Supplementary Material (ESI) for New Journal of Chemistry

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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G T O T H E P A P E R

Investigation of sublimation with and without dissociation in the chloride and nitrate salts of 4-(1-hydroxy-1,2-diphenylethyl)pyridine.

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C o n t e n t s
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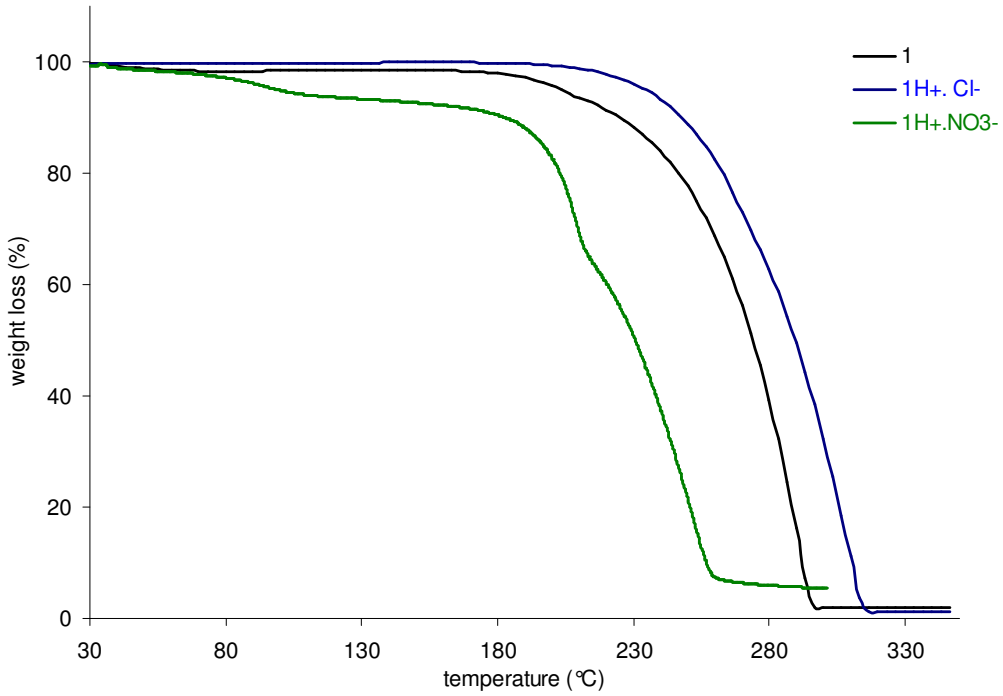

Figure 1 TGA results of compounds 1, $1H^+.Cl^-$ and $1H^+.NO_3^-$ and the first derivative curve of $1H^+.NO_3^-$ to clarify the weight loss calculation.

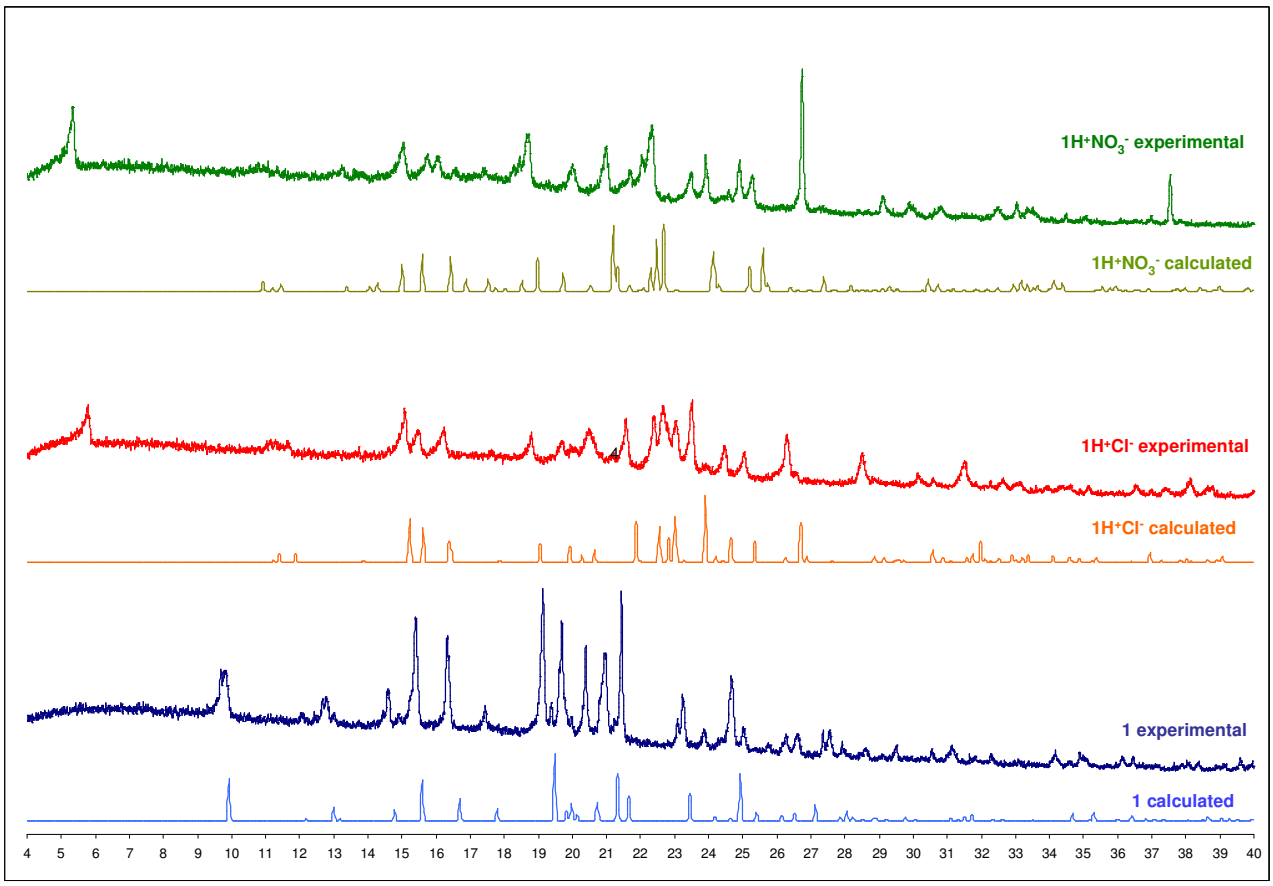

Figure 2 Calculated and measured PXRD traces of **1**, **$1H^+.Cl^-$** and **$1H^+.NO_3^-$.** The peak positions are shifted owing to the different temperatures at which the measured sample was done compared to the calculated pattern. The peak intensities vary, perhaps due to microcrystalline orientation and/or texture effects.

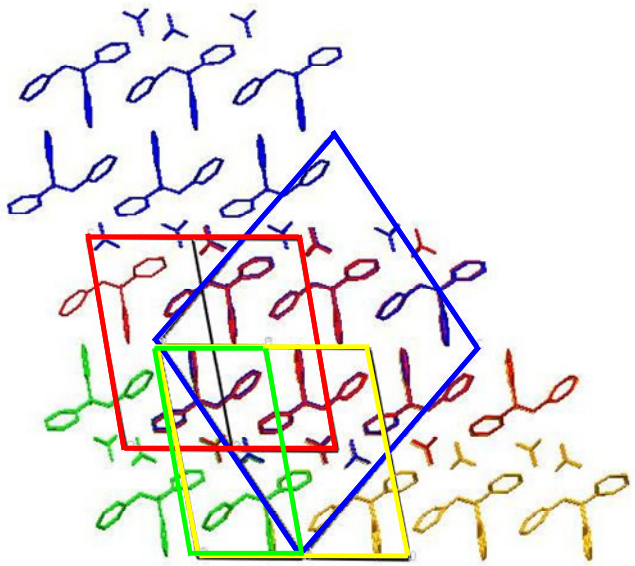

Figure 3 Fitted packing diagrams of sublimed crystals of **$1H^+.NO_3^-$.**

Table I. Cell parameters of sublimed crystal of **$1H^+.NO_3^-$.**

	A	**B**	**C**	**D**
Space group	P-1	P-1	P-1	P-1
a (Å)	6.3168 (13)	9.3876(15)	6.3314(12)	6.3230(13)
b (Å)	8.1971(16)	16.285(3)	19.743(3)	16.379(4)
c (Å)	16.479(3)	16.479(3)	20.854(4)	16.449(5)
α (°)	100.78(3)	94.54(7)	73.17(3)	100.84(2)
β (°)	91.20(3)	100.359(12)	81.74(3)	91.419(15)
γ (°)	100.44(3)	91.385(12)	86.66(1)	100.64(2)
V (Å^3)	823.9(3)	2468.6(8)	2468.9(8)	1641.3(8)
Z	2	6	6	4
colour code on Fig.3	green	blue	red	yellow
comment	original cell		same structures as A	

Table 1 – Crystal Data and Details of the Structure Determination of 1.

Crystal Data			
Formula			C19 H17 N O
Formula Weight			275.34
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	9.3446(19)	10.612(2)	15.267(3)
alpha, beta, gamma [deg]	90	107.70(3)	90
V [Ang**3]			1442.3(5)
Z			4
D(calc) [g/cm**3]			1.268
Mu(MoKa) [/mm]			0.078
F(000)			584
Crystal Size [mm]		0.01 x 0.01 x 0.01	
Data Collection			
Temperature (K)			173
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.4, 26.0
Dataset		-11: 11 ; -13: 13 ; -18: 18	
Tot., Uniq. Data, R(int)		30355, 2835, 0.067	
Observed data [I > 2.0 sigma(I)]			2129
Refinement			
Nref, Npar			2835, 192
R, wR2, S		0.0370, 0.0932, 1.04	
w = 1/[\s^2^(Fo^2^)+(0.0485P)^2^+0.1690P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.19, 0.17

Table 2 – Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms of 1.

Atom	x	y	z	U(eq) [Ang^2]
O8	0.37336(9)	0.18173(8)	0.38465(6)	0.0212(3)
N1	0.41716(12)	0.28226(10)	0.07606(7)	0.0257(3)
C2	0.53275(14)	0.33874(13)	0.13733(9)	0.0257(4)
C3	0.55435(13)	0.33791(12)	0.23096(9)	0.0231(4)
C4	0.45363(13)	0.27399(11)	0.26575(8)	0.0188(4)
C5	0.33489(14)	0.21305(12)	0.20290(9)	0.0238(4)
C6	0.32128(14)	0.22005(12)	0.11040(9)	0.0262(4)
C7	0.46825(13)	0.27833(11)	0.36775(8)	0.0185(3)
C9	0.41213(13)	0.40903(11)	0.38954(9)	0.0206(4)
C10	0.25194(13)	0.43990(11)	0.33521(8)	0.0212(4)
C11	0.22223(15)	0.53026(12)	0.26623(9)	0.0281(4)
C12	0.07553(16)	0.56137(14)	0.21641(10)	0.0346(5)
C13	-0.04380(15)	0.50245(14)	0.23480(10)	0.0344(5)
C14	-0.01642(14)	0.41260(14)	0.30320(10)	0.0328(5)
C15	0.13010(13)	0.38154(13)	0.35305(9)	0.0267(4)
C16	0.63064(13)	0.25196(11)	0.42695(8)	0.0195(4)
C17	0.73016(14)	0.34427(13)	0.47395(9)	0.0253(4)
C18	0.87292(14)	0.31219(13)	0.53063(10)	0.0304(4)
C19	0.91850(15)	0.18829(13)	0.54090(9)	0.0295(4)
C20	0.82145(14)	0.09557(13)	0.49332(9)	0.0300(4)
C21	0.67950(14)	0.12724(12)	0.43704(9)	0.0256(4)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table 3 – Hydrogen Atom Positions and Isotropic Displacement Parameters of 1.

Atom	x	y	z	U(iso) [Ang^2]
H2	0.60400	0.38180	0.11530	0.0310
H3	0.63770	0.38080	0.27140	0.0280
H5	0.26370	0.16700	0.22320	0.0290
H6	0.23880	0.17810	0.06840	0.0310
H8	0.38850	0.18870	0.45000	0.059(5)
H9A	0.47870	0.47490	0.37750	0.0250

H9B	0.42140	0.41220	0.45590	0.0250
H11	0.30340	0.57150	0.25290	0.0340
H12	0.05740	0.62350	0.16950	0.0420
H13	-0.14400	0.52360	0.20060	0.0410
H14	-0.09810	0.37180	0.31630	0.0390
H15	0.14760	0.31960	0.40000	0.0320
H17	0.70050	0.43020	0.46740	0.0300
H18	0.93940	0.37640	0.56250	0.0360
H19	1.01540	0.16660	0.58020	0.0350
H20	0.85240	0.00990	0.49930	0.0360
H21	0.61420	0.06270	0.40470	0.0310

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table 4 - (An)isotropic Displacement Parameters of 1.

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O8	0.0218(5)	0.0240(5)	0.0183(5)	-0.0005(4)	0.0069(4)	-0.0048(3)
N1	0.0274(6)	0.0310(6)	0.0197(6)	0.0004(5)	0.0087(5)	0.0050(5)
C2	0.0244(7)	0.0312(7)	0.0238(7)	0.0036(6)	0.0106(6)	0.0004(6)
C3	0.0200(6)	0.0272(7)	0.0214(7)	0.0006(5)	0.0054(5)	-0.0008(5)
C4	0.0183(6)	0.0197(6)	0.0186(7)	0.0005(5)	0.0058(5)	0.0043(5)
C5	0.0245(7)	0.0270(7)	0.0204(7)	-0.0029(5)	0.0077(5)	-0.0039(5)
C6	0.0259(7)	0.0307(7)	0.0201(7)	-0.0039(5)	0.0044(5)	-0.0012(6)
C7	0.0180(6)	0.0212(6)	0.0166(6)	-0.0012(5)	0.0058(5)	-0.0023(5)
C9	0.0204(6)	0.0224(7)	0.0188(6)	-0.0030(5)	0.0059(5)	-0.0018(5)
C10	0.0224(6)	0.0219(6)	0.0186(7)	-0.0055(5)	0.0050(5)	0.0017(5)
C11	0.0315(7)	0.0252(7)	0.0276(7)	0.0000(6)	0.0091(6)	0.0031(6)
C12	0.0406(8)	0.0328(8)	0.0265(8)	0.0030(6)	0.0044(6)	0.0130(6)
C13	0.0264(7)	0.0405(9)	0.0296(8)	-0.0108(7)	-0.0016(6)	0.0121(6)
C14	0.0214(7)	0.0402(9)	0.0360(9)	-0.0071(7)	0.0074(6)	0.0007(6)
C15	0.0232(7)	0.0303(8)	0.0265(8)	-0.0007(6)	0.0075(6)	0.0021(5)
C16	0.0207(6)	0.0251(7)	0.0138(6)	-0.0008(5)	0.0069(5)	0.0005(5)
C17	0.0240(7)	0.0245(7)	0.0254(7)	-0.0026(6)	0.0047(5)	0.0019(5)
C18	0.0233(7)	0.0350(8)	0.0289(8)	-0.0073(6)	0.0020(6)	-0.0021(6)
C19	0.0219(7)	0.0387(8)	0.0253(8)	0.0024(6)	0.0033(6)	0.0058(6)
C20	0.0282(7)	0.0283(7)	0.0335(8)	0.0031(6)	0.0092(6)	0.0065(6)
C21	0.0250(7)	0.0244(7)	0.0265(7)	-0.0024(6)	0.0067(5)	0.0003(5)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table 5 - Bond Distances (Angstrom) of 1.

O8	-C7	1.4293(15)	C17	-C18	1.394(2)
O8	-H8	0.9700	C18	-C19	1.376(2)
N1	-C6	1.3413(18)	C19	-C20	1.385(2)
N1	-C2	1.3366(17)	C20	-C21	1.3848(19)
C2	-C3	1.3816(19)	C2	-H2	0.9500
C3	-C4	1.3900(18)	C3	-H3	0.9500
C4	-C7	1.5220(17)	C5	-H5	0.9500
C4	-C5	1.3866(18)	C6	-H6	0.9500
C5	-C6	1.3809(19)	C9	-H9A	0.9900
C7	-C16	1.5375(18)	C9	-H9B	0.9900
C7	-C9	1.5542(17)	C11	-H11	0.9500
C9	-C10	1.5103(18)	C12	-H12	0.9500

C10	-C11	1.3885(18)	C13	-H13	0.9500		
C10	-C15	1.3938(18)	C14	-H14	0.9500		
C11	-C12	1.390(2)	C15	-H15	0.9500		
C12	-C13	1.380(2)	C17	-H17	0.9500		
C13	-C14	1.379(2)	C18	-H18	0.9500		
C14	-C15	1.3888(19)	C19	-H19	0.9500		
C16	-C21	1.3933(18)	C20	-H20	0.9500		
C16	-C17	1.3905(18)	C21	-H21	0.9500		

Table 6 – Bond Angles (Degrees) of 1.

C7	-O8	-H8	103.00	C17	-C18	-C19	120.58(13)
C2	-N1	-C6	116.16(11)	C18	-C19	-C20	119.24(13)
N1	-C2	-C3	123.64(13)	C19	-C20	-C21	120.27(13)
C2	-C3	-C4	119.71(12)	C16	-C21	-C20	121.27(12)
C3	-C4	-C7	121.04(11)	N1	-C2	-H2	118.00
C5	-C4	-C7	121.75(12)	C3	-C2	-H2	118.00
C3	-C4	-C5	117.10(12)	C2	-C3	-H3	120.00
C4	-C5	-C6	119.22(13)	C4	-C3	-H3	120.00
N1	-C6	-C5	124.16(13)	C4	-C5	-H5	120.00
O8	-C7	-C4	107.18(10)	C6	-C5	-H5	120.00
O8	-C7	-C16	108.60(10)	N1	-C6	-H6	118.00
C4	-C7	-C9	108.35(10)	C5	-C6	-H6	118.00
C4	-C7	-C16	111.19(11)	C7	-C9	-H9A	109.00
C9	-C7	-C16	111.94(10)	C7	-C9	-H9B	109.00
O8	-C7	-C9	109.46(10)	C10	-C9	-H9A	109.00
C7	-C9	-C10	114.75(11)	C10	-C9	-H9B	109.00
C9	-C10	-C11	120.17(12)	H9A	-C9	-H9B	108.00
C11	-C10	-C15	117.92(12)	C10	-C11	-H11	119.00
C9	-C10	-C15	121.90(11)	C12	-C11	-H11	119.00
C10	-C11	-C12	121.03(13)	C11	-C12	-H12	120.00
C11	-C12	-C13	120.30(14)	C13	-C12	-H12	120.00
C12	-C13	-C14	119.47(14)	C12	-C13	-H13	120.00
C13	-C14	-C15	120.26(13)	C14	-C13	-H13	120.00
C10	-C15	-C14	121.01(13)	C13	-C14	-H14	120.00
C7	-C16	-C17	124.11(11)	C15	-C14	-H14	120.00
C17	-C16	-C21	117.83(12)	C10	-C15	-H15	119.00
C7	-C16	-C21	118.01(11)	C14	-C15	-H15	120.00
C16	-C17	-C18	120.80(13)	C16	-C17	-H17	120.00
C18	-C17	-H17	120.00	C19	-C20	-H20	120.00
C17	-C18	-H18	120.00	C21	-C20	-H20	120.00
C19	-C18	-H18	120.00	C16	-C21	-H21	119.00
C18	-C19	-H19	120.00	C20	-C21	-H21	119.00
C20	-C19	-H19	120.00				

Table 7 – Torsion Angles (Degrees) of 1.

C6	-N1	-C2	-C3	-1.5(2)
C2	-N1	-C6	-C5	0.8(2)
N1	-C2	-C3	-C4	1.1(2)
C2	-C3	-C4	-C5	0.21(19)
C2	-C3	-C4	-C7	-175.95(12)
C3	-C4	-C5	-C6	-0.90(19)
C7	-C4	-C5	-C6	175.24(12)
C3	-C4	-C7	-O8	-166.52(11)
C3	-C4	-C7	-C9	75.45(15)
C3	-C4	-C7	-C16	-47.97(15)
C5	-C4	-C7	-O8	17.50(16)
C5	-C4	-C7	-C9	-100.54(14)
C5	-C4	-C7	-C16	136.05(12)
C4	-C5	-C6	-N1	0.4(2)
O8	-C7	-C9	-C10	-58.26(13)
C4	-C7	-C9	-C10	58.31(14)
C16	-C7	-C9	-C10	-178.72(10)

O8	-C7	-C16	-C17	-138.48(12)
O8	-C7	-C16	-C21	38.96(15)
C4	-C7	-C16	-C17	103.83(14)
C4	-C7	-C16	-C21	-78.73(14)
C9	-C7	-C16	-C17	-17.52(17)
C9	-C7	-C16	-C21	159.93(12)
C7	-C9	-C10	-C11	-108.28(13)
C7	-C9	-C10	-C15	72.87(16)
C9	-C10	-C11	-C12	-179.01(12)
C15	-C10	-C11	-C12	-0.11(19)
C9	-C10	-C15	-C14	179.04(13)
C11	-C10	-C15	-C14	0.2(2)
C10	-C11	-C12	-C13	0.0(2)
C11	-C12	-C13	-C14	0.2(2)
C12	-C13	-C14	-C15	-0.1(2)
C13	-C14	-C15	-C10	-0.1(2)
C7	-C16	-C17	-C18	176.21(12)
C21	-C16	-C17	-C18	-1.24(19)
C7	-C16	-C21	-C20	-176.43(12)
C17	-C16	-C21	-C20	1.18(19)
C16	-C17	-C18	-C19	0.3(2)
C17	-C18	-C19	-C20	0.8(2)
C18	-C19	-C20	-C21	-0.8(2)
C19	-C20	-C21	-C16	-0.2(2)

Table 8 - Contact Distances(Angstrom) of 1.

O8	.C15	3.0380(17)	C14	.H18_f	2.9700
O8	.N1_b	2.8506(15)	C15	.H18_f	3.0300
O8	.H5	2.3700	C16	.H3	2.7600
O8	.H21	2.5200	C17	.H9A	2.7400
O8	.H13_a	2.7200	C17	.H9B	2.9000
O8	.H15	2.6400	C17	.H3	2.9700
N1	.O8_c	2.8506(15)	C20	.H12_i	3.0400
N1	.C7_c	3.4174(17)	C21	.H8	2.8600
N1	.H8_c	1.8900	C21	.H11_i	3.0100
N1	.H9B_c	2.7700	C21	.H2_b	3.0100
C3	.C17	3.572(2)	H2	.C21_c	3.0100
C4	.C11	3.4758(19)	H3	.C16	2.7600
C5	.C10	3.3806(19)	H3	.C17	2.9700
C7	.N1_b	3.4174(17)	H3	.H14_j	2.3500
C10	.C5	3.3806(19)	H5	.O8	2.3700
C11	.C4	3.4758(19)	H5	.C13_a	2.9100
C13	.C19_e	3.514(2)	H5	.H13_a	2.3900
C15	.O8	3.0380(17)	H6	.H15_c	2.4500
C17	.C3	3.572(2)	H8	.C21	2.8600
C19	.C13_h	3.514(2)	H8	.H9B	2.3900
C2	.H21_d	2.7200	H8	.H15	2.5600
C2	.H8_c	2.7800	H8	.N1_b	1.8900
C3	.H9A	2.9300	H8	.C2_b	2.7800
C6	.H8_c	2.8700	H8	.C6_b	2.8700
C6	.H19_e	3.0000	H9A	.C3	2.9300
C9	.H9B_f	3.0600	H9A	.C17	2.7400
C9	.H17	2.6000	H9A	.H11	2.3400
C13	.H5_g	2.9100	H9A	.H17	2.1600
H9B	.C17	2.9000	H15	.O8	2.6400
H9B	.H8	2.3900	H15	.H8	2.5600
H9B	.H17	2.5700	H15	.H6_b	2.4500
H9B	.C9_f	3.0600	H17	.C9	2.6000
H9B	.H9B_f	2.5000	H17	.H9A	2.1600
H9B	.H17_f	2.5100	H17	.H9B	2.5700
H9B	.N1_b	2.7700	H17	.H9B_f	2.5100
H11	.H9A	2.3400	H18	.C14_f	2.9700
H11	.C21_d	3.0100	H18	.C15_f	3.0300

H12	.C20_d	3.0400	H19	.C6_h	3.0000
H13	.O8_g	2.7200	H21	.O8	2.5200
H13	.H5_g	2.3900	H21	.C2_i	2.7200
H14	.H3_k	2.3500			

Table 9 – Hydrogen Bonds (Angstrom, Deg) of 1.

O8	-- H8	.. N1	0.9700	1.8900	2.8506(15)	175.00	4_555
C5	-- H5	.. O8	0.9500	2.3700	2.7079(17)	100.00	.

Translation of Symmetry Code to Equiv.Pos. in crystal 1.

a =[2545.00] = -x,-1/2+y,1/2-z
b =[4555.00] = x,1/2-y,1/2+z
c =[4554.00] = x,1/2-y,-1/2+z
d =[2655.00] = 1-x,1/2+y,1/2-z
e =[4454.00] = -1+x,1/2-y,-1/2+z
f =[3666.00] = 1-x,1-y,1-z
g =[2555.00] = -x,1/2+y,1/2-z
h =[4655.00] = 1+x,1/2-y,1/2+z
i =[2645.00] = 1-x,-1/2+y,1/2-z
j =[1655.00] = 1+x,y,z
k =[1455.00] = -1+x,y,z

Table 10 – Crystal Data and Details of the Structure Determination of $1H^+.Cl^-$.

Crystal Data			
Formula			C19 H18 N O, Cl
Formula Weight			311.79
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	6.3219(13)	8.4477(17)	15.349(3)
alpha, beta, gamma [deg]	102.22(3)	92.54(3)	106.21(3)
V [Ang**3]			764.6(3)
Z			2
D(calc) [g/cm**3]			1.354
Mu(MoKa) [/mm]			0.251
F(000)			328
Crystal Size [mm]		0.50 x 0.50 x 0.50	
Data Collection			
Temperature (K)			100
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.3, 26.3
Dataset		-7: 7 ; -10: 10 ; -19: 18	
Tot., Uniq. Data, R(int)		12756, 3103, 0.032	
Observed data [I > 2.0 sigma(I)]			2637
Refinement			
Nref, Npar			3103, 208
R, wR2, S		0.0333, 0.0895, 1.04	
w = 1/[\s^2^(Fo^2^)+(0.0443P)^2^+0.3508P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.22, 0.27

Table 11 – Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms of $1H^+.Cl^-$.

Atom	x	y	z	U(eq) [Ang^2]
O8	0.47954(16)	0.77556(13)	0.20577(7)	0.0196(3)
N1	-0.1669(2)	0.28393(17)	0.07394(9)	0.0213(4)
C2	0.0337(3)	0.2981(2)	0.11194(10)	0.0225(5)
C3	0.1724(3)	0.45503(19)	0.15523(10)	0.0203(5)
C4	0.1033(2)	0.59981(18)	0.15950(9)	0.0159(4)
C5	-0.1055(2)	0.57852(19)	0.11668(11)	0.0213(4)
C6	-0.2385(3)	0.4187(2)	0.07477(11)	0.0239(5)
C7	0.2550(2)	0.77155(18)	0.21420(10)	0.0161(4)

C9	0.2053(2)	0.92277(18)	0.18447(10)	0.0175(4)
C10	0.3217(2)	1.09351(18)	0.24653(10)	0.0170(4)
C11	0.2011(3)	1.17763(19)	0.30335(10)	0.0204(4)
C12	0.3038(3)	1.3349(2)	0.36069(11)	0.0234(5)
C13	0.5290(3)	1.4096(2)	0.36181(11)	0.0246(5)
C14	0.6509(3)	1.3288(2)	0.30536(11)	0.0249(5)
C15	0.5481(3)	1.17135(19)	0.24776(10)	0.0210(5)
C16	0.2183(2)	0.77920(17)	0.31292(10)	0.0159(4)
C17	0.0134(2)	0.78082(19)	0.34277(10)	0.0201(4)
C18	-0.0154(2)	0.7946(2)	0.43279(11)	0.0224(5)
C19	0.1578(3)	0.8024(2)	0.49389(11)	0.0233(5)
C20	0.3600(3)	0.7986(2)	0.46460(11)	0.0263(5)
C21	0.3910(3)	0.7885(2)	0.37467(11)	0.0220(4)
Cl1	0.68004(6)	0.88693(4)	0.04004(2)	0.0179(1)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table 12 – Hydrogen Atom Positions and Isotropic Displacement Parameters of $1H^{+}.Cl^{-}$.

Atom	x	y	z	U(iso) [Ang^2]
H1	-0.254(3)	0.185(3)	0.0504(14)	0.038(6)
H2	0.08070	0.19980	0.10910	0.0270
H3	0.31520	0.46510	0.18220	0.0240
H5	-0.15580	0.67440	0.11650	0.0260
H6	-0.38150	0.40420	0.04640	0.0290
H8	0.518(4)	0.806(3)	0.1575(16)	0.049(6)
H9A	0.25050	0.92380	0.12360	0.0210
H9B	0.04340	0.90560	0.18080	0.0210
H11	0.04660	1.12680	0.30290	0.0240
H12	0.21970	1.39080	0.39900	0.0280
H13	0.59990	1.51650	0.40140	0.0300
H14	0.80510	1.38070	0.30590	0.0300
H15	0.63260	1.11660	0.20910	0.0250
H17	-0.10720	0.77240	0.30110	0.0240
H18	-0.15430	0.79880	0.45270	0.0270
H19	0.13730	0.81020	0.55540	0.0280
H20	0.47860	0.80290	0.50610	0.0320
H21	0.53160	0.78800	0.35540	0.0260

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table 13 – (An)isotropic Displacement Parameters of $1H^{+}.Cl^{-}$.

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O8	0.0160(5)	0.0234(6)	0.0220(6)	0.0091(5)	0.0054(4)	0.0069(4)
N1	0.0294(7)	0.0133(7)	0.0165(7)	0.0009(5)	0.0039(5)	0.0007(6)
C2	0.0331(9)	0.0169(8)	0.0211(8)	0.0061(6)	0.0096(7)	0.0108(7)
C3	0.0238(8)	0.0199(8)	0.0188(8)	0.0051(6)	0.0038(6)	0.0085(6)
C4	0.0207(7)	0.0153(7)	0.0123(7)	0.0046(6)	0.0051(6)	0.0050(6)
C5	0.0226(8)	0.0163(7)	0.0243(8)	0.0028(6)	-0.0002(6)	0.0063(6)
C6	0.0246(8)	0.0201(8)	0.0240(9)	0.0036(7)	-0.0007(7)	0.0034(6)
C7	0.0149(7)	0.0154(7)	0.0190(8)	0.0050(6)	0.0025(6)	0.0054(6)
C9	0.0187(7)	0.0152(7)	0.0183(8)	0.0049(6)	0.0009(6)	0.0042(6)
C10	0.0217(7)	0.0130(7)	0.0169(7)	0.0060(6)	0.0008(6)	0.0043(6)
C11	0.0213(7)	0.0174(7)	0.0229(8)	0.0064(6)	0.0032(6)	0.0051(6)
C12	0.0292(8)	0.0186(8)	0.0227(8)	0.0038(7)	0.0055(7)	0.0079(7)
C13	0.0303(9)	0.0150(8)	0.0238(9)	0.0019(6)	-0.0017(7)	0.0017(6)
C14	0.0219(8)	0.0201(8)	0.0306(9)	0.0087(7)	0.0019(7)	0.0009(6)
C15	0.0225(8)	0.0184(8)	0.0224(8)	0.0064(6)	0.0047(6)	0.0048(6)
C16	0.0182(7)	0.0096(6)	0.0184(8)	0.0028(6)	0.0015(6)	0.0020(5)

C17	0.0167(7)	0.0197(8)	0.0212(8)	0.0033(6)	-0.0005(6)	0.0028(6)
C18	0.0173(7)	0.0219(8)	0.0258(9)	0.0037(7)	0.0065(6)	0.0029(6)
C19	0.0287(8)	0.0234(8)	0.0169(8)	0.0049(6)	0.0047(6)	0.0059(7)
C20	0.0247(8)	0.0343(9)	0.0219(8)	0.0073(7)	-0.0009(6)	0.0120(7)
C21	0.0188(7)	0.0272(8)	0.0225(8)	0.0063(7)	0.0036(6)	0.0102(6)
Cl1	0.0193(2)	0.0150(2)	0.0196(2)	0.0043(1)	0.0022(1)	0.0051(1)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table 14 – Bond Distances (Angstrom) of $1H^{+}.Cl^{-}$.

O8	-C7	1.4228(17)	C17	-C18	1.386(2)
O8	-H8	0.86(2)	C18	-C19	1.388(2)
N1	-C6	1.335(2)	C19	-C20	1.380(3)
N1	-C2	1.335(2)	C20	-C21	1.391(2)
N1	-H1	0.85(2)	C2	-H2	0.9500
C2	-C3	1.376(2)	C3	-H3	0.9500
C3	-C4	1.399(2)	C5	-H5	0.9500
C4	-C5	1.395(2)	C6	-H6	0.9500
C4	-C7	1.538(2)	C9	-H9A	0.9900
C5	-C6	1.376(2)	C9	-H9B	0.9900
C7	-C16	1.534(2)	C11	-H11	0.9500
C7	-C9	1.548(2)	C12	-H12	0.9500
C9	-C10	1.514(2)	C13	-H13	0.9500
C10	-C15	1.396(2)	C14	-H14	0.9500
C10	-C11	1.395(2)	C15	-H15	0.9500
C11	-C12	1.391(2)	C17	-H17	0.9500
C12	-C13	1.385(3)	C18	-H18	0.9500
C13	-C14	1.383(3)	C19	-H19	0.9500
C14	-C15	1.394(2)	C20	-H20	0.9500
C16	-C21	1.388(2)	C21	-H21	0.9500
C16	-C17	1.3957(19)			

Table 15 – Bond Angles (Degrees) of $1H^{+}.Cl^{-}$.

C7	-O8	-H8	109.4(17)	C17	-C16	-C21	118.80(15)
C2	-N1	-C6	122.12(15)	C16	-C17	-C18	120.47(13)
C6	-N1	-H1	119.1(15)	C17	-C18	-C19	120.28(14)
C2	-N1	-H1	118.7(15)	C18	-C19	-C20	119.52(15)
N1	-C2	-C3	120.01(16)	C19	-C20	-C21	120.37(17)
C2	-C3	-C4	120.04(17)	C16	-C21	-C20	120.54(17)
C5	-C4	-C7	123.52(13)	N1	-C2	-H2	120.00
C3	-C4	-C7	118.78(13)	C3	-C2	-H2	120.00
C3	-C4	-C5	117.65(14)	C2	-C3	-H3	120.00
C4	-C5	-C6	120.04(15)	C4	-C3	-H3	120.00
N1	-C6	-C5	120.10(16)	C4	-C5	-H5	120.00
O8	-C7	-C4	108.78(12)	C6	-C5	-H5	120.00
C4	-C7	-C16	106.95(12)	N1	-C6	-H6	120.00
C9	-C7	-C16	110.58(12)	C5	-C6	-H6	120.00
O8	-C7	-C16	107.40(11)	C7	-C9	-H9A	109.00
C4	-C7	-C9	112.16(12)	C7	-C9	-H9B	109.00
O8	-C7	-C9	110.79(12)	C10	-C9	-H9A	109.00
C7	-C9	-C10	113.92(12)	C10	-C9	-H9B	109.00
C9	-C10	-C11	119.80(13)	H9A	-C9	-H9B	108.00
C11	-C10	-C15	118.54(15)	C10	-C11	-H11	120.00
C9	-C10	-C15	121.65(13)	C12	-C11	-H11	119.00
C10	-C11	-C12	120.95(17)	C11	-C12	-H12	120.00
C11	-C12	-C13	119.80(17)	C13	-C12	-H12	120.00
C12	-C13	-C14	120.06(16)	C12	-C13	-H13	120.00
C13	-C14	-C15	120.18(18)	C14	-C13	-H13	120.00

C10	-C15	-C14	120.45(16)	C13	-C14	-H14	120.00
C7	-C16	-C17	120.95(13)	C15	-C14	-H14	120.00
C7	-C16	-C21	120.24(13)	C10	-C15	-H15	120.00
C14	-C15	-H15	120.00	C20	-C19	-H19	120.00
C16	-C17	-H17	120.00	C19	-C20	-H20	120.00
C18	-C17	-H17	120.00	C21	-C20	-H20	120.00
C17	-C18	-H18	120.00	C16	-C21	-H21	120.00
C19	-C18	-H18	120.00	C20	-C21	-H21	120.00
C18	-C19	-H19	120.00				

Table 16 – Torsion Angles (Degrees) of $1H^{+}.Cl^{-}$.

C6	-N1	-C2	-C3	1.3(2)
C2	-N1	-C6	-C5	-0.8(2)
N1	-C2	-C3	-C4	0.0(2)
C2	-C3	-C4	-C5	-1.7(2)
C2	-C3	-C4	-C7	175.57(14)
C3	-C4	-C5	-C6	2.1(2)
C7	-C4	-C5	-C6	-175.00(15)
C3	-C4	-C7	-O8	35.22(18)
C3	-C4	-C7	-C9	158.12(13)
C3	-C4	-C7	-C16	-80.49(16)
C5	-C4	-C7	-O8	-147.70(14)
C5	-C4	-C7	-C9	-24.80(19)
C5	-C4	-C7	-C16	96.60(16)
C4	-C5	-C6	-N1	-0.9(2)
O8	-C7	-C9	-C10	-68.37(15)
C4	-C7	-C9	-C10	169.87(12)
C16	-C7	-C9	-C10	50.59(15)
O8	-C7	-C16	-C17	178.70(13)
O8	-C7	-C16	-C21	0.15(19)
C4	-C7	-C16	-C17	-64.68(17)
C4	-C7	-C16	-C21	116.77(15)
C9	-C7	-C16	-C17	57.71(18)
C9	-C7	-C16	-C21	-120.84(15)
C7	-C9	-C10	-C11	-106.20(16)
C7	-C9	-C10	-C15	74.72(18)
C9	-C10	-C11	-C12	-179.70(15)
C15	-C10	-C11	-C12	-0.6(2)
C9	-C10	-C15	-C14	179.80(15)
C11	-C10	-C15	-C14	0.7(2)
C10	-C11	-C12	-C13	-0.1(2)
C11	-C12	-C13	-C14	0.7(3)
C12	-C13	-C14	-C15	-0.6(3)
C13	-C14	-C15	-C10	-0.1(2)
C7	-C16	-C17	-C18	-177.41(15)
C21	-C16	-C17	-C18	1.2(2)
C7	-C16	-C21	-C20	178.82(15)
C17	-C16	-C21	-C20	0.2(2)
C16	-C17	-C18	-C19	-1.7(2)
C17	-C18	-C19	-C20	0.9(3)
C18	-C19	-C20	-C21	0.6(3)
C19	-C20	-C21	-C16	-1.1(3)

Table 17 – Contact Distances (Angstrom) of $1H^{+}.Cl^{-}$.

Cl1	.O8	3.0977(13)	C2	.Cl1_e	3.4015(19)
Cl1	.N1_i	3.1400(16)	C2	.Cl1_a	3.4791(19)
Cl1	.C2_i	3.4791(19)	C5	.C17	3.474(2)
Cl1	.Cl1_m	3.6764(9)	C5	.Cl1_f	3.6247(17)
Cl1	.N1_n	3.3884(16)	C6	.Cl1_c	3.3433(19)
Cl1	.C2_o	3.4015(19)	C10	.C17	3.463(2)
Cl1	.C6_n	3.3433(19)	C11	.C16	3.431(2)

Cl1	.C5_l	3.6247(17)	C11	.C2_g	3.518(2)
Cl1	.H9B_l	3.0300	C11	.C17	3.422(2)
Cl1	.H15	2.9700	C13	.C21_g	3.515(3)
Cl1	.H9A	3.1200	C15	.O8	3.168(2)
Cl1	.H1_i	2.40(2)	C15	.N1_i	3.437(2)
Cl1	.H2_i	3.0600	C16	.C11	3.431(2)
Cl1	.H5_l	2.7400	C17	.C11	3.422(2)
Cl1	.H8	2.25(2)	C17	.C5	3.474(2)
Cl1	.H1_n	2.82(2)	C17	.C10	3.463(2)
Cl1	.H2_o	2.8800	C18	.C18_k	3.591(2)
Cl1	.H6_n	2.6800	C20	.C20_h	3.285(2)
O8	.Cl1	3.0977(13)	C21	.C13_d	3.515(3)
O8	.C15	3.168(2)	C4	.H17	2.9400
O8	.H15	2.7600	C5	.H17	2.9600
O8	.H3	2.4800	C5	.H9B	2.6100
O8	.H21	2.2800	C9	.H5	2.6200
N1	.Cl1_a	3.1400(16)	C9	.H2_g	3.0900
N1	.C15_b	3.437(2)	C9	.H17	2.9300
N1	.Cl1_c	3.3884(16)	C10	.H2_g	2.9800
N1	.H15_b	2.9000	C12	.H20_h	3.0100
C2	.C11_d	3.518(2)	C13	.H20_h	2.9700
C14	.H19_h	3.0700	H9B	.H11	2.3400
C15	.H8	3.05(2)	H9B	.C17	2.8900
C17	.H11	3.0600	H9B	.H5	2.0200
C17	.H21_j	3.0800	H9B	.Cl1_f	3.0300
C17	.H9B	2.8900	H9B	.H17	2.4500
C18	.H13_b	2.8100	H11	.H19_k	2.5400
C18	.H21_j	3.0300	H11	.H9B	2.3400
C20	.H18_l	3.0800	H11	.C17	3.0600
C21	.H18_l	3.0400	H13	.C18_i	2.8100
C21	.H13_d	3.0400	H13	.C21_g	3.0400
H1	.Cl1_a	2.40(2)	H13	.H18_i	2.4000
H1	.Cl1_c	2.82(2)	H15	.Cl1	2.9700
H2	.C9_d	3.0900	H15	.H8	2.4600
H2	.C10_d	2.9800	H15	.O8	2.7600
H2	.Cl1_a	3.0600	H15	.N1_i	2.9000
H2	.Cl1_e	2.8800	H17	.C4	2.9400
H3	.O8	2.4800	H17	.H9B	2.4500
H5	.Cl1_f	2.7400	H17	.C5	2.9600
H5	.H9B	2.0200	H17	.C9	2.9300
H5	.C9	2.6200	H17	.H21_j	2.4900
H6	.Cl1_c	2.6800	H18	.H20_j	2.5000
H8	.Cl1	2.25(2)	H18	.H21_j	2.4000
H8	.C15	3.05(2)	H18	.H13_b	2.4000
H8	.H9A	2.2800	H18	.C20_j	3.0800
H8	.H15	2.4600	H18	.C21_j	3.0400
H9A	.Cl1	3.1200	H19	.C14_h	3.0700
H9A	.H8	2.2800	H19	.H11_k	2.5400
H9B	.C5	2.6100	H20	.H18_l	2.5000
H20	.C12_h	3.0100	H21	.C18_l	3.0300
H20	.C13_h	2.9700	H21	.H17_l	2.4900
H21	.C17_l	3.0800	H21	.O8	2.2800
H21	.H18_l	2.4000			

Table 18 – Hydrogen Bonds (Angstrom, Deg) of $1H^{+}.Cl^{-}$.

N1	-- H1	.. Cl1	0.85(2)	2.40(2)	3.1400(16)	144.7(18)	1_445
N1	-- H1	.. Cl1	0.85(2)	2.82(2)	3.3884(16)	125.6(18)	2_565
O8	-- H8	.. Cl1	0.86(2)	2.25(2)	3.0977(13)	170(2)	.
C5	-- H5	.. Cl1	0.9500	2.7400	3.6247(17)	156.00	1_455
C6	-- H6	.. Cl1	0.9500	2.6800	3.3433(19)	128.00	2_565
C21	-- H21	.. O8	0.9500	2.2800	2.663(2)	103.00	.

Translation of Symmetry Code to Equiv.Pos. in crystal $1H^+.Cl^-$.

a =[1445.00] = -1+x,-1+y,z
c =[2565.00] = -x,1-y,-z
d =[1545.00] = x,-1+y,z
e =[2665.00] = 1-x,1-y,-z
f =[1455.00] = -1+x,y,z
g =[1565.00] = x,1+y,z
h =[2676.00] = 1-x,2-y,1-z
i =[1665.00] = 1+x,1+y,z
k =[2576.00] = -x,2-y,1-z
l =[1655.00] = 1+x,y,z
m =[2675.00] = 1-x,2-y,-z
o =[2665.00] = 1-x,1-y,-z

Table 19 – Crystal Data and Details of the Structure Determination of $1H^+.NO_3^-$.

Crystal Data			
Formula			C19 H18 N O, N O3
Formula Weight			338.35
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	6.3168(13)	8.1971(16)	16.497(3)
alpha, beta, gamma [deg]	100.78(3)	91.20(3)	100.44(3)
V [Ang**3]			823.9(3)
Z			2
D(calc) [g/cm**3]			1.364
Mu(MoKa) [/mm]			0.097
F(000)			356
Crystal Size [mm]		0.10 x 0.10 x 0.10	
Data Collection			
Temperature (K)			173
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.2, 25.6
Dataset		0: 7 ; -9: 9 ; -20: 19	
Tot., Uniq. Data, R(int)		3025, 3025, 0.000	
Observed data [I > 2.0 sigma(I)]			1900
Refinement			
Nref, Npar			3025, 229
R, wR2, S		0.0501, 0.1181, 1.04	
w = 1/[\s^2^(Fo^2^)+(0.0419P)^2^+0.2058P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.20, 0.40

Table 20 – Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms of $1H^+.NO_3^-$.

Atom	x	y	z	U(eq) [Ang^2]
O8	0.5183(2)	0.7422(2)	0.28041(10)	0.0239(5)
N1	1.1319(3)	1.1867(2)	0.40682(13)	0.0296(7)
C2	0.9445(4)	1.1930(3)	0.36926(16)	0.0279(8)
C3	0.8164(4)	1.0478(3)	0.32621(15)	0.0261(8)
C4	0.8791(3)	0.8918(3)	0.32166(14)	0.0198(7)
C5	1.0737(4)	0.8919(3)	0.36282(15)	0.0284(8)
C6	1.1978(4)	1.0398(3)	0.40482(16)	0.0345(9)
C7	0.7396(3)	0.7324(3)	0.26980(14)	0.0198(7)
C9	0.7887(4)	0.5692(3)	0.29487(14)	0.0225(8)
C10	0.6715(3)	0.4084(3)	0.24073(15)	0.0214(8)
C11	0.7805(4)	0.3178(3)	0.18068(16)	0.0290(8)
C12	0.6785(4)	0.1682(3)	0.13052(16)	0.0348(9)
C13	0.4636(4)	0.1067(3)	0.13890(17)	0.0350(9)
C14	0.3530(4)	0.1935(3)	0.19855(18)	0.0347(9)
C15	0.4556(4)	0.3431(3)	0.24908(16)	0.0297(9)

C16	0.7804(3)	0.7289(3)	0.17834(14)	0.0186(7)
C17	0.9874(4)	0.7401(3)	0.15099(15)	0.0270(8)
C18	1.0214(4)	0.7282(3)	0.06761(16)	0.0336(9)
C19	0.8504(4)	0.7083(3)	0.01081(16)	0.0322(9)
C20	0.6449(4)	0.6970(3)	0.03773(15)	0.0314(9)
C21	0.6086(4)	0.7057(3)	0.12072(15)	0.0275(8)
O1	0.4844(3)	0.7674(2)	0.44791(11)	0.0355(6)
O2	0.2222(3)	0.5517(2)	0.43076(12)	0.0405(7)
O3	0.4109(3)	0.6354(2)	0.54817(11)	0.0373(7)
N2	0.3706(3)	0.6492(3)	0.47541(12)	0.0258(7)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table 21 – Hydrogen Atom Positions and Isotropic Displacement Parameters of $1H^{+}.NO_3^{-}$.

Atom	x	y	z	U(iso) [Ang^2]
H1	1.23330	1.30120	0.43910	0.084(11)
H2	0.89990	1.29850	0.37240	0.0340
H3	0.68420	1.05360	0.29940	0.0310
H5	1.12140	0.78810	0.36180	0.0340
H6	1.33050	1.03800	0.43250	0.0410
H8	0.49740	0.74220	0.34080	0.062(9)
H9A	0.94570	0.57140	0.29310	0.0270
H9B	0.74930	0.56900	0.35260	0.0270
H11	0.92810	0.35990	0.17400	0.0350
H12	0.75640	0.10790	0.09040	0.0420
H13	0.39200	0.00540	0.10390	0.0420
H14	0.20560	0.15040	0.20500	0.0420
H15	0.37770	0.40150	0.28980	0.0360
H17	1.10660	0.75600	0.18960	0.0320
H18	1.16370	0.73380	0.04930	0.0400
H19	0.87470	0.70250	-0.04620	0.0390
H20	0.52650	0.68320	-0.00100	0.0380
H21	0.46550	0.69570	0.13840	0.0330

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table 22 – (An)isotropic Displacement Parameters of $1H^{+}.NO_3^{-}$.

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O8	0.0186(8)	0.0307(10)	0.0240(10)	0.0076(8)	0.0023(7)	0.0062(7)
N1	0.0357(12)	0.0219(12)	0.0290(13)	0.0032(10)	-0.0036(10)	0.0021(10)
C2	0.0322(14)	0.0207(14)	0.0331(15)	0.0076(12)	0.0064(12)	0.0078(11)
C3	0.0251(13)	0.0263(15)	0.0282(15)	0.0063(12)	-0.0009(11)	0.0075(11)
C4	0.0222(12)	0.0202(13)	0.0177(13)	0.0046(11)	0.0016(10)	0.0048(10)
C5	0.0299(14)	0.0216(14)	0.0333(16)	0.0031(12)	-0.0102(12)	0.0073(11)
C6	0.0350(15)	0.0276(16)	0.0388(17)	0.0051(13)	-0.0129(13)	0.0039(12)
C7	0.0154(11)	0.0231(13)	0.0225(14)	0.0069(11)	-0.0006(10)	0.0054(10)
C9	0.0257(13)	0.0211(13)	0.0211(13)	0.0078(11)	-0.0018(10)	0.0023(10)
C10	0.0241(12)	0.0185(13)	0.0241(14)	0.0094(11)	-0.0003(11)	0.0057(10)
C11	0.0286(13)	0.0241(14)	0.0353(16)	0.0098(13)	0.0040(12)	0.0029(11)
C12	0.0465(17)	0.0263(15)	0.0308(16)	0.0030(13)	0.0039(13)	0.0075(13)
C13	0.0437(17)	0.0212(14)	0.0357(17)	0.0041(13)	-0.0084(14)	-0.0024(12)
C14	0.0274(14)	0.0268(15)	0.0481(18)	0.0096(14)	-0.0027(13)	-0.0012(12)
C15	0.0278(14)	0.0275(15)	0.0362(16)	0.0106(13)	0.0037(12)	0.0064(12)
C16	0.0217(12)	0.0134(12)	0.0199(13)	0.0016(10)	-0.0014(10)	0.0036(9)
C17	0.0204(13)	0.0379(15)	0.0211(14)	0.0054(12)	-0.0017(10)	0.0018(11)
C18	0.0229(13)	0.0447(17)	0.0300(16)	0.0049(14)	0.0043(12)	0.0005(12)
C19	0.0376(15)	0.0380(16)	0.0196(15)	0.0043(13)	0.0042(12)	0.0043(12)

C20	0.0316(14)	0.0398(16)	0.0224(15)	0.0045(13)	-0.0061(12)	0.0084(12)
C21	0.0216(13)	0.0336(15)	0.0283(15)	0.0071(12)	-0.0009(11)	0.0070(11)
O1	0.0407(11)	0.0319(10)	0.0309(11)	0.0100(9)	-0.0012(8)	-0.0049(8)
O2	0.0308(10)	0.0300(11)	0.0563(13)	0.0046(10)	-0.0160(9)	0.0001(8)
O3	0.0453(11)	0.0430(12)	0.0278(11)	0.0109(9)	0.0039(9)	0.0153(9)
N2	0.0267(11)	0.0311(13)	0.0231(13)	0.0058(11)	0.0007(10)	0.0141(10)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table 23 – Bond Distances (Angstrom) of $1H^{+}.NO_3^{-}$.

O8	-C7	1.427(2)	C16	-C21	1.390(3)
O8	-H8	1.0100	C16	-C17	1.385(3)
O1	-N2	1.260(3)	C17	-C18	1.385(4)
O2	-N2	1.241(3)	C18	-C19	1.381(4)
O3	-N2	1.252(3)	C19	-C20	1.374(4)
N1	-C6	1.339(3)	C20	-C21	1.384(3)
N1	-C2	1.338(3)	C2	-H2	0.9500
N1	-H1	1.0800	C3	-H3	0.9500
C2	-C3	1.374(4)	C5	-H5	0.9500
C3	-C4	1.395(3)	C6	-H6	0.9500
C4	-C7	1.533(3)	C9	-H9B	0.9900
C4	-C5	1.392(3)	C9	-H9A	0.9900
C5	-C6	1.372(4)	C11	-H11	0.9500
C7	-C9	1.552(3)	C12	-H12	0.9500
C7	-C16	1.532(3)	C13	-H13	0.9500
C9	-C10	1.504(3)	C14	-H14	0.9500
C10	-C11	1.395(3)	C15	-H15	0.9500
C10	-C15	1.392(3)	C17	-H17	0.9500
C11	-C12	1.384(4)	C18	-H18	0.9500
C12	-C13	1.379(4)	C19	-H19	0.9500
C13	-C14	1.382(4)	C20	-H20	0.9500
C14	-C15	1.388(4)	C21	-H21	0.9500

Table 24 – Bond Angles (Degrees) of $1H^{+}.NO_3^{-}$.

C7	-O8	-H8	105.00	C10	-C15	-C14	120.7(2)
C2	-N1	-C6	121.3(2)	C7	-C16	-C21	120.33(19)
C6	-N1	-H1	119.00	C17	-C16	-C21	118.8(2)
C2	-N1	-H1	120.00	C7	-C16	-C17	120.75(19)
O1	-N2	-O2	119.8(2)	C16	-C17	-C18	120.3(2)
O1	-N2	-O3	118.2(2)	C17	-C18	-C19	120.6(2)
O2	-N2	-O3	122.0(2)	C18	-C19	-C20	119.2(2)
N1	-C2	-C3	120.4(2)	C19	-C20	-C21	120.7(2)
C2	-C3	-C4	120.4(2)	C16	-C21	-C20	120.4(2)
C3	-C4	-C5	116.9(2)	N1	-C2	-H2	120.00
C5	-C4	-C7	123.4(2)	C3	-C2	-H2	120.00
C3	-C4	-C7	119.67(19)	C4	-C3	-H3	120.00
C4	-C5	-C6	120.9(2)	C2	-C3	-H3	120.00
N1	-C6	-C5	120.0(2)	C4	-C5	-H5	120.00
C9	-C7	-C16	109.90(19)	C6	-C5	-H5	120.00
C4	-C7	-C16	108.92(19)	C5	-C6	-H6	120.00
O8	-C7	-C9	110.16(19)	N1	-C6	-H6	120.00
O8	-C7	-C16	107.55(17)	C7	-C9	-H9A	109.00
C4	-C7	-C9	111.74(18)	C7	-C9	-H9B	109.00
O8	-C7	-C4	108.47(18)	C10	-C9	-H9A	109.00
C7	-C9	-C10	114.0(2)	C10	-C9	-H9B	109.00

C9	-C10	-C11	120.0(2)	H9A	-C9	-H9B	108.00
C11	-C10	-C15	117.8(2)	C12	-C11	-H11	119.00
C9	-C10	-C15	122.2(2)	C10	-C11	-H11	119.00
C10	-C11	-C12	121.5(2)	C11	-C12	-H12	120.00
C11	-C12	-C13	119.9(2)	C13	-C12	-H12	120.00
C12	-C13	-C14	119.6(2)	C12	-C13	-H13	120.00
C13	-C14	-C15	120.5(2)	C14	-C13	-H13	120.00
C15	-C14	-H14	120.00	C19	-C18	-H18	120.00
C13	-C14	-H14	120.00	C20	-C19	-H19	120.00
C14	-C15	-H15	120.00	C18	-C19	-H19	120.00
C10	-C15	-H15	120.00	C19	-C20	-H20	120.00
C16	-C17	-H17	120.00	C21	-C20	-H20	120.00
C18	-C17	-H17	120.00	C16	-C21	-H21	120.00
C17	-C18	-H18	120.00	C20	-C21	-H21	120.00

Table 25 – Torsion Angles (Degrees) of $1H^{+}.NO_3^{-}$.

C6	-N1	-C2	-C3	-1.2(4)
C2	-N1	-C6	-C5	0.8(4)
N1	-C2	-C3	-C4	0.5(4)
C2	-C3	-C4	-C5	0.4(4)
C2	-C3	-C4	-C7	-177.0(2)
C3	-C4	-C5	-C6	-0.8(4)
C7	-C4	-C5	-C6	176.5(2)
C3	-C4	-C7	-O8	-39.2(3)
C3	-C4	-C7	-C9	-160.8(2)
C3	-C4	-C7	-C16	77.6(2)
C5	-C4	-C7	-O8	143.6(2)
C5	-C4	-C7	-C9	22.0(3)
C5	-C4	-C7	-C16	-99.6(3)
C4	-C5	-C6	-N1	0.2(4)
O8	-C7	-C9	-C10	64.8(2)
C4	-C7	-C9	-C10	-174.57(18)
C16	-C7	-C9	-C10	-53.5(2)
O8	-C7	-C16	-C17	172.2(2)
O8	-C7	-C16	-C21	-11.1(3)
C4	-C7	-C16	-C17	54.8(3)
C4	-C7	-C16	-C21	-128.5(2)
C9	-C7	-C16	-C17	-67.9(3)
C9	-C7	-C16	-C21	108.8(2)
C7	-C9	-C10	-C11	102.7(3)
C7	-C9	-C10	-C15	-78.5(3)
C9	-C10	-C11	-C12	179.1(2)
C15	-C10	-C11	-C12	0.3(4)
C9	-C10	-C15	-C14	-179.4(2)
C11	-C10	-C15	-C14	-0.6(4)
C10	-C11	-C12	-C13	0.7(4)
C11	-C12	-C13	-C14	-1.3(4)
C12	-C13	-C14	-C15	1.0(4)
C13	-C14	-C15	-C10	-0.1(4)
C7	-C16	-C17	-C18	176.7(2)
C21	-C16	-C17	-C18	0.0(4)
C7	-C16	-C21	-C20	-177.9(2)
C17	-C16	-C21	-C20	-1.1(4)
C16	-C17	-C18	-C19	1.3(4)
C17	-C18	-C19	-C20	-1.3(4)
C18	-C19	-C20	-C21	0.1(4)
C19	-C20	-C21	-C16	1.1(4)

Table 26 – Contact Distances(Angstrom) of $1H^{+}.NO_3^{-}$.

O1	.C6_a	3.282(3)	O2	.H1_m	2.1000
O1	.C7	3.371(3)	O2	.H2_m	2.6500
O1	.C4	3.418(3)	O3	.H1_n	2.2100

O1	.C5_a	3.330(3)	O3	.H2_o	2.4700
O1	.O8	2.748(2)	O3	.H9B_p	2.6400
O1	.C6_n	3.105(3)	O3	.H6_n	2.8300
O2	.N1_m	2.892(2)	O8	.H5_a	2.9200
O2	.O3_i	3.049(3)	O8	.H3	2.5400
O2	.C2_m	3.113(3)	O8	.H15	2.8100
O3	.N2_i	2.889(3)	O8	.H21	2.3100
O3	.O3_i	2.895(3)	N1	.O3_c	3.000(3)
O3	.N1_n	3.000(3)	N1	.O2_b	2.892(2)
O3	.C6_n	3.250(3)	N2	.O3_i	2.889(3)
O3	.C2_o	3.071(3)	N2	.H1_m	2.7700
O3	.O2_i	3.049(3)	N2	.H8	2.5800
O3	.C15_p	3.397(3)	N2	.H5_a	2.9300
O8	.O1	2.748(2)	N2	.H1_n	2.7700
O8	.C15	3.165(3)	C2	.O2_b	3.113(3)
O1	.H5_a	2.7200	C2	.C10_d	3.597(4)
O1	.H8	1.7500	C2	.O3_e	3.071(3)
O1	.H9B	2.8400	C3	.C11_d	3.586(4)
O1	.H6_a	2.6300	C4	.O1	3.418(3)
O1	.H6_n	2.4200	C5	.C17	3.479(4)
O1	.H1_n	2.7500	C5	.O1_f	3.330(3)
O2	.H8	2.7700	C6	.O1_c	3.105(3)
O2	.H5_a	2.5900	C6	.O3_c	3.250(3)
O2	.H9A_a	2.8800	C6	.O1_f	3.282(3)
O2	.H15	2.7100	C7	.O1	3.371(3)
C10	.C21	3.484(4)	C20	.H20_h	3.0500
C10	.C2_g	3.597(4)	C21	.H18_a	3.0900
C11	.C16	3.377(4)	C21	.H13_d	3.0700
C11	.C17	3.599(4)	H1	.N2_c	2.7700
C11	.C3_g	3.586(4)	H1	.O2_b	2.1000
C13	.C21_g	3.531(4)	H1	.N2_b	2.7700
C15	.O8	3.165(3)	H1	.O1_c	2.7500
C15	.O3_i	3.397(3)	H1	.O3_c	2.2100
C16	.C11	3.377(4)	H2	.C10_d	2.9500
C17	.C5	3.479(4)	H2	.O3_e	2.4700
C17	.C11	3.599(4)	H2	.C9_d	2.9400
C20	.C20_h	3.404(4)	H2	.O2_b	2.6500
C21	.C13_d	3.531(4)	H3	.O8	2.5400
C21	.C10	3.484(4)	H5	.C9	2.5800
C3	.H8	2.9700	H5	.H8_k	2.4900
C4	.H17	2.8000	H5	.O1_f	2.7200
C5	.H9A	2.6300	H5	.O2_f	2.5900
C5	.H17	2.8900	H5	.O8_k	2.9200
C5	.H9B	3.0100	H5	.N2_f	2.9300
C9	.H17	3.0700	H5	.H9A	2.0400
C9	.H2_g	2.9400	H6	.O1_f	2.6300
C9	.H5	2.5800	H6	.O1_c	2.4200
C10	.H2_g	2.9500	H6	.O3_c	2.8300
C12	.H20_h	3.0300	H8	.N2	2.5800
C13	.H20_h	3.0900	H8	.C3	2.9700
C17	.H9A	2.9300	H8	.O2	2.7700
C18	.H21_k	3.0900	H8	.O1	1.7500
C18	.H13_j	2.9200	H8	.H9B	2.3400
H8	.H5_a	2.4900	H15	.H9B	2.5800
H9A	.H11	2.3500	H17	.C9	3.0700
H9A	.H5	2.0400	H17	.C4	2.8000
H9A	.O2_f	2.8800	H17	.C5	2.8900
H9A	.C5	2.6300	H17	.H21_k	2.5400
H9A	.C17	2.9300	H17	.H9A	2.5900
H9A	.H17	2.5900	H18	.C21_k	3.0900
H9B	.O3_i	2.6400	H18	.H21_k	2.4800
H9B	.O1	2.8400	H18	.H13_j	2.4200
H9B	.C5	3.0100	H18	.H20_k	2.5300
H9B	.H15	2.5800	H19	.H11_l	2.4900

H9B	.H8	2.3400	H20	.H18_a	2.5300
H11	.H9A	2.3500	H20	.C20_h	3.0500
H11	.H19_l	2.4900	H20	.C12_h	3.0300
H13	.C21_g	3.0700	H20	.C13_h	3.0900
H13	.C18_m	2.9200	H21	.H18_a	2.4800
H13	.H18_m	2.4200	H21	.O8	2.3100
H15	.O8	2.8100	H21	.C18_a	3.0900
H15	.O2	2.7100	H21	.H17_a	2.5400

Table 27 – Hydrogen Bonds (Angstrom, Deg) of $1H^{+}.NO_3^{-}$.

N1	-- H1	.. O2	1.0800	2.1000	2.892(2)	129.00	1_665
N1	-- H1	.. O3	1.0800	2.2100	3.000(3)	129.00	2_776
O8	-- H8	.. O1	1.0100	1.7500	2.748(2)	173.00	.
C2	-- H2	.. O3	0.9500	2.4700	3.071(3)	121.00	2_676
C5	-- H5	.. O2	0.9500	2.5900	3.462(3)	153.00	1_655
C6	-- H6	.. O1	0.9500	2.4200	3.105(3)	129.00	2_776
C21	-- H21	.. O8	0.9500	2.3100	2.681(3)	103.00	.

Translation of Symmetry Code to Equiv.Pos. in crystal of $1H^{+}.NO_3^{-}$.

a =[1455.00] = -1+x,y,z
b =[1665.00] = 1+x,1+y,z
c =[2776.00] = 2-x,2-y,1-z
d =[1565.00] = x,1+y,z
e =[2676.00] = 1-x,2-y,1-z
f =[1655.00] = 1+x,y,z
g =[1545.00] = x,-1+y,z
h =[2665.00] = 1-x,1-y,-z
i =[2666.00] = 1-x,1-y,1-z
l =[2765.00] = 2-x,1-y,-z
m =[1445.00] = -1+x,-1+y,z
p =[2666.00] = 1-x,1-y,1-z