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

Supplementary Information

Chiral Organic-Inorganic Lead Halide Perovskites Based on α-Alanine

Valerii Y. Sirenko,[a] Olesia I. Kucheriv,[a], Dina D. Naumova,[a] Igor V. Fesych,[a] Rostyslav P. Linnik,[a] Ioan-Andrei Dascălu,[b] Sergiu Shova,[b] Igor O. Fritsky,[a] and Il'ya A. Gural'skiy[a]*

[a]Department of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska St. 64, Kyiv 01601, Ukraine

[b]"Petru Poni" Institute of Macromolecular Chemistry, 41A Aleea Gr. Ghica Voda, 700487 Iasi, Romania

*Corresponding author: illia.guralskyi@univ.kiev.ua

Table S1. Crystal data for **I-D**, **I-L**, **Br-D** and **Br-L**

	I-D	**I-L**	**Br-D**	**Br-L**
Formula	$C_3H_{10}I_3NO_3Pb$	$C_3H_{10}Br_3NO_3Pb$	$C_3H_{10}I_3NO_3Pb$	$C_3H_{10}Br_3NO_3Pb$
Formula weight	696.01 g/mol	696.01 g/mol	555.04 g/mol	555.04 g/mol
Temperature/K	293 K	293(2) K	293(2) K	296.0 K
Crystal size/mm^3	0.41×0.24×0.09	0.234×0.163×0.04	0.3×0.1×0.05	0.3×0.15×0.1
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*C*2	*C*2	*C*2	*C*2
a/Å	22.560(3)	22.6435(14)	21.8559(18)	21.836(4)
b/Å	6.4430(5)	6.4529(4)	6.0868(6)	6.0904(11)
c/Å	8.9978(7)	9.0191(6)	8.7692(8)	8.790(3)
β/°	92.204(9)	92.107(6)	93.177(8)	92.41(2)
V/$Å^3$	1306.9(2)	1316.95(14)	1164.80(18)	1167.9(5)
Z	4	4	4	4
Calc. density/g cm^{-3}	3.537	3.510	3.165	3.157
μ/mm^{-1}	19.971	19.818	24.745	24.679
F(000)	1200.0	1200.0	984.0	984.0
Radiation type	Mo *K*α (λ = 0.71073)	Mo *K*α (λ = 0.71073)	Mo *K*α (λ = 0.71073)	Mo *K*α (λ = 0.71073)
2Θ range for data collection/°	4.53 to 52.722	3.6 to 52.704	3.732 to 52.706	3.734 to 52.694
Index ranges	−28 ≤ h ≤ 23, −8 ≤ k ≤ 8, −11 ≤ l ≤ 11	−28 ≤ h ≤ 28, −8 ≤ k ≤ 8, −11 ≤ l ≤ 11	−27 ≤ h ≤ 27, −7 ≤ k ≤ 7, −7 ≤ l ≤ 10	−23 ≤ h ≤ 27, −7 ≤ k ≤ 7, −10 ≤ l ≤ 9
Reflections collected	3595	2684	2397	4219
Independent reflections	3595	2684	2397	2392
R_{sigma}	0.0328	0.0536	0.0734	0.0539

R_{int}	-	-	-	0.0293
Data/restraints/parameters	3595/38/103	2684/1/103	2397/2/101	2392/2/100
Goodness-of-fit on F^2	1.086	1.107	1.049	1.061
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0873, wR_2 = 0.2570	R_1 = 0.0563, wR_2 = 0.1515	R_1 = 0.0603, wR_2 = 0.1401	R_1 = 0.0436, wR_2 = 0.0981
Final R indexes [all data]	R_1 = 0.0946, wR_2 = 0.2665	R_1 = 0.0620, wR_2 = 0.1560	R_1 = 0.0694, wR_2 = 0.1506	R_1 = 0.0513, wR_2 = 0.1037
Largest diff. peak/hole/e $Å^{-3}$	3.37/−3.01	4.57/−3.10	5.17/−4.15	1.33/−0.98
Flack parameter	0.03(2)	0.031(11)	0.06(2)	0.01(3)
CCDC No.				

Table S2. Bond lengths for **I-D**, **I-L**, **Br-D** and **Br-L** (Å) and Σ (°), Δd, σ^2 $(°)^2$ for **I-L** and **Br-L**

I-D			
C1—C2	1.52(7)	I1—Pb1	3.231(3)
C1—O1	1.16(5)	I2—Pb1[2]	3.177(3)
C1—O2	1.34(5)	I2—Pb1	3.214(3)
C2—C3	1.48(6)	I3—Pb1[3]	3.224(6)
C2—N1	1.51(6)	I3—Pb1	3.234(6)
I1—Pb1[1]	3.220(3)		
Symmetry transformations used to generate equivalent atoms:			
[1]1-X,+Y,1-Z; [2]1-X,+Y,2-Z; [3]+X,1+Y,+Z			
I-L			
C1—C2	1.50(4)	I1—Pb1[1]	3.234(4)
C1—O1	1.21(3)	I2—Pb1	3.2200(17)
C1—O2	1.25(3)	I2—Pb1[2]	3.2453(15)
C2—C3	1.50(4)	I3—Pb1	3.1918(15)
C2—N1	1.50(3)	I3—Pb1[3]	3.2265(16)
I1—Pb1	3.233(3)		
Σ, (°)	37.28		
Δd	$2.70 \cdot 10^{-5}$		
σ^2, $(°)^2$	13.87		
Symmetry transformations used to generate equivalent atoms:			
[1]+X,1+Y,+Z; [2]1-X,+Y,-Z; [3]1-X,+Y,1-Z			
Br-D			
Br1—Pb1[1]	3.015(2)	C1—C2	1.52(3)
Br1—Pb1	3.073(2)	C1—O1	1.16(3)
Br2—Pb1	2.959(7)	C1—O2A	1.31(3)
Br2—Pb1[2]	3.140(7)	C1—O2B	1.31(3)

Br3—Pb1[3]	2.991(2)	C2—C3	1.44(3)
Br3—Pb1	3.039(2)	C2—N1	1.43(3)

Symmetry transformations used to generate equivalent atoms:

[1]1-X,+Y,2-Z; [2]+X,-1+Y,+Z; [3]1-X,+Y,1-Z

Br-L

Pb1—Br[1]	3.060(2)	N1—C2	1.47(2)
Pb1—Br1	3.0363(17)	C1—O1	1.15(2)
Pb1—Br2[2]	3.0617(18)	C1—O2B	1.35(2)
Pb1—Br2	2.9713(19)	C1—C2	1.52(3)
Pb1—Br3	2.974(5)	C1—O2A	1.35(2)
Pb1—Br3[3]	3.129(5)	C2—C3	1.48(3)

Σ, (°)	36.24
Δd	$3.23 \cdot 10^{-4}$
σ^2, (°)^2	15.48

Symmetry transformations used to generate equivalent atoms:

[1]1-X,+Y,1-Z; [2]1-X,+Y,-Z; [3]+X,-1+Y,+Z

Table S3. Hydrogen bonding geometry of **I-D**, **I-L**, **Br-D** and **Br-L** (Å, °)

D – H···*A*	d(*D* – H)/Å	d(H···*A*)/Å	d(*D*···*A*)/Å	∠*D* – H···*A*/°
I-D				
N1 – H1A···I1	0.89	2.70	3.54(3)	156.4
N1 – H1A···I3[1]	0.89	3.41	3.77(3)	106.7
N1 – H1B···I1[2]	0.89	2.79	3.60(4)	152.0
N1 – H1C···O1[3]	0.89	2.04	2.77(5)	138.9
N1 – H1C···O1W[3]	0.89	2.63	3.05(5)	109.8
O2 – H2A···O1W	0.85	1.77	2.62(6)	171.2
O1W – H1WA···I2[4]	0.87	2.77	3.61(4)	162.7
O1W – H1WB···I3[4]	0.86	2.73	3.58(4)	169.9
C3 – H3A··· O1[3]	0.97	2.87	3.51	124.7
C3 – H3B··· O2	0.96	2.77	3.54	137.0

Symmetry transformations used to generate equivalent atoms:

[1]1-X,-1+Y,1-Z; [2]+X,-1+Y,+Z; [3]1/2-X,1/2+Y,1-Z; [4]1/2-X,-3/2+Y,1-Z

I-L

N1 – H1A···O1	0.89	1.97	3.85(3)	172.7
N1 – H1B···I2[2]	0.89	2.72	3.52(2)	149.2
N1 – H1C···I1	0.89	3.01	3.741(19)	141.2
N1 – H1C···I2	0.89	3.02	3.62(2)	126.3
O2 – H2A···O1W	0.82	1.79	2.59(3)	166.5
O1W – H1WA···I1[3]	0.86	2.85	3.68(2)	162.3
O1W – H1WB···I3[4]	0.86	2.84	3.68(3)	164.6
C3 – H3C – O2	0.96	2.68	3.51	144.5
C3 – H3A···O1[1]	0.96	3.18	3.61	109.5

Symmetry transformations used to generate equivalent atoms:

[1]3/2-X,-1/2+Y,-Z; [2]+X,1+Y,+Z; [3]1/2+X,1/2+Y,+Z; [4]3/2-X,3/2+Y,1-Z

Br-D

N1 – H1A···Br1	0.89	2.74	3.400(19)	131.7
N1 – H1A···Br2	0.89	2.90	3.590(16)	135.1
N1 – H1B···Br1[1]	0.89	2.49	3.318(19)	154.9
N1 – H1C···O1[2]	0.89	1.98	2.86(3)	168.4
O2A – H2A···O1W	0.86	1.80	2.66(5)	170.3
O2B – H2B···O1W	0.86	1.77	2.61(5)	161.9
O1W – H1WA···Br2[3]	0.87	2.68	3.503(19)	158.7
O1W – H1WB – Br3[4]	0.84	2.54	3.366(18)	169.8
C3 – H3A···O1[2]	0.96	2.65	3.42	138.1
C3 – H3B···O2	0.96	2.68	3.47	138.8

Symmetry transformations used to generate equivalent atoms:

[1]+X,-1+Y,+Z; [2]1/2-X,1/2+Y,2-Z; [3]-1/2+X,-1/2+Y,+Z; [4]1/2-X,-3/2+Y,1-Z

Br-L

N1 – H1A···Br1[1]	0.89	2.65	3.395(14)	142.2
N1 – H1A···Br3[2]	0.89	2.98	3.564(13)	125.0
N1 – H1B···O1[3]	0.89	1.98	2.833(18)	159.4
N1 – H1C···Br1	0.89	2.46	3.320(14)	163.4
O1W – H1WA···Br2[4]	0.86	2.60	3.384(15)	151.6
O1W – H1WB···Br3[3]	0.87	2.63	3.475(14)	166.3
O2B – H2B···O1W	0.87	1.75	2.61(3)	170.5
O2A – H2A ··· O1W	0.86	1.75	2.61(3)	173.9
C3 – H3B ··· O2	0.96	2.69	3.44	134.6
C3 – H3C ··· O1[3]	0.96	2.68	3.44	136.5

Symmetry transformations used to generate equivalent atoms:

[1]+X,-1+Y,+Z; [2]1-X,-1+Y,1-Z; [3]3/2-X,-1/2+Y,1-Z; [4]3/2-X,1/2+Y,1-Z

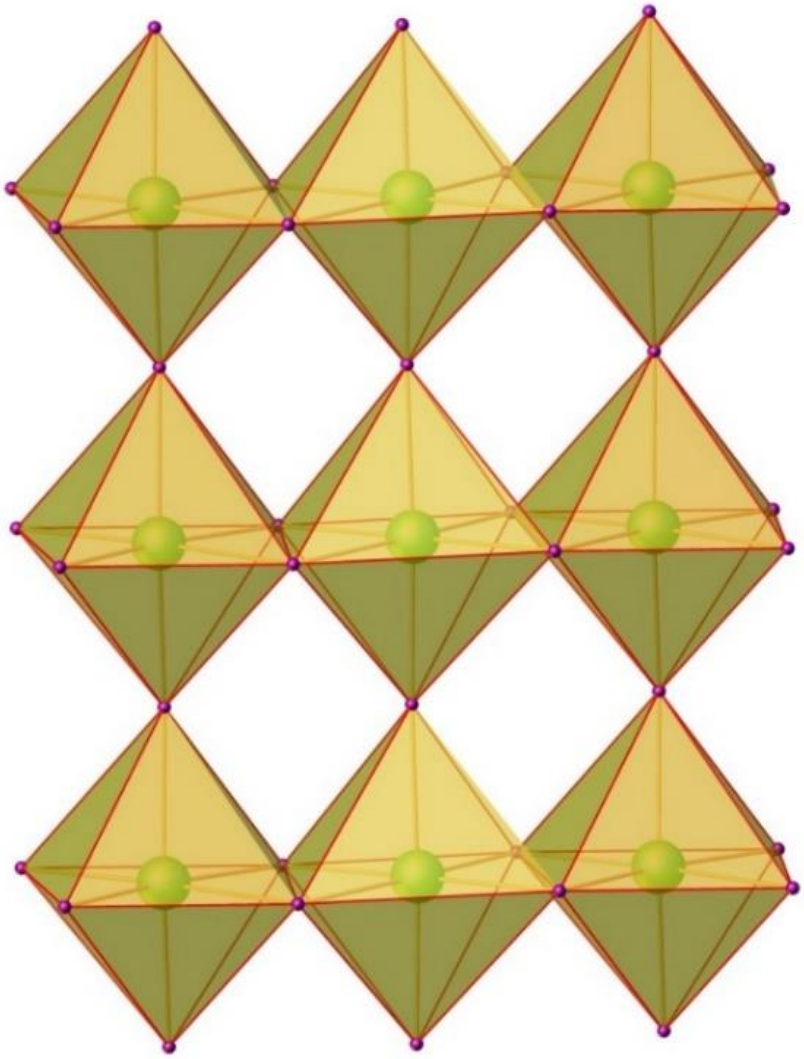

Figure S1. View of the 2D anionic inorganic polymeric $\{[PbBr_3]^-\}_n$ layers.

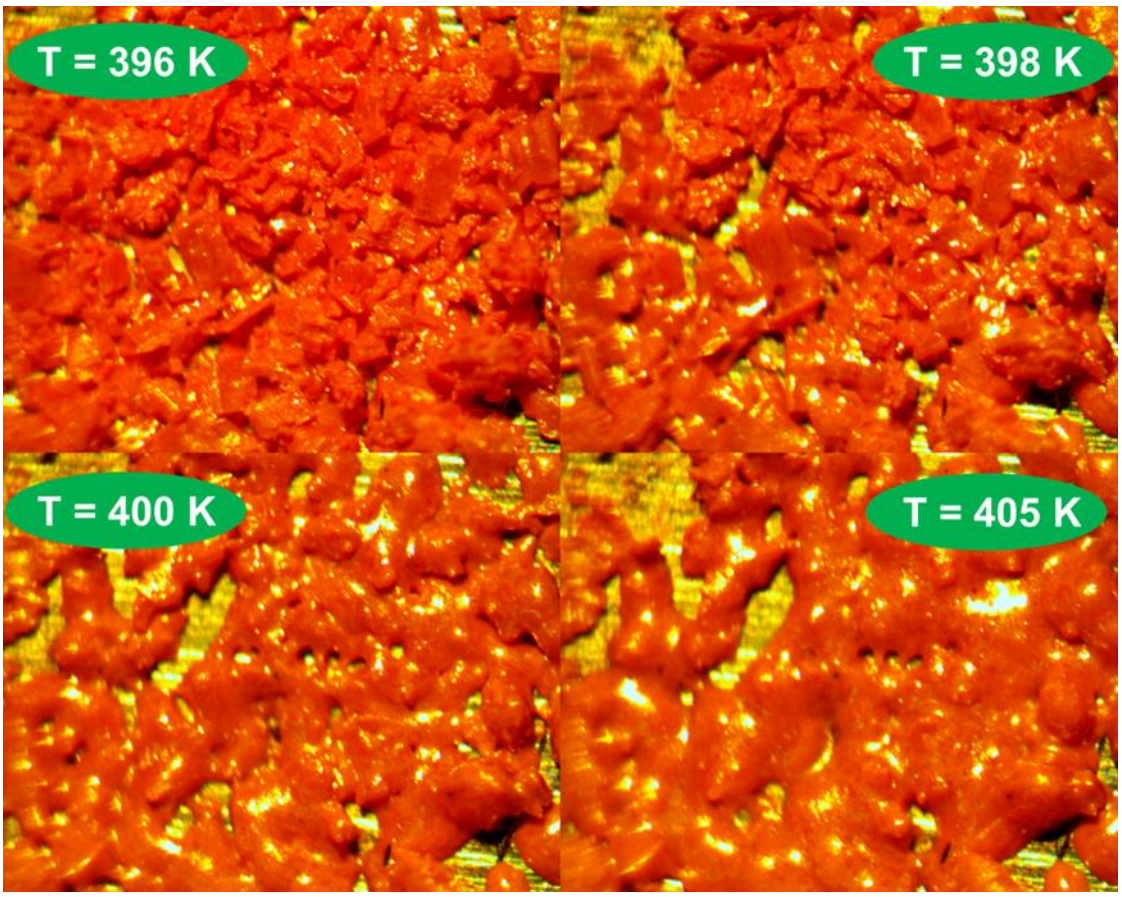

Figure S2. Optical images of **I-L** melting.

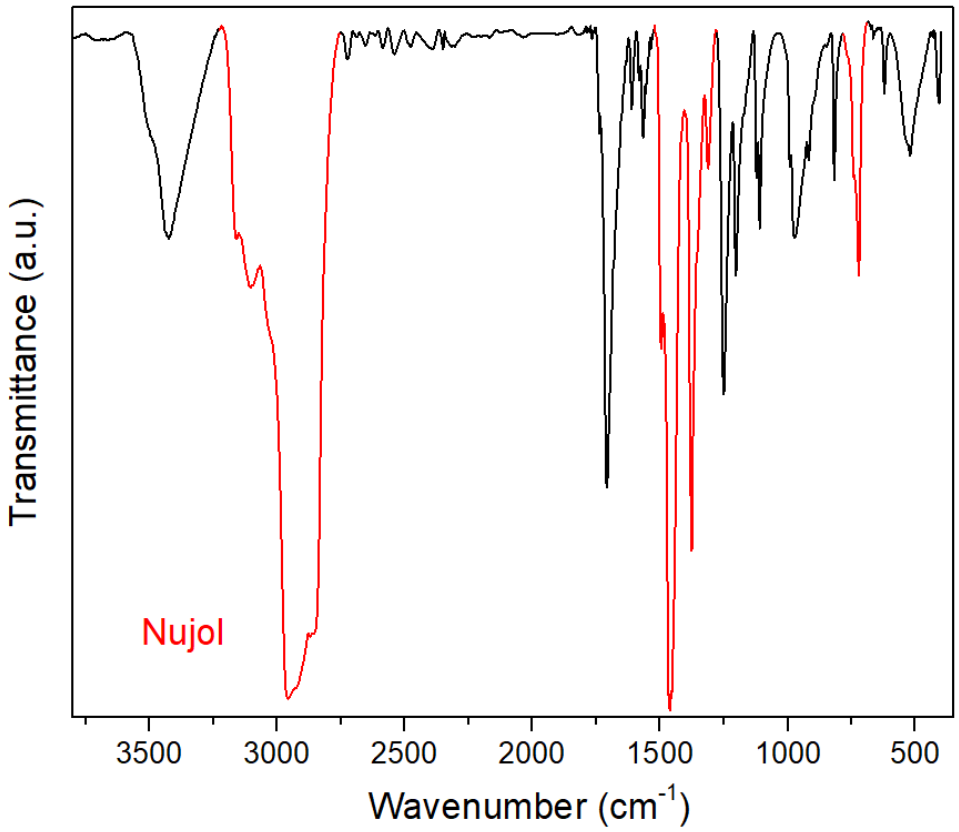

Figure S3. IR spectrum of I-D

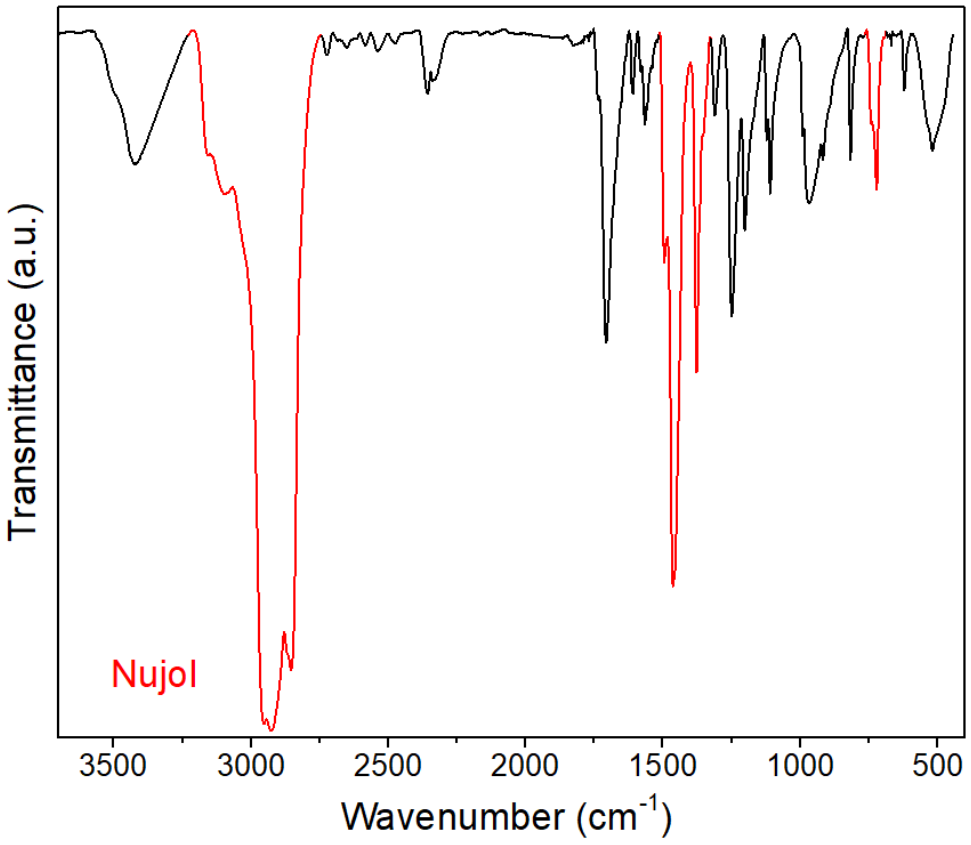

Figure S4. IR spectrum of Br-D

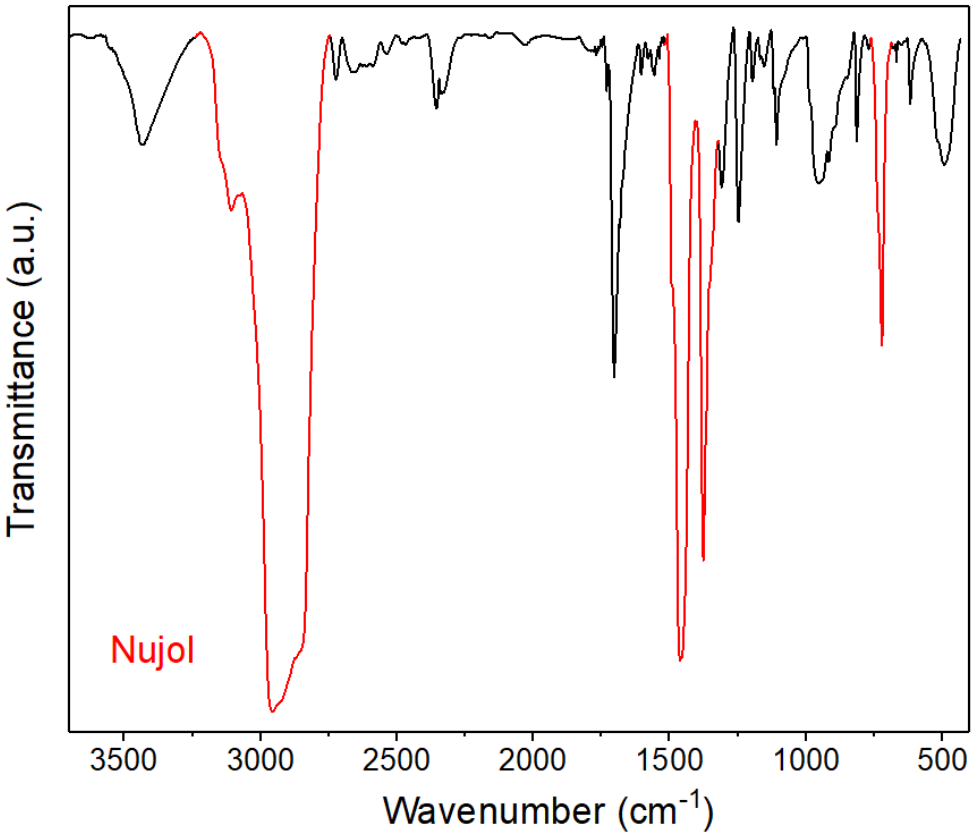

Figure S5. IR spectrum of I-L

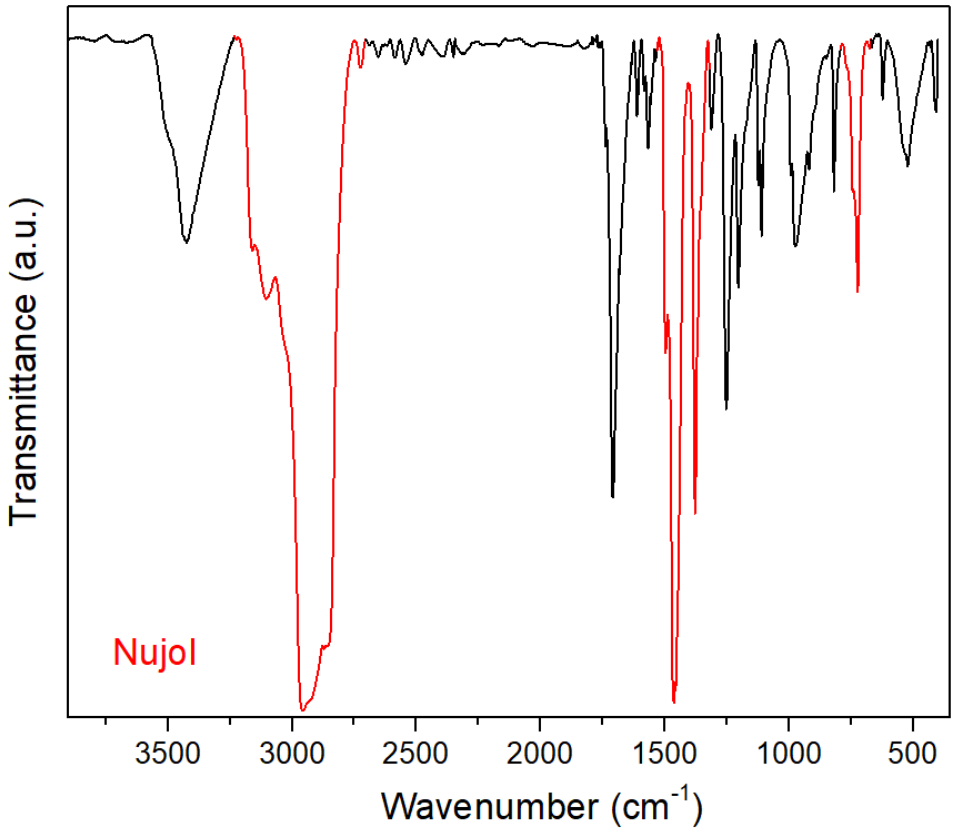

Figure S6. IR spectrum of Br-L

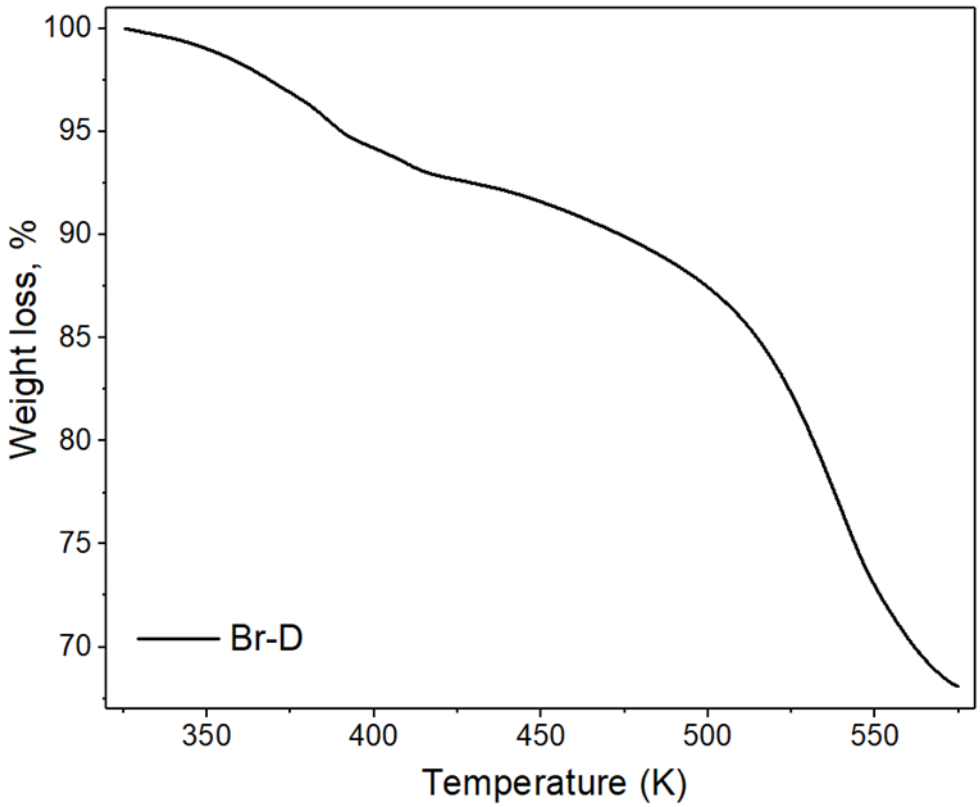

Figure S7. TGA measurements for **Br-D**

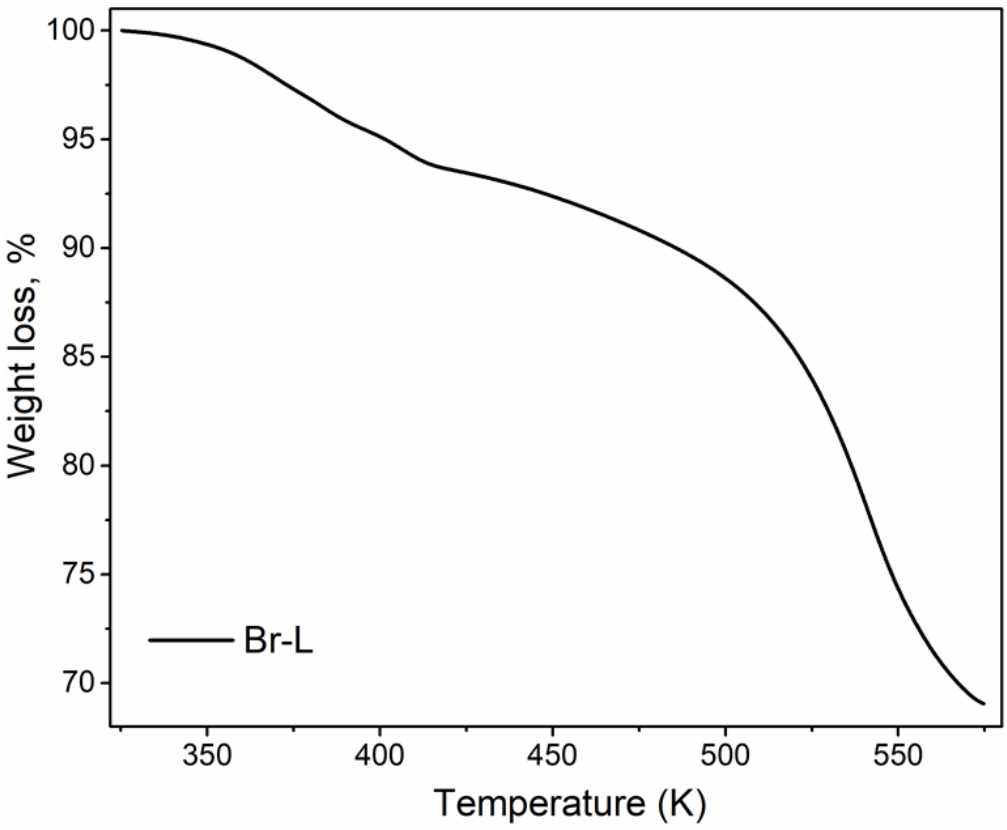

Figure S8. TGA measurements for **Br-L**

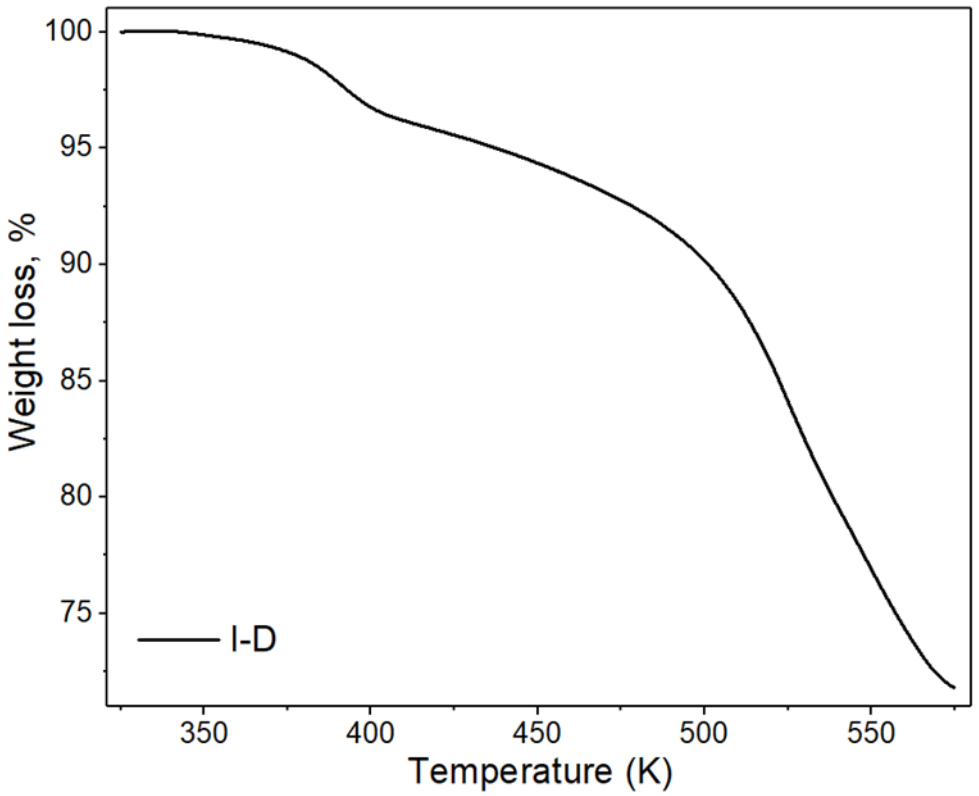

Figure S9. TGA measurements for **I-D**

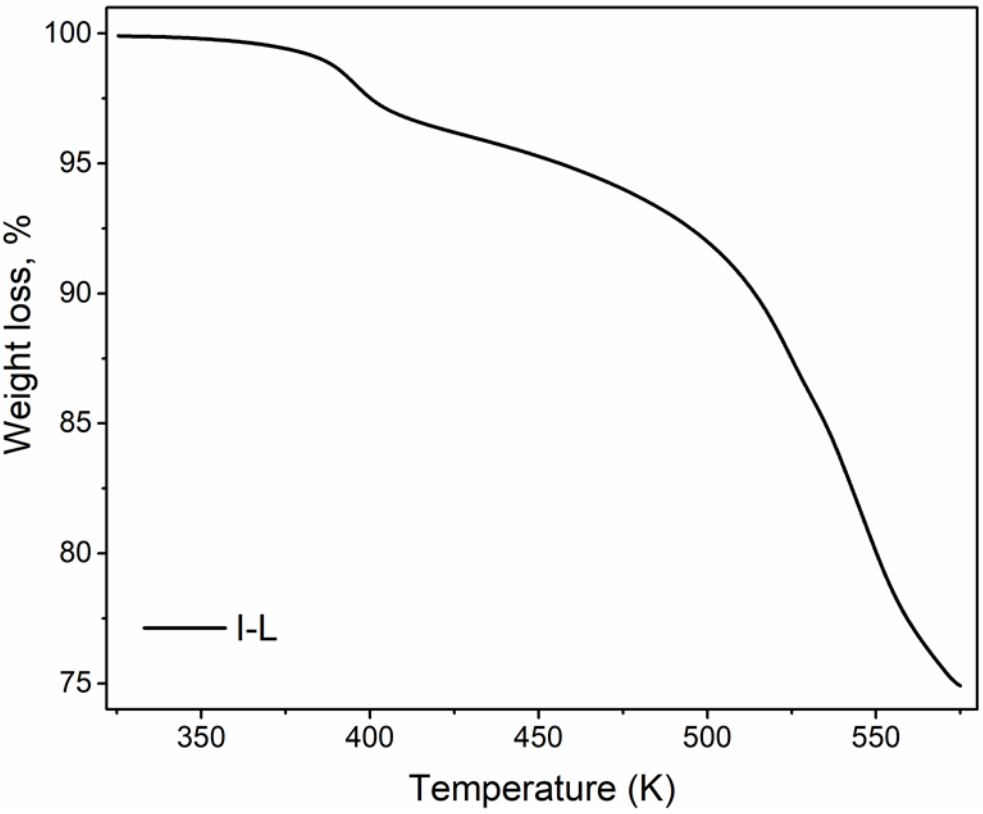

Figure S10 TGA measurements for **I-L**

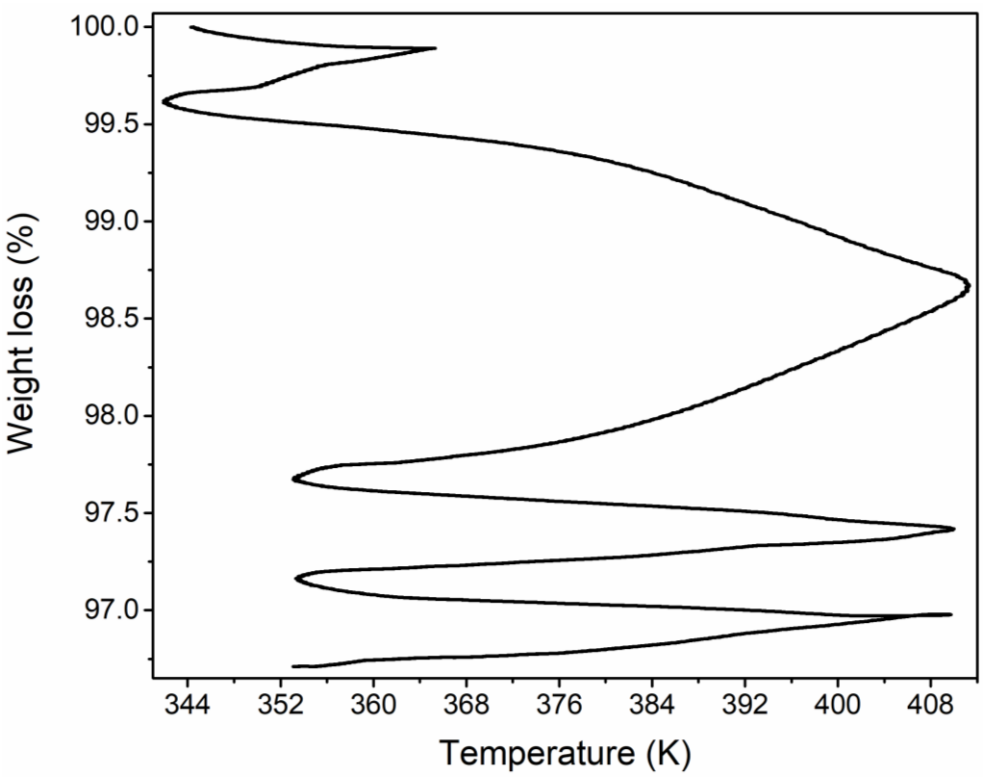

Figure S11. TGA measurements for **I-L** in repeated cycles

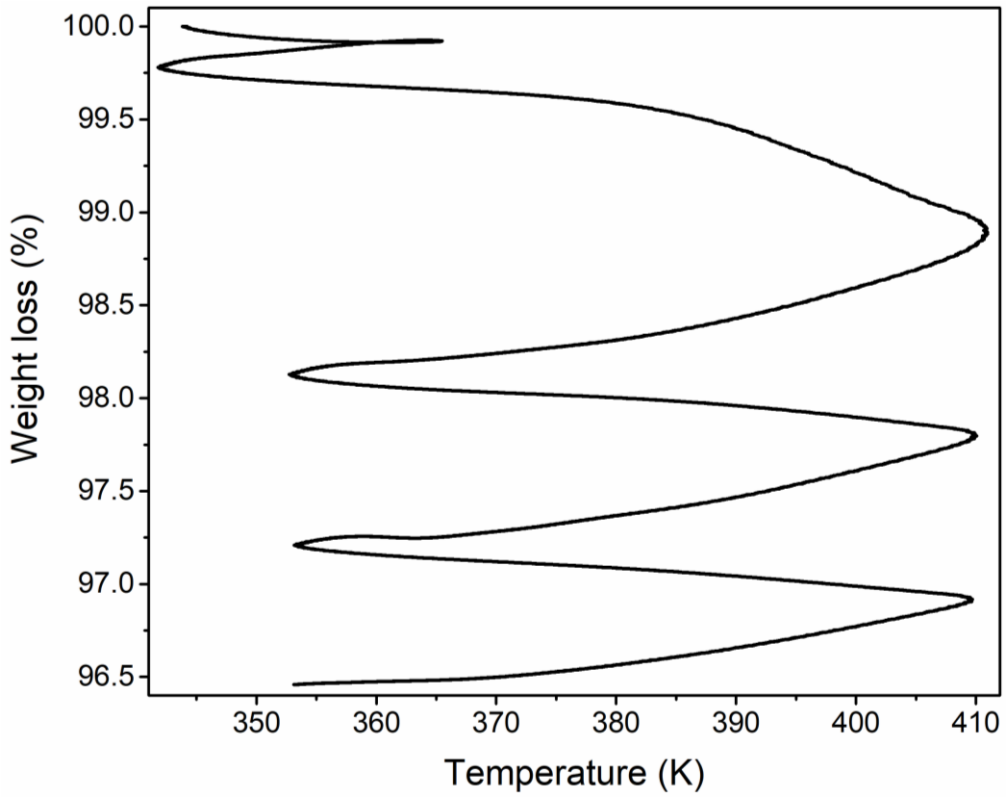

Figure S12. TGA measurements for **Br-L** in repeated cycles