Supporting Information

NMR Study of CO_2 Capture by Fluoroalkylamines: Ammonium ion pK_a Depression via Fluorine Modification and Thermochemistry of Carbamylation

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Stationary Structures Used in the Determination of K_7 at GEN(APFD/6-311+G*, 6-311G*) with Explicit Solvation

Substituent Effect of Adding tF Group to Butylcarbamic Acid

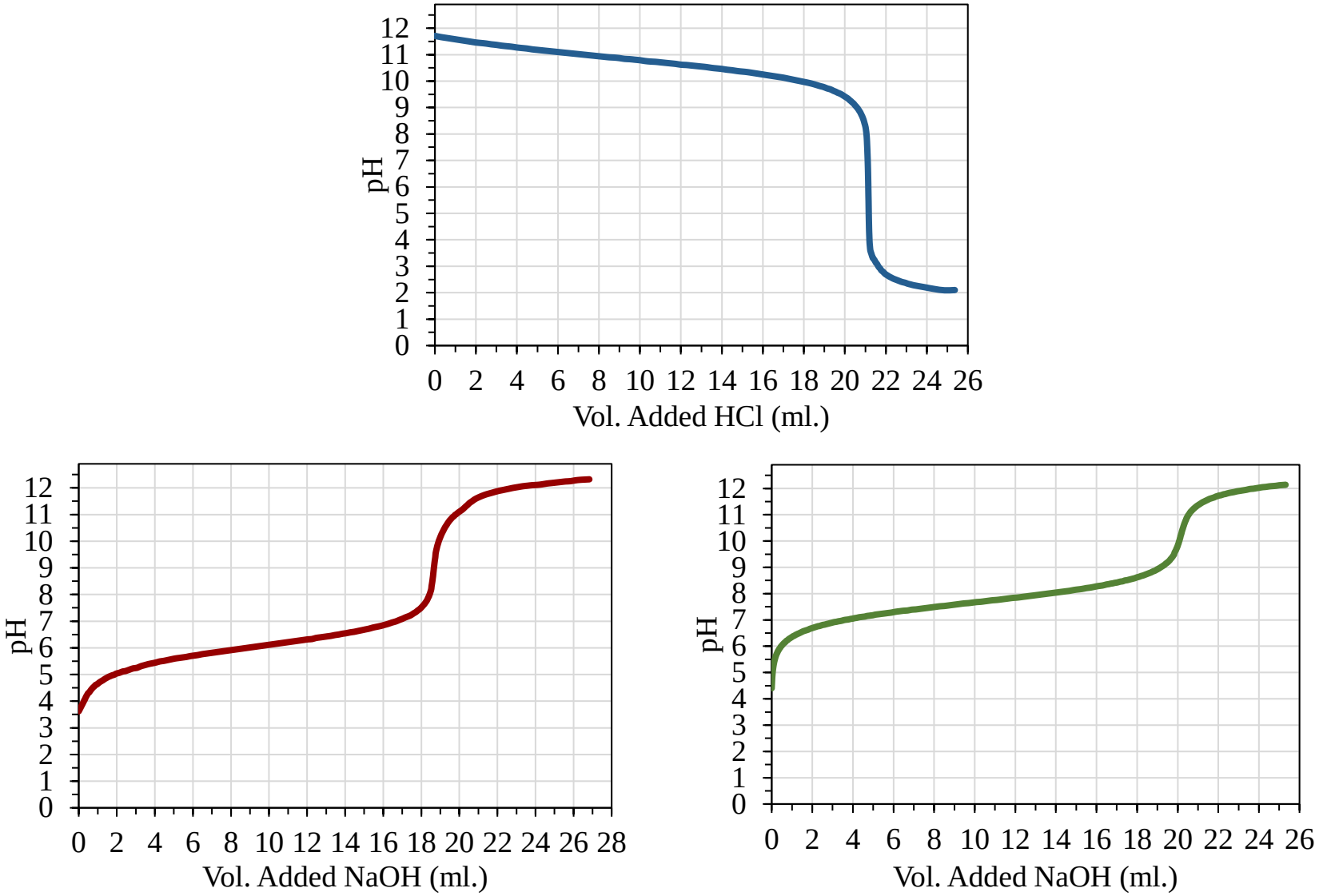

Figure S1. Experimental titration curve of **1a** (blue, pK_a = 10.74), **2a** (red, pK_a = 6.05), and **3a** (green, pK_a = 7.68).

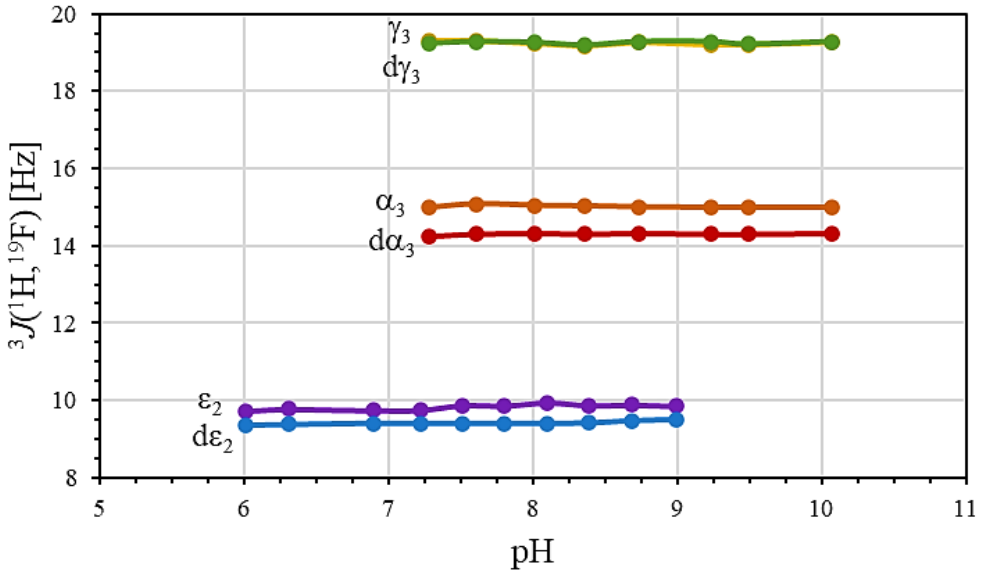

Figure S2. Variation of the $^3J(^1H,^{19}F)$ coupling constant with pH for **2** and **3**.

Table S1. Total Energies and Thermochemical Parameters of Structures Involved in Reactions R6-R8[a-c]

Structure	Method	Total E	VZPE	TE	S	υ	G_{298}	H_{298}
Stationary Structures Used in the Determination of K_7 at APFD/6-311G*								
H_2NCOOH	A	-245.026813	32.00	34.87	68.65	72.4	-245.002913	-244.970298
H_2NCOO^-	A	-244.556677	24.43	26.78	64.30	458.7	-244.543608	-244.513059
(H)(tF)NCOOH	A	-621.219625	53.77	59.13	92.80	56.5	-621.168548	-621.124454
(H)(tF)$NCOO^-$	A	-620.753664	45.69	50.80	91.22	54.9	-620.715098	-620.671759
(Me)(H)NCOOH	A	-284.305789	49.95	53.62	76.88	35.1	-284.255921	-284.219394
(Me)(H)$NCOO^-$	A	-283.836236	42.12	45.41	72.59	136.9	-283.797425	-283.762934
(Me)(tF)NCOOH	A	-660.498553	71.62	77.82	98.79	45.8	-660.420531	-660.373594
(Me)(tF)$NCOO^-$	A	-660.033293	63.51	69.43	96.77	44.5	-659.967686	-659.921709
Stationary Structures Used in the Determination of K_7 at APFD/6-311G* with Explicit Solvation								
$H_2NCOOH•2H_2O$	A	-397.836607	63.79	69.66	93.88	37.7	-397.769267	-397.724660
$H_2NCOO-•2H_2O$	A	-397.367440	55.72	61.39	93.73	31.8	-397.313197	-397.268664
(H)(tF)$NCOOH•2H_2O$	A	-774.028168	85.46	93.89	118.18	27.1	-773.933753	-773.877603

(H)(tF)NCOO$^-$•2H$_2$O	A	-773.563472	77.41	85.81	118.76	25.5	-773.482204	-773.425777
(Me)(H)NCOOH•2H$_2$O	A	-437.117028	81.80	88.57	102.82	31.3	-437.023787	-436.974932
(Me)(H)NCOO$^-$•2H$_2$O	A	-436.647222	73.37	80.06	102.53	24.9	-436.567417	-436.518700
(Me)(tF)NCOOH•2H$_2$O	A	-813.308671	103.31	112.61	123.86	30.5	-813.187118	-813.128268
(Me)(tF)NCOO$^-$•2H$_2$O	A	-812.842991	94.99	104.29	125.70	23.2	-812.735575	-812.675852
Stationary Structures Used in the Determination of K_7 at GEN(APFD/6-311+G*, 6-311G*) with Explicit Solvation								
H$_2$NCOOH•2H$_2$O	B	-397.854260	63.26	69.23	94.88	28.5	-397.788071	-397.742990
H$_2$NCOO$^-$•2H$_2$O	B	-397.396754	55.12	60.90	94.64	33.2	-397.343734	-397.298768
(H)(tF)NCOOH•2H$_2$O	B	-774.054925	84.84	93.43	119.46	28.3	-773.961857	-773.905096
(H)(tF)NCOO$^-$•2H$_2$O	B	-773.600603	76.83	85.32	119.96	25.7	-773.520696	-773.463699
(dF)(H)NCOOH•2H$_2$O	B	-714.138981	107.05	116.15	123.35	13.6	-714.011553	-713.952945
(dF)(H)NCOO$^-$•2H$_2$O	B	-713.682375	99.20	108.16	122.78	21.5	-713.567401	-713.509063
(Me)(H)NCOOH•2H$_2$O	B	-437.134456	81.39	88.23	102.35	35.2	-437.042154	-436.992915
(Me)(H)NCOO$^-$•2H$_2$O	B	-436.675468	72.92	79.68	104.19	19.4	-436.597057	-436.547551
(Me)(tF)NCOOH•2H$_2$O	B	-813.334154	102.18	111.83	130.20	5.9	-813.216866	-813.155004
(Me)(tF)NCOO$^-$•2H$_2$O	B	-812.878403	94.52	103.87	126.18	24.9	-812.771891	-812.711937
(Et)(H)NCOOH•2H$_2$O	B	-476.426011	99.41	106.91	108.90	24.7	-476.306629	-476.254688
(Et)(H)NCOO$^-$•2H$_2$O	B	-475.967113	91.07	98.48	109.86	22.6	-475.861434	-475.809238
(Et)(tF)NCOOH•2H$_2$O	B	-852.625212	120.46	130.73	132.10	24.4	-852.478695	-852.415932
(Et)(tF)NCOO$^-$•2H$_2$O	B	-852.167767	112.67	122.72	131.17	20.8	-852.033573	-851.971251
(Pr)(H)NCOOH•2H$_2$O	B	-515.715264	117.35	125.71	116.88	17.3	-515.569521	-515.513989
(Pr)(H)NCOO$^-$•2H$_2$O	B	-515.256307	109.01	117.25	117.08	15.6	-515.124145	-515.068516
(Pr)(tF)NCOOH•2H$_2$O	B	-891.914876	138.45	149.52	139.17	22.5	-891.741773	-891.675650
(Pr)(tF)NCOO$^-$•2H$_2$O	B	-891.456645	130.34	141.34	139.16	28.0	-891.296577	-891.230460
(Bu)(H)NCOOH•2H$_2$O	B	-555.005133	135.50	144.54	123.98	25.1	-554.831786	-554.773847
(Bu)(H)NCOO$^-$•2H$_2$O	B	-554.545210	127.09	136.07	124.19	16.3	-554.386434	-554.327429
(Bu)(tF)NCOOH•2H$_2$O	B	-931.204312	156.69	168.55	147.56	22.1	-931.003744	-930.934774
(Bu)(tF)NCOO$^-$•2H$_2$O	B	-930.744640	148.43	160.24	147.63	10.7	-930.558486	-930.488341

[a]Method A: SMD[APFD/6-311G*]; Method B: SMD[APFD/6-311G*, 6-311+G*]. [b](tF) = Trifluoroethyl, (dF) = 2,2-Difluoropropyl, (Me) = Methyl, (Et) = Ethyl, (Pr) = Propyl, (Bu) = Butyl, •2H2O = Explicit Water. [c]Total energies (Total E) in Hartree, vibrational zero-point energies (VZPE) and thermal energies (TE) in kcal/mol, and entropy (*S*) in cal/mol^{-1} K^{-1}. Lowest vibrational wavenumber in cm^{-1}.

Table S2. ^{1}H NMR Data for the pH Profile of (2,2,2-trifluoroethyl)butylamine 2b in 90% H_2O : 10% D_2O Solution[a,b]

Peak	pH														
	6.01			6.31			6.9			7.22			7.51		
	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1$
Parent															
α	2.71	t	7.80	2.67	t	7.80	2.57	t	7.35	2.55	t	7.35	2.53	t	7.59
β	1.41	p	7.80	1.39	p	7.57	1.35	p	7.58	1.35	p	7.35	1.33	p	7.69
γ	1.21	sx	7.57	1.20	sx	7.57	1.18	sx	7.35	1.18	sx	7.81	1.18	sx	7.35
δ	0.77	t	7.34	0.75	t	7.46	0.75	t	7.46	0.75	t	7.35	0.76	t	7.35
			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^1$
ε	3.37	q	9.73	3.32	q	9.77	3.18	q	9.74	3.15	q	9.75	3.13	q	9.87
Daughter															
dε	3.80	q	9.36	3.80	q	9.18	3.38	q	9.41	3.80	q	9.41	3.80	q	9.41
Peak	pH														
	7.80			8.10			8.39			8.69			8.99		
	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^1$
Parent															
α	2.53	t	7.58	2.52	t	7.45	2.53	t	7.58	2.52	t	7.52	2.52	t	7.47
β	1.33	p	7.69	1.32	p	7.61	1.33	p	7.54	1.33	p	7.58	1.33	p	7.55
γ	1.18	sx	8.04	1.18	sx	7.58	1.18	sx	8.04	1.17	sx	7.58	1.17	sx	7.81
δ	0.75	t	7.35	0.76	t	7.35	0.76	t	7.37	0.77	t	7.35	0.75	t	7.43
			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^{19}F)$			$^3J(^1H,^1$
ε	3.12	q	9.86	3.12	q	9.94	3.12	q	9.87	3.12	q	9.88	3.12	q	9.85
Daughter															
dε	3.80	q	9.41	3.80	q	9.41	3.80	q	9.42	3.80	q	9.48	3.80	q	9.50

[a]All peaks reported relative to internal standard DSS signal. δ in ppm, *J* in Hz. [b]The $^3J(^1H,^{19}F)$ is the coupling between the ε_2 CH_2 to the CF_3 fluorine.

Table S3. ^{1}H NMR Data for the pH Profile of 2,2-difluoropropylamine 3b in 90% H_2O : 10% D_2O Solution[a,b]

Peak	pH											
	7.28				7.61				8.01			
	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$
Parent												
α	3.35	t	14.98	~	3.25	t	15.08	~	3.14	t	15.04	~
γ	1.72	t	19.30	~	1.70	t	19.32	~	1.66	t	19.24	~
Daughter												
dα	3.43	dt	14.24	6.54	3.43	dt	14.30	6.56	3.43	dt	14.32	6.67
dγ	1.60	t	19.24	~	1.60	t	19.28	~	1.60	t	19.26	~
Peak	pH											
	8.36				8.73				9.03			
	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$
Parent												
α	3.05	t	15.02	~	3.00	t	15.00	~	2.98	t	14.98	~
γ	1.64	t	19.16	~	1.63	t	19.26	~	1.62	t	19.20	~
Daughter												
dα	3.43	dt	14.30	6.68	3.43	dt	14.32	6.68	3.43	dt	14.30	6.68
dγ	1.59	t	19.20	~	1.60	t	19.28	~	1.60	t	19.28	~
	9.49		10.07									
Peak	pH											
	9.23				9.49				10.07			
	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$	δ	Mult.	$^3J(^1H,^{19}F)$	$^3J(^1H,^1H)$
Parent												
α	2.97	t	14.98	~	2.96	t	14.98	~	2.94	t	14.98	~
γ	1.62	t	19.20	~	1.62	t	19.18	~	1.61	t	19.26	~
Daughter												
dα	3.43	dt	14.30	6.68	3.43	dt	14.30	6.69	3.43	dt	14.32	6.69
dγ	1.60	t	19.28	~	1.60	t	19.22	~	1.59	t	19.28	~

[a]All peaks reported relative to internal standard DSS signal. δ in ppm, *J*-coupling in Hz. [b]The $^3J(^1H,^{19}F)$ is coupling between the α_3 CH_2 to the β_3 CF_2 fluorine, and $^3J(^1H,^1H)$ is between the α_3 CH_2 to the NH hydrogen.

Stationary Structures Used in the Determination of K_7 at APFD/6-311G*

Substituent Effect of Adding tF Group to Parent Carbamic Acid

Structure **H_2NCOOH**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.261469	-0.240960	0.006748
2	6	0	-0.030706	0.115361	0.000048
3	8	0	-0.844602	-0.967040	-0.000434
4	1	0	-1.755549	-0.647279	-0.000657
5	8	0	-0.454828	1.263752	-0.000691
6	1	0	1.538916	-1.207527	-0.019346
7	1	0	1.966026	0.475664	-0.018516

Rotational constants (GHZ): 11.6031887 10.8999634 5.6204502
Standard basis: 6-311G(d) (5D, 7F)

Structure **H_2NCOO^-**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.264369	0.000009	-0.088824
2	6	0	0.142530	-0.000000	-0.002952
3	8	0	0.712404	1.127789	0.007882
4	8	0	0.712387	-1.127798	0.007883
5	1	0	-1.701467	0.841357	0.256684
6	1	0	-1.701466	-0.841344	0.256676

Rotational constants (GHZ): 11.9367151 11.2928350 5.8327876
Standard basis: 6-311G(d) (5D, 7F)

Structure **(H)(tF)NCOOH**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.400872	-0.003486	-0.055755
2	6	0	-0.387194	0.093943	1.065005
3	1	0	-0.208263	-0.909067	1.450527
4	1	0	-0.821909	0.699128	1.860972
5	7	0	0.846809	0.671475	0.618247
6	6	0	1.828138	-0.100827	0.095945
7	8	0	2.810663	0.662157	-0.424442
8	1	0	3.501705	0.076397	-0.759371
9	8	0	1.854395	-1.320570	0.109515
10	9	0	-2.544673	-0.564452	0.373818
11	9	0	-0.948565	-0.744121	-1.085619
12	9	0	-1.711394	1.208403	-0.558506
13	1	0	0.881593	1.664271	0.441149

Rotational constants (GHZ): 3.3867167 0.9619400 0.9090947

Standard basis: 6-311G(d) (5D, 7F)

Structure **(H)(tF)NCOO$^-$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.322035	-0.008863	-0.054109
2	6	0	-0.332729	-0.043638	1.090403
3	1	0	-0.133184	-1.087787	1.326624
4	1	0	-0.824468	0.415413	1.951643
5	7	0	0.900217	0.618608	0.781845
6	6	0	1.901792	-0.050205	0.033071
7	8	0	2.734882	0.697813	-0.545382
8	8	0	1.900048	-1.308493	0.050232
9	9	0	-2.463198	-0.658752	0.254910
10	9	0	-0.837899	-0.570986	-1.179709
11	9	0	-1.667719	1.257295	-0.380546
12	1	0	0.813866	1.595779	0.541942

Rotational constants (GHZ): 3.3075597 1.0089166 0.9606413
Standard basis: 6-311G(d) (5D, 7F)

Substituent Effect of Adding tF Group to Methylcarbamic Acid

Structure **(Me)(H)NCOOH**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.612812	-0.668606	0.000003
2	6	0	1.863723	0.063181	-0.000001
3	1	0	2.679624	-0.657386	0.000008
4	1	0	1.958503	0.692440	-0.887363
5	1	0	1.958498	0.692458	0.887348
6	6	0	-0.603096	-0.103456	0.000000
7	8	0	-0.535594	1.248243	0.000000
8	1	0	-1.440047	1.586212	-0.000000
9	8	0	-1.668834	-0.712828	-0.000001
10	1	0	0.625399	-1.675157	-0.000002

Rotational constants (GHZ): 10.5820456 4.2427191 3.0872138
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(H)NCOO$^-$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.573460	-0.648668	-0.205027
2	6	0	-0.635852	0.045048	-0.026307
3	8	0	-0.590665	1.307916	-0.025636
4	8	0	-1.679432	-0.662610	0.087593
5	1	0	0.519070	-1.603714	0.116941

6	6	0	1.823605	0.019972	0.087120
7	1	0	2.652786	-0.660544	-0.115643
8	1	0	1.943079	0.893124	-0.555458
9	1	0	1.905107	0.359240	1.128818

Rotational constants (GHZ): 10.8243196 4.3316931 3.1885812
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(tF)NCOOH**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.498249	-0.104102	-0.060607
2	6	0	-0.452357	0.054511	1.024748
3	1	0	-0.345732	-0.905271	1.527480
4	1	0	-0.825241	0.783270	1.745523
5	7	0	0.819199	0.480434	0.502108
6	6	0	0.989152	1.874921	0.112307
7	1	0	0.286807	2.479273	0.683805
8	1	0	1.998557	2.210247	0.344654
9	1	0	0.799630	2.026554	-0.952837
10	6	0	1.687861	-0.481697	0.098562
11	8	0	2.755815	0.039821	-0.536223
12	1	0	3.351621	-0.688121	-0.756106
13	8	0	1.554202	-1.681862	0.294339
14	9	0	-2.648962	-0.577833	0.449786
15	9	0	-1.103636	-0.953553	-1.027367
16	9	0	-1.785026	1.065335	-0.669338

Rotational constants (GHZ): 2.3195610 0.9354778 0.7974095
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(tF)NCOO^{-}**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428245	-0.104577	-0.056387
2	6	0	-0.392474	0.026677	1.045088
3	1	0	-0.283551	-0.955733	1.500637
4	1	0	-0.807894	0.708989	1.791829
5	7	0	0.887392	0.482379	0.586511
6	6	0	0.970455	1.852502	0.117393
7	1	0	0.319277	2.482021	0.726771
8	1	0	1.991169	2.218975	0.219820
9	1	0	0.675265	1.966969	-0.932756
10	6	0	1.779755	-0.473307	0.031616
11	8	0	2.734947	-0.017606	-0.653355
12	8	0	1.566024	-1.687336	0.295066
13	9	0	-2.543296	-0.719255	0.393368
14	9	0	-0.979070	-0.814578	-1.109367
15	9	0	-1.821049	1.093154	-0.547537

Rotational constants (GHZ): 2.3053033 0.9720384 0.8301668

Standard basis: 6-311G(d) (5D, 7F)

Stationary Structures Used in the Determination of K_7 at APFD/6-311G* with Explicit Solvation

Substituent Effect of Adding tF Group to Parent Carbamic Acid with Explicit Solvation

Structure **$H_2NCOOH•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.506068	-0.147261	-0.107129
2	1	0	2.984989	-0.984770	0.176564
3	1	0	3.043784	0.682297	-0.294549
4	6	0	1.173178	-0.077865	0.045048
5	8	0	0.685857	1.121019	-0.256729
6	8	0	0.487286	-1.040073	0.411958
7	1	0	-0.309615	1.171482	-0.103560
8	1	0	-1.976494	1.551154	1.047258
9	1	0	-2.218854	-1.423466	-1.119511
10	8	0	-1.867999	1.359027	0.110972
11	1	0	-2.145850	0.419325	-0.005652
12	8	0	-2.150976	-1.269854	-0.172663
13	1	0	-1.192849	-1.278955	0.030759

Rotational constants (GHZ): 4.6212269 1.7670245 1.3255410
Standard basis: 6-311G(d) (5D, 7F)

Structure **$H_2NCOO^-•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.507411	-0.108763	0.017450
2	6	0	1.120832	-0.011953	0.023818
3	8	0	0.479358	-1.032360	-0.372933
4	8	0	0.619837	1.061686	0.466842
5	1	0	2.890429	-0.809505	-0.597868
6	1	0	-1.015421	1.367981	-0.058508
7	8	0	-1.949371	1.421558	-0.350445
8	1	0	-1.133137	-1.188155	-0.009548
9	8	0	-2.099951	-1.278819	0.193332
10	1	0	-2.168003	-1.186941	1.147845
11	1	0	-2.251432	0.503154	-0.247916
12	1	0	3.001705	0.770004	0.006571

Rotational constants (GHZ): 4.5967964 1.7797594 1.3514691
Standard basis: 6-311G(d) (5D, 7F)

Structure **(H)(tF)$NCOOH•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.468866	-0.957544	0.908456
2	6	0	0.767083	-0.529086	0.546163
3	8	0	0.910985	0.781680	0.591907
4	8	0	1.655824	-1.329650	0.240815
5	1	0	1.863075	1.070817	0.392479
6	1	0	4.675827	-1.005967	-0.469735
7	8	0	3.291316	1.631700	0.118106
8	1	0	3.678501	0.872195	-0.380551
9	8	0	3.969799	-0.664374	-1.026349
10	1	0	3.138047	-0.988762	-0.625830
11	1	0	3.732537	1.636469	0.972928
12	6	0	-1.607078	-0.097782	1.075245
13	1	0	-2.320744	-0.555517	1.761172
14	1	0	-1.303170	0.861930	1.488648
15	6	0	-2.323397	0.152059	-0.235601
16	9	0	-1.515997	0.696871	-1.164764
17	9	0	-2.807124	-0.989525	-0.766456
18	9	0	-3.364341	0.986794	-0.065682
19	1	0	-0.637894	-1.941620	0.763134

Rotational constants (GHZ): 1.9448920 0.4345249 0.4117476
Standard basis: 6-311G(d) (5D, 7F)

Structure **(H)(tF)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.421921	-0.230470	1.315513
2	6	0	-0.808942	-0.103956	0.662042
3	8	0	-1.042018	0.965571	0.037941
4	8	0	-1.596666	-1.084335	0.805619
5	1	0	-3.280058	-1.003349	-1.738663
6	8	0	-3.732470	1.462858	-0.085527
7	1	0	-3.983265	0.572270	-0.384777
8	8	0	-3.660767	-1.178681	-0.873416
9	1	0	-2.895647	-1.154231	-0.245314
10	1	0	-2.760126	1.388530	-0.016798
11	6	0	1.538813	0.586474	0.940623
12	1	0	1.193711	1.591342	0.702845
13	1	0	2.263063	0.655634	1.755261
14	6	0	2.273499	0.045458	-0.267019
15	9	0	2.801836	-1.175238	-0.025737
16	9	0	1.473518	-0.092828	-1.342531
17	9	0	3.291802	0.851105	-0.628219
18	1	0	0.639619	-1.175414	1.596423

Rotational constants (GHZ): 1.9527039 0.4373992 0.4262068
Standard basis: 6-311G(d) (5D, 7F)

Substituent Effect of Adding tF Group to Methylcarbamic Acid with Explicit Solvation

Structure **(Me)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.021243	-0.467805	-0.127815
2	1	0	2.351859	-1.408074	-0.272367
3	6	0	0.700383	-0.272190	-0.006774
4	8	0	-0.008253	-1.382034	-0.206069
5	8	0	0.208878	0.834363	0.255996
6	1	0	-0.993983	-1.224121	-0.071749
7	1	0	-2.679434	1.957970	0.487116
8	8	0	-2.565746	-1.081814	0.130998
9	1	0	-2.662376	-0.117413	-0.055673
10	8	0	-2.348401	1.530873	-0.308323
11	1	0	-1.396629	1.367088	-0.143994
12	6	0	2.963371	0.607748	0.086702
13	1	0	2.935951	0.970125	1.117793
14	1	0	3.965141	0.238221	-0.125042
15	1	0	2.755611	1.446593	-0.580368
16	1	0	-2.699190	-1.180197	1.078598

Rotational constants (GHZ): 3.9811768 1.1696717 0.9270401
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(H)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.992925	-0.435919	-0.293075
2	1	0	-2.293348	-1.397839	-0.329018
3	6	0	-0.624211	-0.284144	-0.147130
4	8	0	0.092960	-1.283416	-0.454260
5	8	0	-0.201228	0.845872	0.247942
6	1	0	2.457114	1.327686	-1.174631
7	8	0	2.615229	-1.114631	0.528465
8	1	0	2.758299	-0.168674	0.354801
9	8	0	2.322997	1.514393	-0.241208
10	1	0	1.379563	1.269203	-0.061046
11	6	0	-2.909818	0.502334	0.316704
12	1	0	-2.722685	1.510517	-0.054858
13	1	0	-3.930616	0.228002	0.047067
14	1	0	-2.836892	0.527112	1.411145
15	1	0	1.703544	-1.251467	0.193116

Rotational constants (GHZ): 3.9939439 1.1770605 0.9645093
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(tF)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.388368	-0.985292	-0.539265
2	6	0	0.813933	-0.427400	-0.227607
3	8	0	0.972378	0.805633	-0.681395
4	8	0	1.675322	-1.051108	0.401424
5	1	0	1.860185	1.195547	-0.388546
6	1	0	4.736178	-0.624120	0.960142
7	8	0	3.209235	1.870143	0.027918
8	1	0	3.786101	1.068924	0.040430
9	8	0	4.339734	-0.534189	0.088563
10	1	0	3.415660	-0.838160	0.185522
11	6	0	-0.688833	-2.295283	0.019428
12	1	0	-0.864332	-2.250200	1.097428
13	1	0	-1.581537	-2.684735	-0.467170
14	1	0	0.137811	-2.977512	-0.172351
15	1	0	3.089996	2.121887	0.948768
16	6	0	-1.478923	-0.176179	-1.021475
17	1	0	-1.109611	0.622042	-1.661395
18	1	0	-2.166925	-0.789619	-1.605069
19	6	0	-2.269801	0.457515	0.106988
20	9	0	-2.909195	-0.460873	0.861152
21	9	0	-1.486993	1.163090	0.944594
22	9	0	-3.205653	1.295255	-0.374522

Rotational constants (GHZ): 1.5231497 0.4328367 0.3716680
Standard basis: 6-311G(d) (5D, 7F)

Structure **(Me)(tF)NCOO^{-}•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.391032	-0.861744	0.778856
2	6	0	-0.856316	-0.362391	0.375649
3	8	0	-1.089381	0.863612	0.568169
4	8	0	-1.659385	-1.203927	-0.123808
5	1	0	-3.501090	0.441858	-1.925210
6	8	0	-3.758320	1.337254	0.880021
7	1	0	-4.050551	0.803605	0.121164
8	8	0	-3.824334	-0.263449	-1.357423
9	1	0	-3.018472	-0.620838	-0.907205
10	6	0	0.766101	-2.206758	0.380709
11	1	0	0.921792	-2.302673	-0.699572
12	1	0	1.691651	-2.481481	0.888531
13	1	0	-0.008316	-2.913011	0.676860
14	1	0	-2.786245	1.233095	0.841697
15	6	0	1.449729	0.071735	1.039112
16	1	0	1.038913	0.970130	1.495556
17	1	0	2.186353	-0.357586	1.722302
18	6	0	2.194515	0.500237	-0.211585
19	9	0	2.931220	-0.500804	-0.743855
20	9	0	1.367024	0.920651	-1.187354
21	9	0	3.047971	1.510625	0.052864

Rotational constants (GHZ): 1.4528343 0.4297213 0.3948275
Standard basis: 6-311G(d) (5D, 7F)

Stationary Structures Used in the Determination of K_7 at GEN(APFD/6-311+G*, 6-311G*) with Explicit Solvation

Substituent Effect of Adding tF or dF Group to Parent Carbamic Acid

Structure **$H_2NCOOH•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.538956	-0.155422	-0.049599
2	1	0	3.002396	-1.042743	0.053181
3	1	0	3.088576	0.674346	-0.202340
4	6	0	1.201318	-0.095688	0.025286
5	8	0	0.732553	1.139208	-0.130974
6	8	0	0.489045	-1.090435	0.221020
7	1	0	-0.270457	1.180847	-0.058220
8	1	0	-2.097073	1.778325	0.851004
9	1	0	-2.451463	-1.581321	-0.914719
10	8	0	-1.854511	1.394523	0.002409
11	1	0	-2.179094	0.465101	0.007722
12	8	0	-2.220797	-1.258521	-0.038020
13	1	0	-1.243817	-1.290672	0.023363

Rotational constants (GHZ): 4.5957313 1.7300058 1.2738181

Structure **$H_2NCOO^-•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.538513	-0.135404	0.116357
2	6	0	1.166685	-0.003624	-0.012681
3	8	0	0.498947	-1.067917	-0.202640
4	8	0	0.679103	1.160444	0.108331
5	1	0	2.947969	-0.981466	-0.249294
6	1	0	-1.036717	1.400176	-0.034190
7	8	0	-2.016048	1.470447	-0.090927
8	1	0	-1.170714	-1.210977	-0.036302
9	8	0	-2.154860	-1.297856	0.027104
10	1	0	-2.343627	-1.601269	0.920098
11	1	0	-2.310611	0.542472	-0.052422
12	1	0	3.086867	0.699686	-0.021248

Rotational constants (GHZ): 4.5363916 1.7364271 1.2687234

Structure **$(H)(tF)NCOOH•2H_2O$**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.472907	-1.093577	-0.672725
2	6	0	-0.751578	-0.582042	-0.403963

3	8	0	-1.590782	-1.513705	0.028197
4	8	0	-1.040420	0.606068	-0.568712
5	1	0	-2.511786	-1.147644	0.220306
6	1	0	-3.421806	2.434753	0.507261
7	8	0	-3.997459	-0.709457	0.573918
8	1	0	-3.981437	0.254231	0.372470
9	8	0	-3.474646	1.798092	-0.212304
10	1	0	-2.567847	1.457891	-0.350509
11	1	0	-4.124398	-0.790366	1.524644
12	6	0	1.581211	-0.264533	-1.042382
13	1	0	2.269418	-0.818261	-1.682136
14	1	0	1.233360	0.611843	-1.588763
15	6	0	2.361495	0.215224	0.166673
16	9	0	1.599118	0.921036	1.024978
17	9	0	2.884326	-0.810527	0.871661
18	9	0	3.386878	1.006597	-0.201754
19	1	0	0.640931	-2.061241	-0.438912

Rotational constants (GHZ): 1.9157980 0.4292836 0.3921326

Structure **(H)(tF)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.457045	-0.903133	-0.989951
2	6	0	0.787491	-0.423599	-0.587740
3	8	0	0.994225	0.819737	-0.636784
4	8	0	1.626174	-1.310831	-0.242223
5	1	0	3.921347	-0.853131	1.785712
6	8	0	3.505243	1.739859	-0.102295
7	1	0	3.909366	0.939202	0.279283
8	8	0	4.027981	-0.817750	0.830479
9	1	0	3.134247	-0.993320	0.443720
10	1	0	2.592048	1.450311	-0.318627
11	6	0	-1.605179	-0.052265	-1.088621
12	1	0	-1.316107	0.928280	-1.465020
13	1	0	-2.341540	-0.476476	-1.774482
14	6	0	-2.301841	0.148543	0.243343
15	9	0	-2.758756	-1.016696	0.756297
16	9	0	-1.493894	0.683593	1.180655
17	9	0	-3.367561	0.968157	0.124179
18	1	0	-0.629958	-1.872612	-0.766410

Rotational constants (GHZ): 1.9069525 0.4306253 0.4067784

Structure **(dF)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.439945	-1.096782	-0.644773
2	6	0	0.794088	-0.609447	-0.388115
3	8	0	0.952255	0.658803	-0.725557
4	8	0	1.683502	-1.321799	0.097980

5	1	0	1.882576	0.999883	-0.528400
6	1	0	4.447528	-0.690216	1.527828
7	8	0	3.290830	1.671871	-0.271638
8	1	0	3.811478	0.918935	0.092907
9	8	0	4.283396	-0.660830	0.580185
10	1	0	3.366841	-0.979167	0.446127
11	1	0	3.207863	2.317969	0.437212
12	6	0	-1.585192	-0.307540	-1.020273
13	1	0	-1.270667	0.556808	-1.602449
14	1	0	-2.245801	-0.913069	-1.644284
15	6	0	-2.386678	0.174402	0.181792
16	6	0	-1.687912	1.079094	1.153381
17	1	0	-0.823480	0.574284	1.587721
18	1	0	-1.351112	1.981280	0.640970
19	1	0	-0.604372	-2.035077	-0.310321
20	1	0	-2.375495	1.353562	1.956130
21	9	0	-3.515983	0.804388	-0.312070
22	9	0	-2.867510	-0.938958	0.856680

Rotational constants (GHZ): 1.9816694 0.4153194 0.3864887

Structure **(dF)(H)NCOO^{-}•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.439560	-1.257858	-0.641747
2	6	0	-0.828380	-0.741269	-0.404754
3	8	0	-1.613686	-1.482685	0.260929
4	8	0	-1.119760	0.386455	-0.900415
5	1	0	-2.847199	2.347157	0.792168
6	8	0	-4.174565	-0.602211	0.557362
7	1	0	-4.043082	0.352120	0.411482
8	8	0	-3.134070	1.907709	-0.013892
9	1	0	-2.372523	1.353814	-0.315883
10	6	0	1.549189	-0.428753	-1.027690
11	1	0	1.200051	0.353393	-1.701971
12	1	0	2.291490	-1.025633	-1.562963
13	1	0	-3.271575	-0.974510	0.442445
14	6	0	2.255692	0.231266	0.149995
15	6	0	2.881862	-0.691569	1.154784
16	1	0	3.614276	-1.332848	0.660763
17	1	0	3.377884	-0.110905	1.935371
18	1	0	0.660132	-2.077705	-0.094973
19	1	0	2.117612	-1.319975	1.615682
20	9	0	3.228497	1.073309	-0.371909
21	9	0	1.369557	1.076457	0.799045

Rotational constants (GHZ): 1.7837668 0.4621484 0.4178969

Substituent Effect of Adding tF Group to Methylcarbamic Acid

Structure **(Me)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.036225	-0.480621	-0.072491
2	1	0	2.359626	-1.427759	-0.193058
3	6	0	0.716501	-0.265530	-0.005335
4	8	0	-0.000193	-1.382116	-0.145398
5	8	0	0.224242	0.859790	0.167591
6	1	0	-0.987172	-1.216398	-0.057249
7	1	0	-2.681364	2.069046	0.517900
8	8	0	-2.590962	-1.104169	0.058380
9	1	0	-2.713620	-0.130333	-0.019520
10	8	0	-2.374056	1.550974	-0.232485
11	1	0	-1.419716	1.382832	-0.083726
12	6	0	2.988836	0.599917	0.060082
13	1	0	2.910326	1.081937	1.037314
14	1	0	3.991630	0.189542	-0.044871
15	1	0	2.839594	1.354711	-0.714967
16	1	0	-2.857149	-1.341385	0.952421

Rotational constants (GHZ): 3.9482718 1.1521856 0.9066696

Structure **(Me)(H)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.025860	-0.482894	-0.188846
2	1	0	-2.356683	-1.431684	-0.104634
3	6	0	-0.662209	-0.328547	-0.077662
4	8	0	0.049661	-1.377736	-0.189569
5	8	0	-0.214241	0.847657	0.100384
6	1	0	2.526162	1.852592	-0.952392
7	8	0	2.720368	-1.157328	0.234864
8	1	0	2.839893	-0.192678	0.165222
9	8	0	2.349216	1.573289	-0.049222
10	1	0	1.398427	1.296301	-0.022383
11	6	0	-2.942359	0.575712	0.175039
12	1	0	-2.784512	1.457375	-0.448480
13	1	0	-3.962526	0.227053	0.010920
14	1	0	-2.845455	0.877081	1.224222
15	1	0	1.753082	-1.275832	0.093540

Rotational constants (GHZ): 3.9348440 1.1585555 0.9118952

Structure **(Me)(tF)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.451578	1.023430	-0.541988

2	6	0	-0.792202	0.507597	-0.360629
3	8	0	-1.618216	1.355144	0.234205
4	8	0	-1.114715	-0.626786	-0.735871
5	1	0	-2.554494	0.985471	0.308993
6	1	0	-3.725849	-2.440005	-0.673888
7	8	0	-4.059206	0.519928	0.514431
8	1	0	-3.982671	-0.452121	0.377253
9	8	0	-3.313426	-2.015856	0.084956
10	1	0	-2.487204	-1.603752	-0.240632
11	6	0	1.495232	0.148517	-1.007121
12	1	0	1.081288	-0.622923	-1.654805
13	1	0	2.235141	0.714184	-1.575481
14	1	0	-4.597946	0.856971	-0.208483
15	6	0	0.815612	2.324008	0.007821
16	1	0	1.790530	2.603931	-0.387547
17	1	0	0.091862	3.078595	-0.296598
18	1	0	0.870693	2.302993	1.098809
19	6	0	2.220248	-0.547425	0.130960
20	9	0	3.138932	-1.412486	-0.341735
21	9	0	1.381986	-1.245516	0.921965
22	9	0	2.871169	0.319893	0.935141

Rotational constants (GHZ): 1.3759051 0.4461629 0.3739364

Structure **(Me)(tF)NCOO^{-}•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.413183	0.913984	-0.705020
2	6	0	-0.838890	0.370131	-0.408002
3	8	0	-1.049362	-0.839633	-0.713080
4	8	0	-1.682171	1.155239	0.121207
5	1	0	-4.303041	0.595780	1.660245
6	8	0	-3.507225	-1.914809	-0.269181
7	1	0	-3.979436	-1.150809	0.109204
8	8	0	-4.226499	0.578484	0.701660
9	1	0	-3.280676	0.782554	0.492616
10	6	0	0.731702	2.250381	-0.231300
11	1	0	0.811668	2.303186	0.859549
12	1	0	1.684537	2.559451	-0.662212
13	1	0	-0.032155	2.957228	-0.554268
14	1	0	-2.605790	-1.561557	-0.440406
15	6	0	1.505811	0.037170	-1.017808
16	1	0	1.145102	-0.832547	-1.564358
17	1	0	2.243816	0.549051	-1.640047
18	6	0	2.240417	-0.476088	0.209096
19	9	0	2.875769	0.508252	0.884954
20	9	0	1.420250	-1.074002	1.096178
21	9	0	3.183038	-1.381365	-0.132461

Rotational constants (GHZ): 1.4437157 0.4257764 0.3710721

Substituent Effect of Adding tF Group to Ethylcarbamic Acid

Structure **(Et)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.541307	-0.848745	-0.329561
2	6	0	-0.265680	-0.455181	-0.182461
3	8	0	0.546631	-1.463378	0.140663
4	8	0	0.114798	0.712373	-0.351071
5	1	0	1.506011	-1.174389	0.213627
6	1	0	2.928874	2.096978	-0.820714
7	8	0	3.080125	-0.873434	0.374784
8	1	0	3.108050	0.100252	0.232814
9	8	0	2.608228	1.738508	0.012628
10	1	0	1.687916	1.440867	-0.145994
11	1	0	3.554560	-1.272250	-0.361488
12	6	0	-2.625971	0.102824	-0.504975
13	1	0	-2.301345	0.854811	-1.226949
14	1	0	-3.455771	-0.438714	-0.963667
15	6	0	-3.064143	0.757793	0.794749
16	1	0	-2.237367	1.302991	1.259062
17	1	0	-3.875557	1.468381	0.608997
18	1	0	-3.425992	0.012376	1.509396
19	1	0	-1.763713	-1.795252	-0.058070
Rotational constants (GHZ):			3.0682384	0.8305244	0.6981463

Structure **(Et)(H)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.559306	-0.742251	-0.584978
2	6	0	-0.222695	-0.459270	-0.360113
3	8	0	0.550665	-1.456164	-0.196671
4	8	0	0.143947	0.756074	-0.372927
5	1	0	3.005039	1.798277	-0.981673
6	8	0	3.072532	-0.980042	0.691300
7	1	0	3.164906	-0.032755	0.482706
8	8	0	2.647451	1.644455	-0.102211
9	1	0	1.726475	1.302844	-0.229528
10	6	0	-2.590982	0.261939	-0.383887
11	1	0	-2.295852	1.165478	-0.920803
12	1	0	-3.502114	-0.103302	-0.866214
13	1	0	2.162001	-1.191013	0.382661
14	6	0	-2.861098	0.574242	1.080751
15	1	0	-1.961257	0.953243	1.574685
16	1	0	-3.645411	1.332010	1.181026
17	1	0	-3.190104	-0.321472	1.617923
18	1	0	-1.816644	-1.683605	-0.322364
Rotational constants (GHZ):			2.9319737	0.8433368	0.7356037

Structure **(Et)(tF)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.438322	0.758576	-0.105189
2	6	0	0.834318	0.288381	-0.107077
3	8	0	1.696732	1.114238	0.466841
4	8	0	1.144584	-0.806449	-0.595224
5	1	0	2.631856	0.737163	0.488529
6	1	0	3.563089	-2.794794	-0.029359
7	8	0	4.153097	0.283603	0.605014
8	1	0	4.127266	-0.618421	0.211052
9	8	0	3.576122	-2.029948	-0.613142
10	1	0	2.665260	-1.670068	-0.625096
11	6	0	-1.447950	0.015579	-0.813788
12	1	0	-2.157766	0.700067	-1.282024
13	1	0	-1.005604	-0.602240	-1.594921
14	1	0	4.377126	0.171329	1.534352
15	6	0	-0.775986	2.107915	0.357433
16	1	0	-1.827123	2.088553	0.650132
17	1	0	-0.203926	2.315541	1.261353
18	6	0	-0.533682	3.165358	-0.705330
19	6	0	-2.229399	-0.899594	0.108515
20	1	0	0.522091	3.209730	-0.985583
21	1	0	-1.119312	2.961101	-1.606969
22	1	0	-0.827698	4.150568	-0.331139
23	9	0	-1.443082	-1.801438	0.727641
24	9	0	-3.163128	-1.588962	-0.576926
25	9	0	-2.874356	-0.222481	1.082571

Rotational constants (GHZ): 0.9271761 0.4198709 0.3214533

Structure **(Et)(tF)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.371358	0.692710	-0.040617
2	6	0	-0.910282	0.145524	-0.043828
3	8	0	-1.058362	-1.008772	-0.543458
4	8	0	-1.833207	0.845330	0.474319
5	1	0	-4.499452	-0.146806	1.696561
6	8	0	-3.575444	-1.992572	-0.815367
7	1	0	-4.081310	-1.356050	-0.278164
8	8	0	-4.385681	0.124254	0.780824
9	1	0	-3.433641	0.377003	0.679667
10	6	0	0.577354	2.092188	0.319799
11	1	0	-0.027644	2.311932	1.199921
12	1	0	1.621134	2.203873	0.624009
13	1	0	-2.650847	-1.664816	-0.743764
14	6	0	1.421930	0.046132	-0.776820
15	1	0	1.018367	-0.637741	-1.523376
16	1	0	2.044711	0.781324	-1.293414
17	6	0	2.339562	-0.760144	0.119680

18	9	0	2.952427	0.000265	1.054815
19	9	0	1.693276	-1.735387	0.789888
20	9	0	3.316717	-1.357726	-0.597462
21	6	0	0.249607	3.053283	-0.812921
22	1	0	-0.801359	2.972082	-1.104450
23	1	0	0.437755	4.087532	-0.507376
24	1	0	0.863521	2.850516	-1.696476

Rotational constants (GHZ): 0.9918541 0.3937716 0.3168826

Substituent Effect of Adding tF Group to Propylcarbamic Acid

Structure **(Pr)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.894433	-1.240972	-0.311918
2	6	0	0.301408	-0.641255	-0.191804
3	8	0	1.247538	-1.471896	0.250731
4	8	0	0.504976	0.545996	-0.483228
5	1	0	2.150378	-1.034379	0.298548
6	1	0	3.060462	2.394811	-0.841892
7	8	0	3.655591	-0.477657	0.449488
8	1	0	3.519656	0.482020	0.278301
9	8	0	2.752966	2.003722	-0.018309
10	1	0	1.909161	1.548257	-0.221954
11	1	0	4.190736	-0.812071	-0.277228
12	6	0	-2.104689	-0.489977	-0.593076
13	1	0	-1.880188	0.235205	-1.378935
14	1	0	-2.832999	-1.191093	-1.008108
15	6	0	-2.682288	0.213586	0.628272
16	1	0	-1.922170	0.882550	1.048819
17	1	0	-2.906099	-0.532493	1.400489
18	1	0	-0.977678	-2.174876	0.061954
19	6	0	-3.937587	0.997584	0.273069
20	1	0	-4.357534	1.500645	1.149115
21	1	0	-3.727593	1.765428	-0.479357
22	1	0	-4.714739	0.341856	-0.134565

Rotational constants (GHZ): 2.5232090 0.5890891 0.5044853

Structure **(Pr)(H)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.898873	-1.228858	-0.579777
2	6	0	0.354738	-0.694338	-0.339738
3	8	0	1.256318	-1.502883	0.050181
4	8	0	0.529623	0.543618	-0.561941
5	1	0	3.247060	1.896216	-1.207387
6	8	0	3.563219	-0.437256	1.015259
7	1	0	3.526618	0.453536	0.621944
8	8	0	2.832343	1.869128	-0.340011

9	1	0	1.989130	1.360088	-0.448051
10	6	0	-2.078770	-0.385581	-0.650185
11	1	0	-1.867692	0.440990	-1.332846
12	1	0	-2.880231	-0.972498	-1.110085
13	1	0	2.736624	-0.861411	0.691133
14	6	0	-2.540470	0.153528	0.699058
15	1	0	-1.714680	0.704544	1.165097
16	1	0	-2.766317	-0.690675	1.363208
17	6	0	-3.760662	1.053053	0.559038
18	1	0	-4.097409	1.431956	1.528883
19	1	0	-3.544365	1.919364	-0.075807
20	1	0	-4.601611	0.516657	0.105526
21	1	0	-1.036051	-2.137599	-0.160114

Rotational constants (GHZ): 2.3338940 0.6039589 0.5361340

Structure **(Pr)(tF)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.393566	0.549123	-0.085656
2	6	0	-0.773316	-0.132613	-0.199024
3	8	0	-0.808299	-1.254312	0.507946
4	8	0	-1.711270	0.256628	-0.907478
5	1	0	-1.683481	-1.742240	0.393434
6	1	0	-4.654479	0.163432	0.343019
7	8	0	-3.034758	-2.580963	0.334082
8	1	0	-3.686717	-1.874062	0.126446
9	8	0	-4.324607	-0.344871	-0.404680
10	1	0	-3.417631	-0.021602	-0.582931
11	6	0	0.538514	1.866175	-0.707470
12	1	0	1.559119	1.939492	-1.089583
13	1	0	-0.128919	1.901081	-1.568803
14	1	0	-3.240949	-2.897642	1.219318
15	6	0	1.460489	0.086207	0.766020
16	1	0	2.013052	0.939621	1.162467
17	1	0	1.082800	-0.488910	1.609963
18	6	0	2.452316	-0.784096	0.016368
19	9	0	1.879909	-1.870429	-0.535716
20	9	0	3.060789	-0.120485	-0.990126
21	9	0	3.422902	-1.221646	0.843375
22	6	0	0.246018	3.015282	0.250367
23	1	0	0.949065	2.979736	1.091946
24	1	0	0.463885	3.947706	-0.284393
25	6	0	-1.185800	3.031546	0.767908
26	1	0	-1.905680	3.119416	-0.051858
27	1	0	-1.427449	2.120108	1.324117
28	1	0	-1.347831	3.876172	1.444685

Rotational constants (GHZ): 0.7495875 0.3978071 0.2881973

Structure **(Pr)(tF)NCOO$^-$•2H$_2$O** ----------

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.373312	0.477867	-0.080930
2	6	0	0.942807	0.043339	0.027201
3	8	0	1.184675	-0.937069	0.792840
4	8	0	1.808626	0.665755	-0.661931
5	1	0	4.415366	-0.579189	-1.762186
6	8	0	3.768158	-1.654544	1.220782
7	1	0	4.211776	-1.176909	0.496696
8	8	0	4.362981	-0.047667	-0.962262
9	1	0	3.410180	0.201252	-0.854947
10	6	0	-0.705011	1.677755	-0.843681
11	1	0	-0.203317	1.626603	-1.812849
12	1	0	-1.778592	1.647559	-1.047036
13	1	0	2.821851	-1.412993	1.102750
14	6	0	-1.408279	-0.159176	0.681948
15	1	0	-1.002127	-0.627730	1.578307
16	1	0	-2.165928	0.562969	0.991149
17	6	0	-2.126439	-1.237987	-0.107323
18	9	0	-2.728356	-0.751843	-1.216704
19	9	0	-1.303693	-2.220705	-0.525164
20	9	0	-3.092641	-1.822604	0.634682
21	6	0	-0.351013	2.982242	-0.135523
22	1	0	0.732901	3.026028	0.017987
23	1	0	-0.599413	3.807732	-0.814912
24	6	0	-1.072295	3.170077	1.192867
25	1	0	-0.805605	2.389385	1.912389
26	1	0	-2.160343	3.146408	1.065410
27	1	0	-0.815508	4.130891	1.650078
Rotational constants (GHZ):			0.6946880	0.3893205	0.2927312

Substituent Effect of Adding tF Group to Butylcarbamic Acid

Structure **(Bu)(H)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.509146	-1.391304	0.226547
2	1	0	0.786930	-1.932013	-0.579445
3	6	0	-0.672430	-0.755815	0.143287
4	8	0	-1.385282	-1.137608	-0.918332
5	8	0	-1.067658	0.071252	0.977225
6	1	0	-2.294909	-0.711983	-0.936952
7	1	0	-3.591924	1.956612	1.372705
8	8	0	-3.771860	-0.087829	-1.103211
9	1	0	-3.707475	0.694152	-0.508687
10	8	0	-3.063463	1.880040	0.572277
11	1	0	-2.316808	1.283191	0.787344
12	6	0	1.540623	-0.960818	1.157401
13	1	0	1.070163	-0.798420	2.129145
14	1	0	2.233951	-1.797628	1.274894

15	1	0	-4.415396	-0.682376	-0.704831
16	6	0	2.286682	0.288219	0.704523
17	1	0	1.572313	1.113579	0.589604
18	1	0	2.973786	0.584372	1.507900
19	6	0	3.067308	0.094251	-0.590036
20	1	0	3.773951	-0.737244	-0.465184
21	1	0	2.383417	-0.206212	-1.393856
22	6	0	3.817195	1.352683	-1.005940
23	1	0	4.534702	1.660123	-0.237105
24	1	0	4.374494	1.204824	-1.936600
25	1	0	3.128641	2.190180	-1.163842

Rotational constants (GHZ): 1.7747744 0.4710670 0.4469308

Structure **(Bu)(H)NCOO$^-$•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.490727	-0.577925	-1.321665
2	1	0	0.856022	0.123596	-1.949724
3	6	0	-0.678755	-0.187508	-0.692207
4	8	0	-1.305204	0.791821	-1.208693
5	8	0	-1.063651	-0.850498	0.319791
6	1	0	-3.905656	-1.387771	1.374899
7	8	0	-3.749114	1.439739	-0.224311
8	1	0	-3.845404	0.791398	0.496690
9	8	0	-3.388275	-0.611039	1.607996
10	1	0	-2.529713	-0.693108	1.120574
11	6	0	1.488276	-1.378807	-0.629922
12	1	0	0.994161	-2.265249	-0.226688
13	1	0	2.198687	-1.732951	-1.383809
14	1	0	-2.864261	1.230646	-0.602406
15	6	0	2.233823	-0.638883	0.476518
16	1	0	1.517082	-0.314033	1.241773
17	1	0	2.911916	-1.348046	0.970627
18	6	0	3.029884	0.561595	-0.022401
19	1	0	3.728153	0.234420	-0.804942
20	1	0	2.353009	1.281079	-0.500331
21	6	0	3.795842	1.254185	1.097115
22	1	0	4.360599	2.117855	0.731047
23	1	0	3.116732	1.612496	1.878783
24	1	0	4.509118	0.571458	1.572274

Rotational constants (GHZ): 1.8130262 0.4596743 0.4574536

Structure **(Bu)(tF)NCOOH•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.407091	0.341445	-0.188945
2	6	0	-0.675269	-0.470746	-0.090559
3	8	0	-0.544042	-1.427121	0.819187
4	8	0	-1.684059	-0.326225	-0.792798

5	1	0	-1.370767	-1.999620	0.889235
6	1	0	-4.565903	-1.623103	-1.032253
7	8	0	-2.592669	-2.997728	1.107114
8	1	0	-3.175949	-2.777522	0.345064
9	8	0	-3.728552	-2.085224	-1.137620
10	1	0	-3.024943	-1.405482	-1.080669
11	6	0	0.372156	1.507978	-1.072823
12	1	0	1.359997	1.604904	-1.528586
13	1	0	-0.330307	1.292103	-1.877935
14	1	0	-3.070682	-2.743412	1.902821
15	6	0	1.553286	0.181522	0.670231
16	1	0	2.010539	1.153093	0.865036
17	1	0	1.279114	-0.256518	1.628666
18	6	0	2.618796	-0.699995	0.045092
19	9	0	2.164130	-1.929528	-0.261761
20	9	0	3.112806	-0.179587	-1.098909
21	9	0	3.660041	-0.857985	0.887002
22	6	0	-0.008307	2.796420	-0.354192
23	1	0	0.727983	3.016577	0.430219
24	1	0	0.076194	3.614168	-1.081611
25	6	0	-1.408171	2.788580	0.248052
26	1	0	-2.143588	2.590978	-0.541738
27	1	0	-1.500232	1.961614	0.963208
28	6	0	-1.736047	4.101739	0.945998
29	1	0	-2.742837	4.091984	1.375879
30	1	0	-1.031959	4.305228	1.760543
31	1	0	-1.683180	4.946184	0.249887

Rotational constants (GHZ): 0.4871800 0.3826922 0.2472196

Structure **(Bu)(tF)NCOO^{-}•2H$_2$O**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.143459	-0.169598	-0.909584
2	6	0	1.148041	-0.297352	-0.409427
3	8	0	1.452069	-1.377737	0.180929
4	8	0	1.931815	0.683342	-0.589448
5	1	0	4.994385	0.726831	-0.842163
6	8	0	4.000194	-1.730663	1.050245
7	1	0	4.417908	-0.898200	0.763899
8	8	0	4.532615	0.780162	-0.000065
9	1	0	3.565974	0.734871	-0.211021
10	6	0	-0.574388	1.057614	-1.579698
11	1	0	0.061368	1.236993	-2.455658
12	1	0	-1.580965	0.864635	-1.958300
13	1	0	3.068369	-1.631793	0.750347
14	6	0	-0.981655	-1.331870	-0.982858
15	1	0	-1.522273	-1.365649	-1.932830
16	1	0	-0.374575	-2.233693	-0.910624
17	6	0	-2.021151	-1.418458	0.118039
18	9	0	-1.493236	-1.286731	1.349913
19	9	0	-2.984613	-0.478385	0.008550
20	9	0	-2.651251	-2.616035	0.084684
21	6	0	-0.600563	2.313713	-0.711044

22	1	0	0.423080	2.612963	-0.467736
23	1	0	-1.015922	3.121288	-1.329286
24	6	0	-1.407275	2.191094	0.574371
25	1	0	-1.026301	1.350060	1.165477
26	1	0	-2.449513	1.949265	0.336684
27	6	0	-1.350885	3.467620	1.403548
28	1	0	-1.931333	3.378322	2.327798
29	1	0	-0.320731	3.713554	1.684746
30	1	0	-1.749647	4.323094	0.846556

Rotational constants (GHZ): 0.6013128 0.3562698 0.2650171