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4-Nitrophenyl 2-iodobenzoate: sheets built from C—H···O hydrogen bonds and two-centre iodo–nitro interactions

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Molecules of the title compound, $C_{13}H_8INO_4$, are linked into complex sheets by two C—H···O hydrogen bonds and one two-centre iodo–nitro interaction.

Comment

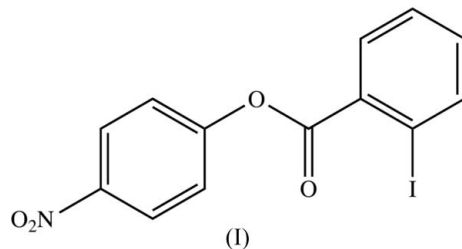We have recently reported the molecular and supramolecular structures of a wide range of iodoaryl–nitroaryl compounds, including sulfonamides (Kelly *et al.*, 2002), benzylideneanilines (Glidewell, Howie *et al.*, 2002; Wardell *et al.*, 2002), benzylanilines (Glidewell, Low *et al.*, 2002; Glidewell, Low, Skakle, Wardell & Wardell, 2004; Ferguson *et al.*, 2005), phenylhydrazones (Glidewell, Low, Skakle & Wardell, 2004; Glidewell *et al.*, 2003), 1,4-diaryl-2,3-diaza-1,3-butadienes (Glidewell, Low, Skakle & Wardell, 2005), N-(iodophenyl)-nitrophthalimides (Glidewell, Low, Skakle, Wardell & Wardell, 2005) and benzoylhydrazones (Glidewell, Low & Wardell, 2005). We have now extended this investigation to include the title ester, 4-nitrophenyl 2-iodobenzoate, (I).

Within the molecule of (I) (Fig. 1), the central ester fragment between atoms C11 and C21 is effectively planar, but the iodinated and nitrated aryl rings make dihedral angles with this plane of 39.9 (2) and 42.7 (2)°, respectively, probably in
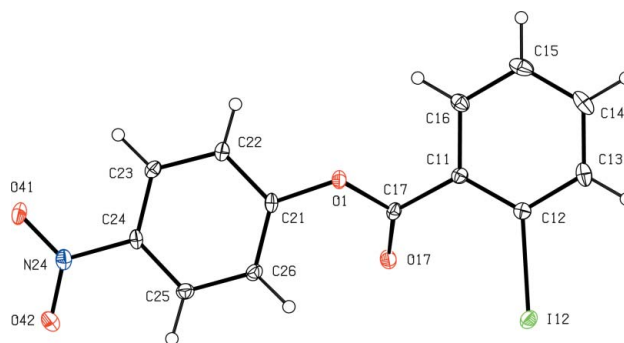

Figure 1
The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

order to minimize the repulsive intramolecular contacts involving the polarized atom O17. The nitro group makes a dihedral angle of 7.4 (2)° with the adjacent aryl ring. The bond distances and inter-bond angles show no unusual values.

The molecules are linked into complex sheets, the formation of which is readily analysed in terms of two one-dimensional substructures. In the simpler of the two substructures, atom C14 in the iodinated ring of the molecule at (x, y, z) acts as hydrogen-bond donor to carbonyl atom O17 in the molecule at $(\frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z)$, thereby forming a $C(7)$ (Bernstein *et al.*, 1995) chain running parallel to the [10$\bar{1}$] direction and generated by the *n*-glide plane at $y = 0.75$ (Fig. 2).

The second substructure is built from a combination of a C—H···O hydrogen bond and an iodo–nitro interaction. Atom C26 in the nitrated ring of the molecule at (x, y, z) acts as hydrogen-bond donor to nitro atom O42 in the molecule at $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z)$, so forming a $C(6)$ chain running parallel to the [010] direction and generated by the 2_1 screw axis along $(\frac{1}{4}, y, \frac{3}{4})$ (Fig. 3). In addition, atom I12 in the molecule at (x, y, z) forms a short contact with atom O41 in the molecule at $(x, 1 + y, z)$, with I···O^i = 3.240 (2) Å and C—I···O^i = 169.8 (2)° [symmetry code: (i) $x, 1 + y, z$], thus generating by translation a $C(11)$ (Starbuck *et al.*, 1999) chain, also running parallel to the [010] direction. The combination of these two interactions then generates a [010] chain of edge-fused $R_3^3(17)$ rings (Fig. 3).

The combination of the [010] and [10$\bar{1}$] chains generates a (101) sheet in the form of a (4,4)-net. If just the C—H···O hydrogen bonds are considered, this sheet is built from two types of $R_4^4(38)$ ring (Fig. 4).

Figure 2
Part of the crystal structure of (I), showing the formation of a $C(7)$ chain along [10$\bar{1}$]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(\frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z)$ and $(-\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z)$, respectively.

Experimental

A solution containing equimolar quantities (2 mmol of each) of 4-nitrophenol and 2-iodobenzoyl chloride in chloroform (50 ml) was heated under reflux for 1 h; the solvent was removed under reduced pressure and the resulting solid residue was recrystallized from ethanol to yield crystals suitable for single-crystal X-ray diffraction.

Crystal data

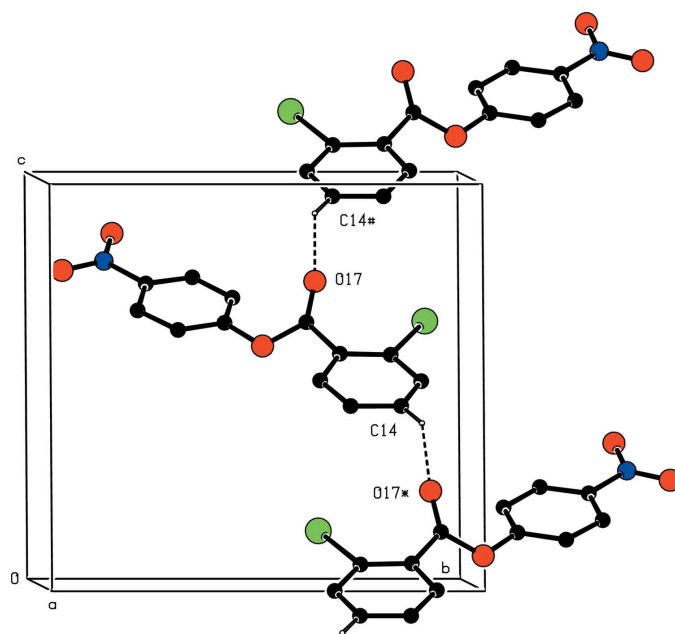|	
$C_{13}H_8INO_4$	$D_x = 1.940$ Mg m^{-3}
$M_r = 369.10$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2905
$a = 9.7231$ (4) Å	reflections
$b = 11.7890$ (3) Å	$\theta = 3.0$–$27.5°$
$c = 11.1187$ (4) Å	$\mu = 2.54$ mm^{-1}
$\beta = 97.363$ (2)°	$T = 120$ (2) K
$V = 1263.98$ (8) Å^3	Plate, colourless
$Z = 4$	$0.10 \times 0.08 \times 0.01$ mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer	2905 independent reflections
	2570 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.036$
Absorption correction: multi-scan	$\theta_{max} = 27.5°$
(*SADABS*; Sheldrick, 2003)	$h = -12 \rightarrow 11$
$T_{min} = 0.814$, $T_{max} = 0.975$	$k = -13 \rightarrow 15$
12630 measured reflections	$l = -14 \rightarrow 14$

Figure 3
Part of the crystal structure of (I), showing the formation of a chain of edge-fused $R_3^3(17)$ rings along [010]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*), a hash (#) or an ampersand (&) are at the symmetry positions $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z)$, $(x, 1 + y, z)$ and $(\frac{1}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z)$, respectively.

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Figure 4
Stereoview of part of the crystal structure of compound (I), showing the formation of a hydrogen-bonded (101) sheet of $R_4^4(38)$ rings. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.026$	$+ 1.8703P]$
$wR(F^2) = 0.058$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
2905 reflections	$\Delta\rho_{max} = 0.80$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.91$ e Å^{-3}
H-atom parameters constrained	

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C14—H14$\cdots$O17[i]	0.95	2.50	3.334 (3)	147
C26—H26$\cdots$O42[ii]	0.95	2.54	3.395 (3)	149

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

All H atoms were located in difference maps and then treated as riding atoms, with C—H distances of 0.95 Å and $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97*

(Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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Wardell, J. L., Wardell, S. M. S. V., Skakle, J. M. S., Low, J. N. & Glidewell, C. (2002). *Acta Cryst.* C**58**, o428–o430.

supporting information

4-Nitrophenyl 2-iodobenzoate: sheets built from C—H···O hydrogen bonds and two-centre iodo–nitro interactions

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S1. Comment

We have recently reported the molecular and supramolecular structures of a wide range of iodoaryl–nitroaryl compounds, including sulfonamides (Kelly *et al.*, 2002), benzylideneanilines (Glidewell, Howie *et al.*, 2002; Wardell *et al.*, 2002), benzylanilines (Glidewell, Low *et al.*, 2002; Glidewell, Low, Skakle, Wardell & Wardell, 2004; Ferguson *et al.*, 2005), phenylhydrazones (Glidewell, Low, Skakle & Wardell, 2004; Glidewell *et al.*, 2003), 1,4-diaryl-2,3-diaza-1,3-butadienes (Glidewell, Low, Skakle & Wardell, 2005), *N*-(iodophenyl)nitrophthalimides (Glidewell, Low, Skakle, Wardell & Wardell, 2005) and benzoylhydrazones (Glidewell, Low & Wardell, 2005). We have now extended this investigation to include the title ester 4-nitrophenyl 2-iodobenzoate, (I).

Within the molecule of (I) (Fig. 1), the central ester fragment between atoms C11 and C21 is effectively planar, but the iodinated and nitrated aryl rings make dihedral angles with this plane of 39.9 (2) and 42.7 (2)°, respectively, probably in order to minimize the repulsive intramolecular contacts involving the polarized atom O17: the nitro group makes a dihedral angle of 7.4 (2)° with the adjacent aryl ring. The bond distances and inter-bond angles show no unusual values.

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The second substructure is built from a combination of a C—H···O hydrogen bond and an iodo–nitro interaction. Atom C26 in the nitrated ring of the molecule at (x, y, z) acts as hydrogen-bond donor to nitro atom O42 in the molecule at $(1/2 − x, 1/2 + y, 1.5 − z)$, so forming a $C(6)$ chain running parallel to the [010] direction and generated by the 2_1 screw axis along $(1/4, y, 3/4)$ (Fig. 3). In addition, atom I12 in the molecule at (x, y, z) forms a short contact with atom O41 in the molecule at $(x, 1 + y, z)$, with I···O^i = 3.240 (2) Å and C—I···O^i = 169.8 (2)° [symmetry code: (i) $x, 1 + y, z$], thus generating by translation a $C(11)$ (Starbuck *et al.*, 1999) chain, also running parallel to the [010] direction. The combination of these two interactions then generates a [010] chain of edge-fused $R_3^3(17)$ rings (Fig. 3)

The combination of the [010] and $[10\overline{1}]$ chains generates a (101) sheet in the form of a (4,4)-net: if just the C—H···O hydrogen bonds are considered, this sheet is built from two types of $R_4^4(38)$ ring (Fig. 4).

S2. Experimental

A solution containing equimolar quantities (2 mmol of each) of 4-nitrophenol and 2-iodobenzoyl chloride in chloroform (50 ml) was heated under reflux for 1 h; the solvent was removed under reduced pressure and the resulting solid residue was recrystallized from ethanol to yield crystals suitable for single-crystal X-ray diffraction.

S3. Refinement

All H atoms were located from difference maps and then treated as riding atoms, with C—H distances of 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.
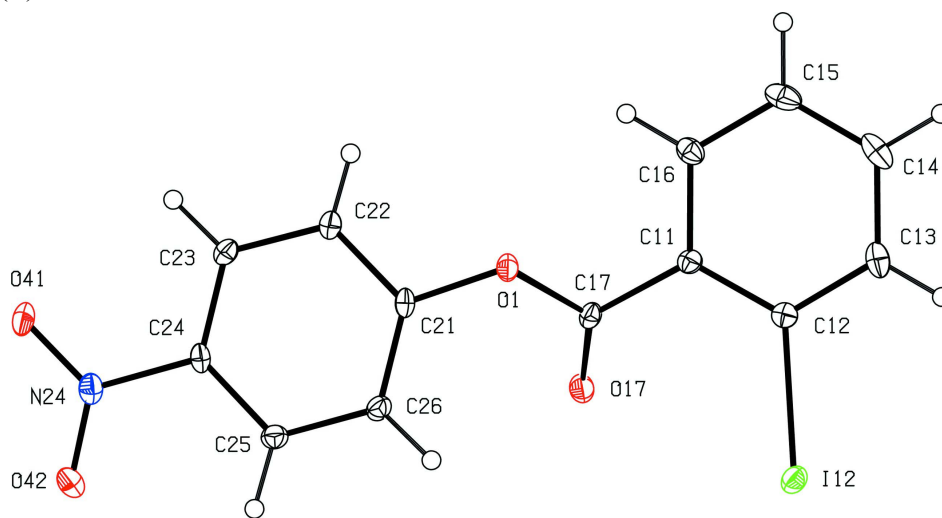
Figure 1

The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.
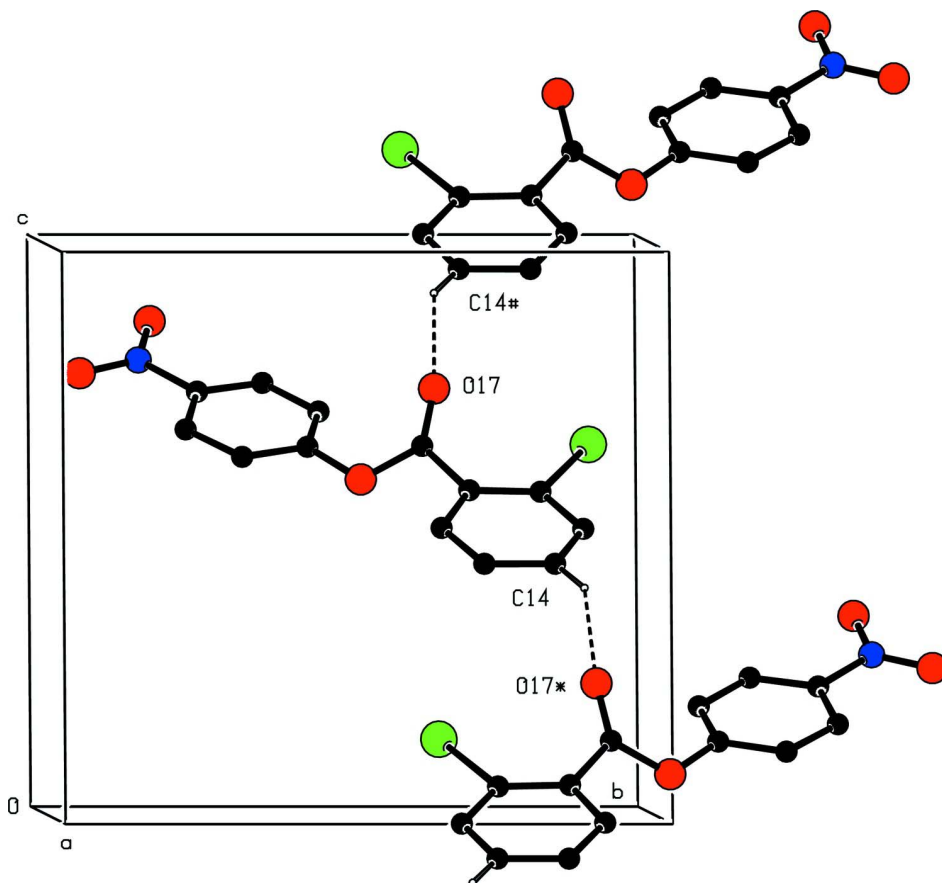
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Part of the crystal structure of (I), showing the formation of a C(7) chain along [10$\bar{1}$]. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions (1/2 + x, 1.5 − y, −1/2 + z) and (−1/2 + x, 1.5 − y, 1/2 + z), respectively.
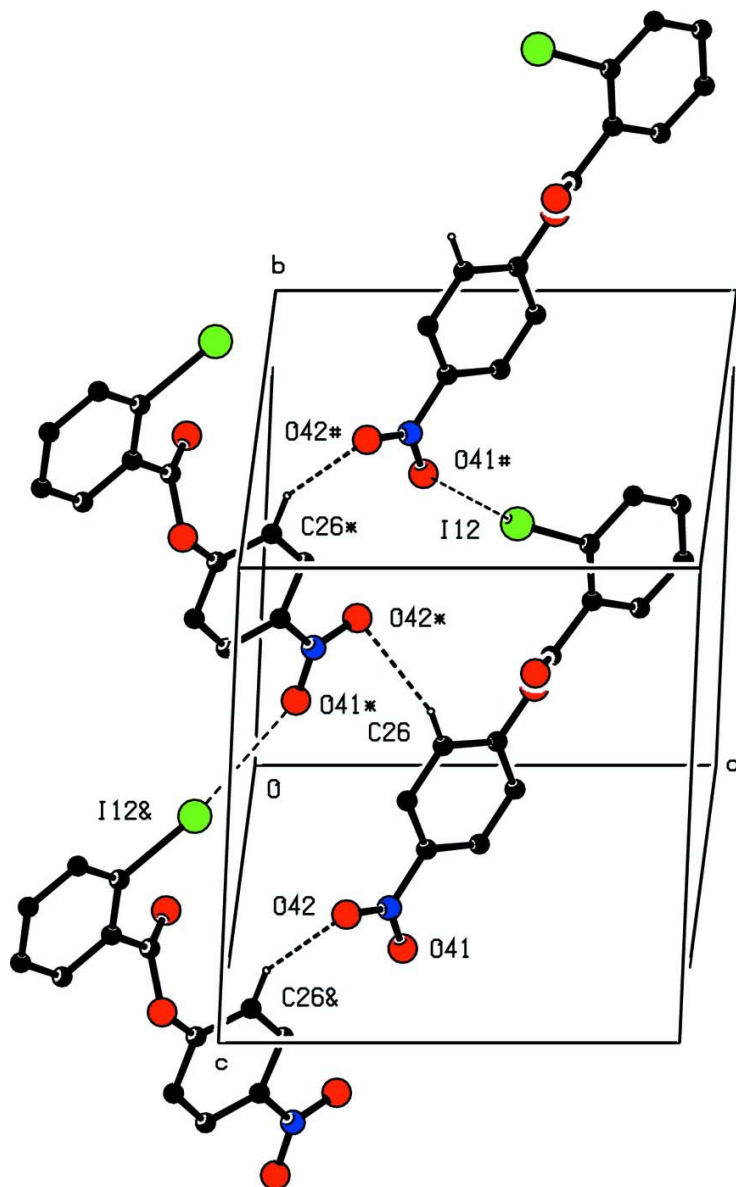
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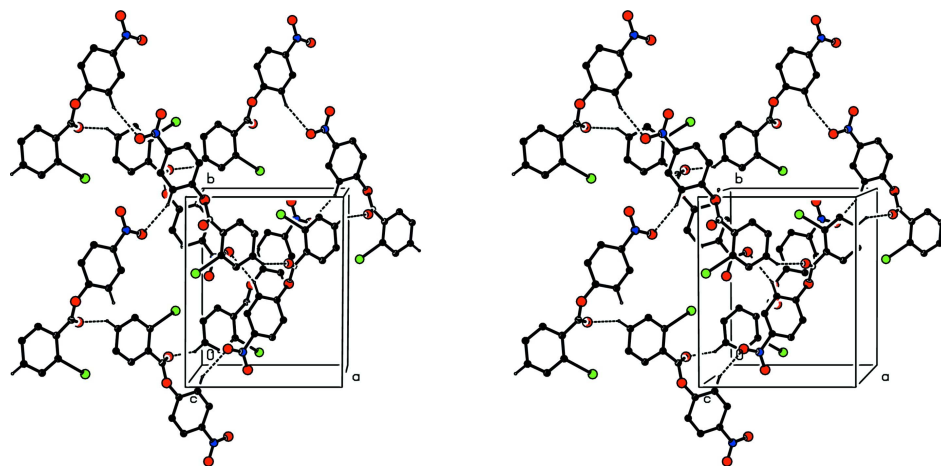
Figure 4

Stereoview of part of the crystal structure of compound (I), showing the formation of a hydrogen-bonded (101) sheet of $R_4^4(38)$ rings. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

4-Nitrophenyl 2-iodobenzoate

Crystal data

$C_{13}H_8INO_4$	$F(000) = 712$
$M_r = 369.10$	$D_x = 1.940$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2905 reflections
$a = 9.7231$ (4) Å	$\theta = 3.0$–27.5°
$b = 11.7890$ (3) Å	$\mu = 2.54$ mm^{-1}
$c = 11.1187$ (4) Å	$T = 120$ K
$\beta = 97.363$ (2)°	Plate, colourless
$V = 1263.98$ (8) Å^3	$0.10 \times 0.08 \times 0.01$ mm
$Z = 4$	

Data collection

Bruker–Nonius 95mm CCD camera on κ goniostat diffractometer	$T_{min} = 0.814$, $T_{max} = 0.975$
	12630 measured reflections
	2905 independent reflections
Radiation source: Bruker-Nonius FR91 rotating anode	2570 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.036$
Graphite monochromator	$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
Detector resolution: 9.091 pixels mm^{-1}	$h = -12 \rightarrow 11$
φ and ω scans	$k = -13 \rightarrow 15$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.026$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.058$	
$S = 1.10$	Hydrogen site location: inferred from neighbouring sites
2905 reflections	
172 parameters	H-atom parameters constrained
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2 + 1.8703P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I12	0.580705 (19)	0.888948 (14)	0.650830 (16)	0.02111 (7)
O1	0.62987 (19)	0.51101 (15)	0.59123 (16)	0.0181 (4)
O17	0.6392 (2)	0.63226 (16)	0.75041 (17)	0.0223 (4)
O41	0.3784 (2)	0.06357 (16)	0.7691 (2)	0.0298 (5)
O42	0.2579 (2)	0.18618 (17)	0.8565 (2)	0.0301 (5)
N24	0.3467 (2)	0.1619 (2)	0.7914 (2)	0.0217 (5)
C11	0.7462 (3)	0.6829 (2)	0.5758 (2)	0.0160 (5)
C12	0.7347 (3)	0.8009 (2)	0.5729 (2)	0.0177 (5)
C13	0.8224 (3)	0.8659 (2)	0.5107 (3)	0.0238 (6)
C14	0.9227 (3)	0.8134 (3)	0.4527 (3)	0.0279 (7)
C15	0.9341 (3)	0.6962 (3)	0.4530 (3)	0.0272 (7)
C16	0.8463 (3)	0.6312 (2)	0.5131 (2)	0.0204 (6)
C17	0.6661 (3)	0.6105 (2)	0.6508 (2)	0.0166 (5)
C21	0.5571 (3)	0.4276 (2)	0.6460 (2)	0.0164 (5)
C22	0.5994 (3)	0.3177 (2)	0.6297 (2)	0.0170 (5)
C23	0.5297 (3)	0.2288 (2)	0.6755 (2)	0.0175 (5)
C24	0.4191 (3)	0.2544 (2)	0.7381 (2)	0.0171 (5)
C25	0.3732 (3)	0.3646 (2)	0.7521 (2)	0.0190 (5)
C26	0.4434 (3)	0.4527 (2)	0.7041 (2)	0.0184 (5)
H13	0.8132	0.9461	0.5082	0.029*
H14	0.9842	0.8579	0.4124	0.033*
H15	1.0022	0.6605	0.4118	0.033*
H16	0.8536	0.5509	0.5121	0.024*
H22	0.6762	0.3032	0.5871	0.020*
H23	0.5567	0.1524	0.6645	0.021*
H25	0.2955	0.3793	0.7936	0.023*
H26	0.4139	0.5290	0.7110	0.022*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I12	0.02273 (11)	0.01574 (11)	0.02471 (11)	0.00248 (7)	0.00243 (8)	0.00048 (7)
O1	0.0217 (10)	0.0145 (9)	0.0183 (9)	−0.0039 (7)	0.0034 (8)	0.0002 (7)
O17	0.0277 (11)	0.0198 (9)	0.0207 (10)	−0.0062 (8)	0.0080 (8)	−0.0028 (8)
O41	0.0316 (12)	0.0136 (9)	0.0453 (13)	−0.0025 (9)	0.0091 (10)	0.0033 (9)
O42	0.0277 (12)	0.0280 (11)	0.0372 (12)	−0.0072 (9)	0.0150 (10)	−0.0014 (9)
N24	0.0205 (12)	0.0184 (11)	0.0254 (12)	−0.0037 (10)	0.0003 (10)	0.0022 (10)
C11	0.0170 (13)	0.0167 (12)	0.0141 (12)	−0.0013 (10)	0.0012 (10)	−0.0036 (10)
C12	0.0173 (13)	0.0195 (13)	0.0161 (12)	−0.0001 (10)	0.0011 (10)	−0.0009 (10)
C13	0.0271 (16)	0.0237 (14)	0.0197 (13)	−0.0088 (12)	−0.0004 (12)	0.0048 (11)
C14	0.0211 (15)	0.0426 (18)	0.0200 (14)	−0.0115 (13)	0.0031 (12)	0.0047 (13)

C15	0.0207 (15)	0.0418 (18)	0.0200 (14)	−0.0022 (13)	0.0058 (11)	−0.0070 (13)
C16	0.0180 (14)	0.0257 (14)	0.0176 (13)	−0.0040 (11)	0.0028 (11)	−0.0022 (11)
C17	0.0172 (13)	0.0122 (12)	0.0199 (13)	0.0008 (10)	−0.0002 (11)	0.0015 (10)
C21	0.0182 (13)	0.0133 (12)	0.0164 (12)	−0.0048 (10)	−0.0021 (10)	0.0017 (10)
C22	0.0178 (13)	0.0142 (12)	0.0180 (12)	−0.0016 (10)	−0.0014 (10)	0.0017 (10)
C23	0.0178 (13)	0.0141 (12)	0.0197 (13)	0.0017 (10)	−0.0009 (11)	−0.0008 (10)
C24	0.0165 (13)	0.0147 (12)	0.0193 (13)	−0.0047 (10)	−0.0008 (10)	0.0033 (10)
C25	0.0165 (13)	0.0191 (13)	0.0217 (13)	0.0013 (11)	0.0031 (11)	−0.0022 (10)
C26	0.0164 (13)	0.0149 (12)	0.0234 (13)	0.0023 (10)	0.0012 (11)	0.0000 (10)

Geometric parameters (Å, º)

C11—C12	1.396 (4)	C17—O17	1.198 (3)
C11—C16	1.406 (4)	C21—C22	1.378 (4)
C11—C17	1.482 (4)	C21—C26	1.382 (4)
C12—C13	1.394 (4)	C22—C23	1.381 (4)
C12—I12	2.098 (3)	C22—H22	0.95
C13—C14	1.383 (4)	C23—C24	1.387 (4)
C13—H13	0.95	C23—H23	0.95
C14—C15	1.386 (4)	C24—C25	1.389 (4)
C14—H14	0.95	C24—N24	1.463 (3)
C15—C16	1.381 (4)	N24—O42	1.229 (3)
C15—H15	0.95	N24—O41	1.233 (3)
C16—H16	0.95	C25—C26	1.388 (4)
O1—C17	1.371 (3)	C25—H25	0.95
O1—C21	1.396 (3)	C26—H26	0.95
C12—C11—C16	118.6 (2)	C22—C21—C26	122.2 (2)
C12—C11—C17	122.7 (2)	C22—C21—O1	115.4 (2)
C16—C11—C17	118.5 (2)	C26—C21—O1	122.2 (2)
C13—C12—C11	120.5 (3)	C21—C22—C23	119.8 (3)
C13—C12—I12	116.6 (2)	C21—C22—H22	120.1
C11—C12—I12	122.87 (19)	C23—C22—H22	120.1
C14—C13—C12	119.8 (3)	C22—C23—C24	117.9 (2)
C14—C13—H13	120.1	C22—C23—H23	121.0
C12—C13—H13	120.1	C24—C23—H23	121.0
C13—C14—C15	120.4 (3)	C23—C24—C25	122.7 (2)
C13—C14—H14	119.8	C23—C24—N24	119.0 (2)
C15—C14—H14	119.8	C25—C24—N24	118.3 (2)
C16—C15—C14	119.9 (3)	O42—N24—O41	123.4 (2)
C16—C15—H15	120.0	O42—N24—C24	118.4 (2)
C14—C15—H15	120.0	O41—N24—C24	118.3 (2)
C15—C16—C11	120.6 (3)	C26—C25—C24	118.4 (3)
C15—C16—H16	119.7	C26—C25—H25	120.8
C11—C16—H16	119.7	C24—C25—H25	120.8
C17—O1—C21	120.4 (2)	C21—C26—C25	118.8 (2)
O17—C17—O1	123.8 (2)	C21—C26—H26	120.6
O17—C17—C11	126.2 (2)	C25—C26—H26	120.6

O1—C17—C11	110.0 (2)		
C16—C11—C12—C13	−1.1 (4)	C17—O1—C21—C22	−139.1 (2)
C17—C11—C12—C13	173.4 (2)	C17—O1—C21—C26	45.9 (3)
C16—C11—C12—I12	175.25 (19)	C26—C21—C22—C23	−2.0 (4)
C17—C11—C12—I12	−10.2 (4)	O1—C21—C22—C23	−177.0 (2)
C11—C12—C13—C14	−0.8 (4)	C21—C22—C23—C24	−0.7 (4)
I12—C12—C13—C14	−177.3 (2)	C22—C23—C24—C25	2.5 (4)
C12—C13—C14—C15	1.9 (4)	C22—C23—C24—N24	−177.8 (2)
C13—C14—C15—C16	−1.0 (4)	C23—C24—N24—O42	173.0 (2)
C14—C15—C16—C11	−0.9 (4)	C25—C24—N24—O42	−7.3 (4)
C12—C11—C16—C15	1.9 (4)	C23—C24—N24—O41	−6.6 (4)
C17—C11—C16—C15	−172.8 (3)	C25—C24—N24—O41	173.0 (2)
C21—O1—C17—O17	0.1 (4)	C23—C24—C25—C26	−1.7 (4)
C21—O1—C17—C11	178.1 (2)	N24—C24—C25—C26	178.6 (2)
C12—C11—C17—O17	−37.8 (4)	C22—C21—C26—C25	2.8 (4)
C16—C11—C17—O17	136.7 (3)	O1—C21—C26—C25	177.5 (2)
C12—C11—C17—O1	144.3 (2)	C24—C25—C26—C21	−0.9 (4)
C16—C11—C17—O1	−41.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O17[i]	0.95	2.50	3.334 (3)	147
C26—H26···O42[ii]	0.95	2.54	3.395 (3)	149

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