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Supporting information for article:

Structural, theoretic and spectroscopic analysis of 2-methyl-5-nitro-aniline salts with various inorganic acids

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Table S1 Experimental details

	(1)	(2)	(3)	(4)
Crystal data				
Chemical formula	$C_7H_9N_2O_2{\cdot}Br$	$C_7H_9N_2O_2{\cdot}I$	$C_7H_9N_2O_2{\cdot}NO_3$	$C_7H_9N_2O_2{\cdot}Cl$
M_r	233.07	280.06	215.17	188.61
Crystal system, space group	Monoclinic, $P12_1/m1$	Triclinic, P-1	Monoclinic, $P12_1/m1$	Triclinic, P-1
Temperature (K)	295	295	295	295
a, b, c (Å)	8.5689 (3), 6.4113 (2), 8.8248 (4)	6.5954 (2), 8.7764 (2), 8.8564 (3)	8.1234 (3), 6.6252 (2), 8.5799 (3)	7.9756 (1), 7.9803 (1), 28.2986 (3)
α, β, γ (°)	90, 110.200 (4), 90	72.140 (2), 84.002 (2), 81.830 (2)	90, 98.712 (3), 90	84.468 (1), 84.229 (1), 89.897 (1)
V (Å^3)	455.00 (3)	481.98 (3)	456.44 (3)	1783.61 (4)
Z	2	2	2	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	4.48	3.29	0.14	0.39
Crystal size (mm)	0.75 × 0.57 × 0.14	0.48 × 0.37 × 0.11	0.37 × 0.34 × 0.06	0.25 × 0.22 × 0.21
Data collection				
Diffractometer	Xcalibur, Atlas	Xcalibur, Atlas	Xcalibur, Atlas	Xcalibur, Atlas
Absorption correction	Gaussian *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Numerical	Gaussian *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Numerical	Multi-scan *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Empirical	Multi-scan *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Empirical

	absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.127, 0.604	0.274, 0.719	0.945, 1.000	0.983, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14243, 1279, 1187	14289, 2472, 2281	16584, 1273, 1078	50750, 7878, 6977
R_{int}	0.038	0.029	0.023	0.020
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.676	0.676	0.676	0.641
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.058, 1.06	0.022, 0.050, 1.08	0.041, 0.119, 1.09	0.052, 0.138, 1.13
No. of reflections	1279	2472	1273	7878
No. of parameters	87	112	102	441
No. of restraints	0	0	0	0
H-atom treatment	H atoms treated by a mixture of independent	H-atom parameters constrained	H atoms treated by a mixture of	H-atom parameters constrained

	and constrained refinement		independent and constrained refinement	
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.34	0.66, −0.79	0.27, −0.23	0.53, −0.42

	(5)	(6)
Crystal data		
Chemical formula	$C_7H_9N_2O_2\cdot HO_4S$	$2(C_7H_9N_2O_2)\cdot 2(I_3)\cdot H_2O$
M_r	250.23	1085.74
Crystal system, space group	Orthorhombic, *Pna*2$_1$	Monoclinic, *P*2$_1$/*c*
Temperature (K)	295	295
a, *b*, *c* (Å)	12.8927 (2), 4.97471 (10), 31.5518 (7)	11.2876 (3), 13.9536 (3), 17.5279 (5)
α, β, γ (°)	90, 90, 90	90, 96.808 (3), 90
V (Å^3)	2023.66 (7)	2741.24 (13)
Z	8	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.34	6.83
Crystal size (mm)	0.46 × 0.21 × 0.06	0.36 × 0.3 × 0.25
Data collection		
Diffractometer	Xcalibur, Atlas	Xcalibur, Atlas
Absorption correction	Gaussian *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Numerical absorption correction based on gaussian integration over a multifaceted crystal model	Gaussian *CrysAlis PRO* 1.171.38.43 (Rigaku Oxford Diffraction, 2015) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption

	Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.874, 0.980	0.186, 0.307
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	84145, 5220, 4577	68555, 5817, 3896
R_{int}	0.060	0.054
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.676	0.633
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.120, 1.06	0.038, 0.070, 1.04
No. of reflections	5220	5817
No. of parameters	295	270
No. of restraints	1	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.51, −0.35	1.12, −0.89
Absolute structure	Flack x determined using 2026 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	
Absolute structure parameter	0.15 (4)	

Computer programs: *CrysAlis PRO* 1.171.38.43 (Rigaku OD, 2015), ShelXT (Sheldrick, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), Olex2 (Dolomanov *et al.*, 2009).

Table S2 Relative energy corresponding to conformation of $H2Me5NA^+$ ion found in crystal structures **1**-**6**. E_1 – energy [kcal/mol] refers to the rotation of nitro group relative to the structure of global minimum, E_2 – energy refers to the simultaneous rotation of ammonio and methyl groups relative to the structure of global minimum, $E_1 + E_2$ – sum of E_1 and E_2 energies, E_{tot} – energy calculated for conformations corresponding to the crystal data.

Compd	Mol. No.	$dihC_4C_5N_2O_1$	E_1,	$dihC_6C_1N_1H$	$dihC_3C_2C_7H$	E_2	$E_1 + E_2$	E_{tot}
(1)		0	0	0	0	0	0	0
(2)		8.31	0.10	-9.04	0.42	0.02	0.12	0.12
(3)		0	0	0	0	0	0	0
(4)	A	-0.41	<0.01	23.03	-21.33	0.35	<0.36	0.36
	B	-6.80	0.07	-17.45	-18.24	0.24	0.31	0.32
	C	-2.57	0.01	-14.03	-25.17	0.36	0.37	0.37
	D	1.67	0.01	-24.78	-4.35	0.13	0.14	0.13
(5)	A	11.37	0.20	-7.44	-30.08	0.43	0.63	0.62
	B	-1.04	<0.01	-0.53	26.31	0.33	<0.34	0.35
(6)	A	15.75	0.38	33.94	5.73	0.23	0.61	0.61
	B	5.29	0.04	18.21	-0.28	0.07	0.11	0.11

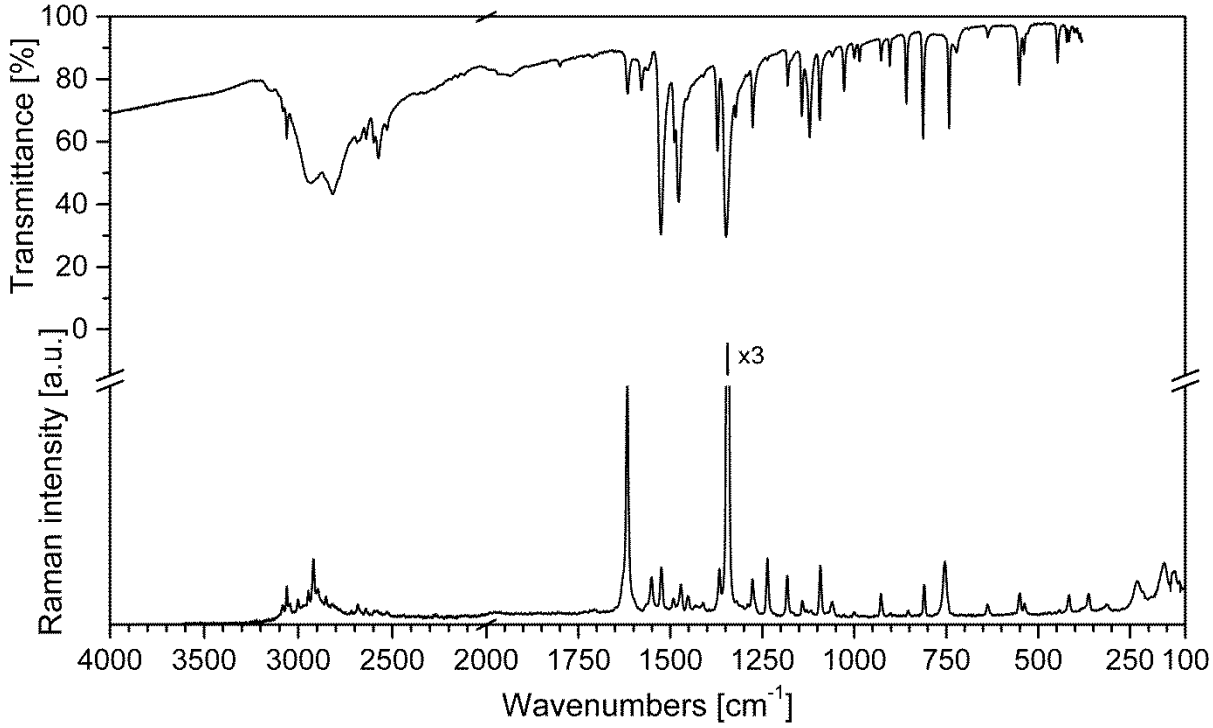

Figure S1 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)Br (**1**).

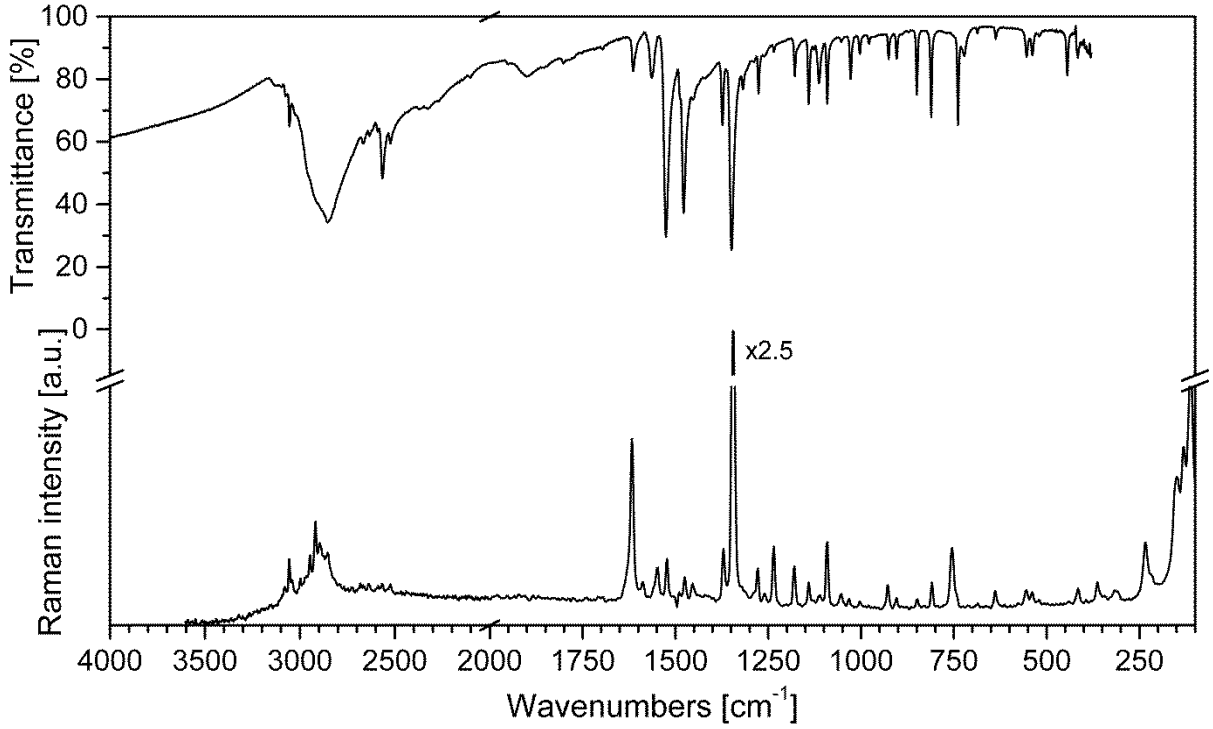

Figure S2 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)I (**2**).

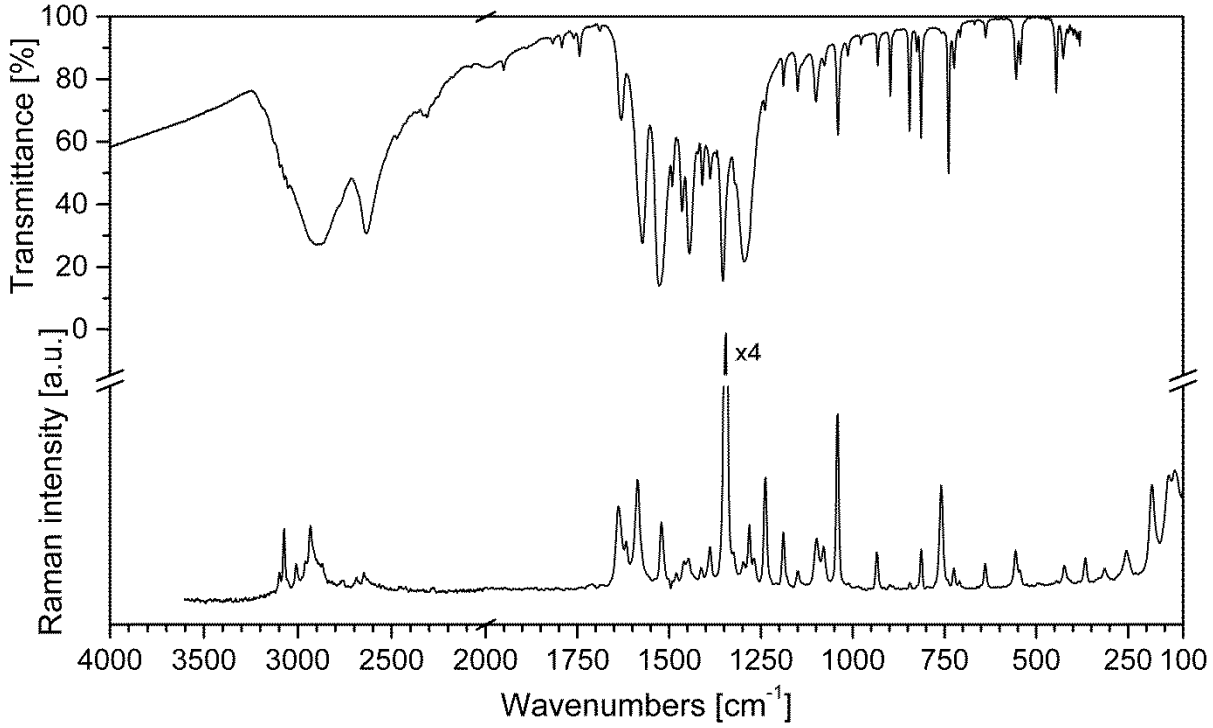

Figure S3 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)NO_3 (**3**).

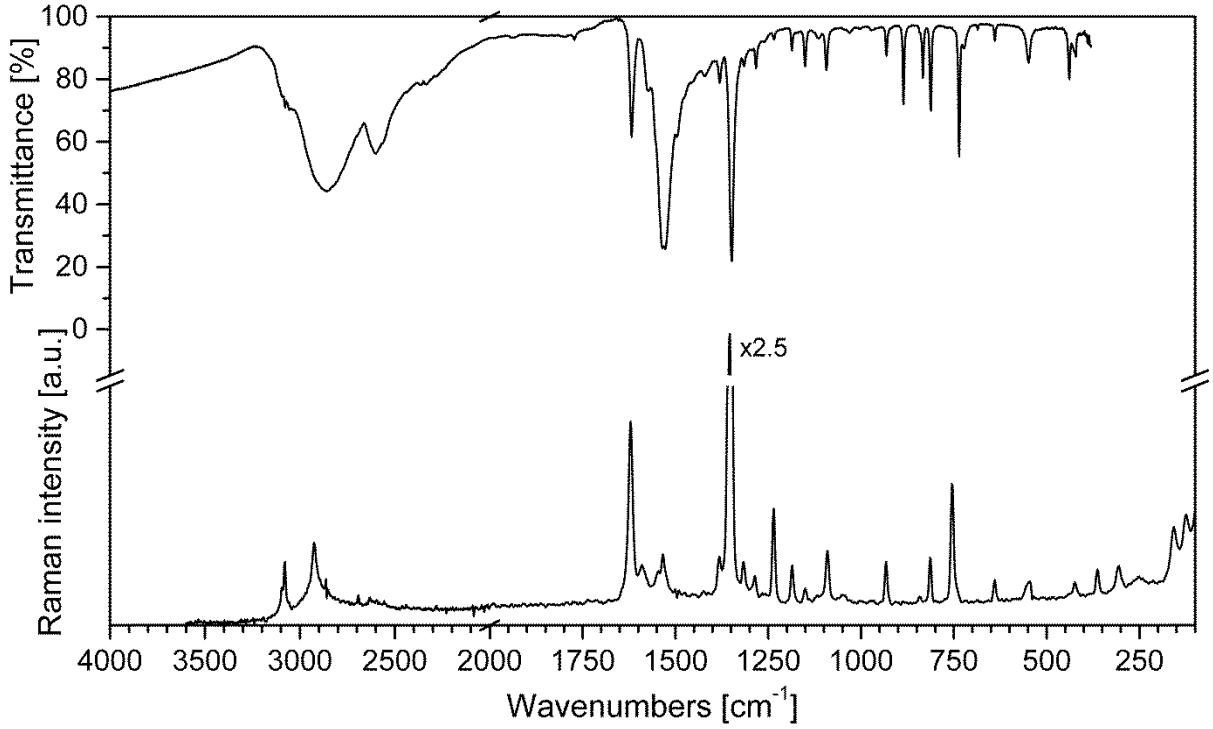

Figure S4 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)Cl (**4**).

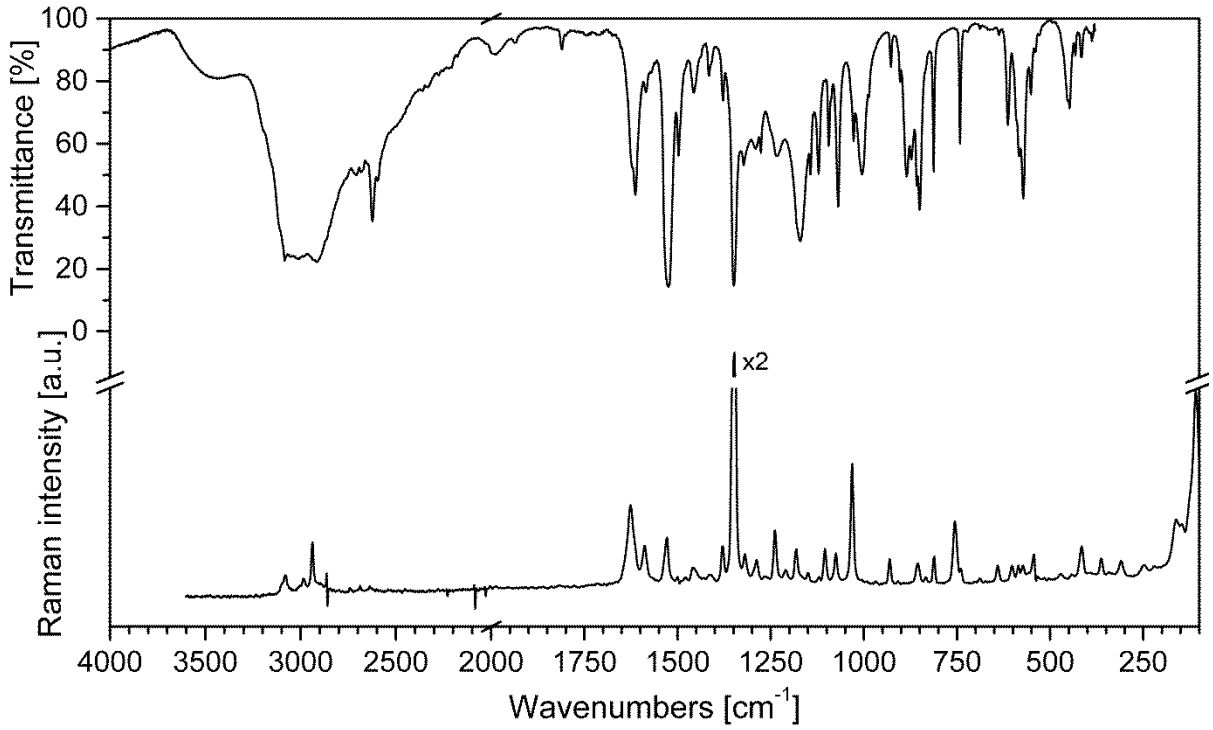

Figure S5 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)HSO_4 (**5**).

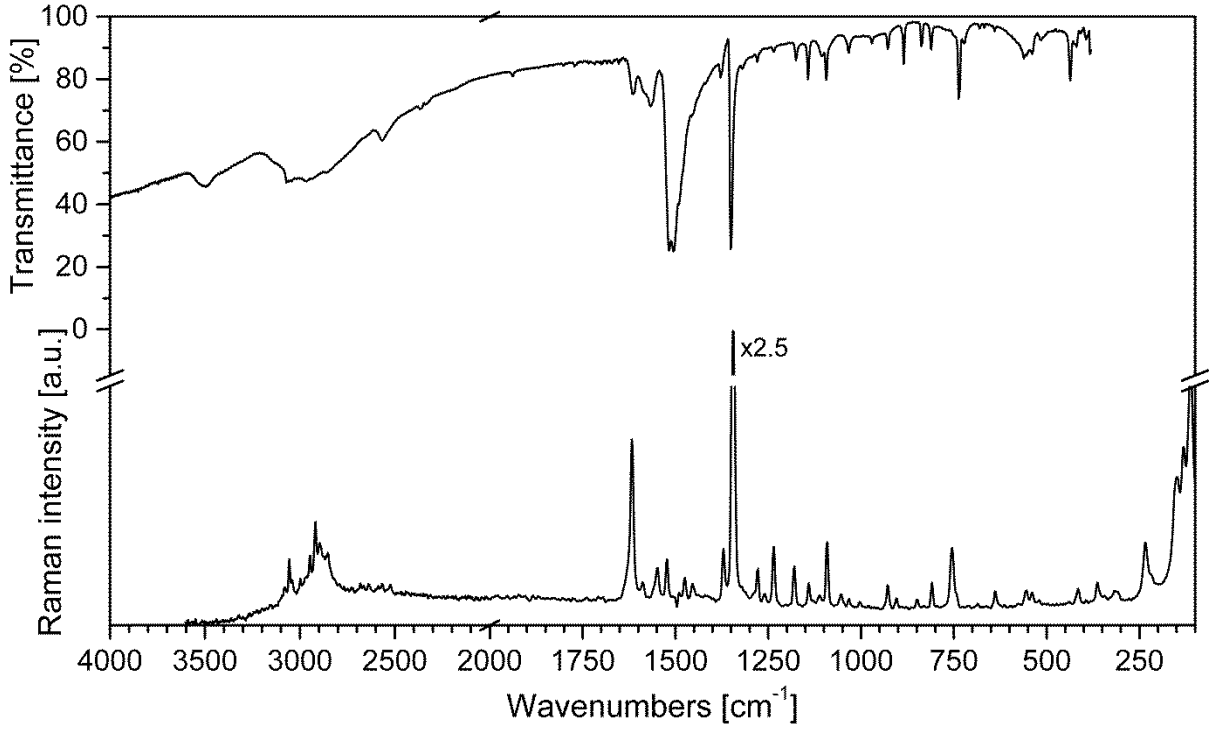

Figure S6 Room temperature powder FT-IR and FT-Raman spectra of (H2Me5NA)I_3·0.5H_2O (**6**).

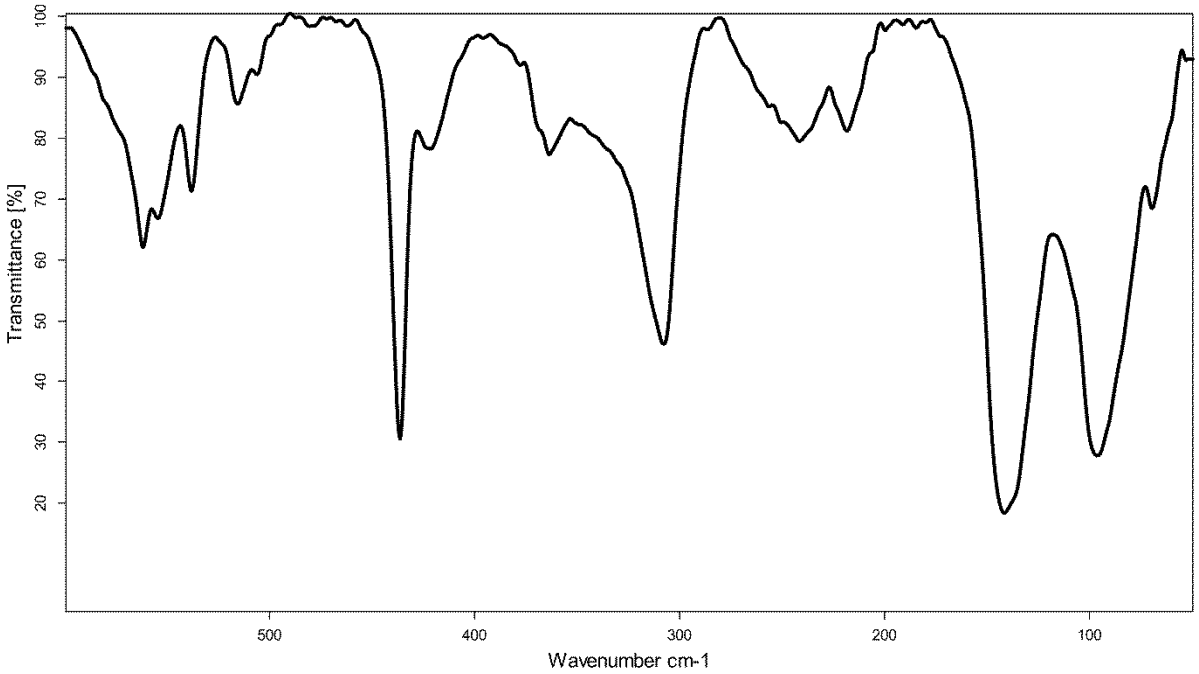

Figure S7 Room temperature powder far-infrared spectra of (H2Me5NA)I_3·0.5H_2O (**6**).