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Propane-1,3-diaminium–2-carboxypyridine-6-carboxylate–pyridine-2,6-dicarboxylic acid–water (1/2/2/8)

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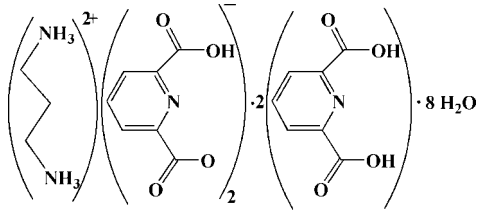
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.139; data-to-parameter ratio = 16.4.

The title proton-transfer compound, $C_3H_{12}N_2^{2+}\cdot 2C_7H_4NO_4^-\cdot\cdot 2C_7H_5NO_4\cdot 8H_2O$ or $(pnH_2)(pydcH)_2.2(pydcH_2)\cdot 8H_2O$, was obtained by the reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) and propane-1,3-diamine (pn) in aqueous solution. Both neutral and monoanionic forms of the diacid are observed in the crystal structure. The negative charge of two monoanions is balanced by the dicationic propane-1,3-diaminium species. In addition, considerable π–π stacking interactions between the aromatic rings of the $(pydcH)^-$ and ($pydcH_2$) fragments [with centroid–centroid distances of 3.5108 (11)–3.5949 (11) Å] are observed. The most important feature of this crystal structure is the presence of a large number of O—H···O, O—H···N, N—H···O, N—H···N, C—H···O and C—H···N hydrogen bonds, with $D\cdots A$ ranging from 2.445 (2) to 3.485 (3) Å. These interactions as well as ion pairing and π–π stacking connect the various fragments into a supramolecular structure.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermazi, Ghasemikhah & Soleimannejad (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah, Ghadermazi & Soleimannejad, 2007; Aghabozorg, Daneshvar *et al.* (2007).



Experimental

Crystal data

$C_3H_{12}N_2^{2+}\cdot 2C_7H_4NO_4^-\cdot\cdot 2C_7H_5NO_4\cdot 8H_2O$
M_r = 886.73
Monoclinic, $P2_1/c$
a = 13.5425 (2) Å
b = 13.5237 (2) Å
c = 21.7538 (3) Å
β = 99.914 (1)°
V = 3924.60 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 150 (2) K
0.26 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.967, T_{max} = 0.985
56174 measured reflections
9031 independent reflections
6702 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.139
S = 1.02
9031 reflections
550 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O19	0.95	1.94	2.830 (2)	154
O5—H5AA···O20	0.95	1.67	2.592 (2)	164
O7—H7A···O3	0.95	1.51	2.455 (2)	177
O7—H7A···O4	0.95	2.57	3.119 (2)	117
O9—H9A···O22	0.95	1.64	2.588 (2)	172
O11—H11A···O13^{i}	0.95	1.50	2.445 (2)	177
O11—H11A···O14^{i}	0.95	2.61	3.181 (2)	119
O16—H16A···O24	0.95	1.60	2.551 (2)	174
O17—H17A···O15	0.95	1.90	2.838 (2)	167
O17—H17A···N4	0.95	2.43	2.956 (2)	115
O17—H17B···O14	0.95	1.87	2.821 (2)	175
O18—H18B···O1	0.95	1.89	2.815 (2)	164
O18—H18A···O17^{ii}	0.95	1.88	2.809 (2)	166
O19—H19B···N1	0.95	2.22	3.092 (2)	152
O19—H19A···O13^{i}	0.95	2.34	3.174 (2)	146
O20—H20B···O12^{iii}	0.95	1.87	2.793 (2)	164
O20—H20A···O22	0.95	1.95	2.875 (3)	165
O21—H21B···O10	0.95	1.89	2.834 (2)	170
O21—H21A···O19^{iii}	0.95	1.85	2.784 (2)	166
O22—H22A···O21	0.95	1.88	2.818 (2)	168
O22—H22B···O17^{iv}	0.95	1.81	2.742 (2)	167
O23—H23B···O6	0.95	1.85	2.749 (2)	157
O23—H23A···O12^{iii}	0.95	1.96	2.899 (2)	170
O24—H24B···O18^{v}	0.95	1.79	2.706 (2)	161
O24—H24A···O12^{vi}	0.95	1.86	2.761 (2)	157
N5—H5A···N2	0.95	2.40	3.342 (3)	171
N5—H5A···O6	0.95	2.61	3.227 (2)	123
N5—H5B···O4	0.95	1.95	2.879 (2)	166
N5—H5C···O23^{vii}	0.95	2.06	2.991 (3)	166
N6—H6A···O14^{i}	0.95	2.01	2.938 (2)	164
N6—H6B···O21^{viii}	0.95	1.90	2.849 (2)	174
N6—H6C···N3	0.95	2.17	3.070 (2)	158

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O18^{iii}	0.95	2.56	3.429 (3)	153
C10—H10···O1^{ix}	0.95	2.50	3.335 (3)	147
C11—H11···O18^{ix}	0.95	2.52	3.427 (3)	159
C19—H19···O15^{x}	0.95	2.46	3.266 (3)	143
C25—H25···O24^{xi}	0.95	2.56	3.485 (3)	165
C26—H26···O16^{xi}	0.95	2.56	3.287 (3)	134
C31—H31A···N2	0.99	2.52	3.391 (3)	146
C31—H31B···O10	0.99	2.54	3.175 (3)	122

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$; (vi) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (vii) $-x+1, -y+2, -z$; (viii) $-x+1, -y+1, -z$; (ix) $x-1, -y+\frac{3}{2}, z-\frac{1}{2}$; (x) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (xi) $-x, -y, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); 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: BQ2048).

References

Aghabozorg, H., Attar Gharamaleki, J., Ghadermazi, M., Ghasemikhah, P. & Soleimannejad, J. (2007). *Acta Cryst.* E**63**, m1803–m1804.
Aghabozorg, H., Attar Gharamaleki, J., Ghasemikhah, P., Ghadermazi, M. & Soleimannejad, J. (2007). *Acta Cryst.* E**63**, m1710–m1711.
Aghabozorg, H., Daneshvar, S., Motyeian, E., Ghadermazi, M. & Attar Gharamaleki, J. (2007). *Acta Cryst.* E**63**, m2468–m2469.
Bruker (1998). *SMART* (Version 5.0), *SAINT* (Version 4.0) and *SADABS* (Version 2.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2008). E**64**, o231-o232 [**doi:10.1107/S1600536807065270**]

Propane-1,3-diaminium-2-carboxypyridine-6-carboxylate-pyridine-2,6-dicarboxylic acid-water (1/2/2/8)

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Comment

Intermolecular interactions, such as hydrogen bonding, π-π stacking, ion pairing and donor-acceptor interactions, are famous for making aggregates of molecules. Hydrogen bonding has been described as the most important interaction in supramolecular chemistry. Dicarboxylic acids possess a good potential to be used as proton donors in the synthesis of proton transfer compounds. Among these diacids, pyridine-2,6-dicarboxylic acid has been used by our research group for preparing of such compounds. For example, (pydaH)(pydcH) in which pyridine-2,6-diamine (pyda) was used as a proton acceptor. The resulting compounds with some remaining sites as electron donors can coordinate to metallic ions (Aghabozorg, Attar Gharamaleki, Ghadermazi, Ghasemikhah & Soleimannejad, 2007; Aghabozorg, Attar Gharamaleki, Ghasemikhah, Ghadermazi & Soleimannejad, 2007; Aghabozorg, Daneshvar *et al.*, 2007).

Here we report a new proton transfer compound obtained from ($pydcH_2$) as a proton donor and propane-1,3-diamine (pn) as an acceptor. The molecular structure of the title compound is shown in Fig. 1. The intermolecular hydrogen bond distances are listed in Table 1.

The structure of this compound contains two neutral $pydcH_2$ molecules, two monoanionic $(pydcH)^-$, one $(pnH_2)^{2+}$ species and eight uncoordinated water molecules. The negative charge of two monoanions is neutralized by dicationic propane-1,3-diaminium fragments.

A considerable π-π stacking interactions between aromatic rings of ($pydcH_2$) and $(pydcH)^-$ fragments with centroid-centroid distances of 3.5108 (11)–3.5949 (11) Å are observed in the prepared compound (Fig. 2). A remarkable feature in the crystal structure of compound (I) is the presence of a large number of O—H···O, O—H···N, N—H···O, N—H···N, C—H···O and C—H···N hydrogen bonds interactions ranging from 2.450 (2) to 3.488 (3) Å. The shortest hydrogen bond is O11—H11A···O13 ($-x + 1, y + 1/2, -z + 1/2$) with D···A = 2.450 (2) Å, a very strong interaction (Table 1). These extensive hydrogen bond interactions as well as ion pairing and π-π stacking connect the different components to form a three-dimensional supramolecular structure (Fig. 3).

Experimental

The reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) (330 mg, 2 mmol) with propane-1,3-diamine (pn) (76 mg, 1 mmol) in a 2:1 molar ratio in tetrahydrofuran (THF) led to the formation of a white precipitate which was filtered off and dried. The resulting powder was dissolved in water to give colorless crystals of the title compound after four weeks.

Figures

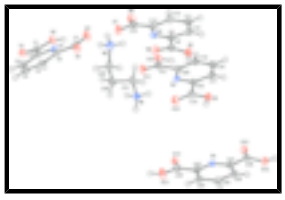

Fig. 1. Molecular structure of the title compound (I), displacement ellipsoids are drawn at the 50% probability level. Water molecules are omitted for clarity.

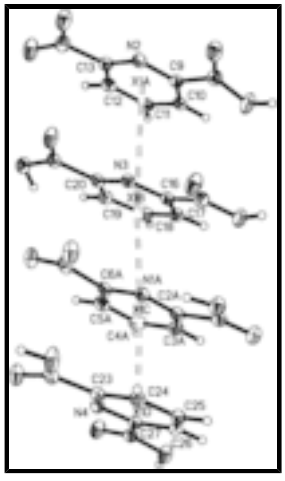

Fig. 2. π-π Stacking interactions between aromatic rings of ($pydcH_2$) and $(pydcH)^-$ fragments with centroid-centroid distances of: X1A····X1B, 3.5949 (11) Å (*x*, *y*, *z*); X1B····X1C, 3.5191 (11) Å (1 − *x*, −1/2 + *y*, 1/2 − *z*); X1C····X1D, 3.5789 (11) Å (1 − *x*, 1/2 + *y*, 1/2 − *z*); X1A····X1D, 3.5108 (11) Å (*x*, 1 + *y*, *z*).

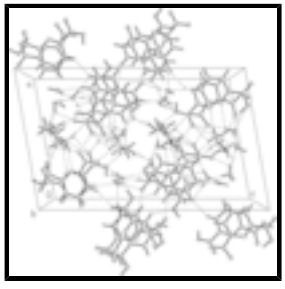

Fig. 3. Unit-cell packing diagram of the compound (I). Hydrogen bonds are indicated by dashed lines.

Propane-1,3-diaminium–2-carboxypyridine-6-carboxylate– pyridine-2,6-dicarboxylic acid–water (1/2/2/8)

Crystal data

$C_3H_{12}N_2^{2+}·2C_7H_4NO_4^-·2C_7H_5NO_4·8H_2O$	F_{000} = 1864
M_r = 886.73	D_x = 1.501 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.5425 (2) Å	Cell parameters from 9156 reflections
b = 13.5237 (2) Å	θ = 2.4–29.1°
c = 21.7538 (3) Å	μ = 0.13 mm^{-1}
β = 99.914 (1)°	*T* = 150 (2) K
V = 3924.60 (10) Å^3	Block, colourless
Z = 4	0.26 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1000 diffractometer	9031 independent reflections
Radiation source: fine-focus sealed tube	6702 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.054$
Detector resolution: 100 pixels mm^{-1}	$\theta_{max} = 27.5^{o}$
$T = 150(2)$ K	$\theta_{min} = 1.5^{o}$
ω scans	$h = -17 \rightarrow 17$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -17 \rightarrow 17$
$T_{min} = 0.967$, $T_{max} = 0.985$	$l = -28 \rightarrow 28$
56174 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 3.5811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
9031 reflections	$\Delta\rho_{max} = 0.84$ e $Å^{-3}$
550 parameters	$\Delta\rho_{min} = -0.51$ e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.90840 (11)	0.77843 (12)	0.54180 (7)	0.0254 (3)
O2	0.74609 (11)	0.79981 (11)	0.51063 (7)	0.0249 (3)
H2A	0.6958	0.8087	0.4748	0.030*
O3	0.60302 (12)	0.87473 (13)	0.31596 (7)	0.0307 (4)

O4	0.68349 (11)	0.88557 (12)	0.23488 (7)	0.0262 (3)
O5	0.18211 (12)	0.78608 (13)	−0.00659 (7)	0.0320 (4)
H5AA	0.2027	0.7723	−0.0453	0.038*
O6	0.33622 (12)	0.84668 (13)	0.02551 (7)	0.0292 (4)
O7	0.45325 (11)	0.89020 (13)	0.23505 (7)	0.0298 (4)
H7A	0.5096	0.8838	0.2675	0.036*
O8	0.35911 (12)	0.86950 (14)	0.30873 (7)	0.0333 (4)
O9	0.15292 (11)	0.52710 (12)	−0.01050 (6)	0.0245 (3)
H9A	0.1799	0.5233	−0.0480	0.029*
O10	0.31288 (12)	0.55101 (13)	0.03474 (7)	0.0315 (4)
O11	0.39207 (11)	0.63847 (12)	0.24320 (6)	0.0262 (3)
H11A	0.4456	0.6339	0.2776	0.031*
O12	0.28767 (11)	0.61399 (11)	0.31033 (6)	0.0235 (3)
O13	0.46668 (11)	0.12691 (14)	0.17039 (7)	0.0322 (4)
O14	0.37185 (11)	0.11228 (12)	0.24412 (6)	0.0258 (3)
O15	0.02539 (11)	0.06135 (12)	0.19062 (7)	0.0255 (3)
O16	−0.04375 (11)	0.02480 (12)	0.09246 (6)	0.0248 (3)
H16A	−0.1019	0.0061	0.1086	0.030*
O17	0.18876 (11)	0.09699 (12)	0.28868 (7)	0.0263 (3)
H17A	0.1416	0.0806	0.2525	0.032*
H17B	0.2490	0.1058	0.2726	0.032*
O18	0.85758 (12)	0.72397 (12)	0.65729 (7)	0.0276 (3)
H18B	0.8642	0.7497	0.6176	0.033*
H18A	0.8308	0.7822	0.6725	0.033*
O19	0.55978 (12)	0.80178 (13)	0.42843 (7)	0.0337 (4)
H19B	0.6221	0.8311	0.4244	0.040*
H19A	0.5239	0.7533	0.4019	0.040*
O20	0.20445 (14)	0.74513 (13)	−0.11979 (8)	0.0385 (4)
H20B	0.2437	0.7866	−0.1413	0.046*
H20A	0.2206	0.6770	−0.1216	0.046*
O21	0.42936 (12)	0.54219 (13)	−0.06159 (7)	0.0338 (4)
H21B	0.3970	0.5418	−0.0262	0.041*
H21A	0.4678	0.6011	−0.0607	0.041*
O22	0.22400 (13)	0.53350 (13)	−0.11351 (7)	0.0348 (4)
H22A	0.2948	0.5373	−0.1021	0.042*
H22B	0.2014	0.4911	−0.1479	0.042*
O23	0.42837 (14)	0.89677 (16)	−0.07328 (8)	0.0464 (5)
H23B	0.3852	0.8938	−0.0432	0.056*
H23A	0.3866	0.8866	−0.1125	0.056*
O24	−0.20133 (11)	−0.03538 (11)	0.13049 (7)	0.0236 (3)
H24B	−0.1884	−0.1000	0.1470	0.028*
H24A	−0.2294	0.0031	0.1597	0.028*
C1	0.83900 (16)	0.79459 (15)	0.49983 (9)	0.0200 (4)
C2	0.85368 (15)	0.80829 (15)	0.43368 (9)	0.0187 (4)
C3	0.94700 (16)	0.79837 (15)	0.41643 (10)	0.0213 (4)
H3	1.0049	0.7844	0.4465	0.026*
C4	0.95318 (17)	0.80945 (16)	0.35423 (10)	0.0244 (5)
H4	1.0156	0.8019	0.3405	0.029*
C5	0.86744 (16)	0.83174 (15)	0.31202 (10)	0.0222 (4)

H5	0.8702	0.8397	0.2690	0.027*
C6	0.77715 (16)	0.84232 (15)	0.33360 (9)	0.0196 (4)
C7	0.68120 (16)	0.86929 (16)	0.29052 (9)	0.0223 (4)
C8	0.25328 (15)	0.82141 (16)	0.03516 (9)	0.0207 (4)
C9	0.22600 (15)	0.82952 (15)	0.09889 (9)	0.0179 (4)
C10	0.12850 (15)	0.81571 (15)	0.10843 (9)	0.0199 (4)
H10	0.0767	0.7994	0.0747	0.024*
C11	0.10811 (15)	0.82621 (15)	0.16848 (10)	0.0215 (4)
H11	0.0417	0.8191	0.1765	0.026*
C12	0.18632 (16)	0.84712 (15)	0.21610 (10)	0.0212 (4)
H12	0.1748	0.8543	0.2577	0.025*
C13	0.28225 (15)	0.85764 (15)	0.20248 (9)	0.0193 (4)
C14	0.36955 (16)	0.87368 (16)	0.25443 (10)	0.0228 (4)
C15	0.22408 (15)	0.54705 (16)	0.03722 (9)	0.0209 (4)
C16	0.18464 (15)	0.56360 (15)	0.09693 (9)	0.0177 (4)
C17	0.08312 (15)	0.55850 (15)	0.09973 (10)	0.0204 (4)
H17	0.0350	0.5465	0.0633	0.024*
C18	0.05401 (16)	0.57144 (16)	0.15715 (10)	0.0224 (4)
H18	−0.0148	0.5680	0.1608	0.027*
C19	0.12607 (15)	0.58934 (15)	0.20898 (9)	0.0197 (4)
H19	0.1079	0.5973	0.2490	0.024*
C20	0.22577 (15)	0.59546 (14)	0.20150 (9)	0.0172 (4)
C21	0.30780 (15)	0.61719 (15)	0.25620 (9)	0.0190 (4)
C22	0.38272 (15)	0.11248 (16)	0.18930 (9)	0.0208 (4)
C23	0.29575 (15)	0.09393 (14)	0.13742 (9)	0.0178 (4)
C24	0.30923 (15)	0.08566 (15)	0.07564 (9)	0.0192 (4)
H24	0.3738	0.0925	0.0647	0.023*
C25	0.22567 (16)	0.06715 (15)	0.03039 (9)	0.0201 (4)
H25	0.2320	0.0614	−0.0123	0.024*
C26	0.13305 (16)	0.05727 (15)	0.04837 (9)	0.0197 (4)
H26	0.0746	0.0452	0.0183	0.024*
C27	0.12751 (15)	0.06546 (14)	0.11150 (9)	0.0173 (4)
C28	0.03140 (15)	0.05113 (15)	0.13594 (9)	0.0193 (4)
C29	0.57849 (17)	0.82728 (18)	0.08483 (10)	0.0278 (5)
H29A	0.6472	0.8472	0.0803	0.033*
H29B	0.5371	0.8245	0.0427	0.033*
C30	0.58164 (16)	0.72587 (18)	0.11447 (10)	0.0266 (5)
H30A	0.6195	0.7297	0.1576	0.032*
H30B	0.6176	0.6798	0.0907	0.032*
C31	0.47782 (16)	0.68576 (17)	0.11606 (10)	0.0255 (5)
H31A	0.4435	0.7295	0.1422	0.031*
H31B	0.4385	0.6861	0.0733	0.031*
N1	0.76996 (13)	0.82962 (13)	0.39359 (8)	0.0192 (4)
N2	0.30298 (13)	0.85093 (12)	0.14479 (8)	0.0185 (3)
N3	0.25553 (12)	0.58254 (12)	0.14653 (7)	0.0172 (3)
N4	0.20715 (12)	0.08387 (12)	0.15546 (7)	0.0172 (3)
N5	0.53588 (15)	0.90263 (15)	0.12309 (8)	0.0285 (4)
H5A	0.4682	0.8858	0.1245	0.034*
H5B	0.5770	0.9026	0.1631	0.034*

H5C	0.5359	0.9684	0.1078	0.034*
N6	0.48067 (13)	0.58346 (14)	0.14140 (8)	0.0230 (4)
H6A	0.5210	0.5842	0.1817	0.028*
H6B	0.5084	0.5374	0.1161	0.028*
H6C	0.4155	0.5676	0.1490	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0257 (8)	0.0309 (9)	0.0189 (7)	0.0012 (6)	0.0019 (6)	0.0031 (6)
O2	0.0228 (8)	0.0324 (9)	0.0200 (7)	0.0025 (6)	0.0051 (6)	0.0006 (6)
O3	0.0221 (8)	0.0496 (11)	0.0201 (8)	−0.0014 (7)	0.0027 (6)	−0.0003 (7)
O4	0.0266 (8)	0.0358 (9)	0.0157 (7)	−0.0062 (7)	0.0017 (6)	0.0001 (6)
O5	0.0288 (9)	0.0478 (11)	0.0183 (8)	−0.0069 (7)	0.0008 (6)	−0.0078 (7)
O6	0.0266 (8)	0.0433 (10)	0.0188 (7)	−0.0046 (7)	0.0074 (6)	−0.0021 (7)
O7	0.0195 (8)	0.0508 (11)	0.0184 (7)	−0.0055 (7)	0.0007 (6)	−0.0019 (7)
O8	0.0287 (9)	0.0554 (11)	0.0162 (8)	0.0009 (8)	0.0048 (6)	−0.0034 (7)
O9	0.0243 (8)	0.0328 (9)	0.0156 (7)	−0.0044 (6)	0.0007 (6)	−0.0031 (6)
O10	0.0249 (8)	0.0493 (11)	0.0212 (8)	−0.0053 (7)	0.0066 (6)	−0.0076 (7)
O11	0.0165 (7)	0.0465 (10)	0.0151 (7)	−0.0009 (7)	0.0014 (6)	−0.0020 (7)
O12	0.0285 (8)	0.0276 (8)	0.0153 (7)	−0.0007 (6)	0.0066 (6)	−0.0005 (6)
O13	0.0181 (8)	0.0608 (12)	0.0173 (7)	−0.0034 (7)	0.0022 (6)	0.0041 (7)
O14	0.0211 (8)	0.0402 (9)	0.0157 (7)	−0.0010 (7)	0.0022 (6)	0.0008 (6)
O15	0.0225 (8)	0.0363 (9)	0.0187 (7)	−0.0022 (6)	0.0065 (6)	−0.0048 (6)
O16	0.0193 (7)	0.0366 (9)	0.0186 (7)	−0.0064 (6)	0.0035 (6)	−0.0035 (6)
O17	0.0251 (8)	0.0379 (9)	0.0163 (7)	−0.0009 (7)	0.0050 (6)	−0.0014 (6)
O18	0.0338 (9)	0.0276 (8)	0.0234 (8)	0.0022 (7)	0.0107 (7)	0.0040 (6)
O19	0.0290 (9)	0.0442 (10)	0.0285 (9)	0.0022 (7)	0.0061 (7)	−0.0040 (7)
O20	0.0527 (11)	0.0310 (9)	0.0367 (10)	−0.0008 (8)	0.0213 (8)	0.0039 (7)
O21	0.0350 (9)	0.0400 (10)	0.0301 (9)	−0.0047 (8)	0.0156 (7)	−0.0063 (7)
O22	0.0425 (10)	0.0408 (10)	0.0223 (8)	−0.0057 (8)	0.0087 (7)	−0.0043 (7)
O23	0.0338 (10)	0.0815 (15)	0.0254 (9)	0.0036 (10)	0.0095 (7)	0.0090 (9)
O24	0.0228 (8)	0.0285 (8)	0.0205 (7)	−0.0024 (6)	0.0060 (6)	−0.0031 (6)
C1	0.0236 (11)	0.0171 (10)	0.0190 (10)	−0.0004 (8)	0.0035 (8)	0.0001 (8)
C2	0.0215 (10)	0.0160 (10)	0.0188 (10)	−0.0015 (8)	0.0043 (8)	−0.0009 (8)
C3	0.0209 (10)	0.0189 (10)	0.0237 (10)	0.0004 (8)	0.0027 (8)	0.0010 (8)
C4	0.0252 (11)	0.0234 (11)	0.0269 (11)	0.0000 (9)	0.0104 (9)	0.0010 (9)
C5	0.0275 (11)	0.0213 (11)	0.0192 (10)	−0.0028 (8)	0.0075 (8)	−0.0014 (8)
C6	0.0258 (11)	0.0158 (10)	0.0169 (9)	−0.0039 (8)	0.0033 (8)	−0.0023 (8)
C7	0.0236 (11)	0.0239 (11)	0.0188 (10)	−0.0064 (8)	0.0019 (8)	−0.0028 (8)
C8	0.0200 (10)	0.0221 (10)	0.0195 (10)	0.0009 (8)	0.0020 (8)	0.0004 (8)
C9	0.0208 (10)	0.0155 (9)	0.0176 (9)	0.0003 (8)	0.0037 (8)	0.0009 (8)
C10	0.0208 (10)	0.0174 (10)	0.0205 (10)	−0.0015 (8)	0.0002 (8)	0.0033 (8)
C11	0.0177 (10)	0.0205 (10)	0.0275 (11)	0.0004 (8)	0.0072 (8)	0.0035 (8)
C12	0.0244 (11)	0.0208 (10)	0.0195 (10)	0.0020 (8)	0.0073 (8)	0.0010 (8)
C13	0.0218 (10)	0.0183 (10)	0.0180 (10)	−0.0006 (8)	0.0034 (8)	0.0001 (8)
C14	0.0217 (11)	0.0268 (11)	0.0202 (10)	0.0008 (9)	0.0042 (8)	−0.0024 (8)
C15	0.0222 (11)	0.0224 (10)	0.0180 (10)	−0.0022 (8)	0.0030 (8)	−0.0009 (8)

C16	0.0190 (10)	0.0168 (10)	0.0172 (9)	0.0004 (8)	0.0030 (7)	0.0012 (8)
C17	0.0197 (10)	0.0174 (10)	0.0226 (10)	−0.0009 (8)	−0.0004 (8)	0.0002 (8)
C18	0.0177 (10)	0.0219 (11)	0.0288 (11)	0.0006 (8)	0.0073 (8)	0.0011 (9)
C19	0.0206 (10)	0.0192 (10)	0.0211 (10)	0.0010 (8)	0.0083 (8)	0.0001 (8)
C20	0.0198 (10)	0.0161 (10)	0.0165 (9)	0.0021 (7)	0.0051 (8)	0.0015 (7)
C21	0.0222 (10)	0.0188 (10)	0.0166 (9)	0.0027 (8)	0.0053 (8)	−0.0003 (8)
C22	0.0184 (10)	0.0261 (11)	0.0176 (10)	0.0006 (8)	0.0023 (8)	0.0032 (8)
C23	0.0198 (10)	0.0162 (10)	0.0171 (9)	0.0002 (8)	0.0023 (8)	0.0009 (8)
C24	0.0210 (10)	0.0188 (10)	0.0188 (10)	0.0000 (8)	0.0059 (8)	0.0002 (8)
C25	0.0272 (11)	0.0190 (10)	0.0146 (9)	−0.0025 (8)	0.0049 (8)	−0.0005 (8)
C26	0.0222 (10)	0.0186 (10)	0.0175 (9)	−0.0028 (8)	0.0014 (8)	−0.0008 (8)
C27	0.0192 (10)	0.0149 (9)	0.0179 (9)	0.0002 (7)	0.0036 (8)	0.0010 (7)
C28	0.0219 (10)	0.0183 (10)	0.0177 (10)	0.0014 (8)	0.0036 (8)	−0.0002 (8)
C29	0.0225 (11)	0.0417 (14)	0.0202 (10)	−0.0082 (10)	0.0064 (9)	−0.0055 (10)
C30	0.0169 (10)	0.0398 (13)	0.0235 (11)	−0.0014 (9)	0.0046 (8)	−0.0042 (10)
C31	0.0187 (10)	0.0327 (12)	0.0249 (11)	0.0005 (9)	0.0033 (8)	0.0008 (9)
N1	0.0226 (9)	0.0185 (9)	0.0168 (8)	−0.0022 (7)	0.0036 (7)	−0.0006 (7)
N2	0.0205 (9)	0.0185 (8)	0.0171 (8)	0.0006 (7)	0.0043 (7)	0.0010 (7)
N3	0.0188 (8)	0.0176 (8)	0.0160 (8)	−0.0001 (7)	0.0053 (6)	0.0001 (7)
N4	0.0183 (8)	0.0179 (8)	0.0153 (8)	0.0010 (6)	0.0028 (6)	0.0002 (6)
N5	0.0297 (10)	0.0355 (11)	0.0199 (9)	−0.0053 (8)	0.0034 (8)	−0.0007 (8)
N6	0.0186 (9)	0.0329 (10)	0.0181 (8)	0.0010 (7)	0.0052 (7)	−0.0035 (7)

Geometric parameters (Å, °)

O1—C1	1.212 (3)	C8—C9	1.499 (3)
O2—C1	1.321 (2)	C9—N2	1.345 (3)
O2—H2A	0.9499	C9—C10	1.384 (3)
O3—C7	1.278 (3)	C10—C11	1.388 (3)
O4—C7	1.236 (2)	C10—H10	0.9500
O5—C8	1.296 (3)	C11—C12	1.377 (3)
O5—H5AA	0.9501	C11—H11	0.9500
O6—C8	1.226 (3)	C12—C13	1.389 (3)
O7—C14	1.295 (3)	C12—H12	0.9500
O7—H7A	0.9501	C13—N2	1.335 (3)
O8—C14	1.215 (3)	C13—C14	1.504 (3)
O9—C15	1.317 (2)	C15—C16	1.504 (3)
O9—H9A	0.9499	C16—N3	1.340 (3)
O10—C15	1.214 (3)	C16—C17	1.388 (3)
O11—C21	1.255 (2)	C17—C18	1.384 (3)
O11—H11A	0.9499	C17—H17	0.9500
O12—C21	1.254 (2)	C18—C19	1.380 (3)
O13—C22	1.289 (2)	C18—H18	0.9500
O14—C22	1.227 (2)	C19—C20	1.390 (3)
O15—C28	1.214 (2)	C19—H19	0.9500
O16—C28	1.314 (2)	C20—N3	1.338 (2)
O16—H16A	0.9500	C20—C21	1.510 (3)
O17—H17A	0.9500	C22—C23	1.505 (3)
O17—H17B	0.9499	C23—N4	1.332 (3)

O18—H18B	0.9501	C23—C24	1.392 (3)
O18—H18A	0.9499	C24—C25	1.389 (3)
O19—H19B	0.9501	C24—H24	0.9500
O19—H19A	0.9500	C25—C26	1.383 (3)
O20—H20B	0.9502	C25—H25	0.9500
O20—H20A	0.9501	C26—C27	1.393 (3)
O21—H21B	0.9500	C26—H26	0.9500
O21—H21A	0.9500	C27—N4	1.336 (3)
O22—H22A	0.9500	C27—C28	1.501 (3)
O22—H22B	0.9500	C29—N5	1.493 (3)
O23—H23B	0.9500	C29—C30	1.513 (3)
O23—H23A	0.9499	C29—H29A	0.9900
O24—H24B	0.9500	C29—H29B	0.9900
O24—H24A	0.9501	C30—C31	1.513 (3)
C1—C2	1.498 (3)	C30—H30A	0.9900
C2—N1	1.337 (3)	C30—H30B	0.9900
C2—C3	1.385 (3)	C31—N6	1.487 (3)
C3—C4	1.378 (3)	C31—H31A	0.9900
C3—H3	0.9500	C31—H31B	0.9900
C4—C5	1.384 (3)	N5—H5A	0.9500
C4—H4	0.9500	N5—H5B	0.9500
C5—C6	1.391 (3)	N5—H5C	0.9500
C5—H5	0.9500	N6—H6A	0.9502
C6—N1	1.336 (3)	N6—H6B	0.9499
C6—C7	1.510 (3)	N6—H6C	0.9500
C1—O2—H2A	115.5	C19—C18—H18	120.4
C8—O5—H5AA	113.4	C17—C18—H18	120.4
C14—O7—H7A	112.3	C18—C19—C20	118.65 (18)
C15—O9—H9A	110.5	C18—C19—H19	120.7
C21—O11—H11A	114.1	C20—C19—H19	120.7
C28—O16—H16A	113.3	N3—C20—C19	123.04 (18)
H17A—O17—H17B	102.8	N3—C20—C21	115.83 (17)
H18B—O18—H18A	96.6	C19—C20—C21	121.13 (17)
H19B—O19—H19A	127.0	O12—C21—O11	124.91 (19)
H20B—O20—H20A	113.5	O12—C21—C20	118.92 (18)
H21B—O21—H21A	108.4	O11—C21—C20	116.17 (17)
H22A—O22—H22B	114.4	O14—C22—O13	124.81 (19)
H23B—O23—H23A	105.7	O14—C22—C23	121.27 (18)
H24B—O24—H24A	108.7	O13—C22—C23	113.92 (17)
O1—C1—O2	120.96 (18)	N4—C23—C24	123.43 (18)
O1—C1—C2	122.15 (19)	N4—C23—C22	115.11 (17)
O2—C1—C2	116.88 (17)	C24—C23—C22	121.44 (18)
N1—C2—C3	123.70 (18)	C25—C24—C23	118.21 (18)
N1—C2—C1	114.54 (17)	C25—C24—H24	120.9
C3—C2—C1	121.76 (18)	C23—C24—H24	120.9
C4—C3—C2	117.9 (2)	C26—C25—C24	119.01 (18)
C4—C3—H3	121.1	C26—C25—H25	120.5
C2—C3—H3	121.1	C24—C25—H25	120.5
C3—C4—C5	119.3 (2)	C25—C26—C27	118.46 (19)

C3—C4—H4	120.4	C25—C26—H26	120.8
C5—C4—H4	120.4	C27—C26—H26	120.8
C4—C5—C6	118.98 (19)	N4—C27—C26	123.16 (18)
C4—C5—H5	120.5	N4—C27—C28	114.39 (17)
C6—C5—H5	120.5	C26—C27—C28	122.43 (18)
N1—C6—C5	122.19 (19)	O15—C28—O16	124.19 (19)
N1—C6—C7	115.94 (18)	O15—C28—C27	122.74 (18)
C5—C6—C7	121.87 (18)	O16—C28—C27	113.06 (17)
O4—C7—O3	125.2 (2)	N5—C29—C30	111.50 (17)
O4—C7—C6	119.12 (19)	N5—C29—H29A	109.3
O3—C7—C6	115.69 (18)	C30—C29—H29A	109.3
O6—C8—O5	125.11 (19)	N5—C29—H29B	109.3
O6—C8—C9	121.12 (18)	C30—C29—H29B	109.3
O5—C8—C9	113.76 (18)	H29A—C29—H29B	108.0
N2—C9—C10	123.73 (18)	C29—C30—C31	112.13 (19)
N2—C9—C8	114.79 (17)	C29—C30—H30A	109.2
C10—C9—C8	121.48 (18)	C31—C30—H30A	109.2
C9—C10—C11	118.47 (19)	C29—C30—H30B	109.2
C9—C10—H10	120.8	C31—C30—H30B	109.2
C11—C10—H10	120.8	H30A—C30—H30B	107.9
C12—C11—C10	118.49 (19)	N6—C31—C30	112.15 (18)
C12—C11—H11	120.8	N6—C31—H31A	109.2
C10—C11—H11	120.8	C30—C31—H31A	109.2
C11—C12—C13	119.14 (19)	N6—C31—H31B	109.2
C11—C12—H12	120.4	C30—C31—H31B	109.2
C13—C12—H12	120.4	H31A—C31—H31B	107.9
N2—C13—C12	123.32 (19)	C6—N1—C2	117.92 (18)
N2—C13—C14	116.79 (18)	C13—N2—C9	116.79 (17)
C12—C13—C14	119.84 (18)	C20—N3—C16	117.42 (17)
O8—C14—O7	125.4 (2)	C23—N4—C27	117.72 (16)
O8—C14—C13	121.05 (19)	C29—N5—H5A	108.8
O7—C14—C13	113.53 (17)	C29—N5—H5B	106.8
O10—C15—O9	124.74 (19)	H5A—N5—H5B	112.7
O10—C15—C16	122.26 (18)	C29—N5—H5C	114.9
O9—C15—C16	113.00 (17)	H5A—N5—H5C	107.1
N3—C16—C17	123.50 (18)	H5B—N5—H5C	106.6
N3—C16—C15	114.34 (17)	C31—N6—H6A	107.8
C17—C16—C15	122.16 (18)	C31—N6—H6B	112.5
C18—C17—C16	118.13 (19)	H6A—N6—H6B	108.7
C18—C17—H17	120.9	C31—N6—H6C	108.0
C16—C17—H17	120.9	H6A—N6—H6C	104.2
C19—C18—C17	119.23 (19)	H6B—N6—H6C	115.1
O1—C1—C2—N1	−177.34 (19)	C18—C19—C20—C21	178.60 (19)
O2—C1—C2—N1	3.4 (3)	N3—C20—C21—O12	−168.41 (18)
O1—C1—C2—C3	3.2 (3)	C19—C20—C21—O12	11.4 (3)
O2—C1—C2—C3	−176.03 (18)	N3—C20—C21—O11	12.3 (3)
N1—C2—C3—C4	−1.2 (3)	C19—C20—C21—O11	−167.82 (19)
C1—C2—C3—C4	178.17 (19)	O14—C22—C23—N4	4.0 (3)
C2—C3—C4—C5	1.3 (3)	O13—C22—C23—N4	−176.68 (19)

C3—C4—C5—C6	0.0 (3)	O14—C22—C23—C24	−174.4 (2)
C4—C5—C6—N1	−1.5 (3)	O13—C22—C23—C24	4.9 (3)
C4—C5—C6—C7	178.33 (19)	N4—C23—C24—C25	0.8 (3)
N1—C6—C7—O4	177.41 (19)	C22—C23—C24—C25	179.11 (19)
C5—C6—C7—O4	−2.4 (3)	C23—C24—C25—C26	−0.3 (3)
N1—C6—C7—O3	−1.6 (3)	C24—C25—C26—C27	−0.6 (3)
C5—C6—C7—O3	178.6 (2)	C25—C26—C27—N4	1.0 (3)
O6—C8—C9—N2	−10.0 (3)	C25—C26—C27—C28	−177.05 (18)
O5—C8—C9—N2	169.95 (18)	N4—C27—C28—O15	4.3 (3)
O6—C8—C9—C10	170.0 (2)	C26—C27—C28—O15	−177.5 (2)
O5—C8—C9—C10	−10.1 (3)	N4—C27—C28—O16	−174.48 (17)
N2—C9—C10—C11	1.2 (3)	C26—C27—C28—O16	3.7 (3)
C8—C9—C10—C11	−178.76 (19)	N5—C29—C30—C31	65.6 (2)
C9—C10—C11—C12	−1.8 (3)	C29—C30—C31—N6	176.28 (17)
C10—C11—C12—C13	0.4 (3)	C5—C6—N1—C2	1.6 (3)
C11—C12—C13—N2	1.7 (3)	C7—C6—N1—C2	−178.23 (18)
C11—C12—C13—C14	−175.90 (19)	C3—C2—N1—C6	−0.2 (3)
N2—C13—C14—O8	−171.6 (2)	C1—C2—N1—C6	−179.62 (17)
C12—C13—C14—O8	6.2 (3)	C12—C13—N2—C9	−2.3 (3)
N2—C13—C14—O7	7.5 (3)	C14—C13—N2—C9	175.36 (18)
C12—C13—C14—O7	−174.77 (19)	C10—C9—N2—C13	0.8 (3)
O10—C15—C16—N3	−0.2 (3)	C8—C9—N2—C13	−179.19 (18)
O9—C15—C16—N3	179.01 (17)	C19—C20—N3—C16	0.5 (3)
O10—C15—C16—C17	−179.6 (2)	C21—C20—N3—C16	−179.69 (17)
O9—C15—C16—C17	−0.4 (3)	C17—C16—N3—C20	1.1 (3)
N3—C16—C17—C18	−1.5 (3)	C15—C16—N3—C20	−178.31 (17)
C15—C16—C17—C18	177.83 (19)	C24—C23—N4—C27	−0.4 (3)
C16—C17—C18—C19	0.4 (3)	C22—C23—N4—C27	−178.80 (17)
C17—C18—C19—C20	1.1 (3)	C26—C27—N4—C23	−0.5 (3)
C18—C19—C20—N3	−1.6 (3)	C28—C27—N4—C23	177.68 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O19	0.95	1.94	2.830 (2)	154
O5—H5AA···O20	0.95	1.67	2.592 (2)	164
O7—H7A···O3	0.95	1.51	2.455 (2)	177
O7—H7A···O4	0.95	2.57	3.119 (2)	117
O9—H9A···O22	0.95	1.64	2.588 (2)	172
O11—H11A···O13^{i}	0.95	1.50	2.445 (2)	177
O11—H11A···O14^{i}	0.95	2.61	3.181 (2)	119
O16—H16A···O24	0.95	1.60	2.551 (2)	174
O17—H17A···O15	0.95	1.90	2.838 (2)	167
O17—H17A···N4	0.95	2.43	2.956 (2)	115
O17—H17B···O14	0.95	1.87	2.821 (2)	175
O18—H18B···O1	0.95	1.89	2.815 (2)	164
O18—H18A···O17^{ii}	0.95	1.88	2.809 (2)	166
O19—H19B···N1	0.95	2.22	3.092 (2)	152

O19—H19A···O13^{i}	0.95	2.34	3.174 (2)	146
O20—H20B···O12^{iii}	0.95	1.87	2.793 (2)	164
O20—H20A···O22	0.95	1.95	2.875 (3)	165
O21—H21B···O10	0.95	1.89	2.834 (2)	170
O21—H21A···O19^{iii}	0.95	1.85	2.784 (2)	166
O22—H22A···O21	0.95	1.88	2.818 (2)	168
O22—H22B···O17^{iv}	0.95	1.81	2.742 (2)	167
O23—H23B···O6	0.95	1.85	2.749 (2)	157
O23—H23A···O12^{iii}	0.95	1.96	2.899 (2)	170
O24—H24B···O18^{v}	0.95	1.79	2.706 (2)	161
O24—H24A···O12^{vi}	0.95	1.86	2.761 (2)	157
N5—H5A···N2	0.95	2.40	3.342 (3)	171
N5—H5A···O6	0.95	2.61	3.227 (2)	123
N5—H5B···O4	0.95	1.95	2.879 (2)	166
N5—H5C···O23^{vii}	0.95	2.06	2.991 (3)	166
N6—H6A···O14^{i}	0.95	2.01	2.938 (2)	164
N6—H6B···O21^{viii}	0.95	1.90	2.849 (2)	174
N6—H6C···N3	0.95	2.17	3.070 (2)	158
C5—H5···O18^{iii}	0.95	2.56	3.429 (3)	153
C10—H10···O1^{ix}	0.95	2.50	3.335 (3)	147
C11—H11···O18^{ix}	0.95	2.52	3.427 (3)	159
C19—H19···O15^{x}	0.95	2.46	3.266 (3)	143
C25—H25···O24^{xi}	0.95	2.56	3.485 (3)	165
C26—H26···O16^{xi}	0.95	2.56	3.287 (3)	134
C31—H31A···N2	0.99	2.52	3.391 (3)	146
C31—H31B···O10	0.99	2.54	3.175 (3)	122

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) *x*, −*y*+1/2, *z*−1/2; (v) *x*−1, −*y*+1/2, *z*−1/2; (vi) −*x*, *y*−1/2, −*z*+1/2; (vii) −*x*+1, −*y*+2, −*z*; (viii) −*x*+1, −*y*+1, −*z*; (ix) *x*−1, −*y*+3/2, *z*−1/2; (x) −*x*, *y*+1/2, −*z*+1/2; (xi) −*x*, −*y*, −*z*.

Fig. 1

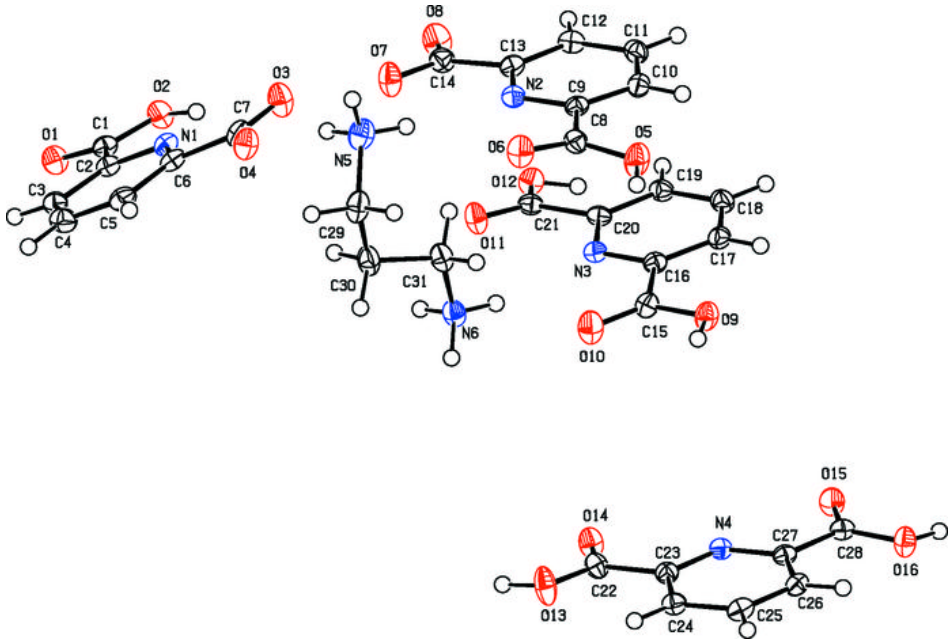
O8
C12
C11
O7
C13
C14
N2
C9
C10
O2
O3
C7
C1
C8
O1
N1
O5
N5
O6
C2
C6
O4
C19
O12
C3
C18
C21
C20
C5
O11
C29
C17
C4
N3
C16
C30
C31
C15
O9
N6
O10
O15
O14
N4
C27
C23
C28
O16
C22
O13
C26
C24
C25

Fig. 2

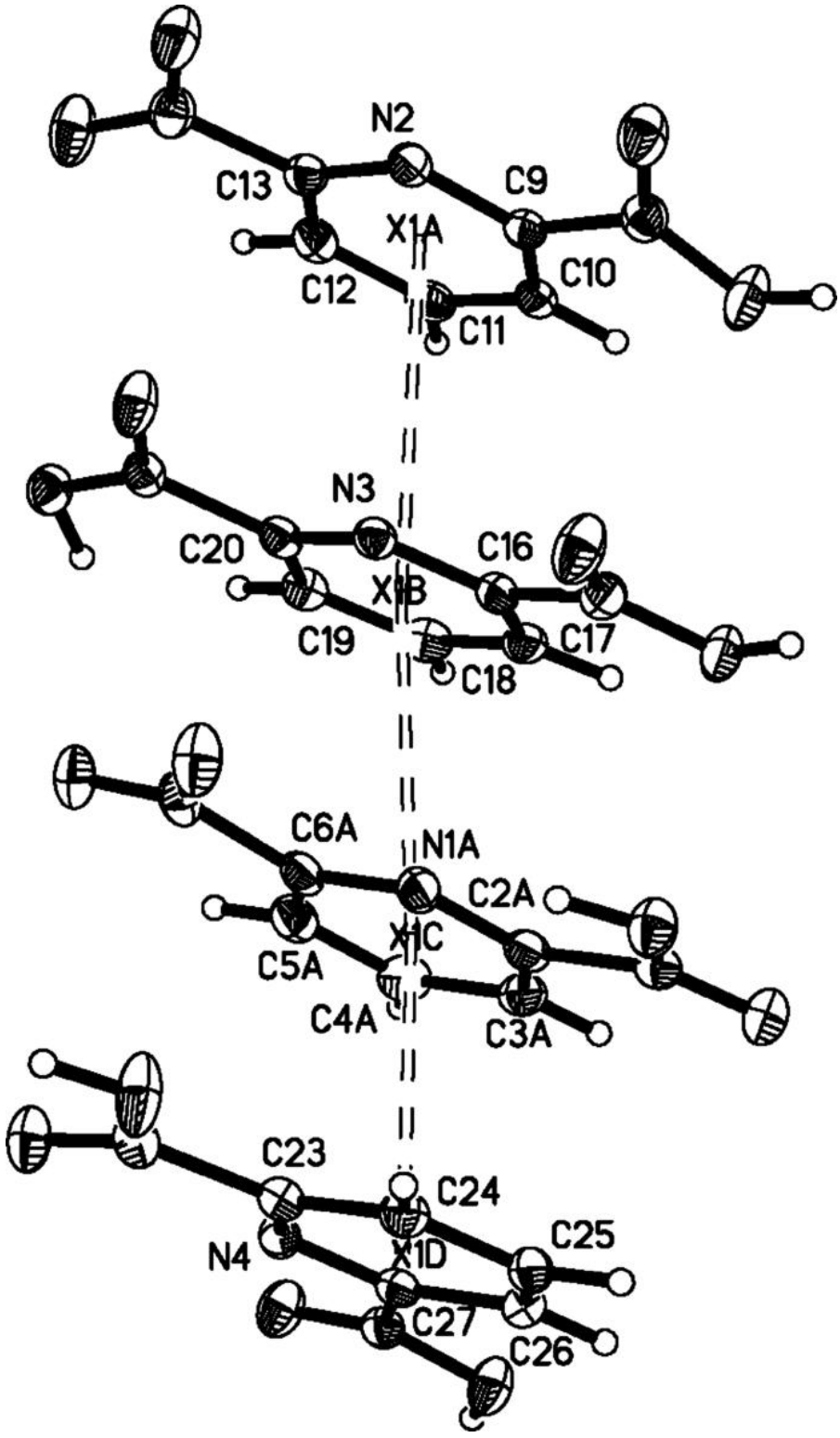
N2
C13
C9
X1A
C10
C12
C11
N3
C20
C16
X1B
C19
C17
C18
C6A
N1A
C2A
X1C
C5A
C4A
C3A
C23
C24
C25
N4
X1D
C27
C26

Fig. 3