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Supporting information for article:

Structural and theoretical analysis of 2-chloro-4-nitroaniline and 2-methyl-6-nitroaniline salts

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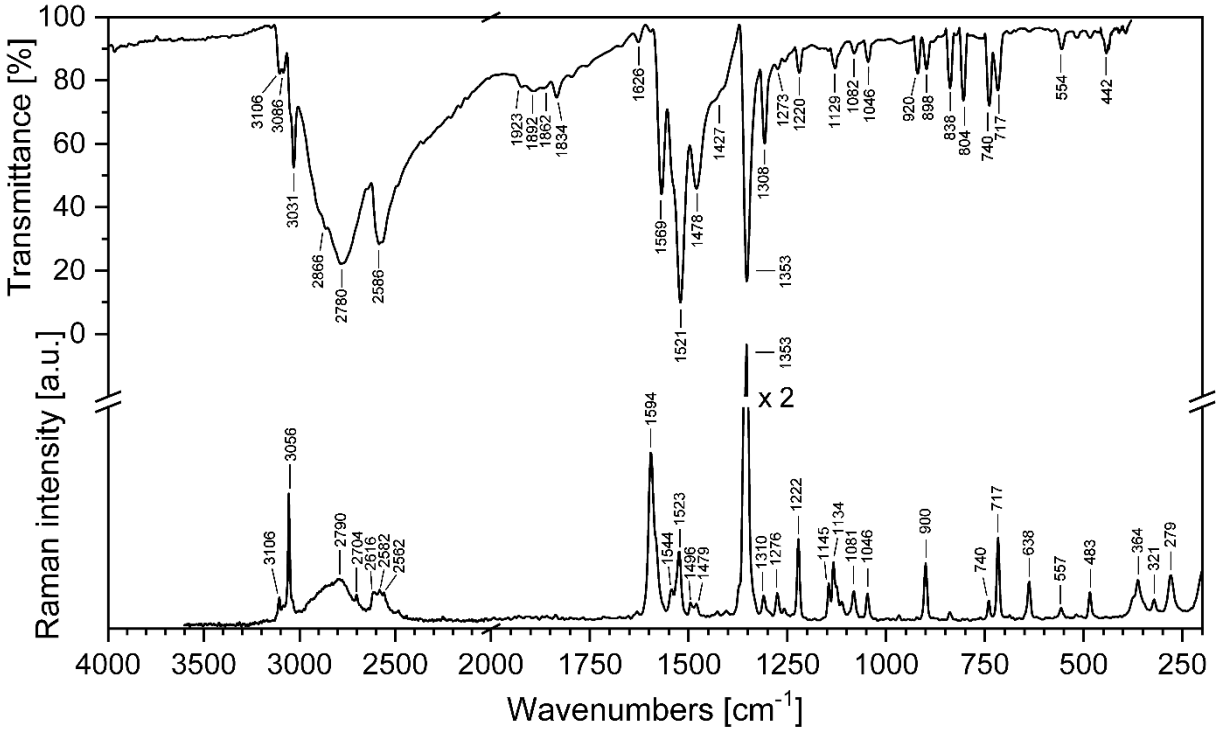

Figure S1. Room temperature FT-IR and FT-Raman spectra of (H2Cl4na)Br (**1**).

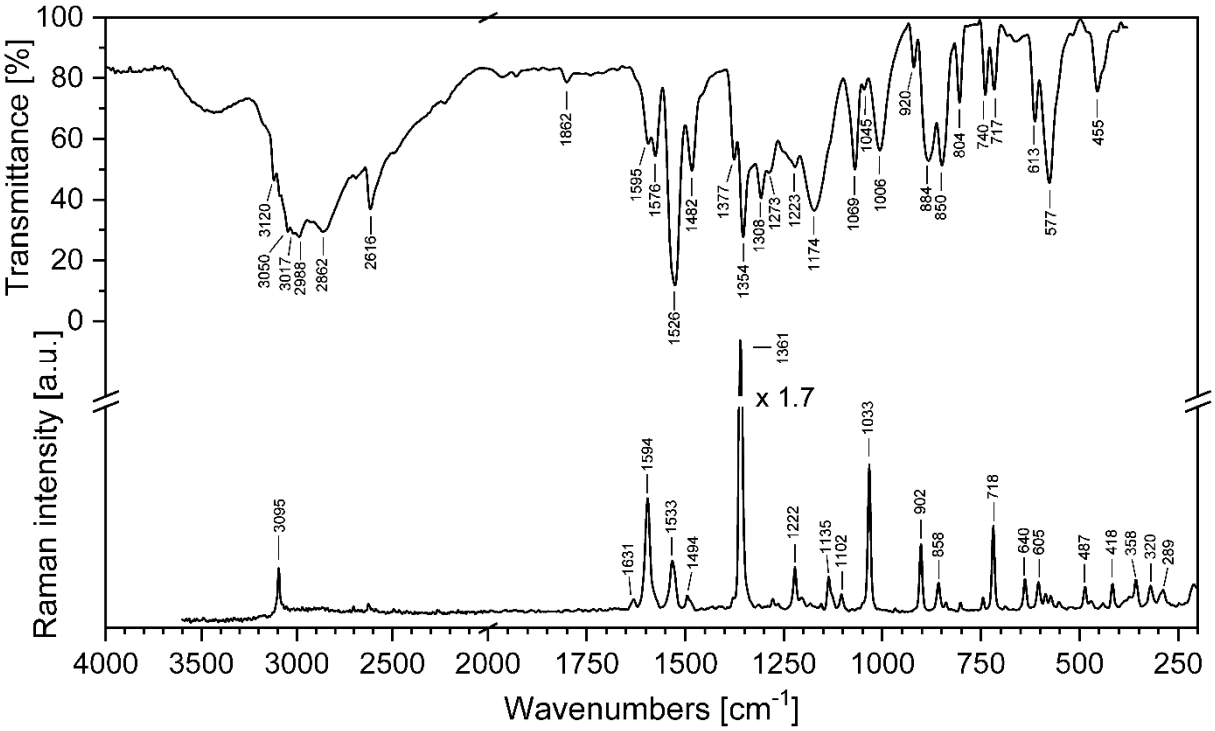

Figure S2. Room temperature FT-IR and FT-Raman spectra of (H2Cl4na)HSO_4 (**2**).

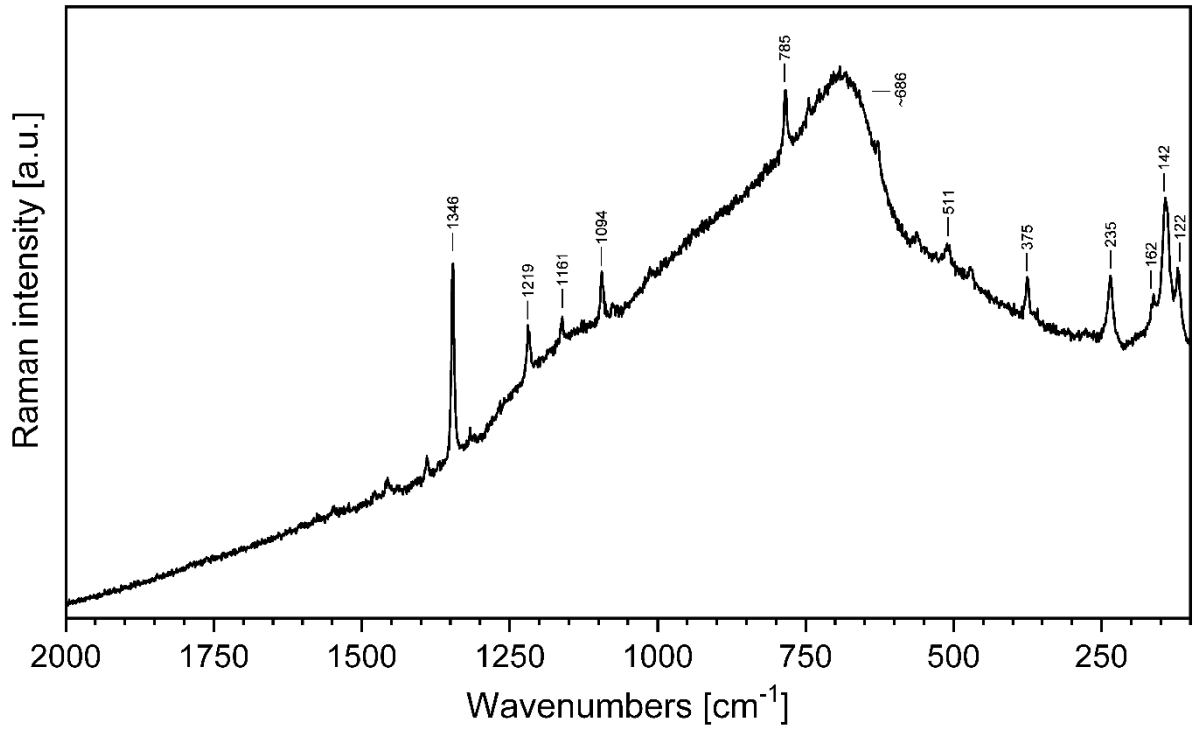

Figure S3. Room temperature FT-Raman spectra of (H2m6na)Br (**3**).

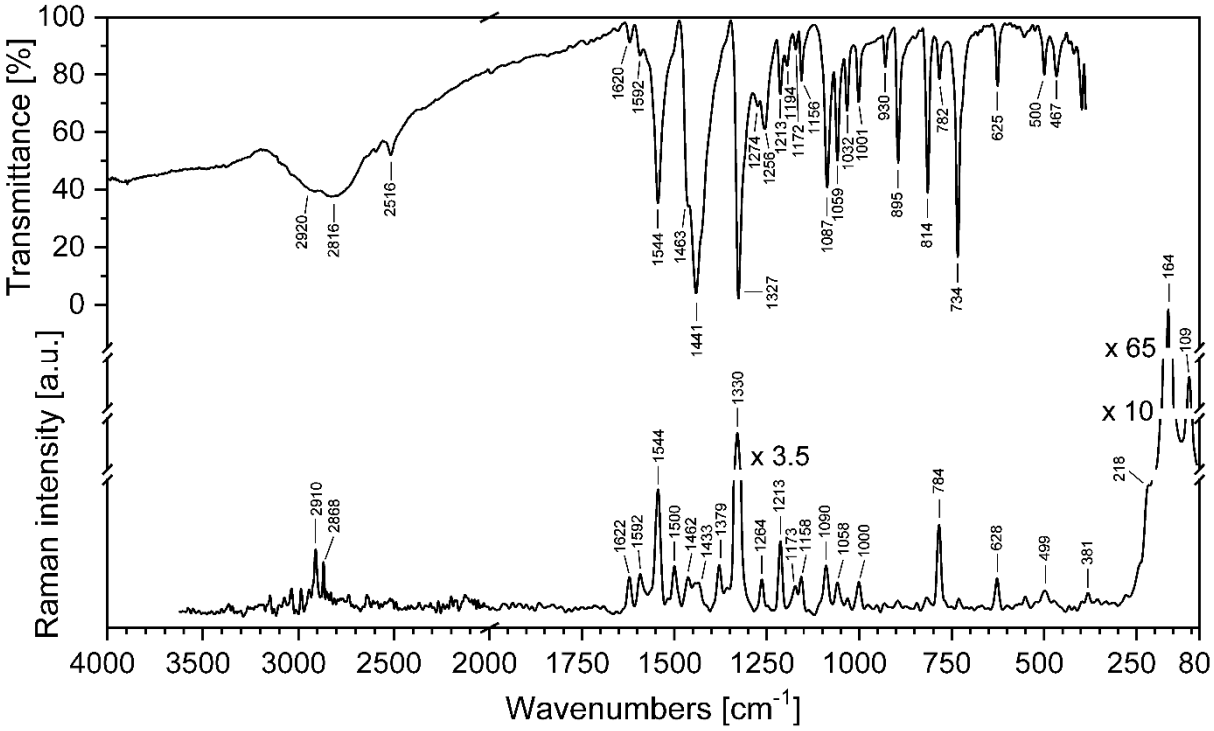

Figure S4. Room temperature FT-IR and FT-Raman spectra of (H2m6na)I_3 (**4**).

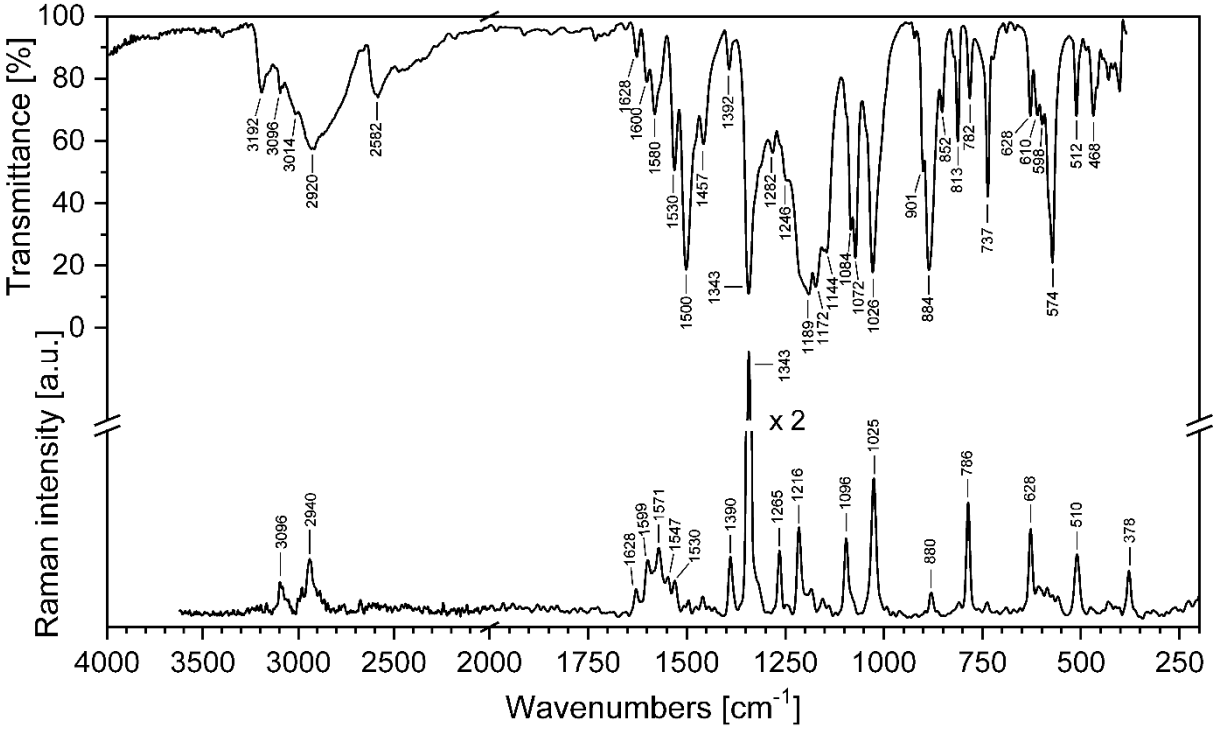

Figure S5. Room temperature FT-IR and FT-Raman spectra of (H2m6na)HSO_4 (**5**).

Table S1. XRD experimental details for studied compounds (H2Cl4na)Br (**1**), (H2Cl4na)HSO_4 (**2**), (H2m6na)Br (**3**), (H2m6na)I_3 (**4**) and (H2m6na)HSO_4 (**5**).

	1	**2**	**3**	**4**	**5**
Chemical formula	$C_6H_6ClN_2O_2\cdot Br$	$C_6H_6ClN_2O_2\cdot HO_4S$	$C_7H_9N_2O_2\cdot Br$	$C_7H_9N_2O_2\cdot I_3$	$C_7H_9N_2O_2\cdot HO_4S$
M_r	253.49	270.65	233.07	533.86	250.23
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
a, b, c (Å)	5.72152 (9), 7.90017 (17), 20.2729 (4)	16.1771 (6), 4.95335 (16), 12.8431 (5)	6.8920 (2), 7.7281 (3), 8.9210 (2)	7.0840 (2), 11.5247 (4), 16.3921 (6)	7.0966 (5), 8.3785 (8), 17.5115 (18)
α, β, γ (°)	90, 90, 90	90, 101.584 (4), 90	76.646 (3), 73.897 (2), 76.045 (2)	90, 98.738 (3), 90	90, 100.185 (9), 90
V (Å^3)	916.35 (3)	1008.17 (7)	436.12 (2)	1322.73 (8)	1024.81 (16)
Z	4	4	2	4	4
F(000)	496	552	232	960	520
D_x (Mg m^{-3})	1.837	1.783	1.775	2.681	1.622
No. of reflections for cell measurement	7548	1898	6602	6876	5045
θ range (°) for cell measurement	2.8–27.4	3.2–31.7	2.8–29.2	3.0–26.6	3.0–30.2
μ (mm^{-1})	4.74	0.60	4.67	7.07	0.33
Crystal shape	Block	Plate	Block	Block	Plate
Colour	Colourless	Colourless	Colourless	Black	Colourless
Crystal size (mm)	0.36 × 0.26 × 0.22	0.56 × 0.46 × 0.06	0.46 × 0.33 × 0.18	0.21 × 0.11 × 0.09	0.42 × 0.32 × 0.09
Absorption correction	Analytical	Multi-scan	Gaussian	Gaussian	Multi-scan
T_{min}, T_{max}	0.300, 0.446	0.967, 1.000	0.947, 0.973	0.966, 0.988	0.939, 1.000

No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18773, 2669, 2340	6028, 2923, 2351	15285, 2299, 1986	5822, 5822, 3181	4495, 4495, 3463
R_{int}	0.035	0.022	0.027	twin	twin
θ values (°)	θ_{max} = 30.0, θ_{min} = 2.8	θ_{max} = 30.0, θ_{min} = 2.6	θ_{max} = 29.0, θ_{min} = 3.1	θ_{max} = 29.7, θ_{min} = 3.1	θ_{max} = 27.5, θ_{min} = 2.7
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.703	0.703	0.682	0.697	0.650
Range of *h*, *k*, *l*	*h* = -8→8, *k* = -11→11, *l* = -28→28	*h* = -22→22, *k* = -6→6, *l* = -9→18	*h* = -9→9, *k* = -10→10, *l* = -12→12	*h* = -9→9, *k* = -15→15, *l* = -22→22	*h* = -9→9, *k* = -10→10, *l* = -22→22
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.028, 0.062, 1.13	0.036, 0.099, 1.07	0.026, 0.061, 1.11	0.031, 0.059, 0.80	0.044, 0.136, 1.07
No. of reflections	2669	2923	2299	5822	4495
No. of parameters	113	161	122	130	149
$(\Delta/\sigma)_{max}$	0.002	0.001	0.001	0.001	0.001
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.33, -0.70	0.52, -0.55	0.33, -0.39	0.70, -0.78	0.66, -0.42
Absolute structure parameter	-0.008 (4)	–	–	–	–

Table S2. Selected hydrogen-bond parameters for studied compounds **1**–**5**.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
(H2Cl4na)Br (**1**)				
N1—H1A···Br1	0.89	2.47	3.329 (2)	162.7
N1—H1B···Br1^{i}	0.89	2.45	3.295 (2)	159.3
N1—H1C···Br1^{ii}	0.89	2.41	3.266 (3)	162.5
C3—H3···Br1^{iii}	0.93	2.79	3.712 (3)	172.0
C5—H5···O2^{iv}	0.93	2.56	3.199 (4)	126.2
(H2Cl4na)HSO_4 (**2**)				
N1—H1A···O3	0.93 (2)	1.96 (2)	2.854 (2)	161 (2)
N1—H1B···O6^{v}	0.90 (3)	1.92 (3)	2.813 (2)	171 (2)
N1—H1C···O3^{vi}	0.87 (3)	2.14 (3)	2.952 (2)	156 (2)
N1—H1C···O5^{vii}	0.87 (3)	2.39 (3)	2.911 (2)	119 (2)
C3—H3···O1^{viii}	0.93	2.41	3.326 (2)	167.6
C6—H6···O3	0.93	2.47	3.184 (2)	134.0
O4—H4···O5^{ix}	0.79 (3)	1.85 (3)	2.6350 (18)	167 (3)
(H2m6na)Br (**3**)				
N1—H1A···O1	0.90 (3)	1.98 (3)	2.693 (2)	135 (2)
N1—H1B···Br1^{x}	0.86 (3)	2.47 (3)	3.2717 (17)	155 (2)
N1—H1C···Br1	0.92 (3)	2.34 (3)	3.2650 (18)	174 (2)
(H2m6na)I_3 (**4**)				
N1—H1A···O1	0.89	1.86	2.591 (6)	138.1
N1—H1B···I1	0.89	2.82	3.598 (4)	146.4
N1—H1C···I1^{xi}	0.89	2.82	3.566 (4)	143.0
C5—H5···O1^{xii}	0.93	2.54	3.304 (6)	140.1
(H2m6na)HSO_4 (**5**)				
O6—H6···O5^{xiii}	0.82	1.75	2.568 (3)	172.9
N1—H1A···O5^{xiv}	0.89	2.39	2.993 (3)	125.6
N1—H1A···O1	0.89	2.01	2.650 (3)	127.5
N1—H1B···O4^{xi}	0.89	1.92	2.802 (3)	168.5
N1—H1C···O3	0.89	1.86	2.731 (3)	167.3

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) *x*-1/2, -*y*+3/2, -*z*+1; (iii) *x*-1, *y*-1, *z*; (iv) -*x*+1, *y*+1/2, -*z*+3/2; (v) *x*, -*y*+1/2, *z*-1/2; (vi) *x*, *y*+1, *z*; (vii) -*x*, -*y*+1, -*z*; (viii) -*x*+1, -*y*+2, -*z*; (ix) -*x*, *y*-1/2, -*z*+1/2; (x) -*x*+1, -*y*, -*z*+2; (xi) *x*+1, *y*, *z*; (xii) -*x*+3/2, *y*+1/2, -*z*+1/2; (xiii) -*x*+1/2, *y*+1/2, -*z*+3/2; (xiv) -*x*+3/2, *y*+1/2, -*z*+3/2.