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1. Introduction

Polymorphism is the phenomenon where materials possess various distinct natures of their physical and chemical properties,¹ including melting point,² hardness, stability,³ dissolution rate⁴ and so on. For example, the chemical compositions of diamond and graphite are both carbon; however, the former is a cubic crystal system that is hard, transparent and non-conductive,⁵ while the latter is a hexagonal system that is soft, opaque and conductive.^{6,7} Magnetic fields can have a great influence on the crystal growth of various alloys,⁸ in order to improve the material properties during material processing.⁹ In particular, the electrons can be offset when the complex contains a large number of conjugated electrons in the presence of a magnetic field.¹⁰

Porphyrins are widely found compounds in animals and plants.¹¹ In recent years, porphyrin compounds have increasingly become prominent in the fields of biochemistry,¹² medicine,¹³ analytical chemistry,¹⁴ synthetic chemistry^{15,16} and materials science. A metal-tetraphenylporphine is a porphyrin complex formed after complexation of a metal ion with a phenyl-substituted metazepine compound.^{17,18} The metalloporphyrin complex as the main molecule has its own unique advantages,

Tuning the crystal structures of metaltetraphenylporphines *via* a magnetic field[†]

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In this work, two new single crystals of copper-tetraphenylporphine (Cu-TPP) (crystals 2 and 3), which were induced by external magnetic fields with strengths of 0.5 and 0.8 T, respectively, have been prepared and characterized by single-crystal X-ray diffraction and Hirshfeld surface analysis. Compared with the original Cu-TPP (crystal 1), crystals 2 and 3 exhibit significant differences in their unit cell parameters, crystalline stacking styles and intermolecular interactions, resulting in a "compressed" crystal packing. Here, the number of closer interactions (H \cdots H, C \cdots H/H \cdots C) increased with the magnetic field strength, accompanied by a decrease in the number of $\pi \cdots \pi$ (C \cdots C) interactions as a sacrifice. On considering the results of our previous work, the results here suggest that a magnetic field has a different influence on the crystallization process of mono-component and multi-component materials, which will certainly provide some suggestions for the design of crystallization strategies for other materials with the presence of an external magnetic field.

such as rigid structure, large surface and so on, which can be used in a variety of organic and biological processes for molecular identification.¹⁹ Metalloporphyrins can be viewed as functional objects; they can be introduced into interlayer compounds, giving many excellent properties, and thus have been shown to have a wide range of applications in optoelectronic materials, such as magnetic materials,^{20,21} and nonlinear optical materials.²²⁻²⁴ The unique structure and properties of the metalloporphyrin compounds make them widely used in the fields of biochemistry, analytical chemistry, synthetic chemistry, pharmaceutical chemistry and biomimetic catalysis, medicine, materials science and energy science.25 It should be noted that the crystallization process can be influenced by external physical stimuli, such as light, pressure, and a magnetic field,²⁶ which can change the properties of semiconductor and NLO materials.²⁷ Xiao's group discovered a kind of up-conversion luminescence of nano-crystals modulated by a magnetic field, and they found an enhancement in the up-conversion intensities induced by the magnetic field, which has been widely applied for optical detection of magnetic fields.²⁷ On considering the large number of conjugated electrons within metalloporphyrin-related compounds, magnetic fields may have a significant influence on their crystallization process.

Asamitsu's group studied the structural phase transition of crystals induced by an external magnetic field in 1995.²⁸ Based on our previous work on the tuning of the intermolecular interactions between co-crystals by an external magnetic field,²⁹ in this work, we performed the crystallization of copper-tetraphenylporphine (Cu-TPP) in the presence of an external magnetic field.



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As a result, two new single crystals of Cu-TPP have been obtained under a magnetic field of 0.5 (crystal 2) and 0.8 T (crystal 3), respectively. We compared in detail the crystal structures and interactions of crystals 2 and 3, along with the original crystal of Cu-TPP (crystal 1, without an external magnetic field), with the help of single-crystal X-ray diffraction and three-dimensional (3-D) Hirshfeld surface analysis. The results revealed that the external magnetic field had a "compressive effect" on the unit cell parameters, crystalline stacking styles and intermolecular interactions. These results may provide some suggestions for the design of crystallization processes with the presence of an external magnetic field.

2. Experimental

2.1 Materials

5,10,15,20-Tetraphenylporphyrin (H₂TPP, purity 98–99%, CAS registry number: 917-23-7), copper nitrate hexahydrate (purity > 98%, CAS registry number: 10402-29-6), nickel acetate (purity > 97%, CAS registry number: 373-02-4) and *N*,*N*-dimethyl-formamide were purchased from SIGMA. All the solvents (reagent grade) used were commercially available from Sinopharm Chemical Reagent and used as received without further purification.

2.2 Preparation of copper tetraphenylporphine (Cu-TPP)

The tetraphenylporphyrin (1 mmol, 0.6147 g) and *N*,*N*-dimethylformamide (50 ml) were put into a round bottom flask, heated and stirred under reflux, after dissolving nickel acetate (0.05 g) into the solution as a catalyst and then adding a few times more copper nitrate (1.2 mmol, 0.2251 g). The reaction was continued, the point plate set the reaction end, and after the reaction, rotatory evaporation gave a purple powder, which was washed with water several times and filtered to give the product.³⁰ Then, the purple powder was dissolved in methanol and slow evaporation was performed under a magnetic field of 0.5 T and 0.8 T, respectively (Scheme 1). Finally, the two new crystals of Cu-TPP 2 and 3 were obtained.

2.3 X-ray crystallographic study

The single-crystal X-ray diffraction data of crystals 2 and 3 were collected with graphite-monochromated Cu-K α radiation at a

Scheme 1 Schematic illustration of the crystallization under an external magnetic field.

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Table 1 Crystal data and structure refinements for crystals 1, 2 and 3

Crystal	1	2	3
Formula	C44H28CuN4	C44H28CuN4	C44H28CuN4
Formula weight	676.24	676.24	676.24
Crystal system	Tetragonal	Tetragonal	Tetragonal
Space group	$I\bar{4}2d$	I42d	$I\bar{4}2d$
Z	4	4	4
a/Å	15.03	15.0159	15.0099
b/Å	15.03	15.0159	15.0099
c/Å	13.99	13.7387	13.6593
$\alpha/^{\circ}$	90	90	90
$\beta/^{\circ}$	90	90	90
γ/°	90	90	90
$V/\text{\AA}^3$	3160.35	3097.76	3077.40
T/K	295	295	295
$\mu (\mathrm{mm}^{-1})$		0.75	1.32
No. of reflns collected		8536	2895
No. of unique reflns		1373	1372
No. of params		111	111
Goodness-of-fit on F^2		1.081	1.081
R_1 , w R_2 $(I > 2\sigma(I))$		0.0501, 0.1269	0.0409, 0.1073
R_1 , w R_2 (all data)		0.0511, 0.1276	0.0417, 0.1079
CCDC	1133854	1829731	1829732

temperature of 295 K, using a SuperNova diffractometer with the ω -scan technique. The lattice parameters were integrated using vector analysis and refined from the diffraction matrix, while the SCALE3 ABSPACK program with the multi-scan method was used for absorption correction. The crystallographic data and refinement parameters for crystals 2 and 3 are summarized in Table 1. Their structures were solved by spherical harmonics methods, and the structure solution and structure refinement were completed by using the SHELXS-2014 and SHELXL-2014 programs, respectively.³¹ All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were inserted at their calculated positions and fixed at their positions. The molecular graphics were prepared by using the mercury and diamond programs (Fig. 1).

2.4 Hirshfeld surface calculations

Molecular Hirshfeld surface calculations were performed by using the CrystalExplorer17 program.³² When the cif files were read into the CrystalExplorer17 program for analysis, all bond lengths to hydrogen were automatically modified to typical standard neutron values. In this study, all the Hirshfeld surfaces were generated using a standard (high) surface resolution. The 3D d_{norm} surfaces were mapped by using a fixed color scale of -0.6311 to 1.2014 Å. Shape index was mapped in the color range of -1.00–1.00 Å, Curvedness was mapped in the range of -4.00–0.40 Å, Fragment Patch was mapped in the color range of -0.008 to -0.008 Å. The 2D fingerprint plots were displayed by using the standard 0.6–2.6 Å view with the d_e and d_i distance scales displayed on the graph axes.

3. Results and discussion

3.1 Crystal structure of crystals 2 and 3

Crystals 2 and 3 were both crystallized in the tetragonal crystal system, with space group $I\bar{4}2d$, identical to crystal 1 (Table 1).

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Fig. 1 The molecular graphics of Cu-TPP ((a) crystal 2, (b) crystal 3).

The unit cell parameters of **2** and **3** are a = 15.0159 Å, b = 15.0159 Å, c = 13.7387 Å, $\alpha = \beta = \gamma = 90^{\circ}$, V = 3097.76 Å³, and a = 15.0099 Å, b = 15.0099 Å, c = 13.6593 Å, $\alpha = \beta = \gamma = 90^{\circ}$, V = 3077.40 Å³, respectively. Compared with crystal **1**, the unit

cell of Cu-TPP exhibited a linear decrease with increasing magnetic field strength, indicating a "compressed" crystal packing induced by the magnetic field. It should be noted that these results were opposite to the influence of a magnetic field



Fig. 2 Molecular connecting and packing styles of crystals 1-3.



Fig. 3 Comparison between the crystal voids of crystals 1-3 along the *a*-axis.

on the crystal structures of co-crystals,²⁹ indicating the different influence of a magnetic field on the crystallization process of mono-component and multi-component materials.

To confirm the "compressive effect" that was induced by the external magnetic field, a detailed comparison was performed between the crystal structures and intermolecular interactions for crystals 1–3. The crystal structures of crystals 1–3 are shown in Fig. 2. Here, all three crystals exhibit similar connecting and stacking styles, their basic unit is the "glyph" motif that is composed of three Cu-TPP molecules (Fig. 2a–c), and the adjacent units in crystals 2 and 3 are connected by $H \cdots C-H$ and $N \cdots H-C$ hydrogen bonding contacts into a one-dimensional (1D) "double-chain" structure (Fig. 2e and f). Meanwhile, in crystal 1, the 1D "double-chain" structure is connected by $H \cdots H$ and $C-H \cdots C$ contacts (Fig. 2d), demonstrating the significant influence of the magnetic field on the crystal structures and intermolecular interactions. Interestingly, in crystals 1–3, the Cu-TPP molecules are stacked into "oval capsule" motifs along

Table 2Selected bond distances of crystals 1, 2, and 3

Bonds	1	2	3
Cu1-N1	1.979	1.985	1.983
N1-C6	1.382	1.371	1.370
N1-C1	1.385	1.375	1.380
C5-C4	1.337	1.349	1.351
C5-C6	1.460	1.443	1.450
C8-C2	1.399	1.385	1.389
C8-C10	1.380	1.387	1.389
C8-C7	1.489	1.502	1.493
C4-C1	1.435	1.446	1.445
C11-C9	1.388	1.381	1.382
C11-C10	1.394	1.391	1.394
C1-C7	1.379	1.389	1.402
C9-C3	1.345	1.375	1.384
C3-C2	1.413	1.401	1.397
C7-C6	1.358	1.395	1.391

the *a*-axis (Fig. 2g–i), and the transverse distances of the "oval capsule" were found to be 12.5178, 10.4625 and 8.2563 Å for crystals **1**, **2** and **3** (respectively), demonstrating clearly the "compressive effect" that was induced by the external magnetic field. It should be noted that the major intermolecular contacts in crystals **2** and **3** were the C–H···C and C–H···N contacts, and their distances were 2.742 and 1.701 Å for **2**, and 2.733 and 2.689 Å for **3**. Meanwhile, for crystal **1**, the main interactions were H···H and C–H···C contacts, with C–H···C distances of 2.884 Å (Fig. 2j–l). It should be noted that the distance of the weak intermolecular C2–H6···C6 contacts decreased with increasing magnetic field strength, from 2.773 Å in crystal **1** to 2.742 Å and 2.733 Å in crystals **2** and **3**, respectively, demonstrating the profound "compressive effect" caused by an external magnetic field.

The "compressive effect" was also derived from the crystal voids, defined as a par value of the procrystal electron density with the isovalue equal to 0.002 *e* a.u. (Fig. 3). With increasing magnetic field strength, the crystal voids of crystals **1–3** tended to get smaller, and their void shape tended to be different. For crystal **1**, the volume and area were calculated to be 403 Å³ and 1313.80 Å², respectively, while for **2** and **3**, the calculated volume and area were decreased to 299.38 Å³ and 1065.28 Å², and 280.83 Å³ and 1027.46 Å², respectively, demonstrating directly the "compressive effect" induced by the external magnetic field.

Selected bond distances and bond angles of the crystals 1–3 are listed in Table 2 and Table S2 (ESI[†]), respectively, to gain a microscopic view of the "compressive effect". When in the presence of a magnetic field, the C–C bond distance in the phenyl and porphine moieties showed a slight increase, especially for C4–C5 and C8–C10 in crystals 1–3, and the Cu1–N1 bond distance under the two different magnetic fields was longer than that without a magnetic field. However, for



Fig. 4 3D d_{norm} Hirshfeld surface (left) and 2D fingerprint plots (right) resolved into H–H, C···H/H···C and $\pi \cdot \cdot \pi$ (C···C) interactions for crystals **2** (upper) and **3** (lower), respectively; the full fingerprint appears beneath each decomposed plot as a grey shadow.

most of the bond distances, such as C3–C2, C11–C9 *etc.*, a decreasing trend was observed in the presence of an external magnetic field.

3.2 Hirshfeld surface analysis of polymorphism

Hirshfeld surface analysis^{33,34} was carried out to compute the intermolecular interaction in the different crystals of Cu-TPP. The 3D d_{norm} Hirshfeld surface and 2D fingerprint plots of crystals 2, 3 and 1 are shown in Fig. 4 and Fig. S1, S2 (ESI[†]), respectively. Here, the different colors represent the strength of the various interactions. For instance, the dark red spots represent sites where moderate hydrogen bonding contacts are formed, while the blue regions correspond to longer contacts.³⁵ In crystal 1, the proportion of $H \cdots H$, $C \cdots H/H \cdots C$ and $\pi \cdots \pi$ (C···C) interactions is 48.4%, 26.5% and 14.3% (Fig. 5 and Table S1, ESI†), respectively, over the entire Hirshfeld surface, with the H...H contacts showing the most significant contribution, as is reflected in the middle region of the 2D fingerprinting plots covering most of the area of the figure (Fig. S1, ESI[†]). However, after applying magnetic fields of different strengths, the proportion of the most significant H...H interactions was increased to 55.0% and 55.4%, according to the total Hirshfeld surfaces of crystal 2 and 3, respectively (Fig. 3). Meanwhile, the proportion of the second strongest C···H/H···C interactions of crystals 2 and 3 was also increased to 26.8% and 30.5%, respectively. On the contrary, the proportion of $\pi \cdots \pi$ (C···C) interactions, which were reflected by the identical d_e and d_i regions on the fingerprint plots, decreased dramatically from 14.3% in 1 to 7.3% in 2 and 3. In addition, other interactions were also changed with the strength of the magnetic field (Fig. 5 and Table S1, ESI[†]). Thus, the mechanical aspects of the influence of a magnetic field on the crystal structures of Cu-TPP can be proposed; on the one hand, the magnetic field induced the compressed packing of the Cu-TPP molecules, which thus led to an increasing number of closer interactions $(H \cdots H, C \cdots H/H \cdots C)$; on the other hand, this compressed packing was accompanied by



Fig. 5 The relative contributions of the various intermolecular interactions to the total Hirshfeld surface of crystals **1–3**.

a decrease in the number of $\pi \cdots \pi$ (C \cdots C) interactions as a sacrifice.

4. Conclusion

In summary, two new crystals of Cu-TPP have been prepared with the help of external magnetic fields with a strength of 0.5 and 0.8 T, respectively. The magnetic fields resulted in a more "compressed" crystal packing for Cu-TPP. It should be noted that this "compressed" packing was evidenced by the increasing number of closer interactions (H···H, C···H/H···C) in the crystals with the magnetic field strength, accompanied by a decrease in the number of $\pi \cdots \pi$ (C···C) interactions as a sacrifice. Along with the results of our previous work, the results here have suggested the opposite influence of a magnetic field on the crystallization process of mono-component and multi-component materials, which will certainly provide some suggestions for the design of crystallization strategies for other materials in the presence of an external magnetic field.

Conflicts of interest

There are no conflicts to declare.

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