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Role of pK_a in establishing the crystal structures of six hydrogen-bonded compounds of 4-methylquinoline with different isomers of chloro- and nitro-substituted benzoic acids

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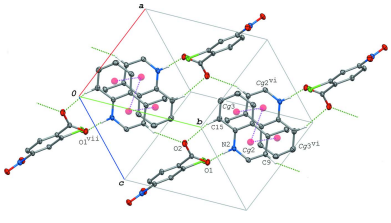
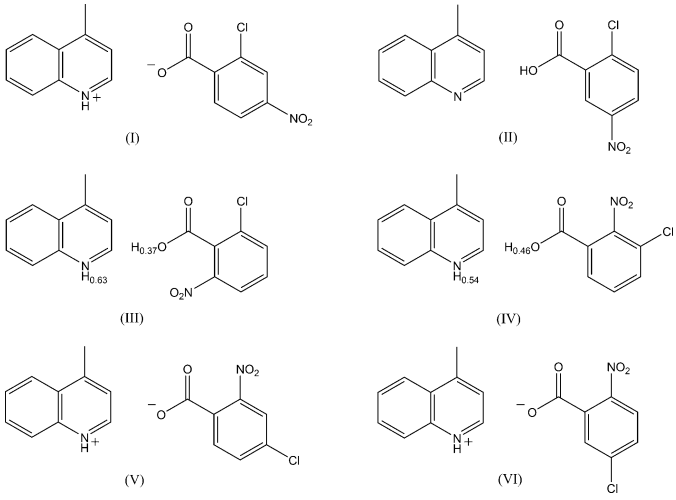
The structures of the six hydrogen-bonded 1:1 compounds of 4-methylquinoline ($C_{10}H_9N$) with chloro- and nitro-substituted benzoic acids ($C_7H_4ClNO_4$), namely, 4-methylquinolinium 2-chloro-4-nitrobenzoate, $C_{10}H_{10}N^+\cdot C_7H_3ClNO_4^-$, (I), 4-methylquinoline–2-chloro-5-nitrobenzoic acid (1/1), $C_{10}H_9N\cdot C_7H_4ClNO_4$, (II), 4-methylquinolinium 2-chloro-6-nitrobenzoate, $C_{10}H_{9.63}N^{0.63+}\cdot C_7H_{3.37}ClNO_4{}^{0.63-}$, (III), 4-methylquinolinium 3-chloro-2-nitrobenzoate, $C_{10}H_{9.54}N^{0.54+}\cdot C_7H_{3.46}ClNO_4{}^{0.54-}$, (IV), 4-methylquinolinium 4-chloro-2-nitrobenzoate, $C_{10}H_{10}N^+\cdot C_7H_3ClNO_4^-$, (V), and 4-methylquinolinium 5-chloro-2-nitrobenzoate, $C_{10}H_{10}N^+\cdot C_7H_3ClNO_4^-$, have been determined at 185–190 K. In each compound, the acid and base molecules are linked by a short hydrogen bond between a carboxy (or carboxylate) O atom and an N atom of the base. The O···N distances are 2.5652 (14), 2.556 (3), 2.5485 (13), 2.5364 (13), 2.5568 (13) and 2.5252 (11) Å, respectively, for compounds (I)–(VI). In the hydrogen-bonded acid–base units of (III) and (IV), the H atoms are each disordered over two positions with O site:N site occupancies of 0.37 (3):0.63 (3) and 0.46 (3):0.54 (4), respectively, for (III) and (IV). The H atoms in the hydrogen-bonded units of (I), (V) and (VI) are located at the N-atom site, while the H atom in (II) is located at the O-atom site. In all the crystals of (I)–(VI), π–π stacking interactions between the quinoline ring systems and C—H···O hydrogen bonds are observed. Similar layer structures are constructed in (IV)–(VI) through these interactions together with π–π interactions between the benzene rings of the adjacent acid molecules. A short Cl···Cl contact and an N—O···π interaction are present in (I), while a C—H···Cl hydrogen bond and a π–π interaction between the benzene ring of the acid molecule and the quinoline ring system in (II), and a C—H···π interaction in (III) are observed. Hirshfeld surfaces for the title compounds mapped over d_{norm} and shape index were generated to visualize the weak intermolecular interactions.



1. Chemical context

The properties of hydrogen bonds formed between organic acids and organic bases depend on the pK_a values of the acids and bases as well as the intermolecular interactions in the crystals. In our ongoing studies of crystal structures for the system of quinoline derivatives–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 (Gotoh & Ishida, 2009), and three compounds of 6-methylquinoline with 2-chloro-4-nitrobenzoic acid, 3-chloro-2-nitrobenzoic acid and 4-chloro-2-nitrobenzoic acid (Gotoh & Ishida, 2020) have a short double-well O—H···N/O···H—N hydrogen bond

between the carboxy O atom and the aromatic N atom. The ΔpK_a [pK_a(base) – pK_a(acid)] values of these compounds are in the range 2.93–3.38. Although the pK_a value of 4-methylquinoline is 5.66, which is slight larger than quinoline (pK_a = 4.90) and 6-methylquinoline (pK_a = 5.20), the system of 4-methylquinoline–chloro- and nitro-substituted benzoic acids is an attractive candidate for studying short hydrogen bonds and also weak intermolecular interactions. We report here crystal structures of six hydrogen-bonded compounds, namely, 4-methylquinolinium 2-chloro-4-nitrobenzoate, (I), 2-chloro-5-nitrobenzoic acid–4-methylquinoline, (II), 2-chloro-6-nitrobenzoic acid–4-methylquinoline, (III), 3-chloro-2-nitrobenzoic acid–4-methylquinoline, (IV), 4-methylquinolinium 4-chloro-2-nitrobenzoate, (V), and 4-methylquinolinium 5-chloro-2-nitrobenzoate, (VI). The ΔpK_a values are 3.62, 3.44, 4.04, 3.84, 3.69 and 3.80, respectively, for (I)–(VI) (Table 1).



2. Structural commentary

The molecular structures of compounds (I)–(VI) are shown in Fig. 1. In each compound, the acid and base molecules are linked by a short hydrogen bond between the O atom of the carboxy (or carboxylate) group and the N atom of the base with O···N distances of 2.5652 (14), 2.556 (3), 2.5485 (13), 2.5364 (13), 2.5568 (13) and 2.5252 (11) Å, respectively, for compounds (1)–(VI) (Tables 2–7). In (III) and (IV), the H atoms in these hydrogen bonds are each disordered over two sites with O site:N site occupancies of 0.37 (3):0.63 (3) and 0.46 (3):0.54 (3), respectively, for (III) and (IV). In (I), (V) and (VI), the H atoms in the hydrogen bonds are located at the N site, while in (II) they are located at the O-atom site. In addition, a weak C—H···O hydrogen bond is observed in each of the acid–base units of (I) and (VI) (C15—H15···O2; Tables 2 and 7). The nitro group in (III) is disordered over two orientations around the N1—C6 bond with occupancies of 0.46 (3) and 0.54 (3).

The dihedral angles made by the benzene C1–C6 ring, the carboxy/carboxylate O1/C7/O2 plane and the nitro O3/N1/O4 plane of the acid, and the quinoline N2/C8–C16 ring system of the base in each hydrogen-bonded acid-base unit of (I)–(VI) are summarized in Table 1, together with those in compounds of other quinoline derivatives with chloro- and nitro-substituted benzoic acids, which contain similar hydrogen-bonded acid-base units (Gotoh & Ishida, 2009, 2011, 2019*a*,*b*, 2020). The H-atom position in the short hydrogen bond and the ΔpK_a value of each compound are also given in Table 1. In each acid–base unit of compounds of (I) and (III)–(VI), the acid C1–C6 ring and the quinoline N2/C8–C16 ring system are considerably twisted with respect to each other with dihedral angles of 58.90 (4)–69.15 (5)°, which are much larger than those of other compounds. In the acid–base unit of (II), the acid ring and the quinoline ring system are slightly twisted by 13.18 (10)°, which is still larger compared with those of quinoline–2-chloro-5-nitrobenzoic acid [1.92 (4)°] and 6-methylquinoline–2-chloro-5-nitrobenzoic acid [2.15 (4)°]. These results suggest that the methyl group substituted to the quinoline ring system at the 4-position has an effect on the molecular packing, which prevents the aromatic rings of the acid and base lying in the same plane in the crystal.

In all the compounds of 3-chloro-2-nitrobenzoic acid and 4-chloro-2-nitrobenzoic acid, the nitro O3/N1/O4 group is approximately perpendicular to the benzene C1–C6 ring with dihedral angles of 74.4 (3)–88.54 (13)°, while in the 2-chloro-6-nitrobenzoic acid molecule of compound (III), where the nitro group and the Cl atom are adjacent to the carboxy group, the carboxy O1/C7/O2 group is almost perpendicular to the benzene ring with a dihedral angle of 84.53 (16)°. In the compounds of 5-chloro-2-nitrobenzoic acid, the nitro and carboxy/carboxylate groups are both twisted by 33.31 (13)–57.13 (11)° out of the benzene ring plane. These large twists are mainly ascribable to intramolecular steric repulsion between the nitro group and the carboxy/carboxylate group.

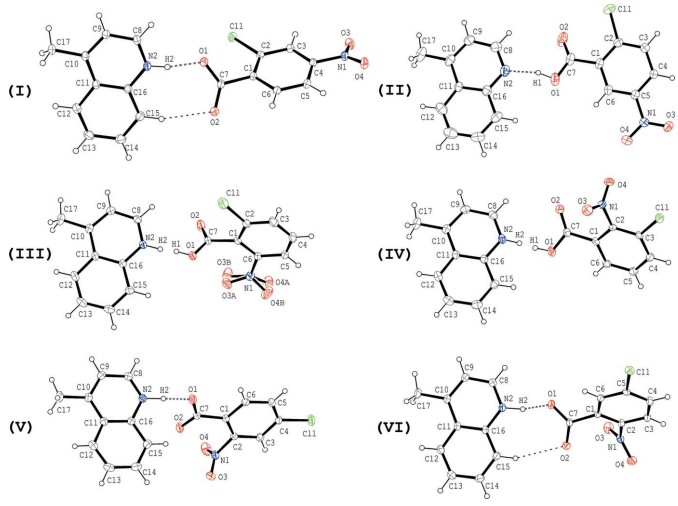


Figure 1
Molecular structures of the title compounds (I)–(VI), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. In the hydrogen bonds between the carboxy O atom and the base N atom of compounds (III) and (IV), the H atoms are each disordered over two positions. The nitro group in (III) is disordered around the N1—C6 bond. Dashed lines in (I), (II), (V) and (VI) indicate the N—H···O, O—H···N and C—H···O hydrogen bonds.

Table 1
Dihedral angles in the acid-base unit (°), hydrogen position and ΔpK_a.

A, *B*, *C*, *D* and *E* are the dihedral angles between the C1–C6 ring and the N2/C8–C16 ring system, between the O1/C7/O2 plane and the N2/C8–C16 ring system, between the C1–C6 ring and the O1/C7/O2 plane, between the C1–C6 ring and the O3/N1/O4 plane, and between the N2/C8–C16 ring system and the nitro group attached to it, respectively.

	A	*B*	*C*	*D*	*E*	H-atom site	ΔpK_a
2-Chloro-4-nitrobenzoic acid							
(I)	69.15 (5)	26.60 (16)	51.29 (17)	17.77 (14)		N	3.62
a	3.15 (7)	43.0 (2)	39.9 (2)	12.2 (2)		O	2.86
b	1.11 (4)	28.59 (12)	29.36 (12)	8.24 (11)		O/N	3.16
c	3.94 (17)	7.5 (5)	4.3 (5)	2.5 (5)	36.2 (5)	O	0.76
2-Chloro-5-nitrobenzoic acid							
(II)	13.81 (10)	14.1 (3)	24.6 (3)	9.7 (3)		O	3.44
a	1.92 (4)	22.48 (14)	21.02 (14)	0.50 (13)		O	2.68
b	2.15 (4)	24.51 (15)	22.63 (15)	0.77 (14)		O	2.98
2-Chloro-6-nitrobenzoic acid							
(III)	61.05 (5)	35.42 (16)	84.53 (16)	21.7 (8), 14.7 (14)		O/N	4.04
3-Chloro-2-nitrobenzoic acid							
(IV)	59.45 (4)	37.30 (13)	22.39 (13)	75.20 (13)		O/N	3.84
a	4.71 (5)	6.18 (16)	9.22 (16)	84.97 (13)		O/N	3.08
b	14.50 (5)	12.55 (18)	3.14 (18)	85.04 (11)		O/N	3.38
c	2.59 (4)	9.95 (12)	9.45 (12)	86.14 (13)	31.67 (11)	O	0.98
d	10.99 (4)	12.08 (13)	2.40 (13)	88.54 (13)	5.58 (12)	O	1.42
4-Chloro-2-nitrobenzoic acid							
(V)	61.21 (5)	67.42 (14)	10.22 (14)	80.76 (15)		N	3.69
a	31.65 (4)	18.77 (13)	13.71 (13)	76.44 (17)		O/N	2.93
b	30.39 (9)	21.7 (3)	16.4 (3)	74.4 (3)		O/N	3.23
5-Chloro-2-nitrobenzoic acid							
(VI)	58.90 (4)	23.54 (13)	35.43 (13)	57.13 (11)		N	3.80
a	54.43 (5)	5.41 (15)	49.95 (15)	33.31 (13)		O/N	3.04
c	37.37 (6)	2.9 (2)	40.3 (2)	47.12 (19)	11.3 (2)	O	0.94

Notes: *a*: quinoline compounds (Gotoh & Ishida, 2009, 2011), *b*: 6-methylquinoline compounds (Gotoh & Ishida, 2020), *c*: 5-nitroquinoline compounds (Gotoh & Ishida, 2019*a*,*b*) and *d*: 6-nitroquinoline–3-chloro-2-nitrobenzoic acid (Gotoh & Ishida, 2019*a*).

The correlation between the H-atom position in the short hydrogen bond and the ΔpK_a value is observed for each system of quinoline and 6-methylquinoline compounds, while for the title compounds (I)–(VI) this correlation is somewhat low.

3. Supramolecular features

In all the crystals of (I)–(VI), π–π interactions between the quinoline ring systems, related by an inversion centre to each other, are observed. The centroid–centroid distances between the quinoline ring systems, namely, *Cg*2···*Cg*2, *Cg*2···*Cg*3 and *Cg*3···*Cg*3, are 3.4323 (7)–3.7751 (8), 3.5878 (7)–3.9304 (9) and 3.7719 (8)–3.9227 (9) Å, respectively, where *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings of the quinoline ring system, respectively. The base molecules in the crystals of (I) and (II) form dimeric units *via* these π–π interactions, while in (III)–(VI) inversion-related base molecules are alternately stacked in column-like structures. On the other hand, π–π interactions between the inversion-related acid molecules are only observed in crystals (IV)–(VI); the centroid-centroid distances, *Cg*1···*Cg*1, are 3.5702 (7)–3.8602 (6) Å, where *Cg*1 is the centroid of the C1–C6 ring. Detailed supramolecular features in the crystals formed through these π–π interactions combined with other weak intermolecular interactions are described below.

In the crystal of (I), the hydrogen-bonded acid–base units, which are related by an inversion centre to each other, are linked into a centrosymmetric dimeric unit *via* π–π interactions between the quinoline ring systems [$Cg2\cdots Cg2^{vi}$ = 3.7318 (7) Å and $Cg2\cdots Cg3^{vi}$ = 3.5955 (7) Å; symmetry code: (vi) $-x+1, -y+2, -z+1$]. The dimeric units are further linked *via* a C—H···O hydrogen bond (C9—H9···O2^{iii}; symmetry code as given in Table 2), forming a ribbon structure propagating along the *b*-axis direction (Fig. 2). The ribbons are

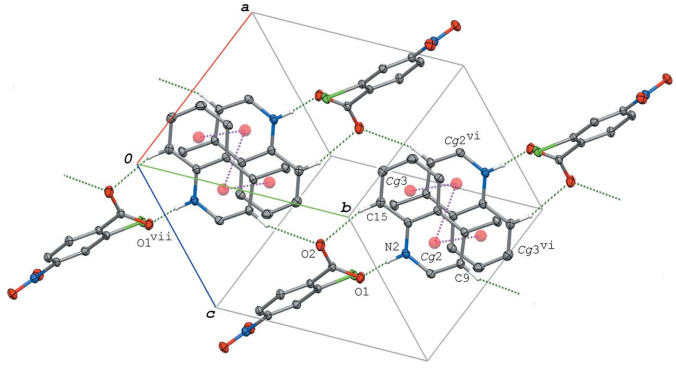


Figure 2
A packing diagram of (I), showing the ribbon structure running along the *b*-axis direction formed *via* the N—H···O and C—H···O hydrogen bonds (green dashed lines) and π–π interactions (magenta dashed lines). H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (vi) $-x+1, -y+2, -z+1$; (vii) $x, y-1, z$.]

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

*Cg*3 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.900 (19)	1.678 (19)	2.5652 (14)	167.7 (18)
C6—H6···O2^{i}	0.95	2.39	3.3066 (16)	163
C8—H8···O3^{ii}	0.95	2.56	3.4199 (16)	151
C9—H9···O2^{iii}	0.95	2.44	3.3360 (16)	158
C15—H15···O2	0.95	2.36	3.2835 (17)	163
N1—O3···*Cg*3^{iv}	1.22 (1)	3.26 (1)	4.3171 (13)	145 (1)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.91 (7)	1.68 (7)	2.556 (3)	162 (7)
C3—H3···O4^{i}	0.95	2.40	3.280 (4)	154
C4—H4···O3^{ii}	0.95	2.54	3.188 (3)	126
C17—H17*A*···O2^{iii}	0.98	2.57	3.479 (4)	155
C17—H17*C*···Cl1^{iv}	0.98	2.81	3.535 (4)	131

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

connected into a layer lying parallel to the (101) plane (Fig. 3) *via* another C—H···O hydrogen bond (C8—H8···O3^{ii}; Table 2). In the layer, the acid molecules are arranged in an antiparallel manner with *Cg*1···*Cg*1^{ii} = 4.0685 (7) Å. Between the layers, an N—O···π interaction (N1—O3···*Cg*3^{iv}; Table 2), a short Cl···Cl contact [Cl1···Cl1^{v} = 3.3391 (5) Å; symmetry code: (v) $-x+1, -y+1, -z+2$] and a C—H···O hydrogen bond (C6—H6···O2^{i}; Table 2) are observed.

In the crystal of (II), the acid–base units are linked *via* C—H···O hydrogen bonds (C3—H3···O4^{i} and C4—H4···O3^{ii}; symmetry codes as given in Table 3), forming a tape structure propagating along the *a*-axis direction (Fig. 4). The tapes are further linked into a three-dimensional network through C—H···O and C—H···Cl hydrogen bonds (C17—H17*A*···O2^{iii} and C17—H17*C*···Cl1^{iv}; Table 3). In addition, π–π interactions are observed between the acid and base aromatic rings and between the base ring systems; the centroid–centroid distances are 3.8339 (16), 3.5056 (15) and 3.8381 (15) Å, respectively, for *Cg*1···*Cg*3^{v}, *Cg*2···*Cg*2^{vi} and *Cg*2···*Cg*3^{vi} [symmetry codes: (v) $x, y+1, z$; (vi) $-x+1, -y+1, -z$]. The acid–base units are linked *via* these π–π interactions, forming a ribbon structure along the *b*-axis direction (Fig. 5).

In the crystal of (III), the acid–base units are linked by C—H···O hydrogen bonds and a C—H···π interaction (C5—H5···O1^{i}, C13—H13···O2^{ii} and C14—H14···*Cg*1^{ii}; symmetry codes as in Table 4), forming a ribbon structure along the *c*-

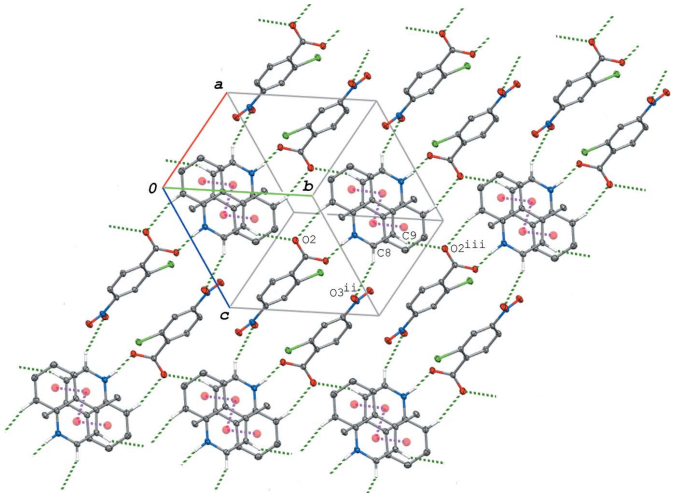


Figure 3
A packing diagram of (I), showing a layer structure parallel to (101) formed *via* the N—H···O and C—H···O hydrogen bonds (green dashed lines) and π–π interactions (magenta dashed lines). H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*1 is the centroid of the C1–C6 ring. [Symmetry codes: (ii) $-x, -y+1, -z+2$; (iii) $x, y+1, z$.]

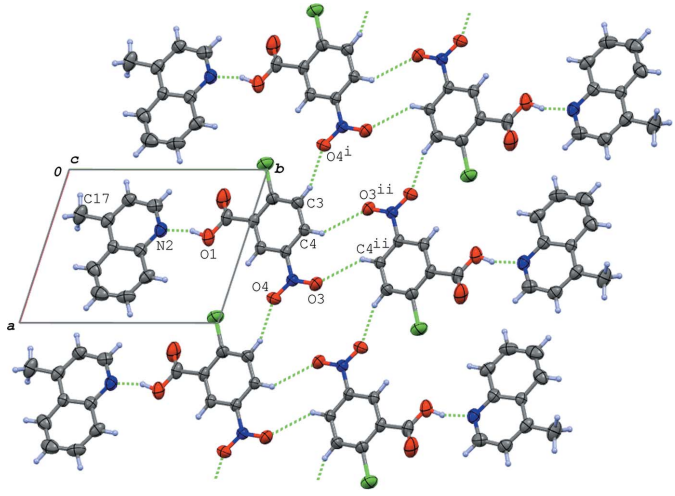


Figure 4
A packing diagram of (II) viewed along the *c* axis, showing the tape structure formed *via* the C—H···O hydrogen bonds (green dashed lines). [Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+3, -z+1$.]

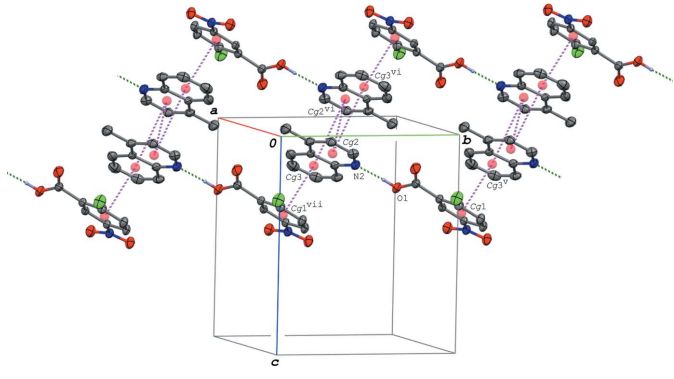


Figure 5
A packing diagram of (II), showing the ribbon structure running along the *b*-axis direction formed *via* the O—H···N hydrogen bonds (green dashed lines) and π–π interactions (magenta dashed lines). H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (v) $x, y+1, z$; (vi) $-x+1, -y+1, -z$; (vii) $x, y-1, z$.]

Table 4
Hydrogen-bond geometry (Å, °) for (III).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84 (4)	1.71 (4)	2.5485 (13)	177 (6)
N2—H2···O1	0.89 (2)	1.66 (2)	2.5485 (13)	176 (2)
C5—H5···O1^{i}	0.95	2.49	3.1489 (15)	126
C13—H13···O2^{ii}	0.95	2.36	3.2889 (17)	165
C14—H14···*Cg*1^{ii}	0.95	2.89	3.6596 (15)	138

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

axis direction (Fig. 6). The base molecules are further stacked in a column along the *a* axis *via* π–π interactions between the

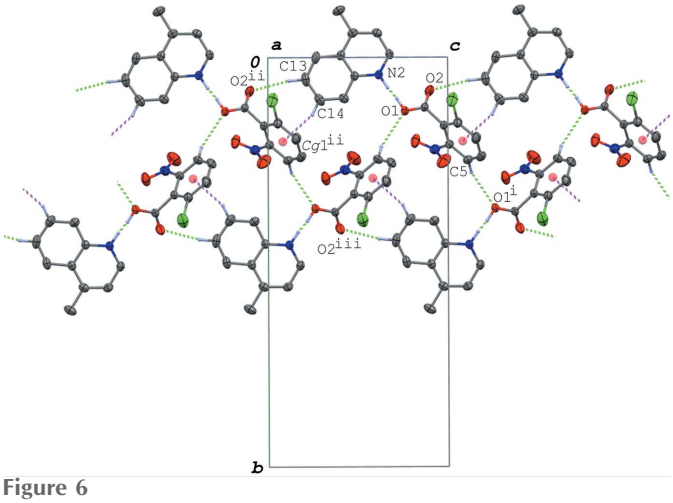


Figure 6
A partial packing diagram of (III) viewed along the *a* axis, showing the ribbon structure formed by the O—H···N/O···H—N and C—H···O hydrogen bonds (green dashed lines), and C—H···π interactions (magenta dashed lines). H atoms not involved in the intermolecular interactions and the disordered O atoms of the minor component of the nitro group are omitted for clarity. [Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, y, z-1$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.]

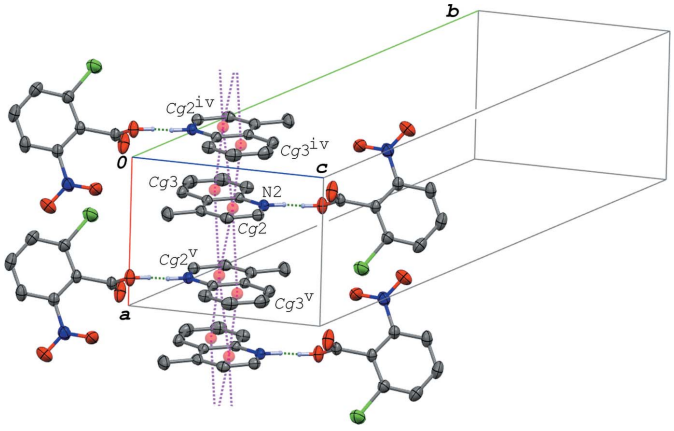


Figure 7
A packing diagram of (III), showing the column structure of the base molecules formed *via* the π–π interactions (magenta dashed lines). H atoms not involved in the O—H···N/O···H—N hydrogen bonds (green dashed lines) and the disordered O atoms of the minor component of the nitro group are omitted for clarity. *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (iv) $-x, -y, -z+1$; (v) $-x+1, -y, -z+1$.]

Table 5
Hydrogen-bond geometry (Å, °) for (IV).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84 (3)	1.70 (3)	2.5364 (13)	175 (3)
N2—H2···O1	0.89 (2)	1.65 (2)	2.5364 (13)	175 (3)
C6—H6···O3^{i}	0.95	2.59	3.4705 (14)	155
C9—H9···O2^{ii}	0.95	2.41	3.1739 (15)	137
C17—H17*C*···O2^{iii}	0.98	2.47	3.4155 (17)	162

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

quinoline ring systems (Fig. 7), and thus the hydrogen-bonded acid–base units form a three-dimensional network. The centroid–centroid distances are 3.4323 (7), 3.4850 (7), 3.6810 (7) and 3.5878 (7) Å, respectively, for *Cg*2···*Cg*2^{iv}, *Cg*2···*Cg*2^{v}, *Cg*2···*Cg*3^{iv} and *Cg*2···*Cg*3^{v} [symmetry codes: (iv) $-x, -y, -z+1$; (v) $-x+1, -y, -z+1$].

In the crystal of (IV), the hydrogen-bonded acid–base units are linked into a ribbon structure along the *a*-axis direction (Fig. 8) *via* C—H···O hydrogen bonds (C6—H3···O3^{i} and C17—H17*C*···O2^{iii}; symmetry codes as in Table 5) and π–π interactions between the quinoline ring systems. The centroid–centroid distances are 3.5037 (8), 3.6022 (8) and 3.9227 (9) Å, respectively, for *Cg*2···*Cg*2^{iii}, *Cg*2···*Cg*3^{iv} and *Cg*3···*Cg*3^{iv} [symmetry codes: (iii) $-x+1, -y, z+1$; (iv) $-x, -y, -z+1$]. The ribbons are further linked into a layer parallel to the (011) plane (Fig. 9) *via* a π–π interaction between the acid rings with a centroid–centroid distance (*Cg*1···*Cg*1^{v}) of 3.6685 (8) Å

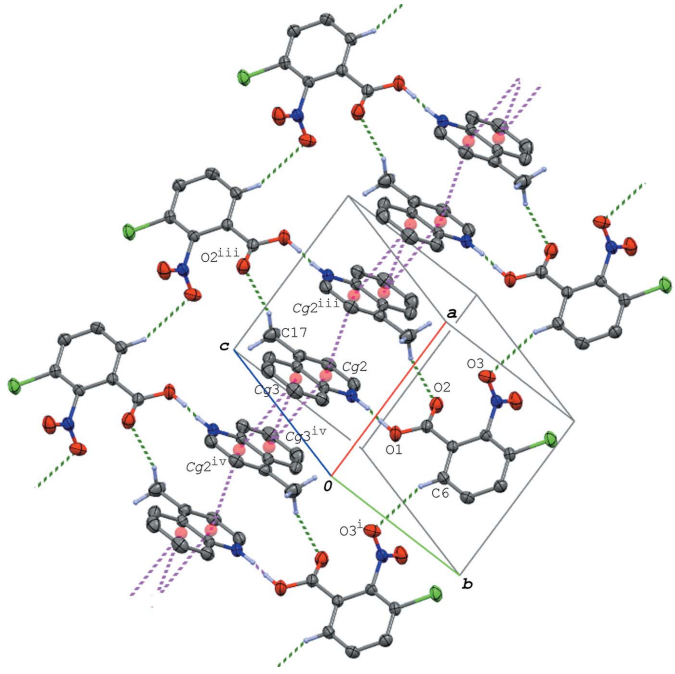


Figure 8
A packing diagram of (IV), showing the ribbon structure formed *via* the π–π interactions (magenta dashed lines), and the O—H···N/O···H—N and C—H···O hydrogen bonds (green dashed lines). Except for the methyl group, H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (i) $x-1, y, z$; (iii) $-x+1, -y, -z+1$; (iv) $-x, -y, -z+1$.]

Table 6
Hydrogen-bond geometry (Å, °) for (V).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	1.06 (2)	1.50 (2)	2.5568 (13)	179 (4)
C8—H8···O2^{i}	0.95	2.56	3.2779 (16)	132
C12—H12···O2^{ii}	0.95	2.52	3.3391 (18)	144

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

[symmetry code: (v) $-x+1, -y+1, -z$]. The layers are linked by a C—H···O hydrogen bond (C9—H9···O2^{ii}; Table 5).

In the crystal of (V), the acid and base molecules are arranged in a similar manner to those in (IV) as shown in Figs. 8 and 9. The hydrogen-bonded acid–base units in (V) are linked into a ribbon structure along the *a*-axis direction (Fig. 10) *via* a C—H···O hydrogen bond (C12—H12···O2^{ii}; symmetry code as in Table 6) and π–π interactions between the quinoline ring systems. The ribbons are further linked into a layer parallel to the (011) plane *via* a π–π interaction between the acid rings. The centroid–centroid distances of the π–π interactions are 3.5702 (7), 3.7751 (8), 3.7870 (8), 3.9304 (9) and 3.7719 (8) Å, respectively, for $Cg1\cdots Cg1^{vi}$, $Cg2\cdots Cg2^{iii}$, $Cg2\cdots Cg3^{ii}$, $Cg2\cdots Cg3^{iii}$ and $Cg3\cdots Cg3^{ii}$ [symmetry codes: (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+2$]. Between the layers, a C—H···O hydrogen bond is observed (C8—H8···O2^{i}; Table 6).

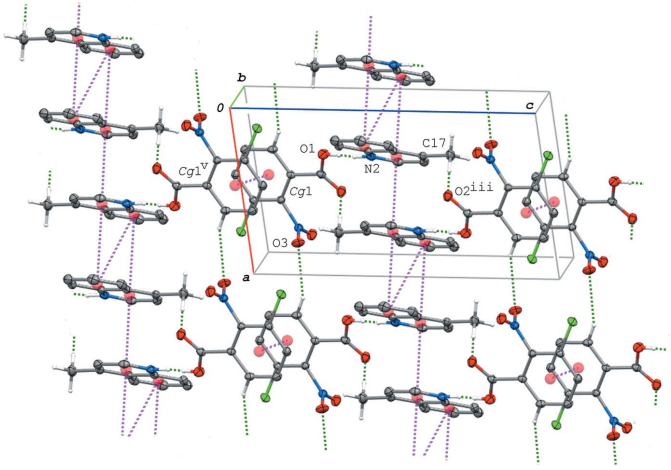


Figure 9
A packing diagram of (IV), showing the layer structure formed *via* the π–π interactions (magenta dashed lines), and the O—H···N/O···H—N and C—H···O hydrogen bonds (green dashed lines). Except for the methyl group, H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*1 is the centroid of the C1–C6 ring. [Symmetry codes: (iii) $-x+1, -y, -z+1$; (v) $-x+1, -y+1, -z+1$.]

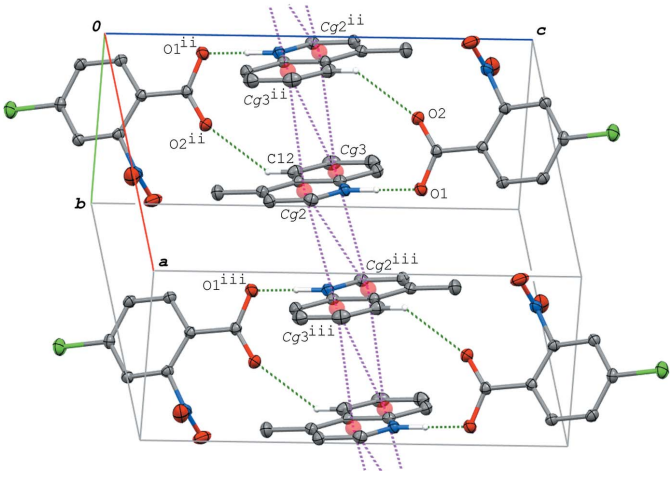


Figure 10
A packing diagram of (V), showing the ribbon structure formed *via* the π–π interactions (magenta dashed lines), and the N—H···O and C—H···O hydrogen bonds (green dashed lines). H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$.]

Table 7
Hydrogen-bond geometry (Å, °) for (VI).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	1.03 (2)	1.52 (2)	2.5252 (11)	165 (2)
C9—H9···O2^{i}	0.95	2.34	3.2856 (13)	171
C12—H12···O3^{ii}	0.95	2.58	3.5065 (14)	166
C15—H15···O2	0.95	2.57	3.4583 (13)	155
C17—H17*A*···O2^{ii}	0.98	2.41	3.3524 (16)	160

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

Although the crystal system of (VI) (monoclinic, *C*2/*c*) is different from those of (IV) and (V) (triclinic, $P\overline{1}$), the molecules in the crystal of (VI) are arranged in a similar manner to those in (IV) and (V). The acid–base units, which are related by an inversion centre to each other, are linked together *via* π–π interactions between the quinoline ring systems and C—H···O hydrogen bonds [$Cg2\cdots Cg3^{ii}$ = 3.8048 (7) Å; C12—H12···O3^{ii} and C17—H17*A*···O2^{ii}; symmetry code as given in Table 7], forming a centrosymmetric dimeric unit. The dimeric units are further linked into a ribbon structure along the *b*-axis direction (Fig. 11) *via* other π–π interactions between the quinoline ring systems with $Cg2\cdots Cg2^{iii}$ = 3.4710 (6) Å and $Cg2\cdots Cg3^{iii}$ = 3.8841 (7) Å [symmetry code: (iii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$]. The ribbons are

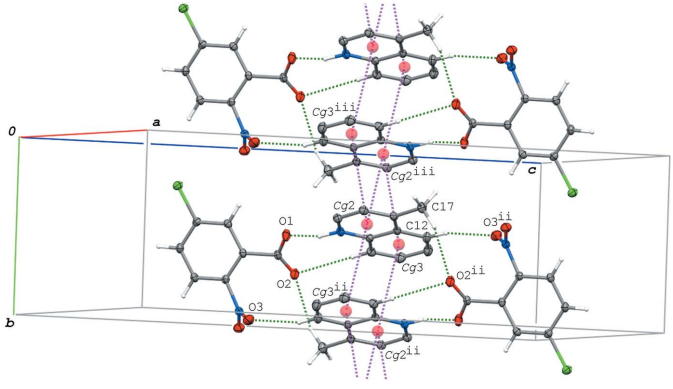


Figure 11
A packing diagram of (VI), showing the ribbon structure formed *via* the π–π interactions (magenta dashed lines), and the N—H···O and C—H···O hydrogen bonds (green dashed lines). H atoms not involved in the hydrogen bonds are omitted for clarity. *Cg*2 and *Cg*3 are the centroids of the N2/C8–C11/C16 and C11–C16 rings, respectively. [Symmetry codes: (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$; (iii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$.]

connected into a layer parallel to (10$\bar{1}$) *via* a weak π–π interaction between adjacent acid rings with $Cg1\cdots Cg1^{iv}$ = 3.8602 (6) Å [symmetry code: (iv) $-x+1, y, -z+\frac{1}{2}$]. Between the layers, a C—H···O hydrogen bond (C9—H9···O2^{i}; Table 7) is observed.

Hirshfeld surfaces for compounds (I)–(VI) mapped over d_{norm} and shape index (Turner *et al.*, 2017; McKinnon *et al.*, 2004, 2007) are shown in Fig. 12. The π–π interactions are indicated by blue and red triangles on the shape-index surfaces (white circles in Fig. 12). On all the surfaces of the quinoline ring systems except one of the back view of (II), the π–π interactions between the quinoline ring systems are observed. On the surfaces of both acid and base molecules of the back view of (II), the π–π interactions between the acid ring and the quinoline ring system are shown, while the interactions between the acid rings are observed on the acid ring surfaces of (IV)–(VI). The C—H···O interactions in (I)–(VI) are indicated by faint-red spots on the d_{norm} surfaces (black arrows). In addition, the short Cl···Cl contact and the N—O···π interaction in (I), and the C—H···Cl interaction in (II) are shown as faint-red spots on the d_{norm} surfaces (green, magenta and cyan arrows, respectively). On the shape-index surfaces of (I) and (III), large red areas corresponding to the N—O···π and C—H···π interactions (magenta and violet arrows, respectively) are observed.

4. Database survey

A search of the Cambridge Structural Database (CSD Version 5.42, last update September 2021; Groom *et al.*, 2016) for organic co-crystals/salts of 4-methylquinoline with carboxylic acid derivatives showed one structure, namely, 4-methylquinoline hydrogensquarate (CSD refcode GUKWAN; Kotov *et al.*, 2018). A search for organic co-crystals/salts of 2-chloro-4-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, 2-chloro-6-nitrobenzoic acid, 3-chloro-2-nitrobenzoic acid, 4-chloro-2-nitrobenzoic acid and 5-chloro-2-nitrobenzoic acid gave 76, 19, 0, 11, 15 and 11 structures, respectively. Limiting the search for

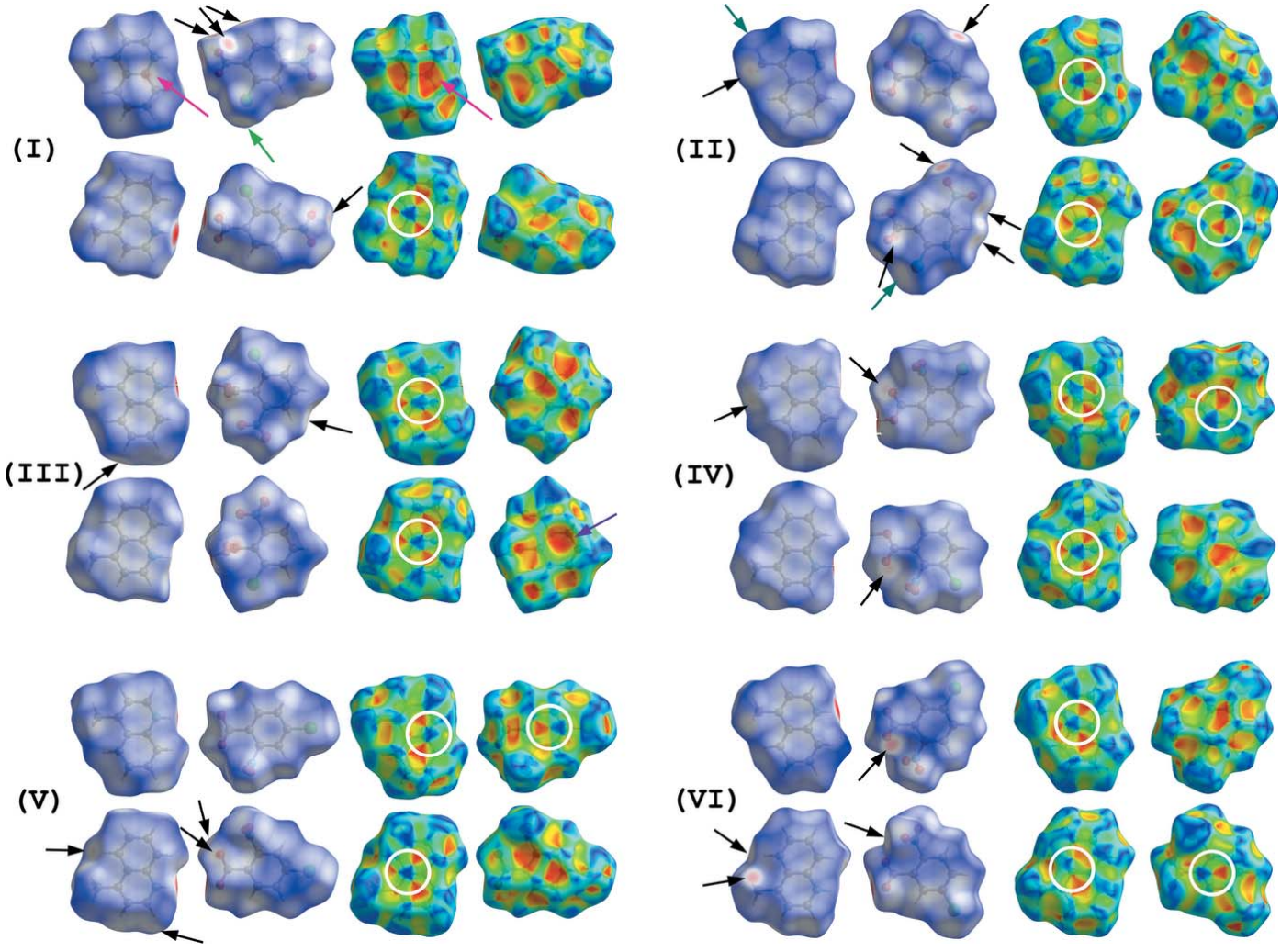


Figure 12
Hirshfeld surfaces [front (top) and back (bottom) views] for compounds (I)–(VI) mapped over d_{norm} and shape index. Each surface is viewed approximately perpendicular to the molecular plane. The π–π interactions are shown by white circles, and the Cl···Cl contacts, the C—H···O, C—H···Cl, N—O···π and C—H···π interactions are indicated by green, black, green cyan, magenta and violet arrows, respectively.

quinoline derivatives of these compounds gave 4, 3, 0, 5, 3 and 2 compounds, namely, for 2-chloro-4-nitrobenzoic acid: 2-chloro-4-nitrobenzoic acid–6-methylquinoline (BUZNIW; Gotoh & Ishida, 2020), 2-chloro-4-nitrobenzoic acid–5-nitroquinoline (NUBHEA; Gotoh & Ishida, 2019*b*), 8-hydroxyquinolinium 2-chloro-4-nitrobenzoate (WOPDEM; Babu & Chandrasekaran, 2014), 2-chloro-4-nitrobenzoic acid–quinoline (YAGFAP; Gotoh & Ishida, 2011), for 2-chloro-5-nitrobenzoic acid: 2-chloro-5-nitrobenzoic acid–6-methylquinoline (BUZNOC; Gotoh & Ishida, 2020), 2-chloro-5-nitrobenzoic acid–quinoline (AJIWIA; Gotoh & Ishida, 2009), 8-hydroxy-2-methylquinolinium 2-chloro-5-nitrobenzoate dihydrate (HIHPIY; Tan, 2007), for 3-chloro-2-nitrobenzoic acid: 3-chloro-2-nitrobenzoic acid–6-methylquinoline (BUZNUI; Gotoh & Ishida, 2020), 3-chloro-2-nitrobenzoic acid–5-nitroquinoline (XOWVUD; Gotoh & Ishida, 2019*a*), 3-chloro-2-nitrobenzoic acid–6-nitroquinoline (XOWWAK, Gotoh & Ishida, 2019*a*), 8-hydroxyquinolin-1-ium 3-chloro-2-nitrobenzoate (XOWWEO; Gotoh & Ishida, 2019*a*), 3-chloro-2-nitrobenzoic acid–quinoline (AJIWOG, Gotoh & Ishida, 2009), for 4-chloro-2-nitrobenzoic acid: 4-chloro-2-nitrobenzoic acid–6-methylquinoline (BUZPAQ; Gotoh & Ishida, 2020), 4-hydroxyquinolin-1-ium 4-chloro-2-nitrobenzoate (WOVZOZ; Gotoh & Ishida, 2019*c*), 4-chloro-2-nitrobenzoic acid–quinoline (AJIWUM; Gotoh & Ishida, 2009), and for 5-chloro-2-nitrobenzoic acid: 5-chloro-2-nitrobenzic acid–quinoline (AJIXAT, Gotoh & Ishida, 2009) and 5-chloro-2-nitrobenzoic acid–5-nitroquinoline (NUBHIE; Gotoh & Ishida, 2019*b*).

Of these compounds, AJIWOG, AJIWUM, AJIXAT, BUZNIW, BUZNUI and BUZPAQ show disordered O—H···N/O···H—N hydrogen bonds, while WOVZOZ shows a disorder structure in the O—H···O hydrogen bond accompanied by a keto-enol tautomerization in the base molecule.

5. Synthesis and crystallization

Single crystals of the title compounds (I)–(VI) were obtained by slow evaporation from acetonitrile solutions of 4-methylquinoline with the appropriate chloro-nitrobenzoic acid in a 1:1 molar ratio at room temperature [120 ml of an acetonitrile solution of 4-methylquinoline (0.20 g) and chloro-nitrobenzoic acid (0.28 g for each acid)].

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 8. All H atoms in compounds (I)–(VI) were found in difference-Fourier maps. The O-bound H atom in (II) and the N-bound H atoms in (I), (V) and (VI) were refined freely; the refined O—H and N—H distances are given in Tables 2, 3, 6 and 7. For (III) and (IV), H atoms in the

Table 8
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{10}H_{10}N^{+}\cdot C_7H_3ClNO_4^{-}$	$C_{10}H_9N\cdot C_7H_4ClNO_4$	$C_{10}H_{9.63}N^{0.63+}\cdot C_7H_{3.37}ClNO_4^{0.63-}$
M_r	344.75	344.75	344.75
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
Temperature (K)	185	185	185
a, b, c (Å)	8.6975 (4), 9.2527 (4), 10.1865 (5)	7.6353 (4), 9.3827 (6), 11.3756 (7)	6.6401 (3), 23.2126 (5), 10.3386 (3)
α, β, γ (°)	72.7483 (15), 86.4281 (16), 74.5728 (15)	91.453 (3), 95.204 (3), 107.773 (3)	90, 99.3926 (15), 90
V (Å^3)	754.55 (6)	771.65 (8)	1572.16 (9)
Z	2	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.28	0.27	0.27
Crystal size (mm)	0.55 × 0.50 × 0.32	0.30 × 0.25 × 0.05	0.35 × 0.28 × 0.25
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}	0.868, 0.915	0.938, 0.986	0.909, 0.935
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22243, 4404, 3822	14544, 4486, 2563	32362, 4588, 3854
R_{int}	0.043	0.038	0.022
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.703	0.704
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.122, 1.13	0.068, 0.257, 1.19	0.044, 0.125, 1.07
No. of reflections	4404	4486	4588
No. of parameters	222	222	244
No. of restraints	0	0	2
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})	0.44, −0.28	0.91, −0.58	0.52, −0.40

	(IV)	(V)	(VI)
Crystal data			
Chemical formula	$C_{10}H_{9.54}N^{0.54+}\cdot C_7H_{3.46}ClNO_4^{0.54-}$	$C_{10}H_{10}N^+\cdot C_7H_3ClNO_4^-$	$C_{10}H_{10}N^+.C_7H_3ClNO_4^-$
M_r	344.75	344.75	344.75
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $C2/c$
Temperature (K)	185	185	190
a, b, c (Å)	7.5234 (10), 7.8017 (11), 13.6341 (17)	7.6858 (3), 8.3615 (3), 13.5746 (5)	16.2625 (10), 7.5099 (4), 25.3105 (15)
α, β, γ (°)	80.934 (4), 80.227 (3), 89.150 (4)	82.5485 (13), 80.8927 (12), 65.0929 (11)	90, 99.4086 (19), 90
V (Å^3)	778.73 (18)	779.33 (5)	3049.6 (3)
Z	2	2	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.27	0.27	0.28
Crystal size (mm)	0.35 × 0.29 × 0.22	0.51 × 0.45 × 0.15	0.30 × 0.21 × 0.12
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}	0.914, 0.942	0.868, 0.960	0.916, 0.968
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16767, 4544, 4017	18635, 3566, 3290	29037, 4457, 3913
R_{int}	0.028	0.027	0.022
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.649	0.703
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.103, 1.07	0.036, 0.102, 1.04	0.036, 0.099, 1.05
No. of reflections	4544	3566	4457
No. of parameters	225	222	222
No. of restraints	2	0	0
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})	0.44, −0.38	0.38, −0.18	0.47, −0.16

Computer programs: *PROCESS-AUTO* (Rigaku, 2006), *CrystalStructure* (Rigaku, 2018), *SHELXS97* (Sheldrick, 2008), *SIR92* (Altomare *et al.*, 1993), *SHELXL2018/3* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *PLATON* (Spek, 2020).

N···H···O hydrogen bonds were found to be disordered over two positions in difference-Fourier maps. The positional parameters and occupancy factors were refined, with bond-length restraints of N—H = 0.88 (1) Å and O—H = 0.84 (1) Å, and with U_{iso}(H) = 1.5U_{eq}(N or O); the refined distances are given in Tables 4 and 5. Other H atoms were positioned geometrically (C—H = 0.95 or 0.98 Å) and treated as riding, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

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supporting information

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Role of pK_a in establishing the crystal structures of six hydrogen-bonded compounds of 4-methylquinoline with different isomers of chloro- and nitro-substituted benzoic acids

Hiroyuki Ishida

Computing details

For all structures, data collection: *PROCESS-AUTO* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 2006); data reduction: *PROCESS-AUTO* (Rigaku, 2006). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for (I), (II), (IV); *SIR92* (Altomare *et al.*, 1993) for (III), (V), (VI). For all structures, program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2018) and *PLATON* (Spek, 2020).

4-Methylquinolinium 2-chloro-4-nitrobenzoate (I)

Crystal data

$C_{10}H_{10}N^+·C_7H_3ClNO_4^-$
M_r = 344.75
Triclinic, $P\overline{1}$
a = 8.6975 (4) Å
b = 9.2527 (4) Å
c = 10.1865 (5) Å
α = 72.7483 (15)°
β = 86.4281 (16)°
γ = 74.5728 (15)°
V = 754.55 (6) Å^3
Z = 2
$F(000)$ = 356.00
D_x = 1.517 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 20962 reflections
θ = 3.2–30.2°
μ = 0.28 mm^{-1}
T = 185 K
Block, colorless
0.55 × 0.50 × 0.32 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} = 0.868, T_{max} = 0.915
22243 measured reflections
4404 independent reflections
3822 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 30.0°, θ_{min} = 3.2°
h = −12→12
k = −13→13
l = −14→14

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.122
S = 1.13
4404 reflections
222 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
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2 + 0.0819P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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	0.32990 (4)	0.49410 (3)	0.93689 (3)	0.03079 (11)
O1	0.14650 (13)	0.72397 (10)	0.67810 (9)	0.0348 (2)
O2	0.17832 (14)	0.56790 (11)	0.54222 (9)	0.0379 (2)
O3	0.06312 (12)	0.05267 (11)	1.18988 (10)	0.0363 (2)
O4	−0.15473 (12)	0.09130 (11)	1.07952 (11)	0.0371 (2)
N1	−0.02872 (13)	0.12105 (11)	1.09235 (11)	0.0273 (2)
N2	0.22641 (12)	0.95808 (11)	0.50904 (10)	0.0252 (2)
H2	0.193 (2)	0.874 (2)	0.558 (2)	0.058 (6)*
C1	0.10772 (13)	0.47157 (12)	0.77222 (11)	0.0220 (2)
C2	0.17864 (13)	0.42010 (12)	0.90230 (11)	0.0222 (2)
C3	0.13592 (13)	0.30429 (12)	1.00803 (11)	0.0239 (2)
H3	0.187120	0.267833	1.095810	0.029*
C4	0.01662 (13)	0.24410 (12)	0.98114 (12)	0.0239 (2)
C5	−0.05810 (14)	0.29108 (13)	0.85435 (12)	0.0259 (2)
H5	−0.140805	0.247959	0.839335	0.031*
C6	−0.00900 (14)	0.40299 (13)	0.74954 (12)	0.0251 (2)
H6	−0.055755	0.433693	0.660379	0.030*
C7	0.14979 (14)	0.59753 (13)	0.65289 (12)	0.0241 (2)
C8	0.18122 (15)	1.08320 (14)	0.55384 (12)	0.0274 (2)
H8	0.108530	1.083030	0.627431	0.033*
C9	0.23804 (14)	1.21539 (13)	0.49531 (12)	0.0268 (2)
H9	0.203126	1.304456	0.528283	0.032*
C10	0.34486 (14)	1.21633 (13)	0.38964 (11)	0.0240 (2)
C11	0.39172 (13)	1.08266 (13)	0.33915 (11)	0.0239 (2)
C12	0.49945 (15)	1.07123 (15)	0.22966 (13)	0.0300 (2)
H12	0.544342	1.156119	0.185742	0.036*
C13	0.53934 (17)	0.93898 (17)	0.18668 (14)	0.0360 (3)
H13	0.611735	0.933167	0.113483	0.043*
C14	0.47410 (17)	0.81181 (17)	0.24992 (15)	0.0361 (3)
H14	0.501707	0.721573	0.218226	0.043*
C15	0.37123 (16)	0.81710 (14)	0.35670 (13)	0.0300 (2)
H15	0.328586	0.730472	0.399948	0.036*
C16	0.32896 (13)	0.95269 (13)	0.40207 (11)	0.0240 (2)
C17	0.41066 (16)	1.35602 (14)	0.32995 (13)	0.0297 (2)
H17A	0.527472	1.321940	0.331657	0.045*

H17B	0.375456	1.429869	0.384385	0.045*
H17C	0.372032	1.407486	0.234819	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03215 (17)	0.03700 (18)	0.02937 (16)	−0.01980 (13)	0.00018 (11)	−0.00912 (12)
O1	0.0553 (6)	0.0235 (4)	0.0299 (4)	−0.0195 (4)	0.0110 (4)	−0.0083 (3)
O2	0.0618 (7)	0.0351 (5)	0.0256 (4)	−0.0271 (5)	0.0103 (4)	−0.0110 (4)
O3	0.0435 (5)	0.0304 (5)	0.0294 (5)	−0.0118 (4)	0.0015 (4)	0.0013 (4)
O4	0.0384 (5)	0.0358 (5)	0.0410 (5)	−0.0222 (4)	0.0093 (4)	−0.0076 (4)
N1	0.0320 (5)	0.0225 (4)	0.0283 (5)	−0.0115 (4)	0.0071 (4)	−0.0059 (4)
N2	0.0284 (5)	0.0233 (4)	0.0237 (4)	−0.0109 (4)	0.0018 (4)	−0.0031 (4)
C1	0.0248 (5)	0.0192 (4)	0.0228 (5)	−0.0082 (4)	0.0023 (4)	−0.0055 (4)
C2	0.0233 (5)	0.0219 (5)	0.0243 (5)	−0.0094 (4)	0.0020 (4)	−0.0078 (4)
C3	0.0262 (5)	0.0228 (5)	0.0224 (5)	−0.0074 (4)	0.0012 (4)	−0.0053 (4)
C4	0.0266 (5)	0.0186 (5)	0.0260 (5)	−0.0087 (4)	0.0048 (4)	−0.0040 (4)
C5	0.0264 (5)	0.0230 (5)	0.0304 (6)	−0.0117 (4)	0.0003 (4)	−0.0062 (4)
C6	0.0283 (5)	0.0229 (5)	0.0248 (5)	−0.0102 (4)	−0.0024 (4)	−0.0044 (4)
C7	0.0273 (5)	0.0223 (5)	0.0240 (5)	−0.0111 (4)	0.0012 (4)	−0.0049 (4)
C8	0.0307 (6)	0.0265 (5)	0.0246 (5)	−0.0113 (4)	0.0052 (4)	−0.0044 (4)
C9	0.0313 (6)	0.0221 (5)	0.0269 (5)	−0.0092 (4)	0.0032 (4)	−0.0056 (4)
C10	0.0246 (5)	0.0220 (5)	0.0235 (5)	−0.0080 (4)	−0.0016 (4)	−0.0016 (4)
C11	0.0240 (5)	0.0245 (5)	0.0217 (5)	−0.0085 (4)	−0.0012 (4)	−0.0024 (4)
C12	0.0294 (6)	0.0327 (6)	0.0265 (5)	−0.0109 (5)	0.0032 (4)	−0.0049 (5)
C13	0.0355 (7)	0.0431 (7)	0.0315 (6)	−0.0110 (6)	0.0085 (5)	−0.0148 (5)
C14	0.0392 (7)	0.0349 (6)	0.0389 (7)	−0.0094 (5)	0.0037 (5)	−0.0184 (5)
C15	0.0336 (6)	0.0262 (5)	0.0324 (6)	−0.0105 (5)	0.0001 (5)	−0.0093 (5)
C16	0.0254 (5)	0.0238 (5)	0.0228 (5)	−0.0083 (4)	−0.0014 (4)	−0.0046 (4)
C17	0.0326 (6)	0.0240 (5)	0.0314 (6)	−0.0128 (5)	0.0027 (5)	−0.0020 (4)

Geometric parameters (Å, º)

Cl1—C2	1.7331 (11)	C8—C9	1.3957 (15)
O1—C7	1.2628 (13)	C8—H8	0.9500
O2—C7	1.2329 (14)	C9—C10	1.3770 (16)
O3—N1	1.2176 (14)	C9—H9	0.9500
O4—N1	1.2221 (14)	C10—C11	1.4294 (16)
N1—C4	1.4674 (14)	C10—C17	1.5007 (15)
N2—C8	1.3236 (16)	C11—C16	1.4155 (15)
N2—C16	1.3686 (15)	C11—C12	1.4213 (17)
N2—H2	0.90 (2)	C12—C13	1.3721 (19)
C1—C2	1.3908 (15)	C12—H12	0.9500
C1—C6	1.3948 (15)	C13—C14	1.408 (2)
C1—C7	1.5169 (14)	C13—H13	0.9500
C2—C3	1.3869 (15)	C14—C15	1.3686 (19)
C3—C4	1.3766 (16)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.4142 (16)

C4—C5	1.3787 (17)	C15—H15	0.9500
C5—C6	1.3846 (15)	C17—H17A	0.9800
C5—H5	0.9500	C17—H17B	0.9800
C6—H6	0.9500	C17—H17C	0.9800

O3—N1—O4	124.18 (10)	C10—C9—C8	119.81 (11)
O3—N1—C4	118.01 (10)	C10—C9—H9	120.1
O4—N1—C4	117.78 (10)	C8—C9—H9	120.1
C8—N2—C16	121.80 (10)	C9—C10—C11	118.97 (10)
C8—N2—H2	115.9 (13)	C9—C10—C17	119.91 (11)
C16—N2—H2	122.1 (13)	C11—C10—C17	121.12 (10)
C2—C1—C6	118.15 (10)	C16—C11—C12	117.55 (11)
C2—C1—C7	124.07 (10)	C16—C11—C10	118.54 (10)
C6—C1—C7	117.78 (10)	C12—C11—C10	123.91 (10)
C3—C2—C1	121.81 (10)	C13—C12—C11	120.75 (12)
C3—C2—Cl1	117.20 (9)	C13—C12—H12	119.6
C1—C2—Cl1	120.94 (8)	C11—C12—H12	119.6
C4—C3—C2	117.58 (10)	C12—C13—C14	120.68 (12)
C4—C3—H3	121.2	C12—C13—H13	119.7
C2—C3—H3	121.2	C14—C13—H13	119.7
C3—C4—C5	123.04 (10)	C15—C14—C13	120.54 (12)
C3—C4—N1	117.88 (10)	C15—C14—H14	119.7
C5—C4—N1	119.05 (10)	C13—C14—H14	119.7
C4—C5—C6	118.01 (10)	C14—C15—C16	119.41 (12)
C4—C5—H5	121.0	C14—C15—H15	120.3
C6—C5—H5	121.0	C16—C15—H15	120.3
C5—C6—C1	121.33 (11)	N2—C16—C15	119.51 (10)
C5—C6—H6	119.3	N2—C16—C11	119.42 (10)
C1—C6—H6	119.3	C15—C16—C11	121.08 (11)
O2—C7—O1	127.32 (10)	C10—C17—H17A	109.5
O2—C7—C1	117.26 (9)	C10—C17—H17B	109.5
O1—C7—C1	115.38 (10)	H17A—C17—H17B	109.5
N2—C8—C9	121.44 (11)	C10—C17—H17C	109.5
N2—C8—H8	119.3	H17A—C17—H17C	109.5
C9—C8—H8	119.3	H17B—C17—H17C	109.5

C6—C1—C2—C3	−0.18 (17)	C16—N2—C8—C9	−0.99 (18)
C7—C1—C2—C3	−179.94 (10)	N2—C8—C9—C10	−0.74 (19)
C6—C1—C2—Cl1	177.53 (8)	C8—C9—C10—C11	1.89 (18)
C7—C1—C2—Cl1	−2.23 (16)	C8—C9—C10—C17	−177.80 (11)
C1—C2—C3—C4	−1.77 (17)	C9—C10—C11—C16	−1.39 (16)
Cl1—C2—C3—C4	−179.56 (8)	C17—C10—C11—C16	178.29 (11)
C2—C3—C4—C5	1.57 (17)	C9—C10—C11—C12	179.23 (11)
C2—C3—C4—N1	179.74 (9)	C17—C10—C11—C12	−1.09 (18)
O3—N1—C4—C3	−17.00 (15)	C16—C11—C12—C13	0.49 (18)
O4—N1—C4—C3	164.68 (11)	C10—C11—C12—C13	179.88 (12)
O3—N1—C4—C5	161.25 (11)	C11—C12—C13—C14	0.1 (2)
O4—N1—C4—C5	−17.08 (16)	C12—C13—C14—C15	−0.9 (2)

C3—C4—C5—C6	0.61 (18)	C13—C14—C15—C16	0.9 (2)
N1—C4—C5—C6	−177.54 (10)	C8—N2—C16—C15	−178.90 (11)
C4—C5—C6—C1	−2.68 (18)	C8—N2—C16—C11	1.46 (17)
C2—C1—C6—C5	2.47 (17)	C14—C15—C16—N2	−179.84 (12)
C7—C1—C6—C5	−177.75 (10)	C14—C15—C16—C11	−0.21 (19)
C2—C1—C7—O2	130.38 (13)	C12—C11—C16—N2	179.17 (10)
C6—C1—C7—O2	−49.38 (16)	C10—C11—C16—N2	−0.25 (16)
C2—C1—C7—O1	−51.76 (16)	C12—C11—C16—C15	−0.47 (17)
C6—C1—C7—O1	128.48 (12)	C10—C11—C16—C15	−179.89 (10)

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.900 (19)	1.678 (19)	2.5652 (14)	167.7 (18)
C6—H6···O2^{i}	0.95	2.39	3.3066 (16)	163
C8—H8···O3^{ii}	0.95	2.56	3.4199 (16)	151
C9—H9···O2^{iii}	0.95	2.44	3.3360 (16)	158
C15—H15···O2	0.95	2.36	3.2835 (17)	163
N1—O3···*Cg*3^{iv}	1.22 (1)	3.26 (1)	4.3171 (13)	145 (1)

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

4-Methylquinoline–2-chloro-5-nitrobenzoic acid (1/1) (II)

Crystal data

$C_{10}H_9N·C_7H_4ClNO_4$
M_r = 344.75
Triclinic, $P\overline{1}$
a = 7.6353 (4) Å
b = 9.3827 (6) Å
c = 11.3756 (7) Å
α = 91.453 (3)°
β = 95.204 (3)°
γ = 107.773 (3)°
V = 771.65 (8) Å^3
Z = 2
F(000) = 356.00
D_x = 1.484 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71075 Å
Cell parameters from 9512 reflections
θ = 3.0–30.1°
μ = 0.27 mm^{-1}
T = 185 K
Platelet, colorless
0.30 × 0.25 × 0.05 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} = 0.938, T_{max} = 0.986
14544 measured reflections
4486 independent reflections
2563 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 30.0°, θ_{min} = 3.0°
h = −9→10
k = −13→13
l = −15→15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.257
S = 1.19
4486 reflections
222 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
$w = 1/[\sigma^2(F_o^2) + (0.1416P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.91$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ 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	−0.03754 (10)	0.97793 (9)	0.28787 (8)	0.0688 (3)
O1	0.4426 (3)	0.8113 (2)	0.27937 (18)	0.0550 (5)
H1	0.401 (10)	0.721 (8)	0.238 (6)	0.17 (3)*
O2	0.1900 (4)	0.8238 (2)	0.1691 (2)	0.0705 (7)
O3	0.7457 (3)	1.4293 (2)	0.54603 (18)	0.0510 (5)
O4	0.8405 (2)	1.2413 (2)	0.50002 (19)	0.0515 (5)
N1	0.7203 (3)	1.3046 (2)	0.49943 (18)	0.0386 (5)
N2	0.3941 (3)	0.5596 (2)	0.1685 (2)	0.0465 (5)
C1	0.3346 (4)	1.0135 (3)	0.3225 (2)	0.0384 (5)
C2	0.1888 (3)	1.0712 (3)	0.3399 (2)	0.0420 (5)
C3	0.2183 (4)	1.2039 (3)	0.4056 (2)	0.0445 (6)
H3	0.117494	1.240795	0.416034	0.053*
C4	0.3935 (3)	1.2831 (3)	0.4562 (2)	0.0384 (5)
H4	0.415578	1.375700	0.499746	0.046*
C5	0.5360 (3)	1.2245 (2)	0.4418 (2)	0.0346 (5)
C6	0.5106 (3)	1.0921 (2)	0.3766 (2)	0.0366 (5)
H6	0.611816	1.054882	0.368761	0.044*
C7	0.3130 (4)	0.8720 (3)	0.2488 (2)	0.0462 (6)
C8	0.2387 (4)	0.4902 (3)	0.1035 (2)	0.0493 (6)
H8	0.146250	0.538936	0.096541	0.059*
C9	0.1990 (4)	0.3519 (3)	0.0444 (2)	0.0467 (6)
H9	0.083758	0.308531	−0.001836	0.056*
C10	0.3317 (4)	0.2774 (3)	0.0539 (2)	0.0460 (6)
C11	0.5048 (3)	0.3480 (2)	0.12444 (19)	0.0352 (5)
C12	0.6504 (4)	0.2871 (4)	0.1402 (3)	0.0545 (7)
H12	0.636763	0.192542	0.102077	0.065*
C13	0.8077 (5)	0.3570 (4)	0.2068 (3)	0.0643 (9)
H13	0.903299	0.311688	0.216432	0.077*
C14	0.8312 (4)	0.4947 (4)	0.2615 (3)	0.0581 (8)
H14	0.944487	0.542707	0.308477	0.070*
C15	0.6987 (4)	0.5661 (3)	0.2515 (2)	0.0494 (6)
H15	0.719222	0.661767	0.289891	0.059*

C16	0.5265 (4)	0.4906 (3)	0.1804 (2)	0.0407 (5)
C17	0.2954 (6)	0.1291 (3)	−0.0083 (3)	0.0663 (9)
H17A	0.308435	0.055894	0.049069	0.099*
H17B	0.384247	0.136518	−0.066635	0.099*
H17C	0.169533	0.096781	−0.048532	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0441 (4)	0.0620 (5)	0.0871 (6)	0.0058 (3)	−0.0173 (4)	−0.0221 (4)
O1	0.0728 (14)	0.0406 (10)	0.0539 (11)	0.0230 (9)	0.0045 (9)	−0.0123 (8)
O2	0.0988 (18)	0.0491 (12)	0.0566 (12)	0.0232 (12)	−0.0230 (12)	−0.0203 (10)
O3	0.0466 (10)	0.0364 (9)	0.0627 (12)	0.0073 (7)	−0.0089 (8)	−0.0114 (8)
O4	0.0359 (9)	0.0534 (11)	0.0668 (12)	0.0176 (8)	0.0023 (8)	−0.0033 (9)
N1	0.0352 (10)	0.0369 (10)	0.0432 (11)	0.0113 (8)	0.0030 (8)	−0.0016 (8)
N2	0.0537 (13)	0.0396 (11)	0.0455 (12)	0.0131 (9)	0.0075 (9)	−0.0053 (9)
C1	0.0492 (13)	0.0284 (10)	0.0344 (11)	0.0085 (9)	0.0017 (9)	−0.0028 (9)
C2	0.0384 (12)	0.0390 (12)	0.0450 (13)	0.0101 (9)	−0.0065 (10)	−0.0047 (10)
C3	0.0371 (12)	0.0416 (12)	0.0542 (14)	0.0138 (10)	−0.0017 (10)	−0.0087 (11)
C4	0.0356 (11)	0.0323 (11)	0.0463 (13)	0.0109 (9)	0.0009 (9)	−0.0079 (9)
C5	0.0390 (12)	0.0291 (10)	0.0338 (10)	0.0084 (8)	0.0017 (8)	−0.0009 (8)
C6	0.0429 (13)	0.0319 (11)	0.0358 (11)	0.0124 (9)	0.0061 (9)	−0.0006 (9)
C7	0.0654 (17)	0.0331 (11)	0.0380 (12)	0.0129 (11)	0.0035 (11)	−0.0028 (10)
C8	0.0437 (14)	0.0566 (16)	0.0452 (13)	0.0122 (12)	0.0048 (11)	0.0001 (12)
C9	0.0461 (14)	0.0491 (14)	0.0397 (12)	0.0094 (11)	−0.0028 (10)	−0.0008 (11)
C10	0.0552 (15)	0.0412 (13)	0.0337 (11)	0.0039 (11)	0.0039 (10)	−0.0050 (10)
C11	0.0413 (12)	0.0340 (11)	0.0300 (10)	0.0109 (9)	0.0050 (9)	−0.0012 (9)
C12	0.0601 (17)	0.0626 (18)	0.0518 (15)	0.0310 (14)	0.0171 (13)	0.0137 (14)
C13	0.0526 (17)	0.084 (2)	0.0628 (19)	0.0265 (16)	0.0152 (15)	0.0222 (18)
C14	0.0385 (14)	0.078 (2)	0.0502 (15)	0.0075 (13)	−0.0007 (11)	0.0121 (15)
C15	0.0504 (15)	0.0489 (14)	0.0374 (12)	−0.0006 (11)	0.0022 (10)	−0.0039 (11)
C16	0.0452 (13)	0.0404 (12)	0.0355 (11)	0.0112 (10)	0.0071 (9)	−0.0006 (10)
C17	0.092 (2)	0.0448 (15)	0.0506 (16)	0.0073 (15)	0.0014 (15)	−0.0109 (13)

Geometric parameters (Å, º)

Cl1—C2	1.723 (2)	C8—C9	1.380 (4)
O1—C7	1.310 (4)	C8—H8	0.9500
O1—H1	0.91 (7)	C9—C10	1.395 (4)
O2—C7	1.214 (3)	C9—H9	0.9500
O3—N1	1.224 (3)	C10—C11	1.440 (3)
O4—N1	1.235 (3)	C10—C17	1.481 (4)
N1—C5	1.462 (3)	C11—C12	1.397 (4)
N2—C8	1.313 (4)	C11—C16	1.423 (3)
N2—C16	1.356 (3)	C12—C13	1.333 (5)
C1—C6	1.397 (3)	C12—H12	0.9500
C1—C2	1.405 (4)	C13—C14	1.373 (5)
C1—C7	1.509 (3)	C13—H13	0.9500

C2—C3	1.383 (3)	C14—C15	1.372 (4)
C3—C4	1.380 (3)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.446 (4)
C4—C5	1.380 (3)	C15—H15	0.9500
C4—H4	0.9500	C17—H17A	0.9800
C5—C6	1.383 (3)	C17—H17B	0.9800
C6—H6	0.9500	C17—H17C	0.9800

C7—O1—H1	102 (4)	C8—C9—H9	120.7
O3—N1—O4	123.8 (2)	C10—C9—H9	120.7
O3—N1—C5	118.12 (19)	C9—C10—C11	118.8 (2)
O4—N1—C5	118.0 (2)	C9—C10—C17	120.4 (3)
C8—N2—C16	118.2 (2)	C11—C10—C17	120.8 (3)
C6—C1—C2	118.0 (2)	C12—C11—C16	118.7 (2)
C6—C1—C7	117.9 (2)	C12—C11—C10	124.7 (2)
C2—C1—C7	124.1 (2)	C16—C11—C10	116.6 (2)
C3—C2—C1	121.4 (2)	C13—C12—C11	122.4 (3)
C3—C2—Cl1	115.90 (19)	C13—C12—H12	118.8
C1—C2—Cl1	122.63 (19)	C11—C12—H12	118.8
C4—C3—C2	120.3 (2)	C12—C13—C14	119.8 (3)
C4—C3—H3	119.9	C12—C13—H13	120.1
C2—C3—H3	119.9	C14—C13—H13	120.1
C5—C4—C3	118.4 (2)	C15—C14—C13	123.1 (3)
C5—C4—H4	120.8	C15—C14—H14	118.5
C3—C4—H4	120.8	C13—C14—H14	118.5
C4—C5—C6	122.6 (2)	C14—C15—C16	117.6 (3)
C4—C5—N1	118.62 (19)	C14—C15—H15	121.2
C6—C5—N1	118.8 (2)	C16—C15—H15	121.2
C5—C6—C1	119.3 (2)	N2—C16—C11	122.8 (2)
C5—C6—H6	120.4	N2—C16—C15	118.7 (2)
C1—C6—H6	120.4	C11—C16—C15	118.5 (2)
O2—C7—O1	125.0 (2)	C10—C17—H17A	109.5
O2—C7—C1	122.6 (3)	C10—C17—H17B	109.5
O1—C7—C1	112.4 (2)	H17A—C17—H17B	109.5
N2—C8—C9	125.2 (3)	C10—C17—H17C	109.5
N2—C8—H8	117.4	H17A—C17—H17C	109.5
C9—C8—H8	117.4	H17B—C17—H17C	109.5
C8—C9—C10	118.5 (2)		

C6—C1—C2—C3	1.9 (4)	C16—N2—C8—C9	−0.8 (4)
C7—C1—C2—C3	−178.0 (2)	N2—C8—C9—C10	0.6 (4)
C6—C1—C2—Cl1	−174.82 (18)	C8—C9—C10—C11	−0.3 (4)
C7—C1—C2—Cl1	5.2 (4)	C8—C9—C10—C17	−179.8 (3)
C1—C2—C3—C4	−0.2 (4)	C9—C10—C11—C12	−179.0 (2)
Cl1—C2—C3—C4	176.8 (2)	C17—C10—C11—C12	0.4 (4)
C2—C3—C4—C5	−1.6 (4)	C9—C10—C11—C16	0.4 (3)
C3—C4—C5—C6	1.6 (4)	C17—C10—C11—C16	179.8 (2)
C3—C4—C5—N1	−177.4 (2)	C16—C11—C12—C13	0.8 (4)

O3—N1—C5—C4	−8.7 (3)	C10—C11—C12—C13	−179.8 (3)
O4—N1—C5—C4	170.1 (2)	C11—C12—C13—C14	−0.8 (4)
O3—N1—C5—C6	172.3 (2)	C12—C13—C14—C15	0.1 (5)
O4—N1—C5—C6	−9.0 (3)	C13—C14—C15—C16	0.5 (4)
C4—C5—C6—C1	0.1 (4)	C8—N2—C16—C11	0.8 (4)
N1—C5—C6—C1	179.15 (19)	C8—N2—C16—C15	179.8 (2)
C2—C1—C6—C5	−1.9 (3)	C12—C11—C16—N2	178.8 (2)
C7—C1—C6—C5	178.1 (2)	C10—C11—C16—N2	−0.6 (3)
C6—C1—C7—O2	−154.9 (3)	C12—C11—C16—C15	−0.1 (3)
C2—C1—C7—O2	25.1 (4)	C10—C11—C16—C15	−179.6 (2)
C6—C1—C7—O1	23.9 (3)	C14—C15—C16—N2	−179.5 (2)
C2—C1—C7—O1	−156.2 (2)	C14—C15—C16—C11	−0.5 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.91 (7)	1.68 (7)	2.556 (3)	162 (7)
C3—H3···O4^{i}	0.95	2.40	3.280 (4)	154
C4—H4···O3^{ii}	0.95	2.54	3.188 (3)	126
C17—H17*A*···O2^{iii}	0.98	2.57	3.479 (4)	155
C17—H17*C*···Cl1^{iv}	0.98	2.81	3.535 (4)	131

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

4-Methylquinolinium 2-chloro-6-nitrobenzoate (III)

Crystal data

$C_{10}H_{9.63}N0.63+·C_7H_{3.37}ClNO_40.63−−$
M_r = 344.75
Monoclinic, $P2_1/c$
a = 6.6401 (3) Å
b = 23.2126 (5) Å
c = 10.3386 (3) Å
β = 99.3926 (15)°
V = 1572.16 (9) Å^3
Z = 4
$F(000)$ = 712.00
D_x = 1.456 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 25957 reflections
θ = 3.1–30.1°
μ = 0.27 mm^{-1}
T = 185 K
Block, colorless
0.35 × 0.28 × 0.25 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} = 0.909, T_{max} = 0.935
32362 measured reflections
4588 independent reflections
3854 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 30.0°, θ_{min} = 3.1°
h = −9→9
k = −32→32
l = −14→14

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.07
4588 reflections
244 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.4164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.71027 (7)	0.10339 (2)	1.02427 (4)	0.05678 (15)	
O1	0.34983 (15)	0.13094 (4)	0.76226 (8)	0.0326 (2)	
H1	0.328 (8)	0.1007 (14)	0.717 (5)	0.049*	0.37 (3)
O2	0.18762 (19)	0.08197 (5)	0.89869 (10)	0.0468 (3)	
O3A	0.0115 (12)	0.2046 (4)	0.8201 (5)	0.0463 (13)	0.54 (3)
O4A	−0.0751 (8)	0.2537 (6)	0.9776 (7)	0.0623 (19)	0.54 (3)
O3B	−0.0248 (19)	0.1914 (7)	0.8468 (19)	0.078 (3)	0.46 (3)
O4B	−0.021 (3)	0.2723 (4)	0.9405 (16)	0.076 (4)	0.46 (3)
N1	0.04842 (19)	0.22525 (5)	0.92742 (12)	0.0376 (3)	
N2	0.28090 (14)	0.04202 (4)	0.61720 (9)	0.02414 (19)	
H2	0.300 (4)	0.0736 (7)	0.666 (2)	0.036*	0.63 (3)
C1	0.36395 (19)	0.16626 (5)	0.97746 (10)	0.0258 (2)	
C2	0.5557 (2)	0.15998 (6)	1.05519 (12)	0.0324 (3)	
C3	0.6290 (2)	0.19756 (7)	1.15678 (14)	0.0401 (3)	
H3	0.761107	0.192060	1.206500	0.048*	
C4	0.5092 (2)	0.24273 (6)	1.18481 (14)	0.0412 (3)	
H4	0.557720	0.268328	1.254673	0.049*	
C5	0.3182 (2)	0.25079 (5)	1.11112 (13)	0.0365 (3)	
H5	0.234047	0.281705	1.130255	0.044*	
C6	0.25041 (19)	0.21305 (5)	1.00842 (11)	0.0283 (2)	
C7	0.28934 (19)	0.12224 (5)	0.87118 (11)	0.0266 (2)	
C8	0.28861 (17)	−0.00796 (5)	0.67783 (11)	0.0266 (2)	
H8	0.308842	−0.008856	0.770917	0.032*	
C9	0.26769 (18)	−0.05958 (5)	0.60825 (12)	0.0283 (2)	
H9	0.273935	−0.095108	0.654330	0.034*	
C10	0.23797 (17)	−0.05958 (5)	0.47294 (12)	0.0272 (2)	
C11	0.22837 (16)	−0.00558 (5)	0.40662 (11)	0.0244 (2)	
C12	0.19706 (19)	0.00027 (6)	0.26760 (12)	0.0335 (3)	
H12	0.180685	−0.033200	0.214019	0.040*	
C13	0.1903 (2)	0.05339 (7)	0.21055 (13)	0.0395 (3)	

H13	0.169884	0.056667	0.117731	0.047*
C14	0.2134 (2)	0.10307 (6)	0.28825 (14)	0.0373 (3)
H14	0.208084	0.139770	0.247145	0.045*
C15	0.24365 (18)	0.09990 (5)	0.42260 (13)	0.0301 (2)
H15	0.258987	0.133966	0.474193	0.036*
C16	0.25156 (16)	0.04526 (5)	0.48282 (11)	0.0233 (2)
C17	0.2150 (2)	−0.11468 (6)	0.39687 (16)	0.0402 (3)
H17A	0.081819	−0.115295	0.339800	0.060*
H17B	0.224727	−0.147324	0.457681	0.060*
H17C	0.323533	−0.117515	0.343293	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0537 (2)	0.0714 (3)	0.0417 (2)	0.0315 (2)	−0.00294 (16)	−0.00849 (18)
O1	0.0511 (5)	0.0267 (4)	0.0208 (4)	−0.0049 (4)	0.0088 (4)	−0.0020 (3)
O2	0.0706 (7)	0.0442 (5)	0.0286 (5)	−0.0253 (5)	0.0173 (5)	−0.0089 (4)
O3A	0.041 (2)	0.064 (3)	0.0298 (17)	0.0180 (18)	−0.0048 (11)	−0.0085 (14)
O4A	0.0501 (18)	0.068 (4)	0.069 (2)	0.0233 (19)	0.0096 (17)	−0.023 (2)
O3B	0.047 (3)	0.086 (6)	0.092 (6)	0.014 (3)	−0.020 (4)	−0.050 (5)
O4B	0.076 (5)	0.048 (3)	0.088 (5)	0.032 (3)	−0.031 (4)	−0.021 (3)
N1	0.0447 (6)	0.0327 (5)	0.0347 (6)	0.0086 (5)	0.0043 (5)	−0.0038 (4)
N2	0.0241 (4)	0.0274 (4)	0.0211 (4)	0.0004 (3)	0.0041 (3)	−0.0024 (3)
C1	0.0332 (6)	0.0250 (5)	0.0191 (5)	−0.0005 (4)	0.0040 (4)	−0.0011 (4)
C2	0.0344 (6)	0.0360 (6)	0.0259 (5)	0.0040 (5)	0.0020 (4)	−0.0015 (5)
C3	0.0396 (7)	0.0467 (7)	0.0306 (6)	−0.0056 (6)	−0.0040 (5)	−0.0030 (6)
C4	0.0567 (9)	0.0334 (6)	0.0308 (6)	−0.0102 (6)	−0.0011 (6)	−0.0079 (5)
C5	0.0545 (8)	0.0237 (5)	0.0308 (6)	0.0003 (5)	0.0052 (5)	−0.0048 (5)
C6	0.0365 (6)	0.0240 (5)	0.0236 (5)	0.0005 (4)	0.0030 (4)	−0.0012 (4)
C7	0.0343 (6)	0.0249 (5)	0.0202 (5)	0.0015 (4)	0.0033 (4)	−0.0026 (4)
C8	0.0253 (5)	0.0323 (6)	0.0225 (5)	0.0015 (4)	0.0050 (4)	0.0023 (4)
C9	0.0253 (5)	0.0272 (5)	0.0330 (6)	0.0007 (4)	0.0068 (4)	0.0035 (4)
C10	0.0214 (5)	0.0273 (5)	0.0340 (6)	−0.0012 (4)	0.0073 (4)	−0.0056 (4)
C11	0.0191 (4)	0.0316 (5)	0.0229 (5)	−0.0006 (4)	0.0042 (4)	−0.0040 (4)
C12	0.0277 (6)	0.0504 (7)	0.0227 (5)	−0.0010 (5)	0.0044 (4)	−0.0072 (5)
C13	0.0325 (6)	0.0636 (9)	0.0226 (5)	0.0020 (6)	0.0047 (5)	0.0072 (6)
C14	0.0334 (6)	0.0450 (7)	0.0343 (6)	0.0041 (5)	0.0076 (5)	0.0147 (5)
C15	0.0288 (5)	0.0300 (6)	0.0321 (6)	0.0010 (4)	0.0063 (4)	0.0043 (4)
C16	0.0200 (5)	0.0281 (5)	0.0222 (5)	0.0003 (4)	0.0044 (4)	−0.0009 (4)
C17	0.0390 (7)	0.0321 (6)	0.0505 (8)	−0.0048 (5)	0.0106 (6)	−0.0155 (6)

Geometric parameters (Å, º)

Cl1—C2	1.7288 (13)	C5—H5	0.9500
O1—C7	1.2720 (14)	C8—C9	1.3928 (17)
O1—H1	0.841 (10)	C8—H8	0.9500
O2—C7	1.2140 (16)	C9—C10	1.3805 (17)
O3A—N1	1.196 (7)	C9—H9	0.9500

O4A—N1	1.232 (4)	C10—C11	1.4251 (16)
O3B—N1	1.190 (9)	C10—C17	1.4961 (17)
O4B—N1	1.201 (5)	C11—C16	1.4134 (15)
N1—C6	1.4879 (17)	C11—C12	1.4248 (16)
N2—C8	1.3157 (15)	C12—C13	1.365 (2)
N2—C16	1.3731 (14)	C12—H12	0.9500
N2—H2	0.887 (10)	C13—C14	1.399 (2)
C1—C6	1.3888 (16)	C13—H13	0.9500
C1—C2	1.3978 (17)	C14—C15	1.3726 (18)
C1—C7	1.5229 (15)	C14—H14	0.9500
C2—C3	1.3908 (19)	C15—C16	1.4100 (16)
C3—C4	1.375 (2)	C15—H15	0.9500
C3—H3	0.9500	C17—H17A	0.9800
C4—C5	1.382 (2)	C17—H17B	0.9800
C4—H4	0.9500	C17—H17C	0.9800
C5—C6	1.3934 (17)		

C7—O1—H1	108 (4)	N2—C8—H8	119.3
O3B—N1—O4B	124.0 (7)	C9—C8—H8	119.3
O3A—N1—O4A	123.7 (4)	C10—C9—C8	120.61 (11)
O3B—N1—C6	119.8 (5)	C10—C9—H9	119.7
O3A—N1—C6	118.4 (3)	C8—C9—H9	119.7
O4B—N1—C6	115.8 (4)	C9—C10—C11	118.37 (10)
O4A—N1—C6	117.8 (3)	C9—C10—C17	121.21 (12)
C8—N2—C16	121.22 (10)	C11—C10—C17	120.42 (12)
C8—N2—H2	117.8 (18)	C16—C11—C12	117.86 (11)
C16—N2—H2	120.9 (18)	C16—C11—C10	118.30 (10)
C6—C1—C2	115.27 (10)	C12—C11—C10	123.84 (11)
C6—C1—C7	124.47 (11)	C13—C12—C11	120.75 (12)
C2—C1—C7	120.22 (10)	C13—C12—H12	119.6
C3—C2—C1	122.86 (12)	C11—C12—H12	119.6
C3—C2—Cl1	118.09 (11)	C12—C13—C14	120.25 (12)
C1—C2—Cl1	119.05 (9)	C12—C13—H13	119.9
C4—C3—C2	119.60 (13)	C14—C13—H13	119.9
C4—C3—H3	120.2	C15—C14—C13	121.39 (12)
C2—C3—H3	120.2	C15—C14—H14	119.3
C3—C4—C5	119.84 (12)	C13—C14—H14	119.3
C3—C4—H4	120.1	C14—C15—C16	118.94 (12)
C5—C4—H4	120.1	C14—C15—H15	120.5
C4—C5—C6	119.24 (13)	C16—C15—H15	120.5
C4—C5—H5	120.4	N2—C16—C15	119.01 (10)
C6—C5—H5	120.4	N2—C16—C11	120.18 (10)
C1—C6—C5	123.18 (12)	C15—C16—C11	120.81 (10)
C1—C6—N1	119.51 (10)	C10—C17—H17A	109.5
C5—C6—N1	117.30 (11)	C10—C17—H17B	109.5
O2—C7—O1	126.71 (11)	H17A—C17—H17B	109.5
O2—C7—C1	118.40 (10)	C10—C17—H17C	109.5
O1—C7—C1	114.82 (10)	H17A—C17—H17C	109.5

N2—C8—C9	121.31 (10)	H17B—C17—H17C	109.5
C6—C1—C2—C3	0.13 (19)	C6—C1—C7—O1	98.00 (14)
C7—C1—C2—C3	−177.61 (12)	C2—C1—C7—O1	−84.49 (14)
C6—C1—C2—Cl1	−179.59 (9)	C16—N2—C8—C9	0.11 (17)
C7—C1—C2—Cl1	2.68 (16)	N2—C8—C9—C10	−0.05 (17)
C1—C2—C3—C4	0.9 (2)	C8—C9—C10—C11	−0.28 (17)
Cl1—C2—C3—C4	−179.40 (12)	C8—C9—C10—C17	−179.94 (11)
C2—C3—C4—C5	−0.7 (2)	C9—C10—C11—C16	0.54 (16)
C3—C4—C5—C6	−0.5 (2)	C17—C10—C11—C16	−179.80 (11)
C2—C1—C6—C5	−1.36 (18)	C9—C10—C11—C12	−179.58 (11)
C7—C1—C6—C5	176.26 (12)	C17—C10—C11—C12	0.08 (17)
C2—C1—C6—N1	177.02 (11)	C16—C11—C12—C13	0.15 (17)
C7—C1—C6—N1	−5.35 (18)	C10—C11—C12—C13	−179.73 (11)
C4—C5—C6—C1	1.6 (2)	C11—C12—C13—C14	−0.2 (2)
C4—C5—C6—N1	−176.84 (12)	C12—C13—C14—C15	0.1 (2)
O3B—N1—C6—C1	8.6 (14)	C13—C14—C15—C16	0.05 (19)
O3A—N1—C6—C1	−19.0 (5)	C8—N2—C16—C15	179.75 (10)
O4B—N1—C6—C1	−164.4 (14)	C8—N2—C16—C11	0.17 (16)
O4A—N1—C6—C1	157.3 (8)	C14—C15—C16—N2	−179.72 (11)
O3B—N1—C6—C5	−172.9 (14)	C14—C15—C16—C11	−0.15 (18)
O3A—N1—C6—C5	159.4 (5)	C12—C11—C16—N2	179.62 (10)
O4B—N1—C6—C5	14.1 (14)	C10—C11—C16—N2	−0.49 (16)
O4A—N1—C6—C5	−24.2 (8)	C12—C11—C16—C15	0.05 (16)
C6—C1—C7—O2	−84.88 (16)	C10—C11—C16—C15	179.94 (10)
C2—C1—C7—O2	92.63 (16)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84 (4)	1.71 (4)	2.5485 (13)	177 (6)
N2—H2···O1	0.89 (2)	1.66 (2)	2.5485 (13)	176 (2)
C5—H5···O1^{i}	0.95	2.49	3.1489 (15)	126
C13—H13···O2^{ii}	0.95	2.36	3.2889 (17)	165
C14—H14···*Cg*1^{ii}	0.95	2.89	3.6596 (15)	138

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

4-Methylquinolinium 3-chloro-2-nitrobenzoate (IV)

Crystal data

$C_{10}H_{9.54}N0.54+·C_7H_{3.46}ClNO_40.54−−$
M_r = 344.75
Triclinic, $P\overline{1}$
a = 7.5234 (10) Å
b = 7.8017 (11) Å
c = 13.6341 (17) Å
α = 80.934 (4)°
β = 80.227 (3)°
γ = 89.150 (4)°
V = 778.73 (18) Å^3
Z = 2
F(000) = 356.00
D_x = 1.470 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 14620 reflections
θ = 3.1–30.2°

μ = 0.27 mm^{-1}
T = 185 K

Block, colorless
0.35 × 0.29 × 0.22 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} = 0.914, T_{max} = 0.942
16767 measured reflections

4544 independent reflections
4017 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 30.0°, θ_{min} = 3.1°
h = −10→10
k = −10→10
l = −19→19

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.103
S = 1.07
4544 reflections
225 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.1388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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}	Occ. (<1)
Cl1	0.86435 (3)	0.88078 (4)	−0.07310 (2)	0.03700 (9)	
O1	0.32371 (11)	0.40966 (11)	0.26115 (7)	0.0398 (2)	
H1	0.318 (6)	0.339 (4)	0.3152 (18)	0.060*	0.46 (3)
O2	0.56467 (12)	0.53822 (11)	0.29489 (6)	0.03676 (18)	
O3	0.87768 (12)	0.52646 (12)	0.12927 (8)	0.0450 (2)	
O4	0.86170 (12)	0.78937 (12)	0.16317 (6)	0.0410 (2)	
N1	0.80578 (11)	0.66730 (12)	0.13027 (7)	0.02921 (18)	
N2	0.30583 (11)	0.21139 (11)	0.42899 (7)	0.02971 (18)	
H2	0.318 (4)	0.278 (3)	0.3693 (12)	0.045*	0.54 (3)
C1	0.47878 (12)	0.61791 (12)	0.13339 (7)	0.02463 (18)	
C2	0.64206 (12)	0.69496 (12)	0.08391 (7)	0.02335 (18)	
C3	0.65928 (13)	0.79149 (12)	−0.01201 (7)	0.02544 (18)	
C4	0.51016 (14)	0.81598 (14)	−0.06009 (8)	0.0305 (2)	
H4	0.520225	0.883772	−0.125138	0.037*	
C5	0.34671 (14)	0.74038 (14)	−0.01204 (9)	0.0318 (2)	
H5	0.244061	0.756140	−0.044445	0.038*	
C6	0.33155 (13)	0.64142 (13)	0.08340 (8)	0.0288 (2)	

H6	0.218788	0.589069	0.114930	0.035*
C7	0.45882 (13)	0.51586 (13)	0.23876 (8)	0.02791 (19)
C8	0.34235 (14)	0.26031 (14)	0.51192 (9)	0.0334 (2)
H8	0.382978	0.376070	0.508800	0.040*
C9	0.32371 (15)	0.14881 (15)	0.60416 (9)	0.0336 (2)
H9	0.350523	0.189658	0.662139	0.040*
C10	0.26665 (13)	−0.01971 (14)	0.61092 (8)	0.0293 (2)
C11	0.23111 (12)	−0.07674 (12)	0.52147 (7)	0.02621 (19)
C12	0.17762 (15)	−0.24889 (14)	0.51777 (9)	0.0347 (2)
H12	0.163822	−0.333039	0.577111	0.042*
C13	0.14562 (17)	−0.29488 (16)	0.42911 (10)	0.0403 (3)
H13	0.110950	−0.410964	0.427749	0.048*
C14	0.16351 (16)	−0.17203 (17)	0.33985 (10)	0.0395 (3)
H14	0.139455	−0.205611	0.279328	0.047*
C15	0.21525 (14)	−0.00529 (15)	0.34041 (8)	0.0329 (2)
H15	0.227352	0.077170	0.280383	0.039*
C16	0.25086 (12)	0.04439 (13)	0.43088 (7)	0.02605 (19)
C17	0.24210 (18)	−0.14002 (17)	0.70976 (9)	0.0420 (3)
H17A	0.116898	−0.182138	0.727282	0.063*
H17B	0.270185	−0.077702	0.762387	0.063*
H17C	0.323199	−0.238764	0.704128	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02892 (13)	0.04837 (17)	0.02927 (14)	−0.01052 (10)	0.00070 (10)	0.00234 (10)
O1	0.0339 (4)	0.0411 (4)	0.0395 (4)	−0.0140 (3)	−0.0068 (3)	0.0110 (3)
O2	0.0414 (4)	0.0382 (4)	0.0302 (4)	−0.0095 (3)	−0.0086 (3)	0.0001 (3)
O3	0.0310 (4)	0.0465 (5)	0.0587 (6)	0.0088 (3)	−0.0142 (4)	−0.0051 (4)
O4	0.0398 (4)	0.0503 (5)	0.0349 (4)	−0.0183 (4)	−0.0104 (3)	−0.0065 (3)
N1	0.0232 (4)	0.0370 (4)	0.0265 (4)	−0.0061 (3)	−0.0045 (3)	−0.0013 (3)
N2	0.0233 (4)	0.0298 (4)	0.0324 (4)	−0.0037 (3)	−0.0010 (3)	0.0027 (3)
C1	0.0232 (4)	0.0226 (4)	0.0273 (4)	−0.0020 (3)	−0.0026 (3)	−0.0029 (3)
C2	0.0211 (4)	0.0241 (4)	0.0254 (4)	−0.0013 (3)	−0.0045 (3)	−0.0049 (3)
C3	0.0240 (4)	0.0259 (4)	0.0255 (4)	−0.0036 (3)	−0.0013 (3)	−0.0040 (3)
C4	0.0318 (5)	0.0327 (5)	0.0265 (4)	0.0001 (4)	−0.0067 (4)	−0.0010 (4)
C5	0.0264 (5)	0.0354 (5)	0.0350 (5)	0.0005 (4)	−0.0103 (4)	−0.0041 (4)
C6	0.0219 (4)	0.0291 (5)	0.0350 (5)	−0.0025 (3)	−0.0043 (4)	−0.0038 (4)
C7	0.0263 (4)	0.0258 (4)	0.0292 (5)	−0.0017 (3)	−0.0010 (4)	−0.0009 (3)
C8	0.0259 (5)	0.0310 (5)	0.0428 (6)	−0.0037 (4)	−0.0042 (4)	−0.0056 (4)
C9	0.0287 (5)	0.0403 (6)	0.0339 (5)	0.0020 (4)	−0.0074 (4)	−0.0103 (4)
C10	0.0244 (4)	0.0352 (5)	0.0261 (4)	0.0056 (4)	−0.0021 (4)	−0.0015 (4)
C11	0.0211 (4)	0.0279 (4)	0.0269 (4)	0.0010 (3)	0.0004 (3)	−0.0007 (3)
C12	0.0340 (5)	0.0270 (5)	0.0388 (6)	−0.0009 (4)	0.0016 (4)	−0.0004 (4)
C13	0.0370 (6)	0.0336 (5)	0.0506 (7)	−0.0034 (4)	−0.0027 (5)	−0.0126 (5)
C14	0.0342 (5)	0.0488 (7)	0.0385 (6)	0.0007 (5)	−0.0064 (5)	−0.0164 (5)
C15	0.0286 (5)	0.0429 (6)	0.0259 (5)	0.0003 (4)	−0.0032 (4)	−0.0029 (4)
C16	0.0190 (4)	0.0299 (5)	0.0268 (4)	−0.0007 (3)	−0.0002 (3)	−0.0009 (3)

C17	0.0474 (7)	0.0469 (7)	0.0275 (5)	0.0104 (5)	−0.0033 (5)	0.0028 (4)

Geometric parameters (Å, º)

Cl1—C3	1.7240 (10)	C8—C9	1.3990 (16)
O1—C7	1.2857 (12)	C8—H8	0.9500
O1—H1	0.843 (10)	C9—C10	1.3735 (16)
O2—C7	1.2261 (13)	C9—H9	0.9500
O3—N1	1.2185 (13)	C10—C11	1.4289 (14)
O4—N1	1.2230 (12)	C10—C17	1.5010 (15)
N1—C2	1.4753 (12)	C11—C12	1.4186 (14)
N2—C8	1.3206 (15)	C11—C16	1.4194 (13)
N2—C16	1.3678 (13)	C12—C13	1.3733 (18)
N2—H2	0.885 (10)	C12—H12	0.9500
C1—C6	1.3913 (14)	C13—C14	1.4137 (19)
C1—C2	1.3922 (13)	C13—H13	0.9500
C1—C7	1.5134 (14)	C14—C15	1.3649 (17)
C2—C3	1.3891 (13)	C14—H14	0.9500
C3—C4	1.3887 (14)	C15—C16	1.4176 (14)
C4—C5	1.3840 (15)	C15—H15	0.9500
C4—H4	0.9500	C17—H17A	0.9800
C5—C6	1.3921 (15)	C17—H17B	0.9800
C5—H5	0.9500	C17—H17C	0.9800
C6—H6	0.9500		
C7—O1—H1	116 (3)	C10—C9—C8	120.01 (10)
O3—N1—O4	125.42 (10)	C10—C9—H9	120.0
O3—N1—C2	117.11 (9)	C8—C9—H9	120.0
O4—N1—C2	117.42 (9)	C9—C10—C11	118.16 (9)
C8—N2—C16	119.82 (9)	C9—C10—C17	120.72 (10)
C8—N2—H2	125 (2)	C11—C10—C17	121.12 (10)
C16—N2—H2	115 (2)	C12—C11—C16	117.78 (9)
C6—C1—C2	117.57 (9)	C12—C11—C10	123.60 (9)
C6—C1—C7	120.60 (8)	C16—C11—C10	118.62 (9)
C2—C1—C7	121.81 (8)	C13—C12—C11	120.54 (10)
C3—C2—C1	121.74 (9)	C13—C12—H12	119.7
C3—C2—N1	117.82 (8)	C11—C12—H12	119.7
C1—C2—N1	120.35 (8)	C12—C13—C14	120.97 (11)
C4—C3—C2	119.89 (9)	C12—C13—H13	119.5
C4—C3—Cl1	119.23 (8)	C14—C13—H13	119.5
C2—C3—Cl1	120.88 (7)	C15—C14—C13	120.16 (11)
C5—C4—C3	119.16 (9)	C15—C14—H14	119.9
C5—C4—H4	120.4	C13—C14—H14	119.9
C3—C4—H4	120.4	C14—C15—C16	119.76 (10)
C4—C5—C6	120.51 (9)	C14—C15—H15	120.1
C4—C5—H5	119.7	C16—C15—H15	120.1
C6—C5—H5	119.7	N2—C16—C15	118.62 (9)
C1—C6—C5	121.11 (9)	N2—C16—C11	120.61 (9)

C1—C6—H6	119.4	C15—C16—C11	120.78 (9)
C5—C6—H6	119.4	C10—C17—H17A	109.5
O2—C7—O1	125.49 (10)	C10—C17—H17B	109.5
O2—C7—C1	120.78 (9)	H17A—C17—H17B	109.5
O1—C7—C1	113.73 (9)	C10—C17—H17C	109.5
N2—C8—C9	122.75 (10)	H17A—C17—H17C	109.5
N2—C8—H8	118.6	H17B—C17—H17C	109.5
C9—C8—H8	118.6		

C6—C1—C2—C3	−0.26 (14)	C16—N2—C8—C9	−1.42 (16)
C7—C1—C2—C3	−178.70 (9)	N2—C8—C9—C10	0.53 (17)
C6—C1—C2—N1	−176.66 (9)	C8—C9—C10—C11	1.18 (15)
C7—C1—C2—N1	4.90 (14)	C8—C9—C10—C17	−178.68 (10)
O3—N1—C2—C3	−101.75 (11)	C9—C10—C11—C12	177.75 (10)
O4—N1—C2—C3	75.67 (12)	C17—C10—C11—C12	−2.39 (15)
O3—N1—C2—C1	74.79 (12)	C9—C10—C11—C16	−1.95 (14)
O4—N1—C2—C1	−107.78 (11)	C17—C10—C11—C16	177.91 (9)
C1—C2—C3—C4	1.32 (15)	C16—C11—C12—C13	−0.30 (15)
N1—C2—C3—C4	177.81 (9)	C10—C11—C12—C13	180.00 (10)
C1—C2—C3—Cl1	−178.25 (7)	C11—C12—C13—C14	−0.57 (18)
N1—C2—C3—Cl1	−1.76 (12)	C12—C13—C14—C15	0.76 (18)
C2—C3—C4—C5	−1.27 (15)	C13—C14—C15—C16	−0.06 (17)
Cl1—C3—C4—C5	178.31 (8)	C8—N2—C16—C15	−179.04 (9)
C3—C4—C5—C6	0.19 (16)	C8—N2—C16—C11	0.56 (14)
C2—C1—C6—C5	−0.84 (15)	C14—C15—C16—N2	178.77 (10)
C7—C1—C6—C5	177.62 (9)	C14—C15—C16—C11	−0.82 (15)
C4—C5—C6—C1	0.89 (16)	C12—C11—C16—N2	−178.59 (9)
C6—C1—C7—O2	−156.92 (10)	C10—C11—C16—N2	1.12 (14)
C2—C1—C7—O2	21.48 (15)	C12—C11—C16—C15	0.99 (14)
C6—C1—C7—O1	22.59 (14)	C10—C11—C16—C15	−179.29 (9)
C2—C1—C7—O1	−159.02 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84 (3)	1.70 (3)	2.5364 (13)	175 (3)
N2—H2···O1	0.89 (2)	1.65 (2)	2.5364 (13)	175 (3)
C6—H6···O3^{i}	0.95	2.59	3.4705 (14)	155
C9—H9···O2^{ii}	0.95	2.41	3.1739 (15)	137
C17—H17*C*···O2^{iii}	0.98	2.47	3.4155 (17)	162

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

4-Methylquinolinium 4-chloro-2-nitrobenzoate (V)

Crystal data

$C_{10}H_{10}N^{+}\cdot C_7H_3ClNO_4^{-}$
M_r = 344.75
Triclinic, $P\overline{1}$

a = 7.6858 (3) Å
b = 8.3615 (3) Å
c = 13.5746 (5) Å

α = 82.5485 (13)°
β = 80.8927 (12)°
γ = 65.0929 (11)°
V = 779.33 (5) Å^3
Z = 2
F(000) = 356.00
D_x = 1.469 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 19686 reflections
θ = 3.0–30.1°
μ = 0.27 mm^{-1}
T = 185 K
Platelet, colorless
0.51 × 0.45 × 0.15 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} = 0.868, T_{max} = 0.960
18635 measured reflections

3566 independent reflections
3290 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −9→9
k = −10→10
l = −17→17

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
3566 reflections
222 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
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.2103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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	0.68899 (5)	−0.41758 (5)	1.09613 (2)	0.04437 (12)
O1	0.55730 (12)	0.11536 (12)	0.67899 (7)	0.0343 (2)
O2	0.27487 (13)	0.08937 (13)	0.70351 (7)	0.0361 (2)
O3	0.04742 (14)	0.09528 (15)	0.90266 (8)	0.0491 (3)
O4	0.12351 (16)	−0.15067 (16)	0.83652 (9)	0.0518 (3)
N1	0.16299 (14)	−0.04644 (15)	0.87379 (8)	0.0336 (2)
N2	0.42785 (14)	0.30577 (13)	0.52175 (7)	0.0270 (2)
H2	0.483 (3)	0.226 (3)	0.5866 (16)	0.075 (6)*
C1	0.49025 (15)	−0.04440 (14)	0.82541 (8)	0.0237 (2)
C2	0.36650 (16)	−0.10303 (15)	0.89062 (8)	0.0255 (2)
C3	0.42201 (17)	−0.21590 (16)	0.97438 (9)	0.0291 (2)
H3	0.334084	−0.253809	1.017135	0.035*
C4	0.61139 (17)	−0.27175 (16)	0.99359 (9)	0.0289 (2)
C5	0.73961 (17)	−0.21407 (16)	0.93296 (9)	0.0294 (2)

H5	0.868057	−0.251966	0.948261	0.035*
C6	0.67764 (16)	−0.10049 (15)	0.84981 (9)	0.0271 (2)
H6	0.764664	−0.059768	0.808401	0.033*
C7	0.43193 (16)	0.06384 (15)	0.72882 (8)	0.0261 (2)
C8	0.50883 (17)	0.25320 (16)	0.43209 (9)	0.0304 (2)
H8	0.615416	0.141673	0.426068	0.036*
C9	0.44242 (18)	0.35661 (17)	0.34601 (9)	0.0314 (3)
H9	0.504996	0.315398	0.282367	0.038*
C10	0.28780 (17)	0.51732 (16)	0.35173 (9)	0.0291 (2)
C11	0.19978 (16)	0.57586 (15)	0.44844 (9)	0.0264 (2)
C12	0.04213 (18)	0.74036 (17)	0.46435 (11)	0.0350 (3)
H12	−0.011398	0.817344	0.408744	0.042*
C13	−0.03350 (19)	0.78908 (18)	0.55913 (12)	0.0400 (3)
H13	−0.138711	0.900418	0.568996	0.048*
C14	0.0424 (2)	0.67651 (19)	0.64235 (10)	0.0393 (3)
H14	−0.012424	0.712464	0.707852	0.047*
C15	0.19339 (18)	0.51667 (17)	0.63033 (9)	0.0327 (3)
H15	0.243434	0.440717	0.686908	0.039*
C16	0.27446 (16)	0.46528 (15)	0.53306 (8)	0.0253 (2)
C17	0.2148 (2)	0.6286 (2)	0.25939 (10)	0.0405 (3)
H17A	0.075011	0.665044	0.263552	0.061*
H17B	0.278616	0.560052	0.200744	0.061*
H17C	0.243044	0.733558	0.253298	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0431 (2)	0.0486 (2)	0.03629 (19)	−0.01563 (16)	−0.01541 (14)	0.01651 (14)
O1	0.0291 (4)	0.0417 (5)	0.0307 (4)	−0.0157 (4)	−0.0063 (3)	0.0105 (4)
O2	0.0291 (4)	0.0476 (5)	0.0321 (4)	−0.0169 (4)	−0.0112 (3)	0.0094 (4)
O3	0.0271 (5)	0.0596 (7)	0.0399 (5)	0.0006 (5)	−0.0017 (4)	0.0002 (5)
O4	0.0427 (6)	0.0587 (7)	0.0673 (7)	−0.0319 (5)	−0.0236 (5)	0.0105 (5)
N1	0.0237 (5)	0.0446 (6)	0.0295 (5)	−0.0139 (5)	−0.0045 (4)	0.0094 (4)
N2	0.0260 (5)	0.0278 (5)	0.0268 (5)	−0.0114 (4)	−0.0037 (4)	0.0016 (4)
C1	0.0229 (5)	0.0244 (5)	0.0231 (5)	−0.0086 (4)	−0.0033 (4)	−0.0019 (4)
C2	0.0213 (5)	0.0285 (5)	0.0254 (5)	−0.0085 (4)	−0.0039 (4)	−0.0018 (4)
C3	0.0275 (6)	0.0331 (6)	0.0257 (5)	−0.0127 (5)	−0.0026 (4)	0.0017 (4)
C4	0.0313 (6)	0.0283 (5)	0.0243 (5)	−0.0089 (5)	−0.0073 (4)	0.0013 (4)
C5	0.0240 (5)	0.0328 (6)	0.0303 (6)	−0.0094 (4)	−0.0079 (4)	0.0000 (5)
C6	0.0244 (5)	0.0298 (5)	0.0277 (5)	−0.0116 (4)	−0.0036 (4)	−0.0010 (4)
C7	0.0252 (5)	0.0262 (5)	0.0245 (5)	−0.0083 (4)	−0.0038 (4)	−0.0003 (4)
C8	0.0270 (6)	0.0286 (5)	0.0333 (6)	−0.0096 (4)	−0.0013 (4)	−0.0035 (5)
C9	0.0334 (6)	0.0371 (6)	0.0255 (5)	−0.0168 (5)	0.0003 (4)	−0.0042 (5)
C10	0.0305 (6)	0.0346 (6)	0.0272 (5)	−0.0189 (5)	−0.0057 (4)	0.0031 (5)
C11	0.0249 (5)	0.0275 (5)	0.0294 (5)	−0.0135 (4)	−0.0044 (4)	0.0007 (4)
C12	0.0295 (6)	0.0293 (6)	0.0450 (7)	−0.0105 (5)	−0.0086 (5)	0.0014 (5)
C13	0.0295 (6)	0.0317 (6)	0.0548 (8)	−0.0079 (5)	−0.0006 (5)	−0.0104 (6)
C14	0.0362 (7)	0.0434 (7)	0.0386 (7)	−0.0168 (6)	0.0054 (5)	−0.0141 (6)

C15	0.0345 (6)	0.0379 (6)	0.0278 (6)	−0.0173 (5)	−0.0010 (5)	−0.0035 (5)
C16	0.0246 (5)	0.0268 (5)	0.0270 (5)	−0.0131 (4)	−0.0027 (4)	−0.0016 (4)
C17	0.0429 (7)	0.0485 (8)	0.0309 (6)	−0.0212 (6)	−0.0104 (5)	0.0106 (6)

Geometric parameters (Å, º)

Cl1—C4	1.7291 (12)	C8—C9	1.3887 (17)
O1—C7	1.2804 (14)	C8—H8	0.9500
O2—C7	1.2313 (14)	C9—C10	1.3699 (18)
O3—N1	1.2127 (15)	C9—H9	0.9500
O4—N1	1.2220 (16)	C10—C11	1.4239 (16)
N1—C2	1.4780 (14)	C10—C17	1.4938 (17)
N2—C8	1.3156 (15)	C11—C16	1.4107 (16)
N2—C16	1.3652 (15)	C11—C12	1.4132 (17)
N2—H2	1.06 (2)	C12—C13	1.364 (2)
C1—C2	1.3936 (15)	C12—H12	0.9500
C1—C6	1.3948 (15)	C13—C14	1.405 (2)
C1—C7	1.5085 (15)	C13—H13	0.9500
C2—C3	1.3790 (16)	C14—C15	1.3601 (19)
C3—C4	1.3859 (17)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.4062 (16)
C4—C5	1.3863 (17)	C15—H15	0.9500
C5—C6	1.3834 (16)	C17—H17A	0.9800
C5—H5	0.9500	C17—H17B	0.9800
C6—H6	0.9500	C17—H17C	0.9800
O3—N1—O4	125.32 (12)	C10—C9—C8	120.82 (11)
O3—N1—C2	117.47 (11)	C10—C9—H9	119.6
O4—N1—C2	117.09 (11)	C8—C9—H9	119.6
C8—N2—C16	120.67 (10)	C9—C10—C11	117.95 (11)
C8—N2—H2	120.5 (12)	C9—C10—C17	121.06 (11)
C16—N2—H2	118.8 (12)	C11—C10—C17	120.99 (11)
C2—C1—C6	116.89 (10)	C16—C11—C12	118.02 (11)
C2—C1—C7	122.38 (10)	C16—C11—C10	118.57 (10)
C6—C1—C7	120.58 (10)	C12—C11—C10	123.40 (11)
C3—C2—C1	123.52 (10)	C13—C12—C11	120.30 (12)
C3—C2—N1	115.15 (10)	C13—C12—H12	119.9
C1—C2—N1	121.33 (10)	C11—C12—H12	119.9
C2—C3—C4	117.23 (10)	C12—C13—C14	120.75 (12)
C2—C3—H3	121.4	C12—C13—H13	119.6
C4—C3—H3	121.4	C14—C13—H13	119.6
C3—C4—C5	121.84 (11)	C15—C14—C13	120.82 (12)
C3—C4—Cl1	118.83 (9)	C15—C14—H14	119.6
C5—C4—Cl1	119.33 (9)	C13—C14—H14	119.6
C6—C5—C4	118.97 (11)	C14—C15—C16	119.15 (12)
C6—C5—H5	120.5	C14—C15—H15	120.4
C4—C5—H5	120.5	C16—C15—H15	120.4
C5—C6—C1	121.49 (11)	N2—C16—C15	118.72 (11)

C5—C6—H6	119.3	N2—C16—C11	120.32 (10)
C1—C6—H6	119.3	C15—C16—C11	120.96 (11)
O2—C7—O1	126.25 (11)	C10—C17—H17A	109.5
O2—C7—C1	118.37 (10)	C10—C17—H17B	109.5
O1—C7—C1	115.33 (10)	H17A—C17—H17B	109.5
N2—C8—C9	121.66 (11)	C10—C17—H17C	109.5
N2—C8—H8	119.2	H17A—C17—H17C	109.5
C9—C8—H8	119.2	H17B—C17—H17C	109.5
C6—C1—C2—C3	−2.12 (17)	C16—N2—C8—C9	−0.01 (17)
C7—C1—C2—C3	173.58 (10)	N2—C8—C9—C10	−0.70 (18)
C6—C1—C2—N1	177.81 (10)	C8—C9—C10—C11	1.00 (17)
C7—C1—C2—N1	−6.48 (16)	C8—C9—C10—C17	−179.56 (11)
O3—N1—C2—C3	97.04 (13)	C9—C10—C11—C16	−0.65 (16)
O4—N1—C2—C3	−79.28 (14)	C17—C10—C11—C16	179.91 (10)
O3—N1—C2—C1	−82.90 (14)	C9—C10—C11—C12	178.67 (11)
O4—N1—C2—C1	100.78 (14)	C17—C10—C11—C12	−0.77 (18)
C1—C2—C3—C4	0.31 (18)	C16—C11—C12—C13	0.21 (17)
N1—C2—C3—C4	−179.63 (10)	C10—C11—C12—C13	−179.11 (11)
C2—C3—C4—C5	1.49 (18)	C11—C12—C13—C14	−0.6 (2)
C2—C3—C4—Cl1	−178.45 (9)	C12—C13—C14—C15	0.2 (2)
C3—C4—C5—C6	−1.37 (18)	C13—C14—C15—C16	0.49 (19)
Cl1—C4—C5—C6	178.58 (9)	C8—N2—C16—C15	−179.53 (11)
C4—C5—C6—C1	−0.58 (18)	C8—N2—C16—C11	0.35 (16)
C2—C1—C6—C5	2.23 (16)	C14—C15—C16—N2	179.02 (11)
C7—C1—C6—C5	−173.56 (10)	C14—C15—C16—C11	−0.86 (18)
C2—C1—C7—O2	−5.64 (16)	C12—C11—C16—N2	−179.37 (10)
C6—C1—C7—O2	169.91 (11)	C10—C11—C16—N2	−0.01 (16)
C2—C1—C7—O1	176.77 (10)	C12—C11—C16—C15	0.51 (16)
C6—C1—C7—O1	−7.68 (15)	C10—C11—C16—C15	179.86 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	1.06 (2)	1.50 (2)	2.5568 (13)	179 (4)
C8—H8···O2^{i}	0.95	2.56	3.2779 (16)	132
C12—H12···O2^{ii}	0.95	2.52	3.3391 (18)	144

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

4-Methylquinolinium 5-chloro-2-nitrobenzoate (VI)

Crystal data

$C_{10}H_{10}N^{+}.C_7H_3ClNO_4^{-}$
M_r = 344.75
Monoclinic, *C*2/*c*
a = 16.2625 (10) Å
b = 7.5099 (4) Å
c = 25.3105 (15) Å
β = 99.4086 (19)°
V = 3049.6 (3) Å^3
Z = 8
F(000) = 1424.00
D_x = 1.502 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71075 Å
Cell parameters from 24067 reflections
θ = 3.0–30.0°

μ = 0.28 mm^{-1}
T = 190 K

Prism, colorless
0.30 × 0.21 × 0.12 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} = 0.916, T_{max} = 0.968
29037 measured reflections

4457 independent reflections
3913 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 30.0°, θ_{min} = 3.0°
h = −22→22
k = −10→10
l = −35→35

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.05
4457 reflections
222 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 1.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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	0.35497 (2)	0.25440 (3)	0.21927 (2)	0.03174 (9)
O1	0.58343 (5)	0.52232 (13)	0.37347 (3)	0.0379 (2)
O2	0.51224 (5)	0.73265 (12)	0.40930 (3)	0.03410 (19)
O3	0.50836 (5)	1.00336 (12)	0.32498 (4)	0.0393 (2)
O4	0.38124 (6)	1.04110 (12)	0.33823 (3)	0.03630 (19)
N1	0.43689 (6)	0.95186 (12)	0.32389 (3)	0.02602 (17)
N2	0.70950 (5)	0.49554 (12)	0.44591 (3)	0.02496 (17)
C1	0.45930 (6)	0.62497 (13)	0.32235 (4)	0.02159 (18)
C2	0.41499 (6)	0.77444 (13)	0.30138 (4)	0.02245 (18)
C3	0.35187 (7)	0.76754 (14)	0.25743 (4)	0.0276 (2)
H3	0.322449	0.872401	0.244702	0.033*
C4	0.33229 (6)	0.60562 (15)	0.23234 (4)	0.0279 (2)
H4	0.289265	0.597431	0.202146	0.033*
C5	0.37668 (6)	0.45573 (13)	0.25212 (4)	0.02356 (18)
C6	0.43909 (6)	0.46287 (13)	0.29667 (4)	0.02320 (18)
H6	0.467928	0.357532	0.309587	0.028*
C7	0.52359 (6)	0.63089 (13)	0.37316 (4)	0.02337 (18)

C8	0.77132 (6)	0.42632 (14)	0.42468 (4)	0.0276 (2)
H8	0.763497	0.406693	0.387111	0.033*
C9	0.84757 (6)	0.38107 (14)	0.45538 (4)	0.0267 (2)
H9	0.890820	0.332639	0.438694	0.032*
C10	0.86007 (6)	0.40684 (13)	0.51013 (4)	0.02478 (19)
C11	0.79365 (6)	0.48165 (13)	0.53362 (4)	0.02323 (18)
C12	0.79902 (7)	0.51180 (16)	0.58948 (4)	0.0313 (2)
H12	0.849207	0.485426	0.613072	0.038*
C13	0.73200 (8)	0.57880 (18)	0.60938 (5)	0.0362 (2)
H13	0.735942	0.596465	0.646879	0.043*
C14	0.65709 (7)	0.62213 (17)	0.57515 (5)	0.0335 (2)
H14	0.611455	0.669217	0.589773	0.040*
C15	0.64983 (6)	0.59662 (15)	0.52088 (4)	0.0283 (2)
H15	0.599673	0.626737	0.497774	0.034*
C16	0.71795 (6)	0.52500 (13)	0.49994 (4)	0.02273 (18)
C17	0.94142 (7)	0.35605 (17)	0.54355 (5)	0.0340 (2)
H17A	0.967677	0.462034	0.561585	0.051*
H17B	0.978265	0.304870	0.520528	0.051*
H17C	0.931537	0.268016	0.570401	0.051*
H2	0.6559 (13)	0.524 (3)	0.4196 (9)	0.074 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03751 (15)	0.02625 (13)	0.03075 (14)	−0.00503 (9)	0.00350 (11)	−0.00484 (9)
O1	0.0330 (4)	0.0476 (5)	0.0287 (4)	0.0189 (4)	−0.0077 (3)	−0.0084 (3)
O2	0.0337 (4)	0.0406 (5)	0.0259 (4)	0.0105 (3)	−0.0015 (3)	−0.0072 (3)
O3	0.0335 (4)	0.0350 (4)	0.0470 (5)	−0.0106 (3)	−0.0008 (4)	−0.0006 (4)
O4	0.0455 (5)	0.0292 (4)	0.0349 (4)	0.0063 (3)	0.0084 (4)	−0.0037 (3)
N1	0.0308 (4)	0.0231 (4)	0.0224 (4)	−0.0004 (3)	−0.0007 (3)	0.0023 (3)
N2	0.0237 (4)	0.0265 (4)	0.0234 (4)	0.0025 (3)	0.0004 (3)	0.0026 (3)
C1	0.0187 (4)	0.0252 (4)	0.0205 (4)	0.0016 (3)	0.0021 (3)	0.0008 (3)
C2	0.0220 (4)	0.0225 (4)	0.0222 (4)	0.0001 (3)	0.0018 (3)	0.0002 (3)
C3	0.0257 (5)	0.0259 (5)	0.0282 (5)	0.0033 (3)	−0.0041 (4)	0.0019 (4)
C4	0.0249 (4)	0.0299 (5)	0.0261 (4)	0.0000 (4)	−0.0044 (4)	−0.0005 (4)
C5	0.0233 (4)	0.0238 (4)	0.0237 (4)	−0.0025 (3)	0.0043 (3)	−0.0021 (3)
C6	0.0218 (4)	0.0238 (4)	0.0240 (4)	0.0022 (3)	0.0038 (3)	0.0015 (3)
C7	0.0220 (4)	0.0262 (4)	0.0208 (4)	0.0016 (3)	0.0001 (3)	0.0020 (3)
C8	0.0283 (5)	0.0294 (5)	0.0248 (4)	0.0018 (4)	0.0038 (4)	0.0015 (4)
C9	0.0234 (4)	0.0270 (5)	0.0300 (5)	0.0023 (3)	0.0049 (4)	0.0009 (4)
C10	0.0213 (4)	0.0212 (4)	0.0303 (5)	−0.0004 (3)	−0.0004 (3)	0.0018 (4)
C11	0.0220 (4)	0.0216 (4)	0.0247 (4)	−0.0012 (3)	−0.0005 (3)	0.0020 (3)
C12	0.0300 (5)	0.0361 (6)	0.0252 (5)	−0.0005 (4)	−0.0028 (4)	−0.0005 (4)
C13	0.0389 (6)	0.0431 (6)	0.0258 (5)	0.0008 (5)	0.0026 (4)	−0.0053 (5)
C14	0.0321 (5)	0.0360 (6)	0.0333 (5)	0.0040 (4)	0.0084 (4)	−0.0044 (4)
C15	0.0247 (4)	0.0290 (5)	0.0307 (5)	0.0040 (4)	0.0029 (4)	0.0001 (4)
C16	0.0226 (4)	0.0208 (4)	0.0238 (4)	0.0002 (3)	0.0008 (3)	0.0021 (3)
C17	0.0226 (5)	0.0376 (6)	0.0387 (6)	0.0040 (4)	−0.0042 (4)	0.0001 (5)

Geometric parameters (Å, º)

Cl1—C5	1.7338 (10)	C8—C9	1.3935 (14)
O1—C7	1.2686 (12)	C8—H8	0.9500
O2—C7	1.2288 (13)	C9—C10	1.3811 (15)
O3—N1	1.2211 (12)	C9—H9	0.9500
O4—N1	1.2277 (12)	C10—C11	1.4303 (14)
N1—C2	1.4698 (13)	C10—C17	1.4985 (14)
N2—C8	1.3215 (13)	C11—C16	1.4159 (13)
N2—C16	1.3700 (13)	C11—C12	1.4204 (14)
N2—H2	1.03 (2)	C12—C13	1.3691 (17)
C1—C2	1.3913 (13)	C12—H12	0.9500
C1—C6	1.3938 (14)	C13—C14	1.4128 (17)
C1—C7	1.5197 (13)	C13—H13	0.9500
C2—C3	1.3858 (14)	C14—C15	1.3726 (16)
C3—C4	1.3847 (15)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.4105 (14)
C4—C5	1.3859 (14)	C15—H15	0.9500
C4—H4	0.9500	C17—H17A	0.9800
C5—C6	1.3893 (14)	C17—H17B	0.9800
C6—H6	0.9500	C17—H17C	0.9800
O3—N1—O4	124.43 (10)	C10—C9—C8	119.80 (9)
O3—N1—C2	117.73 (9)	C10—C9—H9	120.1
O4—N1—C2	117.77 (9)	C8—C9—H9	120.1
C8—N2—C16	120.70 (9)	C9—C10—C11	118.34 (9)
C8—N2—H2	116.0 (12)	C9—C10—C17	120.16 (9)
C16—N2—H2	123.3 (12)	C11—C10—C17	121.50 (9)
C2—C1—C6	117.31 (8)	C16—C11—C12	117.94 (9)
C2—C1—C7	122.75 (9)	C16—C11—C10	118.79 (9)
C6—C1—C7	119.82 (8)	C12—C11—C10	123.27 (9)
C3—C2—C1	123.05 (9)	C13—C12—C11	120.11 (10)
C3—C2—N1	116.47 (9)	C13—C12—H12	119.9
C1—C2—N1	120.40 (8)	C11—C12—H12	119.9
C4—C3—C2	119.06 (9)	C12—C13—C14	121.17 (10)
C4—C3—H3	120.5	C12—C13—H13	119.4
C2—C3—H3	120.5	C14—C13—H13	119.4
C3—C4—C5	118.71 (9)	C15—C14—C13	120.40 (10)
C3—C4—H4	120.6	C15—C14—H14	119.8
C5—C4—H4	120.6	C13—C14—H14	119.8
C4—C5—C6	122.02 (9)	C14—C15—C16	119.00 (10)
C4—C5—Cl1	118.81 (8)	C14—C15—H15	120.5
C6—C5—Cl1	119.16 (8)	C16—C15—H15	120.5
C5—C6—C1	119.83 (9)	N2—C16—C15	118.68 (9)
C5—C6—H6	120.1	N2—C16—C11	119.95 (9)
C1—C6—H6	120.1	C15—C16—C11	121.37 (9)
O2—C7—O1	127.13 (9)	C10—C17—H17A	109.5
O2—C7—C1	118.80 (9)	C10—C17—H17B	109.5

O1—C7—C1	114.03 (8)	H17A—C17—H17B	109.5
N2—C8—C9	122.41 (10)	C10—C17—H17C	109.5
N2—C8—H8	118.8	H17A—C17—H17C	109.5
C9—C8—H8	118.8	H17B—C17—H17C	109.5
C6—C1—C2—C3	1.16 (15)	C16—N2—C8—C9	−0.41 (16)
C7—C1—C2—C3	−174.95 (9)	N2—C8—C9—C10	0.62 (17)
C6—C1—C2—N1	−175.55 (8)	C8—C9—C10—C11	−0.59 (15)
C7—C1—C2—N1	8.33 (14)	C8—C9—C10—C17	179.10 (10)
O3—N1—C2—C3	−120.32 (11)	C9—C10—C11—C16	0.39 (14)
O4—N1—C2—C3	56.69 (13)	C17—C10—C11—C16	−179.29 (10)
O3—N1—C2—C1	56.60 (13)	C9—C10—C11—C12	179.10 (10)
O4—N1—C2—C1	−126.39 (10)	C17—C10—C11—C12	−0.58 (16)
C1—C2—C3—C4	−1.07 (16)	C16—C11—C12—C13	0.76 (16)
N1—C2—C3—C4	175.77 (9)	C10—C11—C12—C13	−177.96 (11)
C2—C3—C4—C5	−0.02 (16)	C11—C12—C13—C14	−1.11 (19)
C3—C4—C5—C6	0.97 (16)	C12—C13—C14—C15	0.4 (2)
C3—C4—C5—Cl1	−177.60 (8)	C13—C14—C15—C16	0.59 (18)
C4—C5—C6—C1	−0.86 (15)	C8—N2—C16—C15	−179.05 (10)
Cl1—C5—C6—C1	177.70 (7)	C8—N2—C16—C11	0.20 (15)
C2—C1—C6—C5	−0.20 (14)	C14—C15—C16—N2	178.31 (10)
C7—C1—C6—C5	176.04 (9)	C14—C15—C16—C11	−0.93 (16)
C2—C1—C7—O2	34.14 (15)	C12—C11—C16—N2	−178.97 (9)
C6—C1—C7—O2	−141.88 (10)	C10—C11—C16—N2	−0.19 (14)
C2—C1—C7—O1	−147.73 (10)	C12—C11—C16—C15	0.25 (15)
C6—C1—C7—O1	36.25 (13)	C10—C11—C16—C15	179.04 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	1.03 (2)	1.52 (2)	2.5252 (11)	165 (2)
C9—H9···O2^{i}	0.95	2.34	3.2856 (13)	171
C12—H12···O3^{ii}	0.95	2.58	3.5065 (14)	166
C15—H15···O2	0.95	2.57	3.4583 (13)	155
C17—H17*A*···O2^{ii}	0.98	2.41	3.3524 (16)	160

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