Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2,4,6-Trinitroanilino)benzoic acid

Graham Smith,[a]* Urs D. Wermuth[b] and Jonathan M. White[c]

[a]School of Physical and Chemical Sciences, Queensland University of Technology, GPO Box 2434, Brisbane, Queensland 4001, Australia, [b]School of Biomolecular and Physical Sciences, Griffith University, Nathan, Queensland 4111, Australia, and [c]BIO-21 Molecular Science and Biotechnology, University of Melbourne, Parkville, Victoria 3052, Australia
Correspondence e-mail: g.smith@qut.edu.au

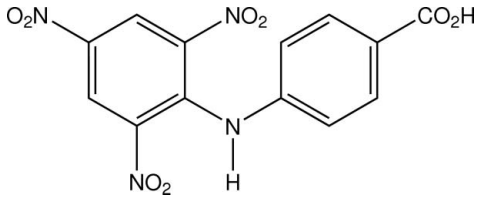
Received 12 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 130 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.100; data-to-parameter ratio = 10.5.

4-(2,4,6-Trinitroanilino)benzoic acid (*p*-picraminobenzoic acid), $C_{13}H_8N_4O_8$, obtained by the reaction of 2,4,6-trinitrobenzenesulfonic acid (picrylsulfonic acid) with 4-aminobenzoic acid in 2-propanol–water, forms a two-dimensional hydrogen-bonded network based on centrosymmetric cyclic $R_2^2(8)$ carboxylic acid dimers which are extended through lateral N—H···$O_{carboxyl}$ interactions. The amino group also makes an intramolecular N—H···O_{nitro} hydrogen bond, while the two aromatic ring systems, are, as expected, non-coplanar, the C—C—N—C torsion angles being 152.0 (2) (picryl) and 136.1 (2)° (benzoic acid)..

Related literature

For the structures of related picryl-substituted compounds, see: Russell & Ward (1997); Smith *et al.* (2006, 2007*a*). For the synthesis of picraminobenzoic acids and their salts, see: Crocker & Matthews (1911). For related literature, see: Goldfarb (1966); Kulkarni *et al.* (2005); Nair *et al.* (2001); Palaiah *et al.* (2000); Smith *et al.* (2007*a*).



Experimental

Crystal data

$C_{13}H_8N_4O_8$
M_r = 348.23
Monoclinic, $P2_1/c$
a = 20.317 (2) Å
b = 5.0919 (5) Å
c = 13.9364 (15) Å
β = 102.903 (2)°
V = 1405.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 130 (2) K
0.45 × 0.06 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.95, T_{max} = 0.99
5876 measured reflections
2462 independent reflections
2057 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.100
S = 1.10
2462 reflections
234 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N14—H14···O21	0.87 (2)	1.96 (2)	2.638 (2)	133 (2)
N14—H14···O711^{i}	0.87 (2)	2.50 (3)	3.177 (3)	135 (2)
O721—H721···O711^{ii}	0.90 (4)	1.74 (4)	2.639 (2)	174 (3)
C31—H31···O62^{iii}	0.95	2.37	3.178 (3)	143

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

The authors acknowledge financial support from the School of Physical and Chemical Sciences, Queensland University of Technology, the School of Biomolecular and Physical Sciences, Griffith University, and the School of Chemistry, University of Melbourne.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2608).

References

Bruker (1999). *SADABS* (Version 2.03) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SMART*. Version 5.55. Bruker AXS Inc., Madison, Wisconsin, USA.
Crocker, J. C. & Matthews, F. (1911). *J. Chem. Soc. Trans.* **99** 301–313.
Goldfarb, A. R. (1966). *Biochem.* **5**, 2570–2574.
Kulkarni, P. B., Reddy, T. S., Nair, J. K., Nazare, A. N., Talawar, M. B., Mukundan, T. & Asthana, S. N. (2005). *J. Hazard. Mater.* **123**, 54–60.
Nair, J. K., Talawar, M. B. & Mukundan, T. (2001). *J. Energetic Mater.* **19**, 155–162.
Palaiah, R. S., Bulakh, N. R., Talawar, M. B. & Mukundan, T. (2000). *J. Energetic Mater.* **18**, 207–217.
Russell, V. A. & Ward, M. D. (1997). *J. Mater. Chem.* **7**, 1123–1133.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Smith, G., Wermuth, U. D. & Healy, P. C. (2006). *Acta Cryst.* E**62**, o5510–o5512.
Smith, G., Wermuth, U. D. & White, J. M. (2007*a*). *Acta Cryst.* E**63**, o3759.
Smith, G., Wermuth, U. D. & White, J. M. (2007*b*). Unpublished data.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

 doi:10.1107/S1600536807058497

supplementary materials

Acta Cryst. (2007). E**63**, o4803 [**doi:10.1107/S1600536807058497**]

4-(2,4,6-Trinitroanilino)benzoic acid

G. Smith, U. D. Wermuth and J. M. White

Comment

Picryl chloride (1-chloro-2,4,6-trinitrobenzene) reacts with the isomeric aminobenzoic acids to give the corresponding picraminobenzoic acids (Crocker & Matthews, 1911). The same reaction products may be obtained using picrylsulfonic acid (2,4,6-trinitrobenzenesulfonic acid) and the metal salts of these three compounds have been investigated for their potential as energetic ballistic modifiers (Palaiah *et al.*, 2000; Nair *et al.*, 2001; Kulkarni *et al.*, 2005). Similar addition compounds are obtained with amino acids and proteins (Goldfarb, 1966) while we have also found that picrylsulfonic acid reacts with guanidine carbonate in methanol to give the analogous picrylguanidine (Smith *et al.*, 2007*a*). This is in contrast to the formation of the proton-transfer salt guanidinium picrylsulfonate (Russell & Ward, 1997) from the reaction of picrylsulfonic acid with guanidinium chloride in methanol-toluene solution. The structures of the salt quinolinium picrylsulfonate (Smith *et al.*, 2006) and the adduct salt 2-carboxyquinolinium-picrylsulfonate-quinolinium-2-carboxylate (1/1/1) (Smith *et al.*, 2007*b*) are also known. Of the three isomeric picraminobenzoic acids synthesized from picrylsulfonic acid, only the *para*-isomer 4-(2,4,6-trinitroanilino)benzoic acid (I) proved suitable for X-ray analysis and the structure is reported here.

The molecules of the title compound (Fig. 1) form centrosymmetric hydrogen-bonded cyclic homodimers [graph set $R^2_2(8)$] which are extended into a two-dimensional network structure through lateral N—$H\cdots O_{carboxyl}$ interactions (Fig. 2; Table 1). The amino-N forms an intramolecular hydrogen bond with an O-acceptor of one of the *ortho*- related nitro groups which is less rotated out of the plane of the benzene ring than the second, more sterically encumbered group [torsion angle C1–C2–N2–O22, −155.43 (19) ° *cf.* C5–C6–N6–O62, 123.1 (2) °]. The third group is essentially coplanar with the ring [C3–C4–N4–O42, 177.4 (2) °]. The carboxylic acid group also lies out of the plane of the benzene ring [torsion angle C21–C11–C71–O721, −165.4 (2) °] while this ring is also rotated out of the plane of the picryl residue [torsion angles C2–C1–N14–C41, 152.0 (2) Å; C1–N14–C41–C51, 136.1 (2) Å].

Experimental

The title compound was synthesized by heating under reflux 1 mmol quantities of 2,4,6-trinitrobenzenesulfonic acid (picrylsulfonic acid) and 4-aminobenzoic acid in 50 ml of 80% propan-2-ol-water for 10 minutes. This reaction is analogous to that of picryl chloride with 4-amimobenzoic acid (Crocker & Matthews, 1911) which gives the same product. After concentration to *ca* 30 ml, partial room temperature evaporation of the hot-filtered solution gave yellow prisms of (I) [m.pt. 558 K (Crocker & Matthews, 1911)].

Refinement

Interactive hydrogen atoms were located by difference methods and their positional and isotropic displacement parameters were refined. The aromatic ring H atoms were included in the refinement in calculated positions (C–H = 0.95 Å) using a riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

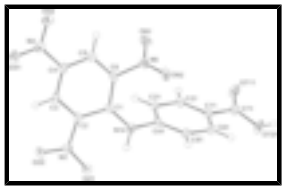


Fig. 1. Molecular configuration and atom naming scheme for (I). Non-H atom displacement ellipsoids are drawn at the 40% probability level.

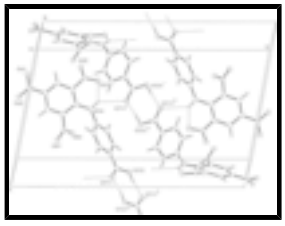


Fig. 2. A perspective view of the two-dimensional network structure of (I) showing the cyclic $R^2_2(8)$ centrosymmetric hydrogen-bonded carboxylic acid homodimers extended through N–H···$O_{carboxyl}$ associations. Hydrogen bonds are shown as dashed lines. Symmetry code (iv): $1 - x$, $1/2 + y$, $3/2 - z$. For other symmetry codes, see Table 1.

4-(2,4,6-Trinitroanilino)benzoic acid

Crystal data

$C_{13}H_8N_4O_8$	F_{000} = 712
M_r = 348.23	D_x = 1.646 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 558 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 20.317 (2) Å	Cell parameters from 1942 reflections
b = 5.0919 (5) Å	θ = 3.0–27.4º
c = 13.9364 (15) Å	μ = 0.14 mm^{-1}
β = 102.903 (2)º	T = 130 (2) K
V = 1405.4 (2) Å^3	Needle, yellow
Z = 4	0.45 × 0.06 × 0.06 mm

Data collection

Bruker CCD area-detector diffractometer	2462 independent reflections
Radiation source: sealed tube	2057 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 130(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −24→22
T_{min} = 0.95, T_{max} = 0.99	k = −5→6
5876 measured reflections	l = −6→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.4928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
2462 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
234 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O21	0.28495 (8)	0.6642 (3)	0.35981 (12)	0.0277 (5)
O22	0.19826 (8)	0.9192 (3)	0.31493 (11)	0.0256 (5)
O41	−0.02274 (8)	0.5879 (4)	0.29940 (13)	0.0373 (6)
O42	−0.03744 (8)	0.2949 (3)	0.40479 (13)	0.0342 (6)
O61	0.16455 (8)	0.0561 (3)	0.66743 (11)	0.0315 (6)
O62	0.22289 (8)	−0.1459 (3)	0.57694 (12)	0.0280 (5)
O711	0.42517 (8)	0.1190 (4)	0.95005 (11)	0.0337 (6)
O721	0.49608 (8)	−0.0810 (4)	0.87222 (13)	0.0362 (6)
N2	0.22466 (9)	0.7173 (4)	0.35345 (13)	0.0203 (6)
N4	−0.00133 (9)	0.4347 (4)	0.36657 (14)	0.0251 (6)
N6	0.18611 (9)	0.0327 (4)	0.59289 (13)	0.0210 (6)
N14	0.28062 (9)	0.3181 (4)	0.49909 (13)	0.0199 (6)
C1	0.21318 (11)	0.3574 (4)	0.47150 (15)	0.0171 (6)
C2	0.18317 (10)	0.5347 (4)	0.39510 (15)	0.0175 (6)
C3	0.11423 (11)	0.5621 (4)	0.36082 (15)	0.0192 (7)
C4	0.07171 (11)	0.4169 (4)	0.40398 (16)	0.0205 (7)
C5	0.09676 (11)	0.2531 (4)	0.48320 (16)	0.0202 (7)
C6	0.16532 (11)	0.2273 (4)	0.51474 (15)	0.0179 (6)
C11	0.39836 (10)	0.1101 (4)	0.77544 (16)	0.0199 (7)
C21	0.34772 (11)	0.2976 (4)	0.76841 (16)	0.0208 (7)
C31	0.30798 (11)	0.3645 (4)	0.67791 (15)	0.0198 (7)
C41	0.31861 (10)	0.2401 (4)	0.59402 (15)	0.0183 (7)

C51	0.36815 (10)	0.0491 (4)	0.60025 (16)	0.0207 (7)
C61	0.40803 (11)	−0.0152 (5)	0.69090 (16)	0.0226 (7)
C71	0.44058 (11)	0.0511 (5)	0.87385 (16)	0.0240 (7)
H3	0.09660	0.67930	0.30830	0.0230*
H5	0.06700	0.16060	0.51490	0.0240*
H14	0.3038 (12)	0.386 (5)	0.4598 (17)	0.026 (7)*
H21	0.34040	0.38020	0.82630	0.0250*
H31	0.27370	0.49410	0.67310	0.0240*
H51	0.37450	−0.03660	0.54250	0.0250*
H61	0.44210	−0.14510	0.69560	0.0270*
H721	0.5209 (17)	−0.101 (7)	0.934 (3)	0.079 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O21	0.0207 (8)	0.0318 (10)	0.0317 (9)	0.0033 (7)	0.0083 (7)	0.0084 (8)
O22	0.0308 (9)	0.0194 (9)	0.0260 (9)	0.0026 (7)	0.0048 (7)	0.0061 (7)
O41	0.0263 (9)	0.0420 (11)	0.0392 (11)	0.0068 (8)	−0.0023 (8)	0.0146 (9)
O42	0.0219 (9)	0.0400 (11)	0.0414 (11)	−0.0048 (8)	0.0084 (8)	0.0058 (9)
O61	0.0345 (10)	0.0403 (11)	0.0203 (9)	−0.0016 (8)	0.0073 (7)	0.0072 (8)
O62	0.0305 (9)	0.0183 (9)	0.0310 (9)	0.0035 (7)	−0.0021 (8)	0.0005 (7)
O711	0.0282 (9)	0.0546 (12)	0.0168 (9)	0.0165 (9)	0.0017 (7)	−0.0008 (8)
O721	0.0270 (10)	0.0586 (13)	0.0202 (9)	0.0228 (9)	−0.0009 (8)	0.0017 (9)
N2	0.0235 (10)	0.0198 (11)	0.0167 (9)	−0.0014 (8)	0.0027 (8)	−0.0010 (8)
N4	0.0213 (10)	0.0267 (12)	0.0266 (11)	0.0017 (9)	0.0037 (9)	−0.0011 (9)
N6	0.0215 (10)	0.0187 (11)	0.0199 (10)	−0.0031 (8)	−0.0017 (8)	0.0025 (8)
N14	0.0177 (10)	0.0243 (11)	0.0169 (10)	0.0021 (8)	0.0022 (8)	0.0029 (8)
C1	0.0218 (11)	0.0144 (11)	0.0149 (11)	0.0019 (9)	0.0035 (9)	−0.0047 (9)
C2	0.0221 (11)	0.0161 (12)	0.0148 (10)	0.0002 (9)	0.0049 (9)	−0.0015 (9)
C3	0.0219 (11)	0.0198 (13)	0.0144 (11)	0.0032 (10)	0.0008 (9)	−0.0004 (9)
C4	0.0182 (11)	0.0232 (13)	0.0187 (11)	0.0008 (10)	0.0011 (9)	−0.0016 (10)
C5	0.0224 (12)	0.0191 (12)	0.0194 (11)	−0.0018 (10)	0.0053 (9)	−0.0020 (9)
C6	0.0221 (11)	0.0155 (12)	0.0145 (10)	0.0021 (9)	0.0006 (9)	0.0009 (9)
C11	0.0161 (11)	0.0228 (13)	0.0198 (11)	0.0012 (9)	0.0018 (9)	0.0041 (10)
C21	0.0218 (12)	0.0202 (12)	0.0188 (11)	−0.0002 (10)	0.0011 (9)	−0.0007 (9)
C31	0.0177 (11)	0.0180 (12)	0.0218 (12)	0.0052 (9)	0.0007 (9)	0.0013 (10)
C41	0.0162 (11)	0.0198 (12)	0.0174 (11)	−0.0017 (9)	0.0007 (9)	0.0030 (9)
C51	0.0209 (11)	0.0235 (13)	0.0177 (11)	0.0008 (10)	0.0043 (9)	−0.0005 (9)
C61	0.0172 (11)	0.0239 (13)	0.0260 (12)	0.0049 (10)	0.0033 (9)	0.0028 (10)
C71	0.0190 (11)	0.0300 (14)	0.0217 (12)	0.0048 (10)	0.0019 (10)	0.0045 (10)

Geometric parameters (Å, °)

O21—N2	1.238 (3)	C2—C3	1.382 (3)
O22—N2	1.227 (3)	C3—C4	1.374 (3)
O41—N4	1.222 (3)	C4—C5	1.387 (3)
O42—N4	1.226 (3)	C5—C6	1.370 (3)
O61—N6	1.220 (2)	C11—C71	1.477 (3)
O62—N6	1.228 (3)	C11—C21	1.391 (3)

O711—C71	1.222 (3)	C11—C61	1.392 (3)
O721—C71	1.318 (3)	C21—C31	1.380 (3)
O721—H721	0.90 (4)	C31—C41	1.388 (3)
N2—C2	1.460 (3)	C41—C51	1.388 (3)
N4—C4	1.462 (3)	C51—C61	1.379 (3)
N6—C6	1.463 (3)	C3—H3	0.9500
N14—C41	1.431 (3)	C5—H5	0.9500
N14—C1	1.353 (3)	C21—H21	0.9500
N14—H14	0.87 (2)	C31—H31	0.9500
C1—C6	1.418 (3)	C51—H51	0.9500
C1—C2	1.425 (3)	C61—H61	0.9500
C71—O721—H721	110 (2)	N6—C6—C5	114.05 (19)
O21—N2—C2	118.84 (18)	C61—C11—C71	122.0 (2)
O22—N2—C2	118.23 (18)	C21—C11—C71	118.2 (2)
O21—N2—O22	122.91 (19)	C21—C11—C61	119.8 (2)
O41—N4—C4	118.19 (18)	C11—C21—C31	120.4 (2)
O42—N4—C4	117.86 (18)	C21—C31—C41	119.2 (2)
O41—N4—O42	123.95 (19)	N14—C41—C31	119.91 (19)
O61—N6—C6	117.96 (18)	N14—C41—C51	119.08 (19)
O62—N6—C6	116.92 (17)	C31—C41—C51	120.92 (19)
O61—N6—O62	125.10 (19)	C41—C51—C61	119.5 (2)
C1—N14—C41	127.36 (18)	C11—C61—C51	120.1 (2)
C41—N14—H14	115.9 (16)	O711—C71—O721	123.1 (2)
C1—N14—H14	114.8 (16)	O711—C71—C11	122.8 (2)
N14—C1—C6	123.88 (19)	O721—C71—C11	114.18 (19)
N14—C1—C2	122.9 (2)	C2—C3—H3	121.00
C2—C1—C6	113.21 (19)	C4—C3—H3	121.00
N2—C2—C1	120.80 (18)	C4—C5—H5	121.00
N2—C2—C3	115.40 (18)	C6—C5—H5	121.00
C1—C2—C3	123.62 (19)	C11—C21—H21	120.00
C2—C3—C4	118.83 (19)	C31—C21—H21	120.00
N4—C4—C5	119.0 (2)	C21—C31—H31	120.00
N4—C4—C3	119.87 (19)	C41—C31—H31	120.00
C3—C4—C5	121.2 (2)	C41—C51—H51	120.00
C4—C5—C6	118.6 (2)	C61—C51—H51	120.00
N6—C6—C1	121.43 (19)	C11—C61—H61	120.00
C1—C6—C5	124.30 (19)	C51—C61—H61	120.00
O21—N2—C2—C1	23.5 (3)	N14—C1—C6—N6	−1.3 (3)
O22—N2—C2—C1	−155.43 (19)	C1—C2—C3—C4	1.9 (3)
O21—N2—C2—C3	−161.37 (19)	N2—C2—C3—C4	−173.13 (19)
O22—N2—C2—C3	19.7 (3)	C2—C3—C4—C5	2.6 (3)
O41—N4—C4—C3	−2.7 (3)	C2—C3—C4—N4	−177.63 (19)
O42—N4—C4—C3	177.4 (2)	C3—C4—C5—C6	−3.5 (3)
O41—N4—C4—C5	177.0 (2)	N4—C4—C5—C6	176.78 (19)
O42—N4—C4—C5	−2.8 (3)	C4—C5—C6—N6	−174.90 (19)
O62—N6—C6—C1	−51.9 (3)	C4—C5—C6—C1	−0.1 (3)
O62—N6—C6—C5	123.1 (2)	C61—C11—C21—C31	−1.5 (3)
O61—N6—C6—C5	−55.2 (3)	C71—C11—C61—C51	−178.9 (2)

O61—N6—C6—C1	129.8 (2)	C71—C11—C21—C31	178.4 (2)
C41—N14—C1—C2	152.0 (2)	C21—C11—C61—C51	0.9 (3)
C1—N14—C41—C51	136.1 (2)	C61—C11—C71—O711	−165.5 (2)
C1—N14—C41—C31	−47.1 (3)	C61—C11—C71—O721	14.4 (3)
C41—N14—C1—C6	−28.2 (3)	C21—C11—C71—O711	14.7 (3)
N14—C1—C2—N2	−10.5 (3)	C21—C11—C71—O721	−165.4 (2)
C2—C1—C6—N6	178.50 (18)	C11—C21—C31—C41	0.8 (3)
C2—C1—C6—C5	4.1 (3)	C21—C31—C41—C51	0.5 (3)
N14—C1—C6—C5	−175.7 (2)	C21—C31—C41—N14	−176.3 (2)
C6—C1—C2—N2	169.77 (18)	N14—C41—C51—C61	175.8 (2)
N14—C1—C2—C3	174.8 (2)	C31—C41—C51—C61	−1.0 (3)
C6—C1—C2—C3	−5.0 (3)	C41—C51—C61—C11	0.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N14—H14···O21	0.87 (2)	1.96 (2)	2.638 (2)	133 (2)
N14—H14···O711^{i}	0.87 (2)	2.50 (3)	3.177 (3)	135 (2)
O721—H721···O711^{ii}	0.90 (4)	1.74 (4)	2.639 (2)	174 (3)
C31—H31···O62^{iii}	0.95	2.37	3.178 (3)	143

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

Fig. 1

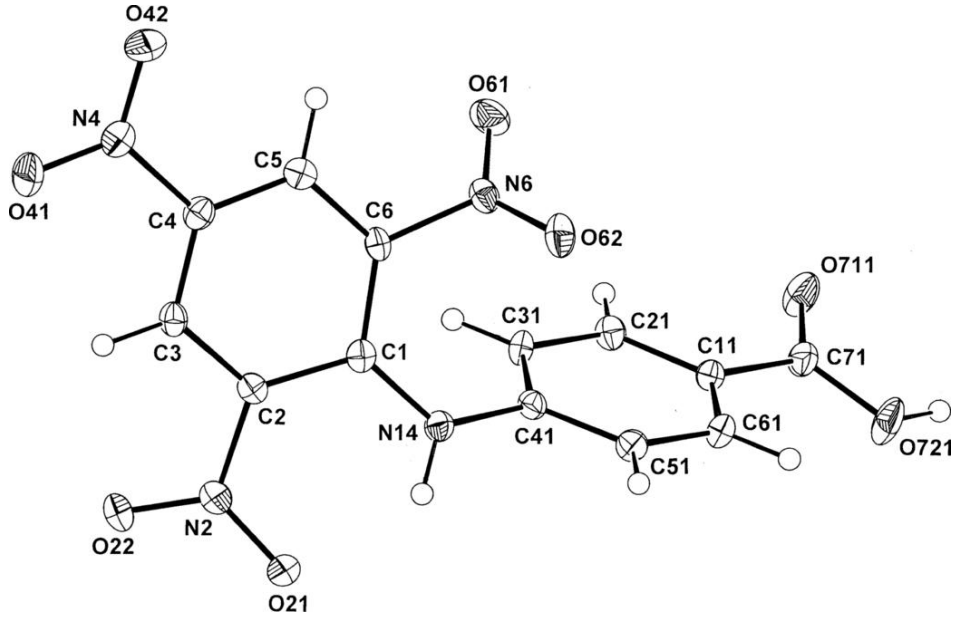
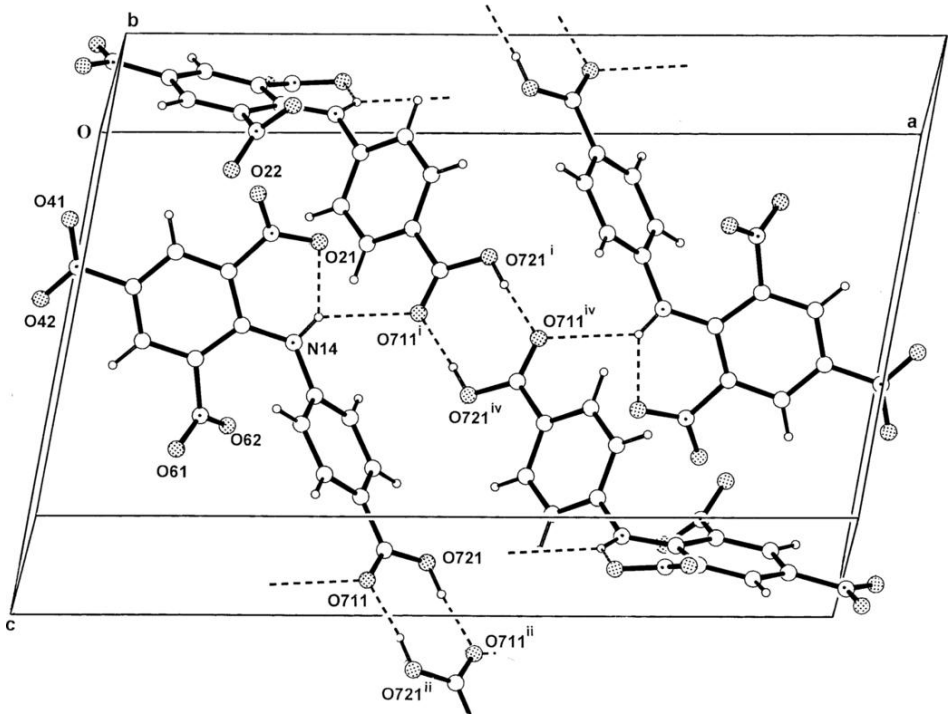

O42
N4
O41
C5
C4
C6
O61
N6
O62
O711
C31
C21
C11
C71
C3
C1
C2
N14
C41
C61
O721
C51
N2
O22
O21

Fig. 2


b
O
a
c
O22
O41
O21
O721 i
O42
O711 iv
O711 i
N14
O721 iv
O62
O61
O721
O711
O711 ii
O721 ii