Relevant and unprecedented C-H/σ supramolecular interactions involving σ-aromatic M_2X_2 cores

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Supporting Information

DFT studies of some relevant complexes

In order to complement the computational study described above characterizing the C–H/σ interaction, we have analyzed previously reported X-ray crystal structures where this interaction is present but not noticed by the original authors. In particular we have selected three examples that clearly illustrate the role of this novel noncovalent interaction in the crystal packing phenomena. The first work was reported by Jes and coworkers,[69] who synthesized a series of different coordination polymers based on a binuclear copper (I) complex and 2,3-dimethylpyrazine ligand, using Cl, Br and I as counter-ions. Among several noncovalent interactions, the C–H/σ interaction also influences the final solid state structure and it is established between a methyl group of a pyrazine moiety of the ligand and the binuclear copper (I) core (Cu_2I_2) as can be observed in Figure **S1**, where a fragment of the polymer is represented. The theoretical model used to evaluate the C–H/σ interaction is also shown.

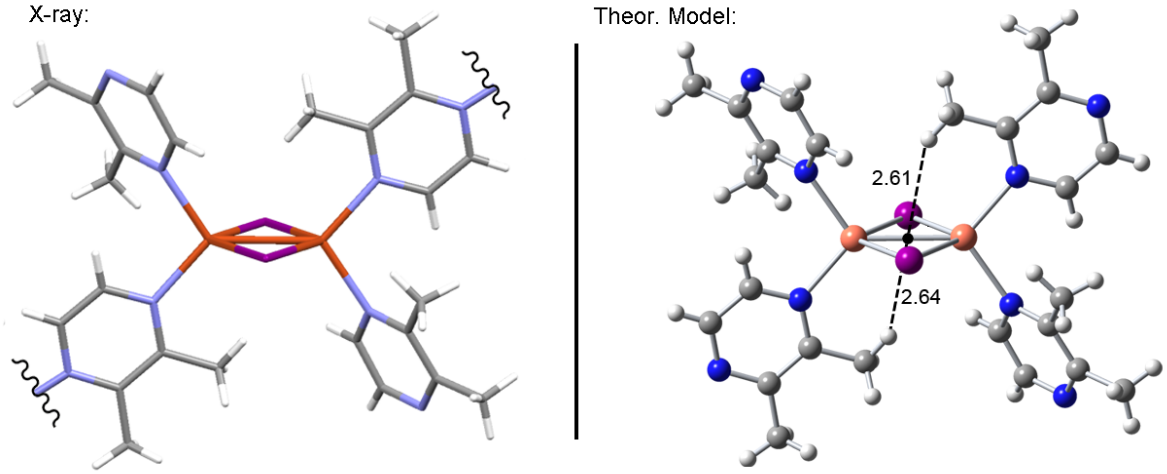


Figure S1. Left: Partial view of the X-ray structure of the coordination polymer reported by Jes and coworkers[69] (only the monomer is shown). Right: Theoretical model (right) used to study the CH/σ interaction observed in the X-ray structure. Distances (in Å) are measured to the ring centroid.

The theoretical model has been used in order to keep a compromise between the size of the system and the computational demands and, moreover, to be able to evaluate the interaction using ligand inter-exchange equations (see Figure **S2**), as has been previously used in compound 2 (see Figure 12). That is, using the first (top) reaction, we have evaluated the reaction energy upon changing one 1,2-dimethylpyrazine (Me_2Pyz) by a pyrazine (Pyz) ligand, denoted as ΔE_1 (one of the C–H/σ interactions). Using the second equation (ΔE_2) we measure both C–H/σ interactions allowing us to evaluate possible cooperativity effects by comparison to ΔE_1. The variation energy for the first equation (ΔE_1) is 5.0 kcal/mol, indicating that the complex with Me_2Pyz ligand is more favorable than that with Pyz, where the interaction is not formed. Therefore a single C-H/σ interaction in this system is approximately -5.0 kcal/mol, which is in reasonably agreement with the energetic value obtained in the preliminary study (complex **15**, Table **4**). The computed value for ΔE_2 where two simultaneous C–H/σ interactions are evaluated is 10 kcal/mol. This value is exactly twice the ΔE_1 energy, indicating that the interaction is additive in this complex and, consequently, cooperativity effects are not present.

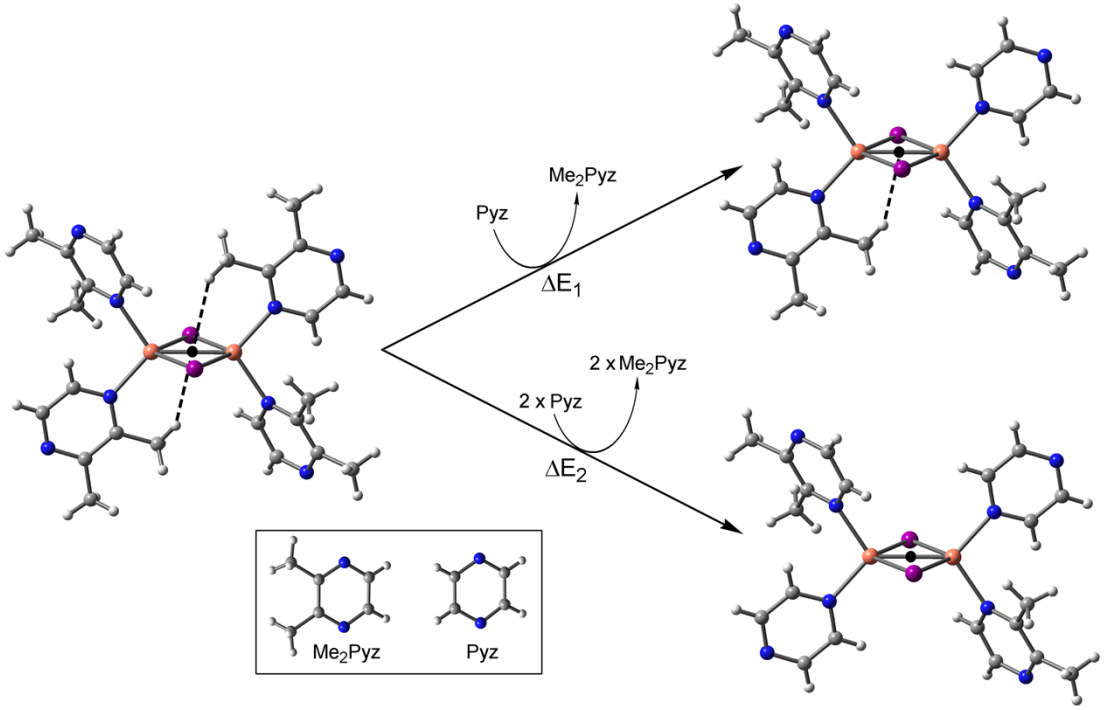


Figure S2. Equations used to compute ΔE_1 and ΔE_2 energies to estimate the C–H/σ interaction in the X-ray structure reported by Jes et al.[69]

The second work we would like to emphasize was reported by Fang and coworkers[70] in 2010, where a series of controllable assemblies of copper (I) iodine coordination polymers were synthesized, using benzotriazol-1-yl-based pyridyl units as ligands. Their results revealed that

the different spatial positions of pyridyl N-donors play an important role in constructing the coordination polymers. The authors demonstrated that the N-donor spatial positions of the pendant pyridyl groups in such bis-heterocyclic ligand are critical to direct the resulting coordination architectures. In this case, the presence of a C–H/σ interaction certainly influence the final arrangement of the ligand since it is established between a methylene group of the ligand and the Cu_2I_2 core, as it can be observed in Figure **S3**. The theoretical model used to compute the CH/σ interaction is also shown in Figure **S3**, where the ligand has been simplified. That is, we have used two methylpyridine and two methylbenzotriazole ligands coordinated to the Cu_2I_2 core.

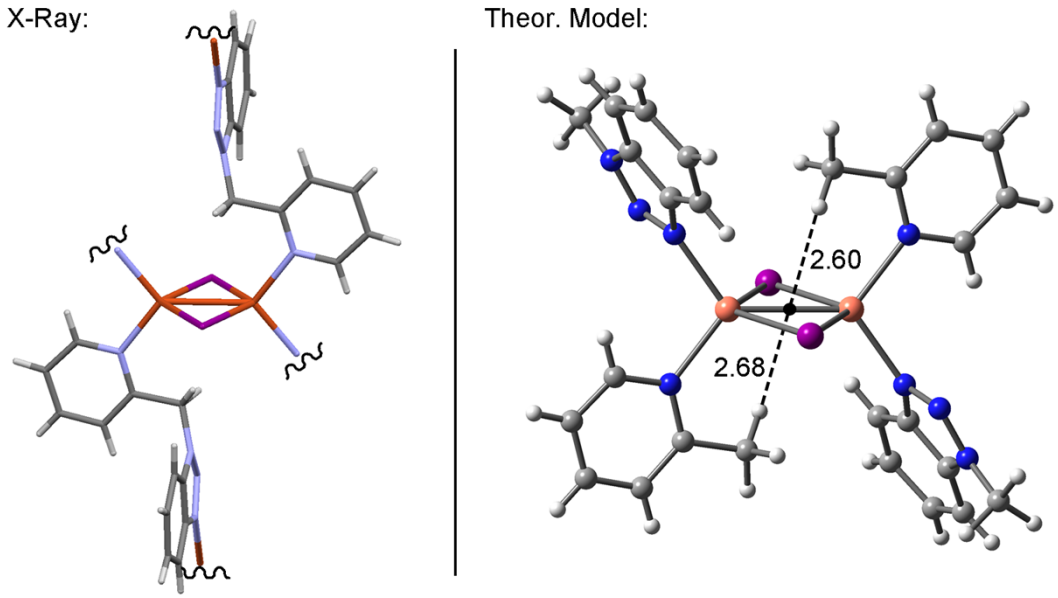


Figure S3 Left: Partial view of the X-ray structure of the coordination polymer reported by Fang and coworkers[70] (only the monomer is shown). Right: Theoretical model (right) used to study the CH/σ interaction observed in the X-ray structure. Distances (in Å) are measured to the ring centroid.

We have used the same energetic scheme described before to evaluate the C–H/σ interaction (see Figure **S4**). In this case the complex where one methylpyridine (MePy) ligand is replaced by a pyridine is 5.4 kcal/mol less favorable (denoted as ΔE_3), which is very similar to the energy value computed above for pyrazine. Therefore, for both cases the interaction energy associated to the C–H/σ interaction is around -5 kcal/mol. In this system the interaction energy is also additive, since the computed value for ΔE_4 is 10.7 kcal/mol, almost twice the value of ΔE_3.

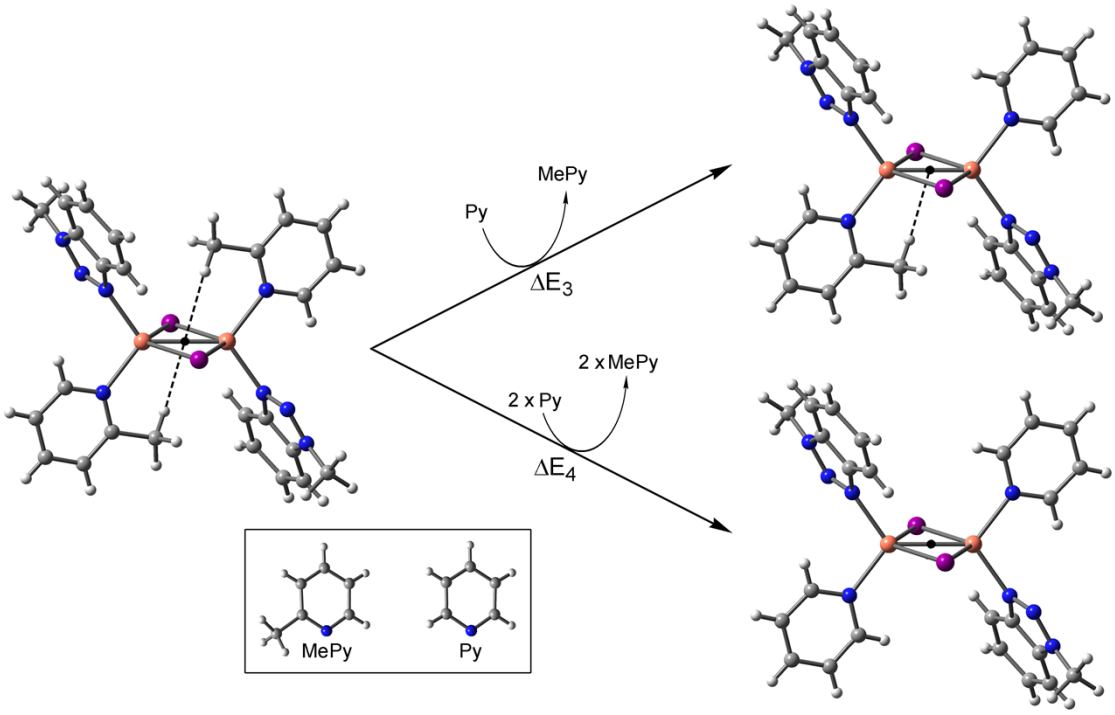


Figure S4. Equations used to compute ΔE_3 and ΔE_4 energies to estimate the C–H/σ interaction in the X-ray structure reported by Fang et al.[70]

Finally, we have also analyzed the structure reported by Knorr and coworkers,[71] who synthesized a coordination polymer based on a binuclear copper (I) core unit containing Br and I as counterions and dithioethers acting as ligands. The C–H/σ interaction is established between a hydrogen atom of the aromatic ring of the sulfur ligand and the Cu_2I_2 core, as it can be observed in Figure **S5**. The theoretical model used to compute the C–H/σ interaction is also represented where thioanisole is used as a ligand.

For this system the computed values of ΔE_5 and ΔE_6 (see Figure **S6**) are 3.4 and 6.9 kcal/mol, indicating that the interaction is approximately additive. In this case we have replaced thioanisol by dimethylsulfide to evaluate the interaction. For this system the C–H/σ interaction energy less favorable (–3.4 kcal/mol) compared to either MePy (–5.4 kcal/mol) or Me_2Pyz (–5.0 kcal/mol) examples studied above. This is due to the larger distance (~0.1 Å), measured from the interacting hydrogen atom to the Cu_2I_2 ring centroid, observed for the thioanisole compared to those observed for the other two structures (methylpyridine and dimethylpyrazine).

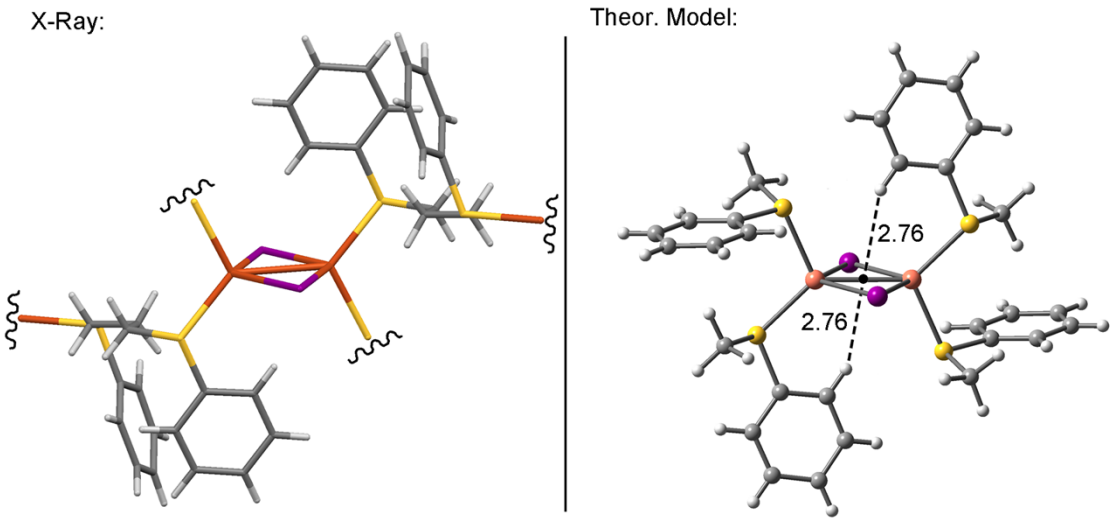


Figure S5. Left: Partial view of the X-ray structure of the coordination polymer reported by Knorr and coworkers[71] (only the monomer is shown). Right: Theoretical model (right) used to study the CH/σ interaction observed in the crystal structure. Distances (in Å) are measured to the ring centroid.

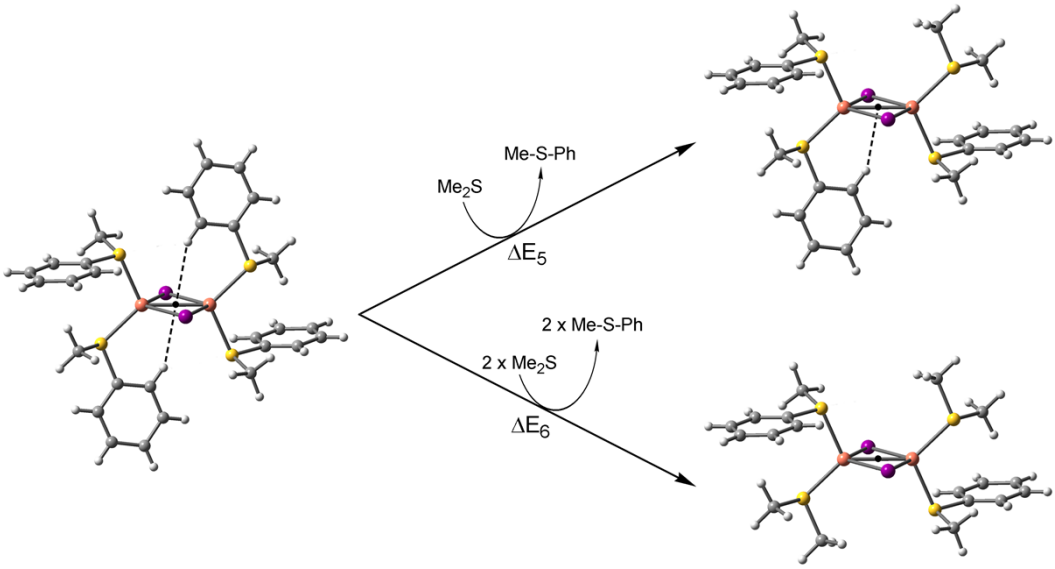


Figure S6. Equations used to compute ΔE_3 and ΔE_4 energies to estimate the C–H/σ interaction in the X-ray structure reported by Knorr *et al*.[71]

References

69. I. Jes, P. Taborsky, J. Pospísil, C. Näther *Dalton Trans.*, **2007**, *22*, 2263–2270.
70. S. M. Fang, Q. Zhang, M. Hu, B. Xiao, L. M. Zhou, G. H. Sun, L. J. Gao, M. Du, C. S. Liu *Cryst. Eng. Comm.*, **2010**, 12, 2203–2212.
71. M. Knorr, F. Guyon, A. Khatyr, C. Strohmann, M. Allain, S. M. Aly, A. Lapprand, D. Fortin, P. D. Harvey *Inorg. Chem.* **2012**, 51, 9917−9934.

TGA study

Thermal stabilities of the three complexes have been studied by thermogravimetric analyses. The TGA curve of **1** shows two-steps degradation (Figure **S7**). The first degradation within the temperature range 208-253˚C correlates to the weight loss of 68.5 % in agreement with the calculated mass loss of 69% corresponding to release of organic ligand. After which it undergoes a second degradation gradually without any sudden change in mass loss up to 600˚C. The thermal behaviour of **2** is similar to that of **1**. The TGA curve for **2** (Figure **S7**) also shows two-steps mass loss within the temperature range 190-262ºC. The first degradation within the temperature range 212-242˚C correlates to the weight loss of 61.7 % in agreement with the calculated mass loss of 62% corresponding to release of organic ligand. After which it undergoes a second degradation gradually without any sudden change in mass loss up to 600˚C. The higher thermal stabilities of the frameworks can be inferred due to the presence of more double bonds in the unsaturated polymer which enhanced the rate of curing and led to the formation of tightly bound frameworks. Finally, The TGA curve for **3** (Figure **S7**) also shows three-steps mass loss within the temperature range 114-127 and 150-245ºC. The first step corresponds to a mass loss of 7 % which agrees well with the calculated value of 7.13% correlated to the release of two acetonitrile molecules, while second steps corresponding to a mass loss of 53.6% agrees well with the calculated value of 54% due to the degradation of the two bridging organic liagnds. In all cases, the last step involves the conversion of metal halide to corresponding metal oxide which is confirmed by qualitative test and quantitative analysis.

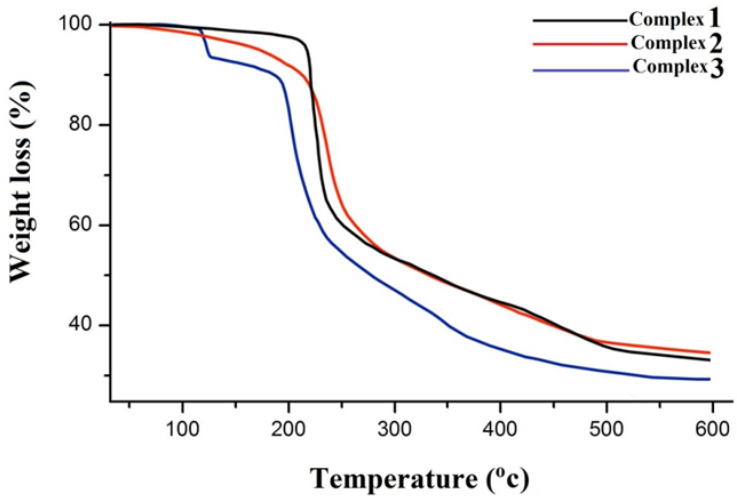
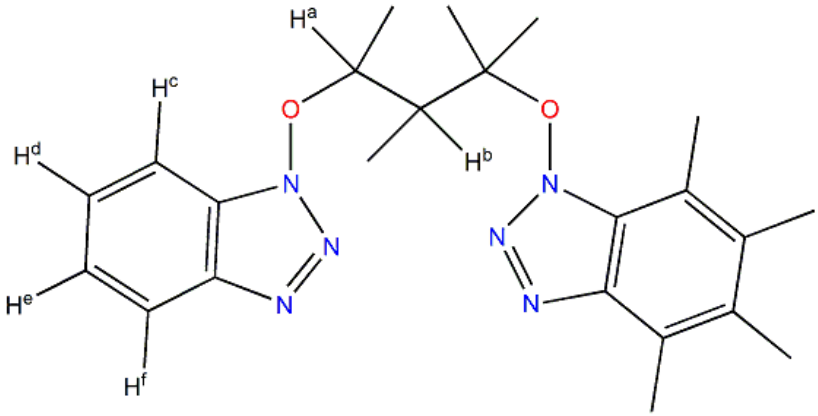


Figure S7. TGA curves for compounds **1**, **2** and **3**



Scheme **SI**: Proton numbering of **L**

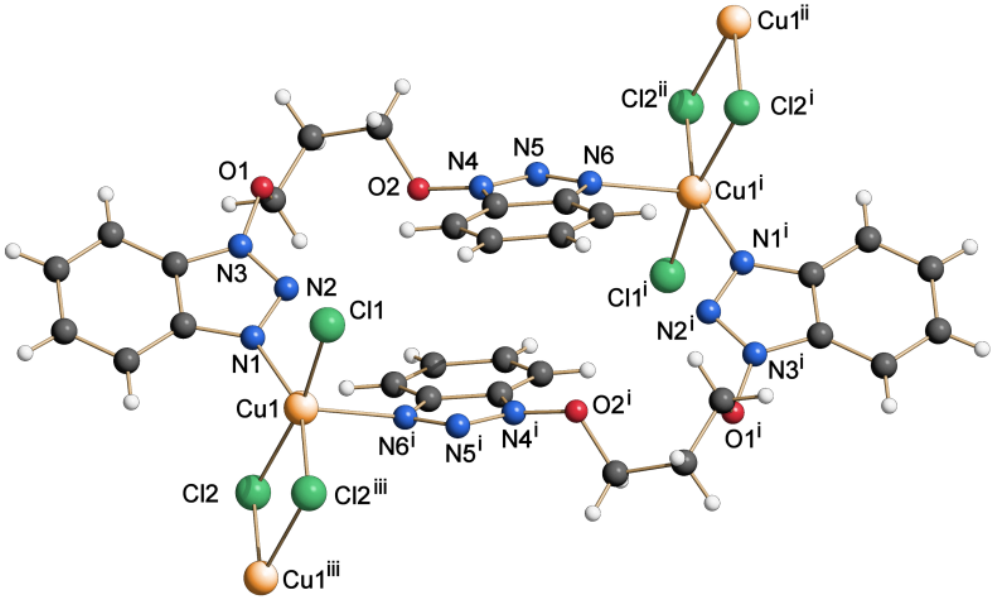


Figure **S8**: The building block of the polymeric chain of complex **1**. Symmetry codes: (i) 2-x, 1-y, 1-z; (ii) 1+x, 1+y, 1+z; (iii) 1-x, -y, -z.

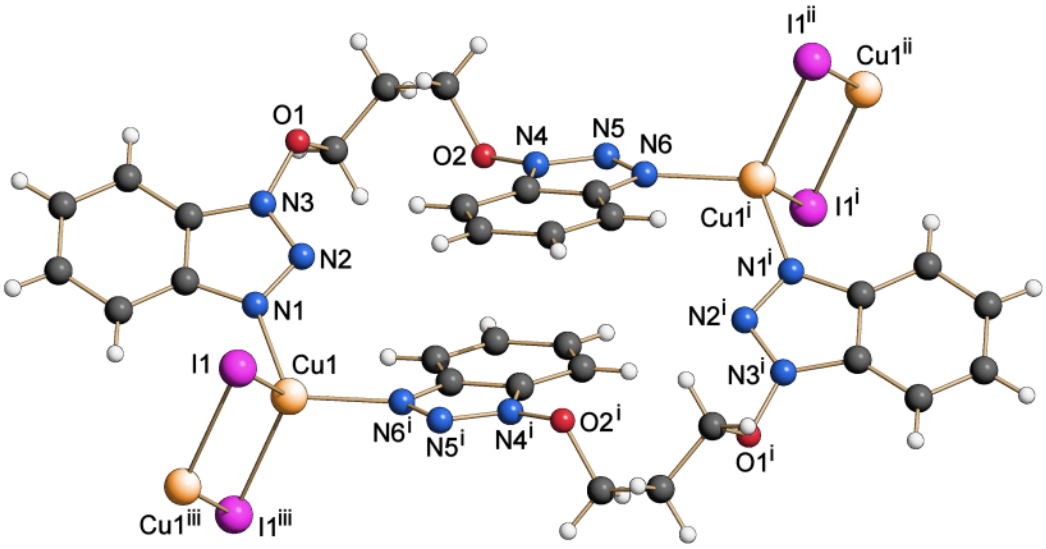


Figure S9: The building block of the polymeric chain of complex **2**. Symmetry codes: (i) 2-x, 1-y, 2-z; (ii) 1+x, 1+y, 1+z; (iii) 1-x, -y, 1-z.

Cartesian coordinates of all optimized compounds and complexes:

4.

Cu	0.0000000	1.2083002	0.0008641
N	0.0000000	2.8566794	1.4139179
H	-0.8237466	2.7907647	2.0188221
C	0.0000000	4.0888918	0.6682195
H	0.0000000	5.0429549	1.2061387
C	0.0000000	4.0883426	-0.6690010
H	0.0000000	5.0420068	-1.2076482
N	0.0000000	2.8555474	-1.4136740
H	0.8237644	2.7890170	-2.0184873
H	-0.8237644	2.7890170	-2.0184873
Cu	0.0000000	-1.2083002	0.0008641
N	0.0000000	-2.8566794	1.4139179
N	0.0000000	-2.8555474	-1.4136740
H	0.8237644	-2.7890170	-2.0184873

C	0.0000000	-4.0883426	-0.6690010
H	0.0000000	-5.0420068	-1.2076482
C	0.0000000	-4.0888918	0.6682195
H	0.0000000	-5.0429549	1.2061387
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H	-0.8237466	-2.7907647	2.0188221
H	0.8237466	2.7907647	2.0188221
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Cl	-2.0038639	0.0000000	0.0005133

5.

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N	0.0000000	2.9915704	1.4254530
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H	0.8249395	2.5441417	-1.9766933
H	-0.8249395	2.5441417	-1.9766933
Cu	0.0000000	-1.2060497	0.2152144
N	0.0000000	-2.9915704	1.4254530
N	0.0000000	-2.6808369	-1.3856284
H	0.8249395	-2.5441417	-1.9766933
C	0.0000000	-3.9874977	-0.7811410
H	0.0000000	-4.8761693	-1.4209922
C	0.0000000	-4.1347125	0.5478304

H	0.0000000	-5.1414138	0.9788113
H	-0.8249395	-2.5441417	-1.9766933
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6.

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N	0.0000000	2.8508879	1.4137360
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H	-0.8250717	2.7833237	-2.0169582
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N	0.0000000	-2.8508879	1.4137360
N	0.0000000	-2.8520968	-1.4138609
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H	-0.8259659	2.8846936	-1.9861009
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N	0.0000000	-3.1198090	1.4132573
N	0.0000000	-2.9981152	-1.3912887
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C	0.0000000	-4.2668508	-0.7108157
H	0.0000000	-5.1920798	-1.2960516
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S	-1.7487197	0.0000000	0.0897357

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C	0.0000000	-3.8912630	0.6998145
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S	1.8240509	0.0000000	0.0461255
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12.

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13.

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Hg	0.0000000	1.8646071	-0.0104605

14.

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15.

Cu	0.0000000	1.2824093	0.0300044
C	0.0000000	3.8912630	0.6998145
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C	0.0000000	3.8668017	-0.7272055
H	0.0000000	4.7881909	-1.3268799
Cu	0.0000000	-1.2824093	0.0300044
C	0.0000000	-3.8668017	-0.7272055
H	0.0000000	-4.7881909	-1.3268799
C	0.0000000	-3.8912630	0.6998145
H	0.0000000	-4.8327625	1.2675390
S	1.8240509	0.0000000	0.0461255
S	-1.8240509	0.0000000	0.0461255
O	0.0000000	2.7351024	-1.3220661
O	0.0000000	2.7804134	1.3326682
O	0.0000000	-2.7351024	-1.3220661
O	0.0000000	-2.7804134	1.3326682

16.

Cu	0.0000000	1.2198923	0.7601805
N	0.0000000	2.9920123	1.9733796
H	-0.8222652	2.9990056	2.5844753
C	0.0000000	4.1408845	1.1000584
H	0.0000000	5.1439962	1.5390102
C	0.0000000	4.0012577	-0.2297369
H	0.0000000	4.8950035	-0.8627420
N	0.0000000	2.7003265	-0.8432654
H	0.8203128	2.5679905	-1.4428663
H	-0.8203128	2.5679905	-1.4428663
Cu	0.0000000	-1.2198923	0.7601805
N	0.0000000	-2.9920123	1.9733796
N	0.0000000	-2.7003265	-0.8432654
H	0.8203128	-2.5679905	-1.4428663
C	0.0000000	-4.0012577	-0.2297369
H	0.0000000	-4.8950035	-0.8627420
C	0.0000000	-4.1408845	1.1000584
H	0.0000000	-5.1439962	1.5390102
H	-0.8203128	-2.5679905	-1.4428663
H	0.8222652	-2.9990056	2.5844753
H	-0.8222652	-2.9990056	2.5844753
H	0.8222652	2.9990056	2.5844753
C	0.0000000	0.0000000	-3.8441691
H	0.0000000	0.0000000	-4.9150221
C	0.0000000	0.0000000	-2.6340133
H	0.0000000	0.0000000	-1.5506662
Cl	1.9915020	0.0000000	0.7518330
Cl	-1.9915020	0.0000000	0.7518330

17.

Cu	0.0000000	1.2151159	0.7561487
N	0.0000000	2.9842431	1.9744540
H	-0.8231996	2.9882841	2.5843016
C	0.0000000	4.1325912	1.1010195
H	0.0000000	5.1358857	1.5393494
C	0.0000000	3.9924795	-0.2285557
H	0.0000000	4.8852136	-0.8626656
N	0.0000000	2.6911613	-0.8425000
H	0.8207356	2.5597383	-1.4419624
H	-0.8207356	2.5597383	-1.4419624
Cu	0.0000000	-1.2151159	0.7561487
N	0.0000000	-2.9842431	1.9744540
N	0.0000000	-2.6911613	-0.8425000
H	0.8207356	-2.5597383	-1.4419624
C	0.0000000	-3.9924795	-0.2285557
H	0.0000000	-4.8852136	-0.8626656
C	0.0000000	-4.1325912	1.1010195
H	0.0000000	-5.1358857	1.5393494
H	-0.8207356	-2.5597383	-1.4419624
H	0.8231996	-2.9882841	2.5843016
H	-0.8231996	-2.9882841	2.5843016
H	0.8231996	2.9882841	2.5843016
C	0.0000000	0.0000000	-3.8591712
H	0.0000000	0.0000000	-4.9300558
C	0.0000000	0.0000000	-2.6490495
H	0.0000000	0.0000000	-1.5657093
Br	2.1426299	0.0000000	0.7800641
Br	-2.1426299	0.0000000	0.7800641

18.

Cu	0.0000000	1.2120626	0.7478189
N	0.0000000	2.9726368	1.9781885
H	-0.8240305	2.9696320	2.5871330
C	0.0000000	4.1267749	1.1129566
H	0.0000000	5.1267247	1.5585302
C	0.0000000	3.9957052	-0.2173562
H	0.0000000	4.8922139	-0.8457741
N	0.0000000	2.6985488	-0.8406316
H	0.8214942	2.5705346	-1.4399490
H	-0.8214942	2.5705346	-1.4399490
Cu	0.0000000	-1.2120626	0.7478189
N	0.0000000	-2.9726368	1.9781885
N	0.0000000	-2.6985488	-0.8406316
H	0.8214942	-2.5705346	-1.4399490
C	0.0000000	-3.9957052	-0.2173562
H	0.0000000	-4.8922139	-0.8457741
C	0.0000000	-4.1267749	1.1129566
H	0.0000000	-5.1267247	1.5585302
H	-0.8214942	-2.5705346	-1.4399490
H	0.8240305	-2.9696320	2.5871330
H	-0.8240305	-2.9696320	2.5871330
H	0.8240305	2.9696320	2.5871330
I	2.3187249	0.0000000	0.7864987
I	-2.3187249	0.0000000	0.7864987
C	0.0000000	0.0000000	-3.8952719
H	0.0000000	0.0000000	-4.9661505
C	0.0000000	0.0000000	-2.6851895
H	0.0000000	0.0000000	-1.6025862

19.

Cu	0.0000000	1.4221052	0.8324072
N	0.0000000	3.2880762	1.9395333
H	-0.8241552	3.3141738	2.5471947
C	0.0000000	4.3820406	1.0001345
H	0.0000000	5.4107046	1.3743053
C	0.0000000	4.1515401	-0.3161485
H	0.0000000	4.9931031	-1.0162134
N	0.0000000	2.8068460	-0.8290391
H	0.8213205	2.6185484	-1.4124553
H	-0.8213205	2.6185484	-1.4124553
Cu	0.0000000	-1.4221052	0.8324072
N	0.0000000	-3.2880762	1.9395333
N	0.0000000	-2.8068460	-0.8290391
H	0.8213205	-2.6185484	-1.4124553
C	0.0000000	-4.1515401	-0.3161485
H	0.0000000	-4.9931031	-1.0162134
C	0.0000000	-4.3820406	1.0001345
H	0.0000000	-5.4107046	1.3743053
H	-0.8213205	-2.6185484	-1.4124553
H	0.8241552	-3.3141738	2.5471947
H	-0.8241552	-3.3141738	2.5471947
H	0.8241552	3.3141738	2.5471947
C	0.0000000	0.0000000	-3.7114661
H	0.0000000	0.0000000	-4.7822427
C	0.0000000	0.0000000	-2.5006015
H	0.0000000	0.0000000	-1.4169268
S	1.7265316	0.0000000	0.9511602
S	-1.7265316	0.0000000	0.9511602

20.

Cu	0.0000000	1.4370932	1.2071503
C	0.0000000	4.2304440	1.3218098
H	0.0000000	5.2493907	1.7454679
C	0.0000000	4.0072621	-0.1419322
H	0.0000000	4.8725612	-0.8326391
Cu	0.0000000	-1.4370932	1.2071503
C	0.0000000	-4.0072621	-0.1419322
H	0.0000000	-4.8725612	-0.8326391
C	0.0000000	-4.2304440	1.3218098
H	0.0000000	-5.2493907	1.7454679
C	0.0000000	0.0000000	-3.5810235
H	0.0000000	0.0000000	-4.6512538
C	0.0000000	0.0000000	-2.3728198
H	0.0000000	0.0000000	-1.3001560
O	0.0000000	2.8424470	-0.5571454
O	0.0000000	3.2303591	2.0692945
O	0.0000000	-3.2303591	2.0692945
O	0.0000000	-2.8424470	-0.5571454
Cl	-1.7427132	0.0000000	1.1406207
Cl	1.7427132	0.0000000	1.1406207

21.

Cu	0.0000000	1.4571472	1.1174105
C	0.0000000	4.2496816	1.3801116
H	0.0000000	5.2571047	1.8318129
C	0.0000000	4.0704541	-0.0894584
H	0.0000000	4.9526959	-0.7573113
Cu	0.0000000	-1.4571472	1.1174105

C	0.0000000	-4.0704541	-0.0894584
H	0.0000000	-4.9526959	-0.7573113
C	0.0000000	-4.2496816	1.3801116
H	0.0000000	-5.2571047	1.8318129
C	0.0000000	0.0000000	-3.6629652
H	0.0000000	0.0000000	-4.7332694
C	0.0000000	0.0000000	-2.4547002
H	0.0000000	0.0000000	-1.3819073
Br	1.8934199	0.0000000	1.0759581
Br	-1.8934199	0.0000000	1.0759581
O	0.0000000	2.9157843	-0.5374117
O	0.0000000	3.2282860	2.0953094
O	0.0000000	-3.2282860	2.0953094
O	0.0000000	-2.9157843	-0.5374117

22.

Cu	0.0000000	1.6713398	0.9777708
C	0.0000000	4.3040540	1.3971376
H	0.0000000	5.2850221	1.8897932
C	0.0000000	4.1476337	0.0025034
H	0.0000000	4.9913176	-0.6992268
Cu	0.0000000	-1.6713398	0.9777708
C	0.0000000	-4.1476337	0.0025034
H	0.0000000	-4.9913176	-0.6992268
C	0.0000000	-4.3040540	1.3971376
H	0.0000000	-5.2850221	1.8897932
C	0.0000000	0.0000000	-3.7500185
H	0.0000000	0.0000000	-4.8204622
C	0.0000000	0.0000000	-2.5422331

H	0.0000000	0.0000000	-1.4706322
O	0.0000000	2.9428752	-0.4894478
O	0.0000000	3.2386497	2.1425839
O	0.0000000	-3.2386497	2.1425839
O	0.0000000	-2.9428752	-0.4894478
I	-1.9955661	0.0000000	1.0705589
I	1.9955661	0.0000000	1.0705589

23.

Cu	0.0000000	1.6731421	0.8760943
C	0.0000000	4.2911638	1.4810224
H	0.0000000	5.2401094	2.0350808
C	0.0000000	4.2318814	0.0654141
H	0.0000000	5.1296602	-0.5678264
Cu	0.0000000	-1.6731421	0.8760943
C	0.0000000	-4.2318814	0.0654141
H	0.0000000	-5.1296602	-0.5678264
C	0.0000000	-4.2911638	1.4810224
H	0.0000000	-5.2401094	2.0350808
C	0.0000000	0.0000000	-3.8320763
H	0.0000000	0.0000000	-4.9024866
C	0.0000000	0.0000000	-2.6240501
H	0.0000000	0.0000000	-1.5512190
O	0.0000000	3.0744618	-0.5010405
O	0.0000000	3.1853284	2.1423459
O	0.0000000	-3.1853284	2.1423459
O	0.0000000	-3.0744618	-0.5010405
S	-1.4200939	0.0000000	0.9238253
S	1.4200939	0.0000000	0.9238253

24.

C	0.0000000	4.8309626	1.2576189
H	0.0000000	5.8709529	1.6132496
C	0.0000000	4.5744756	-0.1477663
H	0.0000000	5.4239562	-0.8463423
C	0.0000000	-4.5744756	-0.1477663
H	0.0000000	-5.4239562	-0.8463423
C	0.0000000	-4.8309626	1.2576189
H	0.0000000	-5.8709529	1.6132496
C	0.0000000	0.0000000	-3.4859476
H	0.0000000	0.0000000	-4.5565808
C	0.0000000	0.0000000	-2.2785659
H	0.0000000	0.0000000	-1.2088882
O	0.0000000	3.3914951	-0.6334534
O	0.0000000	3.8958499	2.1351726
O	0.0000000	-3.8958499	2.1351726
O	0.0000000	-3.3914951	-0.6334534
Cl	-1.7673289	0.0000000	1.2912918
Cl	1.7673289	0.0000000	1.2912918
Hg	0.0000000	1.8534519	1.0952203
Hg	0.0000000	-1.8534519	1.0952203

25.

C	0.0000000	4.8662244	1.2217864
H	0.0000000	5.9150332	1.5514861
C	0.0000000	4.5780774	-0.1776664
H	0.0000000	5.4134247	-0.8935951
C	0.0000000	-4.5780774	-0.1776664
H	0.0000000	-5.4134247	-0.8935951

C	0.0000000	-4.8662244	1.2217864
H	0.0000000	-5.9150332	1.5514861
C	0.0000000	0.0000000	-3.4491493
H	0.0000000	0.0000000	-4.5197842
C	0.0000000	0.0000000	-2.2417489
H	0.0000000	0.0000000	-1.1721799
Br	1.9066791	0.0000000	1.3780288
Br	-1.9066791	0.0000000	1.3780288
O	0.0000000	3.3853585	-0.6385346
O	0.0000000	3.9529444	2.1218403
O	0.0000000	-3.9529444	2.1218403
O	0.0000000	-3.3853585	-0.6385346
Hg	0.0000000	1.8797229	1.1280857
Hg	0.0000000	-1.8797229	1.1280857

26.

C	0.0000000	4.7792457	1.5994386
H	0.0000000	5.7174549	2.1747440
C	0.0000000	4.8486124	0.1719850
H	0.0000000	5.8365038	-0.3124813
C	0.0000000	-4.8486124	0.1719850
H	0.0000000	-5.8365038	-0.3124813
C	0.0000000	-4.7792457	1.5994386
H	0.0000000	-5.7174549	2.1747440
C	0.0000000	0.0000000	-3.9752746
H	0.0000000	0.0000000	-5.0459225
C	0.0000000	0.0000000	-2.7674940
H	0.0000000	0.0000000	-1.6965727
O	0.0000000	3.8096255	-0.5771300

O	0.0000000	3.6726824	2.2419903
O	0.0000000	-3.6726824	2.2419903
O	0.0000000	-3.8096255	-0.5771300
I	-2.1241944	0.0000000	0.7160201
I	2.1241944	0.0000000	0.7160201
Hg	0.0000000	1.8983482	0.7280654
Hg	0.0000000	-1.8983482	0.7280654