Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

From $BaCl_2$ to $Ba(NO_3)Cl$: Birefringence Enhanced Significantly Deriving from the π-conjugated $[NO_3]$

Zhen Chen,[a,b] Hao Zeng,[a] Shujuan Han,[a,b]* Zhihua Yang,[a,b] and Shilie Pan[a,b]*

[a]CAS Key Laboratory of Functional Materials and Devices for Special Environments, Xinjiang Technical Institute of Physics & Chemistry, CAS; Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40–1 South Beijing Road, Urumqi 830011, China.

[b]Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.

*Corresponding author, E-mail: slpan@ms.xjb.ac.cn

Table S1. Crystal data and structure refinement for $Ba(NO_3)Cl$.

Empirical formula	$Ba(NO_3)Cl$
Temperature	273.15 K
Crystal system, space group	Orthorhombic, *Pnma*
Unit cell dimensions (Å)	a = 8.956(17)
	b = 5.297(11)
	c = 8.449(13)
Volume ($Å^3$)	400.8(13)
Z, Calculated density (g/cm^3)	4, 3.891
Absorption coefficient (mm^{-1})	10.423
F(000)	416
Theta range for data collection (°)	3.315 - 25.242
Limiting indices	$-11 \le h \le 11$, $-6 \le k \le 6$, $-9 \le l \le 10$
Reflections collected / unique	2912 / 503 [R(int) = 0.100]
Completeness to theta	99.80%
Goodness-of-fit on F^2	1.100
Final R indices [$F_o^2 > 2\sigma(F_c^2)$][a]	R_1 = 0.0392, wR_2 = 0.0724
R indices (all data)[a]	R_1 = 0.0692, wR_2 = 0.0845
Largest diff. peak and hole ($e \cdot Å^{-3}$)	1.921 and -1.960

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$.

Table S2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $Ba(NO_3)Cl$. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	Y	Z	U(eq)
Ba(1)	7348(1)	7500	3882(1)	24(1)
N(1)	5000(10)	2500	1734(10)	25(2)
O(1)	5681(6)	4531(12)	1507(5)	34(1)
O(2)	3672(8)	2500	2130(8)	31(2)
Cl(1)	6182(3)	2500	5470(3)	26(1)

Table S3. Selected bond lengths (Å) and angles (°) for $Ba(NO_3)Cl$.

Ba(1)-O(1)	2.954(6)	Ba(1)-Cl(1)#7	3.169(5)
Ba(1)-O(1)#1	3.032(6)	Ba(1)-Cl(1)	3.148(5)
Ba(1)-O(1)#2	2.954(6)	Ba(1)-Cl(1)#8	3.148(5)
Ba(1)-O(1)#3	3.032(6)	N(1)-O(1)	1.251(7)
Ba(1)-O(2)#4	3.025(6)	N(1)-O(1)#9	1.251(7)
Ba(1)-O(2)#5	3.025(6)	N(1)-O(2)	1.236(11)
Ba(1)-Cl(1)#6	3.209(7)		
O(1)-Ba(1)-O(1)#2	64.3(3)	O(1)#3-Ba(1)-Cl(1)#8	65.34(14)
O(1)#2-Ba(1)-O(1)#1	168.5(2)	O(1)#2-Ba(1)-Cl(1)#7	65.95(14)
O(1)-Ba(1)-O(1)#1	127.02(12)	O(2)#5-Ba(1)-O(1)#1	106.8(2)
O(1)-Ba(1)-O(1)#3	168.5(2)	O(2)#4-Ba(1)-O(1)#3	106.8(2)
O(1)#2-Ba(1)-O(1)#3	127.02(12)	O(2)#5-Ba(1)-O(1)#3	70.61(19)
O(1)#3-Ba(1)-O(1)#1	41.6(2)	O(2)#4-Ba(1)-O(1)#1	70.61(19)
O(1)#2-Ba(1)-O(2)#5	62.6(2)	O(2)#5-Ba(1)-O(2)#4	122.2(3)
O(1)#2-Ba(1)-O(2)#4	118.2(2)	O(2)#4-Ba(1)-Cl(1)#8	170.85(14)
O(1)-Ba(1)-O(2)#4	62.6(2)	O(2)#5-Ba(1)-Cl(1)	170.85(14)
O(1)-Ba(1)-O(2)#5	118.2(2)	O(2)#5-Ba(1)-Cl(1)#8	60.90(17)
O(1)#1-Ba(1)-Cl(1)#7	115.07(16)	O(2)#5-Ba(1)-Cl(1)#7	65.18(13)
O(1)-Ba(1)-Cl(1)	70.95(15)	O(2)#4-Ba(1)-Cl(1)	60.90(17)
O(1)#1-Ba(1)-Cl(1)#8	100.36(15)	O(2)#4-Ba(1)-Cl(1)#7	65.18(13)
O(1)#3-Ba(1)-Cl(1)	100.36(15)	O(2)#5-Ba(1)-Cl(1)#6	115.74(14)
O(1)-Ba(1)-Cl(1)#7	65.95(14)	O(2)#4-Ba(1)-Cl(1)#6	115.74(14)
O(1)#2-Ba(1)-Cl(1)	124.73(16)	O(1)#9-N(1)-O(1)	118.60(9)
O(1)#1-Ba(1)-Cl(1)	65.34(14)	O(2)-N(1)-O(1)	120.70(5)
O(1)#2-Ba(1)-Cl(1)#6	67.53(13)	O(2)-N(1)-O(1)#9	120.70(5)
O(1)#3-Ba(1)-Cl(1)#7	115.07(16)	Cl(1)#8-Ba(1)-Cl(1)	114.58(14)
O(1)#1-Ba(1)-Cl(1)#6	116.65(13)	Cl(1)#7-Ba(1)-Cl(1)#6	124.38(7)
O(1)-Ba(1)-Cl(1)#6	67.53(13)	Cl(1)-Ba(1)-Cl(1)#6	66.43(7)
O(1)-Ba(1)-Cl(1)#8	124.73(16)	Cl(1)#8-Ba(1)-Cl(1)#7	121.72(7)
O(1)#3-Ba(1)-Cl(1)#6	116.65(13)	Cl(1)-Ba(1)-Cl(1)#7	121.72(7)
O(1)#2-Ba(1)-Cl(1)#8	70.95(15)	Cl(1)#8-Ba(1)-Cl(1)#6	66.43(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2, -y+1, z+1/2 #2 x, -y+3/2, z

#3 -x+3/2, y+1/2, z+1/2

#4 x+1/2, y, -z+1/2

#5 x+1/2, y+1, -z+1/2

#6 -x+1, -y+1, -z+1

#7 -x+3/2, -y+1, z-1/2

#8 x, y+1, z

#9 x, -y+1/2, z

#10 x-1/2, y-1, -z+1/2

#11 x-1/2, y, -z+1/2

#12 x,y-1,z

Table S4. Bonding electron density difference ($\Delta\rho$) and contribution percent *w* (%) of different units in $Ba(NO_3)Cl$ calculated by the REDA method.

Units	$\Delta\rho$ (x 10^4)	*w* (%)
$[NO_3]$	278	93.7
$[BaO_6Cl_4]$	18.6	6.3

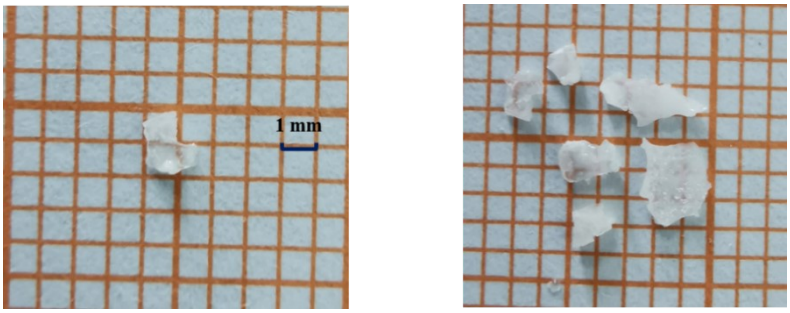

Figure S1. The photograph of the $Ba(NO_3)Cl$ crystal plate.

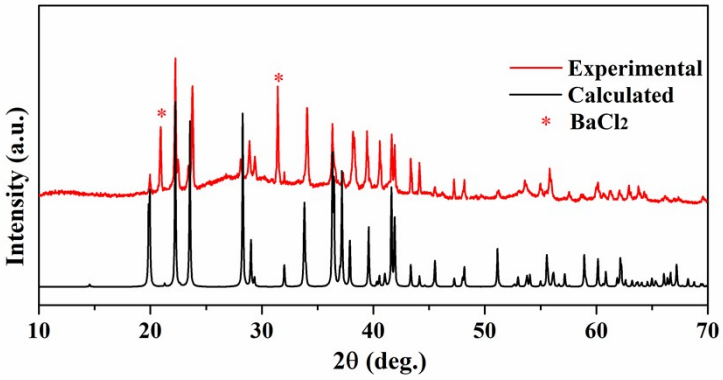

Figure S2. Powder XRD patterns of $Ba(NO_3)Cl$.

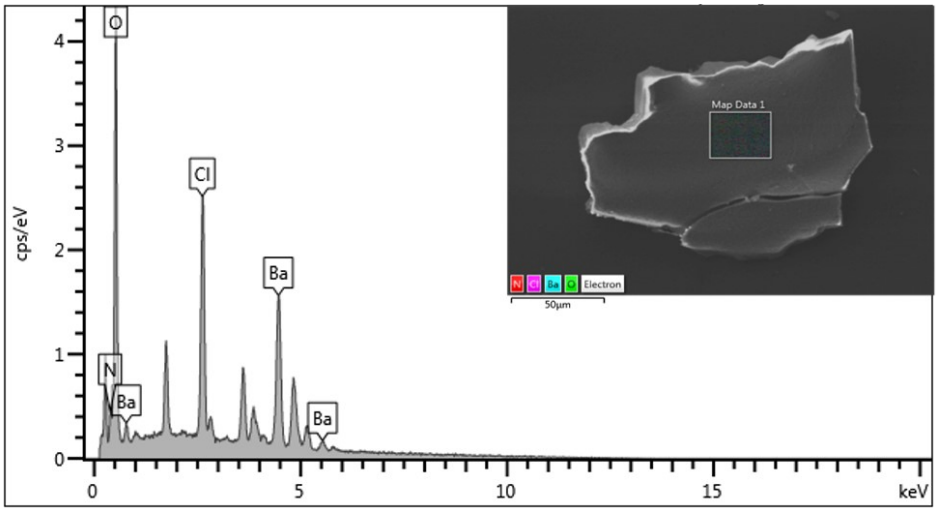

Figure S3. The EDX spectrum of $Ba(NO_3)Cl$.

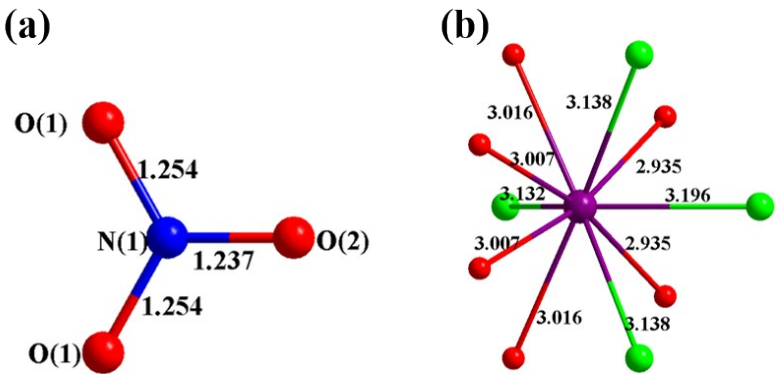

Figure S4. The [NO_3] triangle (a) and [BaO_6Cl_4] polyhedron (b) for $Ba(NO_3)Cl$.

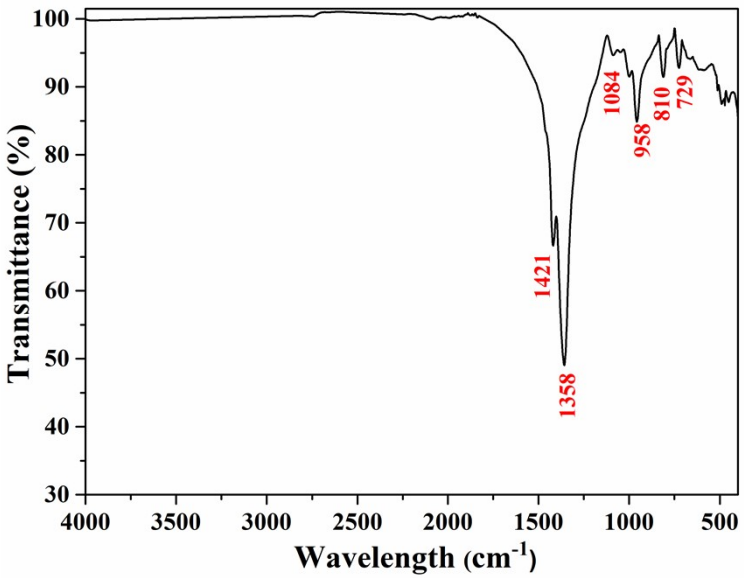

Figure S5. The IR spectrum of $Ba(NO_3)Cl$.