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4-[4-Amino-5-(4-pyridyl)-4*H*-1,2,4-triazol-3-yl]pyridinium 2,4,5-tricarboxybenzoate

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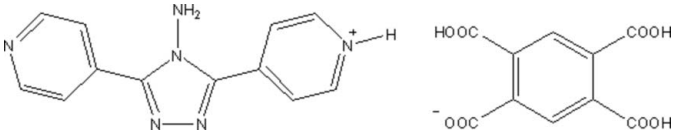
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.071; wR factor = 0.204; data-to-parameter ratio = 10.8.

The solution reaction of 4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole (bpt), benzene-1,2,4,5-tetracarboxylic acid (H_4betc) and $Co(NO_3)_2{\cdot}6H_2O$ led to the formation of the title cocrystal compound Hbpt·H_3betc or $C_{12}H_{11}N_6^+{\cdot}C_{10}H_5O_8^-$, in which strong hydrogen-bonding interactions assemble the ions into a three-dimensional supramolecular framework.

Related literature

For related literature, see: Li *et al.* (2007); Wang *et al.* (2007); Dong *et al.* (2007); Guo & Du (2002).



Experimental

Crystal data

$C_{12}H_{11}N_6^+{\cdot}C_{10}H_5O_8^-$
M_r = 492.41
Triclinic, $P\overline{1}$
a = 9.669 (4) Å
b = 9.892 (4) Å
c = 11.557 (5) Å
α = 78.620 (6)°
β = 78.135 (6)°
γ = 76.979 (6)°
V = 1040.7 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.976
5424 measured reflections
3616 independent reflections
2547 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.204
S = 1.04
3616 reflections
336 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6A···O5^{i}	0.86	2.02	2.757 (4)	143
O6—H6···O1^{ii}	0.82	2.61	3.086 (3)	119
O3—H3···N1^{iii}	0.82	1.82	2.628 (4)	169
O6—H6···O2^{ii}	0.82	1.76	2.573 (3)	170
N6—H6A···O1^{iv}	0.86	2.57	3.138 (4)	124
O8—H8···O1	0.82	1.59	2.413 (3)	179
N5—H5A···O7^{v}	0.905 (10)	2.091 (19)	2.967 (4)	162 (5)
N5—H5B···O4^{vi}	0.907 (10)	2.29 (2)	3.116 (4)	152 (3)
N5—H5B···O7^{vii}	0.907 (10)	2.46 (3)	3.070 (4)	125 (3)

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

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); 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: AT2483).

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supplementary materials

Acta Cryst. (2007). E**63**, o4883 [**doi:10.1107/S1600536807059351**]

4-[4-Amino-5-(4-pyridyl)-4*H*-1,2,4-triazol-3-yl]pyridinium 2,4,5-tricarboxybenzoate

J.-J. Liu, M.-X. Li, M. Shao and X. He

Comment

Organic cocrystals involving hydrogen-bonding and π-π stacking interactions are important in the areas of supramolecular chemistry, crystal engineering, and biological recognition (Wang *et al.*, 2007). Many organic cocrystals have been assembled from N-heterocycle and polycarboxylic acids (Li *et al.*, 2007). In our course of preparing ternary complexes containing 4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole and benzene-1,2,4,5-tetracarboxylic acid (Dong *et al.*, 2007; Guo & Du, 2002), a new cocrystal compound of Hbpt. H~3~betc was prepared unexpectedly. Herein we report the supramolecular framework of the title compound (I).

Experimental

Compound (I) was synthesized in a solution reaction. H_4betc (0.1 mmol) was added to 10 ml hot ethanol solution containing bpt (0.1 mmol) and $Co(NO_3)_2{\cdot}6H_2O$ (0.1 mmol) with stirring. Then NaOH solution was added dropwise into the muddy solution to form a clear pink solution. The solution was kept at room temperature to evaporate slowly. After one week, light yellow crystals suitable for X-ray diffraction were obtained.

Refinement

The H atoms of the NH_2 group were identified in difference Fourier syntheses and refined freely. The other H atoms were located geometrically, with C—H = 0.93, N—H = 0.86 and O—H = 0.82 Å and constrain to ride on their parents atoms, with U_{iso} = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(O).

Figures

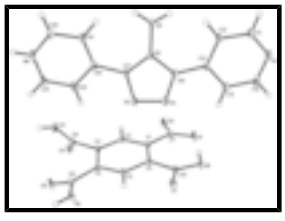

Fig. 1. An *ORTEP* view of the title molecule, with the atom-numbersing scheme.

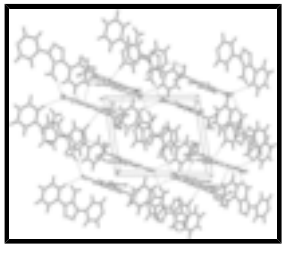

Fig. 2. Packing and hydrogen bonding diagram of the title compound.

4-[4-Amino-5-(4-pyridyl)-4*H*-1,2,4-triazol-3-yl]pyridinium 2,4,5-tricarboxybenzoate

Crystal data

$C_{22}H_{16}N_6O_8$	$Z = 2$
$M_r = 492.41$	$F_{000} = 508$
Triclinic, $P\overline{1}$	$D_x = 1.571$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.669$ (4) Å	Cell parameters from 1502 reflections
$b = 9.892$ (4) Å	$\theta = 2.2$–26.1º
$c = 11.557$ (5) Å	$\mu = 0.12$ mm^{-1}
$\alpha = 78.620$ (6)º	$T = 296$ (2) K
$\beta = 78.135$ (6)º	Block, light-yellow
$\gamma = 76.979$ (6)º	0.30 × 0.30 × 0.20 mm
$V = 1040.7$ (8) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	3616 independent reflections
Radiation source: fine-focus sealed tube	2547 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 296$(2) K	$\theta_{max} = 25.1$º
φ and ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 10$
$T_{min} = 0.964$, $T_{max} = 0.976$	$k = -11 \rightarrow 11$
5424 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.071$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.204$	$w = 1/[\sigma^2(F_o^2) + (0.1223P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3616 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
336 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3322 (3)	0.8520 (3)	0.1415 (3)	0.0268 (7)
C2	0.4104 (3)	0.7976 (3)	0.0394 (3)	0.0311 (8)
H2	0.3610	0.7692	−0.0097	0.037*
C3	0.5588 (3)	0.7842 (3)	0.0084 (3)	0.0288 (7)
C4	0.6323 (3)	0.8310 (3)	0.0802 (3)	0.0273 (7)
C5	0.5564 (3)	0.8803 (3)	0.1826 (3)	0.0291 (7)
H5	0.6067	0.9085	0.2313	0.035*
C6	0.4077 (3)	0.8905 (3)	0.2175 (3)	0.0260 (7)
C7	0.1694 (3)	0.8661 (3)	0.1556 (3)	0.0324 (8)
C8	0.6323 (3)	0.7232 (3)	−0.1027 (3)	0.0319 (8)
C9	0.7885 (3)	0.8363 (4)	0.0439 (3)	0.0341 (8)
C10	0.3530 (3)	0.9423 (3)	0.3371 (3)	0.0314 (8)
C11	−0.0022 (4)	0.4396 (4)	0.7227 (4)	0.0522 (10)
H11	−0.0305	0.3658	0.7794	0.063*
C12	0.1218 (4)	0.4114 (4)	0.6405 (3)	0.0466 (10)
H12	0.1766	0.3209	0.6433	0.056*
C13	0.1635 (3)	0.5187 (3)	0.5543 (3)	0.0345 (8)
C14	0.0788 (4)	0.6515 (4)	0.5562 (3)	0.0410 (9)
H14	0.1033	0.7272	0.4999	0.049*
C15	−0.0431 (4)	0.6701 (4)	0.6434 (3)	0.0447 (9)
H15	−0.0991	0.7597	0.6444	0.054*
C16	0.2958 (4)	0.5033 (3)	0.4658 (3)	0.0347 (8)
C17	0.4936 (3)	0.4228 (3)	0.3530 (3)	0.0330 (8)
C18	0.6221 (3)	0.3351 (4)	0.2942 (3)	0.0336 (8)
C19	0.6714 (3)	0.1944 (4)	0.3361 (3)	0.0401 (9)
H19	0.6186	0.1474	0.4020	0.048*
C20	0.7982 (4)	0.1261 (4)	0.2796 (3)	0.0450 (9)
H20	0.8325	0.0322	0.3077	0.054*
C21	0.8296 (4)	0.3258 (4)	0.1411 (3)	0.0478 (10)
H21	0.8852	0.3687	0.0744	0.057*
C22	0.7032 (4)	0.4010 (4)	0.1932 (3)	0.0440 (9)
H22	0.6717	0.4945	0.1619	0.053*
N1	−0.0829 (3)	0.5666 (3)	0.7248 (3)	0.0459 (8)

N2	0.3819 (3)	0.3821 (3)	0.4343 (2)	0.0303 (6)
N3	0.4787 (3)	0.5603 (3)	0.3354 (3)	0.0526 (9)
N4	0.3522 (3)	0.6111 (3)	0.4076 (3)	0.0531 (9)
N5	0.3484 (3)	0.2474 (3)	0.4713 (3)	0.0406 (7)
N6	0.8729 (3)	0.1925 (3)	0.1852 (3)	0.0457 (8)
H6A	0.9526	0.1471	0.1511	0.055*
O1	0.0868 (2)	0.9087 (3)	0.2452 (2)	0.0506 (7)
O2	0.1228 (2)	0.8334 (3)	0.0740 (2)	0.0451 (7)
O3	0.7241 (3)	0.6058 (3)	−0.0823 (2)	0.0499 (7)
H3	0.7766	0.5890	−0.1453	0.075*
O4	0.6057 (3)	0.7770 (3)	−0.2008 (2)	0.0505 (7)
O5	0.8508 (2)	0.8303 (3)	−0.0578 (2)	0.0521 (7)
O6	0.8478 (2)	0.8557 (3)	0.1290 (2)	0.0496 (7)
H6	0.9336	0.8557	0.1044	0.074*
O7	0.4391 (2)	0.9549 (2)	0.3962 (2)	0.0391 (6)
O8	0.2155 (2)	0.9750 (3)	0.3766 (2)	0.0443 (7)
H8	0.1705	0.9529	0.3328	0.066*
H5A	0.418 (4)	0.202 (5)	0.515 (4)	0.11 (2)*
H5B	0.366 (4)	0.208 (4)	0.404 (2)	0.053 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0186 (16)	0.0331 (17)	0.0240 (16)	−0.0031 (12)	0.0033 (12)	−0.0026 (13)
C2	0.0200 (17)	0.044 (2)	0.0274 (18)	−0.0047 (14)	0.0035 (13)	−0.0115 (15)
C3	0.0233 (17)	0.0357 (18)	0.0216 (16)	−0.0016 (13)	0.0046 (13)	−0.0043 (13)
C4	0.0156 (16)	0.0351 (17)	0.0262 (17)	−0.0023 (12)	0.0016 (12)	−0.0015 (13)
C5	0.0235 (17)	0.0385 (18)	0.0240 (17)	−0.0078 (13)	−0.0001 (13)	−0.0037 (14)
C6	0.0215 (16)	0.0266 (16)	0.0241 (16)	−0.0005 (12)	0.0036 (12)	−0.0030 (13)
C7	0.0207 (17)	0.043 (2)	0.0283 (18)	−0.0036 (14)	0.0032 (14)	−0.0053 (15)
C8	0.0198 (17)	0.043 (2)	0.0278 (18)	−0.0027 (14)	0.0047 (13)	−0.0065 (15)
C9	0.0260 (18)	0.044 (2)	0.0271 (19)	−0.0040 (14)	0.0033 (14)	−0.0061 (15)
C10	0.0322 (19)	0.0315 (18)	0.0257 (17)	−0.0048 (14)	0.0027 (14)	−0.0027 (14)
C11	0.047 (2)	0.048 (2)	0.048 (2)	−0.0057 (18)	0.0194 (18)	−0.0063 (18)
C12	0.039 (2)	0.041 (2)	0.046 (2)	0.0039 (16)	0.0131 (17)	−0.0085 (17)
C13	0.0274 (18)	0.0384 (19)	0.0328 (19)	0.0026 (14)	0.0018 (14)	−0.0112 (15)
C14	0.036 (2)	0.042 (2)	0.037 (2)	0.0000 (16)	0.0035 (16)	−0.0074 (16)
C15	0.033 (2)	0.045 (2)	0.049 (2)	0.0090 (16)	−0.0016 (17)	−0.0149 (19)
C16	0.033 (2)	0.0323 (18)	0.0330 (19)	−0.0002 (15)	0.0033 (15)	−0.0066 (15)
C17	0.0230 (18)	0.040 (2)	0.0269 (18)	−0.0009 (14)	0.0109 (13)	−0.0047 (15)
C18	0.0257 (18)	0.046 (2)	0.0236 (17)	−0.0036 (14)	0.0085 (13)	−0.0102 (15)
C19	0.0277 (19)	0.047 (2)	0.036 (2)	−0.0012 (16)	0.0109 (15)	−0.0080 (16)
C20	0.029 (2)	0.052 (2)	0.048 (2)	−0.0002 (16)	0.0020 (16)	−0.0136 (18)
C21	0.037 (2)	0.067 (3)	0.033 (2)	−0.0131 (19)	0.0168 (16)	−0.0134 (19)
C22	0.037 (2)	0.056 (2)	0.031 (2)	−0.0066 (17)	0.0089 (16)	−0.0059 (17)
N1	0.0358 (18)	0.051 (2)	0.0438 (19)	−0.0011 (15)	0.0075 (14)	−0.0138 (16)
N2	0.0250 (15)	0.0310 (15)	0.0282 (15)	0.0014 (11)	0.0034 (11)	−0.0051 (12)
N3	0.0407 (19)	0.0435 (19)	0.054 (2)	−0.0003 (14)	0.0238 (15)	−0.0046 (16)

N4	0.047 (2)	0.0393 (18)	0.055 (2)	−0.0005 (15)	0.0210 (16)	−0.0057 (15)
N5	0.0312 (17)	0.0373 (18)	0.048 (2)	−0.0031 (13)	0.0068 (14)	−0.0134 (15)
N6	0.0232 (16)	0.067 (2)	0.0425 (19)	−0.0008 (14)	0.0105 (13)	−0.0229 (17)
O1	0.0192 (13)	0.086 (2)	0.0429 (15)	−0.0012 (12)	0.0095 (11)	−0.0262 (14)
O2	0.0226 (13)	0.0788 (18)	0.0374 (14)	−0.0112 (11)	0.0009 (10)	−0.0216 (13)
O3	0.0452 (16)	0.0545 (16)	0.0333 (14)	0.0116 (12)	0.0100 (11)	−0.0093 (12)
O4	0.0493 (17)	0.0682 (18)	0.0256 (14)	0.0039 (13)	−0.0004 (11)	−0.0111 (12)
O5	0.0247 (14)	0.092 (2)	0.0372 (15)	−0.0150 (13)	0.0117 (11)	−0.0177 (14)
O6	0.0195 (13)	0.092 (2)	0.0395 (15)	−0.0144 (13)	0.0031 (10)	−0.0188 (14)
O7	0.0370 (14)	0.0538 (15)	0.0258 (12)	−0.0081 (11)	−0.0003 (10)	−0.0107 (11)
O8	0.0246 (13)	0.0674 (17)	0.0365 (15)	−0.0004 (11)	0.0097 (10)	−0.0231 (13)

Geometric parameters (Å, °)

C1—C2	1.397 (4)	C14—C15	1.388 (5)
C1—C6	1.404 (4)	C14—H14	0.9300
C1—C7	1.526 (4)	C15—N1	1.315 (5)
C2—C3	1.388 (4)	C15—H15	0.9300
C2—H2	0.9300	C16—N4	1.310 (4)
C3—C4	1.396 (4)	C16—N2	1.364 (4)
C3—C8	1.501 (4)	C17—N3	1.314 (4)
C4—C5	1.374 (4)	C17—N2	1.357 (4)
C4—C9	1.492 (4)	C17—C18	1.468 (4)
C5—C6	1.397 (4)	C18—C19	1.389 (5)
C5—H5	0.9300	C18—C22	1.399 (5)
C6—C10	1.520 (4)	C19—C20	1.363 (5)
C7—O2	1.248 (4)	C19—H19	0.9300
C7—O1	1.252 (4)	C20—N6	1.323 (5)
C8—O4	1.206 (4)	C20—H20	0.9300
C8—O3	1.306 (4)	C21—N6	1.322 (5)
C9—O5	1.211 (4)	C21—C22	1.369 (5)
C9—O6	1.299 (4)	C21—H21	0.9300
C10—O7	1.221 (4)	C22—H22	0.9300
C10—O8	1.302 (4)	N2—N5	1.406 (4)
C11—N1	1.323 (5)	N3—N4	1.383 (4)
C11—C12	1.380 (5)	N5—H5A	0.905 (10)
C11—H11	0.9300	N5—H5B	0.907 (10)
C12—C13	1.375 (5)	N6—H6A	0.8600
C12—H12	0.9300	O3—H3	0.8200
C13—C14	1.384 (5)	O6—H6	0.8200
C13—C16	1.464 (4)	O8—H8	0.8200
C2—C1—C6	118.4 (3)	C15—C14—H14	120.5
C2—C1—C7	114.6 (3)	N1—C15—C14	122.9 (3)
C6—C1—C7	127.0 (3)	N1—C15—H15	118.5
C3—C2—C1	122.7 (3)	C14—C15—H15	118.5
C3—C2—H2	118.6	N4—C16—N2	109.7 (3)
C1—C2—H2	118.6	N4—C16—C13	122.3 (3)
C2—C3—C4	118.5 (3)	N2—C16—C13	127.9 (3)
C2—C3—C8	118.3 (3)	N3—C17—N2	110.1 (3)

C4—C3—C8	123.1 (3)	N3—C17—C18	121.0 (3)
C5—C4—C3	118.8 (3)	N2—C17—C18	128.8 (3)
C5—C4—C9	119.8 (3)	C19—C18—C22	118.5 (3)
C3—C4—C9	121.3 (3)	C19—C18—C17	124.3 (3)
C4—C5—C6	123.5 (3)	C22—C18—C17	117.1 (3)
C4—C5—H5	118.3	C20—C19—C18	119.3 (3)
C6—C5—H5	118.3	C20—C19—H19	120.4
C5—C6—C1	117.8 (3)	C18—C19—H19	120.4
C5—C6—C10	112.4 (3)	N6—C20—C19	120.5 (4)
C1—C6—C10	129.8 (3)	N6—C20—H20	119.8
O2—C7—O1	121.8 (3)	C19—C20—H20	119.8
O2—C7—C1	117.0 (3)	N6—C21—C22	120.2 (3)
O1—C7—C1	121.2 (3)	N6—C21—H21	119.9
O4—C8—O3	123.7 (3)	C22—C21—H21	119.9
O4—C8—C3	122.6 (3)	C21—C22—C18	119.0 (4)
O3—C8—C3	113.7 (3)	C21—C22—H22	120.5
O5—C9—O6	123.8 (3)	C18—C22—H22	120.5
O5—C9—C4	122.1 (3)	C15—N1—C11	118.0 (3)
O6—C9—C4	113.9 (3)	C17—N2—C16	105.5 (3)
O7—C10—O8	119.6 (3)	C17—N2—N5	129.1 (3)
O7—C10—C6	119.6 (3)	C16—N2—N5	125.1 (3)
O8—C10—C6	120.9 (3)	C17—N3—N4	107.0 (3)
N1—C11—C12	123.2 (4)	C16—N4—N3	107.7 (3)
N1—C11—H11	118.4	N2—N5—H5A	103 (3)
C12—C11—H11	118.4	N2—N5—H5B	106 (2)
C13—C12—C11	119.2 (3)	H5A—N5—H5B	107 (4)
C13—C12—H12	120.4	C21—N6—C20	122.5 (3)
C11—C12—H12	120.4	C21—N6—H6A	118.7
C12—C13—C14	117.6 (3)	C20—N6—H6A	118.7
C12—C13—C16	124.3 (3)	C8—O3—H3	109.5
C14—C13—C16	118.0 (3)	C9—O6—H6	109.5
C13—C14—C15	119.1 (3)	C10—O8—H8	109.5
C13—C14—H14	120.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6A···O5^{i}	0.86	2.02	2.757 (4)	143
O6—H6···O1^{ii}	0.82	2.61	3.086 (3)	119
O3—H3···N1^{iii}	0.82	1.82	2.628 (4)	169
O6—H6···O2^{ii}	0.82	1.76	2.573 (3)	170
N6—H6A···O1^{iv}	0.86	2.57	3.138 (4)	124
O8—H8···O1	0.82	1.59	2.413 (3)	179
N5—H5A···O7^{v}	0.905 (10)	2.091 (19)	2.967 (4)	162 (5)
N5—H5B···O4^{vi}	0.907 (10)	2.29 (2)	3.116 (4)	152 (3)
N5—H5B···O7^{vii}	0.907 (10)	2.46 (3)	3.070 (4)	125 (3)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) *x*+1, *y*, *z*; (iii) *x*+1, *y*, *z*−1; (iv) *x*+1, *y*−1, *z*; (v) −*x*+1, −*y*+1, −*z*+1; (vi) −*x*+1, −*y*+1, −*z*; (vii) *x*, *y*−1, *z*.

Fig. 1

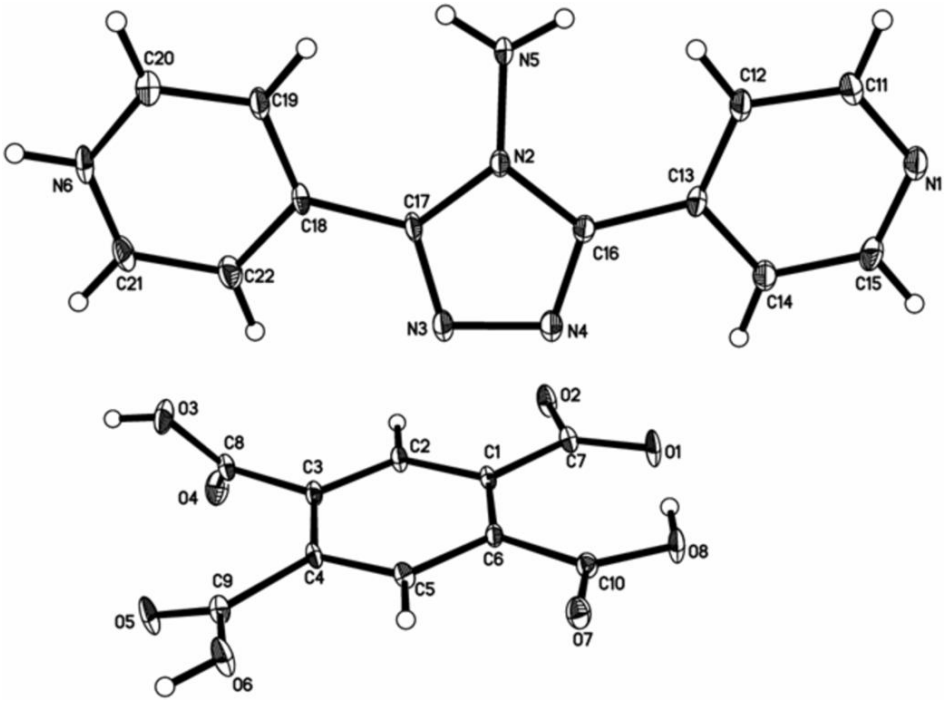
C20
C19
N5
C12
C11
N6
N2
C13
N1
C18
C17
C16
C21
C22
C15
C14
N3
N4
O3
O2
C8
C2
C1
C7
O1
C3
O4
C6
O8
C9
C4
C5
C10
O5
O7
O6

Fig. 2