Supplementary Information

4,5-diiodo-1-H-imidazole-derived linker ligand and Cu(I) and Co(II) coordination polymers based thereupon

Single crystal X-ray Diffractometry. The diffraction data for **1-3** were collected on a Bruker D8 Venture diffractometer (0.5° ω- and ϕ-scans, fixed-χ three circle goniometer, CMOS PHOTON III detector, Mo-IμS 3.0 microfocus source, focusing Montel mirrors, λ = 0.71073 Å MoK_α radiation, N_2-flow thermostat) at 150 K (**1**, **3**) and 200 K (**2**). Absorption correction was applied by SADABS (Bruker Apex3 software suite: Apex3, SADABS-2016/2[1] and SAINT, version 2018.7-2; Bruker AXS Inc.: Madison, WI, 2017.). Structures were solved by SHELXT[2] and refined by full-matrix least-squares treatment against $|F|^2$ in anisotropic approximation with SHELXL 2017/1[3] assisted with OLEX2 1.5 GUI[4]. In **2**, OLEX2 Solvent Mask Procedure was applied due to severe disorder of DMF solvate molecules. The available volume is estimated to be 240 $Å^3$ per $[Co(BimB\text{-}I4)Cl_2]$ formula unit. The structures of **1**-**3** were deposited to the Cambridge Crystallographic Data Centre (CCDC) as a supplementary publication, No. **2313127-2313129**.

(1) Krause, L.; Herbst-Irmer, R.; Sheldrick, G. M.; Stalke, D. Comparison of Silver and Molybdenum Microfocus X-Ray Sources for Single-Crystal Structure Determination. *J. Appl. Crystallogr.* **2015**, *48* (1), 3–10. https://doi.org/10.1107/S1600576714022985.

(2) Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr. Sect. A Found. Adv.* **2015**, *71* (1), 3–8. https://doi.org/10.1107/S2053273314026370.

(3) Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71* (1), 3–8. https://doi.org/10.1107/S2053229614024218.

(4) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2 : A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42* (2), 339–341. https://doi.org/10.1107/S0021889808042726.

Powder X-ray Diffractometry. XRD analysis of polycrystals was performed on Shimadzu XRD-7000 diffractometer (CuK-alpha radiation, Ni – filter, linear One Sight detector, 0.0143° 2θ step, 2s per step). Plotting of PXRD patterns and data treatment was performed using X'Pert Plus software.

Table S1. Crystal data and structure refinement for **1**–**3**.

Identification code	**1**	**2**	**3**
CCDC number	2313127	2313128	2313129
Empirical formula	$C_{10}H_{10}I_4N_4$	$C_{10}H_{10}Cl_2CoI_4N_4$ 1.5[C_3H_7NO]	$C_{10}H_{10}Cu_2I_6N_4$
M, g/mol	693.82	933.29	1074.70
Temperature/K	150	200	150
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	*Pbca*	*C2/c*	$P2_1/n$
a, Å	8.7171 (3)	12.379 (6)	11.0164 (5)
b, Å	12.9296 (5)	16.228 (7)	15.4161 (6)
c, Å	14.2643 (5)	14.155 (10)	12.9223 (5)
α, deg.	90	90	90
β, deg.	90	107.332 (16)	103.359 (2)
γ, deg.	90	90	90
Volume, Å^3	1607.71 (10)	2715 (3)	2135.21 (15)
Z	4	4	4
ρ_{calc}, g/cm^3	2.866	2.284	3.343
μ, mm^{-1}	7.74	5.40	10.67
F(000)	1240	1724	1896
Crystal size, mm	0.17 × 0.14 × 0.1	0.18 × 0.12 × 0.03	0.18 × 0.11 × 0.06
Θ range for data collection, deg.	3.151 to 31.513	28.697 to 2.296	29.592 to 2.090
Tmin, Tmax	0.398, 0.605	0.670, 0.746	0.477, 0.746
Range of h, k, l	-11 ≤ h ≤ 12, -18 ≤ k ≤ 18, -20 ≤ l ≤ 19	-16 ≤ h ≤ 16, -21 ≤ k ≤ 21, -18 ≤ l ≤ 19	-15 ≤ h ≤ 15, -19 ≤ k ≤ 21, -17 ≤ l ≤ 17
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.735	0.676	0.695
R_{int}	0.026	0.049	0.034
Reflections collected/independent	28635, 2606	25734, 3493	40970, 5975
Reflections with I > 2σ(I)	2540	2744	5500
Data/restraints/parameters	2606/0/82	3493/0/100	5975/0/199
Goodness-of-fit on F^2	1.195	1.040	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0134, wR_2 = 0.0311	R_1 = 0.0268, wR_2 = 0.0561	R_1 = 0.0195, wR_2 = 0.0435
Final R indexes [all data]	R_1 = 0.0139, wR_2 = 0.0313	R_1 = 0.0378, wR_2 = 0.0589	R_1 = 0.0221, wR_2 = 0.0447
Weighting scheme	w =1/[σ^2(F_o^2)+(0.0072P)^2 + 1.1732P] where P =(F_o^2 +2F_c^2)/3	w =1/[σ^2(F_o^2)+(0.0233P)^2 + 2.5927P] where P = (F_o^2 +2F_c^2)/3	w =1/[σ^2(F_o^2)+(0.016P)^2 +3.5104P] where P = (F_o^2 +2F_c^2)/3
$(\Delta/\sigma)_{max}$	0.002	0.001	0.003
Largest diff. peak/hole, e/Å^3	0.47, −0.48	0.73, −0.86	1.03, −0.91

Computer programs: SHELXT 2014/5 (Sheldrick, 2014), SHELXL 2017/1 (Sheldrick, 2015), Olex2 1.5 (Dolomanov et al., 2009).

Table S2. Selected bond lengths and angles for **1**.

Bond length, Å			
I1—C1	2.0695 (14)	N2—C4	1.4709 (19)
I2—C2	2.0631 (14)	N2—C3	1.357 (2)
C1—N1	1.3689 (19)	N1—C3	1.324 (2)
C1—C2	1.3745 (19)	C4—C5	1.520 (2)
N2—C2	1.3786 (18)	C5—C5^{i}	1.526 (3)
Bond angle, (º)			
N1—C1—I1	121.53 (10)	C1—C2—I2	130.79 (11)
N1—C1—C2	111.42 (13)	C1—C2—N2	105.11 (12)
C2—C1—I1	127.02 (11)	N2—C2—I2	123.95 (10)
C2—N2—C4	128.39 (13)	N2—C4—C5	113.14 (12)
C3—N2—C2	106.53 (12)	C4—C5—C5^{i}	109.61 (15)
C3—N2—C4	124.99 (13)	N1—C3—N2	112.89 (13)
C3—N1—C1	104.05 (13)		

Symmetry code(s): (i) −x+2, −y+1, −z+1.

Table S3. Selected bond lengths and angles for **2**.

Bond length, Å			
I2—C2	2.073 (3)	N2—C3	1.342 (4)
I1—C1	2.068 (3)	N2—C2	1.378 (4)
Co1—Cl1	2.2528 (14)	N2—C4	1.473 (4)
Co1—Cl1^{i}	2.2528 (14)	C1—C2	1.361 (4)
Co1—N1^{i}	2.014 (3)	C1—I1A	2.034 (6)
Co1—N1	2.014 (3)	C5—C5^{ii}	1.542 (6)
N1—C3	1.333 (4)	C5—C4	1.521 (5)
N1—C1	1.385 (4)		
Bond angle, (º)			
Cl1^{i}—Co1—Cl1	113.88 (6)	N1—C3—N2	111.4 (3)
N1—Co1—Cl1i	114.78 (8)	N1—C1—I1	122.2 (2)
N1^{i}—Co1—Cl1	114.78 (8)	N1—C1—I1A	123.7 (3)
N1^{i}—Co1—Cl1i	104.23 (8)	C2—C1—I1	127.8 (2)
N1—Co1—Cl1	104.23 (8)	C2—C1—N1	109.9 (3)
N1^{i}—Co1—N1	104.89 (17)	C2—C1—I1A	122.9 (3)
C3—N1—Co1	124.9 (2)	N2—C2—I2	123.0 (2)
C3—N1—C1	105.1 (3)	C1—C2—I2	131.0 (2)
C1—N1—Co1	129.6 (2)	C1—C2—N2	105.9 (3)
C3—N2—C2	107.6 (3)	C4—C5—C5^{ii}	110.2 (4)
C3—N2—C4	124.8 (3)	N2—C4—C5	110.9 (3)
C2—N2—C4	127.5 (3)		

Symmetry code(s): (i) −x+1, y, −z+3/2; (ii) −x+3/2, −y+3/2, −z+1.

Table S4. Selected bond lengths and angles for **3**.

Bond length, Å			
I1—C1	2.064 (3)	I6—Cu2	2.5557 (4)
I2—C2	2.069 (3)	I6—Cu2^{i}	2.6102 (4)
I3—C9	2.052 (3)	Cu1—Cu2	2.8620 (6)
I4—C8	2.066 (3)	Cu1—N1^{ii}	1.988 (2)
I5—Cu1	2.6533 (4)	Cu1—N4	1.973 (2)
I5—Cu2	2.5076 (4)	Cu2—Cu2^{i}	2.6264 (8)
I6—Cu1	3.0411 (5)		
Bond angle, (º)			
Cu2—I5—Cu1	67.290 (14)	I5—Cu2—I6^{i}	116.177 (16)
Cu2—I6—Cu1	60.777 (12)	I5—Cu2—I6	124.843 (17)
Cu2^{i}—I6—Cu1	120.691 (13)	I5—Cu2—Cu1	58.784 (12)
Cu2—I6—Cu2^{i}	61.105 (15)	I5—Cu2—Cu2^{i}	173.91 (3)
I5—Cu1—I6	103.815 (15)	I6—Cu2—I6^{i}	118.895 (15)
I5—Cu1—Cu2	53.925 (12)	I6^{i}—Cu2—Cu1	166.865 (18)
Cu2—Cu1—I6	51.198 (11)	I6—Cu2—Cu1	68.026 (13)
N1^{ii}—Cu1—I5	109.28 (7)	I6—Cu2—Cu2^{i}	60.473 (15)
N1^{ii}—Cu1—I6	96.81 (7)	I6^{i}—Cu2—Cu2^{i}	58.422 (15)
N1^{ii}—Cu1—Cu2	120.80 (7)	Cu2^{i}—Cu2—Cu1	127.14 (2)
N4—Cu1—I5	111.08 (7)	C1—N1—Cu1^{iii}	126.80 (18)
N4—Cu1—I6	106.26 (7)	C3—N1—Cu1^{iii}	127.4 (2)
N4—Cu1—Cu2	111.35 (7)	C8—N4—Cu1	130.06 (18)
N4—Cu1—N1^{ii}	126.26 (10)	C10—N4—Cu1	124.83 (19)

Symmetry code(s): (i) −x+1, −y, −z+2; (ii) x, y, z+1; (iii) x, y, z−1.

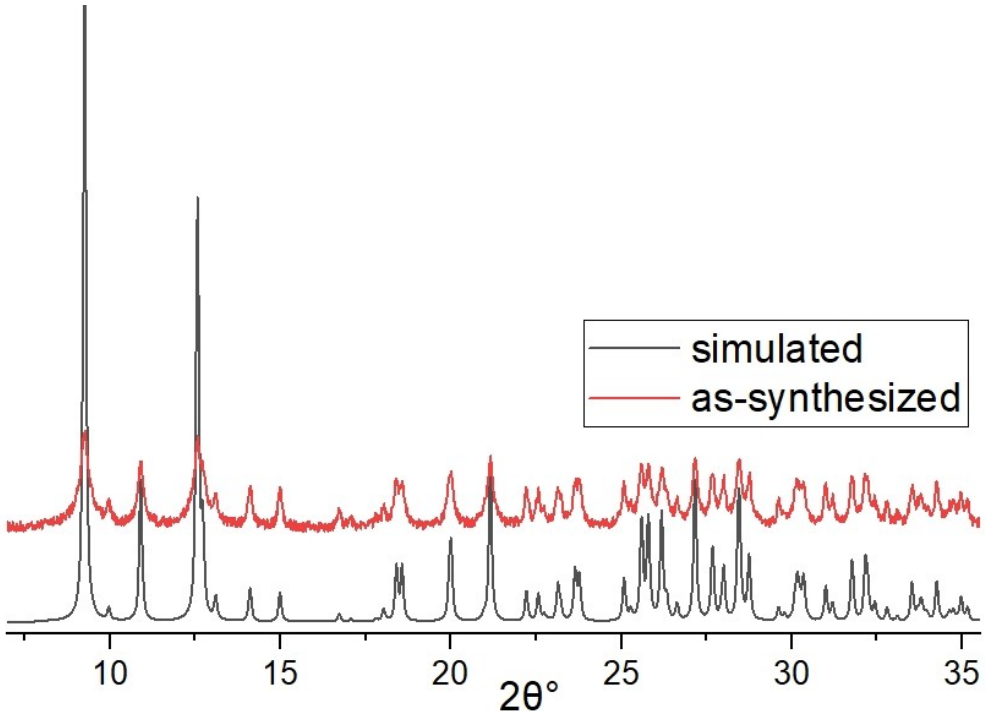

Figure 1S. PXRD data for **2**

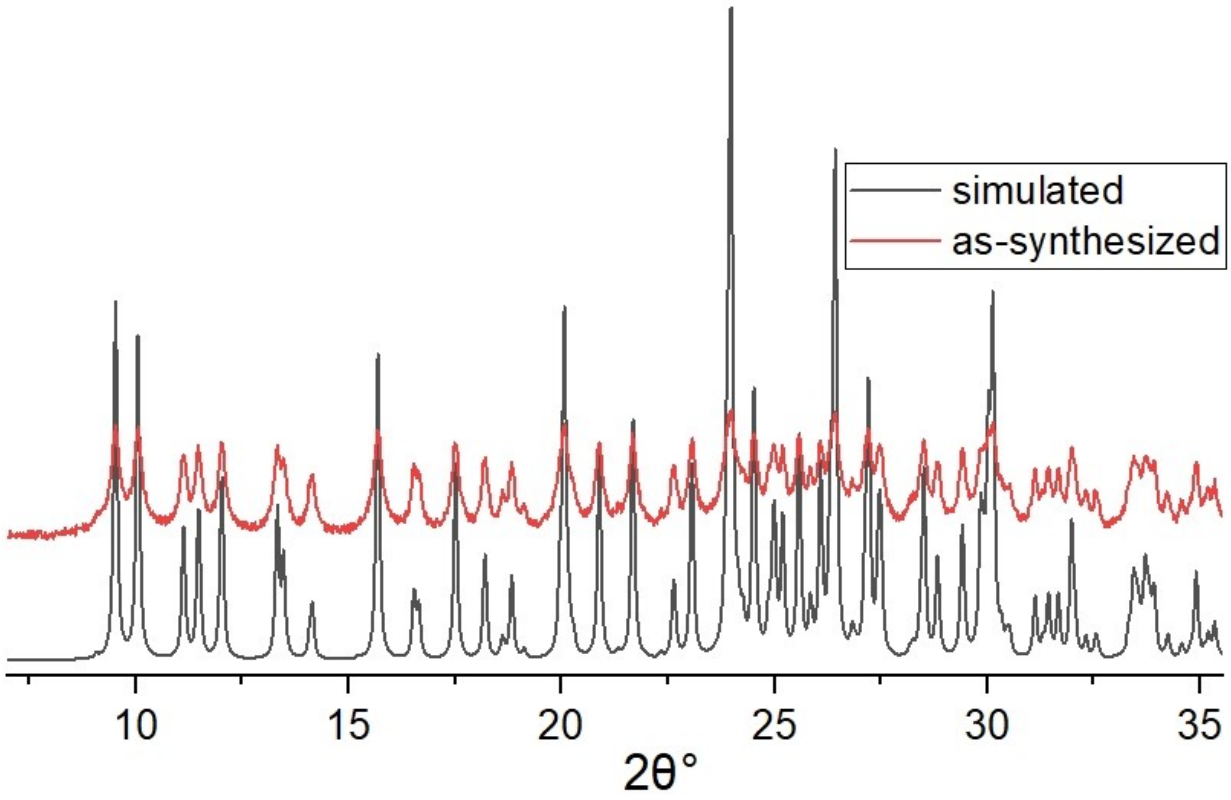

Figure 2S. PXRD data for **3**

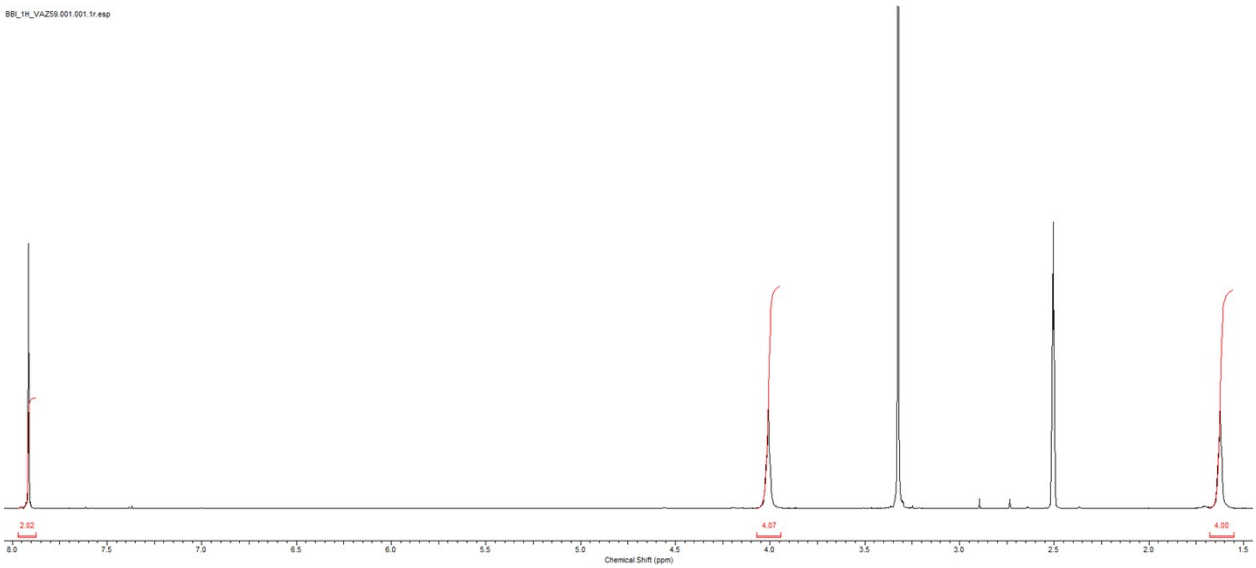

Figure 3S. ^{1}H NMR spectrum of 1 (d^{6}-DMSO)

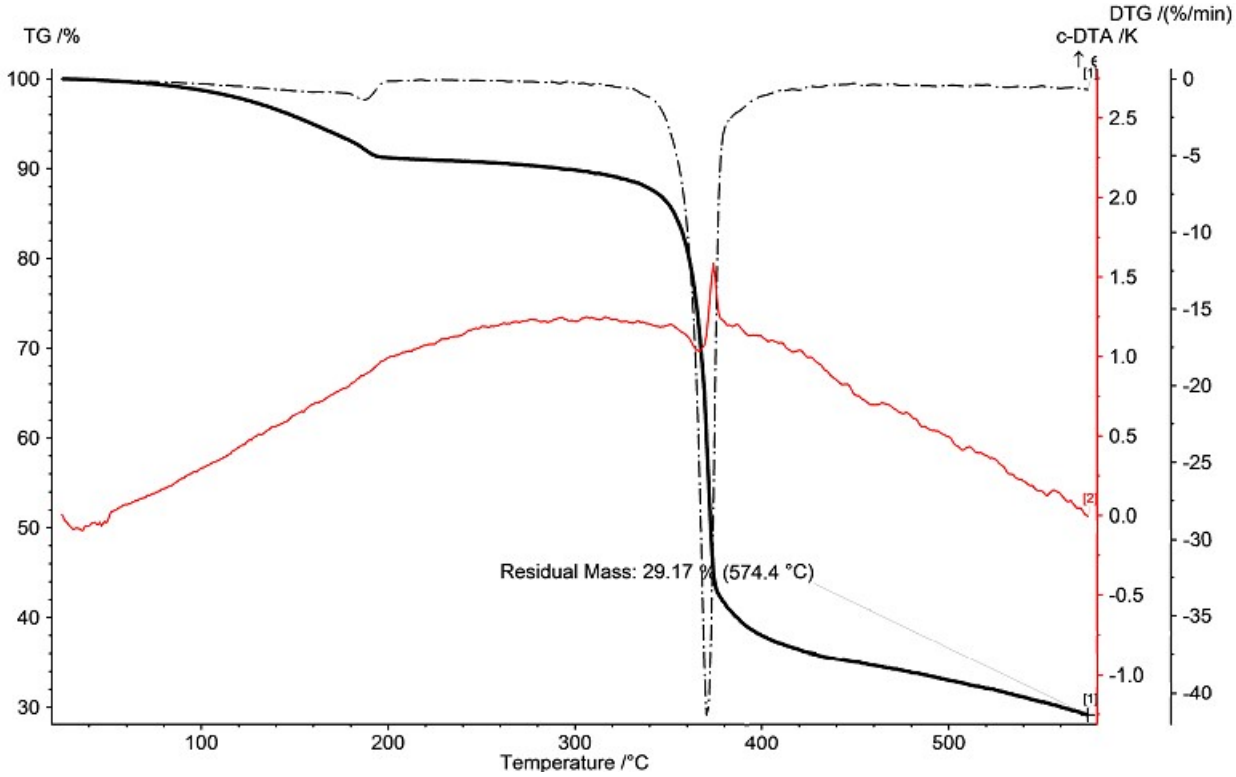

Figure 4S. TGA experiment for **2**

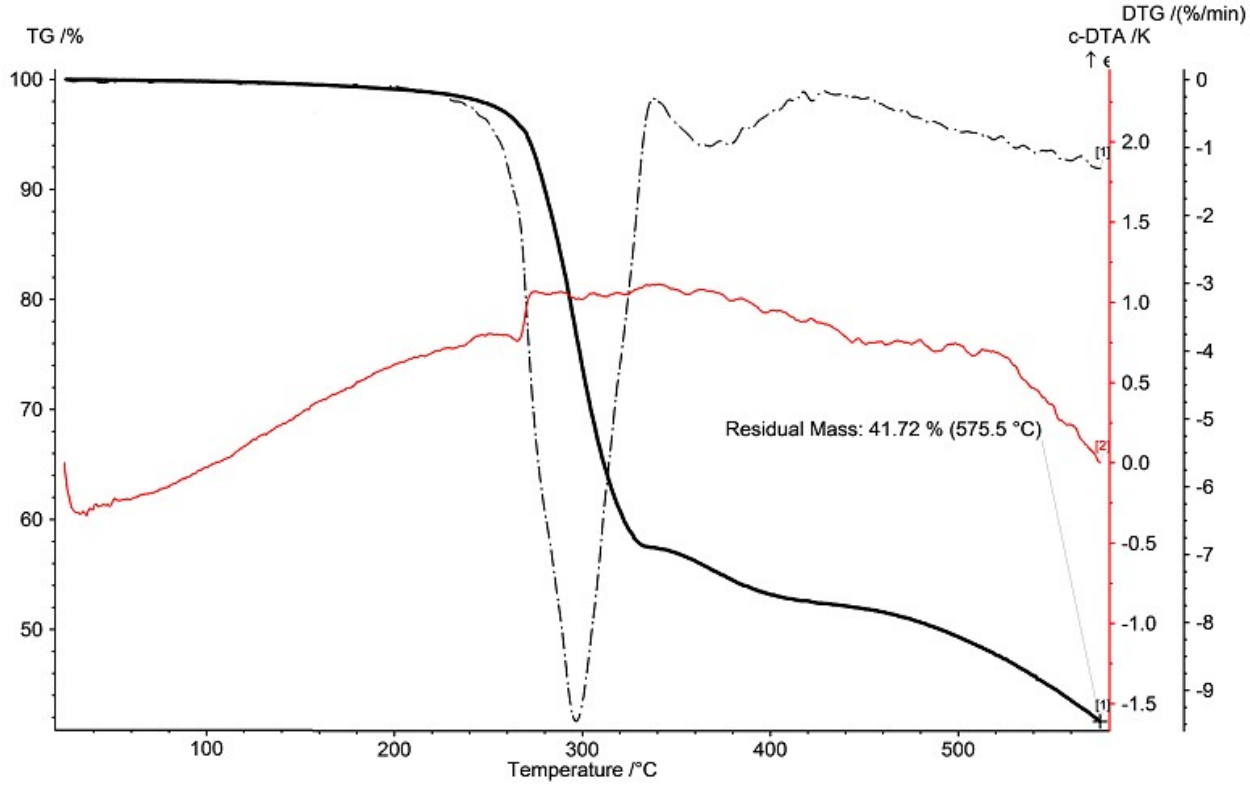

Figure 5S. TGA experiment for **3**

Computational details

The single point calculations based on the experimental X-ray geometries of **1**–**3** have been carried out at the DFT level of theory using the dispersion-corrected hybrid functional ωB97XD [Phys. Chem. Chem. Phys. 2008, 10, 6615.] with the help of Gaussian-09 [M. J. Frisch et al. Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT, 2010.] program package. The Douglas–Kroll–Hess 2nd order scalar relativistic calculations requested relativistic core Hamiltonian were carried out using the DZP-DKH basis sets [Mol. Phys. 2010, 108, 1965. || J. Chem. Phys. 2009, 130, 064108. || Chem. Phys. Lett. 2013, 582, 158. || J. Mol. Struct. - Theochem 2010, 961, 107.] for all atoms. The topological analysis of the electron density distribution has been performed by using the Multiwfn program (version 3.7) [J. Comput. Chem. 2012, 33, 580.]. The Cartesian atomic coordinates for model supramolecular associates are presented in **Table S5**, Supporting Information.

Table S5. Values of the density of all electrons – $\rho(\mathbf{r})$, Laplacian of electron density – $\nabla^2\rho(\mathbf{r})$ and appropriate λ_2 eigenvalues, energy density – H_b, potential energy density – $V(\mathbf{r})$, and Lagrangian kinetic energy – $G(\mathbf{r})$ (a.u.) at the bond critical points (3, –1) corresponding to various halogen bonds I···I, I···Cl, and I···Cu in the X-ray structures **1**–**3**, and estimated strength for these noncovalent interactions E_{int} (kcal/mol).

Contact*	$\%_{vdw\ sum}$	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_2	H_b	$V(\mathbf{r})$	$G(\mathbf{r})$	E_{int}**
1								
I30···I1 3.784 Å	96	0.009	0.033	-0.009	0.001	-0.006	0.007	2.6
2								
I60···Cl31 3.246 Å	87	0.016	0.051	-0.016	0.001	-0.011	0.012	4.7
I30···I1 3.909 Å	99	0.007	0.028	-0.007	0.002	-0.004	0.006	1.7
I93···Cl4 4.031 Å	108	0.004	0.014	-0.004	0.001	-0.002	0.003	0.9
3								
I68···I5 3.681 Å	93	0.013	0.050	-0.013	0.001	-0.011	0.012	4.7
I3···I38 3.796 Å	96	0.009	0.033	-0.009	0.001	-0.006	0.007	2.6
I66···I33 3.793 Å	96	0.010	0.033	-0.010	0.001	-0.006	0.007	2.6
I37···I2 4.033 Å	102	0.004	0.013	-0.004	0.001	-0.001	0.002	0.4
I66···Cu8 3.485 Å	103	0.009	0.028	-0.009	0.001	-0.006	0.007	2.6

* The Bondi's (shortest) van der Waals radii for iodine, chlorine, and copper atoms are 1.98, 1.75, and 1.40 Å, respectively [J. Phys. Chem. 1966, 70, 3006.]. The numeration of atoms corresponds to their ordering in attached xyz-files for model supramolecular associates.

** $E_{int} = 0.68(-V(\mathbf{r}))$ (this empirical correlation between the interaction energy and the potential energy density of electrons at the bond critical points (3, –1) was specifically developed for halogen bonds involving iodine atoms) [Russ. Chem. Rev. 2014, 83, 1181.]

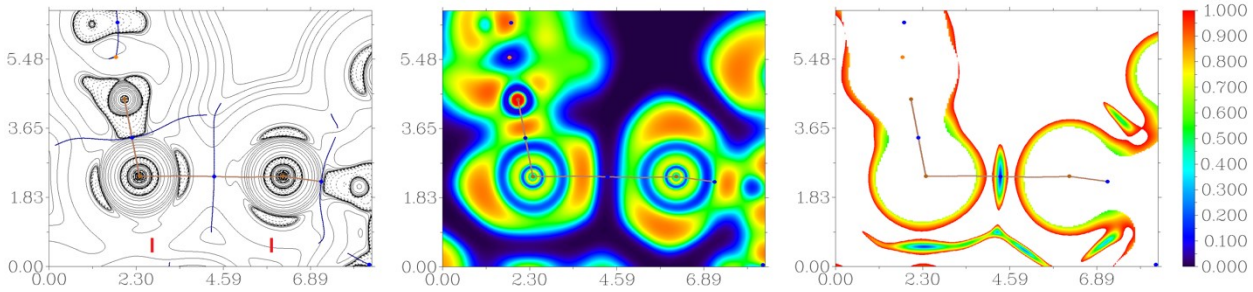

Figure 6S. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function (ELF, center panel) and reduced density gradient (RDG, right panel) analyses for halogen bonds I···I in **1**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) – in pale brown, ring critical points (3, +1) – in orange, length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

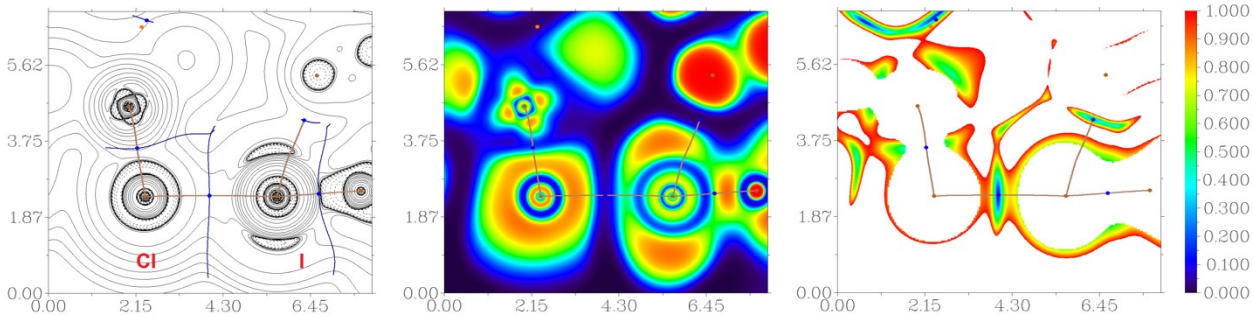

Figure 7S. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function (ELF, center panel) and reduced density gradient (RDG, right panel) analyses for halogen bonds I···Cl in **2**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) – in pale brown, ring critical points (3, +1) – in orange, length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

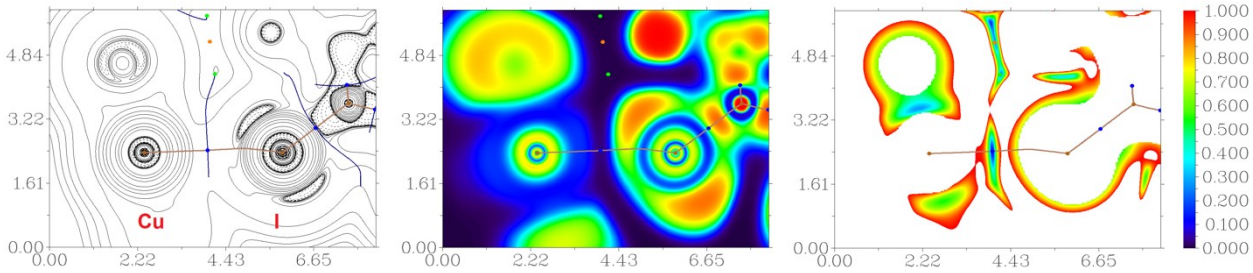

Figure 8S. Contour line diagram of the Laplacian of electron density distribution $\nabla^2\rho(\mathbf{r})$, bond paths, and selected zero-flux surfaces (left panel), visualization of electron localization function (ELF, center panel) and reduced density gradient (RDG, right panel) analyses for halogen bonds I···Cu in **3**. Bond critical points (3, –1) are shown in blue, nuclear critical points (3, –3) – in pale brown, ring critical points (3, +1) – in orange, cage critical points (3, +3) – in light green, length units – Å, and the color scale for the ELF and RDG maps is presented in a.u.

The QTAIM analysis of model supramolecular associates demonstrates the presence of bond critical points (3, –1) for various halogen bonds I···I, I···Cl, and I···Cu in the X-ray structures **1**–**3**. The low magnitude of the electron density (0.004–0.016 a.u.), positive values of the Laplacian of electron density (0.013–0.051 a.u.), and very close to zero positive energy density (0.001–0.002 a.u.) in these bond critical points (3, –1) and estimated strength for appropriate short contacts (0.4–4.7 kcal/mol) are typical for noncovalent interactions involving halogen atoms in similar chemical systems [Zeitschrift für Kristallographie-Crystalline Materials 2018 233 (6), 371-377; Crystal Growth & Design 2011 21 (2), 1136-1147; CrystEngComm 2019 21 (5), 850-856; CrystEngComm 2020 22 (3), 554-563; CrystEngComm 2019 21 (43), 6666-6670]. The balance between the Lagrangian kinetic energy G(**r**) and potential energy density V(**r**) at the bond critical points (3, –1) reveals the nature of these interactions, if the ratio –G(**r**)/V(**r**) > 1 is satisfied, than the nature of appropriate interaction is purely non-covalent, in case the –G(**r**)/V(**r**) < 1 some covalent component takes place [J. Chem. Phys. 2002, 117, 5529.]; based on this criterion one can state that a covalent contribution in all halogen bonds I···I, I···Cl, and I···Cu in the X-ray structures **1**–**3** is absent. The Laplacian of electron density is typically decomposed into the sum of contributions along the three principal axes of maximal variation, giving the three eigenvalues of the Hessian matrix (λ_1, λ_2 and λ_3), and the sign of λ_2 can be utilized to distinguish bonding (attractive, $\lambda_2 < 0$) weak interactions from non-bonding ones (repulsive, $\lambda_2 > 0$).[J. Am. Chem. Soc. 2010, 132, 6498. || J. Chem. Theory Comput. 2011, 7, 625.] Thus, all discussed intermolecular interactions I···I, I···Cl, and I···Cu in the X-ray structures **1**–**3** are attractive .

Table S6. Cartesian atomic coordinates for model supramolecular associates.

Atom	X	Y	Z
1			
I	2.856855	8.697483	3.903711
I	5.087910	5.554815	4.867978
C	4.383045	8.583056	5.296620
N	5.970516	7.889642	6.629619
N	4.770171	9.675220	6.025811
C	5.100985	7.464905	5.647807
C	6.927654	7.090722	7.410161
H	6.510741	6.222215	7.638333
H	7.124756	7.562911	8.257703
C	8.232168	6.833681	6.673267
H	8.630356	7.694095	6.388067
H	8.057913	6.290173	5.864325
C	5.729488	9.212728	6.812772
H	6.199514	9.750263	7.439332
I	14.577345	4.232117	10.360589
I	12.346290	7.374785	9.396322
C	13.051155	4.346544	8.967680
N	11.463684	5.039958	7.634681
N	12.664029	3.254380	8.238489
C	12.333215	5.464695	8.616493
C	10.506546	5.838878	6.854139
H	10.923459	6.707385	6.625967
H	10.309444	5.366689	6.006597
C	9.202032	6.095919	7.591033
H	8.803844	5.235505	7.876233
H	9.376287	6.639427	8.399975

C	11.704712	3.716872	7.451528
H	11.234686	3.179337	6.824968
I	5.860245	15.162283	3.228439
I	3.629190	12.019615	2.264172
C	4.334055	15.047856	1.835530
N	2.746584	14.354442	0.502531
N	3.946929	16.140020	1.106339
C	3.616115	13.929705	1.484343
C	1.789446	13.555522	-0.278011
H	2.206359	12.687015	-0.506183
H	1.592344	14.027711	-1.125553
C	0.484932	13.298481	0.458883
H	0.086744	14.158895	0.744083
H	0.659187	12.754973	1.267825
C	2.987612	15.677528	0.319378
H	2.517586	16.215063	-0.307182
I	-5.860245	10.696917	-3.228439
I	-3.629190	13.839585	-2.264172
C	-4.334055	10.811344	-1.835530
N	-2.746584	11.504758	-0.502531
N	-3.946929	9.719180	-1.106339
C	-3.616115	11.929495	-1.484343
C	-1.789446	12.303678	0.278011
H	-2.206359	13.172185	0.506183
H	-1.592344	11.831489	1.125553
C	-0.484932	12.560719	-0.458883
H	-0.086744	11.700305	-0.744083
H	-0.659187	13.104227	-1.267825
C	-2.987612	10.181672	-0.319378
H	-2.517586	9.644137	0.307182
I	10.218795	4.232117	-3.228439
I	7.987740	7.374785	-2.264172
C	8.692605	4.346544	-1.835530
N	7.105134	5.039958	-0.502531
N	8.305479	3.254380	-1.106339
C	7.974665	5.464695	-1.484343
C	6.147996	5.838878	0.278011
H	6.564909	6.707385	0.506183
H	5.950894	5.366689	1.125553
C	4.843482	6.095919	-0.458883
H	4.445294	5.235505	-0.744083
H	5.017737	6.639427	-1.267825
C	7.346162	3.716872	-0.319378
H	6.876136	3.179337	0.307182
I	-1.501695	8.697483	3.228439
I	0.729360	5.554815	2.264172
C	0.024495	8.583056	1.835530
N	1.611966	7.889642	0.502531
N	0.411621	9.675220	1.106339
C	0.742435	7.464905	1.484343
C	2.569104	7.090722	-0.278011
H	2.152191	6.222215	-0.506183

H	2.766206	7.562911	-1.125553
C	3.873618	6.833681	0.458883
H	4.271806	7.694095	0.744083
H	3.699363	6.290173	1.267825
C	1.370938	9.212728	0.319378
H	1.840964	9.750263	-0.307182
2_part1			
I	7.285618	12.294171	11.046024
I	4.203584	10.377481	12.713710
Co	3.026833	7.880966	10.134215
Cl	3.092667	6.652019	8.247359
N	4.615712	9.108614	9.981391
N	6.260543	10.241491	9.034450
C	5.365323	9.251907	8.888382
H	5.277634	8.720830	8.105872
C	5.078912	10.067851	10.865229
C	6.095739	10.770524	10.296362
C	6.706076	11.971396	7.333118
H	6.677015	12.697712	8.005286
H	5.789513	11.836022	6.985352
C	7.196835	10.689384	7.989815
H	7.287963	9.981940	7.303012
H	8.088613	10.844750	8.390143
I	7.065993	12.047829	2.466262
I	10.148028	13.964519	0.798576
N	9.735899	15.233386	3.530895
N	8.091069	14.100509	4.477836
C	8.986288	15.090093	4.623904
H	9.073977	15.621170	5.406414
C	9.272700	14.274149	2.647057
C	8.255872	13.571476	3.215924
C	7.645535	12.370604	6.179168
H	7.674596	11.644288	5.507000
H	8.562098	12.505978	6.526934
C	7.154776	13.652616	5.522471
H	7.063649	14.360060	6.209274
H	6.262998	13.497250	5.122143
Cl	2.961000	6.652019	12.021070
N	1.437955	9.108614	10.287039
I	-1.231951	12.294171	9.222405
I	1.850083	10.377481	7.554719
N	-0.206876	10.241491	11.233980
C	0.688344	9.251907	11.380047
H	0.776033	8.720830	12.162557
C	0.974755	10.067851	9.403200
C	-0.042072	10.770524	9.972067
C	-0.652409	11.971396	12.935311
H	-0.623348	12.697712	12.263143
H	0.264154	11.836022	13.283077
C	-1.143168	10.689384	12.278614
H	-1.234296	9.981940	12.965417
H	-2.034946	10.844750	11.878286

I	-1.012326	12.047829	17.802167
I	-4.094361	13.964519	19.469853
N	-3.682232	15.233386	16.737534
N	-2.037402	14.100509	15.790593
C	-2.932621	15.090093	15.644525
H	-3.020310	15.621170	14.862015
C	-3.219033	14.274149	17.621372
C	-2.202206	13.571476	17.052505
C	-1.591868	12.370604	14.089261
H	-1.620929	11.644288	14.761429
H	-2.508431	12.505978	13.741495
C	-1.101109	13.652616	14.745958
H	-1.009982	14.360060	14.059155
H	-0.209331	13.497250	15.146286
I	11.502507	12.294171	-2.466262
I	8.420472	10.377481	-0.798576
Co	7.243722	7.880966	-3.378072
Cl	7.309556	6.652019	-5.264927
N	8.832601	9.108614	-3.530895
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C	9.582212	9.251907	-4.623904
H	9.494523	8.720830	-5.406414
C	9.295800	10.067851	-2.647057
C	10.312628	10.770524	-3.215924
C	10.922965	11.971396	-6.179168
H	10.893904	12.697712	-5.507000
H	10.006402	11.836022	-6.526934
C	11.413724	10.689384	-5.522471
H	11.504851	9.981940	-6.209274
H	12.305502	10.844750	-5.122143
I	11.282882	12.047829	-11.046024
I	14.364916	13.964519	-12.713710
N	13.952788	15.233386	-9.981391
N	12.307957	14.100509	-9.034450
C	13.203177	15.090093	-8.888382
H	13.290866	15.621170	-8.105872
C	13.489588	14.274149	-10.865229
C	12.472761	13.571476	-10.296362
C	11.862424	12.370604	-7.333118
H	11.891485	11.644288	-8.005286
H	12.778987	12.505978	-6.985352
C	11.371665	13.652616	-7.989815
H	11.280537	14.360060	-7.303012
H	10.479887	13.497250	-8.390143
Cl	7.177889	6.652019	-1.491216
N	5.654844	9.108614	-3.225248
I	2.984937	12.294171	-4.289881
I	6.066972	10.377481	-5.957567
N	4.010013	10.241491	-2.278307
C	4.905233	9.251907	-2.132239
H	4.992922	8.720830	-1.349729
C	5.191644	10.067851	-4.109086

C	4.174817	10.770524	-3.540219
C	3.564480	11.971396	-0.576975
H	3.593540	12.697712	-1.249143
H	4.481042	11.836022	-0.229209
C	3.073721	10.689384	-1.233672
H	2.982593	9.981940	-0.546869
H	2.181942	10.844750	-1.634000
I	3.204563	12.047829	4.289881
I	0.122528	13.964519	5.957567
N	0.534656	15.233386	3.225248
N	2.179487	14.100509	2.278307
C	1.284267	15.090093	2.132239
H	1.196578	15.621170	1.349729
C	0.997856	14.274149	4.109086
C	2.014683	13.571476	3.540219
C	2.625020	12.370604	0.576975
H	2.595960	11.644288	1.249143
H	1.708458	12.505978	0.229209
C	3.115779	13.652616	1.233672
H	3.206907	14.360060	0.546869
H	4.007558	13.497250	1.634000
2_part2			
I	7.285618	12.294171	11.046024
I	4.203584	10.377481	12.713710
Co	3.026833	7.880966	10.134215
Cl	3.092667	6.652019	8.247359
N	4.615712	9.108614	9.981391
N	6.260543	10.241491	9.034450
C	5.365323	9.251907	8.888382
H	5.277634	8.720830	8.105872
C	5.078912	10.067851	10.865229
C	6.095739	10.770524	10.296362
C	6.706076	11.971396	7.333118
H	6.677015	12.697712	8.005286
H	5.789513	11.836022	6.985352
C	7.196835	10.689384	7.989815
H	7.287963	9.981940	7.303012
H	8.088613	10.844750	8.390143
I	7.065993	12.047829	2.466262
I	10.148028	13.964519	0.798576
N	9.735899	15.233386	3.530895
N	8.091069	14.100509	4.477836
C	8.986288	15.090093	4.623904
H	9.073977	15.621170	5.406414
C	9.272700	14.274149	2.647057
C	8.255872	13.571476	3.215924
C	7.645535	12.370604	6.179168
H	7.674596	11.644288	5.507000
H	8.562098	12.505978	6.526934
C	7.154776	13.652616	5.522471
H	7.063649	14.360060	6.209274
H	6.262998	13.497250	5.122143

Cl	2.961000	6.652019	12.021070
N	1.437955	9.108614	10.287039
I	-1.231951	12.294171	9.222405
I	1.850083	10.377481	7.554719
N	-0.206876	10.241491	11.233980
C	0.688344	9.251907	11.380047
H	0.776033	8.720830	12.162557
C	0.974755	10.067851	9.403200
C	-0.042072	10.770524	9.972067
C	-0.652409	11.971396	12.935311
H	-0.623348	12.697712	12.263143
H	0.264154	11.836022	13.283077
C	-1.143168	10.689384	12.278614
H	-1.234296	9.981940	12.965417
H	-2.034946	10.844750	11.878286
I	-1.012326	12.047829	17.802167
I	-4.094361	13.964519	19.469853
N	-3.682232	15.233386	16.737534
N	-2.037402	14.100509	15.790593
C	-2.932621	15.090093	15.644525
H	-3.020310	15.621170	14.862015
C	-3.219033	14.274149	17.621372
C	-2.202206	13.571476	17.052505
C	-1.591868	12.370604	14.089261
H	-1.620929	11.644288	14.761429
H	-2.508431	12.505978	13.741495
C	-1.101109	13.652616	14.745958
H	-1.009982	14.360060	14.059155
H	-0.209331	13.497250	15.146286
I	1.096118	4.180171	11.046024
I	-1.985916	2.263481	12.713710
N	-1.573788	0.994614	9.981391
N	0.071043	2.127491	9.034450
C	-0.824177	1.137907	8.888382
H	-0.911866	0.606830	8.105872
C	-1.110588	1.953851	10.865229
C	-0.093761	2.656524	10.296362
C	0.516576	3.857396	7.333118
H	0.487515	4.583712	8.005286
H	-0.399987	3.722022	6.985352
C	1.007335	2.575384	7.989815
H	1.098463	1.867940	7.303012
H	1.899113	2.730750	8.390143
I	0.876493	3.933829	2.466262
I	3.958528	5.850519	0.798576
N	3.546399	7.119386	3.530895
N	1.901569	5.986509	4.477836
C	2.796788	6.976093	4.623904
H	2.884477	7.507170	5.406414
C	3.083200	6.160149	2.647057
C	2.066372	5.457476	3.215924
C	1.456035	4.256604	6.179168

H	1.485096	3.530288	5.507000
H	2.372598	4.391978	6.526934
C	0.965276	5.538616	5.522471
H	0.874149	6.246060	6.209274
H	0.073498	5.383250	5.122143
Co	5.135278	8.347034	3.378072
Cl	5.069444	9.575981	5.264927
Cl	5.201111	9.575981	1.491216
N	6.724156	7.119386	3.225248
I	9.394063	3.933829	4.289881
I	6.312028	5.850519	5.957567
N	8.368987	5.986509	2.278307
C	7.473767	6.976093	2.132239
H	7.386078	7.507170	1.349729
C	7.187356	6.160149	4.109086
C	8.204183	5.457476	3.540219
C	8.814520	4.256604	0.576975
H	8.785460	3.530288	1.249143
H	7.897958	4.391978	0.229209
C	9.305279	5.538616	1.233672
H	9.396407	6.246060	0.546869
H	10.197058	5.383250	1.634000
I	9.174437	4.180171	-4.289881
I	12.256472	2.263481	-5.957567
N	11.844344	0.994614	-3.225248
N	10.199513	2.127491	-2.278307
C	11.094733	1.137907	-2.132239
H	11.182422	0.606830	-1.349729
C	11.381144	1.953851	-4.109086
C	10.364317	2.656524	-3.540219
C	9.753980	3.857396	-0.576975
H	9.783040	4.583712	-1.249143
H	10.670542	3.722022	-0.229209
C	9.263221	2.575384	-1.233672
H	9.172093	1.867940	-0.546869
H	8.371442	2.730750	-1.634000
3_part1			
I	1.156525	5.870451	-0.629135
I	-0.339658	6.422039	3.046477
I	4.981606	7.394024	10.131915
I	3.369303	5.920553	13.453606
I	-0.472069	1.609441	10.839377
I	2.750357	1.722749	13.961290
Cu	0.848658	3.401254	12.283596
Cu	1.527013	0.635452	11.998449
N	2.681010	4.017281	1.207728
N	1.833197	4.300167	3.228403
N	2.862829	5.388235	9.283890
N	1.981869	4.540504	11.137977
C	1.664571	4.930994	1.136567
C	1.126119	5.123695	2.378744
C	2.752583	3.659165	2.474296

H	3.374672	3.027506	2.814776
C	1.682773	4.134598	4.678280
H	1.904330	3.200244	4.918317
H	0.735675	4.291503	4.921573
C	2.558280	5.069893	5.486701
H	2.284436	6.009350	5.336068
H	3.504836	4.971276	5.215257
C	2.390330	4.700523	6.963986
H	1.429188	4.729182	7.200918
H	2.712175	3.775634	7.108345
C	3.154212	5.641522	7.866702
H	4.125353	5.530788	7.708136
H	2.913505	6.575737	7.645235
C	2.916844	5.496456	11.482593
C	3.468083	6.026462	10.353570
C	1.982360	4.517688	9.809175
H	1.424896	3.950669	9.289761
I	2.294603	-1.722749	11.183993
Cu	3.517947	-0.635452	13.146834
I	5.517029	-1.609441	14.305906
Cu	4.196302	-3.401254	12.861687
I	-1.156525	9.545649	0.629135
I	0.339658	8.994061	-3.046477
I	-4.981606	8.022076	-10.131915
I	-3.369303	9.495547	-13.453606
N	-2.681010	11.398819	-1.207728
N	-1.833197	11.115933	-3.228403
N	-2.862829	10.027865	-9.283890
N	-1.981869	10.875596	-11.137977
C	-1.664571	10.485106	-1.136567
C	-1.126119	10.292405	-2.378744
C	-2.752583	11.756935	-2.474296
H	-3.374672	12.388594	-2.814776
C	-1.682773	11.281502	-4.678280
H	-1.904330	12.215856	-4.918317
H	-0.735675	11.124597	-4.921573
C	-2.558280	10.346207	-5.486701
H	-2.284436	9.406750	-5.336068
H	-3.504836	10.444824	-5.215257
C	-2.390330	10.715577	-6.963986
H	-1.429188	10.686918	-7.200918
H	-2.712175	11.640466	-7.108345
C	-3.154212	9.774578	-7.866702
H	-4.125353	9.885312	-7.708136
H	-2.913505	8.840363	-7.645235
C	-2.916844	9.919644	-11.482593
C	-3.468083	9.389638	-10.353570
C	-1.982360	10.898412	-9.809175
H	-1.424896	11.465431	-9.289761
I	-2.858815	1.837599	-6.915456
I	-4.354998	1.286011	-3.239844
I	0.966266	0.314026	3.845594

I	-0.646037	1.787497	7.167286
N	-1.334330	3.690769	-5.078593
N	-2.182143	3.407883	-3.057918
N	-1.152511	2.319815	2.997569
N	-2.033471	3.167546	4.851657
C	-2.350769	2.777056	-5.149754
C	-2.889221	2.584355	-3.907577
C	-1.262757	4.048885	-3.812025
H	-0.640668	4.680544	-3.471545
C	-2.332567	3.573452	-1.608041
H	-2.111010	4.507806	-1.368004
H	-3.279665	3.416547	-1.364748
C	-1.457060	2.638157	-0.799620
H	-1.730904	1.698700	-0.950253
H	-0.510504	2.736774	-1.071063
C	-1.625010	3.007527	0.677665
H	-2.586152	2.978868	0.914597
H	-1.303165	3.932416	0.822024
C	-0.861128	2.066528	1.580381
H	0.110013	2.177262	1.421815
H	-1.101835	1.132313	1.358914
C	-1.098496	2.211594	5.196273
C	-0.547257	1.681588	4.067250
C	-2.032980	3.190362	3.522854
H	-2.590444	3.757381	3.003441
3_part2			
I	1.156525	5.870451	-0.629135
I	-0.339658	6.422039	3.046477
I	4.981606	7.394024	10.131915
I	3.369303	5.920553	13.453606
I	-0.472069	1.609441	10.839377
I	2.750357	1.722749	13.961290
Cu	0.848658	3.401254	12.283596
Cu	1.527013	0.635452	11.998449
N	2.681010	4.017281	1.207728
N	1.833197	4.300167	3.228403
N	2.862829	5.388235	9.283890
N	1.981869	4.540504	11.137977
C	1.664571	4.930994	1.136567
C	1.126119	5.123695	2.378744
C	2.752583	3.659165	2.474296
H	3.374672	3.027506	2.814776
C	1.682773	4.134598	4.678280
H	1.904330	3.200244	4.918317
H	0.735675	4.291503	4.921573
C	2.558280	5.069893	5.486701
H	2.284436	6.009350	5.336068
H	3.504836	4.971276	5.215257
C	2.390330	4.700523	6.963986
H	1.429188	4.729182	7.200918
H	2.712175	3.775634	7.108345
C	3.154212	5.641522	7.866702

H	4.125353	5.530788	7.708136
H	2.913505	6.575737	7.645235
C	2.916844	5.496456	11.482593
C	3.468083	6.026462	10.353570
C	1.982360	4.517688	9.809175
H	1.424896	3.950669	9.289761
I	2.294603	-1.722749	11.183993
Cu	3.517947	-0.635452	13.146834
I	5.517029	-1.609441	14.305906
Cu	4.196302	-3.401254	12.861687
I	6.874155	9.545649	13.201776
I	8.370339	8.994061	9.526165
I	3.049074	8.022076	2.440727
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N	5.349670	11.398819	11.364914
N	6.197483	11.115933	9.344239
N	5.167851	10.027865	3.288752
N	6.048812	10.875596	1.434664
C	6.366109	10.485106	11.436075
C	6.904561	10.292405	10.193898
C	5.278097	11.756935	10.098346
H	4.656008	12.388594	9.757866
C	6.347907	11.281502	7.894362
H	6.126350	12.215856	7.654325
H	7.295005	11.124597	7.651068
C	5.472400	10.346207	7.085941
H	5.746244	9.406750	7.236574
H	4.525844	10.444824	7.357384
C	5.640350	10.715577	5.608655
H	6.601492	10.686918	5.371724
H	5.318505	11.640466	5.464296
C	4.876468	9.774578	4.705940
H	3.905327	9.885312	4.864506
H	5.117175	8.840363	4.927407
C	5.113836	9.919644	1.090048
C	4.562597	9.389638	2.219071
C	6.048320	10.898412	2.763467
H	6.605784	11.465431	3.282880
I	5.171865	1.837599	5.657186
I	3.675682	1.286011	9.332798
I	8.996946	0.314026	16.418235
I	7.384643	1.787497	19.739927
N	6.696350	3.690769	7.494049
N	5.848537	3.407883	9.514724
N	6.878169	2.319815	15.570211
N	5.997209	3.167546	17.424298
C	5.679911	2.777056	7.422888
C	5.141459	2.584355	8.665065
C	6.767923	4.048885	8.760617
H	7.390012	4.680544	9.101096
C	5.698113	3.573452	10.964601
H	5.919670	4.507806	11.204638

H	4.751015	3.416547	11.207894
C	6.573620	2.638157	11.773021
H	6.299776	1.698700	11.622389
H	7.520176	2.736774	11.501578
C	6.405670	3.007527	13.250307
H	5.444528	2.978868	13.487238
H	6.727515	3.932416	13.394666
C	7.169552	2.066528	14.153023
H	8.140693	2.177262	13.994456
H	6.928845	1.132313	13.931555
C	6.932184	2.211594	17.768914
C	7.483423	1.681588	16.639891
C	5.997700	3.190362	16.095496
H	5.440236	3.757381	15.576082