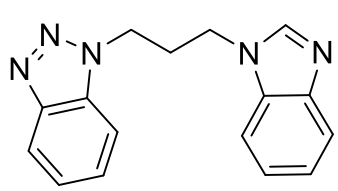
Supporting Information

Highly efficient and very robust blue-excitable yellow phosphors built on multiple-stranded one-dimensional inorganic-organic hybrid chains

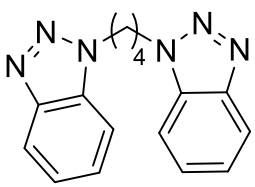
*Yang Fang, Christopher A. Sojdak, Gangotri Dey, Simon J. Teat, Mingxing Li, Mircea Cotlet, Kun Zhu, Wei Liu, Lu Wang, Deirdre M. O´Carroll and Jing Li**

Table of Contents

S1. Characterization of ligands



biprbt



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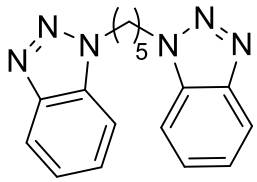
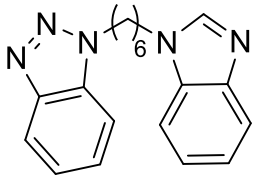
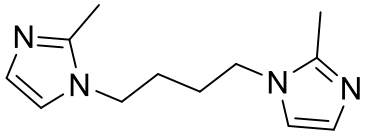


bbtpe



bihebt



bmibu

Figure S1. Ligand structures.

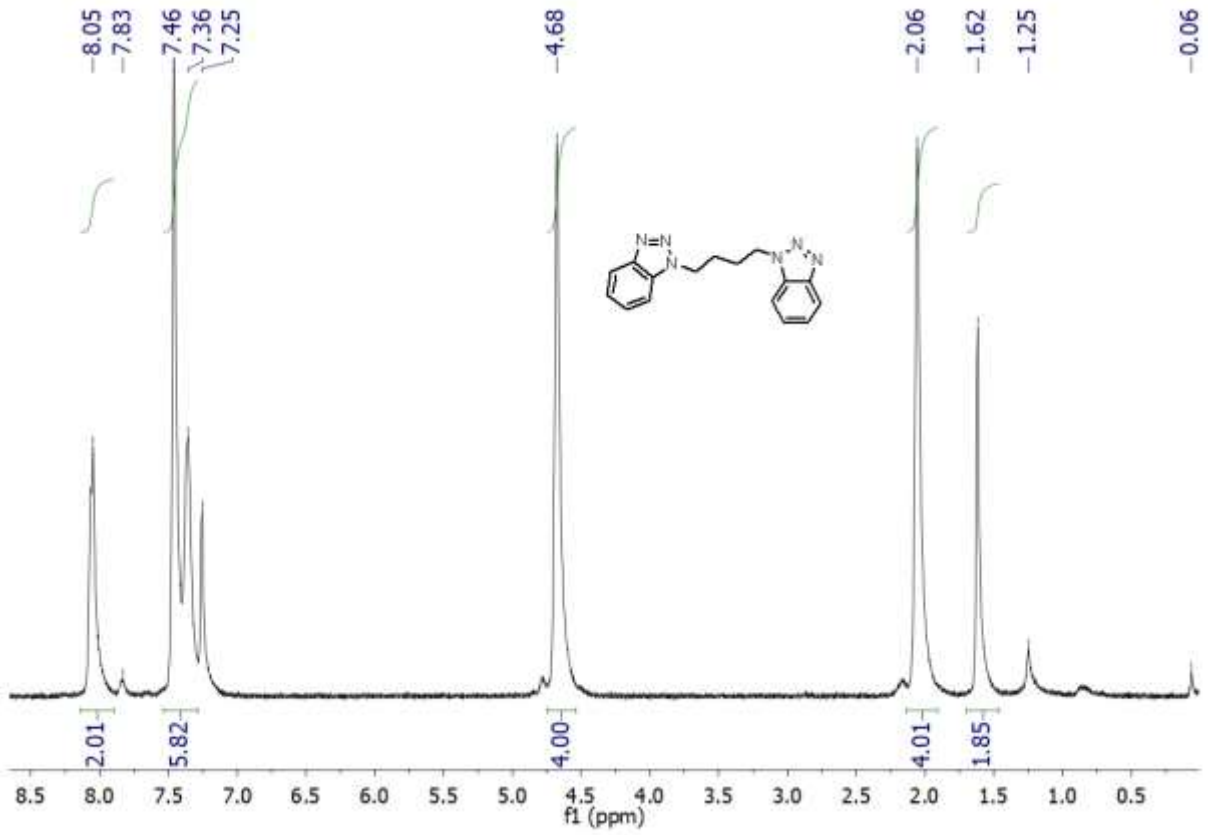


Figure S2. ^{1}H NMR spectrum of *bbtbu*.

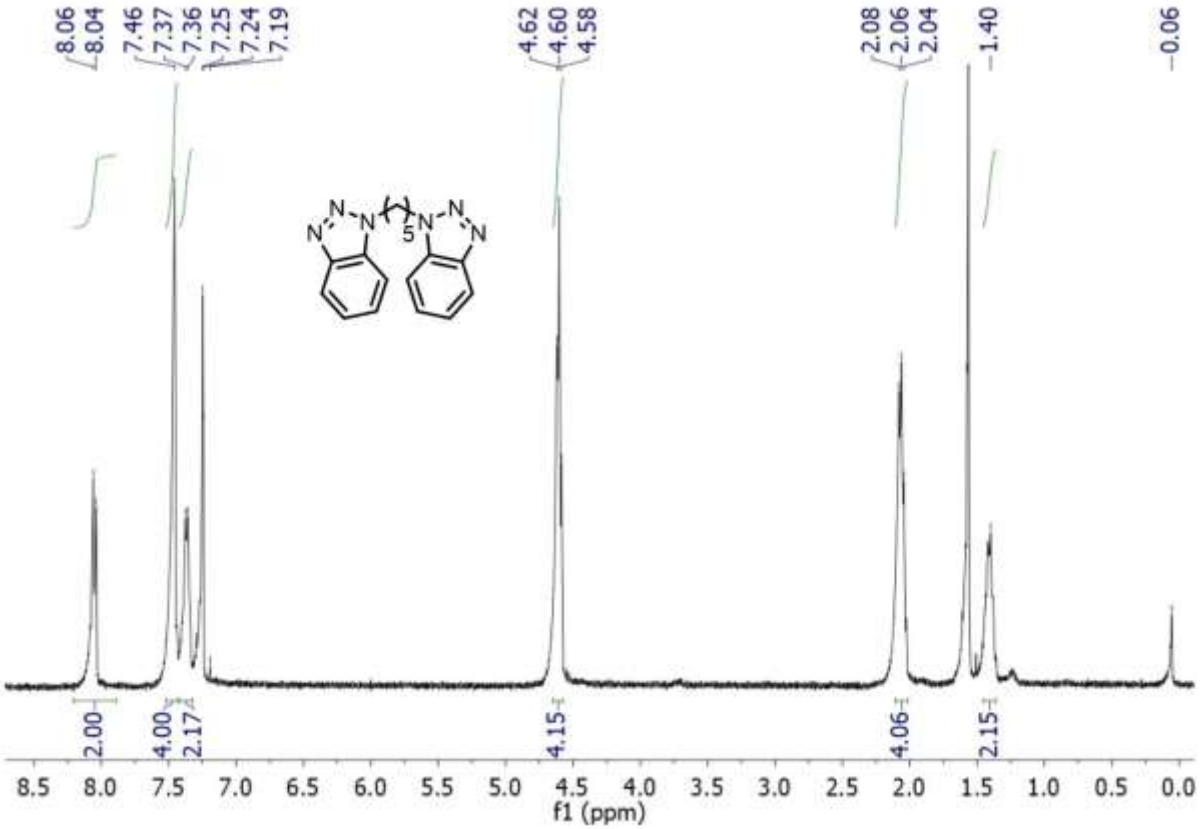


Figure S3. ^{1}H NMR spectrum of *bbtpe*.

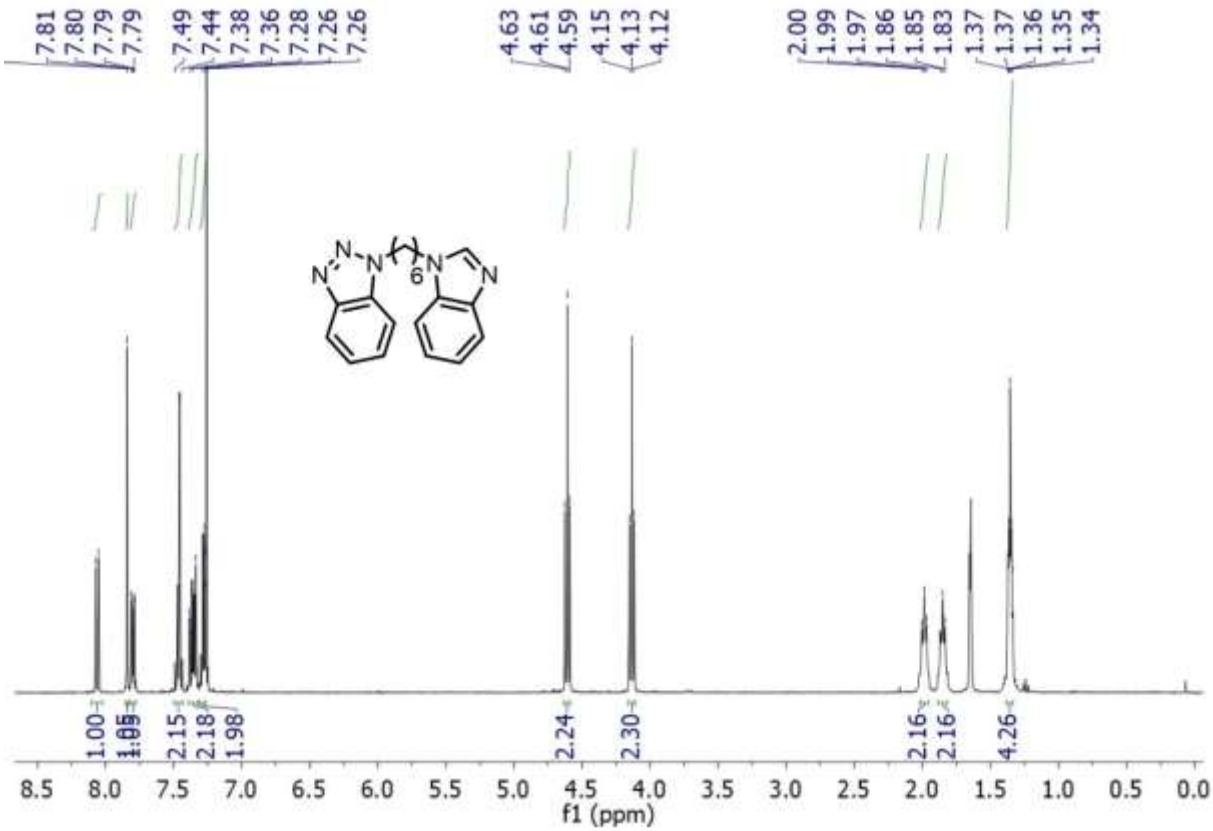


Figure S4. ^{1}H NMR spectrum of *bihebt*.

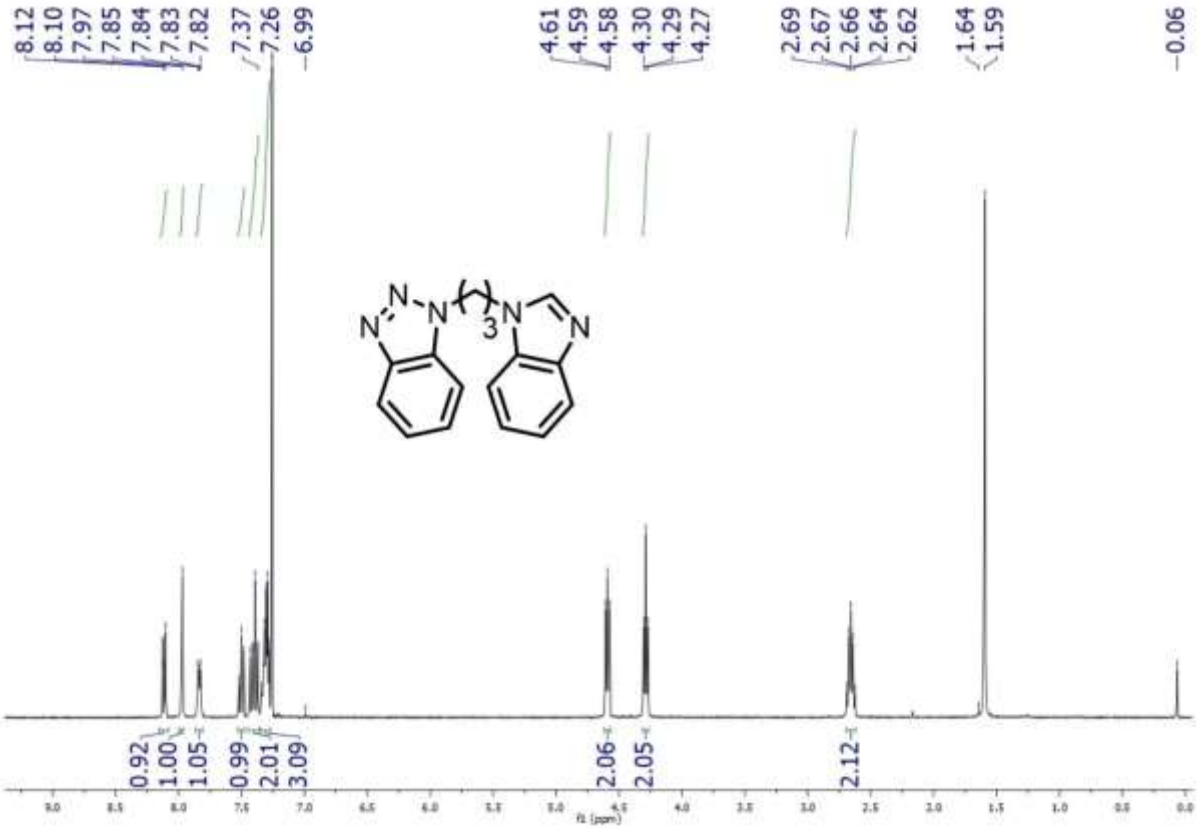


Figure S5. ^{1}H NMR spectrum of *biprbt*.

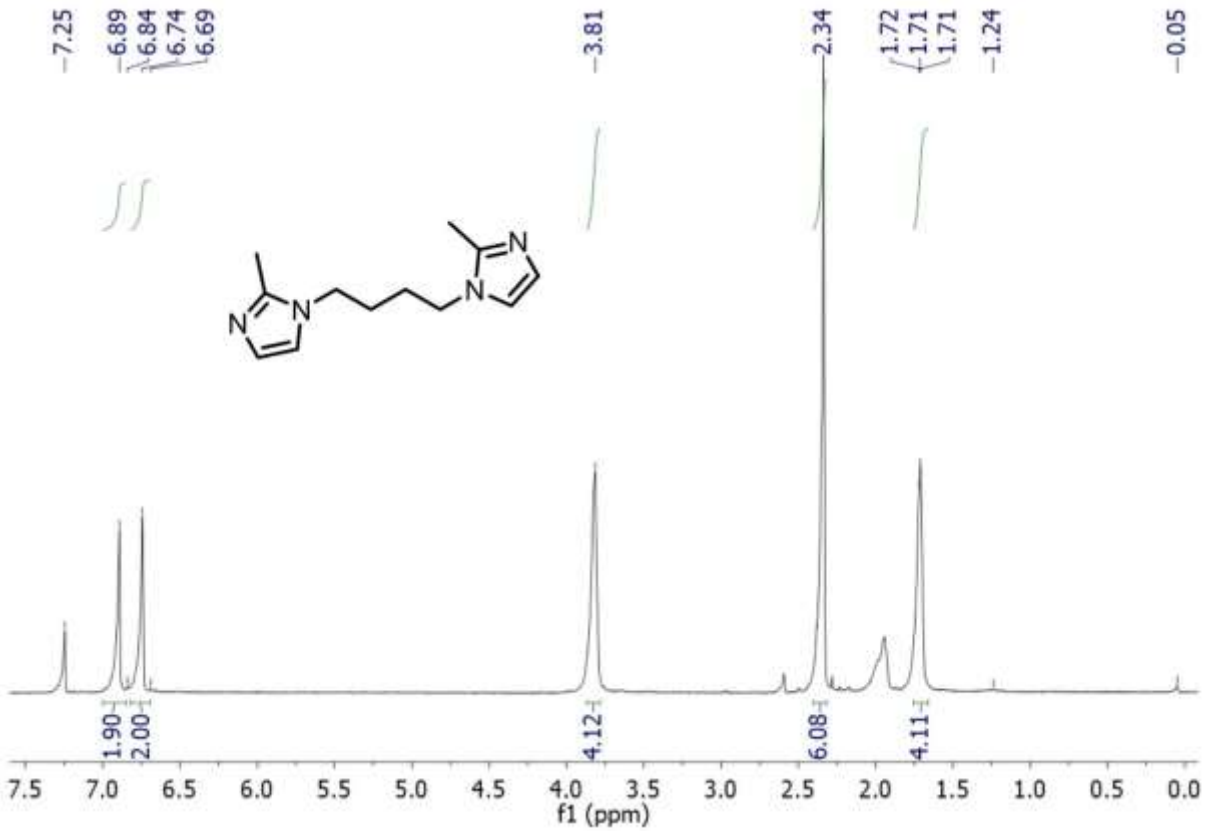


Figure S6. ^{1}H NMR spectrum of *bmibu*.

S2. Crystal images

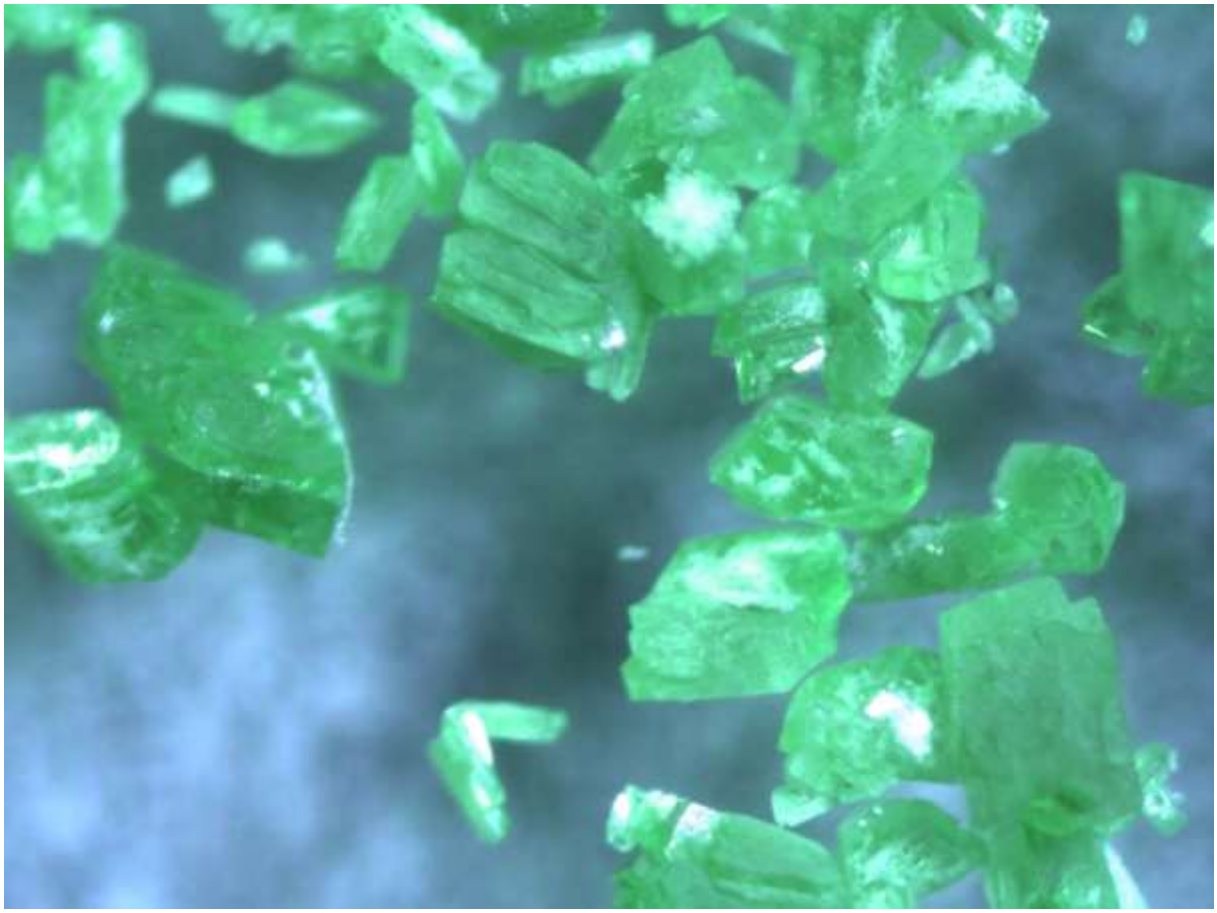


Figure S7. Crystal image of 1D-Cu_2I_2(*biprbt*)$_2$ (**1**).

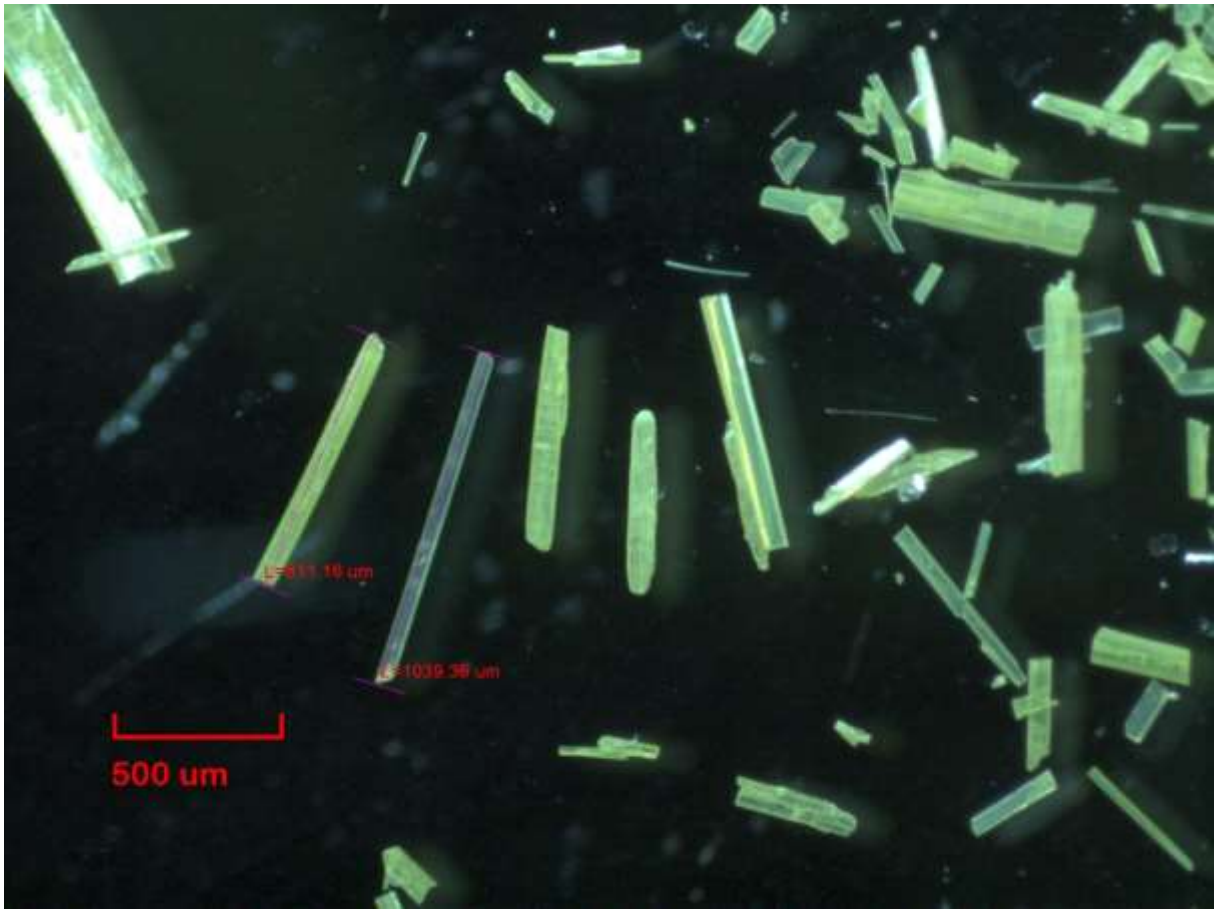


Figure S8. Crystal image of 1D-Cu_2I_2(*bbtbu*)$_2$ (**2**).

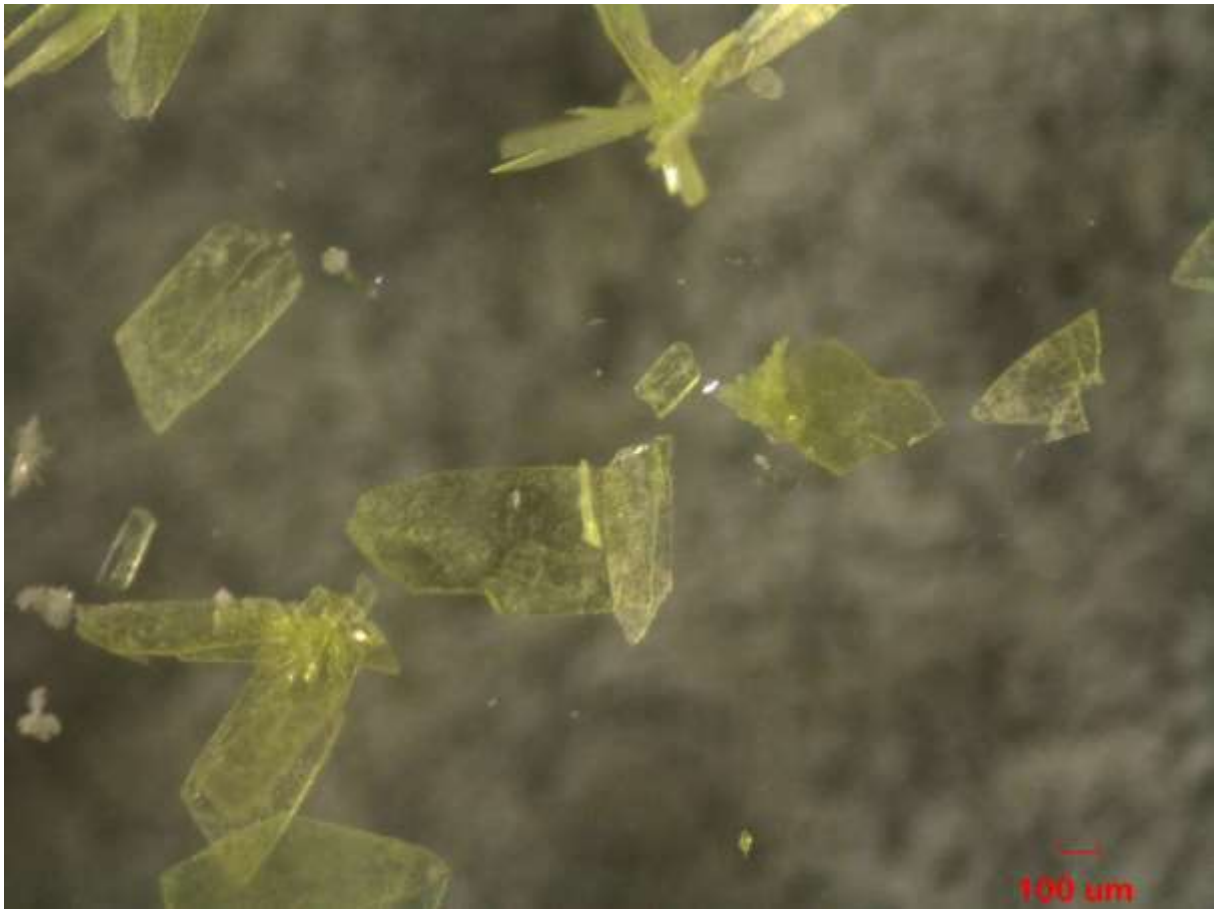


Figure S9. Crystal image of 1D-Cu_2I_2(*bihebt*)$_2$ (**3**).

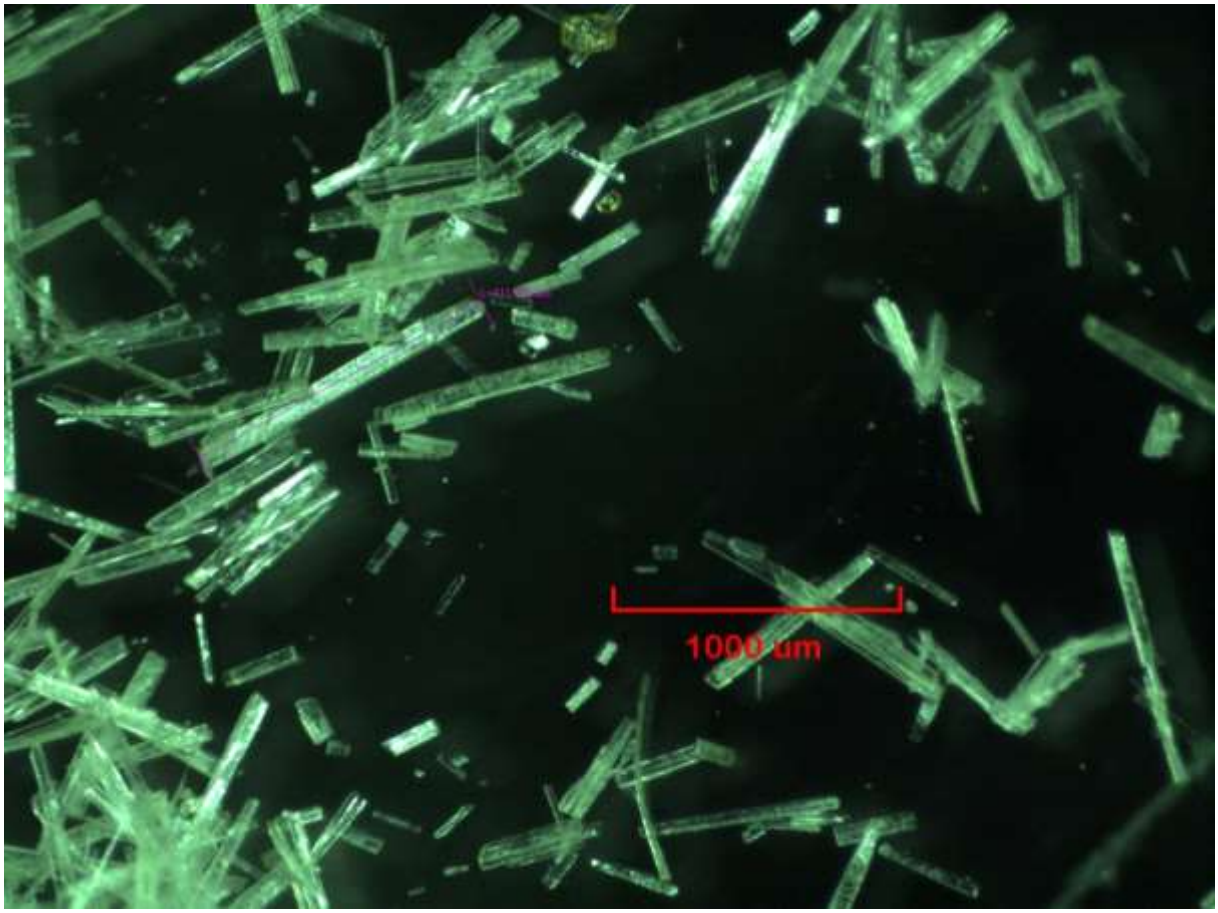


Figure S10. Crystal image of 1D-Cu_2I_2(*bbtpe*)$_2$ (**4**).

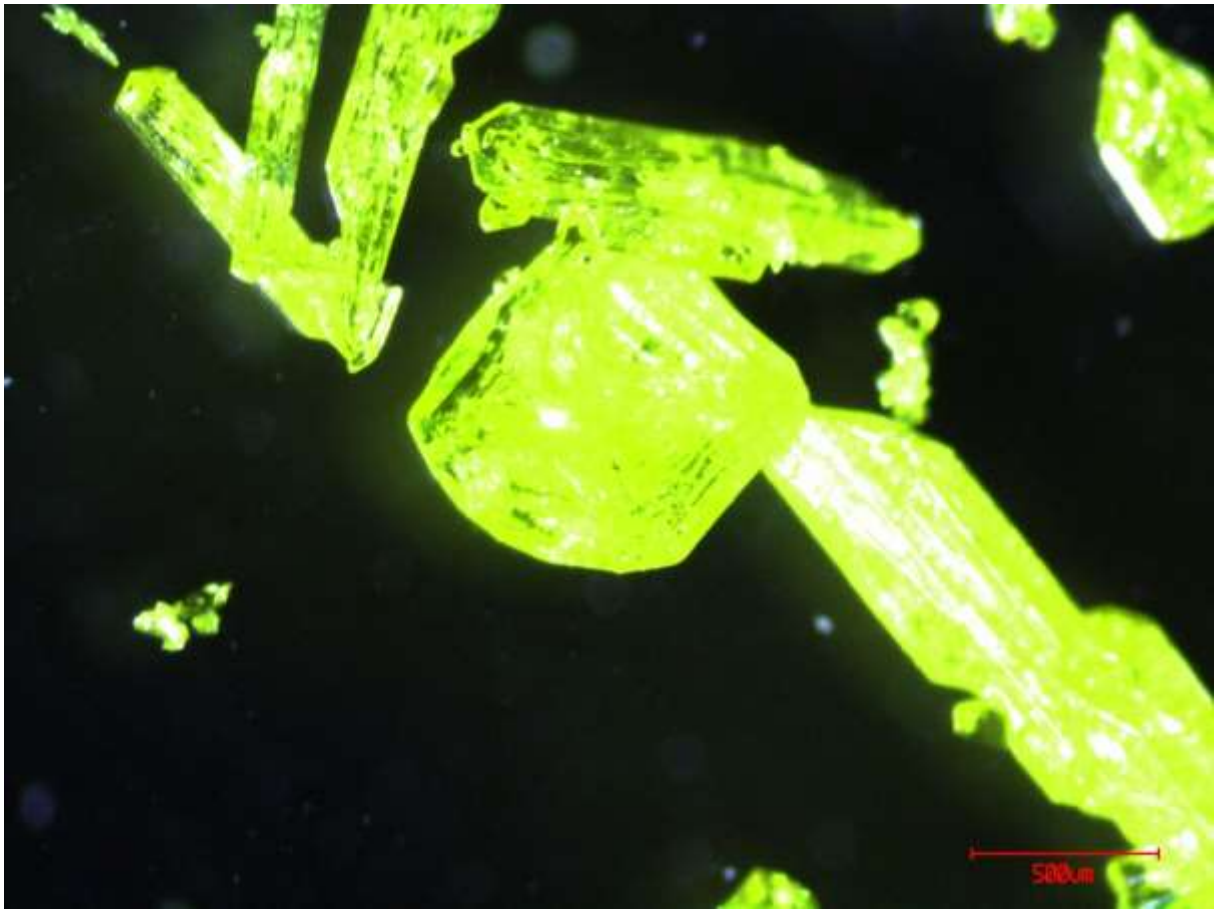


Figure S11. Crystal image of 1D-Cu_4I_4(*bbtpe*)$_2$ (**5**).

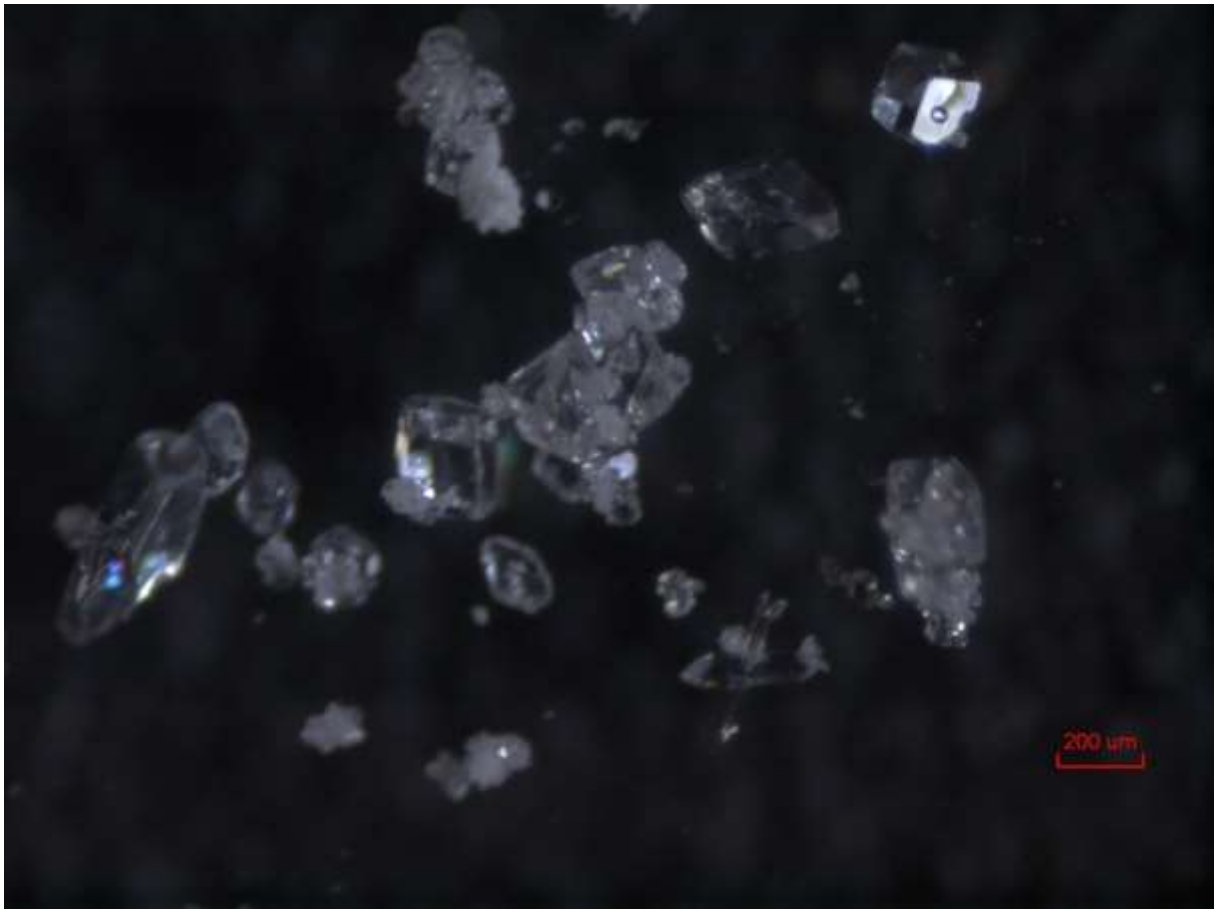


Figure S12. Crystal image of 1D-Cu_6I_6(*bmibu*)$_3$ (**6**).

S3. Structural plots of compounds **1**, **3**, **4**

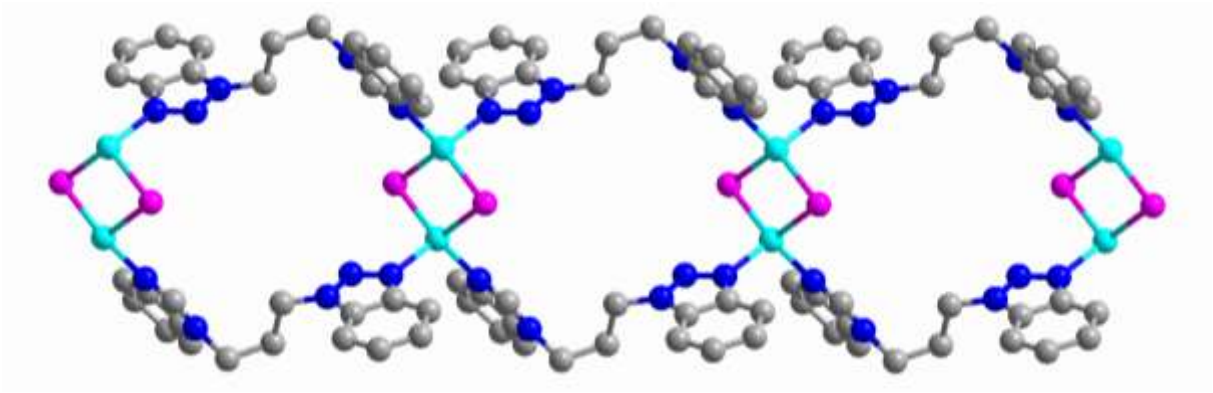


Figure 13. Structure of 1D-Cu_2I_2(*biprbt*) (**1**).

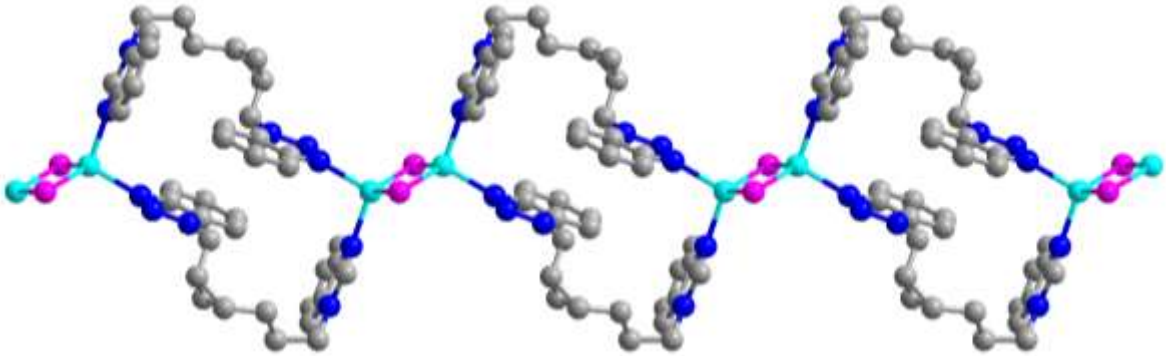


Figure 14. Structure of 1D-Cu_2I_2(*bihebt*) (**3**).

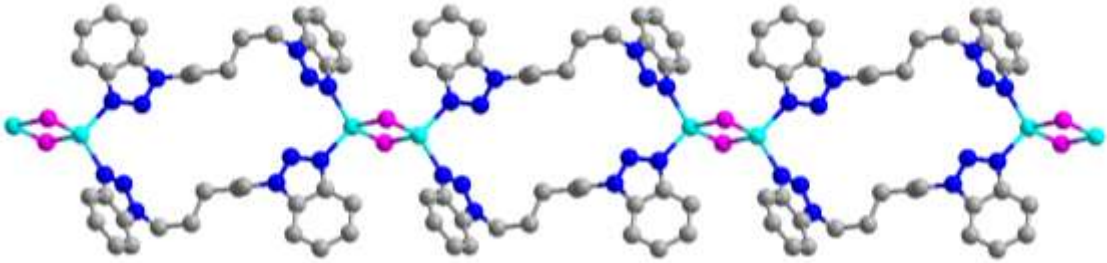


Figure 15. Structure of 1D-Cu_2I_2(*bbtpe*)$_2$ (**4**).

Table S1. Shortest Cu-Cu distances in compounds **1-6**.

Structure	Cu-Cu distance (Å)
1D-Cu_2I_2(*biprbt*)$_2$ (**1**)	2.89
1D-Cu_2I_2(*bbtbu*)$_2$ (**2**)	2.69
1D-Cu_2I_2(*bihebt*)$_2$ (**3**)	2.72
1D-Cu_2I_2(*bbtpe*)$_2$ (**4**)	2.93
1D-Cu_4I_4(*bbtpe*)$_2$ (**5**)	2.61,2.78
1D-Cu_6I_6(*bmibu*)$_3$ (**6**)	2.59, 2.81, 3.06

S4. Powder X-ray diffraction (PXRD) patterns of compounds **1-6**

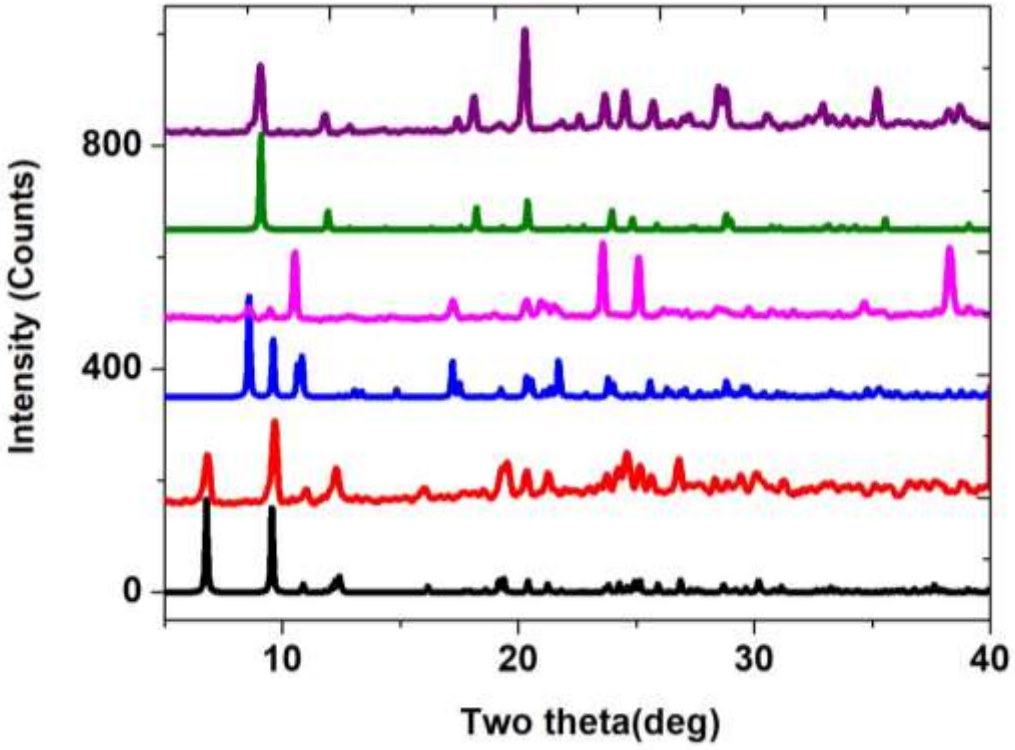


Figure S16. PXRD patterns of compounds **2**, **4**, **5**. From bottom to top: simulated **5**, experimental **5**, simulated **4**, experimental **4**, simulated **2**, and experimental **2**.

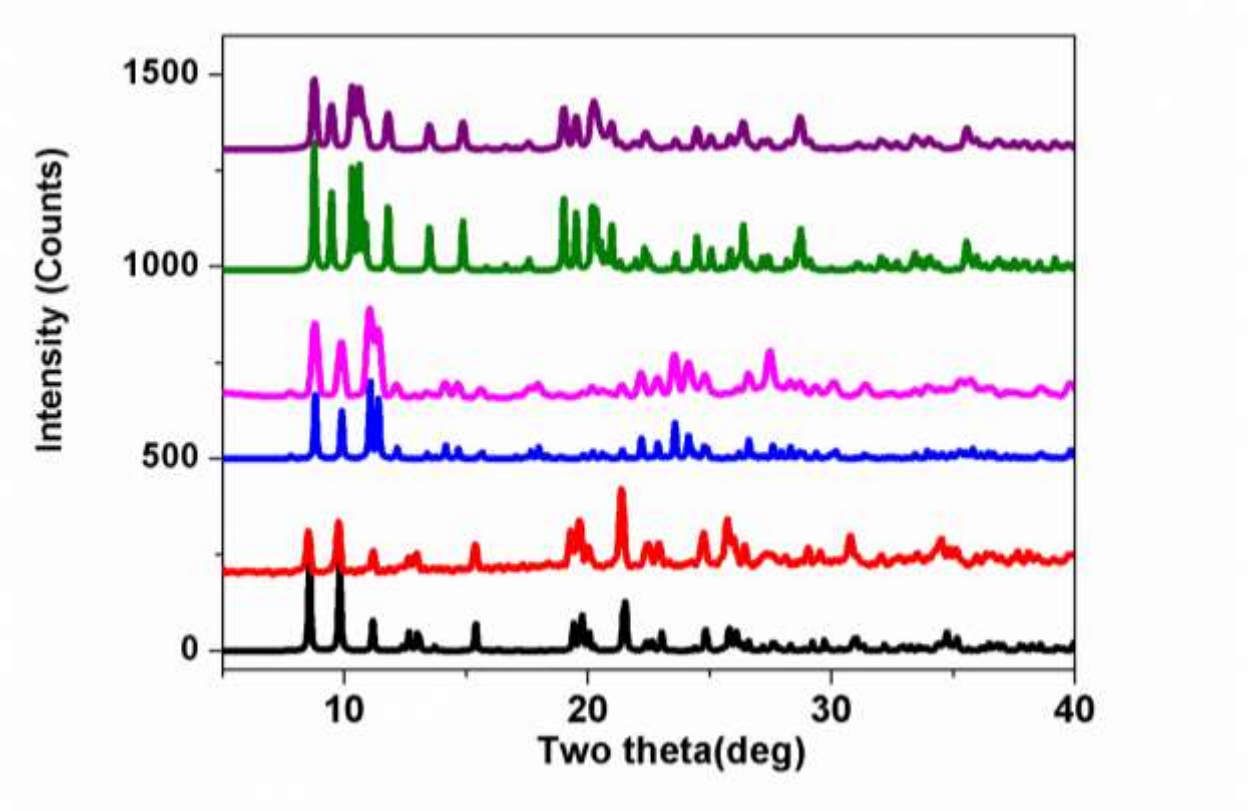


Figure S17. PXRD patterns of compounds **1**, **3**, **6**. From bottom to top: simulated **1**, experimental **1**, simulated **6**, experimental **6**, simulated **3**, and experimental **3**.

S5. Thermogravimetric (TG) analysis of compounds **1**-**6**

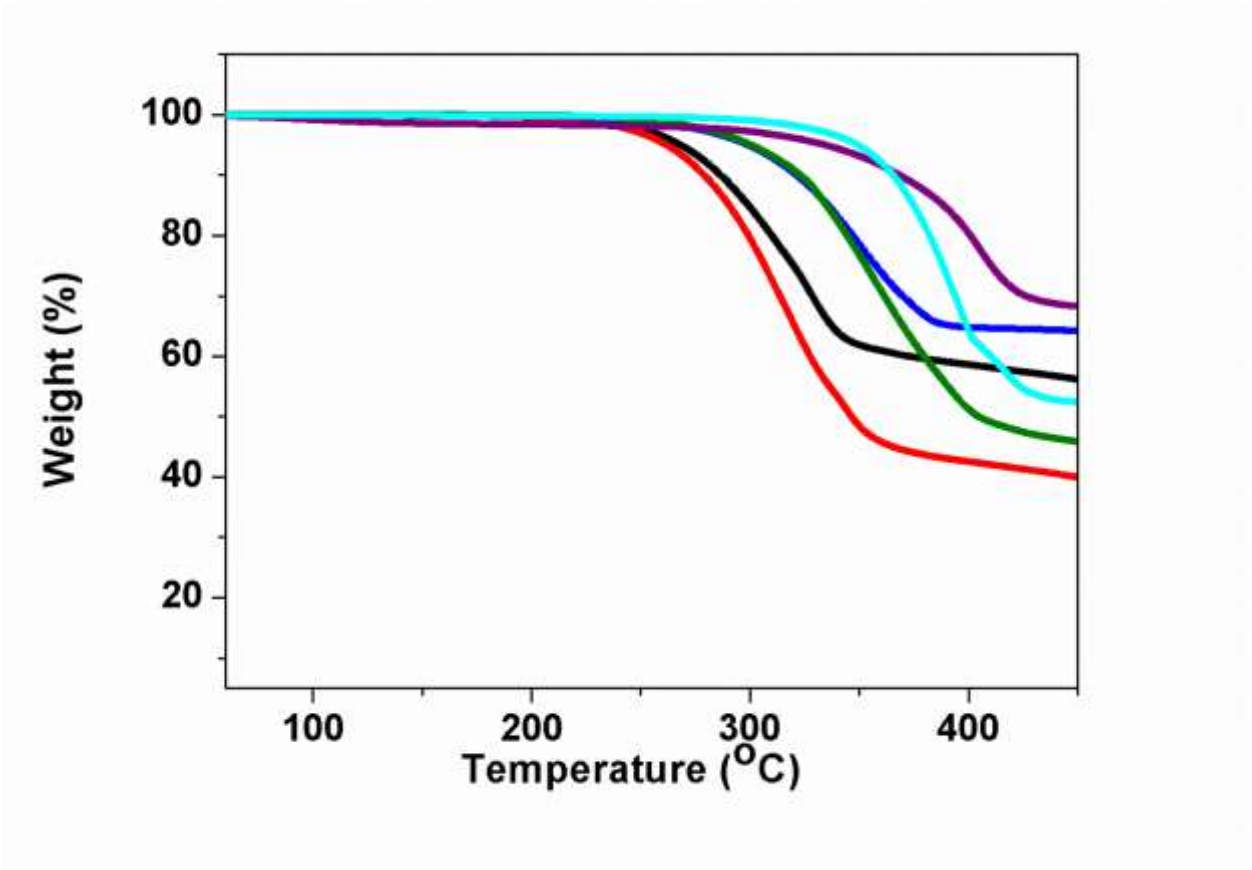


Figure S18. TG plots of **1** (olive), **2** (blue), **3** (cyan), **4** (red), **5** (black), **6** (purple).

S6. Long-term stability tests of compounds **1** and **5**

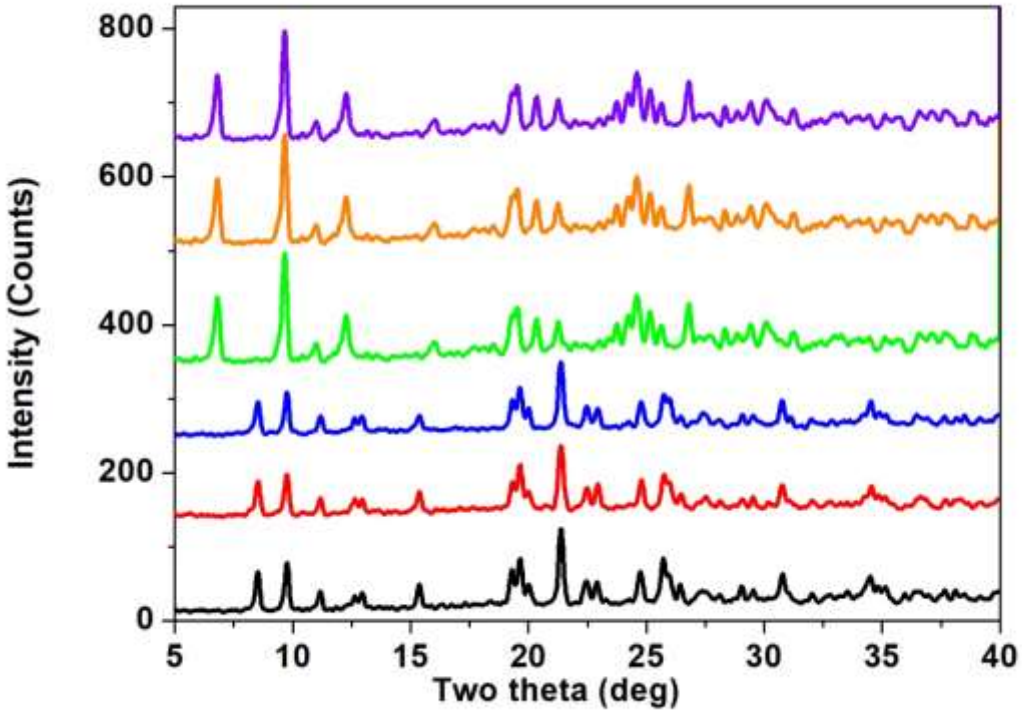


Figure S19. PXRD patterns of compounds **1**, **5** after long-term stability tests. From bottom to top: Sample **1** before and after thermal stability tests, **1** after photostability test; sample **5** before and after thermal stability tests, and **5** after photostability test.

S7. Electronic band structure (BS) and density of states (DOS) calculations of selected structures

The BS and DOS of selected structures were calculated using CASTEP package (Materials Studio 5.1). Generalized gradient approximations (GGA) with Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional (xc) were used in all calculations.

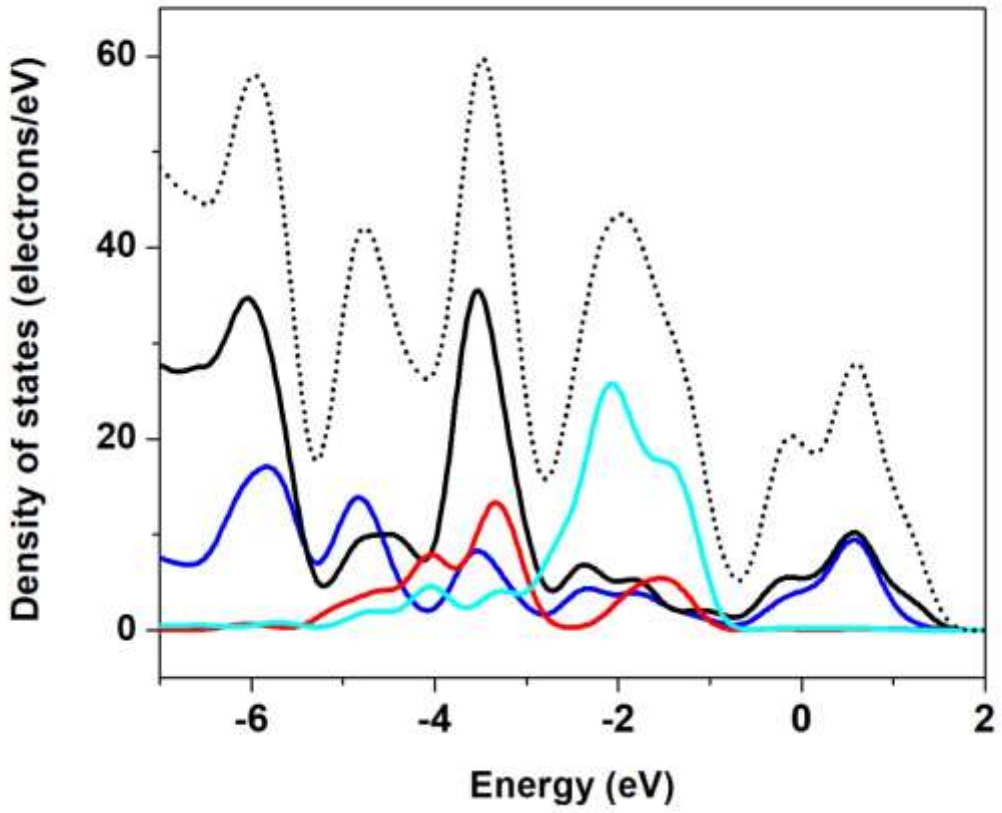


Figure S20. Calculated density of states (DOS) for 1D-Cu_2I_2(*bbtbu*)$_2$ (**2**). Line color scheme: total DOS (dashed black), Cu 3d orbitals (cyan), I 5p orbitals (red), N 2p orbitals (blue), C 2p orbitals (black).

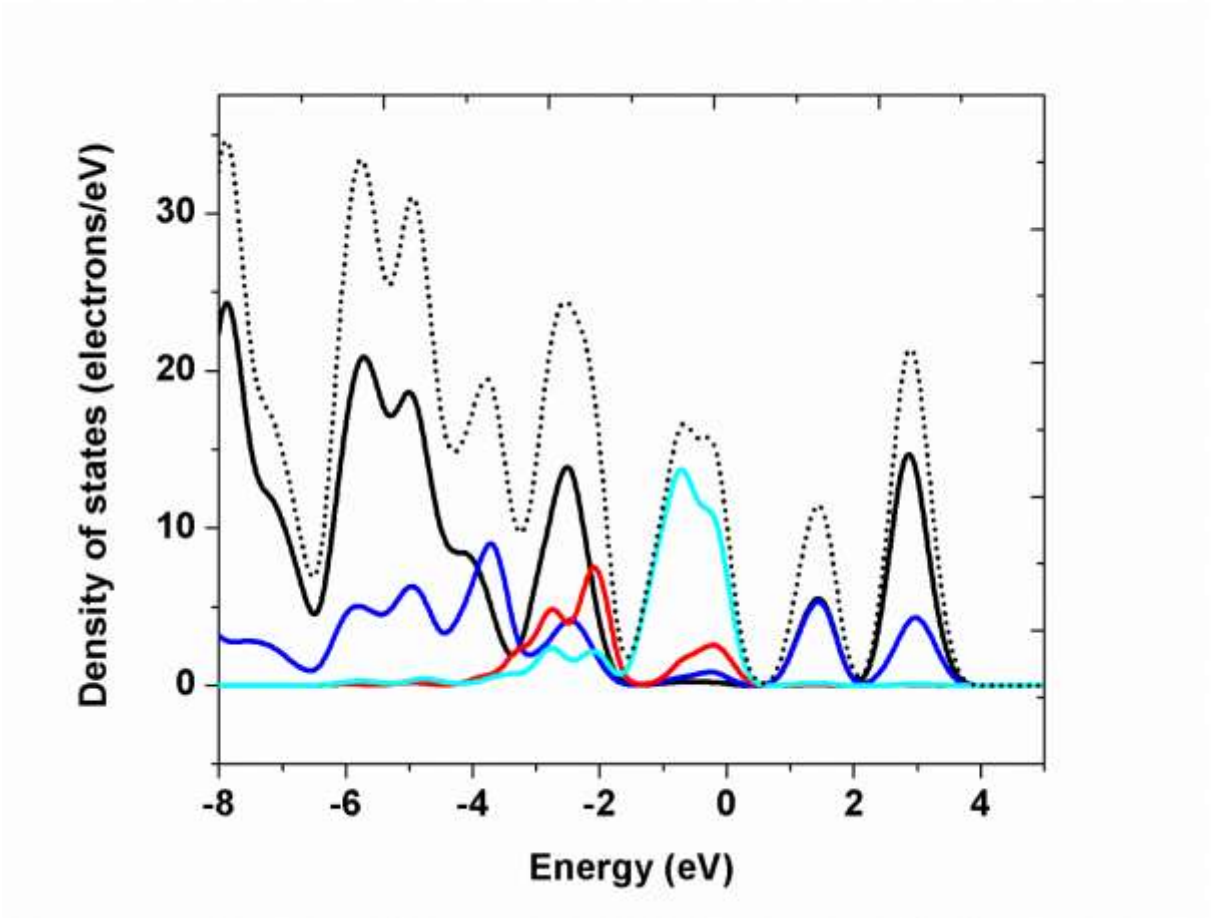


Figure S21. Calculated density of states (DOS) for 1D-Cu_2I_2(*bbtpe*)$_2$ (**4**). Line color scheme: total DOS (dashed black), Cu 3d orbitals (cyan), I 5p orbitals (red), N 2p orbitals (blue), C 2p orbitals (black).

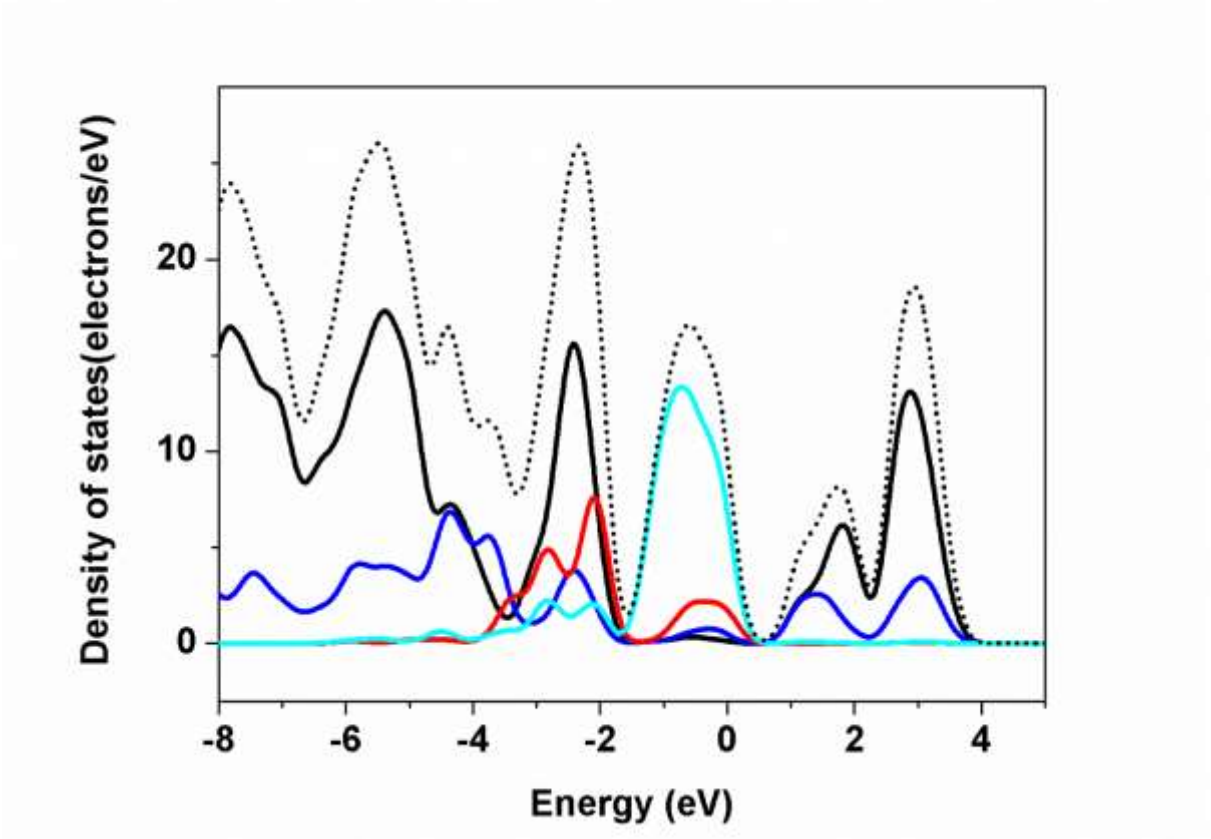


Figure S22. Calculated density of states (DOS) for 1D-Cu_2I_2(*biprbt*)$_2$ (**1**). Line color scheme: total DOS (dashed black), Cu 3d orbitals (cyan), I 5p orbitals (red), N 2p orbitals (blue), C 2p orbitals (black).

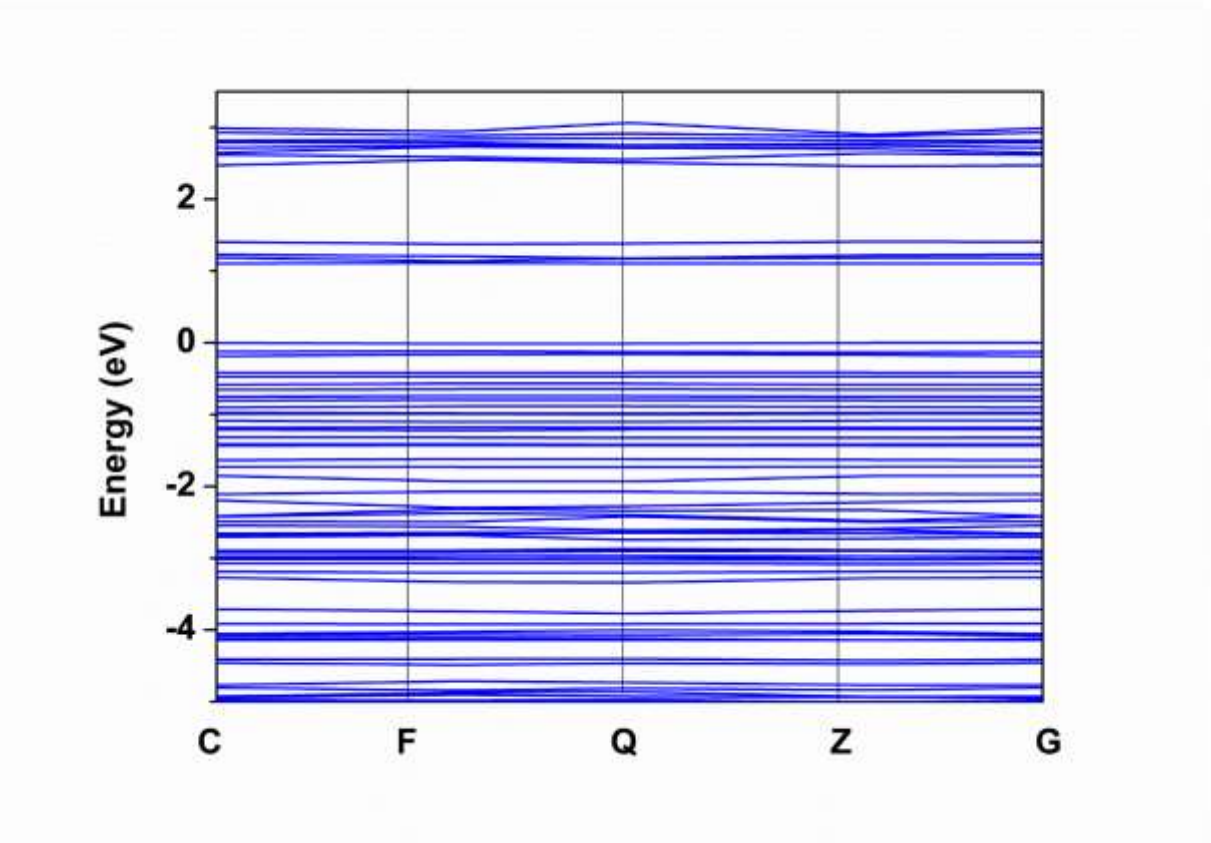


Figure S23. Calculated band structure (BS) for 1D-Cu_4I_4(*bbtpe*)$_2$ (**5**).

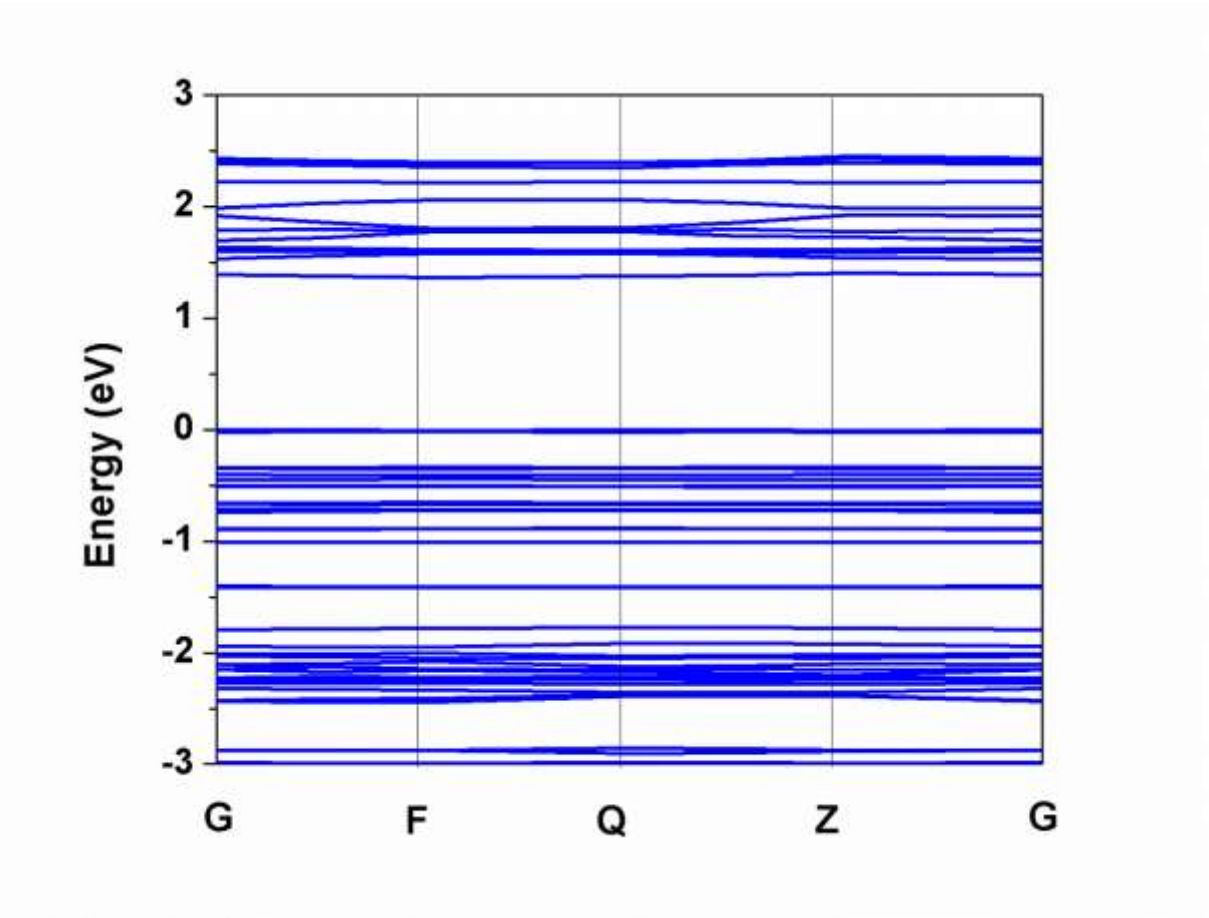


Figure S24. Calculated band structure (BS) for 1D-Cu_2I_2(*bbtpe*)$_2$ (**4**).

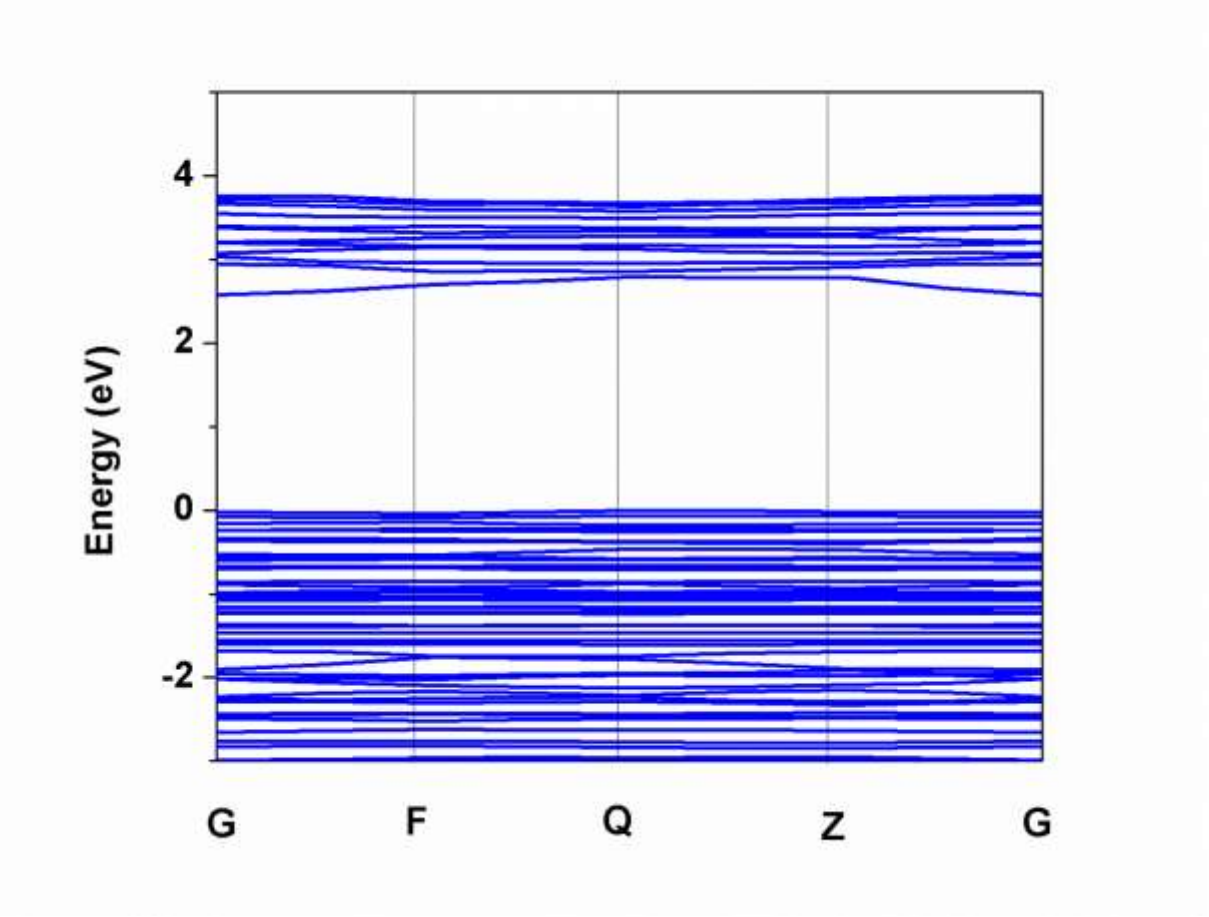


Figure S25. Calculated band structure (BS) for 1D-Cu_6I_6(*bmibu*)$_3$ (**6**).

Table S2. Binding energy calculation summary.

Compound	Total Energy (eV)	E(Cu_2I_2) (eV)	E(Ligand) (eV)	E(tpp) (eV)	E(B.E) (eV)
1D-Cu_2I_2(*bbtpe*)$_2$	-21249.38	-2975.97	-4566.75	/	-1.60 (Cu-N)
1D-Cu_2I_2(*tpp*)$_2$(*4,4'-bpy*)	-13796.18	-2975.43	-2208.07	-3198.70	-1.29 (Cu-N)
1D-Cu_2I_2(*tpp*)$_2$(*pz*)	-11814.78	-2975.43	-1217.30	-3198.70	-1.36 (Cu-N)
0D-Cu_2I_2(*tpp*)$_3$	-12578.74	-2975.70	/	-3198.70	-2.31 (Cu-P)

S8. Emission spectra, luminescence decay profiles and related data

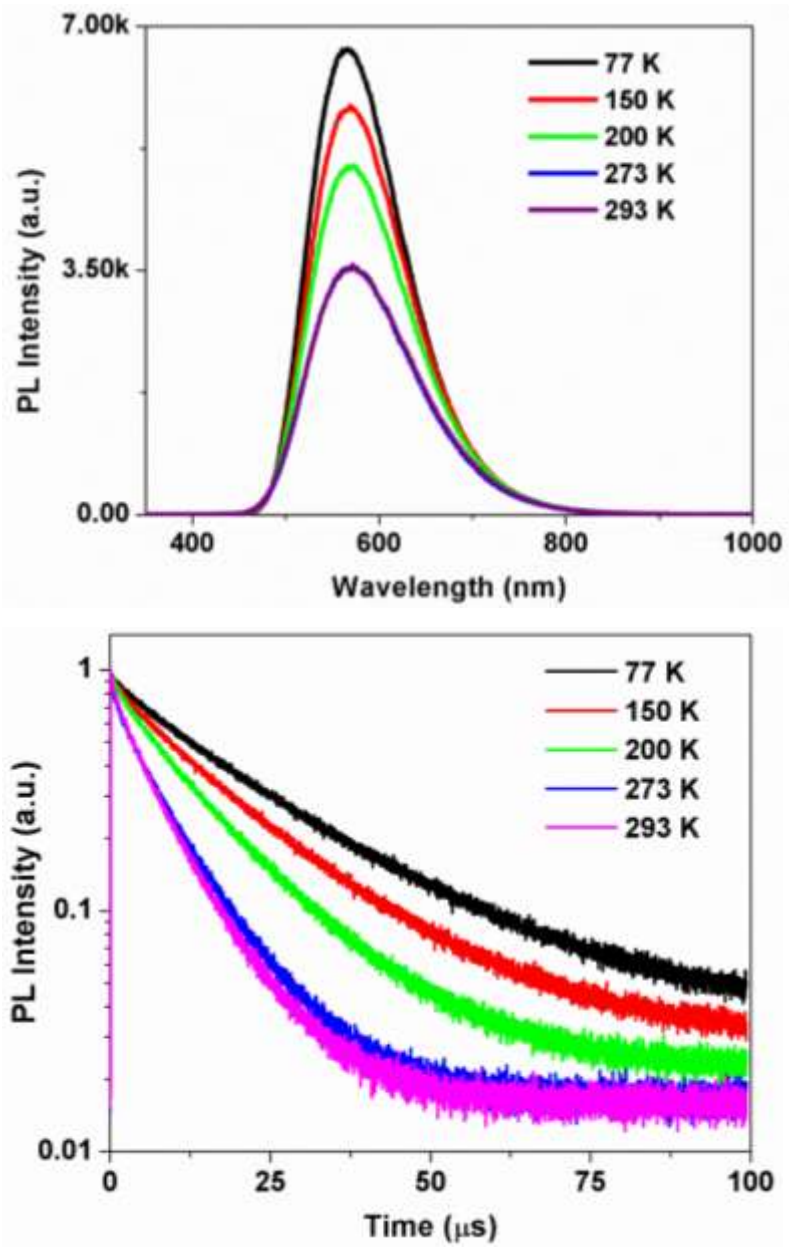


Figure S26. Top: emission spectra of compounds **1**; Bottom: luminescence decay profiles of **1** at various temperatures (λ_{ex} = 380 nm).

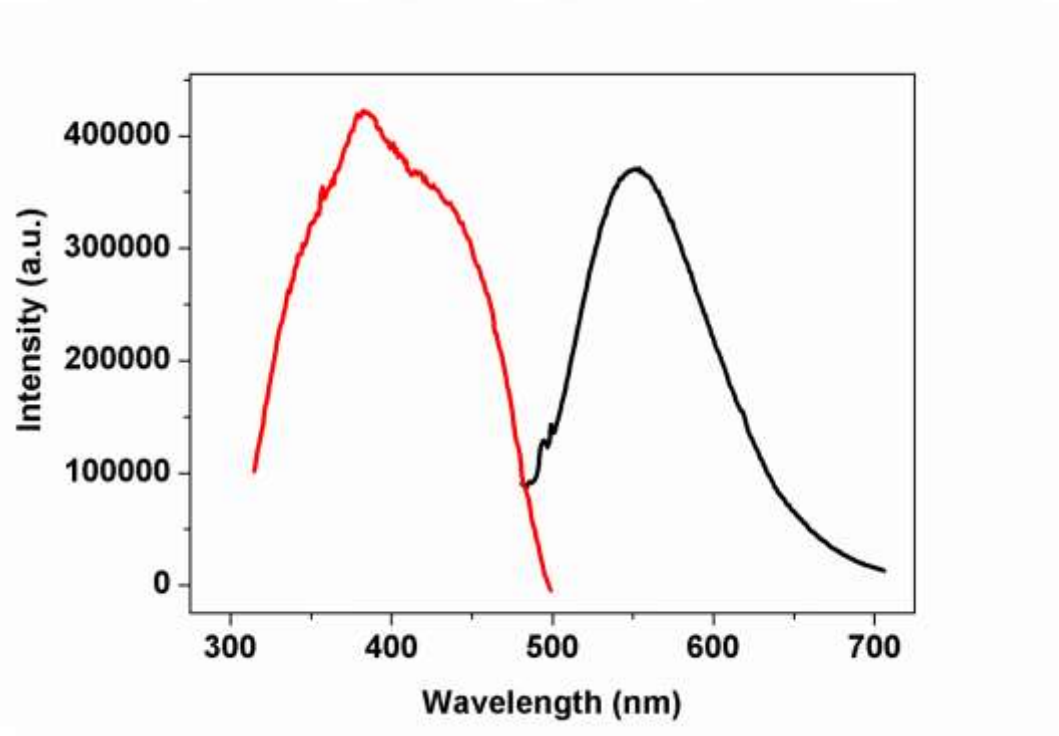


Figure S27. Excitation (red) and emission (black, excited at 450 nm) spectra of 1D-Cu_4I_4(*bbtpe*)$_2$ (**5**).

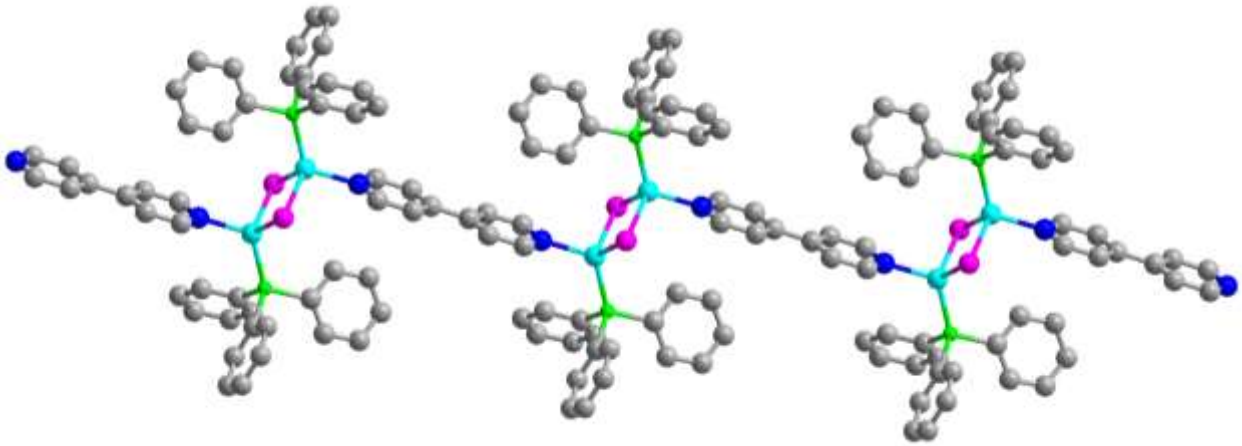


Figure 28. Structure of 1D-Cu_2I_2(*tpp*)$_2$(*4,4'-bpy*).

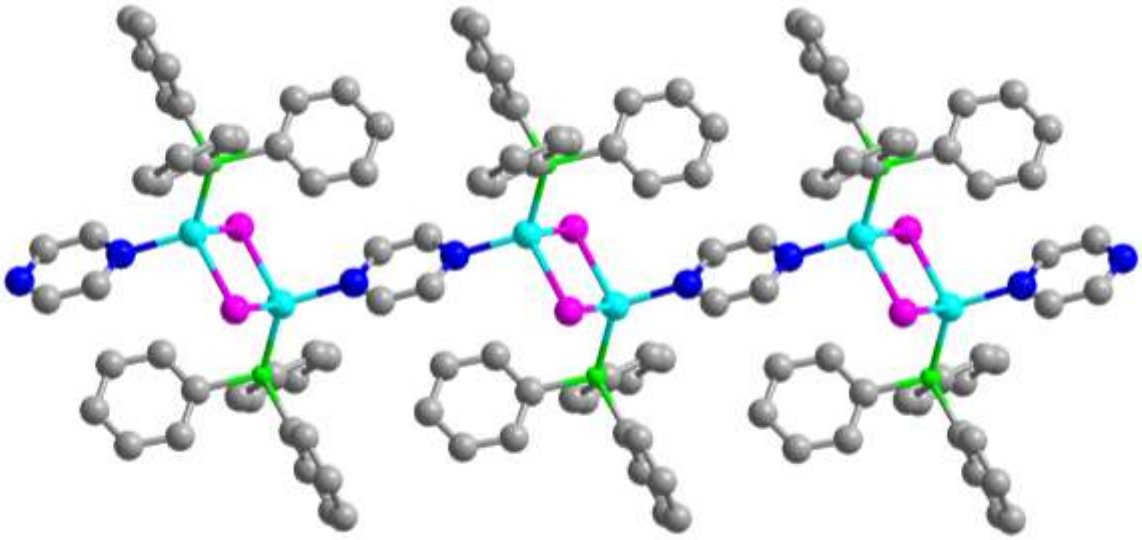


Figure 29. Structure of 1D-Cu_2I_2(*tpp*)$_2$(*pz*).

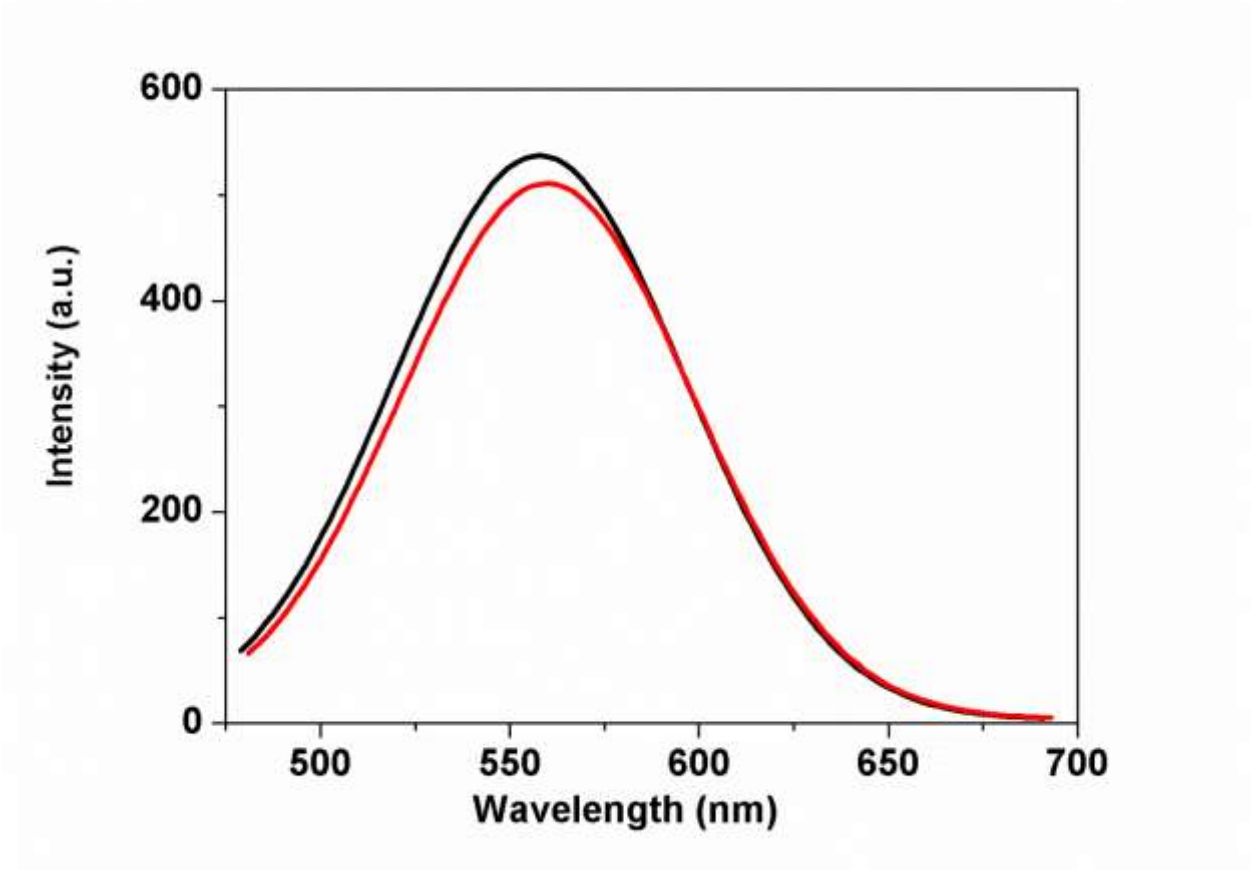


Figure S30. Room temperature PL spectra of isolated compound **5** before (black) and after (red) continuous illumination for one monthillumination.

Table S3. Lifetime values of **1** at various temperatures.

Temperature (K)	Average Amplitude Weighted τ (μs)	τ1 (μs)	τ2 (μs)
77	20.65	23.24 (85.5%)	5.39 (14.5%)
150	16.08	18.80 (81.0%)	4.50 (19.0%)
200	12.14	14.46 (78.5%)	3.67 (21.5%)
273	7.54	9.54 (71.9%)	2.44 (28.1%)
293	6.64	8.78 (66.8%)	2.33 (33.2%)

Table S4. Lifetime values of **5** at various temperatures.

Temperature (K)	Average Amplitude Weighted τ (μs)	τ1 (μs)	τ2 (μs)
77	33.85	40.44 (81.5%)	4.89 (18.5%)
150	12.94	18.18 (60.6%)	4.90 (39.4%)
200	5.98	9.78 (46.0%)	2.75 (54.0%)
273	2.41	4.86 (31.9%)	1.26 (68.1%)
293	2.26	4.34 (29.3%)	1.10 (70.7%)

S9. HOMO-LUMO energy calculations of ligands

The electronic properties of ligands were evaluated with the DFT computation using Gaussian 09 at B3LYP/6-311++G(3df,3pd).

Table S5. Calculated HOMO-LUMO energy levels of ligands

Ligand	HOMO		LUMO	
	DGDZVP	6-311++G(3df,3pd)	DGDZVP	6-311++G(3df,3pd)
bbtpe	-6.704	-6.763	-1.563	-1.601
bbtbu	-6.751	-6.808	-1.621	-1.654
biprbt	-6.411	-6.484	-1.661	-1.692
bihebt	-6.309	-	-1.565	-
bmibu	-6.495	-6.551	-0.457	-0.690

S10. Phosphor performance in prototype WLED devise

Table S6. IQYs and EQYs of compound **5** before and after one month of continuous illumination.

Status	IQY % (EQY %) (λ_{ex}: 450 nm)
Before Test	70 (40)
After Test	67 (36)