ELECTRONIC SUPPORTING INFORMATION

Synthesis, Crystal structures and Characterization of two non-metal cation tetrafluoroborates

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Table S1

Atomic coordinates, equivalent isotropic displacement parameters in $[H_3tren]\cdot(BF_4)_3\cdot$(**I**)

Atom	**Site**	**x**	**y**	**z**	**B_{eq}(Å^2)**
B(1)	4a	0.8109(4)	0.3109(4)	0.1891(4)	3.5(1)
B(2)	4a	0.4728(3)	0.5272(3)	0.0272(3)	2.8(1)
B(3)	4a	0.7053(4)	0.2947(4)	-0.2053(4)	3.(1)
F(1)	4a	0.8807(2)	0.3807(2)	0.1193(2)	3.45(8)
F(2)	12b	0.7001(2)	0.3478(3)	0.1768(3)	5.84(8)
F(3)	4a	0.5409(2)	0.4591(2)	-0.0409(2)	4.07(8)
F(4)	12b	0.4265(3)	0.4611(3)	0.1137(3)	5.56(7)
F(5)	12b	0.7377(4)	0.2890(5)	-0.0951(3)	9.7(2)
F(6)	4a	0.7706(3)	0.2294(3)	-0.2706(3)	7.3(2)
N(1)	4a	1.0308(2)	0.5308(2)	-0.0308(2)	1.96(7)
N(2)	12b	1.0059(4)	0.2727(3)	-0.0631(3)	3.71(7)
C(1)	12b	1.0969(3)	0.4574(3)	-0.1086(3)	2.61(6)
C(2)	12b	1.0294(4)	0.3583(3)	-0.1546(3)	3.13(7)

Table S2

Selected inter-atomic distances (Å) in $[H_3tren]\cdot(BF_4)_3\cdot$(**I**)

B(1)-F(2)	3×1.373(8)	N(1)-C(1)	1.469(4)
B(1)-F(1)	1.383(4)	N(2)-C(2)	1.495(5)
<B-F>	1.375	C(1)-C(2)	1.502(5)
B(2)-F(3)	1.378(4)		
B(2)-F(4)	3×1.373(4)		
<B-F>	1.374		
B(3)-F(6)	1.32(1)		
B(3)-F(5)	3×1.343(5)		
<B-F>	1.337		

Table S3

Hydrogen bond distances (Å) and X-H…F angles (°) in $[H_3tren]\cdot(BF_4)_3\cdot$(**I**)

X-H…F	d(H..F)	d(N..F)	X-H…F
N(2)-H1C...F(4)	2.143	2.946(?)	150
N(2)-H1D...F(1)	1.989	2.878(?)	176

Table S4

Atomic coordinates, equivalent isotropic displacement parameters in $[H_3tren]\cdot(BF_4)_3\cdot$HF (I**I**)

Atom	S.O.F	x	y	z	B_{eq}(Å^2)
B		-0.0416(3)	0.4291(3)	0.1059(4)	3.11(6)
F(1)		0.0496(3)	0.3735(5)	0.1537(6)	8.1(2)
F(2)	0.50	0.1149(9)	0.502(1)	0.166(2)	9.1(6)
F(2P)	0.50	0.087(2)	0.463(1)	0.211(2)	11.4(8)
F(3)		0.0837(4)	0.3739(3)	0.0671(5)	7.0(1)

F(4)	0.50	0.027(1)	0.479(1)	0.0119(8)	7.6(4)
F(4P)	0.50	0.068(1)	0.5129(9)	0.054(1)	8.4(4)
F(5)		-1/3	1/3	-0.2001(3)	2.92(6)
N(1)		-1/3	1/3	0.0094(3)	1.89(6)
N(2)		-0.1401(3)	0.4852(3)	-0.1257(3)	3.48(6)
C(1)		-0.2261(2)	0.3949(2)	0.0502(2)	2.77(5)
C(2)		-0.1643(2)	0.4955(2)	-0.4955(2)	2.99(6)

Table S5

Selected inter-atomic distances (Å) in $[H_3tren]\cdot(BF_4)_3\cdot HF$ (I**I**)

B- F(4p)	1.293(9)	N(1)-C(1)$^{\$1}$	1.507(3)	C(1)-C(2)	1.517(2)
B- F(2)	1.33(1)	N(1)-C(1)	1.507(3)		
B- F(1)	1.346(6)	N(1)-C(1)$^{\$2}$	1.507(3)		
B- F(3)	1.374(5)	N(2)-C(2)	1.486(4)		
B- F(2p)	1.41(2)	<N-C>	1.496		
B- F(4)	1.439(9)				
<B-F>	1.36				

Symmetry transformation codes: $^{\$1}$ -y, x-y+1, z ; $^{\$2}$ -x+y-1, -x, z

Table S6

Hydrogen bond distances (Å) and X-H…F angles (°) in $[H_3tren]\cdot(BF_4)_3\cdot HF$ (I**I**)

X-H…F	d(H..F)	d(N..F)	X-H…F
N(1)-H2D...F(5)	2.04	2.84(?)	148
N(1)-H...F(5)	1.820	2.516(?)	180

Table s7: Assignment of vibration modes in $[H_3tren](BF_4)_3$

Stretching Frequency	**Intensity**	**Assignment**	**Expected from literature**	**Ref.**
3255, 3200, 3173	m-s	$-NH_3^+$ (symmetric and asymmetric)	2800-300	[33-35]
3046, 2978, 2876	w	$-CH_2-$ stretching symmetric and asymmetric	2930/2850	
1469, 1451, 1405, 1387, 1369	m-s	$-CH_2-$ scissoring	1465	
1323-1298	w	$-CH_2-$ wagging $-CH_2-$ twisting	1300-1305	
724	s	$-CH_2-$ rocking	720	
1210, 1026, 1118, 1149	m-s	C-N stretching	1220-1020	
1607, 1638, 1505, 1525	m-s	NH_2 scissoring, N–H bending	1615	
855, 832	m-s	NH_2 wagging and twisting	850–750	
768	w	B-F ν_1 (symmetric stretching)	777 cm^{-1}	[36,37]
-	m	B-F ν_2 (symmetric	360 cm^{-1}	

		deformation)		
993-947-903-1026	m-s	B-F ν_3 (asymmetric stretching)	1070 cm^{-1}	
-	m-s	B-F ν_4 (asymmetric deformation)	533 cm^{-1}	

[a] intensities : s = strong, m = medium, w = weak, br = broad, var = varies.

Table s8: assignment of vibration modes in $[H_3tren]\cdot(BF_4)_3\cdot HF$

Stretching Frequency	**Intensity**	**Assignment**	**Expected from literature**	**Ref.**
3262, 3215	m-s	$-NH_3^+$ (symmetric and asymmetric)	2800-3000	[33-35]
3066-3022	w	$-CH_2-$ stretching symmetric and asymmetric	2930/2850	
1468, 1375, 1379	m-s	$-CH_2-$ scissoring	1465	
1355, 1313, 1335, 1298, 1281	w	$-CH_2-$ wagging $-CH_2-$ twisting	1300-1305	
743	s	$-CH_2-$ rocking	720	
1194,	m-s	C-N stretching	1220-1020	
1608-1504	m-s	NH_2 scissoring, N–H bending	1615	
847	m-s	NH_2 wagging and twisting	850–750	
760-	w	B-F ν_1 (symmetric stretching)	777 cm^{-1}	[36,37]
-	m	B-F ν_2 (symmetric deformation)	360 cm^{-1}	
981, 1026	m-s	B-F ν_3 (asymmetric stretching)	1070 cm^{-1}	
-	m-s	B-F ν_4 (asymmetric deformation)	533 cm^{-1}	

[a] intensities : s = strong, m = medium, w = weak, br = broad, var = varies.

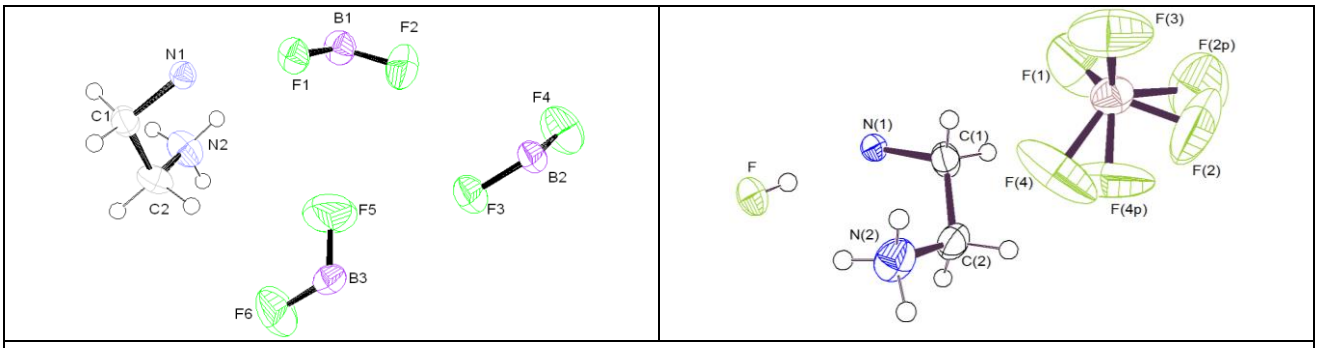

Fig. S1 : The asymmetric unit and the atom numbering scheme of $[H_3tren]\cdot(BF_4)_3$ showing the atom labelling and 50% probability displacement for I (left) and II (right)

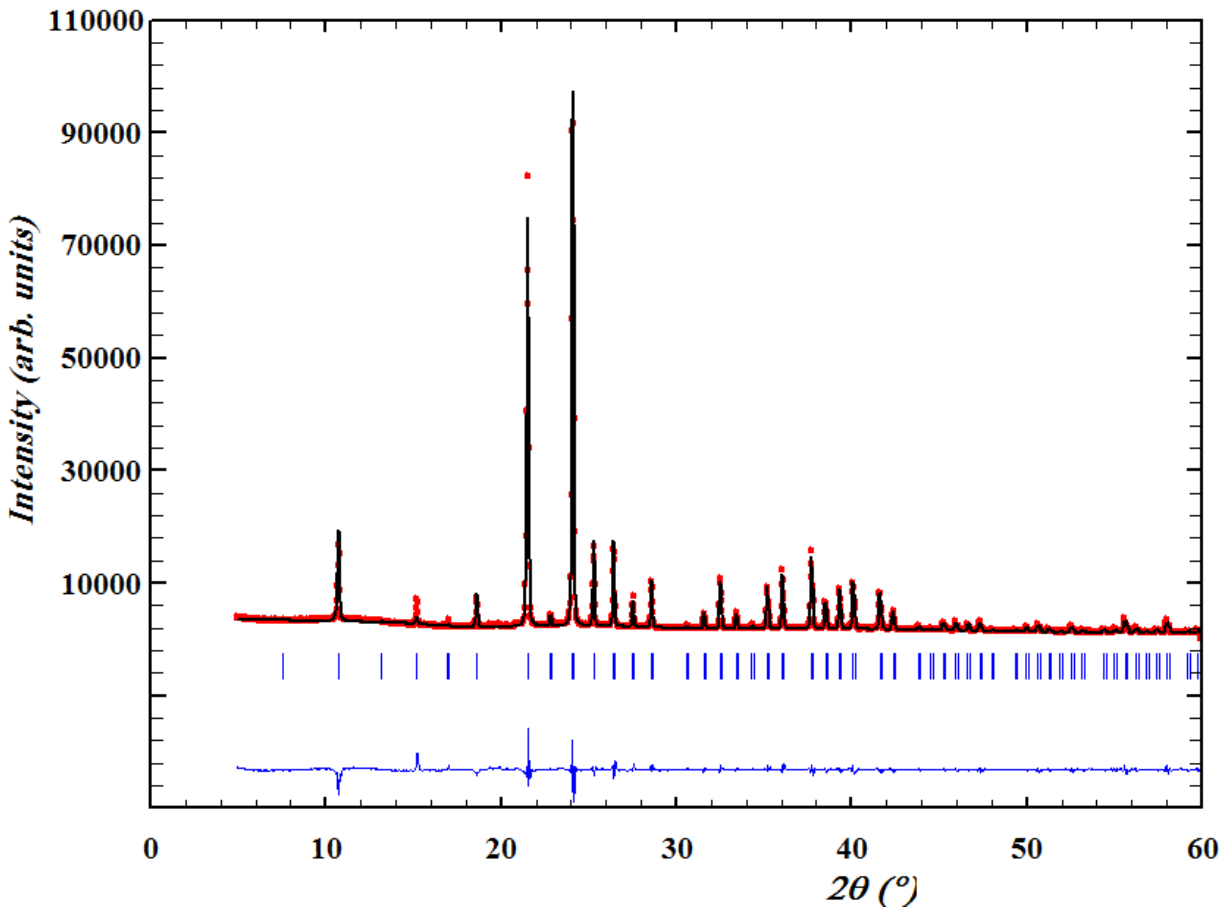

Fig. S2: X-ray diffraction patterns simulation, in Full pattern matching mode, of $[H_3tren]\cdot(BF_4)_3$ phase, experimental (red) calculated (black) and difference (blue).

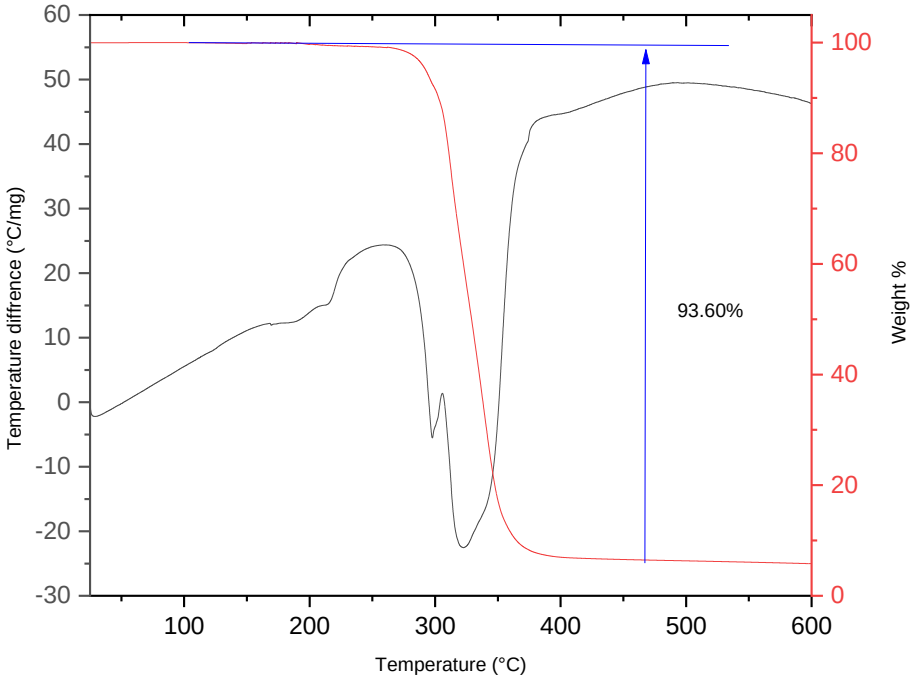

Fig. S3: DTA and TGA curves of $[H_3tren]\cdot(BF_4)_3$

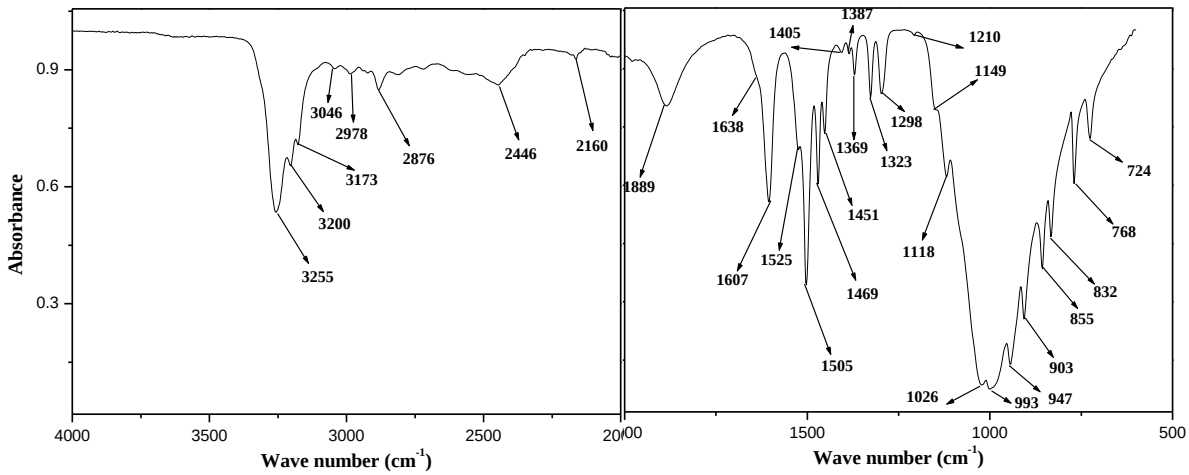

Fig. S4: Infra-red absorption spectrum of $[H_3tren](BF_4)_3$

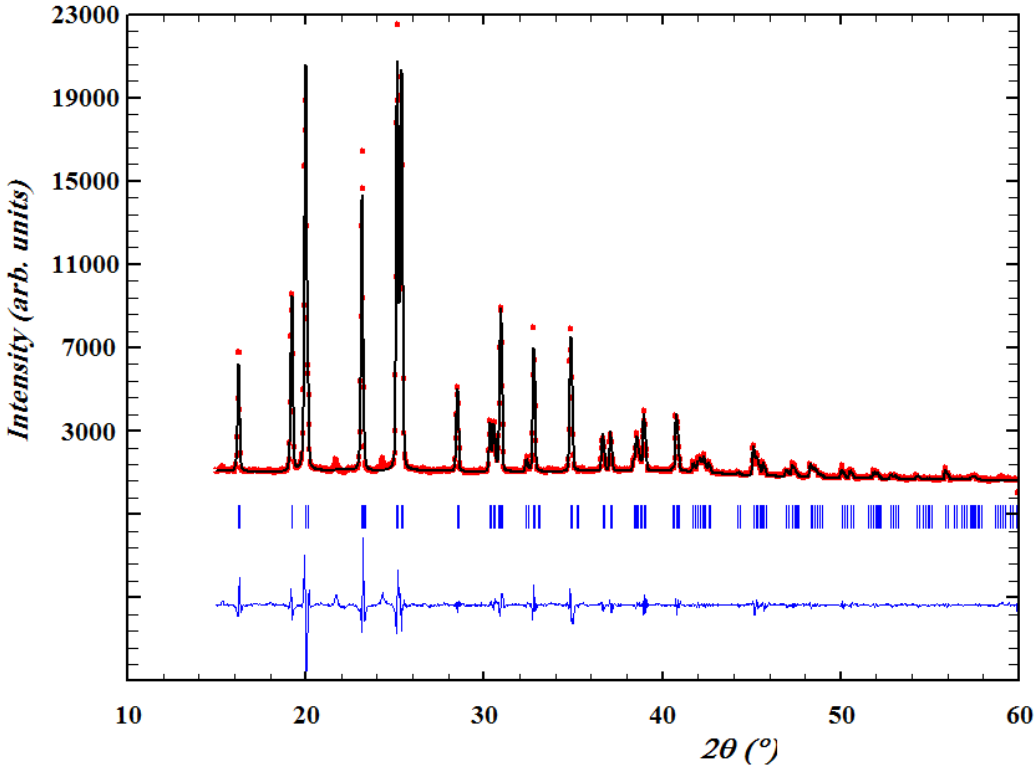

Fig. S5: X-ray diffraction patterns simulation, in Full pattern matching mode, of [H_3*tren*]·(BF_4)$_3$.HF phase, experimental (red) calculated (black) and difference (blue).

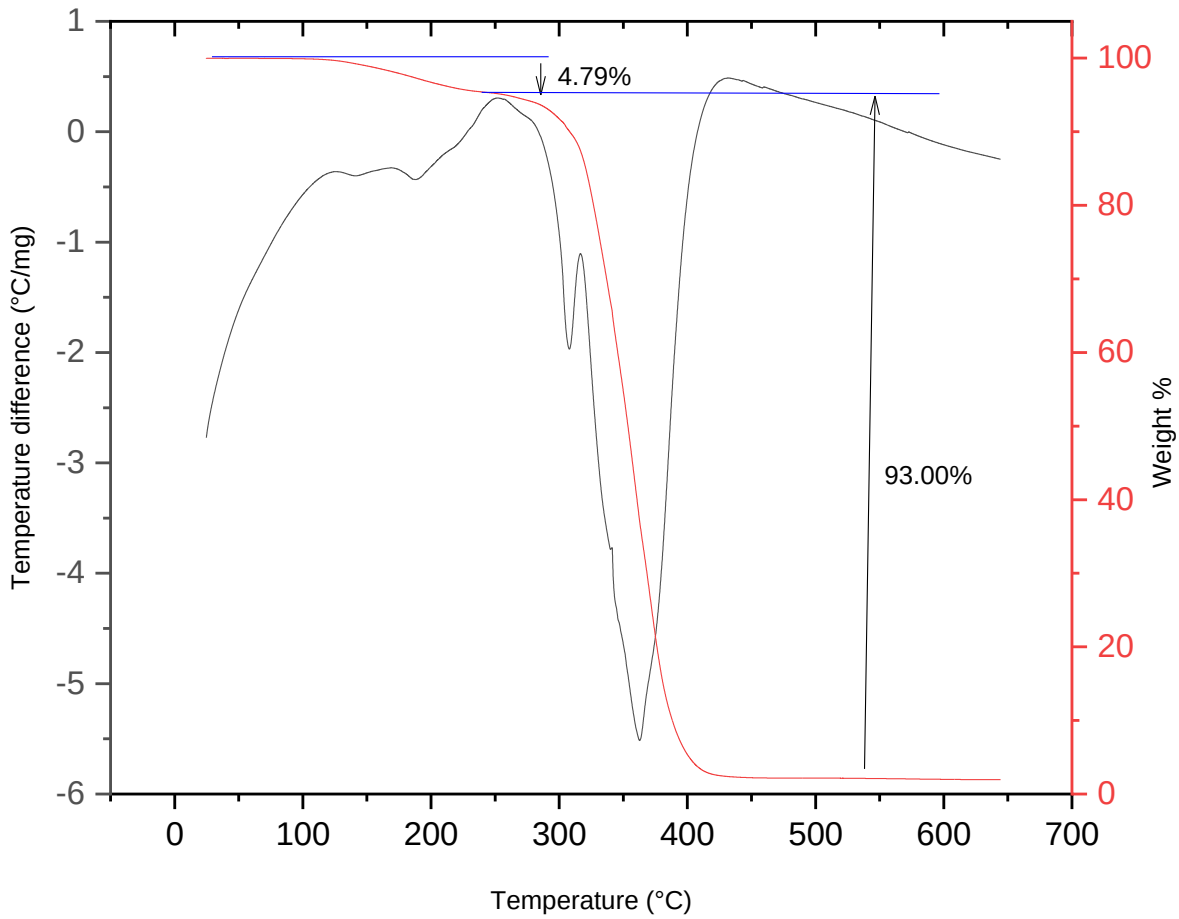

Fig. S6: DTA and TGA curves of [H_3*tren*]·(BF_4)$_3$·HF

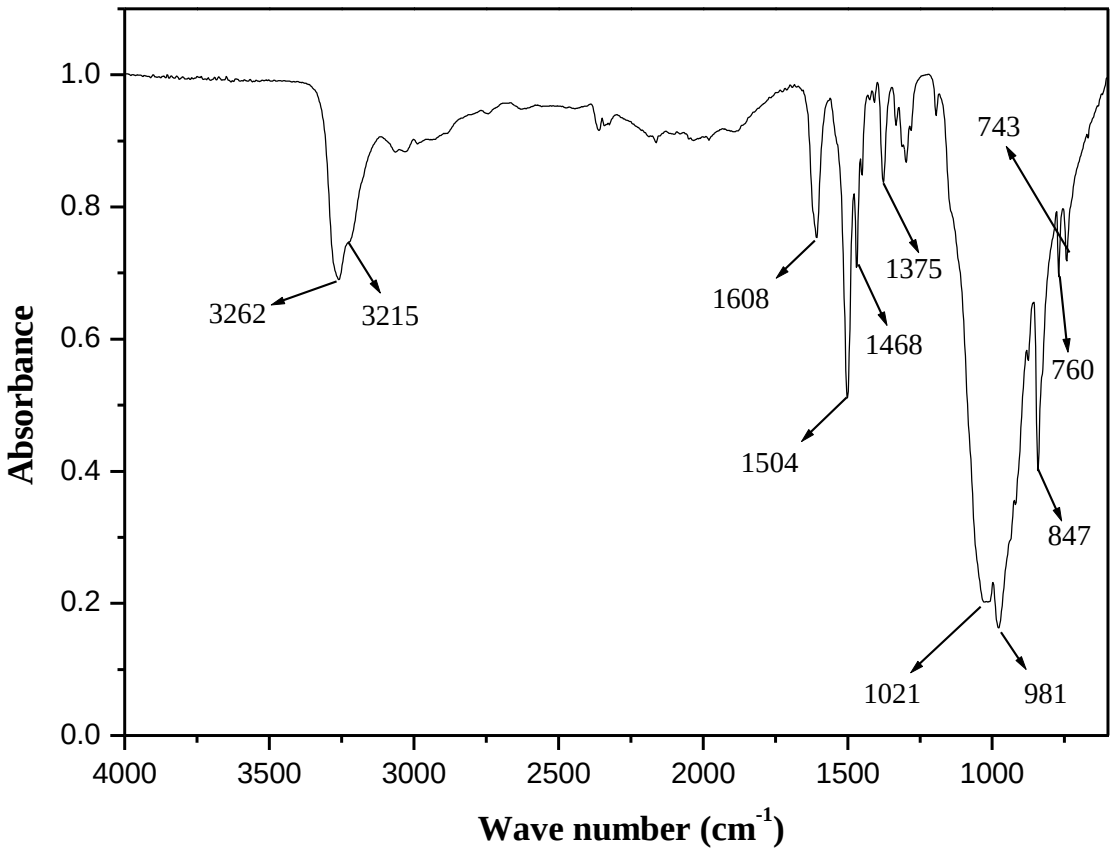

Fig. S7: Infra-red absorption spectrum of $[H_3tren]\cdot(BF_4)_3\cdot HF$

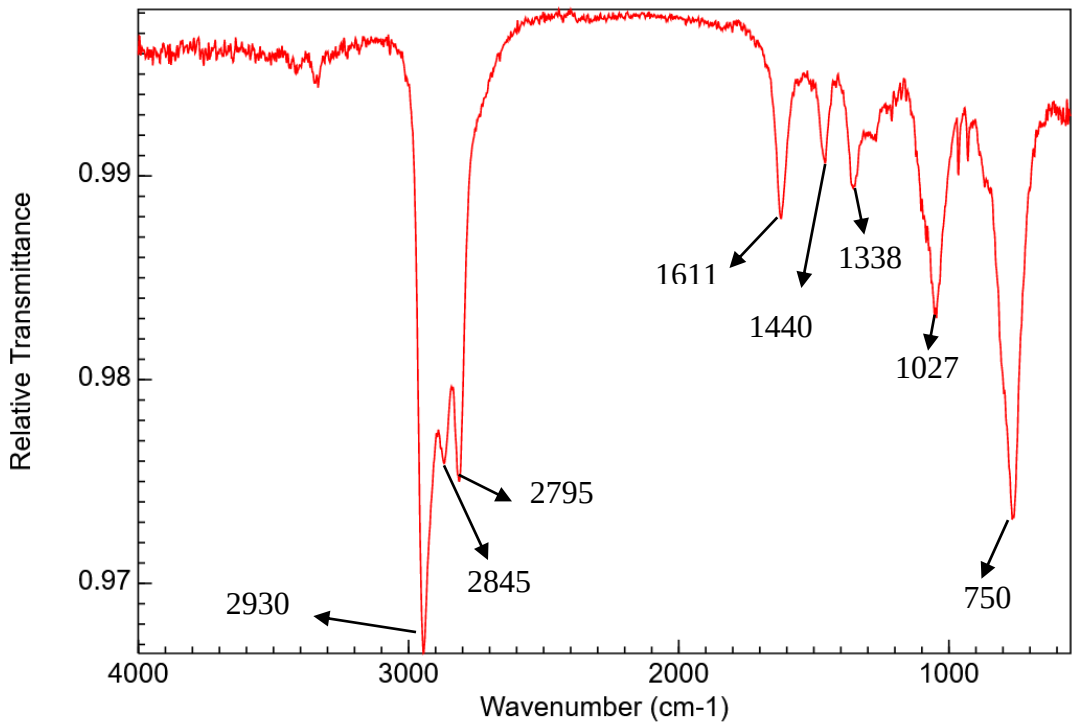

Fig. S8: Infra-red absorption spectrum of tris-(2-aminoethyl)amine (tren) (from https://webbook.nist.gov/cgi/cbook.cgi?ID=C4097896&Mask=80)