 1.23934100 -4.36423900

H 4.71656100 1.06410300 -4.90112500

C 5.77544600 -0.83260800 -4.71331200

H 6.11562000 -0.83436700 -5.74813800

H 6.55476100 -1.28361800 -4.09958700

H 4.88918700 -1.46333200 -4.64752900

C 5.96896000 1.44184700 1.63052700

O 6.23701100 0.67747700 0.64837500

O 4.82092100 2.02094000 1.60832200

C 6.90736900 1.66467500 2.75751200

H 6.35425600 1.40415300 3.66684300

H 7.04598700 2.74954900 2.82419600

C 8.22354600 0.92112800 2.65285700

H 8.84249300 1.14629600 3.52048400

H 8.07027500 -0.15720400 2.61730300

H 8.77564100 1.21185200 1.75934400

F 3.50458200 3.45263300 -0.67113700

H 3.66676500 3.73890000 -1.54206600

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acrylic Acid

Structure II

1 3

U 1.29142400 2.84187900 -3.26580500

F 0.20006500 3.94554800 -4.56339500

F 3.27522800 2.83849100 -3.66261100

C -0.00185400 -0.47153500 -2.90360000

H -0.36597500 -1.48836000 -2.89899400

C 0.41714400 0.68786300 -2.92196700

C 0.22831400 2.54138000 -0.05271900

O 0.73243400 3.08548300 -1.09088800

C 0.12799200 3.28891600 1.18273800

H 0.50521500 4.31148500 1.14505900

C -0.39655600 2.74996200 2.29563500

H -0.46230500 3.33288900 3.21682000

H -0.77005100 1.72329000 2.31612000

O -0.19825700 1.32252900 -0.08507700

H -0.07258800 0.92171300 -0.99147300

Transition State I

1 3

U -1.68946700 1.02065900 -1.50862700

F -3.44004000 1.82802100 -2.06786900

F 0.17666400 1.25136600 -2.21122300

C -1.99661900 -1.19187800 -0.40011700

C -2.14724100 -1.90652700 -1.37394400

H -2.28723100 -2.58498300 -2.19205900

C -1.53840500 1.19433600 1.72610500

C -1.35424800 2.09233600 2.85170400

C -1.15309900 3.39932800 2.70032500

O -1.50449900 1.69037600 0.49812800

O -1.72484800 -0.01679800 1.90217900

H -1.39342600 1.61651900 3.82293200

H -1.01933700 4.04344700 3.56010200

H -1.11653400 3.86062800 1.72138400

H -1.86390600 -0.62636400 0.76270900

Structure III

1 3

C 2.48985300 -1.13314300 -0.27771700

O 3.27584800 -0.32424500 -0.92151600

O 3.04122300 -1.79994900 0.67766000

U 5.07433200 -0.72283400 0.38749300

C 1.08451400 -1.27754500 -0.59166400

H 0.52547100 -1.98262900 0.02516700

C 0.52953700 -0.57044000 -1.58907700

H -0.53025200 -0.67670700 -1.82986200

H 1.12274100 0.12839500 -2.18432000

F 5.21854600 0.50798900 1.98129800

F 6.78161900 -0.48781400 -0.68935300

C 5.54228100 -3.51041700 0.96239300

H 4.64391700 -3.85743600 1.45314800

C 6.58548100 -3.21601700 0.40769800

H 7.52885600 -3.00233700 -0.07446200

Structure V

1 3

C 2.98226000 0.57698700 0.07433600

O 3.52768500 1.55120700 0.70347500

O 3.71424400 -0.01450200 -0.80752400

U 5.51549000 1.31041800 -0.42421400

C 1.61902400 0.17671900 0.35464900

H 1.10458400 0.74994500 1.11490600

C 1.05621700 -0.83963900 -0.29717800

H 0.03739200 -1.14136400 -0.08979600

H 1.60282600 -1.39208900 -1.05221300

F 7.04602200 0.14690000 0.18124900

F 5.63872800 2.49211600 -2.14298600

C 6.49296900 4.48465400 0.13914200

O 6.22438800 3.30133000 0.47653900

C 6.89420000 5.50627800 1.08457600

H 7.09284100 6.48519300 0.66864000

C 7.01025500 5.23596900 2.38341500

H 6.80823100 4.24635100 2.77472800

H 7.31265500 6.00182000 3.08609200

O 6.43023400 4.87112800 -1.09593900

H 6.15657700 4.13766300 -1.68843800

Transition State II

1 3

U 5.78565600 1.29680800 -0.46741600

F 7.08481300 -0.22208600 -0.53388700

F 6.50089200 2.54714500 -2.27829400

C 3.29571900 0.55497600 0.14222300

O 4.20524000 0.70298200 1.04079600

O 3.65141100 0.82318800 -1.06630400

C 1.96752300 0.10746700 0.49522700

H 1.79736000 -0.08968400 1.54563900

C 1.02900100 -0.04735400 -0.43866600

H 0.03317200 -0.38384500 -0.17931800

H 1.23672300 0.15819000 -1.48212600

C 6.11229800 4.00207900 0.41113200

O 6.58962700 2.94174700 0.92288600

C 6.20753700 5.29919400 1.04091500

H 5.75188600 6.12221100 0.50616800

C 6.83695800 5.44975300 2.20725300

H 7.28603500 4.60499100 2.71609600

H 6.91851100 6.42237500 2.67588000

O 5.47898200 3.88754500 -0.71810700

H 6.08162500 3.39113600 -1.70569400

Structure VI

1 3

C 6.33381400 2.91855500 -1.82545600

O 6.01234600 3.70003300 -0.85779600

C 6.91096700 3.39342300 -3.06717700

H 7.13359300 2.63435500 -3.80574600

C 7.14417900 4.68996000 -3.26192200

H 6.90778900 5.42148700 -2.49838700

H 7.57633200 5.04791100 -4.18771000

O 6.11295000 1.66697200 -1.64220600

C 7.00381400 0.58150200 1.83731900

O 6.01983600 0.01584700 1.23376500

C 7.99666300 -0.15970400 2.58799600

H 8.77379900 0.42994700 3.05658100

C 7.93505800 -1.48745700 2.67687100

H 7.14235900 -2.04438300 2.19149700

H 8.67594900 -2.04552500 3.23518600

O 7.07383900 1.86188100 1.74405200

U 5.21212100 1.98074000 0.41735600

F 3.23194700 1.72008500 0.11566000

F 4.11571300 3.19658000 2.40126100

H 3.22304800 3.34615200 2.61608600

Structure VIII

1 3

C 6.40542200 2.63451700 -2.03101800

O 5.85853500 2.73946200 -0.87504200

C 6.99454600 3.76720400 -2.72385200

H 7.43322300 3.55378000 -3.68994300

C 6.98064900 4.98403000 -2.18491200

H 6.52906000 5.15938600 -1.21572800

H 7.41792000 5.83002000 -2.69970100

O 6.40788400 1.46932300 -2.56246600

C 6.77164100 -0.19805600 1.33902600

O 7.22091500 -0.28900700 0.13800900

C 7.56900200 -0.55225500 2.50032800

H 7.07967600 -0.43929700 3.45911400

C 8.82250400 -0.98009100 2.36982500

H 9.28035300 -1.07657900 1.39256400

H 9.41832700 -1.24059200 3.23532000

O 5.57288700 0.22834000 1.47686900

U 5.28569400 0.52568100 -0.78649100

F 3.23203100 0.77018500 -1.03539400

C 3.63659100 -2.12633300 -2.12079400

O 4.65358000 -1.52666600 -1.69556900

C 3.68115100 -3.45990600 -2.69345200

H 2.73356200 -3.86799100 -3.01951000

C 4.82939400 -4.12315500 -2.80524500

H 5.76448400 -3.68959500 -2.47185000

H 4.85949100 -5.11616200 -3.23486200

O 2.45625100 -1.58972600 -2.07674500

H 2.49562400 -0.68563300 -1.69443100

Transition State III

1 3

U 5.46968700 0.49206400 -1.03100100

F 3.08159300 0.65089300 -0.80649200

C 6.62668200 2.67704500 -2.08415400

O 5.54170000 2.74610300 -1.39973200

C 7.24471500 3.83399000 -2.70128500

H 8.15433000 3.64502300 -3.25647500

C 6.70699200 5.04556300 -2.57321700

H 5.79533600 5.19500600 -2.00687500

H 7.16603800 5.91301200 -3.03014400

O 7.14661800 1.51069000 -2.20143700

C 6.58353700 -0.24351500 1.29656700

O 6.98346900 -0.71182400 0.16947700

C 7.18490700 -0.61310000 2.56351100

H 6.75413600 -0.15259600 3.44310100

C 8.20371600 -1.46865800 2.61451000

H 8.60862900 -1.90904200 1.71110400

H 8.65492500 -1.74655500 3.55850600

O 5.61011900 0.58746800 1.24745000

C 4.28530700 -1.98103800 -1.81364100

O 4.99621900 -1.15321200 -2.49823000

C 4.03716900 -3.33501100 -2.27164400

H 3.43726900 -3.95038700 -1.61383100

C 4.51418700 -3.77125000 -3.43610600

H 5.10910800 -3.12876400 -4.07412000

H 4.31804900 -4.77957800 -3.77798200

O 3.82569600 -1.58085300 -0.69507500

H 3.09279900 -0.35207500 -0.70030400

Structure IX

1 3

C 2.37686600 0.81642500 0.39707900

O 3.33296900 0.05140100 0.01668600

C 1.00531500 0.35422300 0.51481200

H 0.28362100 1.08881800 0.84793700

C 0.67729300 -0.90202300 0.22137400

H 1.42646500 -1.61039800 -0.11169600

H -0.34462000 -1.24904100 0.30620900

O 2.69134700 2.02463100 0.67197000

C 5.97434400 2.84132400 -2.01908300

O 6.34209800 3.19806000 -0.84711300

C 6.50719100 3.43630300 -3.23098400

H 6.12053600 3.04187600 -4.16166400

C 7.41543000 4.40789600 -3.17333900

H 7.77702200 4.77776000 -2.22121900

H 7.81617600 4.85402500 -4.07462200

O 5.08677800 1.91016300 -2.08917500

C 6.58252100 0.45302100 1.95647800

O 6.58027600 0.11524600 0.72057800

C 7.42839800 -0.18765700 2.94745500

H 7.34349300 0.19043900 3.95793500

C 8.25089900 -1.17758400 2.60801000

H 8.30782800 -1.52907400 1.58465500

H 8.88385300 -1.65736800 3.34360300

O 5.78765000 1.40261900 2.29320600

U 4.96572300 1.64887000 0.16725400

F 4.36982400 3.90648400 1.21467500

H 3.46496500 3.90118500 1.44000500

M06L

cc-pVTZ-PP and MWD60 (U) / maug-cc-pVTZ (light atoms)

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Formic Acid

Structure II

1 3

U 0.11304800 1.24367300 -0.01337000

F -1.89451200 1.32383900 0.16304400

F 2.09679700 1.44870300 -0.30459200

C 0.24783400 -2.26981500 0.11656800

H 0.30251800 -3.33442900 0.10194100

C 0.18470600 -1.05025400 0.12829000

C 0.22709700 1.18806000 3.46755300

H 0.55111800 1.81491700 4.30453000

O 0.31509200 1.58658000 2.31263200

O -0.25364700 0.01198500 3.72505100

H -0.26645100 -0.17767900 4.67469000

Transition State I

1 3

U -0.34656800 0.93352600 0.55706800

F -0.96304300 0.51599200 -1.31094300

F 1.55847500 1.38111400 0.10224000

C -0.02533600 -1.26519200 1.57918000

C -0.24314200 -1.93020200 0.57421200

H -0.42768600 -2.54495000 -0.28198400

C 0.39033200 0.94553100 3.78566800

H 0.53071100 1.59165800 4.65587000

O 0.02027000 1.50871100 2.69091700

O 0.58877400 -0.27297300 3.90604800

H 0.33030000 -0.79222700 2.86010500

Structure III

1 3

C 1.57976200 -0.14767800 -0.27843700

H 0.53969000 -0.46890300 -0.39525800

O 1.87052200 1.08171800 -0.19090200

O 2.51356200 -1.01152400 -0.22910900

U 4.13668600 0.60115000 0.00768600

F 4.53452700 0.75490600 -1.96875000

F 4.13912000 0.55563100 2.02908100

C 4.34960100 3.37452500 0.76219300

H 4.23293800 3.38280900 1.82409700

C 4.48042100 3.43010200 -0.43506800

H 4.59460700 3.53510200 -1.49205500

Structure V

1 3

C 1.52980800 0.46303100 -0.06701400

H 0.47352000 0.75306900 -0.08180100

O 2.42446300 1.32770700 0.17850000

O 1.86015400 -0.73816700 -0.29479500

U 4.13542100 -0.27465900 -0.03679100

F 4.30653100 0.22706400 -1.98192100

F 4.12442000 -0.84817300 1.89443500

C 5.17841900 2.92214700 0.75488100

H 4.22352200 3.44984100 0.64926700

O 5.27933000 1.71998600 0.54237800

O 6.22243900 3.59994400 1.11586000

H 6.01650100 4.53571200 1.25306000

Transition State II

1 3

U 3.87157100 0.49711300 -0.90612300

F 3.07857300 -0.29850100 -2.55698300

F 3.13659200 2.76923500 -0.93050300

C 6.17218900 0.11114100 0.43022800

H 7.09127500 -0.02651100 1.00876100

O 5.94147200 -0.57461000 -0.60514700

O 5.31251900 0.98334300 0.80770100

C 1.16995900 0.52135500 0.27124600

H 0.25633500 0.11831400 0.71893600

O 2.26907500 -0.11740400 0.50645300

O 1.12634800 1.53251900 -0.44419000

H 2.18796200 2.49859600 -0.73111100

Structure VI

1 3

C 1.62331200 0.41110800 0.41719000

H 0.76015100 0.31611100 1.08433600

C 5.77668300 0.15759000 0.55561400

H 6.55490100 0.01080300 1.31201500

O 1.91744300 1.52697900 -0.10511000

O 2.34232600 -0.60508100 0.15986300

O 5.62756900 -0.65851200 -0.39226700

O 5.00489700 1.17859900 0.64014100

U 3.77814400 0.56955800 -1.20791800

F 3.10180300 -0.17707900 -2.94143200

F 3.60431200 3.05331300 -1.65042400

H 2.95586400 3.60266000 -1.26548000

Structure VIII

1 3

C 1.41557800 0.36097600 0.33918500

H 0.57834000 0.42184400 1.04344300

C 5.59197400 0.46424700 0.48035600

H 6.40064800 0.54410200 1.21543500

O 2.19769300 1.36495300 0.21263300

O 1.61242000 -0.68234200 -0.33887200

O 4.84074900 -0.55828600 0.47442000

O 5.40400200 1.39175400 -0.36309500

U 3.56725300 0.26144300 -1.30517700

F 4.26622800 -0.99130000 -2.72104400

C 3.11507800 2.69052600 -3.94562600

H 3.66395300 3.63446800 -4.03353100

O 3.26849000 1.94929200 -2.98630100

O 2.28504000 2.37424300 -4.89334000

H 2.25929500 3.04390100 -5.59213000

Transition State III

1 3

U 3.81660400 0.79650000 -0.71484600

F 3.08628400 2.68503400 -2.10120800

C 1.68831900 0.57126000 0.90589800

H 0.84412100 0.50007900 1.59954400

C 5.81779400 -0.02349300 0.88220100

H 6.63122300 -0.35348500 1.53699100

O 4.89803800 -0.83018400 0.54537300

O 5.78566900 1.17216700 0.45220800

O 2.60507600 1.44240200 1.11496200

O 1.77497000 -0.18727400 -0.09719500

C 3.58161900 -0.13856300 -3.46339400

H 3.67854700 -0.80843500 -4.32483500

O 4.52656700 -0.19336800 -2.57464100

O 2.60721800 0.61222800 -3.32858700

H 2.74362500 2.12202800 -2.81615300

Structure IX

1 3

C 1.35799000 0.45072100 0.50409400

H 0.36972500 0.46365500 0.97651600

C 6.11333500 0.28201000 0.64545000

H 7.03446000 0.19565000 1.23144600

O 1.99356400 1.52631800 0.30406900

O 1.87872100 -0.65171500 0.14731100

O 5.08673700 -0.41146600 0.98702600

O 6.04085800 1.04337300 -0.35164800

U 3.78875600 0.34046400 -0.72965500

C 3.37635300 -0.33996600 -3.30696300

H 3.17308000 -0.60469900 -4.34997500

O 2.99346700 0.79041200 -2.85370000

O 3.98506700 -1.13989000 -2.54154900

F 3.92964200 2.87746600 -0.86866600

H 3.18383300 3.36548800 -0.59562300

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acetic Acid

Structure II

1 3

U 0.78444900 0.50799200 0.40809100

F -0.50817800 1.98349500 -0.07798700

F 2.43992900 0.83186200 -0.70932500

C -0.90243700 -2.53733000 -0.24011100

H -1.41898900 -3.42991000 -0.51248900

C -0.30622200 -1.51448700 0.06731000

C 1.85848100 -0.31770600 3.69656600

O 1.29874500 0.11825600 2.68243100

O 3.04719600 -0.83941200 3.53347400

H 3.42859400 -1.15412800 4.36492400

C 1.23286600 -0.29179700 5.03593500

H 0.85265800 -1.29015200 5.25845100

H 1.95493200 -0.03995700 5.80901800

H 0.40141800 0.40150200 5.06137100

Transition State I

1 3

U 0.37007600 0.73866500 0.92929100

F -0.58703100 1.27769800 -0.77285500

F 2.26369000 1.02147000 0.31330400

C 0.13832000 -1.71606100 0.94898600

C -0.49132600 -1.85534700 -0.09007700

H -1.03172000 -2.00564500 -1.00071900

C 1.31834600 -0.75380100 3.73732800

O 0.97027700 0.26941000 2.99601300

O 1.20096900 -1.91570100 3.30881600

H 0.72302300 -1.87705000 2.18300900

C 1.85778400 -0.47428700 5.08145000

H 2.00170500 -1.38979000 5.64107600

H 2.81089800 0.04269400 4.97427900

H 1.19587500 0.20400700 5.61432600

Structure III

1 3

C 2.43776800 0.46870400 -0.09661700

O 2.86397300 1.27953900 -1.00814000

O 3.31903000 -0.05891600 0.66282500

C 1.00625300 0.15297700 0.02696700

H 0.76598500 -0.61904400 -0.70573900

H 0.77885000 -0.23335300 1.01384100

H 0.39937000 1.01968500 -0.21510400

U 5.07519300 0.95346100 -0.47241200

F 5.55477300 0.11477100 -2.25106000

F 6.81333600 0.81670600 0.55115800

C 4.82775000 3.85149000 -0.47805600

H 3.91251500 4.05065000 -0.99153000

C 5.87014900 3.71075000 0.10988300

H 6.79907200 3.62264200 0.62980400

Structure V

1 3

C 2.59696400 0.19265500 0.15007700

O 3.46053900 1.07980600 0.47517700

O 3.01845700 -1.00111200 -0.02569800

C 1.17166300 0.52982300 -0.03709200

H 0.96800600 0.57490600 -1.10684900

H 0.54338200 -0.25665200 0.36990000

H 0.93197600 1.48976500 0.40423600

U 5.22094000 -0.44846700 0.43832900

F 5.57487800 0.02673500 -1.50116400

F 5.05069600 -1.04820900 2.36359600

C 6.59022600 2.63214900 1.46915700

O 6.37212600 1.46112700 1.14493800

O 7.77931800 2.89254600 1.95080400

H 7.87777600 3.82549100 2.18366100

C 5.59584300 3.71957300 1.32146700

H 5.52031800 4.29923500 2.23955500

H 5.92641400 4.40062600 0.53672400

H 4.62482300 3.31942100 1.05497200

Transition State II

1 3

U 5.11369700 0.44912200 1.45913700

F 5.66077300 -0.48929500 3.14244100

F 6.62636000 2.24004600 1.71372900

C 2.91932200 0.39472200 -0.11748500

O 3.01635000 -0.41104000 0.85958200

O 3.90663100 1.22290100 -0.29230000

C 1.76655700 0.41430300 -1.03062100

H 1.37622700 1.42709500 -1.10538900

H 2.10470800 0.14420100 -2.03047300

H 0.99681700 -0.27329900 -0.70278500

C 7.18839500 0.02221900 -0.57575400

O 6.46320700 -0.76405000 0.14939000

O 7.20604100 1.26368200 -0.34418200

C 7.98391400 -0.55231400 -1.67683900

H 7.43564700 -1.34332300 -2.17879800

H 8.30133900 0.21581000 -2.37145400

H 8.87173500 -1.01386200 -1.24219600

H 7.04879500 1.94288800 0.79202100

Structure VI

1 3

C 3.09680200 0.41985700 -0.01322400

O 3.50053600 1.63269200 -0.03677400

O 3.84712100 -0.42569900 0.59255300

C 1.82127000 0.00625000 -0.62400200

H 1.89760600 -0.99995900 -1.02304100

H 1.06251500 -0.01710500 0.15921700

H 1.50316600 0.71200600 -1.38252600

U 5.44844500 1.09748900 1.18732600

C 7.29406200 -0.10212200 -0.39045600

O 7.20430200 -0.41295800 0.83934500

O 6.49528600 0.82078200 -0.82397700

F 4.95386200 1.19083500 3.13971500

C 8.24037900 -0.75967300 -1.30742700

H 7.68148500 -1.45519800 -1.93419400

H 8.68976000 -0.02980000 -1.97464900

H 8.99378900 -1.31145000 -0.75820200

F 5.22363300 3.53431700 0.51845000

H 4.45231600 3.67917700 0.01123300

Structure VIII

1 3

C 2.77249100 0.11070800 -0.07639500

O 3.56681600 0.77354000 -0.84612100

O 3.06916300 0.03780000 1.15771700

C 1.57970600 -0.55807100 -0.63392000

H 1.89340200 -1.51438600 -1.05322000

H 0.84706200 -0.75261600 0.14082600

H 1.15622400 0.02412900 -1.44590100

U 5.07531700 1.23572000 0.84229800

C 6.97744300 -0.18620200 -0.48735800

O 6.22179600 -0.73999500 0.38282800

O 6.81281500 1.06371700 -0.70617800

F 5.92090600 1.57189600 2.65815800

C 8.02031700 -0.95730100 -1.19500900

H 7.73292100 -1.99884100 -1.28861200

H 8.23871900 -0.51640600 -2.16127200

H 8.93234900 -0.92097700 -0.59869600

C 4.57889500 4.64049500 1.44104500

O 4.78399100 3.63130000 0.76608400

O 4.06703400 4.46465800 2.64121200

H 3.93944100 5.29984700 3.11064100

C 4.88132100 6.01114600 0.96946300

H 4.00414800 6.64930800 1.06273300

H 5.66272300 6.44559300 1.59289800

H 5.21547600 5.99793500 -0.05994400

Transition State III

1 3

C 2.64767400 0.54315600 -0.14040000

O 3.41921400 0.83501700 -1.10634000

O 3.14141900 0.63595300 1.05399500

C 1.25433200 0.10679800 -0.33605200

H 1.16385200 -0.93010900 -0.01419900

H 0.59423000 0.68490100 0.30614900

H 0.95862300 0.19399000 -1.37420100

U 5.19626600 1.30321100 0.35182400

C 7.15722900 -0.10474300 -0.84419500

O 6.36915000 -0.68091100 -0.02543300

O 6.96134600 1.15507300 -1.06469000

F 6.74887500 1.54679800 2.19098600

C 8.26393000 -0.81456500 -1.50672300

H 8.15919300 -1.88746600 -1.40049000

H 8.32294300 -0.52289300 -2.55161000

H 9.19853300 -0.50047000 -1.04132900

C 4.81752200 3.98297000 1.59862800

O 4.94785700 3.53354100 0.38763800

O 5.12829400 3.25421200 2.57282400

H 6.19319400 2.32309100 2.54164900

C 4.29199300 5.35071500 1.78959500

H 4.01068800 5.51980500 2.82175300

H 5.07811100 6.05641600 1.51972700

H 3.46095000 5.54223000 1.11724800

Structure IX

1 3

C 2.54766700 0.01338300 -0.35345100

O 3.17436600 1.08423100 -0.65276200

O 3.17553900 -0.84222300 0.36365600

C 1.17357500 -0.25018600 -0.82199900

H 1.22425600 -0.95409500 -1.65290800

H 0.59421600 -0.73150900 -0.03987100

H 0.69245100 0.65776200 -1.16557600

U 5.11068700 0.41297300 0.57969500

C 7.35093000 -0.17207100 -0.84081900

O 6.30133600 -0.93470900 -0.80699400

O 7.29660800 0.91615600 -0.19419500

C 8.53705200 -0.58632500 -1.61222000

H 8.25921100 -0.70574000 -2.65798900

H 9.33680500 0.13785600 -1.51901500

H 8.86715300 -1.56510700 -1.27015700

C 5.00224400 0.84896200 3.25544200

O 5.55031200 -0.20334300 2.79345300

O 4.52987900 1.68845800 2.39777100

C 4.91264600 1.12370700 4.70130900

H 5.57665100 1.95420300 4.93937000

H 3.90756300 1.44970100 4.95563500

H 5.19939800 0.25614700 5.28285000

F 5.09095500 2.75877600 -0.43981200

H 4.23852400 2.89228500 -0.79775900

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Propionic Acid

Structure II

1 3

U 1.20803800 2.87519300 -3.35911900

F 0.00372500 3.91696900 -4.60758400

F 3.15528800 3.01757300 -3.89078200

C 0.15120200 -0.52204000 -2.84472300

H -0.14222400 -1.54631100 -2.77508400

C 0.49077800 0.64960500 -2.94165800

C 0.24404300 2.58485800 -0.07644500

O 0.68732900 3.11645900 -1.13186800

C 0.11219600 3.36134600 1.17524200

H -0.48230800 4.24231600 0.91797500

H 1.10590400 3.77257200 1.37477700

C -0.44939900 2.61227800 2.36265400

H -0.50300800 3.27242300 3.22231000

H -1.45108600 2.24118600 2.16394900

H 0.17362700 1.76379800 2.63166900

O -0.11037100 1.34564100 -0.04635400

H 0.01566900 0.91305200 -0.93000400

Transition State I

1 3

U 0.37274900 0.73272000 0.91138500

F -0.40412900 1.29360800 -0.86349200

F 2.30475600 0.74168800 0.33431300

C -0.01705800 -1.69751200 0.99997400

C -0.47973000 -1.78976900 -0.12947200

H -0.88964400 -1.91327600 -1.10971900

C 1.21644500 -0.74030100 3.76316000

O 0.96704300 0.27690700 2.97399100

O 0.99336800 -1.90407900 3.38274800

C 1.76853000 -0.44629200 5.10698100

H 2.68893600 0.11925000 4.93593900

H 1.09534000 0.28193800 5.56661000

C 1.99282000 -1.66078200 5.97864900

H 1.06532700 -2.19675200 6.16113600

H 2.69152300 -2.35508200 5.52020800

H 2.40024500 -1.35906500 6.93846800

H 0.51949400 -1.86746800 2.26764800

Structure III

1 3

C 2.55454000 -0.63572000 -0.12035300

O 3.31266500 -0.17004700 -1.03622900

O 3.13811600 -1.23438200 0.86978900

U 5.24353400 -0.78426300 0.10120000

C 1.08297200 -0.49797300 -0.15475700

H 0.80919100 0.02055600 0.76869700

H 0.67617500 -1.50298300 -0.01465100

C 0.53835900 0.18791600 -1.38729600

H -0.54375200 0.25043700 -1.33059000

H 0.92661400 1.19798100 -1.48582200

H 0.79450700 -0.35508900 -2.29317800

F 5.71033500 0.43908000 1.64690800

F 6.87688500 -0.61002100 -1.07916700

C 5.36179300 -3.64858500 0.60730800

H 4.51551000 -3.85569400 1.22520700

C 6.33569600 -3.49491800 -0.08538200

H 7.20843100 -3.39493600 -0.69305300

Structure V

1 3

C 2.48563000 0.69528600 -0.56308900

O 2.95326300 1.88331900 -0.39347700

O 3.31714300 -0.21506400 -0.89373000

U 5.09263300 1.28053500 -0.92299700

C 1.04151500 0.41861300 -0.37869500

H 0.51116200 1.12168700 -1.02568300

H 0.79409800 0.75475600 0.63147500

C 0.63371800 -1.01610900 -0.62592700

H -0.43382100 -1.13556900 -0.46873600

H 0.85761900 -1.32357800 -1.64404700

H 1.14907300 -1.69819300 0.04512600

F 5.43767700 0.81582700 1.07638400

F 4.96673400 1.81481000 -2.86839600

C 5.58662500 4.00098100 1.04620800

O 5.58208700 3.39003300 -0.04698900

C 5.68992600 5.47694200 1.10732100

H 4.83680600 5.85302100 0.53561200

H 6.55116400 5.74381900 0.49033200

C 5.75972600 6.08087500 2.49201900

H 5.83016800 7.16159700 2.42055800

H 4.87658000 5.84210900 3.07813500

H 6.62820800 5.72582800 3.04034000

O 5.49995500 3.37685700 2.18312300

H 5.45059600 2.40793900 2.04891500

Transition State II

1 3

U 4.76249200 -0.19340600 -0.01123400

F 5.91479600 1.26108700 0.76696300

F 4.21052700 -2.31082300 0.88582900

C 4.95295100 -0.25204100 -2.70030600

O 4.19711900 0.58983200 -2.09750900

O 5.57536100 -1.09328400 -1.95139900

C 5.10477800 -0.24166600 -4.17093100

H 5.43347800 0.76791000 -4.43292200

H 4.09266500 -0.29648200 -4.58037800

C 6.01716500 -1.31084000 -4.72826500

H 6.07210800 -1.22838400 -5.80918000

H 7.02624900 -1.21902200 -4.33546500

H 5.65762300 -2.30763400 -4.48711700

C 1.91528900 -0.61377900 -0.14719200

O 2.56569600 0.27109100 0.49481700

O 2.56968900 -1.63156100 -0.60199600

C 0.46892900 -0.48213000 -0.41859800

H 0.35627300 -0.57475900 -1.50249800

H 0.00428000 -1.39552300 -0.03623400

C -0.17495600 0.77131800 0.12890900

H -1.23298300 0.78440700 -0.11288400

H -0.07925900 0.82901700 1.20991900

H 0.27491200 1.66666300 -0.29196800

H 3.33469400 -2.23373300 0.25500400

Structure VI

1 3

C 2.03039900 -0.51093000 -0.03573800

O 2.60930000 0.57364400 -0.39315900

O 2.79349800 -1.47550600 0.32864000

U 4.74030000 -0.19673000 -0.02797500

F 5.05772800 0.86812100 1.65524800

C 0.55615000 -0.65074900 -0.03386000

H 0.28147400 -0.94556000 0.98243700

H 0.33238200 -1.53799100 -0.63170000

C -0.20183000 0.57064600 -0.50292400

H -1.27080500 0.38481600 -0.46833700

H 0.00790400 1.43398800 0.12281900

H 0.05839700 0.83329500 -1.52493900

C 5.32668500 -0.03680300 -2.66319800

O 5.60555900 0.92604100 -1.87242200

O 4.79089900 -1.08908300 -2.13829000

C 5.59915200 0.04934700 -4.11607200

H 6.65218700 0.32596200 -4.21119300

H 5.06679000 0.93811000 -4.46595300

C 5.24689900 -1.18608600 -4.91307900

H 5.47612300 -1.03143400 -5.96280500

H 5.80722300 -2.05373600 -4.57457100

H 4.18938400 -1.42411400 -4.83461700

F 5.08728400 -2.58756500 0.75086900

H 4.24220600 -2.98383200 0.81965600

Structure VIII

1 3

C 1.51982500 -0.17230900 -0.34885400

O 1.52531400 1.07075900 -0.64913400

O 2.65563000 -0.76506000 -0.27765400

U 3.84874200 1.13393100 -0.84075700

F 4.60124600 1.45611500 1.08277700

C 0.26199400 -0.91468500 -0.08835000

H 0.36651000 -1.34950900 0.90882700

H 0.27545300 -1.78155000 -0.75326200

C -1.00146300 -0.09674200 -0.23033900

H -1.87303800 -0.71055000 -0.02396000

H -1.01284000 0.74203000 0.46088300

H -1.10536900 0.30456000 -1.23513200

C 4.79061300 0.11959700 -3.17457000

O 3.67758900 0.77172600 -3.09876200

O 5.47143300 -0.00103800 -2.10612000

C 5.22750800 -0.45999200 -4.46772400

H 5.21914800 0.35878400 -5.19128600

H 4.41305000 -1.10910900 -4.79938800

C 6.55584400 -1.18049400 -4.42051500

H 6.80220400 -1.57861800 -5.40013000

H 7.36028400 -0.51483100 -4.11852000

H 6.53440100 -2.00917200 -3.71776800

C 4.72929200 4.37507100 -0.11411700

O 4.31901000 3.45839700 -0.86003900

C 4.79812800 5.78110600 -0.58018600

H 3.79411100 6.02553300 -0.93603800

H 5.39899600 5.76323500 -1.49287700

C 5.31128400 6.78895300 0.42378100

H 5.31999400 7.78033000 -0.01825000

H 4.68477000 6.82491200 1.31085800

H 6.32382800 6.55692400 0.74258500

O 5.11780600 4.14906600 1.10576500

H 5.03104700 3.19633700 1.32732300

Transition State III

1 3

U 4.03092200 1.45231400 -0.68431200

F 4.46053100 3.61998800 -1.72252200

C 1.95080300 -0.09818400 0.07755300

O 1.78589600 1.13502600 -0.22718700

O 3.14407900 -0.56336800 -0.00440700

C 0.82418400 -0.96058400 0.50582100

H 1.11592200 -1.38651200 1.46909300

H 0.82582700 -1.82001100 -0.16942800

C -0.52031000 -0.27127300 0.56095800

H -1.28784400 -0.96961300 0.88023500

H -0.51343200 0.56064400 1.26030800

H -0.80806200 0.11923700 -0.41165900

C 5.57731800 1.56004400 1.52525200

O 5.99427600 0.95233800 0.49107800

O 4.41004100 2.12192000 1.44562800

C 6.35864700 1.64733700 2.77956700

H 5.71061200 1.25777600 3.56901400

H 6.44170500 2.71176700 3.01408200

C 7.70188600 0.95481800 2.73647000

H 8.20970500 1.06345800 3.68981300

H 7.59580100 -0.10740000 2.53274100

H 8.34267100 1.37604800 1.96634900

C 5.34447100 1.04181000 -3.26634300

O 5.93384600 2.01185800 -2.72231700

O 4.22941500 0.61196400 -2.75240800

C 5.90985000 0.36447400 -4.46052000

H 6.95147300 0.14198100 -4.21835900

H 5.98337800 1.13769800 -5.23031300

C 5.15334600 -0.85114200 -4.94570300

H 5.63772900 -1.26876500 -5.82306600

H 5.11572800 -1.62814300 -4.18627500

H 4.13031000 -0.60360500 -5.21667500

H 5.16784700 3.19103200 -2.28134000

Structure IX

1 3

C 1.76107700 -0.20144300 0.11913700

O 1.92982400 0.89351900 -0.53640600

O 2.80449400 -0.74686400 0.61477700

U 4.21244700 0.89910000 -0.23953300

C 0.41806000 -0.80457300 0.29361000

H 0.28202400 -0.93244400 1.37040400

H 0.49461100 -1.82795700 -0.08230700

C -0.71750900 -0.03730600 -0.34483100

H -1.66020500 -0.54613800 -0.16837400

H -0.79906800 0.96701900 0.06255800

H -0.58366200 0.05312500 -1.41967900

C 4.95644100 0.71690500 -2.89048400

O 4.66944100 1.85377600 -2.37544000

O 4.89592100 -0.29748000 -2.11528900

C 5.34096500 0.59436600 -4.31780300

H 6.18870800 1.26867600 -4.46360600

H 4.53624700 1.05760100 -4.89411400

C 5.64230500 -0.81410200 -4.77807800

H 5.91722000 -0.81642900 -5.82841400

H 6.46443700 -1.24917600 -4.21598300

H 4.78084100 -1.46566500 -4.65696800

C 5.96270800 1.47168000 1.74989200

O 6.24656800 0.67985400 0.76656400

O 4.81411700 2.01898800 1.74181000

C 6.94032500 1.72818300 2.83503300

H 6.41839200 1.51189800 3.77033000

H 7.08354800 2.81147800 2.86125700

C 8.24680800 0.97705900 2.71308600

H 8.90038300 1.22494700 3.54383400

H 8.09144700 -0.09862100 2.72060700

H 8.76766000 1.22814000 1.79278500

F 3.74365800 3.39325800 -0.58546800

H 3.90981900 3.54420300 -1.49301000

$[UF_2(C{\equiv}CH)]^+$ + 3 eq. Acrylic Acid

Structure II

1 3

U -1.51080000 1.93321300 -1.93739600

F -3.50342500 2.22979800 -1.86820900

F 0.49441100 1.90668400 -2.14484800

C -1.82888300 -1.57125300 -1.34439900

H -1.90458200 -2.63080700 -1.24313800

C -1.74289300 -0.35916300 -1.47046900

C -1.51890900 1.52411800 1.42142400

O -1.41506900 2.12694500 0.31605700

C -1.37357300 2.18893600 2.69699600

H -1.48800200 1.55962200 3.56742100

C -1.11379300 3.49133800 2.78341900

H -1.00095700 4.10575200 1.90063700

H -1.00516300 3.97989400 3.74012600

O -1.76579300 0.25462800 1.48388600

H -1.82634900 -0.14501800 0.57980700

Transition State I

1 3

U 0.37007600 0.73866500 0.92929100

F -0.58703100 1.27769800 -0.77285500

F 2.26369000 1.02147000 0.31330400

C 0.13832000 -1.71606100 0.94898600

C -0.49132600 -1.85534700 -0.09007700

H -1.03172000 -2.00564500 -1.00071900

C 1.31834600 -0.75380100 3.73732800

O 0.97027700 0.26941000 2.99601300

O 1.20096900 -1.91570100 3.30881600

H 0.72302300 -1.87705000 2.18300900

C 1.85778400 -0.47428700 5.08145000

H 2.00170500 -1.38979000 5.64107600

H 2.81089800 0.04269400 4.97427900

H 1.19587500 0.20400700 5.61432600

Structure III

1 3

C 2.74818800 1.39717300 0.32646700

O 3.09968600 2.09608500 1.35869900

O 3.69329200 1.02634800 -0.46354100

U 5.33734200 1.91252300 0.88960500

C 1.36320900 1.05489600 0.11006100

H 0.66526300 1.41495300 0.85212600

C 0.99160900 0.33062600 -0.94525200

H -0.04251500 0.06717600 -1.11178500

H 1.71698500 -0.01781400 -1.66842900

F 5.73270200 0.77363600 2.51742300

F 7.13581400 1.99571800 -0.03751500

C 4.93005600 4.76794100 1.31623700

H 3.98724900 4.84005600 1.81270400

C 5.99805900 4.76319300 0.75841900

H 6.94760200 4.79897600 0.27087200

Structure V

1 3

C 2.99583800 0.67268500 -0.13659100

O 3.43730800 1.88373000 -0.23725700

O 3.86180100 -0.27018200 -0.22465600

U 5.62102200 1.22996200 -0.55846900

C 1.58455500 0.42545200 0.06385700

H 0.95367600 1.30086800 0.11990500

C 1.11320100 -0.81586100 0.16637900

H 0.06103000 -1.00978200 0.31395200

H 1.77376300 -1.67041600 0.10342300

F 7.31542400 0.14762600 -0.77447800

F 5.74473100 2.49802700 -2.22032900

C 6.43509800 4.41668800 0.23417000

O 6.23593500 3.20610600 0.51653100

C 6.79429500 5.41167500 1.22193500

H 6.93230800 6.41604700 0.84901400

C 6.94645300 5.09588000 2.50558600

H 6.80567200 4.08279700 2.85703000

H 7.21735000 5.84032200 3.23920600

O 6.33305100 4.87045900 -0.98147600

H 6.10431100 4.15499900 -1.61427600

Transition State II

1 3

U 6.07178300 1.11863600 -0.59339300

F 7.23136600 -0.46951100 -0.15100700

F 6.27724100 2.61851100 -2.41356900

C 3.49363300 0.75818100 0.11084900

O 4.37731200 1.10128300 0.97305400

O 3.91022500 0.62550200 -1.10844900

C 2.11906600 0.52887400 0.48774200

H 1.88748400 0.66516800 1.53429600

C 1.20811900 0.17242200 -0.41681500

H 0.17756100 0.00063900 -0.14304900

H 1.47505300 0.04399600 -1.45733400

C 6.00047800 3.83996500 0.35045600

O 6.83733600 2.90679700 0.61247700

C 5.89906900 5.03680000 1.15046500

H 5.15000200 5.74990500 0.83789000

C 6.69725700 5.23996300 2.19837400

H 7.44136600 4.50930900 2.48606200

H 6.62993200 6.14002000 2.79161800

O 5.20082700 3.66827200 -0.65105200

H 5.76586100 3.31408400 -1.76421300

Structure VI

1 3

C 6.30555400 2.89433300 -1.72044600

O 5.97350100 3.72664800 -0.79724600

C 6.95460200 3.30874100 -2.94661200

H 7.18299300 2.51936000 -3.64827200

C 7.24368500 4.58752600 -3.17606900

H 6.99997400 5.35261600 -2.45112800

H 7.72842300 4.90257500 -4.08829700

O 6.03423200 1.65482500 -1.51020900

C 7.02265300 0.61061000 1.77172600

O 5.94237500 0.05593000 1.36324300

C 8.09709500 -0.12763100 2.39895400

H 8.95574800 0.45300100 2.70397100

C 8.01149800 -1.44469700 2.57573200

H 7.13678800 -1.99462600 2.25486400

H 8.80886600 -2.00488200 3.04139700

O 7.12678300 1.88995800 1.59926200

U 5.10118100 2.05953700 0.54448500

F 3.16442300 1.78428300 0.00352400

F 3.82507600 3.24279300 2.44754000

H 2.92066300 3.39746500 2.60081000

Structure VIII

1 3

C 6.41571600 2.60722600 -1.97895600

O 5.82311400 2.70386800 -0.84247100

C 7.04747200 3.74549500 -2.61896700

H 7.52287600 3.54738200 -3.56902500

C 7.02901400 4.95156500 -2.05765500

H 6.54023800 5.11416300 -1.10633100

H 7.49642400 5.80301600 -2.52984300

O 6.42810300 1.45184900 -2.53772400

C 6.79302000 -0.14982100 1.35100200

O 7.22979300 -0.24078100 0.13610900

C 7.64316500 -0.43904700 2.48896800

H 7.17638500 -0.33768200 3.45843600

C 8.91442600 -0.79921700 2.33186600

H 9.35054100 -0.88783500 1.34582900

H 9.55044800 -1.01193300 3.17840600

O 5.57744200 0.20990300 1.51036500

U 5.24893000 0.46076400 -0.79478300

F 3.21089200 0.77316700 -1.14056100

C 3.57213300 -2.18102000 -2.20270800

O 4.58412300 -1.61060600 -1.72960500

C 3.59986700 -3.52081300 -2.75409800

H 2.65848400 -3.89874100 -3.12557800

C 4.72522400 -4.22903800 -2.79649100

H 5.65586700 -3.82684300 -2.41945800

H 4.74696600 -5.22649300 -3.20923700

O 2.40102200 -1.60610900 -2.23467200

H 2.44871400 -0.70153400 -1.85876400

Transition State III

1 3

U 5.46968700 0.49206400 -1.03100100

F 3.08159300 0.65089300 -0.80649200

C 6.62668200 2.67704500 -2.08415400

O 5.54170000 2.74610300 -1.39973200

C 7.24471500 3.83399000 -2.70128500

H 8.15433000 3.64502300 -3.25647500

C 6.70699200 5.04556300 -2.57321700

H 5.79533600 5.19500600 -2.00687500

H 7.16603800 5.91301200 -3.03014400

O 7.14661800 1.51069000 -2.20143700

C 6.58353700 -0.24351500 1.29656700

O 6.98346900 -0.71182400 0.16947700

C 7.18490700 -0.61310000 2.56351100

H 6.75413600 -0.15259600 3.44310100

C 8.20371600 -1.46865800 2.61451000

H 8.60862900 -1.90904200 1.71110400

H 8.65492500 -1.74655500 3.55850600

O 5.61011900 0.58746800 1.24745000

C 4.28530700 -1.98103800 -1.81364100

O 4.99621900 -1.15321200 -2.49823000

C 4.03716900 -3.33501100 -2.27164400

H 3.43726900 -3.95038700 -1.61383100

C 4.51418700 -3.77125000 -3.43610600

H 5.10910800 -3.12876400 -4.07412000

H 4.31804900 -4.77957800 -3.77798200

O 3.82569600 -1.58085300 -0.69507500

H 3.09279900 -0.35207500 -0.70030400

Structure IX

1 3

C 2.43845000 0.82957300 0.39477500

O 3.36185200 0.06034000 -0.05970600

C 1.06807000 0.38269200 0.55000900

H 0.37506500 1.11115600 0.94636900

C 0.70201600 -0.85230400 0.21608100

H 1.42085900 -1.55650900 -0.18103200

H -0.31751500 -1.19049100 0.32817800

O 2.78527400 2.02217200 0.70744700

C 6.00110200 2.88495400 -2.08673800

O 6.35575500 3.29158300 -0.93190600

C 6.46916100 3.48835400 -3.31841400

H 6.09920200 3.04622300 -4.23239800

C 7.30354900 4.52491700 -3.30075200

H 7.65176000 4.94301900 -2.36562900

H 7.65835400 4.98059400 -4.21334300

O 5.17833600 1.88107500 -2.13372000

C 6.56497100 0.36881900 2.00518800

O 6.70784600 0.08905200 0.76404000

C 7.32354600 -0.28770200 3.05087900

H 7.11615600 0.03689900 4.06044900

C 8.21737700 -1.23050400 2.76253400

H 8.39914200 -1.53029600 1.73904000

H 8.78751100 -1.72460300 3.53530600

O 5.69950400 1.27965100 2.30379300

U 5.06672900 1.61593100 0.12125300

F 4.46205600 3.86292400 1.19798500

H 3.55813700 3.78010300 1.42133700