

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 4-(2-Carboxybenzoyl)benzoic acid–4,4'-bipyridine (1/1)

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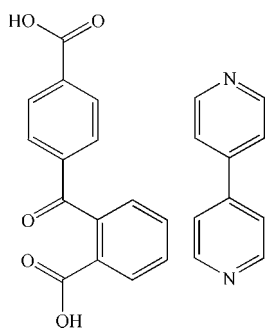
Received 6 November 2008; accepted 14 November 2008

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  
 $R$  factor = 0.045;  $wR$  factor = 0.128; data-to-parameter ratio = 12.4.

In the heteromolecular title compound,  $\text{C}_{15}\text{H}_{10}\text{O}_5 \cdot \text{C}_{10}\text{H}_8\text{N}_2$ , the two components are linked by  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds to form four-component ring supramolecular assemblies. These are further interconnected with neighbouring molecules by weak intermolecular  $\text{C}-\text{H} \cdots \pi$  interactions and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds to generate a three-dimensional network.

## Related literature

For details of the  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bond, see: Bhogala *et al.* (2005); Wang *et al.* (2008). For details of the  $\text{C}-\text{H} \cdots \pi$  interaction, see: Fun & Kia (2008).



## Experimental

## Crystal data

$\text{C}_{15}\text{H}_{10}\text{O}_5 \cdot \text{C}_{10}\text{H}_8\text{N}_2$   
 $M_r = 426.41$

Monoclinic,  $P2_1/n$   
 $a = 7.6883$  (6) Å

$b = 24.1886$  (18) Å  
 $c = 10.9560$  (8) Å  
 $\beta = 95.873$  (1)°  
 $V = 2026.8$  (3) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.35 \times 0.28 \times 0.16$  mm

## Data collection

Bruker CCD area detector  
diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 1997)  
 $T_{\min} = 0.957$ ,  $T_{\max} = 0.984$

10190 measured reflections  
3607 independent reflections  
2177 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.128$   
 $S = 1.02$   
3607 reflections

292 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C19–C24 ring.

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{C8}-\text{H8} \cdots \text{O4}^i$	0.93	2.51	3.282 (3)	141
$\text{O5}-\text{H5} \cdots \text{N2}^{ii}$	0.82	1.84	2.641 (2)	166
$\text{O2}-\text{H2} \cdots \text{N1}^{iii}$	0.82	1.79	2.595 (2)	168
$\text{C1}-\text{H1} \cdots \text{Cg1}^{iv}$	0.93	2.54	3.449 (3)	165

Symmetry codes: (i)  $x+1, y, z+1$ ; (ii)  $x-1, y, z$ ; (iii)  $-x+1, -y, -z+2$ ; (iv)  $x-\frac{1}{2}, -y-\frac{1}{2}, z-\frac{1}{2}$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Luoyang Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2130).

## References

- Bhogala, B. R., Basavoju, S. & Nangia, A. (2005). *Cryst. Growth Des.* **5**, 1683–1686.  
Bruker (1997). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Fun, H.-K. & Kia, R. (2008). *Acta Cryst.* **E64**, m1116–m1117.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Wang, Y.-T., Tang, G.-M., Zhang, Y.-C. & Wan, W.-Z. (2008). *Acta Cryst.* **E64**, o1753.

**supplementary materials**

*Acta Cryst.* (2008). E64, o2399 [ doi:10.1107/S1600536808037823 ]

## 4-(2-Carboxybenzoyl)benzoic acid-4,4'-bipyridine (1/1)

J.-G. Wang and J.-H. Qin

### Comment

The asymmetric unit consists of one 4,4'-bipyridine molecule and one 4-(2-carboxylbenzoyl)benzoic acid molecule (Fig. 1). The two components are linked by O—H $\cdots$ N hydrogen bonds to form four-component ring supramolecular adducts (Tab. 1 & Fig. 2). The four-component ring supramolecular adducts interact with neighboring molecules *via* weak intermolecular C—H $\cdots$  $\pi$  interactions and C—H $\cdots$ O hydrogen bonds (Tab. 1). The C—H $\cdots$  $\pi$  interactions link the four-component ring supramolecular adducts into two-dimensional layers (Fig. 3), which are further connected by weak intermolecular C—H $\cdots$ O hydrogen bonds to generate a three-dimensional supramolecular structure (Fig. 4).

### Experimental

4,4'-bipyridine (0.1 mmol), 4-(2-carboxylbenzoyl)benzoic acid (0.1 mmol), and NaOH (0.2 mmol) were added to a H<sub>2</sub>O solution (15 ml) in a Teflon-lined stainless steel reactor. The mixture was heated at 473 K for 3 d, and then slowly cooled down to room temperature. Colorless crystals of the title compound were obtained.

### Refinement

All hydrogen atoms were positioned geometrically and treated as riding, with C—H bond lengths constrained to 0.93 Å (aromatic CH) and O—H bond lengths constrained to 0.82 Å (OH), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

### Figures

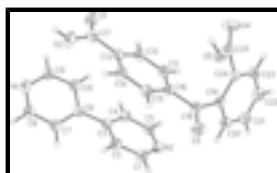


Fig. 1. A view of the heteromolecular components of the title compound with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

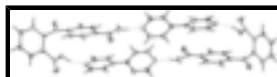


Fig. 2. A view of the four-component ring supramolecular adducts, formed by O—H $\cdots$ N hydrogen bonds.

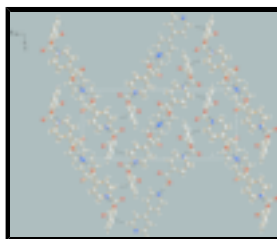


Fig. 3. A packing section of the title compound viewed down the *a* axis, indicating the C—H $\cdots$  $\pi$  contacts by dashed lines.

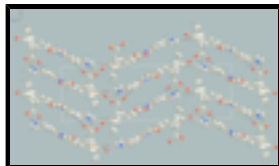


Fig. 4. A view of the molecular packing down the *c* axis.

## 4-(2-Carboxybenzoyl)benzoic acid–4,4'-bipyridine (1/1)

### Crystal data

$C_{15}H_{10}O_5 \cdot C_{10}H_8N_2$

$M_r = 426.41$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P2_1/n$

$a = 7.6883$  (6) Å

$b = 24.1886$  (18) Å

$c = 10.9560$  (8) Å

$\beta = 95.8730$  (10)°

$V = 2026.8$  (3) Å<sup>3</sup>

$Z = 4$

$F_{000} = 888$

$D_x = 1.397$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 1385 reflections

$\theta = 2.5$ – $21.2$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 296$  (2) K

Block, colorless

$0.35 \times 0.28 \times 0.16$  mm

### Data collection

Bruker CCD area detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 1997)

$T_{\min} = 0.957$ ,  $T_{\max} = 0.984$

10190 measured reflections

3607 independent reflections

2177 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\text{max}} = 25.1$ °

$\theta_{\text{min}} = 1.7$ °

$h = -9 \rightarrow 9$

$k = -28 \rightarrow 28$

$l = -13 \rightarrow 7$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.128$

$S = 1.02$

3607 reflections

292 parameters

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

Extinction correction: SHELXL,

$$F_c^* = kF_c [1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods Extinction coefficient: 0.0131 (14)

Secondary atom site location: difference Fourier map

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.7560 (3)	0.00682 (8)	0.99002 (17)	0.0561 (5)
N2	0.9586 (2)	0.15564 (8)	0.46655 (17)	0.0512 (5)
O1	0.2912 (3)	-0.00260 (8)	0.69911 (15)	0.0779 (6)
O2	0.3035 (3)	0.06365 (7)	0.84053 (15)	0.0671 (5)
H2	0.2837	0.0379	0.8859	0.101*
O3	0.5482 (2)	0.25808 (7)	0.42728 (14)	0.0659 (5)
O4	0.0942 (2)	0.13238 (8)	0.19022 (17)	0.0789 (6)
O5	0.1584 (2)	0.20365 (7)	0.31530 (14)	0.0532 (4)
H5	0.0822	0.1908	0.3541	0.080*
C1	0.9364 (3)	0.18081 (10)	0.5716 (2)	0.0557 (7)
H1	0.9493	0.2190	0.5754	0.067*
C2	0.8955 (3)	0.15357 (10)	0.6751 (2)	0.0530 (6)
H2A	0.8810	0.1733	0.7463	0.064*
C3	0.8761 (3)	0.09687 (9)	0.67290 (19)	0.0426 (5)
C4	0.8951 (3)	0.07078 (10)	0.5629 (2)	0.0521 (6)
H4	0.8804	0.0327	0.5560	0.062*
C5	0.9359 (3)	0.10128 (11)	0.4632 (2)	0.0556 (6)
H5A	0.9480	0.0828	0.3901	0.067*
C6	0.8351 (3)	0.06565 (9)	0.7835 (2)	0.0436 (6)
C7	0.8857 (3)	0.08447 (10)	0.9015 (2)	0.0515 (6)
H7	0.9477	0.1174	0.9134	0.062*
C8	0.8436 (3)	0.05426 (11)	1.0008 (2)	0.0571 (7)
H8	0.8781	0.0677	1.0791	0.069*
C9	0.7071 (3)	-0.01128 (10)	0.8773 (2)	0.0618 (7)
H9	0.6445	-0.0442	0.8682	0.074*
C10	0.7445 (3)	0.01621 (10)	0.7733 (2)	0.0561 (7)
H10	0.7089	0.0016	0.6962	0.067*
C11	0.4552 (3)	0.11251 (9)	0.44658 (19)	0.0472 (6)
H11	0.4816	0.1016	0.3692	0.057*
C12	0.4068 (3)	0.07337 (9)	0.5287 (2)	0.0503 (6)
H12	0.4006	0.0363	0.5060	0.060*
C13	0.3673 (3)	0.08886 (9)	0.64455 (19)	0.0441 (6)
C14	0.3797 (3)	0.14392 (10)	0.6772 (2)	0.0497 (6)
H14	0.3544	0.1548	0.7548	0.060*
C15	0.4293 (3)	0.18291 (9)	0.59573 (19)	0.0481 (6)
H15	0.4392	0.2198	0.6194	0.058*
C16	0.4644 (3)	0.16755 (9)	0.47894 (19)	0.0416 (5)
C17	0.3161 (3)	0.04481 (11)	0.7299 (2)	0.0518 (6)
C18	0.5073 (3)	0.21165 (10)	0.3914 (2)	0.0455 (6)
C19	0.5114 (3)	0.19699 (9)	0.25883 (18)	0.0408 (5)
C20	0.6710 (3)	0.20203 (9)	0.2104 (2)	0.0499 (6)
H20	0.7674	0.2158	0.2592	0.060*

## supplementary materials

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C21	0.6878 (3)	0.18689 (10)	0.0910 (2)	0.0561 (6)
H21	0.7957	0.1898	0.0602	0.067*
C22	0.5460 (3)	0.16750 (10)	0.0174 (2)	0.0565 (7)
H22	0.5575	0.1576	-0.0634	0.068*
C23	0.3861 (3)	0.16268 (9)	0.0633 (2)	0.0499 (6)
H23	0.2902	0.1496	0.0129	0.060*
C24	0.3669 (3)	0.17700 (9)	0.18334 (19)	0.0419 (5)
C25	0.1923 (3)	0.16868 (10)	0.2289 (2)	0.0491 (6)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0681 (14)	0.0556 (14)	0.0461 (12)	0.0026 (11)	0.0131 (10)	0.0071 (10)
N2	0.0492 (12)	0.0565 (14)	0.0486 (12)	-0.0050 (10)	0.0086 (9)	0.0031 (10)
O1	0.1202 (17)	0.0535 (12)	0.0602 (12)	-0.0246 (11)	0.0108 (10)	0.0006 (10)
O2	0.1031 (15)	0.0560 (11)	0.0451 (10)	-0.0019 (10)	0.0217 (10)	0.0098 (8)
O3	0.0921 (14)	0.0547 (12)	0.0515 (11)	-0.0205 (10)	0.0106 (9)	-0.0029 (9)
O4	0.0604 (12)	0.0931 (15)	0.0854 (14)	-0.0297 (11)	0.0174 (10)	-0.0236 (11)
O5	0.0504 (10)	0.0576 (11)	0.0538 (11)	-0.0020 (8)	0.0153 (8)	0.0034 (8)
C1	0.0671 (17)	0.0449 (15)	0.0563 (17)	-0.0067 (12)	0.0129 (13)	0.0014 (12)
C2	0.0642 (16)	0.0476 (15)	0.0489 (15)	-0.0051 (12)	0.0143 (12)	-0.0005 (11)
C3	0.0406 (13)	0.0469 (14)	0.0412 (13)	-0.0016 (10)	0.0077 (10)	0.0003 (11)
C4	0.0633 (16)	0.0447 (14)	0.0505 (15)	-0.0066 (12)	0.0167 (12)	-0.0025 (11)
C5	0.0612 (16)	0.0587 (17)	0.0487 (15)	-0.0053 (13)	0.0149 (12)	-0.0048 (12)
C6	0.0427 (13)	0.0447 (14)	0.0439 (13)	0.0025 (10)	0.0063 (10)	0.0029 (11)
C7	0.0580 (15)	0.0504 (15)	0.0466 (15)	-0.0050 (12)	0.0083 (12)	0.0004 (12)
C8	0.0671 (17)	0.0623 (18)	0.0425 (14)	0.0015 (14)	0.0075 (12)	0.0006 (13)
C9	0.0805 (19)	0.0502 (16)	0.0550 (16)	-0.0103 (13)	0.0090 (14)	0.0087 (13)
C10	0.0767 (18)	0.0499 (16)	0.0413 (14)	-0.0090 (13)	0.0050 (12)	0.0010 (11)
C11	0.0587 (15)	0.0484 (15)	0.0351 (12)	0.0046 (12)	0.0070 (11)	-0.0012 (11)
C12	0.0643 (16)	0.0406 (14)	0.0457 (14)	0.0020 (11)	0.0039 (12)	0.0001 (11)
C13	0.0472 (14)	0.0500 (15)	0.0347 (13)	0.0023 (11)	0.0018 (10)	0.0037 (11)
C14	0.0601 (15)	0.0511 (15)	0.0387 (13)	0.0014 (12)	0.0092 (11)	-0.0031 (11)
C15	0.0606 (15)	0.0421 (14)	0.0421 (14)	-0.0018 (11)	0.0068 (11)	0.0010 (11)
C16	0.0427 (13)	0.0462 (14)	0.0360 (12)	0.0002 (10)	0.0044 (10)	0.0022 (10)
C17	0.0573 (16)	0.0556 (17)	0.0418 (15)	-0.0004 (13)	0.0019 (12)	0.0065 (12)
C18	0.0449 (14)	0.0508 (16)	0.0409 (13)	-0.0018 (11)	0.0054 (10)	0.0017 (11)
C19	0.0438 (13)	0.0427 (13)	0.0365 (12)	-0.0013 (10)	0.0067 (10)	0.0052 (10)
C20	0.0435 (14)	0.0578 (16)	0.0485 (14)	-0.0035 (11)	0.0052 (11)	0.0032 (12)
C21	0.0468 (15)	0.0667 (17)	0.0566 (16)	0.0037 (12)	0.0144 (12)	0.0023 (13)
C22	0.0624 (17)	0.0642 (17)	0.0448 (14)	0.0070 (13)	0.0150 (13)	-0.0036 (12)
C23	0.0516 (15)	0.0510 (15)	0.0461 (14)	-0.0025 (11)	0.0012 (11)	-0.0041 (11)
C24	0.0458 (14)	0.0396 (13)	0.0408 (13)	0.0003 (10)	0.0064 (11)	0.0046 (10)
C25	0.0494 (15)	0.0539 (16)	0.0439 (14)	-0.0026 (12)	0.0041 (11)	0.0024 (12)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N1—C9	1.328 (3)	C9—H9	0.9300
N1—C8	1.330 (3)	C10—H10	0.9300

N2—C5	1.327 (3)	C11—C16	1.378 (3)
N2—C1	1.328 (3)	C11—C12	1.383 (3)
O1—C17	1.205 (3)	C11—H11	0.9300
O2—C17	1.308 (3)	C12—C13	1.387 (3)
O2—H2	0.8200	C12—H12	0.9300
O3—C18	1.220 (3)	C13—C14	1.380 (3)
O4—C25	1.205 (3)	C13—C17	1.497 (3)
O5—C25	1.315 (3)	C14—C15	1.379 (3)
O5—H5	0.8200	C14—H14	0.9300
C1—C2	1.376 (3)	C15—C16	1.385 (3)
C1—H1	0.9300	C15—H15	0.9300
C2—C3	1.379 (3)	C16—C18	1.493 (3)
C2—H2A	0.9300	C18—C19	1.499 (3)
C3—C4	1.382 (3)	C19—C20	1.391 (3)
C3—C6	1.489 (3)	C19—C24	1.402 (3)
C4—C5	1.380 (3)	C20—C21	1.377 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—H5A	0.9300	C21—C22	1.371 (3)
C6—C10	1.383 (3)	C21—H21	0.9300
C6—C7	1.388 (3)	C22—C23	1.380 (3)
C7—C8	1.376 (3)	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.383 (3)
C8—H8	0.9300	C23—H23	0.9300
C9—C10	1.375 (3)	C24—C25	1.493 (3)
C9—N1—C8	117.3 (2)	C14—C13—C12	118.8 (2)
C5—N2—C1	116.7 (2)	C14—C13—C17	122.7 (2)
C17—O2—H2	109.5	C12—C13—C17	118.4 (2)
C25—O5—H5	109.5	C15—C14—C13	120.6 (2)
N2—C1—C2	123.7 (2)	C15—C14—H14	119.7
N2—C1—H1	118.1	C13—C14—H14	119.7
C2—C1—H1	118.1	C14—C15—C16	120.5 (2)
C1—C2—C3	119.7 (2)	C14—C15—H15	119.8
C1—C2—H2A	120.2	C16—C15—H15	119.8
C3—C2—H2A	120.2	C11—C16—C15	119.2 (2)
C2—C3—C4	116.7 (2)	C11—C16—C18	122.3 (2)
C2—C3—C6	121.4 (2)	C15—C16—C18	118.6 (2)
C4—C3—C6	121.9 (2)	O1—C17—O2	124.5 (2)
C5—C4—C3	119.9 (2)	O1—C17—C13	123.2 (2)
C5—C4—H4	120.0	O2—C17—C13	112.3 (2)
C3—C4—H4	120.0	O3—C18—C16	121.2 (2)
N2—C5—C4	123.2 (2)	O3—C18—C19	119.9 (2)
N2—C5—H5A	118.4	C16—C18—C19	118.8 (2)
C4—C5—H5A	118.4	C20—C19—C24	118.8 (2)
C10—C6—C7	116.7 (2)	C20—C19—C18	117.1 (2)
C10—C6—C3	121.3 (2)	C24—C19—C18	124.02 (18)
C7—C6—C3	122.0 (2)	C21—C20—C19	120.7 (2)
C8—C7—C6	119.7 (2)	C21—C20—H20	119.6
C8—C7—H7	120.1	C19—C20—H20	119.6
C6—C7—H7	120.1	C22—C21—C20	120.2 (2)

## supplementary materials

N1—C8—C7	123.1 (2)	C22—C21—H21	119.9
N1—C8—H8	118.4	C20—C21—H21	119.9
C7—C8—H8	118.4	C21—C22—C23	120.0 (2)
N1—C9—C10	123.3 (2)	C21—C22—H22	120.0
N1—C9—H9	118.4	C23—C22—H22	120.0
C10—C9—H9	118.4	C22—C23—C24	120.7 (2)
C9—C10—C6	119.8 (2)	C22—C23—H23	119.6
C9—C10—H10	120.1	C24—C23—H23	119.6
C6—C10—H10	120.1	C23—C24—C19	119.49 (19)
C16—C11—C12	120.3 (2)	C23—C24—C25	118.1 (2)
C16—C11—H11	119.9	C19—C24—C25	122.33 (19)
C12—C11—H11	119.9	O4—C25—O5	124.0 (2)
C11—C12—C13	120.6 (2)	O4—C25—C24	122.1 (2)
C11—C12—H12	119.7	O5—C25—C24	113.9 (2)
C13—C12—H12	119.7		
C5—N2—C1—C2	1.3 (3)	C14—C15—C16—C18	176.4 (2)
N2—C1—C2—C3	0.2 (4)	C14—C13—C17—O1	173.8 (2)
C1—C2—C3—C4	-1.7 (3)	C12—C13—C17—O1	-7.4 (3)
C1—C2—C3—C6	178.9 (2)	C14—C13—C17—O2	-6.8 (3)
C2—C3—C4—C5	1.6 (3)	C12—C13—C17—O2	172.1 (2)
C6—C3—C4—C5	-179.0 (2)	C11—C16—C18—O3	-165.6 (2)
C1—N2—C5—C4	-1.5 (3)	C15—C16—C18—O3	15.8 (3)
C3—C4—C5—N2	0.0 (4)	C11—C16—C18—C19	10.3 (3)
C2—C3—C6—C10	151.9 (2)	C15—C16—C18—C19	-168.35 (19)
C4—C3—C6—C10	-27.6 (3)	O3—C18—C19—C20	59.3 (3)
C2—C3—C6—C7	-28.2 (3)	C16—C18—C19—C20	-116.6 (2)
C4—C3—C6—C7	152.4 (2)	O3—C18—C19—C24	-123.0 (2)
C10—C6—C7—C8	-0.5 (3)	C16—C18—C19—C24	61.1 (3)
C3—C6—C7—C8	179.6 (2)	C24—C19—C20—C21	-0.9 (3)
C9—N1—C8—C7	-0.4 (4)	C18—C19—C20—C21	176.9 (2)
C6—C7—C8—N1	0.3 (4)	C19—C20—C21—C22	1.1 (4)
C8—N1—C9—C10	0.7 (4)	C20—C21—C22—C23	-0.5 (4)
N1—C9—C10—C6	-0.9 (4)	C21—C22—C23—C24	-0.3 (4)
C7—C6—C10—C9	0.7 (3)	C22—C23—C24—C19	0.4 (3)
C3—C6—C10—C9	-179.3 (2)	C22—C23—C24—C25	-177.6 (2)
C16—C11—C12—C13	-0.2 (3)	C20—C19—C24—C23	0.2 (3)
C11—C12—C13—C14	-0.9 (3)	C18—C19—C24—C23	-177.5 (2)
C11—C12—C13—C17	-179.8 (2)	C20—C19—C24—C25	178.1 (2)
C12—C13—C14—C15	0.4 (3)	C18—C19—C24—C25	0.4 (3)
C17—C13—C14—C15	179.3 (2)	C23—C24—C25—O4	30.4 (3)
C13—C14—C15—C16	1.2 (3)	C19—C24—C25—O4	-147.5 (2)
C12—C11—C16—C15	1.7 (3)	C23—C24—C25—O5	-150.7 (2)
C12—C11—C16—C18	-176.9 (2)	C19—C24—C25—O5	31.3 (3)
C14—C15—C16—C11	-2.2 (3)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8 $\cdots$ O4 <sup>i</sup>	0.93	2.51	3.282 (3)	141



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O5—H5 $\cdots$ N2 <sup>ii</sup>	0.82	1.84	2.641 (2)	166
O2—H2 $\cdots$ N1 <sup>iii</sup>	0.82	1.79	2.595 (2)	168
C1—H1 $\cdots$ Cg1 <sup>iv</sup>	0.93	2.54	3.449 (3)	165

Symmetry codes: (i)  $x+1, y, z+1$ ; (ii)  $x-1, y, z$ ; (iii)  $-x+1, -y, -z+2$ ; (iv)  $x-1/2, -y-1/2, z-1/2$ .

Fig. 1

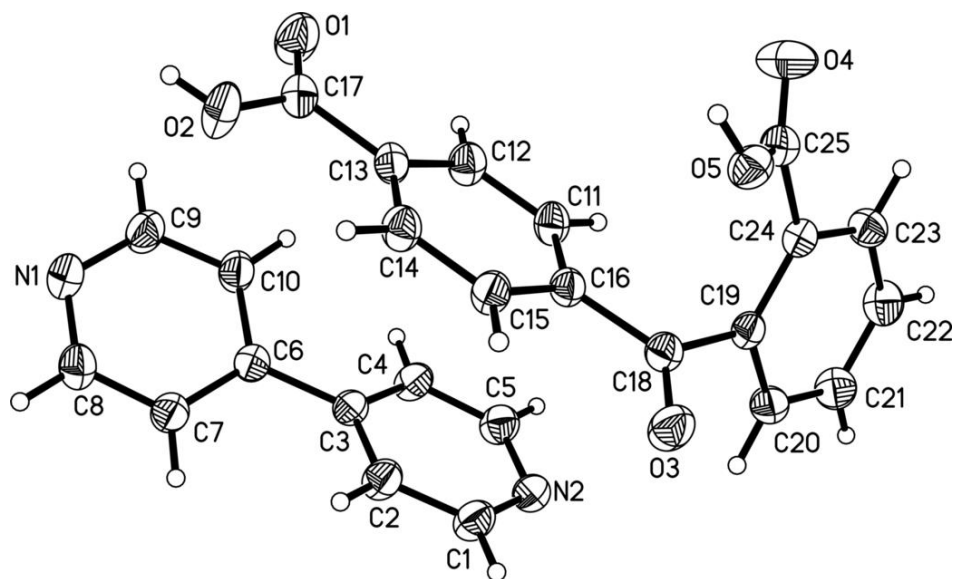


Fig. 2

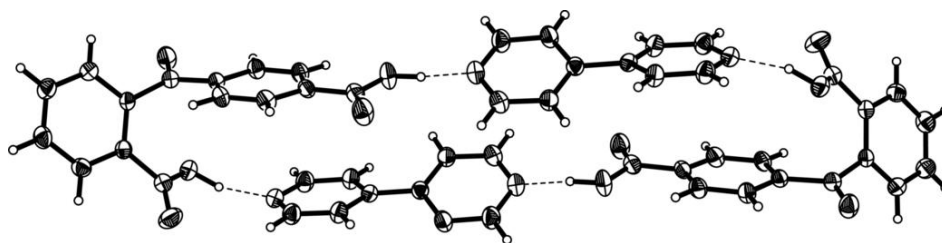


Fig. 3

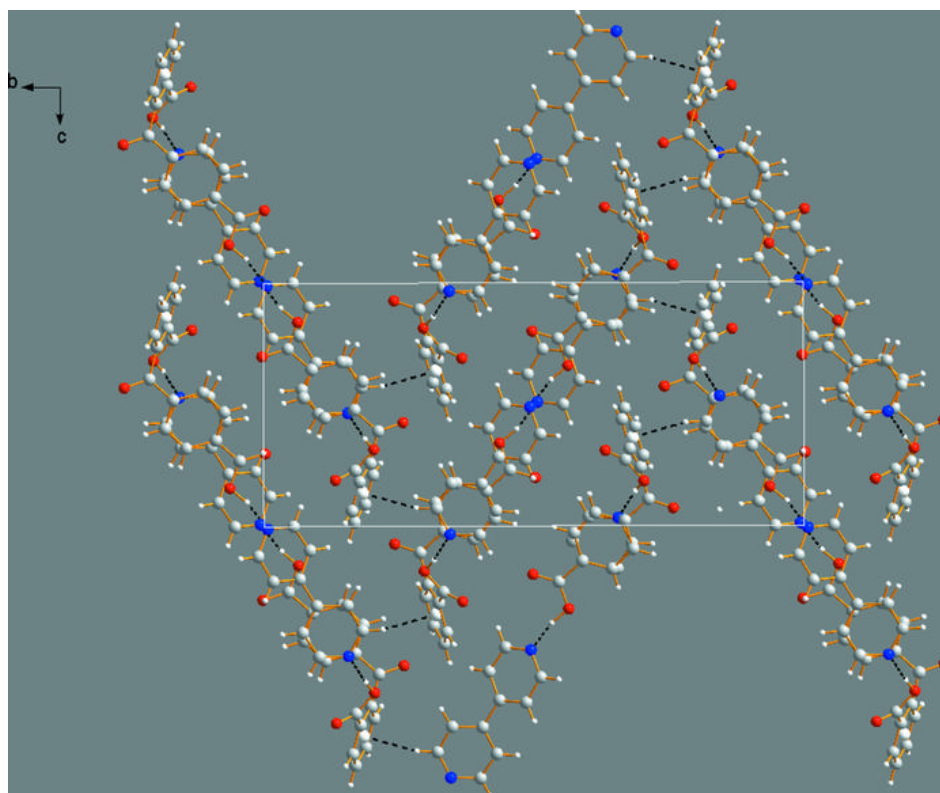


Fig. 4

