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10,11,12,13-Tetrahydro-4,5,9,14-tetraazadibenz[*a,c*]anthracene–benzene-1,4-dicarboxylic acid (2/1)

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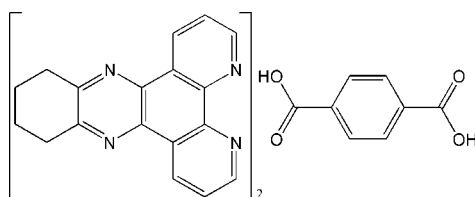
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 Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.059; wR factor = 0.181; data-to-parameter ratio = 13.6.

In the title adduct, $2\text{C}_{18}\text{H}_{14}\text{N}_4 \cdot \text{C}_8\text{H}_6\text{O}_4$, the centrosymmetric benzene-1,4-dicarboxylic acid molecule makes two $\text{O} \cdots \text{H} \cdots \text{N}$ hydrogen bonds to adjacent 10,11,12,13-tetrahydro-4,5,9,14-tetraazadibenzo[*a,c*]anthracene (TTBT) molecules. Aromatic π - π stacking interactions occur between TTBT rings [centroid-centroid distance = $3.570(3)$ Å], leading to a two-dimensional supramolecular structure in the crystal.

Related literature

 For related literature, see: Che *et al.* (2006, 2008); Stephenson & Hardie (2006); Xu *et al.* (2008); Yao *et al.* (2008).


Experimental

Crystal data

 $2\text{C}_{18}\text{H}_{14}\text{N}_4 \cdot \text{C}_8\text{H}_6\text{O}_4$
 $M_r = 738.80$
 Triclinic, $P\bar{1}$
 $a = 7.266(4)$ Å

 $b = 9.917(5)$ Å
 $c = 13.564(9)$ Å
 $\alpha = 101.469(9)^\circ$
 $\beta = 97.429(9)^\circ$
 $\gamma = 109.697(6)^\circ$
 $V = 881.2(9)$ Å³
 $Z = 1$
 Mo $K\alpha$ radiation

 $\mu = 0.09$ mm⁻¹
 $T = 292(2)$ K
 $0.32 \times 0.21 \times 0.08$ mm

Data collection

 Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.978$, $T_{\max} = 0.992$

 7636 measured reflections
 3444 independent reflections
 1394 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.180$
 $S = 0.93$
 3444 reflections

 253 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---|-------|--------------|--------------|----------------|
| $\text{O2}-\text{H2A} \cdots \text{N2}$ | 0.82 | 2.02 | 2.694 (4) | 139 |

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2788).

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supplementary materials

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10,11,12,13-Tetrahydro-4,5,9,14-tetraazadibenz[*a,c*]anthracene-benzene-1,4-dicarboxylic acid (2/1)

C.-B. Liu, J. Wang, X.-Y. Li, G.-B. Che and Y. Liu

Comment

Current crystal engineering on the basis of the supramolecular architectures assembled from various noncovalent interactions, such as hydrogen bonds and π - π stacking interactions have been extensively studied owing to their novel topologies and potential applications as functional materials (Stephenson & Hardie, 2006; Yao *et al.*, 2008). 1,10-Phenanthroline (phen) and its derivatives have been widely used to build novel supramolecular architectures (Xu, Li *et al.*, 2008; Che, Liu *et al.*, 2008). As a continuation of our studies in this area, we have prepared the title compound, (I), using the phen derivative 10,11,12,13-tetrahydro-4,5,9,14-tetraazadibenz[*a,c*]anthracene (TTBA).

The asymmetric unit of (I) consists of one TTBA molecule and half of a centrosymmetric 1,4-benzenedicarboxylic acid molecule (Fig. 1). The two components of (I) interact by way of O—H \cdots N hydrogen bonds (Table 1). Furthermore, there are π - π aromatic stacking interactions involving TTBA ligands of adjacent units [centroid-centroid distance = 3.570 (3) \AA], forming an intriguing two-dimensional supramolecular motif (Fig. 2).

Experimental

The TTBA was synthesized according to the literature method (Che, Li *et al.*, 2006). TTBA (1.0 mmol) and 1,4-benzenedicarboxylic acid (0.5 mmol) were dissolved in aqueous solution and the mixture was sealed in a Teflon-lined autoclave and heated to 433 K for 4 d. Upon cooling and opening the bomb, colorless blocks of (I) were obtained.

Refinement

The hydrogen atoms were positioned geometrically (C—H = 0.93 \AA , O—H = 0.82 \AA) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Figures

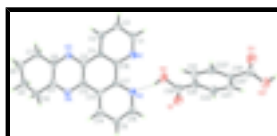


Fig. 1. View of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry code: (i) 1 - *x*, -*y*, 3 - *z*.]

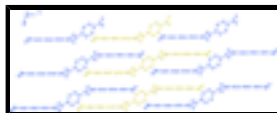


Fig. 2. Packing diagram of the two-dimensional supramolecular structure of (I) formed *via* π - π interactions and hydrogen bonds. H atoms have been omitted.

10,11,12,13-Tetrahydro-4,5,9,14-tetraazadibenz[a,c]anthracene– benzene-1,4-dicarboxylic acid (2/1)

Crystal data

| | |
|--|---|
| $2\text{C}_{18}\text{H}_{14}\text{N}_4\cdot\text{C}_8\text{H}_6\text{O}_4$ | $Z = 1$ |
| $M_r = 738.80$ | $F_{000} = 386$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.392 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation |
| $a = 7.266 (4) \text{ \AA}$ | $\lambda = 0.71073 \text{ \AA}$ |
| $b = 9.917 (5) \text{ \AA}$ | Cell parameters from 2386 reflections |
| $c = 13.564 (9) \text{ \AA}$ | $\theta = 2.3\text{--}26.0^\circ$ |
| $\alpha = 101.469 (9)^\circ$ | $\mu = 0.09 \text{ mm}^{-1}$ |
| $\beta = 97.429 (9)^\circ$ | $T = 292 (2) \text{ K}$ |
| $\gamma = 109.697 (6)^\circ$ | Block, colorless |
| $V = 881.2 (9) \text{ \AA}^3$ | $0.32 \times 0.21 \times 0.08 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker SMART CCD diffractometer | 3444 independent reflections |
| Radiation source: fine-focus sealed tube | 1394 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.047$ |
| $T = 292(2) \text{ K}$ | $\theta_{\text{max}} = 26.1^\circ$ |
| ω scans | $\theta_{\text{min}} = 2.3^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $h = -8 \rightarrow 8$ |
| $T_{\text{min}} = 0.978, T_{\text{max}} = 0.992$ | $k = -12 \rightarrow 12$ |
| 7636 measured reflections | $l = -16 \rightarrow 16$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | H-atom parameters constrained |
| $wR(F^2) = 0.180$ | $w = 1/[\sigma^2(F_o^2) + (0.0762P)^2]$ |
| $S = 0.93$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3444 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 253 parameters | $\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|------------|------------|------------|----------------------------------|
| C1 | 0.7589 (5) | 0.5815 (4) | 1.2595 (3) | 0.0603 (10) |
| H1 | 0.7594 | 0.6000 | 1.3295 | 0.072* |
| C2 | 0.7631 (5) | 0.6947 (4) | 1.2121 (3) | 0.0593 (9) |
| H2 | 0.7692 | 0.7861 | 1.2495 | 0.071* |
| C3 | 0.7581 (4) | 0.6668 (4) | 1.1082 (3) | 0.0534 (9) |
| H3 | 0.7589 | 0.7394 | 1.0739 | 0.064* |
| C4 | 0.7517 (4) | 0.5297 (3) | 1.0542 (2) | 0.0411 (8) |
| C5 | 0.7492 (4) | 0.4942 (3) | 0.9448 (2) | 0.0418 (8) |
| C6 | 0.7476 (4) | 0.5624 (4) | 0.7934 (3) | 0.0473 (8) |
| C7 | 0.7508 (5) | 0.6785 (4) | 0.7365 (2) | 0.0607 (10) |
| H7A | 0.8810 | 0.7585 | 0.7590 | 0.073* |
| H7B | 0.6518 | 0.7193 | 0.7543 | 0.073* |
| C8 | 0.7086 (6) | 0.6201 (4) | 0.6202 (3) | 0.0773 (12) |
| H8A | 0.5654 | 0.5694 | 0.5943 | 0.093* |
| H8B | 0.7534 | 0.7030 | 0.5898 | 0.093* |
| C9 | 0.8103 (6) | 0.5164 (4) | 0.5882 (3) | 0.0779 (12) |
| H9A | 0.9537 | 0.5678 | 0.6125 | 0.093* |
| H9B | 0.7826 | 0.4845 | 0.5137 | 0.093* |
| C10 | 0.7414 (6) | 0.3822 (4) | 0.6306 (2) | 0.0669 (10) |
| H10A | 0.6063 | 0.3186 | 0.5940 | 0.080* |
| H10B | 0.8271 | 0.3265 | 0.6187 | 0.080* |
| C11 | 0.7453 (4) | 0.4230 (4) | 0.7430 (2) | 0.0485 (8) |
| C12 | 0.7473 (4) | 0.3561 (3) | 0.8947 (2) | 0.0433 (8) |
| C13 | 0.7493 (4) | 0.2468 (3) | 0.9524 (2) | 0.0439 (8) |
| C14 | 0.7547 (4) | 0.1100 (4) | 0.9065 (3) | 0.0535 (9) |
| H14 | 0.7545 | 0.0847 | 0.8367 | 0.064* |
| C15 | 0.7602 (5) | 0.0130 (4) | 0.9645 (3) | 0.0578 (9) |
| H15 | 0.7664 | -0.0782 | 0.9355 | 0.069* |
| C16 | 0.7563 (5) | 0.0539 (4) | 1.0681 (3) | 0.0622 (10) |
| H16 | 0.7582 | -0.0131 | 1.1071 | 0.075* |
| C17 | 0.7489 (4) | 0.2799 (3) | 1.0574 (2) | 0.0431 (8) |
| C18 | 0.7504 (4) | 0.4245 (3) | 1.1102 (2) | 0.0429 (8) |
| C19 | 0.7010 (6) | 0.0878 (4) | 1.3406 (3) | 0.0611 (10) |

supplementary materials

| | | | | |
|-----|------------|-------------|--------------|-------------|
| C20 | 0.5949 (5) | 0.0433 (3) | 1.4226 (2) | 0.0527 (9) |
| C21 | 0.4077 (6) | 0.0460 (4) | 1.4252 (3) | 0.0597 (10) |
| H21 | 0.3439 | 0.0761 | 1.3747 | 0.072* |
| C22 | 0.6860 (5) | -0.0042 (4) | 1.4971 (3) | 0.0611 (10) |
| H22 | 0.8116 | -0.0082 | 1.4950 | 0.073* |
| N1 | 0.7543 (4) | 0.4499 (3) | 1.2122 (2) | 0.0533 (7) |
| N2 | 0.7502 (4) | 0.1824 (3) | 1.1147 (2) | 0.0513 (7) |
| N3 | 0.7496 (4) | 0.5981 (3) | 0.89318 (19) | 0.0472 (7) |
| N4 | 0.7442 (4) | 0.3203 (3) | 0.79299 (19) | 0.0491 (7) |
| O1 | 0.8422 (4) | 0.0570 (3) | 1.3217 (2) | 0.0853 (9) |
| O2 | 0.6271 (4) | 0.1674 (3) | 1.29255 (18) | 0.0766 (8) |
| H2A | 0.6112 | 0.1355 | 1.2302 | 0.115* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C1 | 0.067 (2) | 0.068 (3) | 0.049 (2) | 0.028 (2) | 0.0207 (18) | 0.014 (2) |
| C2 | 0.070 (2) | 0.053 (2) | 0.057 (3) | 0.0253 (19) | 0.0208 (19) | 0.0101 (19) |
| C3 | 0.054 (2) | 0.053 (2) | 0.058 (2) | 0.0230 (18) | 0.0178 (18) | 0.0190 (19) |
| C4 | 0.0385 (18) | 0.0422 (19) | 0.043 (2) | 0.0169 (15) | 0.0081 (15) | 0.0082 (16) |
| C5 | 0.0338 (18) | 0.046 (2) | 0.045 (2) | 0.0133 (15) | 0.0059 (15) | 0.0148 (17) |
| C6 | 0.0439 (19) | 0.050 (2) | 0.049 (2) | 0.0188 (17) | 0.0066 (16) | 0.0151 (18) |
| C7 | 0.069 (2) | 0.065 (2) | 0.051 (2) | 0.0243 (19) | 0.0119 (19) | 0.0243 (19) |
| C8 | 0.106 (3) | 0.082 (3) | 0.053 (3) | 0.043 (3) | 0.015 (2) | 0.026 (2) |
| C9 | 0.100 (3) | 0.093 (3) | 0.057 (2) | 0.047 (3) | 0.025 (2) | 0.029 (2) |
| C10 | 0.084 (3) | 0.070 (3) | 0.043 (2) | 0.027 (2) | 0.0104 (19) | 0.0135 (19) |
| C11 | 0.049 (2) | 0.052 (2) | 0.041 (2) | 0.0161 (17) | 0.0074 (16) | 0.0106 (18) |
| C12 | 0.0388 (18) | 0.047 (2) | 0.042 (2) | 0.0156 (15) | 0.0067 (15) | 0.0103 (17) |
| C13 | 0.0391 (18) | 0.044 (2) | 0.048 (2) | 0.0137 (15) | 0.0108 (15) | 0.0134 (17) |
| C14 | 0.058 (2) | 0.050 (2) | 0.052 (2) | 0.0230 (18) | 0.0093 (17) | 0.0091 (19) |
| C15 | 0.070 (2) | 0.043 (2) | 0.064 (2) | 0.0256 (19) | 0.0160 (19) | 0.0128 (19) |
| C16 | 0.072 (2) | 0.049 (2) | 0.067 (3) | 0.0211 (19) | 0.015 (2) | 0.023 (2) |
| C17 | 0.0412 (18) | 0.0398 (19) | 0.049 (2) | 0.0132 (15) | 0.0120 (15) | 0.0146 (17) |
| C18 | 0.0401 (18) | 0.048 (2) | 0.043 (2) | 0.0173 (16) | 0.0116 (15) | 0.0135 (17) |
| C19 | 0.079 (3) | 0.053 (2) | 0.057 (2) | 0.025 (2) | 0.024 (2) | 0.0211 (19) |
| C20 | 0.067 (2) | 0.043 (2) | 0.050 (2) | 0.0207 (18) | 0.0185 (18) | 0.0124 (17) |
| C21 | 0.074 (3) | 0.059 (2) | 0.054 (2) | 0.030 (2) | 0.0161 (19) | 0.0227 (19) |
| C22 | 0.069 (2) | 0.060 (2) | 0.066 (2) | 0.0287 (19) | 0.023 (2) | 0.025 (2) |
| N1 | 0.0634 (18) | 0.0523 (19) | 0.0464 (18) | 0.0224 (15) | 0.0166 (14) | 0.0131 (15) |
| N2 | 0.0600 (18) | 0.0427 (17) | 0.0547 (18) | 0.0202 (14) | 0.0139 (14) | 0.0171 (15) |
| N3 | 0.0502 (16) | 0.0494 (17) | 0.0433 (17) | 0.0193 (13) | 0.0087 (13) | 0.0143 (14) |
| N4 | 0.0541 (17) | 0.0485 (17) | 0.0435 (18) | 0.0194 (14) | 0.0095 (13) | 0.0098 (14) |
| O1 | 0.099 (2) | 0.097 (2) | 0.101 (2) | 0.0578 (18) | 0.0578 (18) | 0.0550 (17) |
| O2 | 0.101 (2) | 0.0836 (19) | 0.0687 (17) | 0.0465 (16) | 0.0330 (15) | 0.0399 (15) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------|-----------|----------|-----------|
| C1—N1 | 1.323 (4) | C10—H10B | 0.9700 |
| C1—C2 | 1.393 (4) | C11—N4 | 1.329 (4) |

| | | | |
|------------|-----------|----------------------|-----------|
| C1—H1 | 0.9300 | C12—N4 | 1.349 (4) |
| C2—C3 | 1.375 (4) | C12—C13 | 1.461 (4) |
| C2—H2 | 0.9300 | C13—C14 | 1.392 (4) |
| C3—C4 | 1.393 (4) | C13—C17 | 1.397 (4) |
| C3—H3 | 0.9300 | C14—C15 | 1.366 (4) |
| C4—C18 | 1.405 (4) | C14—H14 | 0.9300 |
| C4—C5 | 1.452 (4) | C15—C16 | 1.389 (4) |
| C5—N3 | 1.355 (3) | C15—H15 | 0.9300 |
| C5—C12 | 1.398 (4) | C16—N2 | 1.322 (4) |
| C6—N3 | 1.327 (4) | C16—H16 | 0.9300 |
| C6—C11 | 1.408 (4) | C17—N2 | 1.357 (4) |
| C6—C7 | 1.504 (4) | C17—C18 | 1.466 (4) |
| C7—C8 | 1.520 (4) | C18—N1 | 1.351 (4) |
| C7—H7A | 0.9700 | C19—O1 | 1.208 (4) |
| C7—H7B | 0.9700 | C19—O2 | 1.317 (4) |
| C8—C9 | 1.486 (5) | C19—C20 | 1.488 (5) |
| C8—H8A | 0.9700 | C20—C21 | 1.375 (4) |
| C8—H8B | 0.9700 | C20—C22 | 1.381 (4) |
| C9—C10 | 1.511 (4) | C21—C22 ⁱ | 1.384 (4) |
| C9—H9A | 0.9700 | C21—H21 | 0.9300 |
| C9—H9B | 0.9700 | C22—C21 ⁱ | 1.384 (4) |
| C10—C11 | 1.491 (4) | C22—H22 | 0.9300 |
| C10—H10A | 0.9700 | O2—H2A | 0.8200 |
| N1—C1—C2 | 124.8 (3) | N4—C11—C6 | 121.7 (3) |
| N1—C1—H1 | 117.6 | N4—C11—C10 | 116.5 (3) |
| C2—C1—H1 | 117.6 | C6—C11—C10 | 121.8 (3) |
| C3—C2—C1 | 117.8 (3) | N4—C12—C5 | 121.5 (3) |
| C3—C2—H2 | 121.1 | N4—C12—C13 | 118.5 (3) |
| C1—C2—H2 | 121.1 | C5—C12—C13 | 120.1 (3) |
| C2—C3—C4 | 119.9 (3) | C14—C13—C17 | 118.3 (3) |
| C2—C3—H3 | 120.1 | C14—C13—C12 | 122.0 (3) |
| C4—C3—H3 | 120.1 | C17—C13—C12 | 119.7 (3) |
| C3—C4—C18 | 117.4 (3) | C15—C14—C13 | 119.6 (3) |
| C3—C4—C5 | 122.5 (3) | C15—C14—H14 | 120.2 |
| C18—C4—C5 | 120.1 (3) | C13—C14—H14 | 120.2 |
| N3—C5—C12 | 121.2 (3) | C14—C15—C16 | 118.3 (3) |
| N3—C5—C4 | 118.5 (3) | C14—C15—H15 | 120.8 |
| C12—C5—C4 | 120.3 (3) | C16—C15—H15 | 120.8 |
| N3—C6—C11 | 121.7 (3) | N2—C16—C15 | 124.0 (3) |
| N3—C6—C7 | 116.9 (3) | N2—C16—H16 | 118.0 |
| C11—C6—C7 | 121.4 (3) | C15—C16—H16 | 118.0 |
| C6—C7—C8 | 113.5 (3) | N2—C17—C13 | 122.2 (3) |
| C6—C7—H7A | 108.9 | N2—C17—C18 | 117.4 (3) |
| C8—C7—H7A | 108.9 | C13—C17—C18 | 120.4 (3) |
| C6—C7—H7B | 108.9 | N1—C18—C4 | 123.4 (3) |
| C8—C7—H7B | 108.9 | N1—C18—C17 | 117.1 (3) |
| H7A—C7—H7B | 107.7 | C4—C18—C17 | 119.4 (3) |
| C9—C8—C7 | 112.1 (3) | O1—C19—O2 | 123.7 (4) |

supplementary materials

| | | | |
|---------------|-----------|---------------------------|-----------|
| C9—C8—H8A | 109.2 | O1—C19—C20 | 123.6 (4) |
| C7—C8—H8A | 109.2 | O2—C19—C20 | 112.6 (4) |
| C9—C8—H8B | 109.2 | C21—C20—C22 | 119.2 (3) |
| C7—C8—H8B | 109.2 | C21—C20—C19 | 121.8 (3) |
| H8A—C8—H8B | 107.9 | C22—C20—C19 | 119.0 (4) |
| C8—C9—C10 | 111.6 (3) | C20—C21—C22 ⁱ | 120.1 (3) |
| C8—C9—H9A | 109.3 | C20—C21—H21 | 119.9 |
| C10—C9—H9A | 109.3 | C22 ⁱ —C21—H21 | 119.9 |
| C8—C9—H9B | 109.3 | C20—C22—C21 ⁱ | 120.6 (3) |
| C10—C9—H9B | 109.3 | C20—C22—H22 | 119.7 |
| H9A—C9—H9B | 108.0 | C21 ⁱ —C22—H22 | 119.7 |
| C11—C10—C9 | 112.4 (3) | C1—N1—C18 | 116.7 (3) |
| C11—C10—H10A | 109.1 | C16—N2—C17 | 117.6 (3) |
| C9—C10—H10A | 109.1 | C6—N3—C5 | 117.0 (3) |
| C11—C10—H10B | 109.1 | C11—N4—C12 | 116.9 (3) |
| C9—C10—H10B | 109.1 | C19—O2—H2A | 109.5 |
| H10A—C10—H10B | 107.9 | | |

Symmetry codes: (i) $-x+1, -y, -z+3$.

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

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O2—H2A \cdots N2 | 0.82 | 2.02 | 2.694 (4) | 139 |

Fig. 1

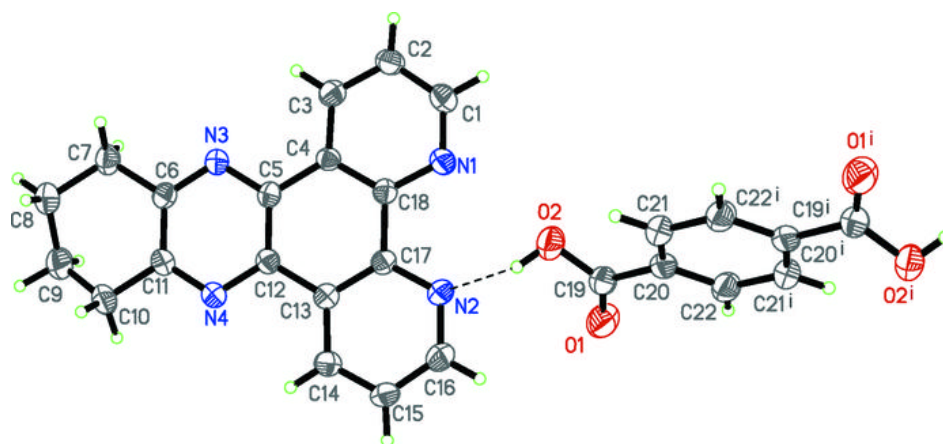


Fig. 2

