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8-(Carboxymethoxy)quinolinium nitrate monohydrate

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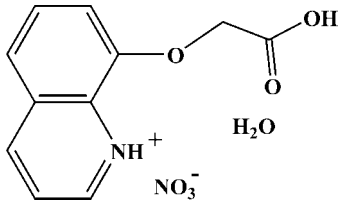
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 11.0.

In the title compound, $C_{11}H_{10}NO_3^+\cdot NO_3^-\cdot H_2O$, the planar 8-carboxymethoxyquinolinium cation, the nitrate anion and the water molecule are dimerized by hydrogen bonds into square building-block units, and then further assembled into two-dimensional gently undulating supramolecular layers.

Related literature

For general background, see Czugler & Kalman (1981); Das *et al.* (1987); Song *et al.* (2004); Wang & Lu (2004).



Experimental

Crystal data

$C_{11}H_{10}NO_3^+\cdot NO_3^-\cdot H_2O$
M_r = 284.23
Monoclinic, $P2_1/n$
a = 5.3577 (5) Å
b = 19.5100 (17) Å
c = 11.8959 (11) Å
β = 94.663 (3)°
V = 1239.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 298 (2) K
0.25 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.980
6235 measured reflections
2071 independent reflections
1376 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.01
2071 reflections
189 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O7	0.86	1.81	2.652 (2)	166
O7—H7B···O5^{i}	0.841 (9)	2.610 (18)	3.140 (2)	122.3 (19)
O7—H7B···O2^{ii}	0.841 (9)	2.085 (16)	2.852 (2)	152 (2)
O7—H7A···O1	0.852 (9)	2.52 (2)	2.943 (2)	111.6 (18)
O7—H7A···O2	0.852 (9)	1.929 (11)	2.776 (2)	172 (3)
O3—H3···O6^{iii}	0.82	2.63	3.192 (2)	127
O3—H3···N2^{iii}	0.82	2.55	3.301 (3)	154
O3—H3···O5^{iii}	0.82	1.77	2.587 (2)	175

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+2, -y+2, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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: RN2043).

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supplementary materials

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8-(Carboxymethoxy)quinolinium nitrate monohydrate

F. Sun, L. Chen, H.-C. Fang, X.-M. Lin and Y.-P. Cai

Comment

There are no reports of the title compound but there are several reports on metal compounds involving the ligand 2-(quinolin-8-yloxy)acetate and its derivatives (Czugler & Kalman, 1981; Das *et al.*, 1987; Wang & Lu, 2004; Song *et al.*, 2004). The title compound (Scheme I) contains one cation, one nitrate anion and one water molecule (Fig.1).

Fig. 2 shows that the cation, the nitrate anion and water molecule are dimerized by the hydrogen bonds (Table 1) into stable square building block units, and then further assembled into 2D supramolecular layers which are gently undulating.

Experimental

A solution of $Cu(NO_3)_2$ (363 mg, 1.00 mmol) in CH_3OH (20 ml) was slowly added to a solution of 2-(quinolin-8-yloxy)acetic acid (410 mg, 1.95 mmol) in CH_3OH (10 ml). The resultant blue solution was stirred for 2 h at room temperature and then filtered. Colorless crystals suitable for X-ray diffraction were obtained in two day by slow diffusion of diethyl ether into a dilute solution of the title complex in methanol. The assigned structure was substantiated by elemental analysis; calculated for $C_{11}H_{12}N_2O_7$: C 46.44, H 4.22, N 9.85%; found: C 46.36, H 4.28, N 9.82%.

Refinement

The structure was solved using direct methods followed by Fourier synthesis. Non-H atoms were refined anisotropically. All of H atoms except water molecule were placed in idealized positions (C—H = 0.93 or 0.97 Å, O—H = 0.82 Å, N—H = 0.86 Å), forced to ride on the atom to which they are bonded, and were included in the refinement in the riding-model approximation. U_{iso} values were set equal to $1.5U_{eq}$(parent atom) for methyl H atoms and to $1.2U_{eq}$(parent atom)for all other H atoms. The water H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.84 (1) and H···H 1.43 (2) Å, but their U_{iso} values were set equal to 1.5 U_{eq}(parent atom O).

Figures

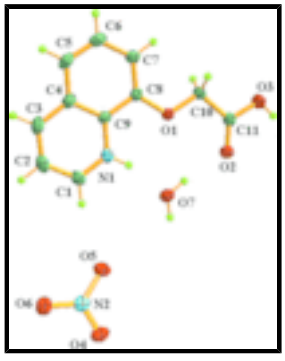


Fig. 1. The structure of the title compound (I). The atom-numbering scheme is shown and ellipsoids are drawn at the 30% probability level.

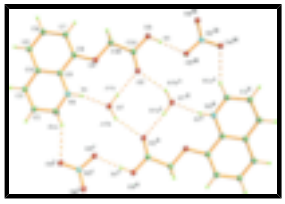


Fig. 2. A view of the dimerized supramolecular sheet constructed by hydrogen bonding interactions. Symmetry codes i: 1.5-x, 0.5+y, 0.5-z; ii: 2-x, 2-y, 1-z; iii: 0.5+x, 1.5-y, 0.5+z.

8-(Carboxymethoxy)quinolinium nitrate monohydrate

Crystal data

$C_{11}H_{10}NO_3^+ \cdot NO_3^- \cdot H_2O$	$F_{000} = 592$
$M_r = 284.23$	$D_x = 1.523$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P2yn	Cell parameters from 1544 reflections
$a = 5.3577$ (5) Å	$\theta = 2.7$–22.5º
$b = 19.5100$ (17) Å	$\mu = 0.13$ mm^{-1}
$c = 11.8959$ (11) Å	$T = 298$ (2) K
$\beta = 94.663$ (3)º	Block, yellow
$V = 1239.3$ (2) Å^3	0.25 × 0.22 × 0.16 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2071 independent reflections
Radiation source: fine-focus sealed tube	1376 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 298$(2) K	$\theta_{max} = 25.5$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 6$
$T_{min} = 0.968$, $T_{max} = 0.980$	$k = -23 \rightarrow 22$
6235 measured reflections	$l = -14 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.237P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2071 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}

189 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
3 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0044 (12)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3857 (3)	1.04106 (6)	0.31886 (12)	0.0504 (4)
O2	0.7769 (3)	1.08262 (7)	0.45561 (14)	0.0639 (5)
O3	0.6421 (3)	1.19011 (7)	0.44971 (15)	0.0717 (5)
H3	0.7765	1.1975	0.4856	0.107*
O4	0.7649 (4)	0.21455 (8)	0.17156 (19)	0.0945 (7)
O5	0.5562 (3)	0.28962 (8)	0.07269 (16)	0.0761 (6)
O6	0.4361 (4)	0.18475 (9)	0.07206 (17)	0.0943 (7)
O7	0.7613 (3)	0.94258 (8)	0.41435 (15)	0.0697 (5)
H7A	0.766 (4)	0.9861 (5)	0.420 (2)	0.105*
H7B	0.893 (3)	0.9224 (10)	0.439 (2)	0.105*
N1	0.3815 (3)	0.90790 (8)	0.26857 (14)	0.0478 (5)
H1	0.4942	0.9259	0.3150	0.057*
N2	0.5863 (4)	0.22855 (10)	0.10544 (17)	0.0595 (5)
C1	0.3960 (5)	0.84190 (10)	0.24671 (19)	0.0585 (6)
H1A	0.5251	0.8159	0.2820	0.070*
C2	0.2210 (5)	0.81128 (12)	0.1718 (2)	0.0678 (7)
H2	0.2335	0.7649	0.1552	0.081*
C3	0.0298 (5)	0.84926 (12)	0.1222 (2)	0.0633 (7)
H3A	−0.0890	0.8285	0.0719	0.076*
C4	0.0098 (4)	0.91954 (11)	0.14604 (17)	0.0491 (6)
C5	−0.1837 (5)	0.96193 (13)	0.09874 (19)	0.0597 (6)
H5	−0.3112	0.9434	0.0503	0.072*
C6	−0.1842 (5)	1.02966 (12)	0.12375 (19)	0.0592 (6)
H6	−0.3134	1.0571	0.0923	0.071*
C7	0.0059 (4)	1.05930 (11)	0.19611 (18)	0.0503 (6)
H7	0.0039	1.1062	0.2103	0.060*
C8	0.1930 (4)	1.01977 (9)	0.24550 (16)	0.0428 (5)
C9	0.1954 (4)	0.94906 (10)	0.22072 (16)	0.0415 (5)

C10	0.4012 (4)	1.11253 (9)	0.34252 (17)	0.0480 (6)
H10A	0.2518	1.1275	0.3764	0.058*
H10B	0.4137	1.1380	0.2732	0.058*
C11	0.6279 (4)	1.12555 (11)	0.42193 (17)	0.0482 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0499 (10)	0.0361 (7)	0.0612 (9)	0.0015 (7)	−0.0185 (8)	−0.0028 (6)
O2	0.0534 (11)	0.0450 (9)	0.0881 (11)	0.0037 (8)	−0.0256 (9)	−0.0097 (8)
O3	0.0775 (14)	0.0385 (8)	0.0930 (13)	−0.0001 (8)	−0.0295 (10)	−0.0109 (8)
O4	0.0822 (14)	0.0620 (11)	0.1291 (16)	0.0015 (10)	−0.0530 (13)	0.0185 (11)
O5	0.0753 (13)	0.0433 (9)	0.1048 (13)	0.0006 (8)	−0.0219 (10)	0.0184 (9)
O6	0.0987 (16)	0.0594 (10)	0.1156 (15)	−0.0244 (11)	−0.0464 (13)	0.0157 (10)
O7	0.0638 (12)	0.0514 (9)	0.0877 (12)	0.0058 (8)	−0.0320 (10)	−0.0014 (9)
N1	0.0471 (12)	0.0411 (10)	0.0533 (10)	−0.0052 (9)	−0.0074 (9)	0.0001 (8)
N2	0.0587 (14)	0.0471 (12)	0.0697 (13)	0.0000 (11)	−0.0124 (11)	0.0048 (10)
C1	0.0633 (17)	0.0381 (12)	0.0723 (15)	−0.0001 (11)	−0.0047 (14)	0.0011 (11)
C2	0.077 (2)	0.0438 (13)	0.0808 (17)	−0.0116 (13)	−0.0052 (15)	−0.0090 (12)
C3	0.0669 (18)	0.0577 (14)	0.0630 (15)	−0.0201 (13)	−0.0083 (14)	−0.0099 (12)
C4	0.0439 (14)	0.0542 (13)	0.0474 (12)	−0.0082 (11)	−0.0059 (11)	−0.0006 (10)
C5	0.0461 (16)	0.0749 (17)	0.0552 (14)	−0.0107 (13)	−0.0143 (12)	−0.0008 (12)
C6	0.0450 (15)	0.0719 (16)	0.0579 (14)	0.0072 (13)	−0.0120 (12)	0.0073 (12)
C7	0.0455 (15)	0.0474 (12)	0.0562 (13)	0.0041 (11)	−0.0061 (12)	0.0045 (10)
C8	0.0405 (14)	0.0433 (12)	0.0429 (11)	−0.0027 (10)	−0.0068 (11)	0.0010 (9)
C9	0.0361 (13)	0.0434 (11)	0.0437 (11)	−0.0018 (10)	−0.0038 (10)	0.0036 (9)
C10	0.0508 (15)	0.0347 (11)	0.0560 (13)	0.0005 (10)	−0.0102 (11)	0.0011 (9)
C11	0.0506 (15)	0.0400 (12)	0.0528 (13)	−0.0033 (11)	−0.0038 (11)	−0.0008 (10)

Geometric parameters (Å, °)

O1—C8	1.362 (2)	C2—H2	0.9300
O1—C10	1.424 (2)	C3—C4	1.406 (3)
O2—C11	1.203 (2)	C3—H3A	0.9300
O3—C11	1.303 (2)	C4—C9	1.402 (3)
O3—H3	0.8200	C4—C5	1.407 (3)
O4—N2	1.219 (2)	C5—C6	1.355 (3)
O5—N2	1.260 (2)	C5—H5	0.9300
O6—N2	1.218 (2)	C6—C7	1.403 (3)
O7—H7A	0.852 (9)	C6—H6	0.9300
O7—H7B	0.841 (9)	C7—C8	1.360 (3)
N1—C1	1.317 (2)	C7—H7	0.9300
N1—C9	1.368 (2)	C8—C9	1.411 (3)
N1—H1	0.8600	C10—C11	1.498 (3)
C1—C2	1.377 (3)	C10—H10A	0.9700
C1—H1A	0.9300	C10—H10B	0.9700
C2—C3	1.359 (3)		
C8—O1—C10	117.04 (15)	C4—C5—H5	120.0

C11—O3—H3	109.5	C5—C6—C7	121.5 (2)
H7A—O7—H7B	114.9 (13)	C5—C6—H6	119.2
C1—N1—C9	122.98 (19)	C7—C6—H6	119.2
C1—N1—H1	118.5	C8—C7—C6	120.3 (2)
C9—N1—H1	118.5	C8—C7—H7	119.9
O6—N2—O4	121.1 (2)	C6—C7—H7	119.9
O6—N2—O5	119.9 (2)	C7—C8—O1	126.71 (18)
O4—N2—O5	119.1 (2)	C7—C8—C9	118.90 (19)
N1—C1—C2	120.3 (2)	O1—C8—C9	114.39 (17)
N1—C1—H1A	119.9	N1—C9—C4	118.56 (18)
C2—C1—H1A	119.9	N1—C9—C8	120.38 (18)
C3—C2—C1	119.6 (2)	C4—C9—C8	121.06 (19)
C3—C2—H2	120.2	O1—C10—C11	108.78 (16)
C1—C2—H2	120.2	O1—C10—H10A	109.9
C2—C3—C4	120.7 (2)	C11—C10—H10A	109.9
C2—C3—H3A	119.6	O1—C10—H10B	109.9
C4—C3—H3A	119.6	C11—C10—H10B	109.9
C9—C4—C3	117.8 (2)	H10A—C10—H10B	108.3
C9—C4—C5	118.3 (2)	O2—C11—O3	124.4 (2)
C3—C4—C5	123.9 (2)	O2—C11—C10	125.03 (19)
C6—C5—C4	120.0 (2)	O3—C11—C10	110.57 (19)
C6—C5—H5	120.0		
C9—N1—C1—C2	0.8 (3)	C1—N1—C9—C4	0.8 (3)
N1—C1—C2—C3	−1.4 (4)	C1—N1—C9—C8	−178.5 (2)
C1—C2—C3—C4	0.4 (4)	C3—C4—C9—N1	−1.7 (3)
C2—C3—C4—C9	1.1 (3)	C5—C4—C9—N1	178.85 (19)
C2—C3—C4—C5	−179.4 (2)	C3—C4—C9—C8	177.63 (19)
C9—C4—C5—C6	1.5 (3)	C5—C4—C9—C8	−1.8 (3)
C3—C4—C5—C6	−177.9 (2)	C7—C8—C9—N1	179.70 (19)
C4—C5—C6—C7	0.3 (4)	O1—C8—C9—N1	−0.3 (3)
C5—C6—C7—C8	−1.8 (3)	C7—C8—C9—C4	0.4 (3)
C6—C7—C8—O1	−178.6 (2)	O1—C8—C9—C4	−179.64 (18)
C6—C7—C8—C9	1.4 (3)	C8—O1—C10—C11	−178.52 (17)
C10—O1—C8—C7	−3.3 (3)	O1—C10—C11—O2	3.0 (3)
C10—O1—C8—C9	176.72 (17)	O1—C10—C11—O3	−177.08 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O7	0.86	1.81	2.652 (2)	166
O7—H7B···O5^{i}	0.841 (9)	2.610 (18)	3.140 (2)	122.3 (19)
O7—H7B···O2^{ii}	0.841 (9)	2.085 (16)	2.852 (2)	152 (2)
O7—H7A···O1	0.852 (9)	2.52 (2)	2.943 (2)	111.6 (18)
O7—H7A···O2	0.852 (9)	1.929 (11)	2.776 (2)	172 (3)
O3—H3···O6^{iii}	0.82	2.63	3.192 (2)	127
O3—H3···N2^{iii}	0.82	2.55	3.301 (3)	154
O3—H3···O5^{iii}	0.82	1.77	2.587 (2)	175

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) *x*+1/2, −*y*+3/2, *z*+1/2.

Fig. 1

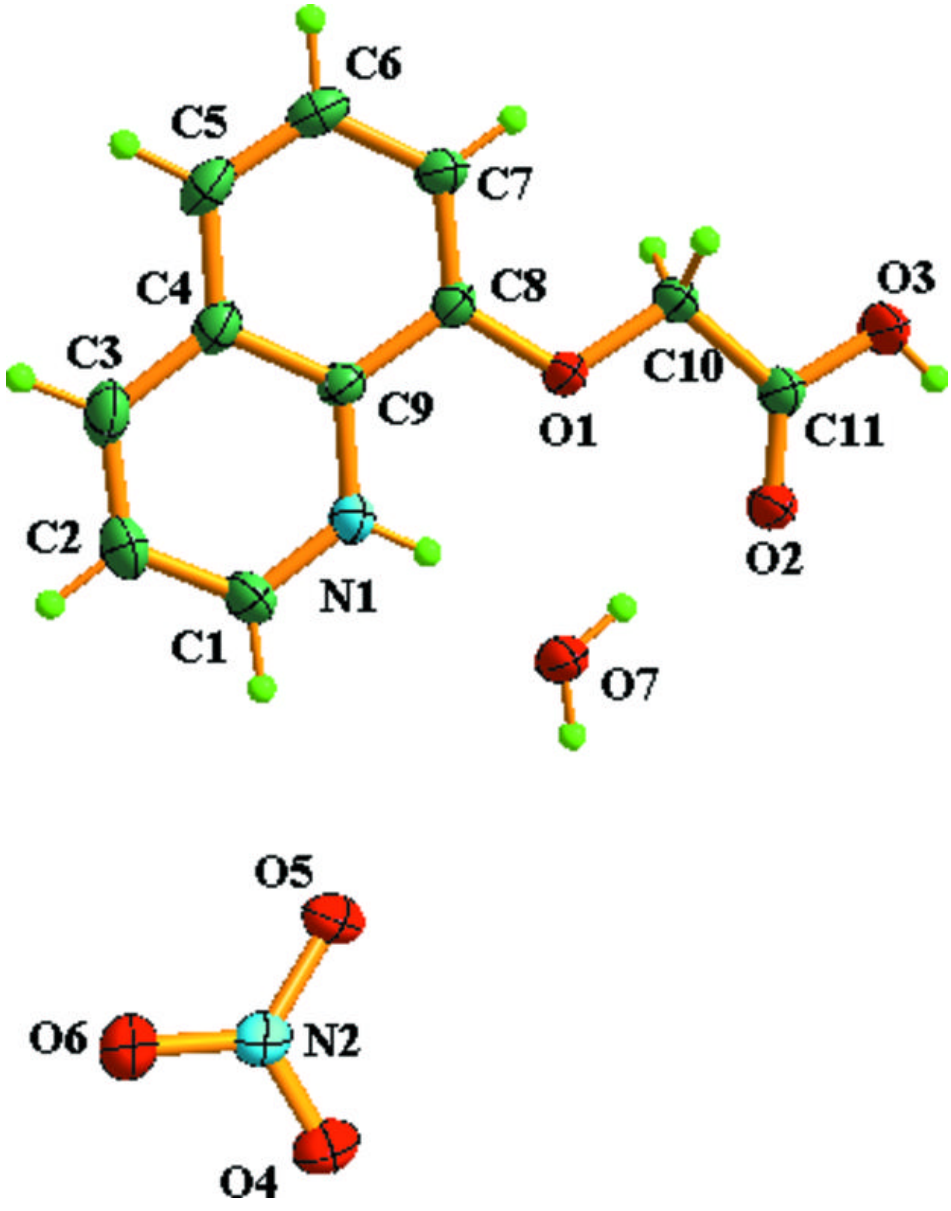
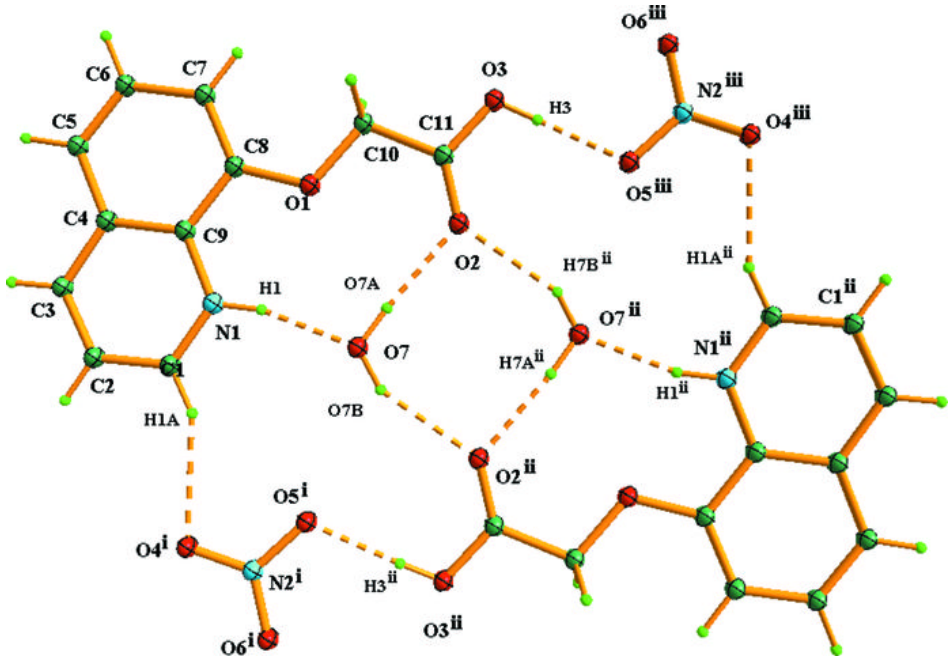


Fig. 2


O6iii
N2iii
O4iii
O3
H3
O5iii
C6
C7
C5
C8
C11
C10
O1
C4
C9
O2
H7Bii
H1Aii
C1ii
C3
H1
O7A
O7ii
N1
O7
H7Aii
N1ii
C2
C1
H1ii
H1A
O7B
O2ii
O5i
O4i
N2i
H3ii
O3ii
O6i