CRYSTALLOGRAPHIC
COMMUNICATIONS

ISSN 2056-9890

Crystal structures of 3-chloro-2-nitrobenzoic acid with quinoline derivatives: 3-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1), 3-chloro-2-nitrobenzoic acid–6-nitroquinoline (1/1) and 8-hydroxyquinolinium 3-chloro-2-nitrobenzoate

Received 10 September 2019
Accepted 14 September 2019

Edited by A. J. Lough, University of Toronto, Canada

Keywords: crystal structure; 3-chloro-2-nitrobonzoic acid; 5-nitroquinoline; 6-nitroquinoline; 8-hydroxyqunoline; hydrogen bond.

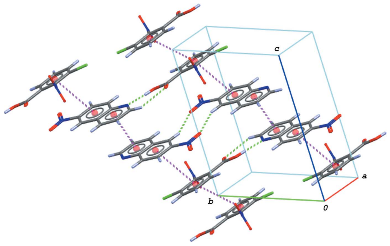
CCDC references: 1953605; 1953604; 1953603

Supporting information: this article has supporting information at journals.iucr.org/e

Kazuma Gotoh and Hiroyuki Ishida*

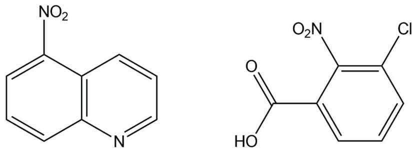
Department of Chemistry, Faculty of Science, Okayama University, Okayama 700-8530, Japan. *Correspondence e-mail: ishidah@cc.okayama-u.ac.jp

The structures of three compounds of 3-chloro-2-nitrobenzoic acid with 5-nitroquinoline, (I), 6-nitroquinoline, (II), and 8-hydroxyquinoline, (III), have been determined at 190 K. In each of the two isomeric compounds, (I) and (II), $C_7H_4ClNO_4 \cdot C_9H_6N_2O_2$, the acid and base molecules are held together by O—H···N and C—H···O hydrogen bonds. In compound (III), $C_9H_8NO^+ \cdot C_7H_3ClNO_4^-$, an acid–base interaction involving H-atom transfer occurs and the H atom is located at the N site of the base molecule. In the crystal of (I), the hydrogen-bonded acid–base units are linked by C—H···O hydrogen bonds, forming a tape structure along the *b*-axis direction. Adjacent tapes, which are related by a twofold rotation axis, are linked by a third C—H···O hydrogen bond, forming wide ribbons parallel to the ($\overline{1}03$) plane. These ribbons are stacked *via* π–π interactions between the quinoline ring systems [centroid–centroid distances = 3.4935 (5)–3.7721 (6) Å], forming layers parallel to the *ab* plane. In the crystal of (II), the hydrogen-bonded acid–base units are also linked into a tape structure along the *b*-axis direction *via* C—H···O hydrogen bonds. Inversion-related tapes are linked by further C—H···O hydrogen bonds to form wide ribbons parallel to the ($\overline{3}08$) plane. The ribbons are linked by weak π–π interactions [centroid–centroid distances = 3.8016 (8)–3.9247 (9) Å], forming a three-dimensional structure. In the crystal of (III), the cations and the anions are alternately linked *via* N—H···O and O—H···O hydrogen bonds, forming a 2_1 helix running along the *b*-axis direction. The cations and the anions are further stacked alternately in columns along the *a*-axis direction *via* π–π interactions [centroid–centroid distances = 3.8016 (8)–3.9247 (9) Å], and the molecular chains are linked into layers parallel to the *ab* plane through these interactions.

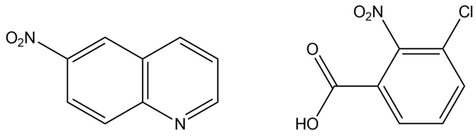


1. Chemical context

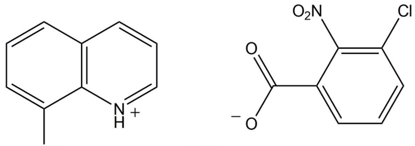
The hydrogen bonds formed between organic acids and organic bases vary from an O—H···N type to an $O^- \cdots H—N^+$ type depending on the pK_a values of the acids and bases as well as intermolecular interactions in the crystals, and at an appropriate ΔpK_a [pKa(base) − pKa(acid)] value, a short strong hydrogen bond with a broad single minimum potential energy curve for the H atom or a double-minimum potential is observed (Schmidtmann & Wilson, 2008; Gilli & Gilli, 2009). For the system of quinoline–chloro- and nitro-substituted benzoic acids, we have shown that three compounds of quinoline with 3-chloro-2-nitrobenzoic acid, 4-chloro-2-nitrobenzoic acid and 5-chloro-2-nitrobenzoic acid, the ΔpK_a values of which are 3.08, 2.93 and 3.04, respectively, have a short double-well O···H···N hydrogen bond between the carboxy O atom and the aromatic N atom (Gotoh & Ishida, 2009). Similar O···H···N hydrogen bonds have been also observed in compounds of phthalazine with 3-chloro-2-nitrobenzoic acid and 4-chloro-2-nitrobenzoic acid with ΔpK_a values of 1.65 and 1.50, respectively (Gotoh & Ishida, 2011), and of isoquinoline with 3-chloro-2-nitrobenzoic acid with ΔpK_a = 3.58 (Gotoh & Ishida, 2015).



(I)



(II)



(III)

We report here the crystal structures of the title compounds in order to extend our studies of short hydrogen bonding in pyridine derivative–chloro- and nitro-substituted benzoic acid systems. The ΔpK_a values are 0.98 and 1.42 and 3.02 for 3-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1), (I), 3-chloro-2-nitrobenzoic acid–6-nitroquinoline (1/1), (II), and 8-hydroxyquinolium 3-chloro-2-nitrobenzoate, (III), respectively.

2. Structural commentary

The molecular structure of (I) is shown in Fig. 1. The acid and base molecules are held together by an O—H···N hydrogen bond between the carboxy group and the N atom of the base. In addition, a weak C—H···O interaction is formed between the acid and base molecules (Table 1). In the hydrogen-bonded acid–base unit, the quinoline ring system (N2/C8–C16), the carboxy group (O1/C7/O2) and the benzene ring (C1–C6) are almost coplanar with each other; the carboxy group makes dihedral angles of 9.95 (12) and 9.45 (12)°, respectively, with the quinoline ring system and the benzene ring, and the dihedral angle between the quinoline ring system and the benzene ring is 2.59 (4)°. On the other hand, the benzene ring and the nitro group (O3/N1/O4) in the acid molecule is almost perpendicular, with a dihedral angle of 86.14 (13)°. The quinoline ring system and the attached nitro group (O5/N3/O6) are somewhat twisted with a dihedral angle of 31.67 (11)°.

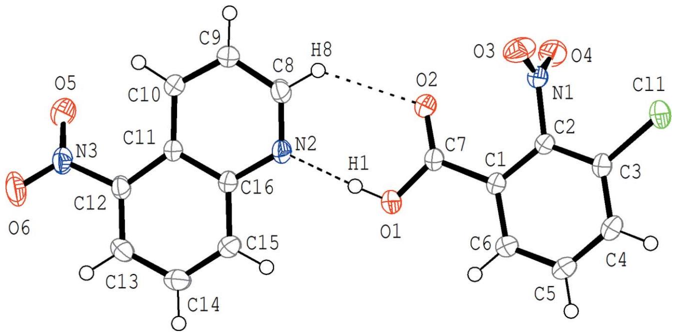


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The O—H···N and C—H···O hydrogen bonds are indicated by dashed lines (Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.88 (2)	1.80 (2)	2.6727 (12)	178 (2)
C8—H8···O2	0.95	2.48	3.1820 (13)	131
C5—H5···O2^{i}	0.95	2.57	3.4860 (14)	163
C14—H14···O5^{i}	0.95	2.56	3.4644 (14)	159
C13—H13···O6^{ii}	0.95	2.32	3.1495 (14)	146

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.87 (3)	1.76 (3)	2.6310 (14)	176 (3)
C8—H8···O2	0.95	2.53	3.2082 (16)	128
C8—H8···O6^{i}	0.95	2.41	3.2387 (15)	145
C12—H12···O5^{ii}	0.95	2.37	3.2526 (16)	155
C14—H14···O4^{iii}	0.95	2.52	3.3226 (16)	142

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

The molecular structure of (II) is shown in Fig. 2. Similar to (I), the acid and base molecules are held together by an O—H···N hydrogen bond and an additional C—H···O interaction (Table 2). In the acid–base unit, the quinoline ring

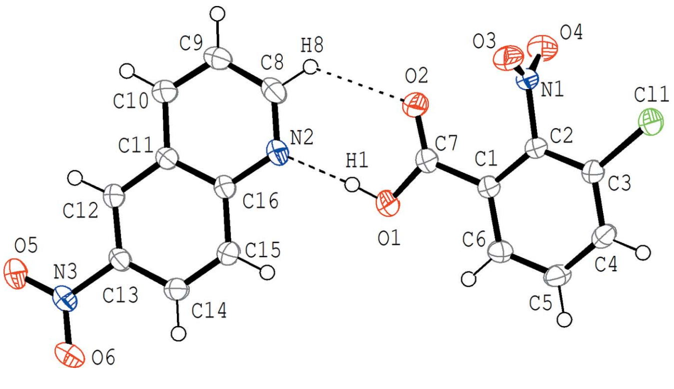


Figure 2
The molecular structure of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The O—H···N and C—H···O hydrogen bonds are indicated by dashed lines (Table 2).

Table 3
Hydrogen-bond geometry (Å, °) for (III).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N2—H2$\cdots$O1	0.880 (16)	1.776 (16)	2.6355 (12)	164.7 (14)
O5—H5*O*$\cdots$O2^{i}	0.872 (19)	1.756 (19)	2.6247 (12)	173.2 (19)
C4—H4$\cdots$O3^{ii}	0.95	2.49	3.1082 (12)	123

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

system, the carboxy group and the benzene ring of the acid are slightly twisted to each other; the carboxy group makes dihedral angles of 12.08 (13) and 2.40 (13)°, respectively, with the quinoline ring system and the benzene ring, and the dihedral angle between the quinoline ring system and the benzene ring is 10.99 (4)°. In the acid molecule, the benzene ring and the nitro group (O3/N1/O4) are almost perpendicular with a dihedral angle of 88.54 (13)°. On the other hand, in the base molecule the quinoline ring system and the nitro group (O5/N3/O6) are almost coplanar with a dihedral angle of 5.58 (12)°.

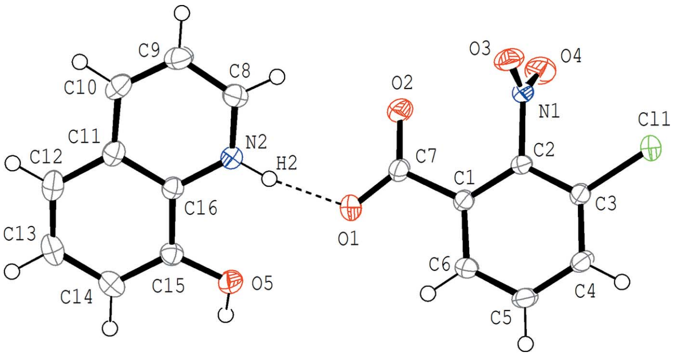


Figure 3
The molecular structure of (III), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The N—H$\cdots$O hydrogen bond is indicated by a dashed line (Table 3).

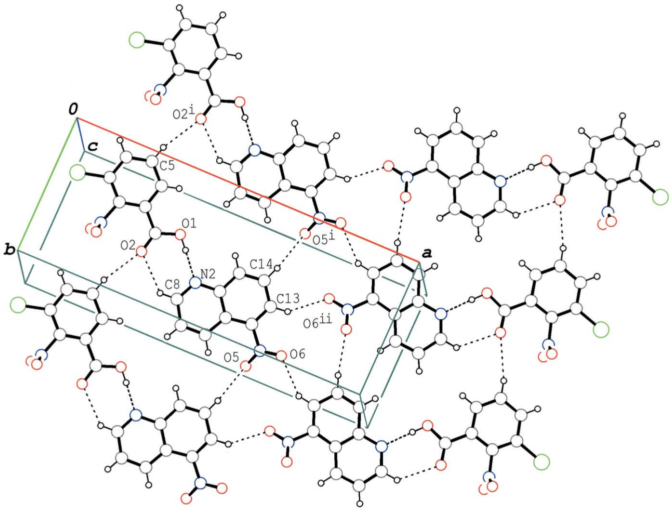


Figure 4
A packing diagram of (I), showing the hydrogen-bonded tape structure along the *b*-axis direction. Adjacent tapes, related by a twofold rotation axis, are linked by further C—H$\cdots$O hydrogen bonds, forming wide ribbons parallel to ($\overline{1}03$). The dashed lines indicate the O—H$\cdots$N and C—H$\cdots$O hydrogen bonds. [Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.]

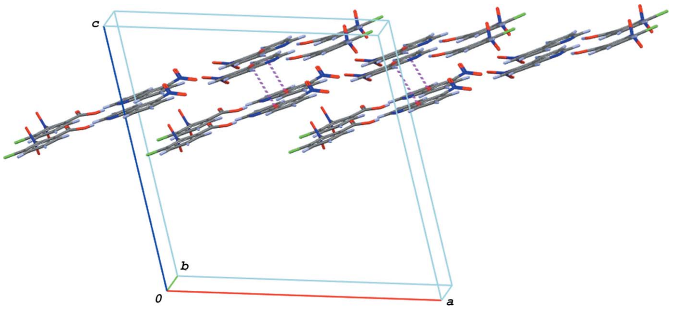


Figure 5
A partial packing diagram of (I), showing the ribbons linked by π–π stacking interactions (magenta dashed lines).

The molecular structure of (III) is shown in Fig. 3. An acid–base interaction involving H-atom transfer occurs and the acid and base molecules are linked by an N^{+}—H$\cdots$$O^{-}$ hydrogen bond (Table 3). In the hydrogen-bonded unit, the quinoline ring system makes dihedral angles of 34.96 (13) and 30.80 (14)°, respectively, with the carboxylate group and the benzene ring of the acid. In the acid molecule, the benzene ring makes dihedral angles of 4.71 (13) and 86.12 (11)°, respectively, with the carboxylate and nitro groups.

3. Supramolecular features

In the crystal of (I), the hydrogen-bonded acid–base units are linked by C—H$\cdots$O hydrogen bonds (C5—H5$\cdots$O2^{i} and C14—H14$\cdots$O5^{i}; symmetry codes as in Table 1), forming a tape structure along the *b*-axis direction. Adjacent tapes, which are related by a twofold rotation axis, are linked by a third C—H$\cdots$O hydrogen bond (C13—H13$\cdots$O6^{ii}), forming wide ribbons parallel to the ($\overline{1}03$) plane (Fig. 4). These ribbons are stacked *via* π–π interactions between the quinoline ring

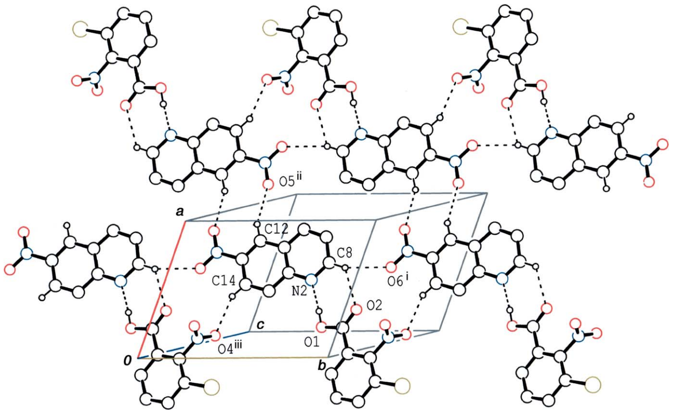


Figure 6
A packing diagram of (II), showing the ribbon structure along the *b*-axis direction formed by O—H$\cdots$N and C—H$\cdots$O hydrogen bonds (dashed lines). H atoms not involved in the hydrogen bonds have been omitted. [Symmetry codes: (i) $x, y+1, z$; (ii) $-x+2, -y, -z+1$; (iii) $x, y-1, z$.]

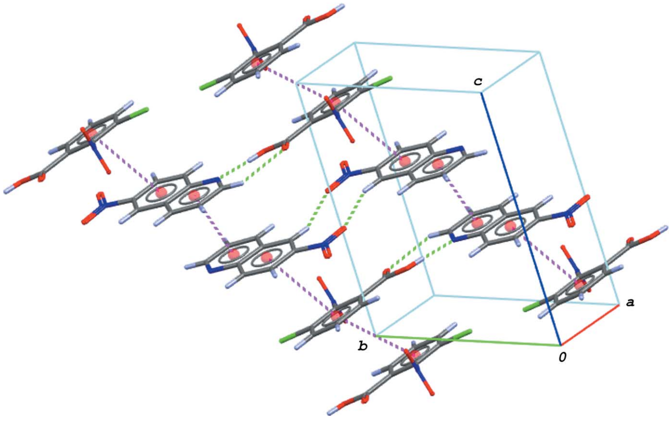


Figure 7
A partial packing diagram of (II), showing the column structure along [$\overline{1}$11] formed by weak *π*–*π* interactions (magenta dashed lines). The O—H⋯N and C—H⋯O hydrogen bonds in the hydrogen-bonded acid–base units are indicated by green dashed lines. The *π*–*π* interactions including the centroid of the ten-membered quinoline ring system (*Cg*4) are omitted for clarity.

systems, forming layers parallel to the *ab* plane (Fig. 5). The centroid–centroid distances are 3.4935 (5), 3.6761 (6) and 3.7721 (6) Å, respectively, for $Cg4\cdots Cg4^{iii}$, $Cg2\cdots Cg2^{iii}$ and $Cg2\cdots Cg3^{iii}$, where *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N2/C8–C11/C16, C11–C16 and N2/C8–C16 rings, respectively, of the base molecule [symmetry code: (iii) $-x + 1, y, -z + 2$].

In the crystal of (II), the hydrogen-bonded acid–base units are also linked into a tape structure along the *b*-axis direction *via* C—H⋯O hydrogen bonds (C8—H8⋯O6^{i} and C14—H14⋯O4^{iii}; symmetry codes as in Table 2). Inversion-related tapes are linked by a further C—H⋯O hydrogen bond (C12—H12⋯O5^{ii}; Table 2), forming wide ribbons parallel to the ($\overline{3}$08) plane (Fig. 6). The acid and base molecules are further stacked in a column along [$\overline{1}$11] in an ⋯*A*⋯*A*⋯*B*⋯*B*⋯*A*⋯*A*⋯*B*⋯*B*⋯ manner (*A*: acid and *B*: base) *via* weak *π*–*π* interactions (Fig. 7), so forming a three-dimensional structure. The centroid–centroid distances are 3.8016 (8), 3.8666 (8), 3.9247 (9) and 3.8225 (8) Å, respectively, for $Cg1\cdots Cg1^{iv}$, $Cg1\cdots Cg3^{v}$, $Cg2\cdots Cg2^{vi}$ and $Cg2\cdots Cg4^{vi}$, where *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are, respectively, the centroids of the C1–C6 ring of the acid molecule, and the N2/C8–C11/C16, C11–C16 and N2/C8–C16 rings of the base molecule [symmetry codes: (iv) $-x, -y + 2, -z$; (v) $x - 1, y + 1, z$; (vi) $-x + 1, -y + 1, -z + 1$]. A pair of short O⋯N contacts [O6⋯N3^{vii} = 2.8453 (13) Å; symmetry code: (vii) $-x + 1, -y, -x + 1$] between the nitro groups of the base molecule are alsso observed.

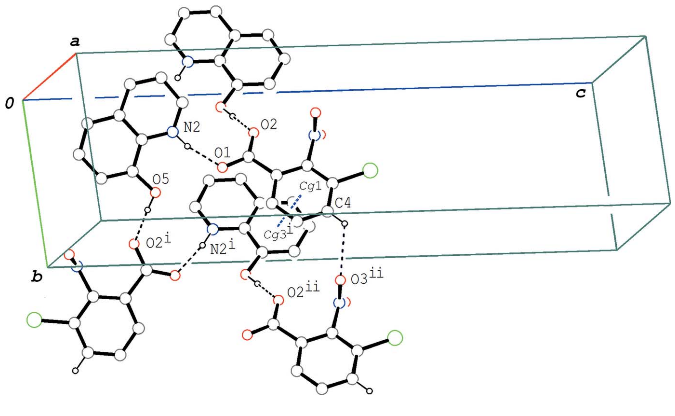


Figure 8
A partial packing diagram of (III), showing the 2_1 helix running along the *b*-axis direction formed by O—H⋯O and N—H⋯O hydrogen bonds (black dashed lines). The C—H⋯O and *π*–*π* interactions observed in the chain are indicated by black and blue dashed lines, respectively. *Cg*1 and *Cg*3 are the centroids of the C1–C6 and C11–C16 rings, respectively. H atoms not involved in the hydrogen bonds have been omitted. [Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, y + 1, z$.]

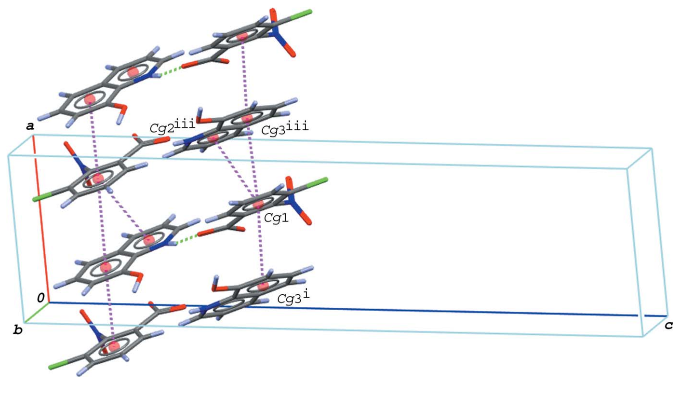


Figure 9
A partial packing diagram of (III), showing the *π*–*π* interactions (magenta dashed lines). The N—H⋯O hydrogen bonds in the hydrogen-bonded acid–base units are indicated by green dashed lines. *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, N2/C8–C11/C16 and C11–C16 rings, respectively. The *π*–*π* interactions including the centroid of the ten-membered quinoline ring system (*Cg*4) are omitted for clarity. [Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, y + 1, z$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.]

In the crystal of compound (III), the cations and the anions are alternately linked *via* N—H⋯O and O—H⋯O hydrogen bonds (N2—H2⋯O1 and O5—H5*O*⋯O2^{i}; symmetry code as in Table 3), forming a 2_1 helical chain running along the *b*-axis direction (Fig. 8). In the chain, a C—H⋯O (C4—H4⋯O3^{ii}; Table 3) interaction formed between the anions and a *π*–*π* interaction between the C1–C6 ring and the C11–C16 ring are observed [$Cg1\cdots Cg3^{i}$ = 3.5570 (6) Å]; *Cg*1 and *Cg*3 are, respectively, the centroids of the C1–C6 ring of the anion and the C11–C16 ring of the cation. In addition to the *π*–*π* interaction ($Cg1\cdots Cg3^{i}$), other *π*–*π* interactions are observed; the centroid–centroid distances are 3.5469 (6), 3.8550 (6) and 3.5133 (6) Å, respectively, for $Cg1\cdots Cg2^{iii}$, $Cg1\cdots Cg3^{iii}$ and $Cg1\cdots Cg4^{iii}$, where *Cg*2 and *Cg*4 are the centroids of the N2/C8–C11/C16 and N2/C8–C16 rings of the cation, respectively [symmetry code: (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$]. The cations and the anions are stacked alternately in columns along the *a*-axis direction *via* the *π*–*π* interactions (Fig. 9), and the molecular chains are linked into layers parallel to the *ab* plane through these interactions. A short Cl⋯O contact [Cl1⋯O3^{iv} = 3.0669 (10) Å; symmetry code: (iv) $-x + 2, -y + 1, -z + 1$] is observed between the layers.

Table 4
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_7H_4ClNO_4{\cdot}C_9H_6N_2O_2$	$C_7H_4ClNO_4{\cdot}C_9H_6N_2O_2$	$C_7H_3ClNO_4{\cdot}C_9H_8NO$
M_r	375.72	375.72	346.73
Crystal system, space group	Monoclinic, $C2/c$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	190	190	190
a, b, c (Å)	20.5876 (4), 7.6889 (3), 20.4312 (4)	7.7282 (10), 10.2839 (14), 11.2828 (16)	7.3409 (5), 7.4689 (4), 27.0427 (14)
α, β, γ (°)	90, 104.5338 (7), 90	71.990 (4), 79.724 (4), 69.051 (3)	90, 95.7158 (19), 90
V (Å^3)	3130.70 (16)	794.08 (19)	1475.33 (15)
Z	8	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.29	0.28	0.29
Crystal size (mm)	0.45 × 0.40 × 0.30	0.38 × 0.35 × 0.30	0.45 × 0.30 × 0.26
Data collection			
Diffractometer	Rigaku R-AXIS RAPIDII	Rigaku R-AXIS RAPIDII	Rigaku R-AXIS RAPIDII
Absorption correction	Numerical (*NUMABS*; Higashi, 1999)	Numerical (*NUMABS*; Higashi, 1999)	Numerical (*NUMABS*; Higashi, 1999)
$T_{\min}$, $T_{\max}$	0.837, 0.918	0.887, 0.919	0.844, 0.927
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30107, 4549, 4077	16549, 4622, 4029	29560, 4311, 3937
$R_{\rm int}$	0.022	0.026	0.019
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.703	0.703	0.703
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.104, 1.05	0.039, 0.113, 1.07	0.033, 0.092, 1.06
No. of reflections	4549	4622	4311
No. of parameters	239	239	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.30, −0.35	0.50, −0.33	0.39, −0.30

Computer programs: *RAPID-AUTO* (Rigaku, 2006), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006), *CrystalStructure* (Rigaku, 2018) and *PLATON* (Spek, 2015).

4. Database survey

A search of the Cambridge Structural Database (Version 5.40, last update May 2019; Groom *et al.*, 2016) for organic co-crystals of 3-chloro-2-nitrobonzoic acid with base molecules gave six hits (five compounds), namely, 4-benzpylpyridine (1/1) (refcode UHAQUP; Sugiyama *et al.*, 2002), quinolone (1/1) (AJIWOG; Gotoh & Ishida, 2009), phthalazine (1/1) (CALJUW; Gotoh & Ishida, 2011), isoquinoline (1/1) (NOVLAN; Gotoh & Ishida, 2015) and 4,4′-bipyridine (2/1) (XICGUO and XICGUO01; Rawat *et al.*, 2018). The structure of 3-chloro-2-nitrobonzoic acid itself (XICHAV) was also reported by Rawat *et al.* (2018). There is no structure for a salt of 3-chloro-2-nitrobonzoic acid with an organic base molecule. In the acid molecules of the above compounds, the dihedral angles between the benzene ring and the nitro group, and between the benzene ring and the carboxy group are in the ranges 79.1 (3)–89.9 (3)° and 1.4 (3)–14.2 (3)°, respectively, which agree with those in the three title compounds. The ΔpK_a values for UHAQUP, AJIWOG, CALJUW, NOVLAN and XICGUO are 1.32, 3.08, 1.65, 3.58 and 3.27, respectively, and these compounds show short O···N distances in the O—H···N hydrogen bonds of 2.600 (3), 2.561 (1), 2.540 (2)–2.571 (2), 2.573 (1) and 2.613 (3) Å, respectively. Furthermore, in the short hydrogen bonds of AJIWOG, CALJUW and NOVLAN, the H atom is disordered over two positions. On the other hand, the compounds (I), (II) and (III) with ΔpK_a values of 0.98, 1.42 and 3.02, respectively, show longer O···N distances of 2.673 (1), 2.631 (1) and 2.636 (1) Å, which suggests that the ΔpK_a value is not an effective measure of hydrogen-bond strength in the 3-chloro-2-nitrobenzoic acid–organic base system.

A search for organic co-crystals/salts of 5-nitroquinoline showed six structures. Limiting the search to benzoic acid derivatives gave two hits, namely, 3-aminobenzoic acid–5-nitroquinoline (1/1) (PANYIM; Lynch *et al.*, 1997) and 4-animobenzoic acid–5-nitroquinoline (1/2) (PANZEJ; Lynch *et al.*, 1997). No structure was found in the CSD for organic co-crystals/salts of 6-nitroquinoline. A search for organic co-crystals/salts of 8-hydroxyquinoline gave 17 hits. Of these compounds, one related compound is 8-hydroxyquinolinium 2-chloro-4-nitrobenzoate (WOPDEM; Babu & Chandrasekaran, 2014; ΔpK_a = 2.80), in which the O···N distance of the N—H···O hydrogen bond is 2.644 (3) Å.

5. Synthesis and crystallization

Crystals of all three compounds, (I)–(III), were obtained by slow evaporation from acetonitrile solutions of 3-chloro-2-nitrobenzoic acid with quinoline derivatives in a 1:1 molar ratio at room temperature [100 ml acetonitrile solution of 3-

chloro-2-nitrobenzoic acid (0.39 g) and 5-nitroquinoline (0.34 g) for (I), 150 ml acetonitrile solution of 3-chloro-2-nitrobenzoic acid (0.45 g) and 6-nitroquinoline (0.39 g) for (II), and 120 ml acetonitrile solution of 3-chloro-2-nitrobenzoic acid (0.55 g) and 8-hydroxyqunoline (0.40 mg) for (III)] .

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms in compounds (I)–(III) were found in difference-Fourier maps. O- and N-bound H atoms in (I)–(III) were refined freely [refined distances: O1—H1 = 0.88 (2) Å in (I), N1—H1 = 0.87 (3) Å in (II), and N2—H2 = 0.880 (16) and O5—H5*O* = 0.872 (19) Å in (III),]. Other H atoms were positioned geometrically (C—H = 0.95 Å) and treated as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

References

Babu, B. & Chandrasekaran, J. (2014). Private Communication (refcode WOPDEM). CCDC, Cambridge, England.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Gilli, G. & Gilli, P. (2009). *The Nature of the Hydrogen Bond.* Oxford University Press.

Gotoh, K. & Ishida, H. (2009). *Acta Cryst.* C**65**, o534–o538.

Gotoh, K. & Ishida, H. (2011). *Acta Cryst.* C**67**, o473–o478.

Gotoh, K. & Ishida, H. (2015). *Acta Cryst.* E**71**, 31–34.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.

Lynch, D. E., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1997). *Aust. J. Chem.* **50**, 977–986.

Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.

Rawat, H., Samanta, R., Bhattacharya, B., Deolka, S., Dutta, A., Dey, S., Raju, K. B. & Reddy, C. M. (2018). *Cryst. Growth Des.* **18**, 2918–2923.

Rigaku (2006). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku (2018). *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.

Schmidtmann, M. & Wilson, C. C. (2008). *CrystEngComm*, **10**, 177–183.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2015). *Acta Cryst.* C**71**, 9–18.

Sugiyama, T., Meng, J. & Matsuura, T. (2002). *J. Mol. Struct.* **611**, 53–64.

supporting information

Acta Cryst. (2019). E**75**, 1552-1557   [https://doi.org/10.1107/S2056989019012799]

Crystal structures of 3-chloro-2-nitrobenzoic acid with quinoline derivatives: 3-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1), 3-chloro-2-nitrobenzoic acid–6-nitroquinoline (1/1) and 8-hydroxyquinolinium 3-chloro-2-nitrobenzoate

Kazuma Gotoh and Hiroyuki Ishida

Computing details

For all structures, data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO* (Rigaku, 2006); data reduction: *RAPID-AUTO* (Rigaku, 2006); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2018) and *PLATON* (Spek, 2015).

3-Chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1) (I)

Crystal data

$C_7H_4ClNO_4{\cdot}C_9H_6N_2O_2$
$M_r = 375.72$
Monoclinic, $C2/c$
$a = 20.5876$ (4) Å
$b = 7.6889$ (3) Å
$c = 20.4312$ (4) Å
$\beta = 104.5338$ (7)°
$V = 3130.70$ (16) Å^3
$Z = 8$
$F(000) = 1536.00$
$D_x = 1.594$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 25710 reflections
$\theta = 3.1$–30.1°
$\mu = 0.29$ mm^{-1}
$T = 190$ K
Block, colorless
0.45 × 0.40 × 0.30 mm

Data collection

Rigaku R-AXIS RAPIDII diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.837$, $T_{max} = 0.918$
30107 measured reflections
4549 independent reflections
4077 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.1°$
$h = -26 \rightarrow 28$
$k = -10 \rightarrow 10$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.104$
$S = 1.05$
4549 reflections
239 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 1.2587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.03434 (2)	0.24994 (4)	0.50043 (2)	0.03753 (9)
O1	0.34832 (4)	0.34621 (10)	0.61778 (4)	0.03292 (17)
O2	0.27238 (4)	0.55880 (10)	0.60848 (5)	0.03766 (19)
O3	0.14558 (5)	0.57618 (11)	0.50150 (4)	0.0412 (2)
O4	0.12329 (5)	0.55420 (11)	0.59855 (5)	0.0414 (2)
O5	0.64633 (4)	0.97971 (11)	0.75715 (4)	0.03764 (19)
O6	0.72372 (4)	0.82403 (14)	0.73078 (5)	0.0472 (2)
N1	0.14396 (4)	0.49673 (11)	0.55218 (5)	0.02666 (17)
N2	0.43699 (4)	0.60692 (11)	0.64264 (4)	0.02613 (17)
N3	0.66566 (4)	0.84775 (12)	0.73417 (4)	0.02984 (18)
C1	0.23369 (5)	0.26976 (12)	0.58259 (5)	0.02307 (18)
C2	0.16614 (4)	0.31430 (12)	0.55708 (5)	0.02215 (17)
C3	0.11699 (5)	0.18860 (13)	0.53478 (5)	0.02620 (19)
C4	0.13470 (5)	0.01433 (14)	0.53907 (6)	0.0320 (2)
H4	0.101547	−0.072633	0.523966	0.038*
C5	0.20130 (6)	−0.03225 (14)	0.56561 (6)	0.0344 (2)
H5	0.213441	−0.151718	0.569282	0.041*
C6	0.25043 (5)	0.09415 (13)	0.58689 (6)	0.0296 (2)
H6	0.295828	0.060186	0.604524	0.035*
C7	0.28632 (5)	0.40747 (12)	0.60433 (5)	0.02479 (18)
C8	0.41075 (5)	0.76300 (13)	0.63187 (5)	0.0281 (2)
H8	0.363528	0.772862	0.614770	0.034*
C9	0.44900 (5)	0.91633 (13)	0.64438 (5)	0.0290 (2)
H9	0.427911	1.026448	0.634382	0.035*
C10	0.51692 (5)	0.90588 (12)	0.67109 (5)	0.02615 (19)
H10	0.543243	1.008630	0.680454	0.031*
C11	0.54753 (5)	0.74008 (11)	0.68461 (5)	0.02182 (17)
C12	0.61745 (5)	0.70585 (13)	0.71097 (5)	0.02475 (18)
C13	0.64371 (5)	0.54231 (14)	0.71854 (6)	0.0311 (2)
H13	0.690681	0.525741	0.735325	0.037*
C14	0.60078 (6)	0.39830 (14)	0.70133 (6)	0.0356 (2)
H14	0.618748	0.283873	0.706670	0.043*
C15	0.53282 (6)	0.42258 (13)	0.67677 (6)	0.0313 (2)
H15	0.504064	0.324562	0.665699	0.038*

C16	0.50536 (5)	0.59203 (12)	0.66783 (5)	0.02310 (18)
H1	0.3780 (11)	0.430 (3)	0.6264 (10)	0.073 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02113 (13)	0.03817 (16)	0.04799 (17)	−0.00501 (9)	−0.00126 (11)	−0.00276 (10)
O1	0.0197 (3)	0.0265 (4)	0.0495 (5)	−0.0024 (3)	0.0029 (3)	−0.0014 (3)
O2	0.0245 (4)	0.0230 (3)	0.0615 (5)	−0.0035 (3)	0.0033 (3)	−0.0040 (3)
O3	0.0537 (5)	0.0289 (4)	0.0359 (4)	0.0016 (3)	0.0018 (4)	0.0084 (3)
O4	0.0421 (5)	0.0322 (4)	0.0559 (5)	0.0007 (3)	0.0237 (4)	−0.0094 (4)
O5	0.0346 (4)	0.0320 (4)	0.0431 (4)	−0.0071 (3)	0.0037 (3)	−0.0078 (3)
O6	0.0214 (4)	0.0566 (6)	0.0631 (6)	−0.0097 (4)	0.0097 (4)	−0.0088 (5)
N1	0.0211 (4)	0.0221 (4)	0.0344 (4)	−0.0018 (3)	0.0025 (3)	−0.0014 (3)
N2	0.0195 (4)	0.0268 (4)	0.0299 (4)	−0.0039 (3)	0.0020 (3)	0.0007 (3)
N3	0.0221 (4)	0.0337 (4)	0.0314 (4)	−0.0067 (3)	0.0022 (3)	−0.0007 (3)
C1	0.0209 (4)	0.0210 (4)	0.0265 (4)	−0.0031 (3)	0.0044 (3)	−0.0008 (3)
C2	0.0215 (4)	0.0196 (4)	0.0248 (4)	−0.0018 (3)	0.0047 (3)	−0.0002 (3)
C3	0.0216 (4)	0.0260 (4)	0.0294 (4)	−0.0046 (3)	0.0036 (3)	−0.0019 (3)
C4	0.0300 (5)	0.0237 (5)	0.0405 (5)	−0.0075 (4)	0.0057 (4)	−0.0040 (4)
C5	0.0341 (5)	0.0196 (4)	0.0477 (6)	−0.0026 (4)	0.0068 (5)	−0.0018 (4)
C6	0.0259 (4)	0.0221 (4)	0.0391 (5)	0.0000 (3)	0.0050 (4)	−0.0001 (4)
C7	0.0200 (4)	0.0239 (4)	0.0290 (4)	−0.0032 (3)	0.0035 (3)	0.0002 (3)
C8	0.0197 (4)	0.0304 (5)	0.0321 (5)	−0.0014 (3)	0.0025 (4)	0.0042 (4)
C9	0.0245 (4)	0.0241 (4)	0.0369 (5)	0.0014 (3)	0.0053 (4)	0.0051 (4)
C10	0.0230 (4)	0.0216 (4)	0.0332 (5)	−0.0019 (3)	0.0059 (4)	0.0017 (3)
C11	0.0186 (4)	0.0219 (4)	0.0243 (4)	−0.0020 (3)	0.0042 (3)	−0.0004 (3)
C12	0.0187 (4)	0.0275 (4)	0.0267 (4)	−0.0030 (3)	0.0032 (3)	−0.0015 (3)
C13	0.0223 (4)	0.0319 (5)	0.0368 (5)	0.0049 (4)	0.0032 (4)	0.0004 (4)
C14	0.0325 (5)	0.0246 (5)	0.0470 (6)	0.0061 (4)	0.0047 (5)	−0.0010 (4)
C15	0.0287 (5)	0.0218 (4)	0.0409 (5)	−0.0016 (3)	0.0038 (4)	−0.0022 (4)
C16	0.0203 (4)	0.0220 (4)	0.0259 (4)	−0.0027 (3)	0.0037 (3)	−0.0007 (3)

Geometric parameters (Å, º)

Cl1—C3	1.7352 (10)	C5—C6	1.3913 (14)
O1—C7	1.3231 (12)	C5—H5	0.9500
O1—H1	0.88 (2)	C6—H6	0.9500
O2—C7	1.2065 (13)	C8—C9	1.4051 (14)
O3—N1	1.2099 (12)	C8—H8	0.9500
O4—N1	1.2150 (12)	C9—C10	1.3699 (13)
O5—N3	1.2256 (13)	C9—H9	0.9500
O6—N3	1.2282 (12)	C10—C11	1.4182 (13)
N1—C2	1.4708 (12)	C10—H10	0.9500
N2—C8	1.3118 (13)	C11—C16	1.4205 (12)
N2—C16	1.3768 (12)	C11—C12	1.4290 (13)
N3—C12	1.4711 (13)	C12—C13	1.3621 (14)
C1—C6	1.3909 (13)	C13—C14	1.4053 (16)

C1—C2	1.3997 (13)	C13—H13	0.9500
C1—C7	1.5002 (13)	C14—C15	1.3755 (16)
C2—C3	1.3909 (12)	C14—H14	0.9500
C3—C4	1.3857 (14)	C15—C16	1.4138 (13)
C4—C5	1.3889 (16)	C15—H15	0.9500
C4—H4	0.9500		

C7—O1—H1	111.7 (14)	O1—C7—C1	113.43 (8)
O3—N1—O4	125.03 (10)	N2—C8—C9	123.28 (9)
O3—N1—C2	117.71 (9)	N2—C8—H8	118.4
O4—N1—C2	117.21 (9)	C9—C8—H8	118.4
C8—N2—C16	118.56 (8)	C10—C9—C8	119.51 (9)
O5—N3—O6	123.97 (9)	C10—C9—H9	120.2
O5—N3—C12	118.67 (8)	C8—C9—H9	120.2
O6—N3—C12	117.33 (9)	C9—C10—C11	119.32 (9)
C6—C1—C2	117.92 (8)	C9—C10—H10	120.3
C6—C1—C7	121.16 (9)	C11—C10—H10	120.3
C2—C1—C7	120.92 (8)	C10—C11—C16	117.28 (8)
C3—C2—C1	121.68 (9)	C10—C11—C12	126.54 (8)
C3—C2—N1	116.90 (8)	C16—C11—C12	116.12 (8)
C1—C2—N1	121.41 (8)	C13—C12—C11	123.12 (9)
C4—C3—C2	119.53 (9)	C13—C12—N3	115.57 (9)
C4—C3—Cl1	120.28 (7)	C11—C12—N3	121.28 (9)
C2—C3—Cl1	120.18 (8)	C12—C13—C14	119.48 (9)
C3—C4—C5	119.50 (9)	C12—C13—H13	120.3
C3—C4—H4	120.3	C14—C13—H13	120.3
C5—C4—H4	120.3	C15—C14—C13	120.17 (10)
C4—C5—C6	120.72 (10)	C15—C14—H14	119.9
C4—C5—H5	119.6	C13—C14—H14	119.9
C6—C5—H5	119.6	C14—C15—C16	120.63 (9)
C1—C6—C5	120.61 (10)	C14—C15—H15	119.7
C1—C6—H6	119.7	C16—C15—H15	119.7
C5—C6—H6	119.7	N2—C16—C15	117.59 (8)
O2—C7—O1	124.25 (9)	N2—C16—C11	121.96 (8)
O2—C7—C1	122.32 (9)	C15—C16—C11	120.46 (9)

C6—C1—C2—C3	−1.77 (14)	C8—C9—C10—C11	1.01 (15)
C7—C1—C2—C3	178.02 (9)	C9—C10—C11—C16	1.49 (14)
C6—C1—C2—N1	178.69 (9)	C9—C10—C11—C12	178.64 (9)
C7—C1—C2—N1	−1.53 (14)	C10—C11—C12—C13	−175.60 (10)
O3—N1—C2—C3	−92.47 (11)	C16—C11—C12—C13	1.57 (14)
O4—N1—C2—C3	85.14 (11)	C10—C11—C12—N3	6.67 (15)
O3—N1—C2—C1	87.09 (12)	C16—C11—C12—N3	−176.16 (8)
O4—N1—C2—C1	−95.29 (11)	O5—N3—C12—C13	−148.03 (10)
C1—C2—C3—C4	1.39 (15)	O6—N3—C12—C13	30.14 (14)
N1—C2—C3—C4	−179.05 (9)	O5—N3—C12—C11	29.86 (14)
C1—C2—C3—Cl1	−177.45 (7)	O6—N3—C12—C11	−151.97 (10)
N1—C2—C3—Cl1	2.11 (12)	C11—C12—C13—C14	−1.45 (16)

C2—C3—C4—C5	0.03 (16)	N3—C12—C13—C14	176.40 (10)
Cl1—C3—C4—C5	178.87 (9)	C12—C13—C14—C15	0.27 (18)
C3—C4—C5—C6	−1.02 (18)	C13—C14—C15—C16	0.68 (18)
C2—C1—C6—C5	0.76 (16)	C8—N2—C16—C15	−177.79 (10)
C7—C1—C6—C5	−179.03 (10)	C8—N2—C16—C11	2.30 (14)
C4—C5—C6—C1	0.62 (18)	C14—C15—C16—N2	179.60 (10)
C6—C1—C7—O2	−171.24 (11)	C14—C15—C16—C11	−0.50 (16)
C2—C1—C7—O2	8.99 (15)	C10—C11—C16—N2	−3.23 (14)
C6—C1—C7—O1	9.12 (14)	C12—C11—C16—N2	179.32 (8)
C2—C1—C7—O1	−170.66 (9)	C10—C11—C16—C15	176.87 (9)
C16—N2—C8—C9	0.41 (16)	C12—C11—C16—C15	−0.58 (14)
N2—C8—C9—C10	−2.09 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.88 (2)	1.80 (2)	2.6727 (12)	178 (2)
C8—H8···O2	0.95	2.48	3.1820 (13)	131
C5—H5···O2$^{\text{i}}$	0.95	2.57	3.4860 (14)	163
C14—H14···O5$^{\text{i}}$	0.95	2.56	3.4644 (14)	159
C13—H13···O6$^{\text{ii}}$	0.95	2.32	3.1495 (14)	146

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

3-Chloro-2-nitrobenzoicacid–6-nitroquinoline (1/1) (II)

Crystal data

$C_7H_4ClNO_4\cdot C_9H_6N_2O_2$
M_r = 375.72
Triclinic, $P\overline{1}$
a = 7.7282 (10) Å
b = 10.2839 (14) Å
c = 11.2828 (16) Å
α = 71.990 (4)°
β = 79.724 (4)°
γ = 69.051 (3)°
V = 794.08 (19) Å^3

Z = 2
F(000) = 384.00
D_x = 1.571 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 14524 reflections
θ = 3.1–30.1°
μ = 0.28 mm^{-1}
T = 190 K
Block, colorless
0.38 × 0.35 × 0.30 mm

Data collection

Rigaku R-AXIS RAPIDII diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{\min}$ = 0.887, $T_{\max}$ = 0.919
16549 measured reflections

4622 independent reflections
4029 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
$\theta_{\max}$ = 30.0°, $\theta_{\min}$ = 3.1°
h = −10→10
k = −14→14
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.113$
$S = 1.07$
4622 reflections
239 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.0976P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.21217 (4)	1.44247 (3)	−0.00166 (3)	0.04778 (11)
O1	0.17321 (12)	0.77718 (8)	0.24868 (9)	0.03883 (19)
O2	0.30609 (12)	0.94833 (9)	0.20949 (10)	0.0464 (2)
O3	0.23107 (11)	1.23134 (10)	0.01395 (9)	0.0439 (2)
O4	0.12561 (13)	1.25965 (10)	0.19770 (10)	0.0477 (2)
O5	0.83957 (13)	−0.07571 (9)	0.45563 (10)	0.0469 (2)
O6	0.58065 (12)	−0.04120 (8)	0.38490 (8)	0.03651 (18)
N1	0.12435 (12)	1.22061 (9)	0.10689 (9)	0.03234 (19)
N2	0.50541 (13)	0.60187 (9)	0.31357 (9)	0.03239 (19)
N3	0.69185 (13)	0.00332 (9)	0.41169 (8)	0.03128 (18)
C1	−0.00331 (13)	1.01631 (10)	0.15345 (9)	0.02609 (18)
C2	−0.02570 (12)	1.16317 (10)	0.10624 (9)	0.02667 (18)
C3	−0.18851 (13)	1.26120 (10)	0.05510 (10)	0.0299 (2)
C4	−0.33392 (14)	1.21363 (12)	0.04976 (10)	0.0325 (2)
H4	−0.445873	1.280397	0.015146	0.039*
C5	−0.31344 (14)	1.06810 (12)	0.09541 (10)	0.0318 (2)
H5	−0.411793	1.034696	0.091986	0.038*
C6	−0.14952 (13)	0.97031 (11)	0.14634 (9)	0.02906 (19)
H6	−0.137031	0.870569	0.176756	0.035*
C7	0.17485 (14)	0.91108 (10)	0.20737 (10)	0.0302 (2)
C8	0.62786 (17)	0.65774 (11)	0.32741 (12)	0.0382 (2)
H8	0.593373	0.759863	0.309365	0.046*
C9	0.80676 (17)	0.57424 (13)	0.36745 (13)	0.0413 (3)
H9	0.890518	0.619663	0.374699	0.050*
C10	0.85796 (16)	0.42727 (12)	0.39567 (12)	0.0367 (2)
H10	0.977047	0.368770	0.424193	0.044*
C11	0.73037 (14)	0.36326 (10)	0.38169 (9)	0.02805 (19)
C12	0.77423 (14)	0.21193 (10)	0.40730 (10)	0.02926 (19)

H12	0.890452	0.148054	0.437393	0.035*
C13	0.64508 (14)	0.16024 (10)	0.38761 (9)	0.02718 (19)
C14	0.47039 (14)	0.24888 (11)	0.34310 (10)	0.0302 (2)
H14	0.385636	0.207883	0.329622	0.036*
C15	0.42557 (14)	0.39522 (11)	0.31976 (10)	0.0310 (2)
H15	0.307926	0.457014	0.290674	0.037*
C16	0.55426 (13)	0.45484 (10)	0.33887 (9)	0.02686 (18)
H1	0.285 (3)	0.723 (3)	0.270 (2)	0.089 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03623 (16)	0.02349 (14)	0.0773 (2)	−0.00733 (10)	−0.02054 (14)	0.00154 (12)
O1	0.0321 (4)	0.0222 (3)	0.0574 (5)	−0.0076 (3)	−0.0081 (3)	−0.0028 (3)
O2	0.0339 (4)	0.0274 (4)	0.0765 (6)	−0.0091 (3)	−0.0234 (4)	−0.0020 (4)
O3	0.0315 (4)	0.0410 (4)	0.0603 (5)	−0.0196 (3)	−0.0013 (4)	−0.0068 (4)
O4	0.0429 (5)	0.0451 (5)	0.0664 (6)	−0.0136 (4)	−0.0170 (4)	−0.0240 (4)
O5	0.0430 (4)	0.0235 (4)	0.0679 (6)	−0.0034 (3)	−0.0177 (4)	−0.0047 (4)
O6	0.0471 (4)	0.0304 (4)	0.0395 (4)	−0.0196 (3)	−0.0002 (3)	−0.0132 (3)
N1	0.0246 (4)	0.0221 (4)	0.0508 (5)	−0.0070 (3)	−0.0109 (4)	−0.0065 (3)
N2	0.0329 (4)	0.0204 (4)	0.0417 (5)	−0.0051 (3)	−0.0079 (3)	−0.0066 (3)
N3	0.0368 (4)	0.0225 (4)	0.0340 (4)	−0.0100 (3)	−0.0023 (3)	−0.0066 (3)
C1	0.0231 (4)	0.0236 (4)	0.0311 (4)	−0.0078 (3)	−0.0029 (3)	−0.0060 (3)
C2	0.0217 (4)	0.0244 (4)	0.0349 (4)	−0.0085 (3)	−0.0041 (3)	−0.0071 (3)
C3	0.0250 (4)	0.0238 (4)	0.0389 (5)	−0.0071 (3)	−0.0065 (4)	−0.0042 (4)
C4	0.0220 (4)	0.0342 (5)	0.0401 (5)	−0.0080 (4)	−0.0063 (4)	−0.0075 (4)
C5	0.0255 (4)	0.0365 (5)	0.0374 (5)	−0.0152 (4)	−0.0011 (4)	−0.0099 (4)
C6	0.0273 (4)	0.0282 (4)	0.0335 (4)	−0.0132 (4)	0.0008 (3)	−0.0075 (4)
C7	0.0287 (4)	0.0229 (4)	0.0370 (5)	−0.0068 (3)	−0.0050 (4)	−0.0054 (3)
C8	0.0433 (6)	0.0228 (4)	0.0506 (6)	−0.0102 (4)	−0.0097 (5)	−0.0097 (4)
C9	0.0420 (6)	0.0310 (5)	0.0588 (7)	−0.0157 (4)	−0.0144 (5)	−0.0122 (5)
C10	0.0328 (5)	0.0294 (5)	0.0518 (6)	−0.0100 (4)	−0.0144 (4)	−0.0099 (4)
C11	0.0282 (4)	0.0229 (4)	0.0343 (5)	−0.0078 (3)	−0.0074 (3)	−0.0071 (3)
C12	0.0269 (4)	0.0218 (4)	0.0373 (5)	−0.0048 (3)	−0.0091 (4)	−0.0054 (3)
C13	0.0303 (4)	0.0204 (4)	0.0307 (4)	−0.0082 (3)	−0.0044 (3)	−0.0055 (3)
C14	0.0298 (4)	0.0270 (4)	0.0359 (5)	−0.0115 (4)	−0.0083 (4)	−0.0055 (4)
C15	0.0270 (4)	0.0258 (4)	0.0385 (5)	−0.0068 (3)	−0.0103 (4)	−0.0041 (4)
C16	0.0275 (4)	0.0210 (4)	0.0309 (4)	−0.0064 (3)	−0.0054 (3)	−0.0053 (3)

Geometric parameters (Å, º)

Cl1—C3	1.7257 (10)	C5—C6	1.3921 (14)
O1—C7	1.3142 (12)	C5—H5	0.9500
O1—H1	0.87 (3)	C6—H6	0.9500
O2—C7	1.2117 (13)	C8—C9	1.4096 (16)
O3—N1	1.2153 (13)	C8—H8	0.9500
O4—N1	1.2132 (13)	C9—C10	1.3646 (15)
O5—N3	1.2243 (12)	C9—H9	0.9500

O6—N3	1.2244 (12)	C10—C11	1.4193 (14)
N1—C2	1.4796 (12)	C10—H10	0.9500
N2—C8	1.3218 (14)	C11—C12	1.4142 (13)
N2—C16	1.3688 (12)	C11—C16	1.4175 (13)
N3—C13	1.4682 (12)	C12—C13	1.3637 (14)
C1—C2	1.3940 (13)	C12—H12	0.9500
C1—C6	1.3947 (13)	C13—C14	1.4088 (13)
C1—C7	1.5044 (13)	C14—C15	1.3671 (14)
C2—C3	1.3873 (13)	C14—H14	0.9500
C3—C4	1.3934 (13)	C15—C16	1.4163 (14)
C4—C5	1.3832 (15)	C15—H15	0.9500
C4—H4	0.9500		

C7—O1—H1	107.0 (16)	O1—C7—C1	113.28 (9)
O4—N1—O3	125.19 (9)	N2—C8—C9	123.66 (10)
O4—N1—C2	117.34 (9)	N2—C8—H8	118.2
O3—N1—C2	117.37 (9)	C9—C8—H8	118.2
C8—N2—C16	118.54 (9)	C10—C9—C8	119.08 (10)
O5—N3—O6	123.52 (9)	C10—C9—H9	120.5
O5—N3—C13	118.83 (9)	C8—C9—H9	120.5
O6—N3—C13	117.64 (9)	C9—C10—C11	118.90 (10)
C2—C1—C6	117.80 (9)	C9—C10—H10	120.5
C2—C1—C7	120.79 (8)	C11—C10—H10	120.5
C6—C1—C7	121.39 (8)	C12—C11—C16	119.20 (9)
C3—C2—C1	121.41 (9)	C12—C11—C10	122.22 (9)
C3—C2—N1	117.24 (8)	C16—C11—C10	118.57 (9)
C1—C2—N1	121.35 (8)	C13—C12—C11	118.16 (9)
C2—C3—C4	120.06 (9)	C13—C12—H12	120.9
C2—C3—Cl1	120.21 (7)	C11—C12—H12	120.9
C4—C3—Cl1	119.73 (8)	C12—C13—C14	123.80 (9)
C5—C4—C3	119.26 (9)	C12—C13—N3	118.24 (9)
C5—C4—H4	120.4	C14—C13—N3	117.95 (8)
C3—C4—H4	120.4	C15—C14—C13	118.50 (9)
C4—C5—C6	120.36 (9)	C15—C14—H14	120.8
C4—C5—H5	119.8	C13—C14—H14	120.8
C6—C5—H5	119.8	C14—C15—C16	120.10 (9)
C5—C6—C1	121.10 (9)	C14—C15—H15	120.0
C5—C6—H6	119.4	C16—C15—H15	119.9
C1—C6—H6	119.4	N2—C16—C15	118.54 (9)
O2—C7—O1	124.46 (9)	N2—C16—C11	121.22 (9)
O2—C7—C1	122.25 (9)	C15—C16—C11	120.23 (9)

C6—C1—C2—C3	0.76 (15)	N2—C8—C9—C10	−1.0 (2)
C7—C1—C2—C3	179.34 (9)	C8—C9—C10—C11	1.07 (19)
C6—C1—C2—N1	−178.31 (9)	C9—C10—C11—C12	179.07 (11)
C7—C1—C2—N1	0.27 (15)	C9—C10—C11—C16	−0.01 (17)
O4—N1—C2—C3	90.22 (12)	C16—C11—C12—C13	1.04 (15)
O3—N1—C2—C3	−86.34 (12)	C10—C11—C12—C13	−178.04 (10)

O4—N1—C2—C1	−90.67 (12)	C11—C12—C13—C14	0.05 (16)
O3—N1—C2—C1	92.76 (12)	C11—C12—C13—N3	178.77 (9)
C1—C2—C3—C4	−0.19 (16)	O5—N3—C13—C12	4.41 (15)
N1—C2—C3—C4	178.92 (9)	O6—N3—C13—C12	−174.69 (9)
C1—C2—C3—Cl1	179.61 (8)	O5—N3—C13—C14	−176.79 (10)
N1—C2—C3—Cl1	−1.28 (14)	O6—N3—C13—C14	4.11 (14)
C2—C3—C4—C5	−0.26 (16)	C12—C13—C14—C15	−0.97 (16)
Cl1—C3—C4—C5	179.94 (8)	N3—C13—C14—C15	−179.70 (9)
C3—C4—C5—C6	0.12 (16)	C13—C14—C15—C16	0.76 (15)
C4—C5—C6—C1	0.48 (15)	C8—N2—C16—C15	−177.77 (10)
C2—C1—C6—C5	−0.90 (14)	C8—N2—C16—C11	1.38 (15)
C7—C1—C6—C5	−179.48 (9)	C14—C15—C16—N2	179.46 (9)
C2—C1—C7—O2	−1.69 (16)	C14—C15—C16—C11	0.30 (15)
C6—C1—C7—O2	176.84 (11)	C12—C11—C16—N2	179.64 (9)
C2—C1—C7—O1	179.50 (9)	C10—C11—C16—N2	−1.25 (15)
C6—C1—C7—O1	−1.96 (14)	C12—C11—C16—C15	−1.22 (15)
C16—N2—C8—C9	−0.26 (18)	C10—C11—C16—C15	177.89 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.87 (3)	1.76 (3)	2.6310 (14)	176 (3)
C8—H8···O2	0.95	2.53	3.2082 (16)	128
C8—H8···O6^{i}	0.95	2.41	3.2387 (15)	145
C14—H14···O4^{ii}	0.95	2.52	3.3226 (16)	142
C12—H12···O5^{iii}	0.95	2.37	3.2526 (16)	155

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

8-Hydroxyquinoliniumb 3-chloro-2-nitrobenzoate (III)

Crystal data

$C_7H_3ClNO_4{\cdot}C_9H_8NO$
$M_r = 346.73$
Monoclinic, $P2_1/n$
$a = 7.3409\ (5)$ Å
$b = 7.4689\ (4)$ Å
$c = 27.0427\ (14)$ Å
$\beta = 95.7158\ (19)°$
$V = 1475.33\ (15)$ Å^3
$Z = 4$

$F(000) = 712.00$
$D_x = 1.561$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71075$ Å
Cell parameters from 25520 reflections
$\theta = 3.0$–$30.0°$
$\mu = 0.29$ mm^{-1}
$T = 190$ K
Block, pale yellow
0.45 × 0.30 × 0.26 mm

Data collection

Rigaku R-AXIS RAPIDII diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.844$, $T_{max} = 0.927$
29560 measured reflections

4311 independent reflections
3937 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -37 \rightarrow 37$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.092$
$S = 1.06$
4311 reflections
225 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.86076 (4)	0.71237 (3)	0.49827 (2)	0.03111 (8)
O1	0.49893 (14)	0.57049 (11)	0.27915 (3)	0.0388 (2)
O2	0.50879 (12)	0.37292 (10)	0.34157 (3)	0.03253 (18)
O3	0.81650 (12)	0.34758 (10)	0.42238 (3)	0.03453 (19)
O4	0.56116 (14)	0.41075 (12)	0.45203 (3)	0.0406 (2)
O5	0.25608 (11)	0.64218 (10)	0.18109 (3)	0.03011 (17)
N1	0.68835 (12)	0.44696 (11)	0.42827 (3)	0.02456 (17)
N2	0.41002 (11)	0.32651 (12)	0.21056 (3)	0.02279 (16)
C1	0.63355 (12)	0.66248 (12)	0.35750 (3)	0.02025 (17)
C2	0.69708 (12)	0.62802 (12)	0.40684 (3)	0.01940 (16)
C3	0.77981 (12)	0.76019 (13)	0.43755 (3)	0.02089 (17)
C4	0.80144 (13)	0.93180 (13)	0.41926 (4)	0.02407 (18)
H4	0.857461	1.022784	0.440109	0.029*
C5	0.74011 (14)	0.96853 (13)	0.37014 (4)	0.02617 (19)
H5	0.754706	1.085267	0.357150	0.031*
C6	0.65741 (13)	0.83530 (13)	0.33982 (4)	0.02399 (18)
H6	0.616164	0.862693	0.306263	0.029*
C7	0.53938 (13)	0.52246 (13)	0.32319 (4)	0.02389 (18)
C8	0.47845 (15)	0.17222 (14)	0.22785 (4)	0.0276 (2)
H8	0.530731	0.164820	0.261364	0.033*
C9	0.47520 (16)	0.02008 (14)	0.19773 (4)	0.0314 (2)
H9	0.520396	−0.091226	0.210789	0.038*
C10	0.40556 (15)	0.03461 (14)	0.14900 (4)	0.0292 (2)
H10	0.404556	−0.067323	0.127964	0.035*
C11	0.33516 (13)	0.19899 (13)	0.12955 (4)	0.02402 (19)
C12	0.26151 (15)	0.22187 (16)	0.07953 (4)	0.0303 (2)
H12	0.260234	0.124767	0.056813	0.036*
C13	0.19225 (15)	0.38479 (17)	0.06420 (4)	0.0317 (2)

H13	0.145274	0.400180	0.030447	0.038*
C14	0.18881 (14)	0.53056 (16)	0.09724 (4)	0.0287 (2)
H14	0.138468	0.641773	0.085598	0.034*
C15	0.25798 (13)	0.51294 (13)	0.14634 (4)	0.02325 (18)
C16	0.33572 (12)	0.34640 (13)	0.16246 (3)	0.02087 (17)
H2	0.421 (2)	0.417 (2)	0.2315 (6)	0.044 (4)*
H5O	0.173 (3)	0.722 (2)	0.1717 (7)	0.049 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.04386 (16)	0.02719 (13)	0.02051 (12)	−0.00200 (9)	−0.00565 (9)	−0.00222 (8)
O1	0.0621 (6)	0.0278 (4)	0.0233 (4)	−0.0053 (4)	−0.0116 (3)	−0.0018 (3)
O2	0.0403 (4)	0.0219 (3)	0.0328 (4)	−0.0084 (3)	−0.0092 (3)	0.0002 (3)
O3	0.0389 (4)	0.0186 (3)	0.0436 (5)	0.0042 (3)	−0.0082 (3)	0.0010 (3)
O4	0.0546 (5)	0.0327 (4)	0.0368 (4)	−0.0104 (4)	0.0154 (4)	0.0047 (3)
O5	0.0389 (4)	0.0219 (3)	0.0282 (4)	0.0071 (3)	−0.0033 (3)	−0.0022 (3)
N1	0.0342 (4)	0.0172 (3)	0.0211 (4)	−0.0033 (3)	−0.0036 (3)	0.0004 (3)
N2	0.0267 (4)	0.0202 (4)	0.0214 (4)	0.0002 (3)	0.0019 (3)	−0.0013 (3)
C1	0.0217 (4)	0.0178 (4)	0.0206 (4)	0.0009 (3)	−0.0011 (3)	−0.0016 (3)
C2	0.0219 (4)	0.0152 (4)	0.0208 (4)	0.0006 (3)	0.0008 (3)	0.0002 (3)
C3	0.0228 (4)	0.0187 (4)	0.0206 (4)	0.0012 (3)	−0.0007 (3)	−0.0023 (3)
C4	0.0256 (4)	0.0165 (4)	0.0292 (5)	−0.0006 (3)	−0.0022 (3)	−0.0030 (3)
C5	0.0300 (5)	0.0161 (4)	0.0315 (5)	0.0002 (3)	−0.0013 (4)	0.0023 (3)
C6	0.0277 (4)	0.0194 (4)	0.0240 (4)	0.0016 (3)	−0.0016 (3)	0.0025 (3)
C7	0.0263 (4)	0.0205 (4)	0.0236 (4)	0.0007 (3)	−0.0040 (3)	−0.0032 (3)
C8	0.0318 (5)	0.0250 (5)	0.0259 (4)	0.0026 (4)	0.0025 (4)	0.0029 (4)
C9	0.0361 (5)	0.0219 (5)	0.0368 (5)	0.0044 (4)	0.0066 (4)	0.0014 (4)
C10	0.0321 (5)	0.0219 (4)	0.0348 (5)	−0.0013 (4)	0.0090 (4)	−0.0065 (4)
C11	0.0228 (4)	0.0249 (4)	0.0249 (4)	−0.0035 (3)	0.0053 (3)	−0.0040 (3)
C12	0.0300 (5)	0.0367 (6)	0.0246 (5)	−0.0062 (4)	0.0042 (4)	−0.0083 (4)
C13	0.0289 (5)	0.0450 (6)	0.0207 (4)	−0.0029 (4)	0.0002 (3)	−0.0003 (4)
C14	0.0272 (4)	0.0335 (5)	0.0251 (5)	0.0015 (4)	0.0012 (4)	0.0054 (4)
C15	0.0232 (4)	0.0229 (4)	0.0237 (4)	−0.0004 (3)	0.0024 (3)	0.0006 (3)
C16	0.0202 (4)	0.0212 (4)	0.0214 (4)	−0.0019 (3)	0.0030 (3)	−0.0010 (3)

Geometric parameters (Å, º)

Cl1—C3	1.7268 (10)	C5—C6	1.3898 (14)
O1—C7	1.2511 (12)	C5—H5	0.9500
O2—C7	1.2519 (13)	C6—H6	0.9500
O3—N1	1.2211 (12)	C8—C9	1.3969 (15)
O4—N1	1.2154 (12)	C8—H8	0.9500
O5—C15	1.3483 (12)	C9—C10	1.3695 (16)
O5—H5O	0.872 (19)	C9—H9	0.9500
N1—C2	1.4751 (12)	C10—C11	1.4132 (15)
N2—C8	1.3236 (13)	C10—H10	0.9500
N2—C16	1.3676 (12)	C11—C16	1.4154 (13)

N2—H2	0.880 (16)	C11—C12	1.4161 (14)
C1—C2	1.3930 (12)	C12—C13	1.3671 (17)
C1—C6	1.3935 (13)	C12—H12	0.9500
C1—C7	1.5180 (13)	C13—C14	1.4103 (16)
C2—C3	1.3902 (12)	C13—H13	0.9500
C3—C4	1.3887 (13)	C14—C15	1.3798 (14)
C4—C5	1.3870 (14)	C14—H14	0.9500
C4—H4	0.9500	C15—C16	1.4189 (13)

C15—O5—H5O	109.9 (12)	N2—C8—C9	121.23 (10)
O4—N1—O3	125.17 (9)	N2—C8—H8	119.4
O4—N1—C2	118.51 (9)	C9—C8—H8	119.4
O3—N1—C2	116.22 (9)	C10—C9—C8	118.66 (10)
C8—N2—C16	122.14 (9)	C10—C9—H9	120.7
C8—N2—H2	115.9 (11)	C8—C9—H9	120.7
C16—N2—H2	121.9 (11)	C9—C10—C11	120.97 (9)
C2—C1—C6	117.27 (8)	C9—C10—H10	119.5
C2—C1—C7	123.14 (8)	C11—C10—H10	119.5
C6—C1—C7	119.58 (8)	C10—C11—C16	117.63 (9)
C3—C2—C1	121.72 (8)	C10—C11—C12	123.44 (9)
C3—C2—N1	116.73 (8)	C16—C11—C12	118.92 (9)
C1—C2—N1	121.48 (8)	C13—C12—C11	119.49 (10)
C4—C3—C2	120.08 (9)	C13—C12—H12	120.3
C4—C3—Cl1	119.26 (7)	C11—C12—H12	120.3
C2—C3—Cl1	120.64 (7)	C12—C13—C14	121.63 (10)
C5—C4—C3	119.08 (9)	C12—C13—H13	119.2
C5—C4—H4	120.5	C14—C13—H13	119.2
C3—C4—H4	120.5	C15—C14—C13	120.53 (10)
C4—C5—C6	120.29 (9)	C15—C14—H14	119.7
C4—C5—H5	119.9	C13—C14—H14	119.7
C6—C5—H5	119.9	O5—C15—C14	125.04 (9)
C5—C6—C1	121.56 (9)	O5—C15—C16	116.43 (8)
C5—C6—H6	119.2	C14—C15—C16	118.52 (9)
C1—C6—H6	119.2	N2—C16—C11	119.30 (9)
O1—C7—O2	126.78 (9)	N2—C16—C15	119.84 (8)
O1—C7—C1	115.77 (9)	C11—C16—C15	120.85 (9)
O2—C7—C1	117.44 (8)		

C6—C1—C2—C3	0.47 (14)	C16—N2—C8—C9	−1.11 (16)
C7—C1—C2—C3	−178.81 (9)	N2—C8—C9—C10	2.40 (16)
C6—C1—C2—N1	−176.32 (8)	C8—C9—C10—C11	−1.12 (16)
C7—C1—C2—N1	4.41 (14)	C9—C10—C11—C16	−1.33 (15)
O4—N1—C2—C3	85.64 (11)	C9—C10—C11—C12	−179.99 (10)
O3—N1—C2—C3	−91.03 (11)	C10—C11—C12—C13	178.41 (10)
O4—N1—C2—C1	−97.42 (11)	C16—C11—C12—C13	−0.23 (14)
O3—N1—C2—C1	85.91 (11)	C11—C12—C13—C14	−1.28 (16)
C1—C2—C3—C4	−0.17 (14)	C12—C13—C14—C15	0.76 (16)
N1—C2—C3—C4	176.76 (8)	C13—C14—C15—O5	−177.90 (10)

C1—C2—C3—Cl1	−178.87 (7)	C13—C14—C15—C16	1.27 (15)
N1—C2—C3—Cl1	−1.94 (12)	C8—N2—C16—C11	−1.46 (14)
C2—C3—C4—C5	−0.23 (14)	C8—N2—C16—C15	177.62 (9)
Cl1—C3—C4—C5	178.49 (8)	C10—C11—C16—N2	2.62 (13)
C3—C4—C5—C6	0.32 (15)	C12—C11—C16—N2	−178.66 (9)
C4—C5—C6—C1	−0.01 (15)	C10—C11—C16—C15	−176.45 (9)
C2—C1—C6—C5	−0.38 (14)	C12—C11—C16—C15	2.27 (14)
C7—C1—C6—C5	178.92 (9)	O5—C15—C16—N2	−2.60 (13)
C2—C1—C7—O1	−176.23 (9)	C14—C15—C16—N2	178.16 (9)
C6—C1—C7—O1	4.51 (14)	O5—C15—C16—C11	176.47 (8)
C2—C1—C7—O2	4.37 (14)	C14—C15—C16—C11	−2.77 (14)
C6—C1—C7—O2	−174.89 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.880 (16)	1.776 (16)	2.6355 (12)	164.7 (14)
O5—H5*O*···O2^{i}	0.872 (19)	1.756 (19)	2.6247 (12)	173.2 (19)
C4—H4···O3^{ii}	0.95	2.49	3.1082 (12)	123

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