

Electronic Supplementary Information

Cationic and Anionic 1-D Chains Based on $\text{NH}^+ \cdots \text{N}$ Charge-Assisted Hydrogen Bond in Bipyridyls Derivatives and Polyiodides

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Figure S1. View of the packing diagram of $(\text{Q}_2\text{S}_2 \cdot \text{I}_2)_n$ along [010]. pg. S2

Figure S2. View of the asymmetric unit of compound $(\text{HL2})\text{IBr}_2$. S3

Table S1. Selected bond distances (Å) for compounds $\text{L1} \cdot 2\text{I}_2$, $(\text{HL1})\text{I}_3$, $(\text{HL2})\text{I}_3$, $(\text{HL1})\text{IBr}_2$, $(\text{HL2})\text{IBr}_2$, and $(\text{HL1})\text{I}_5$. S4

Table S2. Selected bond angles (°) for compounds $\text{L1} \cdot 2\text{I}_2$, $(\text{HL1})\text{I}_3$, $(\text{HL2})\text{I}_3$, $(\text{HL1})\text{IBr}_2$, $(\text{HL2})\text{IBr}_2$, and $(\text{HL1})\text{I}_5$. S5

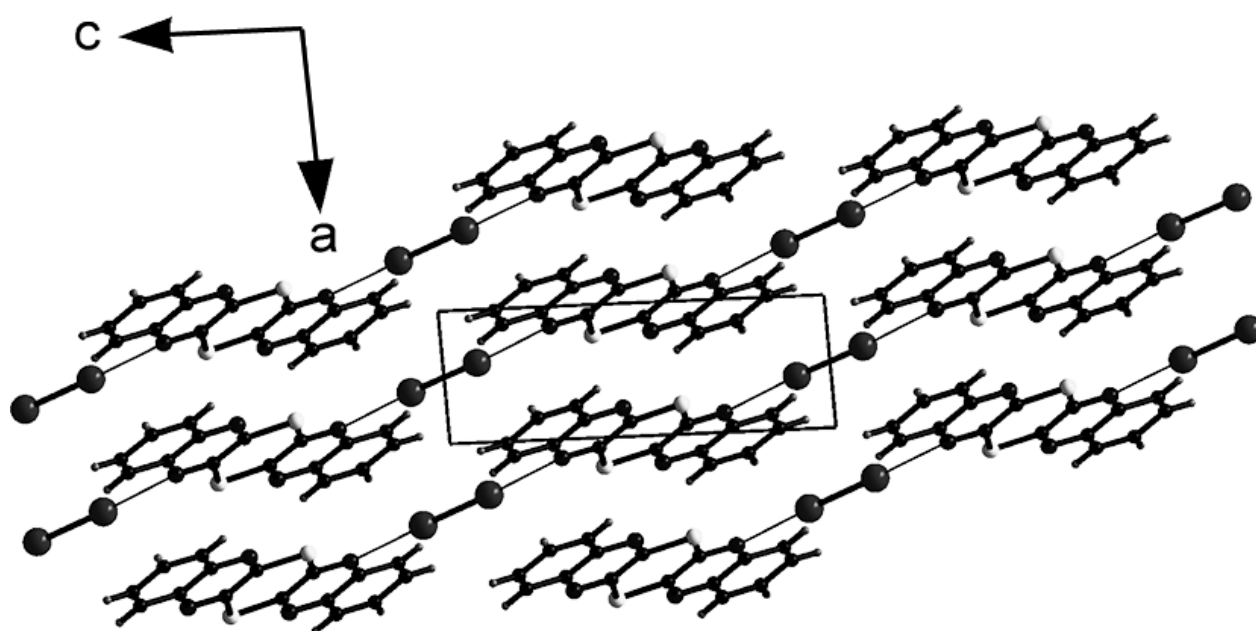


Figure S1 View of the packing diagram of $(Q_2S_2 \cdot I_2)_n$ along $[010]$. [$Q_2S_2 = bis(\text{quinoxaline})\text{-}2,2',3,3'\text{-disulfide}$]. F. Isaia et al., *Eur. J. Inorg. Chem.*, 2009 2667–2672.

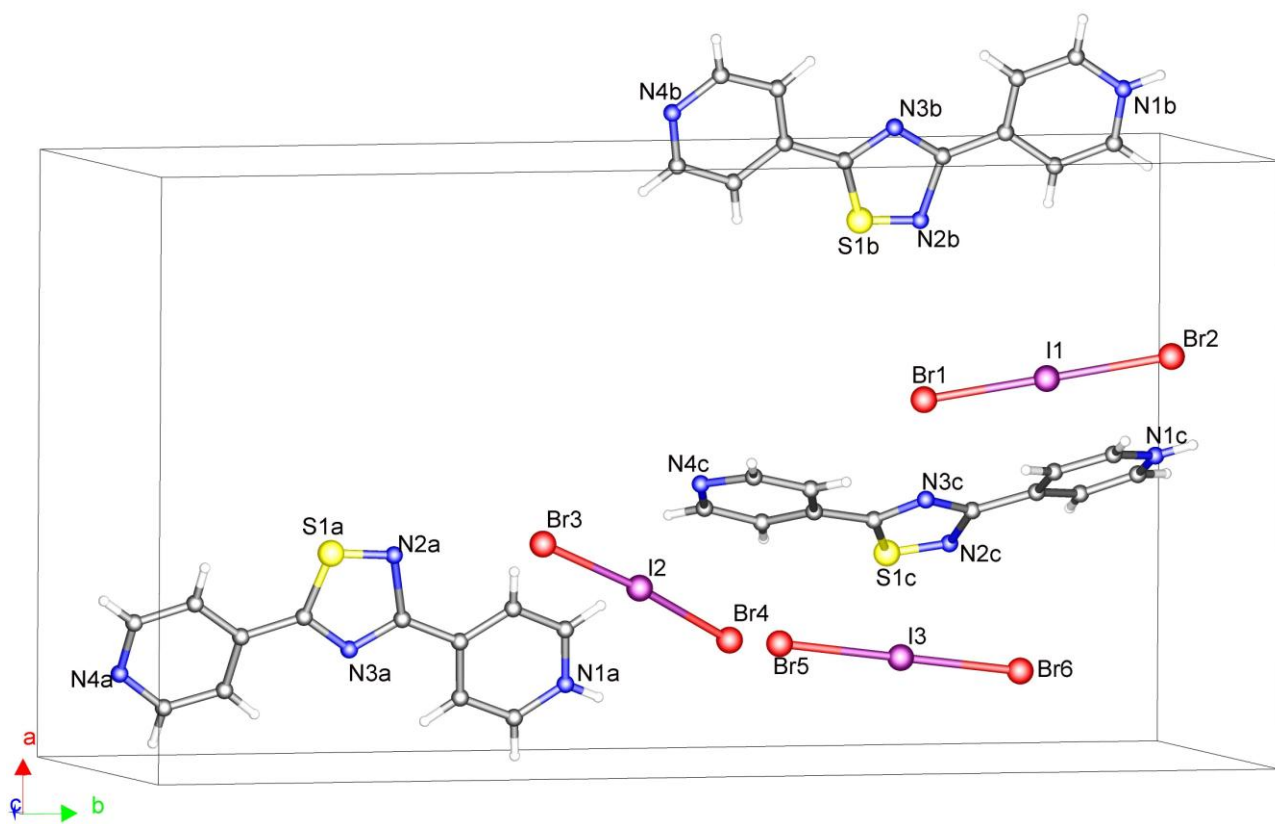


Figure S2 View of the asymmetric unit of compound **(HL2)IBr₂**.

Table S1 Selected bond distances (Å) for compounds **L1-2I₂**, **(HL1)I₃**, **(HL2)I₃**, **(HL1)IBr₂**, **(HL2)IBr₂**, and **(HL1)I₅**.

	L1-2I₂	(HL1)I₃	(HL2)I₃	(HL1)IBr₂	(HL2)IBr₂	(HL1)I₅
N1—C1/C3 ^b	1.336(7)	1.320(7)	1.307(7) ^a	1.335(7)	1.355(13) ^a	1.308(6)
N1—C2	1.328(7)	1.331(8)	1.331(7) ^a	1.334(7)	1.332(13) ^a	1.334(6)
N2/S'—C6	1.578(6)	1.387(7)	1.666(5) ^a	1.526(6)	1.656(11) ^a	1.501(6)
N3—C6	1.345(7)	1.363(7)	1.318(6) ^a	1.344(7)	1.350(12) ^a	1.340(6)
N3—C7		1.314(7)	1.354(6) ^a	1.343(7)	1.341(13) ^a	1.315(6)
N4—C11		1.344(8)	1.346(6) ^a	1.342(8)	1.352(14) ^a	1.330(7)
N4—C12/C10 ^b		1.321(7)	1.317(7) ^a	1.338(7)	1.355(14) ^a	1.305(6)
N1—H		0.86		0.86	0.86	0.86
N1—I1	2.505(5)					
S—N2	1.505(5)	1.573(5)	1.520(3) ^a	1.520(4)	1.379(7) ^a	1.482(4)
S—C7		1.713(5)	1.487(6) ^a	1.668(6)	1.637(11) ^a	1.662(5)
I1—I2	2.761(1)	2.931(1)	2.919(2)			2.864(1)
I2—I3			2.891(2)			2.968(1)
I3—I4		2.932(1)				3.232(1)
I4—I5			2.872(2)			2.761(1)
I5—I6			2.969(2)			
I1—Br1				2.733(1)	2.717(1)	
I1—Br2				2.695(1)	2.761(1)	
I2—Br3					2.713(1)	
I2—Br4					2.738(1)	
I3—Br5					2.805(1)	
I3—Br6					2.747(1)	

^a Average of the corresponding distances in the different independent molecules; ^b Numbering scheme relative to **L2**

Table S2 Selected bond angles (°) for compounds **L1-2I₂**, **(HL1)I₃**, **(HL2)I₃^a**, **(HL1)IBr₂**, **(HL2)IBr₂^a**, and **(HL1)I₅**.

	L1-2I₂	(HL1)I₃	(HL2)I₃^a	(HL1)IBr₂	(HL2)IBr₂^a	(HL1)I₅
N1—C2—C3/N1—C2—C1 ^b	122.2(6)	121.7(6)	121.9(5) ^a	119.2(6)	122.1(10) ^a	118.9(6)
N1—C1—C5/N1—C3—C4 ^b	122.3(6)	123.4(6)	124.15(4) ^a	120.8(5)	121.0(9) ^a	121.9(5)
N2—C6—C5	126.2(4)	123.3(5)	125.9(4) ^a	123.7(5)	125.5(8) ^a	124.4(5)
N2—C6—N3	114.4(4)	116.7(5)	113.0(3) ^a	115.0(5)	112.2(7) ^a	114.6(5)
N3—C6—C5	119.4(5)	120.0(5)	121.0(4) ^a	121.3(5)	122.4(8) ^a	121.0(4)
N3—C7—C8	-	123.0(5)	117.0(4) ^a	125.6(4)	121.9(9) ^a	123.3(5)
N4—C11—C10/N4—C11—C12 ^b	-	121.8(6)	120.8(4) ^a	122.8(6)	122.0(9) ^a	122.4(6)
N4—C12—C8/N4—C10—C9 ^b	-	121.7(5)	123.7(5) ^a	122.9(5)	120.3(9) ^a	123.8(5)
N2—S—C7	-	93.7(3)	106.0(2) ^a	99.6(3)	105.3(5) ^a	98.6(3)
C1—N1—C2/C3—N1—C2 ^b	118.9(5)	119.3(5)	119.1(4) ^a	122.4(5)	119.2(8) ^a	121.8(5)
C6—N3—C7	107.1(6)	108.4(5)	108.0(4) ^a	109.4(5)	108.3(8) ^a	108.5(5)
C11—N4—C12/C11—N4—C10 ^b	-	120.1(5)	119.7(4) ^a	118.4(5)	119.7(8) ^a	118.6(5)
S—C7—C8	-	124.7(4)	122.9(4) ^a	123.7(5)	126.6(8) ^a	124.5(4)
S—C7—N3	-	112.2(4)	115.1(4) ^a	115.0(5)	111.5(8) ^a	112.2(5)
S—N2—C6	102.1(3)	108.9(3)	97.4(2) ^a	104.5(3)	102.8(5) ^a	106.1(3)
N1—I1—I2	179.65(12)	-	-	-	-	-
I2—I1—I2 _a		180.00				
I4—I3—I4 _b		180.00				
I1—I2—I3			176.57(5) ^a			174.38(2)
I2—I3—I4						94.4
Br1—I—Br2				176.91(3)	179.04(5)	
Br3—I2—Br4					174.55(5)	
Br5—I3—Br6					178.49(5)	

^a Average of the crystallographic units; ^b Numbering scheme relative to **L2**