Structure-property relationships in Tris(2-amino-5-methylpyridinium) hexabromobismuthate monohydrate with focus on optical and electrical behavior for optoelectronics applications

Rima Altalib[1], Imen Ibrahmi[1*], Arafet Ghoudi[1], Sami Znaidia[2], Walid Rekik[3], Jerome Lhoste[4], Abderrazek Oueslati[1]

[1]*Laboratory of spectroscopic characterization and optical materials, Faculty of Sciences, University of Sfax, B.P. 1171, 3000 Sfax, Tunisia*
[2] Department of Physics, Faculty of Science, King Khalid University, Abha, Saudi Arabia
[3]*Laboratory Physical-Chemistry of Solid State, Chemistry department, Faculty of Sciences of Sfax, University of Sfax, BP 1171, 3000, Sfax, Tunisia*
[4.]*Institut des Molécules et Matériaux du Mans (IMMM)– UMR-6283 CNRS, Le Mans Université, Avenue Olivier Messiaen, F-72085 Le Mans Cedex 9, France*
* *Corresponding author. E-mail address:* arafetghoudi199@gmail.com

Table S1: Fractional atomic coordinates and equivalent isotropic temperature factors (Å²).

	x	*y*	*z*	U_{eq}
Bi1	0.5000	0.71499(3)	0.2500	0.03908(11)
Br1	0.60149(3)	0.71239(6)	0.37780(4)	0.0603(2)
Br2	0.43375(3)	0.72248(6)	0.33817(4)	0.0613(2)
Br3	0.5000	0.92713(7)	0.2500	0.0625(3)
Br4	0.5000	0.48510(8)	0.2500	0.0830(4)
Bi2	0.7500	0.2500	0.5000	0.03855(11)
Br5	0.66150(3)	0.24916(5)	0.55591(4)	0.05435(19)
Br6	0.66397(3)	0.24736(5)	0.35596(4)	0.0571(2)
Br7	0.74994(3)	0.46915(5)	0.48869(4)	0.0576(2)
C5	1.0083(5)	0.6756(7)	0.3626(5)	0.106(3)
N2	0.8976(3)	0.5421(6)	0.5438(4)	0.096(2)
C1	0.9789(3)	0.6377(6)	0.4101(4)	0.065(2)
C2	0.9420(4)	0.5533(6)	0.3917(4)	0.082(3)
C3	0.9146(3)	0.5205(6)	0.4345(4)	0.077(2)
C4	0.9873(3)	0.6805(6)	0.4741(4)	0.069(2)
N11	0.9597(3)	0.6486(5)	0.5166(3)	0.0715(19)
C6	0.9231(3)	0.5702(6)	0.4993(5)	0.067(2)
C7	0.7901(3)	0.5351(5)	0.7223(3)	0.0418(15)
N10	0.7446(2)	0.5657(4)	0.8037(3)	0.0517(14)
C9	0.7484(3)	0.4604(4)	0.6897(3)	0.0449(16)
C10	0.7866(3)	0.5868(5)	0.7789(3)	0.0482(17)
C11	0.7056(3)	0.4396(4)	0.7140(3)	0.0441(16)
C12	0.7033(3)	0.4948(5)	0.7736(3)	0.0472(16)
N4	0.6635(3)	0.4805(5)	0.8009(3)	0.0719(18)
C8	0.8365(3)	0.5561(6)	0.6938(4)	0.074(2)
C14	0.6664(4)	0.6447(6)	0.5570(4)	0.070(2)
N9	0.6247(4)	0.5769(6)	0.5476(5)	0.111(4)
C13	0.6814(4)	0.7121(6)	0.6099(5)	0.084(3)
N	0.5550(5)	0.5023(15)	0.5774(16)	0.45(2)
C18	0.5982(6)	0.5736(13)	0.5917(11)	0.186(12)
C15	0.7297(6)	0.7887(9)	0.6189(8)	0.203(8)
C16	0.6103(10)	0.6409(19)	0.6466(11)	0.227(19)
C17	0.6523(7)	0.7080(12)	0.6550(6)	0.150(8)
O	0.5827(4)	0.4335(5)	0.4316(5)	0.180(5)

Table S2: Hydrogen bonding geometry (Å, °)

D—H···A	**D—H**	**H···A**	**D···A**	**D—H···A**
N2-H2A□□□Br1^{I}	0.86	2.89	3.544(7)	134.6
N2-H2B□□□Br7	0.86	2.92	3.582(7)	135.3
N11-H11□□□Br1^{I}	0.86	2.87	3.538(6)	136.2
N11-H11□□□Br2^{I}	0.86	2.88	3.525(6)	133.4
N10-H10□□□Br6^{II}	0.86	2.93	3.566(5)	131.8
N10-H10□□□Br7^{II}	0.86	3.02	3.656(5)	132.1

C10-H10A□□□Br5^{III}	0.93	3.03	3.695(6)	130.2
C11-H11A□□□Br2^{IV}	0.93	3.03	3.881(6)	153.3
N4-H4A□□□Br6^{II}	0.86	3.09	3.697(6)	129.6
N4-H4A□□□Br7^{II}	0.86	2.96	3.590(6)	131.6
N4-H4B□□□Br1^{II}	0.86	3.07	3.588(6)	121.1
N4-H4B…Br2^{IV}	0.86	3.13	3.926(6)	154.1
C14-H14□□□Br7	0.93	3.04	3.695(8)	129.1
N9-H9A□□□O	0.86	1.98	2.834(11)	171.3
N-HB□□□Br2^{IV}	0.86	2.73	3.324(11)	127.3
O-HC□□□Br6	0.85	3.05	3.827(11)	153.2
O-HD□□□Br4	0.85	2.72	3.476(7)	149.7

Symmetry codes : ^{I} –x+3/2, -y+3/2, -z+1; ^{II} x, -y+1, z+1/2 ;
^{III} –x+3/2, y+1/2, -z+3/2 ; ^{IV} –x+1, -y+1, -z+1.

Table S3: Parameters of the equivalent circuit at various temperatures.

T (K)	R1 (×10^{5} Ω)	Q_1 (×10^{-8} F)	α_1	R_2 (×10^{7} Ω)	C (×10^{-11} F)	Q_2 (×10^{-9} F)	α_2
318	21.499	3.0519	0.720	1.885	3.717	2.070	0.393
323	14.274	6.9550	0.673	1.497	3.682	2.611	0.381
328	8.6971	6.3910	0.675	1.171	3.700	3.878	0.353
333	5.0656	4.1626	0.699	0.8607	3.724	5.829	0.332
338	0.5503	6.3302	0.683	5.985	3.678	7.775	0.336
343	33.301	3.7520 10^{-3}	0.690	0.0279	3.454	18.999	0.749
348	6.1882	1.7484 10^{-2}	0.957	0.297	5.564	10.844	0.387
353	2.1372	1.4598 10^{-2}	0.966	0.113	5.695	26.958	0.401
358	1.6578	1.0419 10^{-2}	0.965	0.731	7.490	25.846	0.482
363	1.0543	1.1335 10^{-2}	0.955	0.544	8.159	24.161	0.519

Table S4: The list of parameters obtained by fitting the modified KWW function to the frequency-dependent modulus (M'') data.

T (K)	M''_{max}	β	ω_{max}
313	0.0049	0.65062	2207.77281
318	0.00492	0.67214	2163.41111
323	0.00502	0.69027	2849.93939
328	0.00508	0.69575	3687.8195
333	0.00511	0.69871	5112.03084
338	0.00511	0.69819	7783.86198
343	0.00508	0.6901	13041.99717
348	0.00506	0.68557	23358.60064
353	0.00505	0.6821	45097.80746
358	0.00503	0.67595	88095.69313

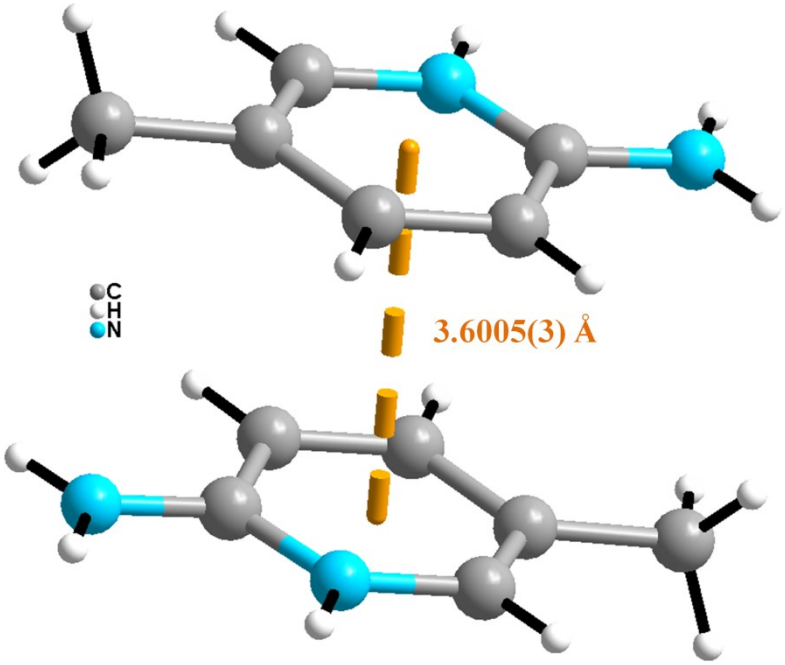

Figure S1: π…π interactions in the structure of $(C_6H_9N_2)_3[BiBr_6].H_2O$.

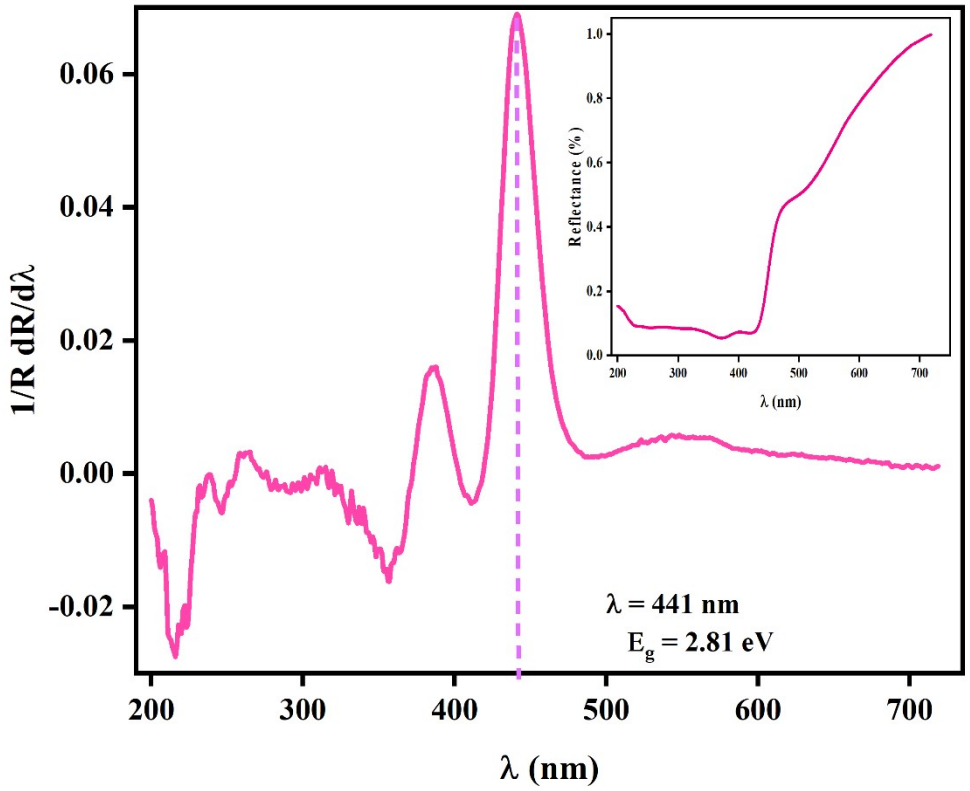

Figure S2: Variation of (1/R(λ))(dR(λ)/dλ) as a function of wavelength, insert: variation of reflectance as a function of wavelength.