Binary and ternary charge-transfer complexes using 1,3,5-trinitrobenzene

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Three binary and one ternary charge-transfer complexes have been made using 1,3,5-trinitrobenzene, *viz.* 1,3,5-trinitrobenzene–2-acetylnaphthalene (1/1), $C_6H_3N_3O_6 \cdot C_{12}H_{10}O$, (I), 1,3,5-trinitrobenzene–9-bromoanthracene (1/1), $C_{14}H_9Br \cdot C_6H_3N_3O_6$, (II), 1,3,5-trinitrobenzene–methyl red (1/1), $C_{15}H_{15}N_3O_2 \cdot C_6H_3N_3O_6$, (III) (systematic name for methyl red: 2-{(*E*)-[4-(dimethylamino)phenyl]diazenyl}benzoic acid), and 1,3,5-trinitrobenzene–1-naphthoic acid–2-amino-5-nitropyridine (1/1/1), $C_6H_3N_3O_6 \cdot C_{11}H_8O_2 \cdot C_5H_5N_3O_2$, (IV). All charge-transfer complexes show alternating donor and acceptor stacks, which have weak C—H···O hydrogen bonds perpendicular to the stacking axis. In addition, complex (IV) is a crystal engineering attempt to modify the packing of the stacks by inserting a third molecule into the structure. This third molecule is stabilized by strong hydrogen bonds between the carboxylic acid group of the donor molecule and the pyridine acceptor molecule.

1. Chemical context

The crystal structure of 1,3,5-trinitrobenzene (TNB), an energetic or high-explosive material, was first reported as far back as 1930 (Hertel & Romer, 1930). A number of structures of pure TNB have appeared since then, including a neutron diffraction study in 1972 (Choi & Abel, 1972). More recently, polymorphs (Thallapally *et al.*, 2004) and pseudo-polymorphs of TNB (Jetti *et al.*, 2003) have been reported.

Crystal engineering, the conception and synthesis of molecular solid-state structures, is fundamentally based upon the discernment and subsequent exploitation of intermolecular interactions. Thus, primarily non-covalent bonding is used to achieve the organization of molecules and ions in the solid state in order to produce materials with desired properties. The stability of an energetic material is one of the decisive factors in determining the viability of the final product, be it for fuels, propellants, pyrotechnics or explosives. If the energetic cannot be safely synthesized, handled and stored before its ultimate use, it is regarded as a failure, discarded and forgotten. Although not a forgotten but rather an old energetic material, 1,3,5-trinitrobenzene (TNB) falls into the class of energetics that are shock and heat sensitive, especially when in powdered dry form. Co-crystallization presents an opportunity to re-look at these problems for example, Guo *et al.* (2013*a*) have shown that taking 2,4,6,8,10,12-hexanitrohexa-azaisowurtzitane (CL-20) and co-crystallizing it with caprolactam (CPL) has lead to new and interesting effects on the relevant properties. The importance of crystal engineering in the stabilization of explosive materials, such as trinitrotoluene (TNT) and ethylenedinitramine, was described recently (Landenberger *et al.*, 2010; Aakeröy *et al.*, 2015). Recently,
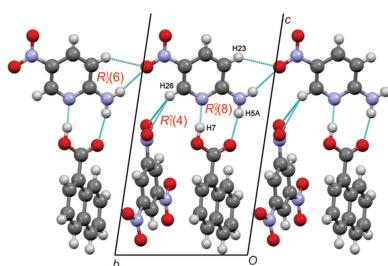
research communications

Chen *et al.* (2017) isolated a novel co-crystal of 1,3,5-trinitro-benzene (TNB) and 1-nitronaphthalene (NNAP), synthesized by using both solution and mechanochemical methods. The TNB/NNAP co-crystal has the largest proportion of π–π stacking interaction (12.7%). A charge-transfer complex of TNT and TNB has also been reported (Guo *et al.*, 2013*b*). The results indicate that the electronic effect has an influence on the intermolecular interactions in the co-crystal. Our study comprises of an investigation of TNB as a model energetic with various polycyclic aromatic hydrocarbons in order to observe their effect on the structural aspects of the solid state. The structure and properties of many charge-transfer (CT) complexes of TNB with a variety of aromatic molecules have been investigated (Brown *et al.*, 1964; Herbstein & Kaftory, 1975), and reviewed by Herbstein in different sections of his book (Herbstein, 2005). To this end, we have synthesized four new charge-transfer co-crystals, three binary (I)–(III), and one ternary (IV): trinitrobenzene–2-acetylnaphthalene, (I), tri-nitrobenzene–9-bromoanthracene, (II), trinitrobenzene–methyl red, (III), and trinitrobenzene–1-naphthoic acid–2-amino-5-nitropyridine, (IV).

(I)

(II)

(III)

(IV)
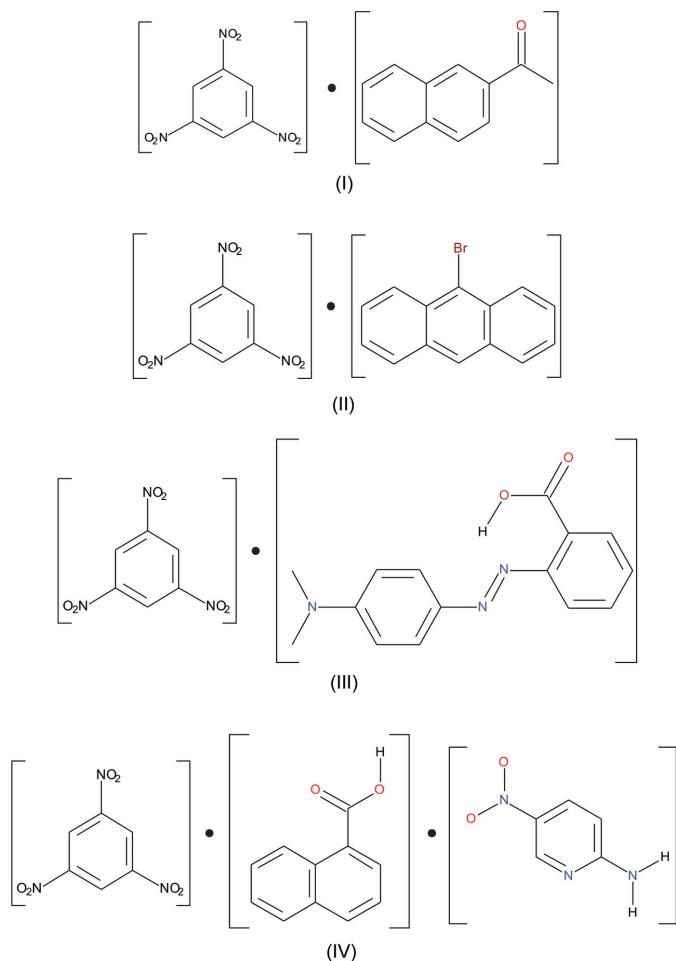
2. Structural commentary

The asymmetric units and atom-labelling schemes for the title charge-transfer complexes are shown in Fig. 1. All compounds

Table 1
Centroid distances (Å) between the trinitrobenzene and the ring centroids (*Cg*) of the aromatic polycyclics.

Structure	Donor	Acceptor	$Cg\cdots Cg$	Symmetry operator
(I)	C1–C6	C11–C20	3.3745 (2)	x, y, z
(II)	C1–C6	C11–C24	3.5173 (11)	x, y, z
(III)	C1–C6	C11–C16	3.6587 (14)	$1 - x, 1 - y, 1 - z$
(III)	C1–C6	C19–C24	4.6432 (18)	x, y, z
(IV)	C1–C6	C11–C20	4.0417 (8)	$x, y + 1, z$

have $Z' = 1$ with all molecules in general positions. As a result of the strong polarizing effect of the nitro groups, TNB has an electron-poor π-system. On the other hand, the donor molecules (polycyclic aromatic hydrocarbons) have an electron-rich π-system. The packing of the unit cell of the complexes follows a donor (*D*) acceptor (*A*) π–π interaction, which is the major driving force in the formation of these complexes, as seen in Fig. 2 (donor molecules shown in blue and acceptors in green), resulting in a general face-to-face π-stacking, with Table 1 summarizing the closest centroid–centroid distances between the TNB acceptor and aromatic donor systems. The intermolecular interactions of the $D\cdots A$ stacks can be quantified using Hirschfeld surface analysis as well as the resulting fingerprint plots using the programme *Crystal-Explorer17.5* (Spackman & McKinnon, 2002). In the paper by Chen *et al.* (2017), the authors describe the regions of blue and red triangles on the Hirshfeld surface using the shape index as evidence of π–π interactions. Fig. 3 shows such surfaces plotted for the TNB molecules in (I)–(IV). The red triangles show concave regions indicative of ring carbons of the π-stacked molecule above it. (I) and (II) show the most triangles, indicative that they have the greatest proportion of π–π stacking of the four structures. This can be quantified by looking at the contribution that $C\cdots C$ contacts make up in the fingerprint plots. (I) and (II) have values of 12.0 and 12.6%, respectively, much greater than the 4.4 and 7.5% for (III) and (IV), respectively. Table 2 summarizes the percentages of $C\cdots C$, $H\cdots H$ and $C\cdots H$ contacts and the relevant fingerprint plots are given in the supporting information. In terms of the molecular geometry, the TNB molecules show some changes from the geometries encountered in the pure compound. The pure compound has torsion angles of the nitro group to the benzene ring in the range from 0 to 28.17°, whereas in the CT complexes described here they range from −20.0 (4) to +20.0 (5)°. The packing and hydrogen-bonding interactions are further described below individually for each compound.

Table 2
Proportion (%) of intermolecular contacts between donor and acceptor molecules in the Hirshfeld fingerprint plots.

Structure	$C\cdots C$	$H\cdots H$	$C\cdots H$
(I)	12.0	10.7	1.5
(II)	12.6	6.6	0.9
(III)	4.4	11.0	5.4
(IV)	7.5	8.8	4.6
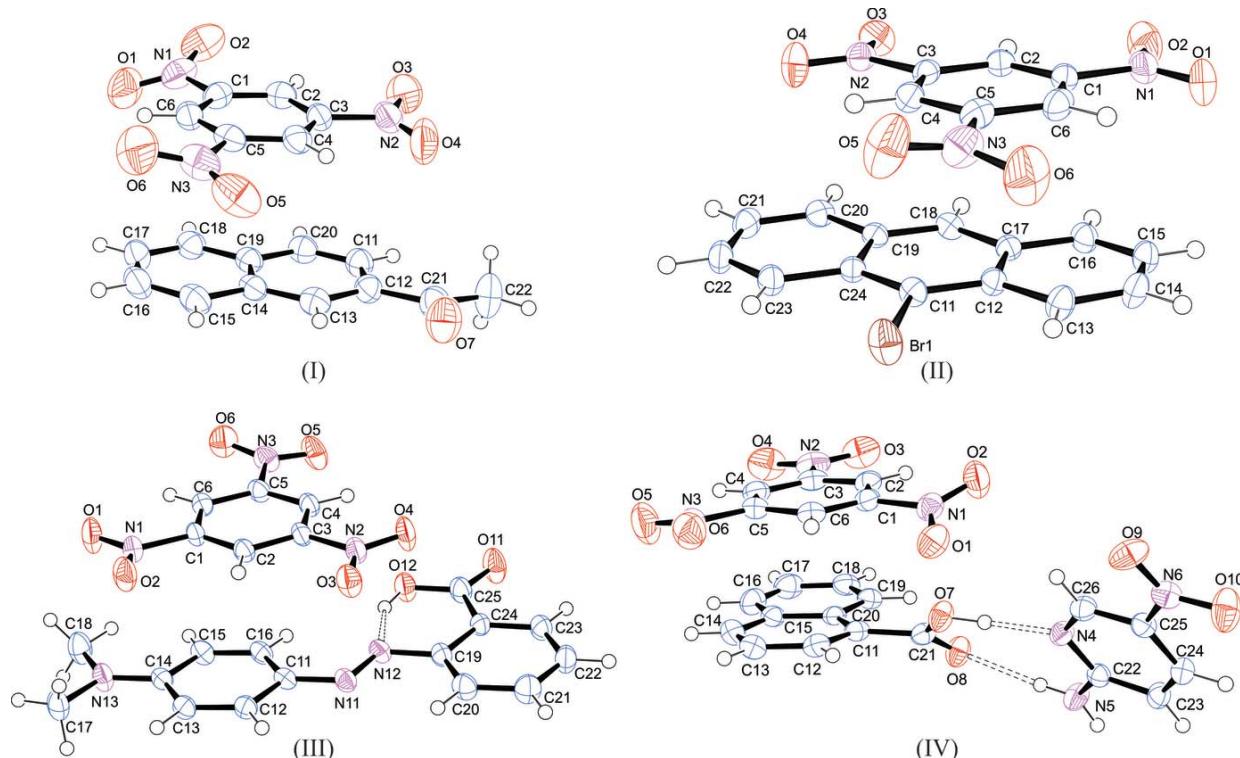
Figure 1
Perspective views of compounds (I)–(IV), showing the atom-numbering schemes. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The dashed lines indicate the symmetry-independent N—H···O and O—H···N hydrogen bonds.
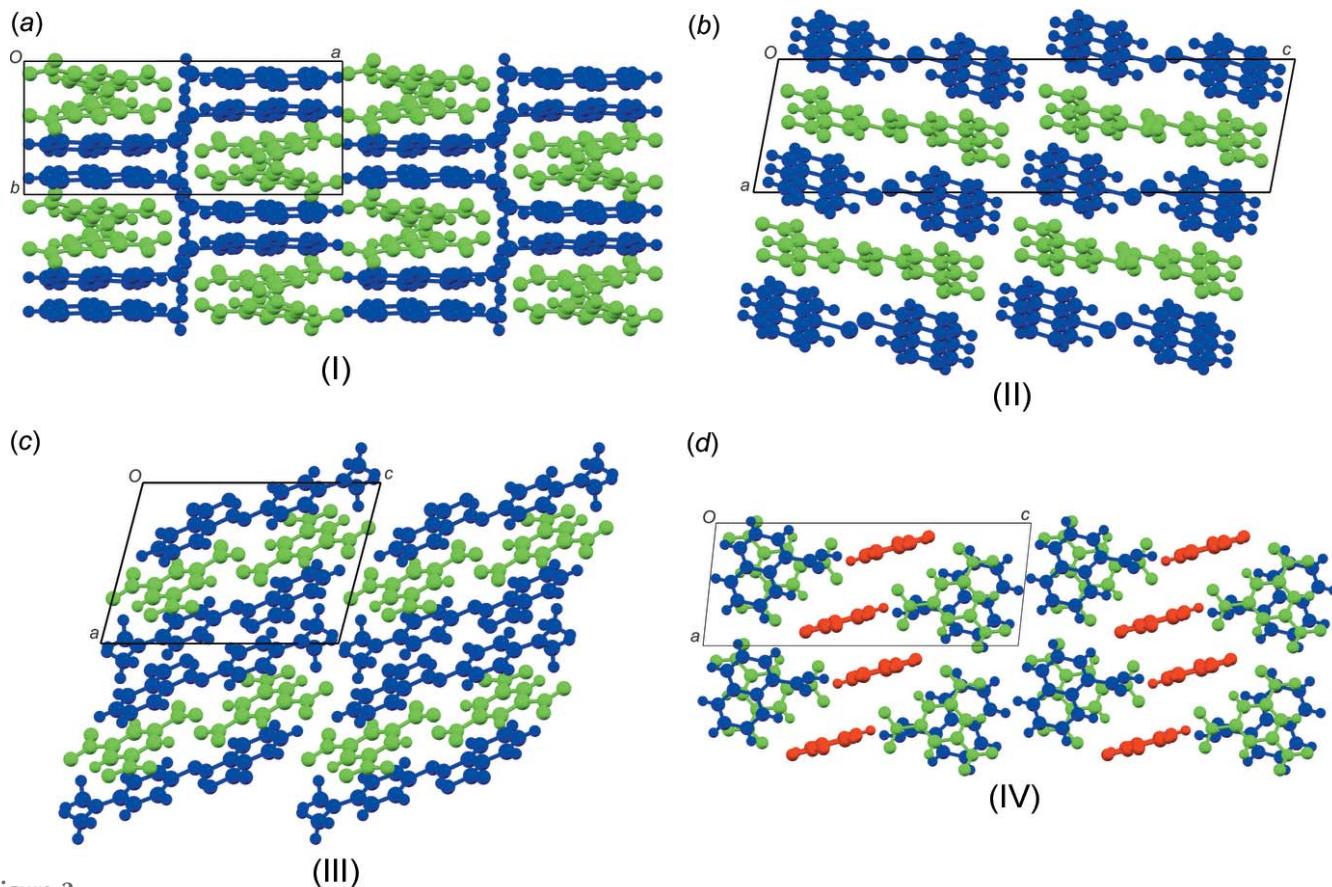
Figure 2
The packing diagrams for all four compounds (I)–(IV). The acceptor molecules are shown in green and the donor molecules in blue. The third molecule of 2-amino-5-nitropyridine is shown in red in (IV).

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4$\cdots$O2^i	0.93	2.4	3.189 (3)	143
C11—H11$\cdots$O3^{ii}	0.93	2.48	3.323 (4)	150
C22—H22A$\cdots$O4^{iii}	0.96	2.64	3.554 (4)	159

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4$\cdots$O6^i	0.95	2.5	3.287 (3)	140
C6—H6$\cdots$O5^{ii}	0.95	2.68	3.593 (3)	162
C14—H14$\cdots$O4^{iii}	0.95	2.57	3.255 (3)	129
C21—H21$\cdots$O1^{iv}	0.95	2.65	3.364 (3)	132

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4$\cdots$O4^i	0.95	2.35	3.285 (4)	169
C15—H15$\cdots$O11^{ii}	0.95	2.34	3.254 (4)	161
C18—H18A$\cdots$O11^{ii}	0.98	2.55	3.519 (4)	170
C20—H20$\cdots$O3^{iii}	0.95	2.64	3.574 (4)	167
O12—H12$\cdots$N12	0.95 (6)	1.70 (6)	2.577 (3)	153 (5)
C21—H21$\cdots$O2^{iii}	0.95	2.56	3.469 (4)	161

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5A$\cdots$O8	0.90 (5)	2.03 (5)	2.919 (5)	168 (5)
N5—H5B$\cdots$O9^i	0.86 (4)	2.24 (4)	3.069 (5)	161 (4)
O7—H7$\cdots$N4	0.95 (5)	1.71 (5)	2.650 (4)	171 (5)
C23—H23$\cdots$O9^i	0.95	2.5	3.272 (5)	139
C26—H26$\cdots$O1	0.95	2.69	3.530 (5)	147
C26—H26$\cdots$O2	0.95	2.72	3.477 (5)	138

Symmetry code: (i) $x, y-1, z$.

3. Supramolecular features

Structure (I) crystallizes in the $P2_1/c$ space group with both the TNB and 2-acetylnaphthalene molecules in the asymmetric unit. The donor and acceptor molecules pack in a checkerboard fashion parallel to the ab plane (Fig. 2a). In the plane perpendicular to the stacking, the ac plane, there are C—H$\cdots$O interactions between TNB and 2-acetylnaphthalene molecules (Table 3, Fig. 4a), forming an $R_3^3(17)$ ring described using graph set notation (Bernstein et $al.$, 1995).

Structure (II) crystallizes in the $P2_1/c$ space group with both the TNB and 9-bromoanthracene in the asymmetric unit. The packing of the structure displays a clear separation of the donor (blue) and acceptor (green) layers (Fig. 2b). The

alternating DA stacks show that the bromine atom of the 9-bromoanthracene packs in a head-to-head stacked fashion; however, the distance between the nearest Br atoms is very long [4.981 (1) Å], much longer than the sum of their van der Waals radii, and as a result Br$\cdots$Br interactions are not involved in the molecular aggregation. In the plane perpendicular to the stacking, there are C—H$\cdots$O interactions (Table 4) between TNB molecules forming an $R_2^2(10)$ ring, and a discrete hydrogen bond between the TNB and 9-bromoanthracene molecules (Fig. 4b).

Structure (III) crystallizes in the $P\overline{1}$ space group with both the TNB and the methyl red in the asymmetric unit. The packing of the structure illustrates that for each phenyl ring on the methyl red molecule, there is an associated TNB molecule. The two TNB molecules are at different distances from the ring centroids, with a variation of ca 0.98 Å (Table 2). Along the bc plane, the TNB molecules display similar hydrogen-bonded rings as those observed for (II) (Fig. 2c), and an additional six-membered intramolecular $S(6)$ hydrogen bond is found (Fig. 1c). The TNB and methyl red molecules are again joined by C—H$\cdots$O hydrogen bonds (Table 5) to the nitro oxygen atoms, forming an $R_2^2(11)$ ring (Fig. 4c).

Structure (IV) crystallizes in the $P\overline{1}$ space group with the TNB, 1-naphthoic and 2-amino-5-nitropyridine molecules in the asymmetric unit. The addition of a third molecule into this charge-transfer complex results in groups of alternating DA stacks separated by the added pyridine component (Fig. 2d). The TNB molecules are joined by $R_2^1(6)$ rings, whereas a strong hydrogen-bonding interaction between the DA stacks and the 2-amino-5-nitropyridine molecule was found, forming an $R_2^2(8)$ ring, as well as a weaker bifurcated C—H$\cdots$O $R_1^2(4)$ ring (Table 6, Fig. 4d); interestingly there is no additional DA stacking with the 1-naphthoic and the pyridine components.

Figure 3
The molecular Hirshfeld surfaces mapped with shape index for the TNB acceptor molecule in (I)–(IV).
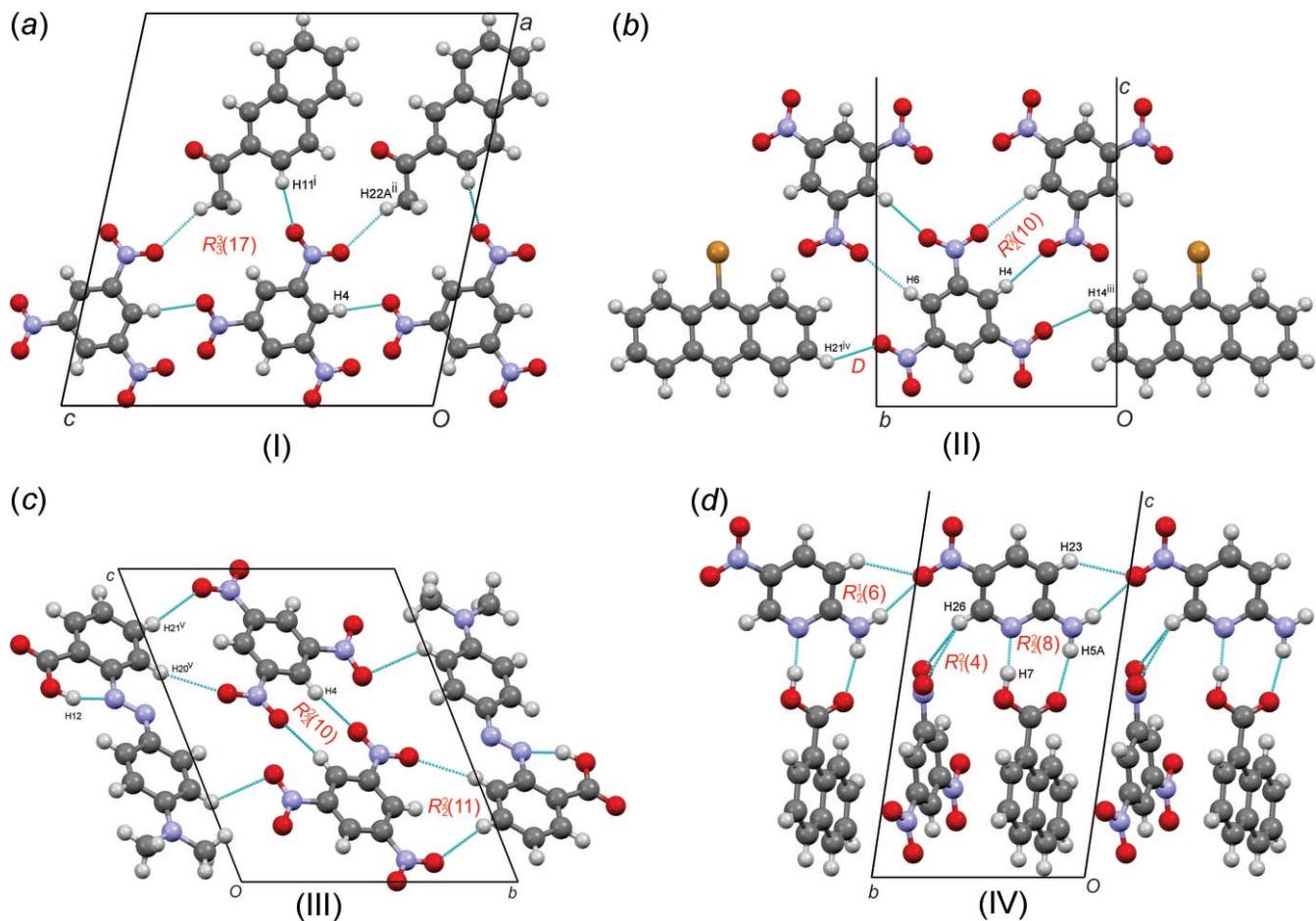
Figure 4
The hydrogen-bonding diagrams for all four compounds. Atoms with superscripts (i)–(v) are at the symmetry positions $(-x + 1, -y + 1, -z + 1)$, $(-x + 1, y - \frac{1}{2}, -z + \frac{1}{2})$, $(x, y - 1, z)$, $(x - 1, y + 1, z)$ and $(1 - x, -y, -z + 1)$ respectively.

In summary, we have contributed to the field of CT complexes using TNB, presenting further evidence that TNB is an ideal acceptor and, when paired with a donor that has hydrogen-bonding functionality, can be used to make ternary complexes.

4. Database survey

A database survey in the Cambridge Structural Database (CSD, Version 5.38; April 2017 update; Groom *et al.*, 2016) was undertaken for any structures containing the 1,3,5-trinitrobenzene moiety. A total of 135 hits where found, which was then reduced to 95 by evaluating if there is evidence of π–π interactions as indicative for a CT complex.

5. Synthesis and crystallization

All chemicals were purchased from commercial sources (Sigma Aldrich) and used as received without further purification. The 1,3,5-trinitrobenzene charge-transfer complexes were prepared in a 10 mL ethanolic solution with a 1:1 or 1:1:1 stoichiometric ratio of the donor to the acceptor molecule (based on 0.469 mmol of TNB), which was then heated until total dissolution took place (approx. 4 h). The solution was then cooled very slowly to obtain crystals suitable for X-ray diffraction. Detailed masses are as follows: (I): 0.100 g of 1,3,5-trinitrobenzene and 0.080 g of 2-acetylnaphthalene; (II): 0.100 g of 1,3,5-trinitrobenzene and 0.121 g of 9-bromo-anthracene; (III): 0.100 g of 1,3,5-trinitrobenzene and 0.127 g of methyl red; and (IV): 0.100 g of 1,3,5-trinitrobenzene, 0.081 of 1-naphthoic acid and 0.065 g of 2-amino-5-nitropyridine.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 7. For all compounds, the C-bound H atoms were placed geometrically [C—H bond lengths of 0.96 (methyl CH_3), and 0.95 Å (Ar—H)] and refined as riding with $U_{iso}(H) = 1.2U_{eq}(Ar-C)$ or $U_{iso}(H) = 1.5U_{eq}(methyl-C)$. The O and N–bound H atoms were located in the difference map and their coordinates and isotropic displacement parameters allowed to refine freely.

Table 7
Experimental details.

	(I)	(II)	(III)	(IV)
Crystal data				
Chemical formula	$C_6H_3N_3O_6 \cdot C_{12}H_{10}O$	$C_{14}H_9Br \cdot C_6H_3N_3O_6$	$C_{15}H_{15}N_3O_2 \cdot C_6H_3N_3O_6$	$C_6H_3N_3O_6 \cdot C_{11}H_8O_2 \cdot$ $C_5H_5N_3O_2$
M_r	383.31	470.24	482.41	524.41
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	293	173	173	173
a, b, c (Å)	16.6728 (10), 6.8197 (3), 15.4419 (7)	7.0928 (2), 9.7701 (3), 27.0563 (7)	8.550 (3), 10.437 (3), 13.072 (5)	7.5365 (15), 7.9003 (16), 19.153 (4)
α, β, γ (°)	90, 102.217 (3), 90	90, 100.674 (1), 90	110.689 (10), 103.510 (12), 90.730 (12)	97.580 (7), 94.667 (6), 99.547 (7)
V (Å³)	1716.03 (15)	1842.49 (9)	1055.2 (7)	1108.5 (4)
Z	4	4	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm⁻¹)	0.12	2.28	0.12	0.13
Crystal size (mm)	$0.15 \times 0.12 \times 0.07$	$0.33 \times 0.12 \times 0.11$	$0.29 \times 0.13 \times 0.12$	$0.63 \times 0.33 \times 0.06$
Data collection				
Diffractometer	Bruker D8 Venture Photon CCD area detector	Bruker D8 Venture Photon CCD area detector	Bruker D8 Venture Photon CCD area detector	Bruker D8 Venture Photon CCD area detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)	Multi-scan (*SADABS*; Sheldrick, 1996)	Multi-scan (*SADABS*; Sheldrick, 1996)	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.9, 0.95	0.56, 0.77	0.9, 0.95	0.9, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15612, 3195, 1874	28424, 4450, 3758	39527, 5072, 3262	12982, 3988, 3368
R_{int}	0.063	0.048	0.072	0.034
Refinement				
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.053, 0.152, 1.01	0.040, 0.096, 1.08	0.078, 0.249, 1.07	0.072, 0.168, 1.22
No. of reflections	3195	4450	5072	3988
No. of parameters	254	271	322	355
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	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)	0.40, −0.29	1.42, −0.94	0.49, −0.43	0.32, −0.37

Computer programs: *APEX3*, *SAINT-Plus* and *XPREP* (Bruker, 2016), *SHELXS97* (Sheldrick, 2015), *SHELXL2017/1* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

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supporting information

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Computing details

For all structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT-Plus* (Bruker, 2016); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2016). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for (I); *SHELXS97* (Sheldrick, 2015) for (II), (III), (IV). For all structures, program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015). Molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) for (I); *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006) for (II), (III), (IV). For all structures, software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

1,3,5-Trinitrobenzene–1-(naphthalen-2-yl)ethan-1-one (1/1) (I)

Crystal data

$C_6H_3N_3O_6 \cdot C_{12}H_{10}O$	$F(000) = 792$
$M_r = 383.31$	$D_x = 1.484$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1787 reflections
$a = 16.6728$ (10) Å	$\theta = 2.5$–19.9°
$b = 6.8197$ (3) Å	$\mu = 0.12$ mm^{-1}
$c = 15.4419$ (7) Å	$T = 293$ K
$\beta = 102.217$ (3)°	Plate, yellow
$V = 1716.03$ (15) Å^3	$0.15 \times 0.12 \times 0.07$ mm
$Z = 4$	

Data collection

Bruker D8 Venture Photon CCD area detector diffractometer	3195 independent reflections
	1874 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.063$
ω scans	$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -18 \rightarrow 20$
	$k = -8 \rightarrow 8$
$T_{min} = 0.9$, $T_{max} = 0.95$	$l = -18 \rightarrow 18$
15612 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.4622P]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3195 reflections	$(\Delta/\sigma)_{max} < 0.001$
254 parameters	$\Delta\rho_{max} = 0.40$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.28$ e Å^{-3}
0 constraints	

Special details

Experimental. (SADABS; Sheldrick, 1996)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.21511 (18)	0.3392 (4)	0.53179 (17)	0.0389 (7)
C2	0.29340 (17)	0.3382 (4)	0.51644 (18)	0.0405 (7)
H2	0.338939	0.313665	0.561495	0.049*
C3	0.30078 (16)	0.3753 (4)	0.43143 (18)	0.0375 (6)
C4	0.23515 (17)	0.4104 (3)	0.36307 (17)	0.0380 (7)
H4	0.242162	0.435636	0.305949	0.046*
C5	0.15851 (17)	0.4066 (3)	0.38276 (17)	0.0373 (6)
C6	0.14629 (17)	0.3724 (3)	0.46663 (17)	0.0393 (7)
H6	0.093996	0.371735	0.478805	0.047*
N1	0.2053 (2)	0.3015 (4)	0.62306 (17)	0.0552 (7)
N2	0.38409 (17)	0.3748 (3)	0.4122 (2)	0.0530 (7)
N3	0.08572 (17)	0.4407 (4)	0.31102 (18)	0.0552 (7)
O1	0.14078 (18)	0.3516 (4)	0.64216 (16)	0.0780 (8)
O2	0.26172 (18)	0.2195 (3)	0.67273 (14)	0.0753 (8)
O3	0.44113 (14)	0.3279 (3)	0.47247 (19)	0.0778 (8)
O4	0.39003 (15)	0.4197 (4)	0.33769 (17)	0.0748 (7)
O5	0.09752 (15)	0.5061 (3)	0.24181 (15)	0.0707 (7)
O6	0.01788 (16)	0.4066 (4)	0.32863 (18)	0.0871 (8)
C11	0.37425 (18)	0.8616 (4)	0.44847 (17)	0.0416 (7)
H11	0.431199	0.855588	0.46446	0.05*
C12	0.33560 (17)	0.8871 (4)	0.35789 (17)	0.0386 (6)
C13	0.25164 (17)	0.9004 (4)	0.33542 (18)	0.0399 (7)
H13	0.225873	0.918682	0.276412	0.048*
C14	0.20357 (16)	0.8866 (3)	0.40060 (17)	0.0355 (6)
C15	0.11648 (17)	0.8960 (4)	0.37776 (19)	0.0447 (7)
H15	0.090008	0.917791	0.319232	0.054*
C16	0.07171 (19)	0.8732 (4)	0.4412 (2)	0.0491 (8)
H16	0.014733	0.878211	0.425528	0.059*
C17	0.11022 (19)	0.8425 (4)	0.5296 (2)	0.0490 (8)
H17	0.078694	0.827225	0.572177	0.059*
C18	0.19420 (19)	0.8348 (4)	0.55427 (19)	0.0437 (7)
H18	0.2192	0.815473	0.61345	0.052*
C19	0.24309 (17)	0.8560 (3)	0.49009 (17)	0.0363 (6)
C20	0.32950 (17)	0.8457 (4)	0.51201 (18)	0.0402 (7)
H20	0.356146	0.827898	0.57077	0.048*
C21	0.3838 (2)	0.8968 (4)	0.2863 (2)	0.0473 (7)
C22	0.4755 (2)	0.9057 (5)	0.3127 (2)	0.0672 (10)
H22A	0.498045	0.917132	0.260632	0.101*

H22B	0.495732	0.788375	0.344169	0.101*
H22C	0.491439	1.017472	0.350196	0.101*
O7	0.34871 (15)	0.8966 (3)	0.20881 (14)	0.0650 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0476 (19)	0.0333 (14)	0.0369 (15)	−0.0045 (12)	0.0118 (14)	−0.0014 (11)
C2	0.0381 (18)	0.0357 (14)	0.0434 (16)	0.0008 (12)	−0.0011 (14)	−0.0009 (12)
C3	0.0303 (16)	0.0325 (13)	0.0510 (17)	0.0010 (11)	0.0114 (14)	−0.0037 (12)
C4	0.0447 (19)	0.0346 (14)	0.0363 (14)	0.0034 (12)	0.0121 (14)	−0.0028 (11)
C5	0.0352 (17)	0.0306 (13)	0.0421 (15)	0.0039 (11)	−0.0007 (13)	−0.0036 (11)
C6	0.0346 (17)	0.0345 (14)	0.0502 (17)	−0.0023 (12)	0.0121 (14)	−0.0070 (12)
N1	0.073 (2)	0.0471 (15)	0.0475 (16)	−0.0166 (14)	0.0164 (16)	−0.0030 (12)
N2	0.0416 (17)	0.0424 (14)	0.078 (2)	0.0023 (12)	0.0204 (16)	−0.0066 (13)
N3	0.0462 (19)	0.0524 (15)	0.0570 (17)	0.0066 (13)	−0.0114 (14)	−0.0043 (13)
O1	0.095 (2)	0.0840 (17)	0.0698 (16)	−0.0071 (15)	0.0500 (16)	−0.0035 (13)
O2	0.097 (2)	0.0782 (16)	0.0457 (13)	−0.0164 (15)	0.0035 (14)	0.0144 (12)
O3	0.0317 (14)	0.0797 (16)	0.118 (2)	0.0058 (12)	0.0062 (15)	0.0163 (15)
O4	0.0642 (18)	0.0922 (18)	0.0813 (17)	−0.0031 (13)	0.0449 (15)	−0.0105 (14)
O5	0.0794 (19)	0.0802 (16)	0.0436 (12)	0.0271 (13)	−0.0073 (13)	0.0002 (12)
O6	0.0373 (16)	0.101 (2)	0.112 (2)	−0.0084 (14)	−0.0087 (15)	0.0112 (16)
C11	0.0329 (16)	0.0417 (15)	0.0488 (17)	0.0003 (12)	0.0056 (14)	−0.0014 (12)
C12	0.0349 (17)	0.0365 (14)	0.0451 (16)	−0.0017 (12)	0.0102 (13)	−0.0027 (12)
C13	0.0406 (18)	0.0362 (14)	0.0407 (15)	0.0010 (12)	0.0038 (13)	−0.0014 (12)
C14	0.0290 (16)	0.0292 (12)	0.0461 (16)	0.0018 (11)	0.0032 (13)	−0.0040 (11)
C15	0.0361 (18)	0.0404 (15)	0.0538 (17)	0.0053 (12)	0.0010 (15)	−0.0034 (13)
C16	0.0349 (18)	0.0454 (16)	0.068 (2)	0.0061 (13)	0.0131 (16)	−0.0054 (15)
C17	0.044 (2)	0.0430 (16)	0.066 (2)	0.0039 (13)	0.0249 (17)	−0.0054 (14)
C18	0.049 (2)	0.0382 (15)	0.0456 (16)	0.0023 (13)	0.0137 (15)	−0.0019 (12)
C19	0.0359 (17)	0.0307 (14)	0.0413 (15)	0.0020 (11)	0.0063 (13)	−0.0026 (11)
C20	0.0381 (18)	0.0401 (14)	0.0396 (15)	0.0016 (12)	0.0016 (13)	0.0004 (12)
C21	0.052 (2)	0.0463 (16)	0.0466 (18)	0.0000 (14)	0.0180 (16)	−0.0048 (14)
C22	0.046 (2)	0.095 (3)	0.067 (2)	−0.0053 (19)	0.0274 (18)	−0.0026 (19)
O7	0.0648 (16)	0.0863 (16)	0.0466 (13)	−0.0020 (13)	0.0180 (12)	−0.0060 (11)

Geometric parameters (Å, °)

C1—C2	1.375 (4)	C12—C13	1.372 (4)
C1—C6	1.375 (4)	C12—C21	1.500 (4)
C1—N1	1.475 (4)	C13—C14	1.416 (4)
C2—C3	1.368 (4)	C13—H13	0.93
C2—H2	0.93	C14—C19	1.415 (4)
C3—C4	1.371 (4)	C14—C15	1.421 (4)
C3—N2	1.481 (4)	C15—C16	1.361 (4)
C4—C5	1.375 (4)	C15—H15	0.93
C4—H4	0.93	C16—C17	1.396 (4)
C5—C6	1.373 (4)	C16—H16	0.93

C5—N3	1.478 (4)	C17—C18	1.372 (4)
C6—H6	0.93	C17—H17	0.93
N1—O2	1.217 (4)	C18—C19	1.418 (4)
N1—O1	1.222 (3)	C18—H18	0.93
N2—O4	1.214 (3)	C19—C20	1.410 (4)
N2—O3	1.224 (3)	C20—H20	0.93
N3—O5	1.212 (3)	C21—O7	1.215 (3)
N3—O6	1.240 (3)	C21—C22	1.497 (4)
C11—C20	1.357 (4)	C22—H22A	0.96
C11—C12	1.422 (4)	C22—H22B	0.96
C11—H11	0.93	C22—H22C	0.96
C2—C1—C6	123.4 (2)	C12—C13—C14	121.1 (3)
C2—C1—N1	117.7 (3)	C12—C13—H13	119.5
C6—C1—N1	118.9 (3)	C14—C13—H13	119.5
C3—C2—C1	116.5 (3)	C19—C14—C13	119.2 (2)
C3—C2—H2	121.8	C19—C14—C15	119.3 (2)
C1—C2—H2	121.8	C13—C14—C15	121.5 (2)
C2—C3—C4	123.5 (2)	C16—C15—C14	120.2 (3)
C2—C3—N2	118.1 (3)	C16—C15—H15	119.9
C4—C3—N2	118.4 (2)	C14—C15—H15	119.9
C3—C4—C5	117.0 (2)	C15—C16—C17	120.8 (3)
C3—C4—H4	121.5	C15—C16—H16	119.6
C5—C4—H4	121.5	C17—C16—H16	119.6
C6—C5—C4	122.8 (3)	C18—C17—C16	120.5 (3)
C6—C5—N3	118.1 (3)	C18—C17—H17	119.7
C4—C5—N3	119.0 (2)	C16—C17—H17	119.7
C5—C6—C1	116.8 (3)	C17—C18—C19	120.4 (3)
C5—C6—H6	121.6	C17—C18—H18	119.8
C1—C6—H6	121.6	C19—C18—H18	119.8
O2—N1—O1	125.4 (3)	C20—C19—C14	118.9 (2)
O2—N1—C1	117.0 (3)	C20—C19—C18	122.4 (2)
O1—N1—C1	117.6 (3)	C14—C19—C18	118.7 (3)
O4—N2—O3	125.5 (3)	C11—C20—C19	120.8 (3)
O4—N2—C3	117.2 (3)	C11—C20—H20	119.6
O3—N2—C3	117.3 (3)	C19—C20—H20	119.6
O5—N3—O6	126.0 (3)	O7—C21—C22	121.3 (3)
O5—N3—C5	117.3 (3)	O7—C21—C12	120.2 (3)
O6—N3—C5	116.6 (3)	C22—C21—C12	118.4 (3)
C20—C11—C12	121.1 (3)	C21—C22—H22A	109.5
C20—C11—H11	119.4	C21—C22—H22B	109.5
C12—C11—H11	119.4	H22A—C22—H22B	109.5
C13—C12—C11	118.9 (2)	C21—C22—H22C	109.5
C13—C12—C21	119.2 (3)	H22A—C22—H22C	109.5
C11—C12—C21	121.9 (3)	H22B—C22—H22C	109.5
C6—C1—C2—C3	0.9 (4)	C20—C11—C12—C13	1.5 (4)
N1—C1—C2—C3	−179.4 (2)	C20—C11—C12—C21	−177.5 (2)

C1—C2—C3—C4	−0.6 (4)	C11—C12—C13—C14	−0.8 (4)
C1—C2—C3—N2	−179.8 (2)	C21—C12—C13—C14	178.3 (2)
C2—C3—C4—C5	−0.3 (4)	C12—C13—C14—C19	−0.9 (3)
N2—C3—C4—C5	178.9 (2)	C12—C13—C14—C15	−178.7 (2)
C3—C4—C5—C6	0.9 (4)	C19—C14—C15—C16	−0.9 (4)
C3—C4—C5—N3	−179.1 (2)	C13—C14—C15—C16	176.9 (2)
C4—C5—C6—C1	−0.7 (4)	C14—C15—C16—C17	0.7 (4)
N3—C5—C6—C1	179.4 (2)	C15—C16—C17—C18	0.0 (4)
C2—C1—C6—C5	−0.2 (4)	C16—C17—C18—C19	−0.6 (4)
N1—C1—C6—C5	−179.9 (2)	C13—C14—C19—C20	1.8 (3)
C2—C1—N1—O2	−20.0 (4)	C15—C14—C19—C20	179.6 (2)
C6—C1—N1—O2	159.7 (3)	C13—C14—C19—C18	−177.6 (2)
C2—C1—N1—O1	161.3 (3)	C15—C14—C19—C18	0.3 (3)
C6—C1—N1—O1	−19.0 (4)	C17—C18—C19—C20	−178.9 (2)
C2—C3—N2—O4	−175.6 (2)	C17—C18—C19—C14	0.4 (4)
C4—C3—N2—O4	5.2 (4)	C12—C11—C20—C19	−0.6 (4)
C2—C3—N2—O3	4.9 (4)	C14—C19—C20—C11	−1.1 (3)
C4—C3—N2—O3	−174.4 (2)	C18—C19—C20—C11	178.2 (2)
C6—C5—N3—O5	166.6 (2)	C13—C12—C21—O7	−7.3 (4)
C4—C5—N3—O5	−13.4 (3)	C11—C12—C21—O7	171.7 (3)
C6—C5—N3—O6	−10.7 (4)	C13—C12—C21—C22	173.0 (3)
C4—C5—N3—O6	169.3 (3)	C11—C12—C21—C22	−8.0 (4)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2[i]	0.93	2.4	3.189 (3)	143
C11—H11···O3[ii]	0.93	2.48	3.323 (4)	150
C22—H22A···O4[iii]	0.96	2.64	3.554 (4)	159

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

1,3,5-Trinitrobenzene–9-bromoanthracene (1/1) (II)

Crystal data

$C_{14}H_9Br·C_6H_3N_3O_6$
$M_r = 470.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.0928 (2)$ Å
$b = 9.7701 (3)$ Å
$c = 27.0563 (7)$ Å
$\beta = 100.674 (1)°$
$V = 1842.49 (9)$ Å^3
$Z = 4$

$F(000) = 944$
$D_x = 1.695$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8164 reflections
$\theta = 2.2–27.9°$
$\mu = 2.28$ mm^{-1}
$T = 173$ K
Needle, yellow
$0.33 × 0.12 × 0.11$ mm

Data collection

Bruker D8 Venture Photon CCD area detector diffractometer
Graphite monochromator
ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.56$, $T_{max} = 0.77$
28424 measured reflections

4450 independent reflections
3758 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.5°$

$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -35 \rightarrow 35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.096$
$S = 1.08$
4450 reflections
271 parameters
0 restraints
0 constraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 2.1935P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.42$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}

Special details

Experimental. (SADABS; Sheldrick, 1996)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3620 (3)	0.7554 (2)	0.10545 (9)	0.0275 (5)
C2	0.3965 (3)	0.6350 (2)	0.08161 (9)	0.0256 (5)
H2	0.369113	0.62674	0.046011	0.031*
C3	0.4723 (3)	0.5280 (2)	0.11194 (9)	0.0236 (4)
C4	0.5164 (3)	0.5366 (2)	0.16372 (9)	0.0267 (5)
H4	0.568061	0.460884	0.183771	0.032*
C5	0.4822 (4)	0.6599 (3)	0.18498 (9)	0.0293 (5)
C6	0.4047 (4)	0.7724 (2)	0.15702 (10)	0.0303 (5)
H6	0.382248	0.856585	0.172517	0.036*
N1	0.2782 (3)	0.8716 (2)	0.07398 (10)	0.0370 (5)
N2	0.5097 (3)	0.3967 (2)	0.08822 (8)	0.0290 (4)
N3	0.5319 (4)	0.6732 (2)	0.24030 (8)	0.0401 (6)
O1	0.2533 (3)	0.9777 (2)	0.09572 (9)	0.0543 (6)
O2	0.2376 (3)	0.8538 (2)	0.02904 (9)	0.0519 (6)
O3	0.4729 (3)	0.3904 (2)	0.04231 (7)	0.0396 (4)
O4	0.5756 (3)	0.30406 (19)	0.11577 (8)	0.0434 (5)
O5	0.5774 (5)	0.5714 (2)	0.26496 (8)	0.0654 (7)
O6	0.5271 (4)	0.7868 (3)	0.25776 (9)	0.0634 (7)
C11	0.9660 (3)	0.6511 (2)	0.16436 (8)	0.0235 (4)
C12	0.8864 (3)	0.7691 (2)	0.13900 (8)	0.0231 (4)
C13	0.8514 (4)	0.8940 (2)	0.16310 (9)	0.0305 (5)
H13	0.883923	0.900938	0.198681	0.037*
C14	0.7719 (4)	1.0031 (2)	0.13575 (10)	0.0338 (6)
H14	0.748685	1.084959	0.15261	0.041*
C15	0.7233 (4)	0.9972 (3)	0.08274 (10)	0.0319 (5)

H15	0.668981	1.074876	0.064272	0.038*
C16	0.7543 (3)	0.8804 (2)	0.05821 (9)	0.0285 (5)
H16	0.721939	0.877421	0.02255	0.034*
C17	0.8346 (3)	0.7622 (2)	0.08509 (8)	0.0223 (4)
C18	0.8607 (3)	0.6406 (2)	0.06047 (8)	0.0239 (5)
H18	0.824385	0.636703	0.024888	0.029*
C19	0.9385 (3)	0.5241 (2)	0.08641 (8)	0.0226 (4)
C20	0.9636 (3)	0.4002 (2)	0.06075 (9)	0.0274 (5)
H20	0.924336	0.396003	0.02525	0.033*
C21	1.0428 (4)	0.2876 (3)	0.08608 (10)	0.0322 (5)
H21	1.058174	0.205658	0.068314	0.039*
C22	1.1019 (4)	0.2928 (3)	0.13873 (10)	0.0319 (5)
H22	1.159053	0.214283	0.156067	0.038*
C23	1.0789 (3)	0.4077 (2)	0.16519 (9)	0.0282 (5)
H23	1.118668	0.408027	0.200702	0.034*
C24	0.9956 (3)	0.5283 (2)	0.14027 (8)	0.0224 (4)
Br1	1.03399 (4)	0.65915 (3)	0.23592 (2)	0.03853 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0215 (11)	0.0233 (11)	0.0390 (13)	0.0012 (9)	0.0088 (10)	0.0050 (10)
C2	0.0224 (11)	0.0255 (12)	0.0296 (11)	−0.0013 (9)	0.0067 (9)	0.0014 (9)
C3	0.0203 (10)	0.0211 (11)	0.0306 (11)	−0.0022 (8)	0.0075 (9)	−0.0027 (9)
C4	0.0268 (12)	0.0232 (11)	0.0307 (12)	−0.0006 (9)	0.0068 (9)	0.0009 (9)
C5	0.0297 (12)	0.0287 (12)	0.0301 (12)	−0.0045 (10)	0.0071 (10)	−0.0041 (10)
C6	0.0309 (13)	0.0228 (12)	0.0393 (13)	−0.0013 (10)	0.0121 (10)	−0.0064 (10)
N1	0.0296 (11)	0.0304 (12)	0.0515 (14)	0.0040 (9)	0.0094 (10)	0.0117 (10)
N2	0.0264 (10)	0.0259 (10)	0.0353 (11)	−0.0005 (8)	0.0076 (8)	−0.0060 (9)
N3	0.0492 (14)	0.0377 (13)	0.0331 (12)	−0.0039 (11)	0.0068 (10)	−0.0095 (10)
O1	0.0568 (14)	0.0288 (11)	0.0759 (16)	0.0161 (10)	0.0087 (12)	0.0048 (10)
O2	0.0588 (14)	0.0489 (13)	0.0476 (13)	0.0129 (11)	0.0091 (10)	0.0208 (10)
O3	0.0412 (11)	0.0416 (11)	0.0347 (10)	0.0031 (9)	0.0040 (8)	−0.0129 (8)
O4	0.0580 (13)	0.0250 (9)	0.0485 (12)	0.0132 (9)	0.0136 (10)	0.0009 (8)
O5	0.116 (2)	0.0441 (13)	0.0327 (11)	−0.0039 (13)	0.0041 (12)	0.0036 (10)
O6	0.0894 (19)	0.0487 (13)	0.0455 (13)	0.0123 (13)	−0.0048 (12)	−0.0221 (11)
C11	0.0252 (11)	0.0260 (11)	0.0195 (10)	0.0006 (9)	0.0044 (8)	0.0025 (8)
C12	0.0239 (11)	0.0214 (11)	0.0242 (11)	0.0001 (9)	0.0047 (9)	0.0014 (8)
C13	0.0406 (14)	0.0230 (11)	0.0279 (12)	0.0002 (10)	0.0061 (10)	−0.0032 (9)
C14	0.0423 (15)	0.0183 (11)	0.0409 (14)	0.0006 (10)	0.0077 (11)	−0.0026 (10)
C15	0.0334 (13)	0.0232 (12)	0.0388 (13)	0.0023 (10)	0.0062 (10)	0.0078 (10)
C16	0.0297 (12)	0.0277 (12)	0.0275 (11)	0.0021 (10)	0.0042 (9)	0.0061 (9)
C17	0.0199 (10)	0.0233 (11)	0.0245 (10)	−0.0006 (8)	0.0060 (8)	0.0031 (8)
C18	0.0225 (11)	0.0290 (12)	0.0207 (10)	0.0019 (9)	0.0053 (8)	0.0003 (8)
C19	0.0188 (10)	0.0242 (11)	0.0260 (11)	0.0005 (8)	0.0071 (8)	−0.0003 (9)
C20	0.0249 (11)	0.0286 (12)	0.0300 (12)	−0.0002 (9)	0.0086 (9)	−0.0047 (10)
C21	0.0301 (13)	0.0227 (11)	0.0465 (15)	0.0021 (10)	0.0146 (11)	−0.0055 (10)
C22	0.0309 (13)	0.0219 (11)	0.0443 (14)	0.0046 (10)	0.0103 (11)	0.0073 (10)

C23	0.0274 (12)	0.0252 (12)	0.0319 (12)	0.0020 (9)	0.0056 (10)	0.0057 (9)
C24	0.0197 (10)	0.0216 (11)	0.0267 (11)	0.0000 (8)	0.0061 (8)	0.0019 (8)
Br1	0.05475 (19)	0.03823 (16)	0.02111 (13)	0.01206 (12)	0.00313 (10)	0.00126 (10)

Geometric parameters (Å, º)

C1—C6	1.382 (4)	C12—C17	1.438 (3)
C1—C2	1.385 (3)	C13—C14	1.359 (3)
C1—N1	1.477 (3)	C13—H13	0.95
C2—C3	1.376 (3)	C14—C15	1.413 (4)
C2—H2	0.95	C14—H14	0.95
C3—C4	1.381 (3)	C15—C16	1.358 (4)
C3—N2	1.480 (3)	C15—H15	0.95
C4—C5	1.376 (3)	C16—C17	1.426 (3)
C4—H4	0.95	C16—H16	0.95
C5—C6	1.388 (3)	C17—C18	1.391 (3)
C5—N3	1.479 (3)	C18—C19	1.396 (3)
C6—H6	0.95	C18—H18	0.95
N1—O2	1.209 (3)	C19—C20	1.423 (3)
N1—O1	1.221 (3)	C19—C24	1.439 (3)
N2—O4	1.210 (3)	C20—C21	1.362 (4)
N2—O3	1.222 (3)	C20—H20	0.95
N3—O5	1.208 (3)	C21—C22	1.409 (4)
N3—O6	1.209 (3)	C21—H21	0.95
C11—C24	1.400 (3)	C22—C23	1.358 (4)
C11—C12	1.405 (3)	C22—H22	0.95
C11—Br1	1.908 (2)	C23—C24	1.430 (3)
C12—C13	1.426 (3)	C23—H23	0.95
C6—C1—C2	123.2 (2)	C12—C13—H13	119.6
C6—C1—N1	118.6 (2)	C13—C14—C15	121.3 (2)
C2—C1—N1	118.1 (2)	C13—C14—H14	119.4
C3—C2—C1	116.8 (2)	C15—C14—H14	119.4
C3—C2—H2	121.6	C16—C15—C14	119.9 (2)
C1—C2—H2	121.6	C16—C15—H15	120
C2—C3—C4	123.3 (2)	C14—C15—H15	120
C2—C3—N2	118.8 (2)	C15—C16—C17	121.1 (2)
C4—C3—N2	117.9 (2)	C15—C16—H16	119.4
C5—C4—C3	117.0 (2)	C17—C16—H16	119.4
C5—C4—H4	121.5	C18—C17—C16	121.6 (2)
C3—C4—H4	121.5	C18—C17—C12	119.6 (2)
C4—C5—C6	123.2 (2)	C16—C17—C12	118.8 (2)
C4—C5—N3	118.2 (2)	C17—C18—C19	122.1 (2)
C6—C5—N3	118.6 (2)	C17—C18—H18	119
C1—C6—C5	116.4 (2)	C19—C18—H18	119
C1—C6—H6	121.8	C18—C19—C20	121.5 (2)
C5—C6—H6	121.8	C18—C19—C24	119.8 (2)
O2—N1—O1	125.3 (2)	C20—C19—C24	118.8 (2)

O2—N1—C1	117.7 (2)	C21—C20—C19	121.3 (2)
O1—N1—C1	117.0 (2)	C21—C20—H20	119.4
O4—N2—O3	125.0 (2)	C19—C20—H20	119.4
O4—N2—C3	117.4 (2)	C20—C21—C22	119.8 (2)
O3—N2—C3	117.6 (2)	C20—C21—H21	120.1
O5—N3—O6	124.3 (2)	C22—C21—H21	120.1
O5—N3—C5	118.4 (2)	C23—C22—C21	121.4 (2)
O6—N3—C5	117.2 (2)	C23—C22—H22	119.3
C24—C11—C12	123.9 (2)	C21—C22—H22	119.3
C24—C11—Br1	118.43 (16)	C22—C23—C24	120.8 (2)
C12—C11—Br1	117.69 (17)	C22—C23—H23	119.6
C11—C12—C13	124.5 (2)	C24—C23—H23	119.6
C11—C12—C17	117.4 (2)	C11—C24—C23	124.9 (2)
C13—C12—C17	118.0 (2)	C11—C24—C19	117.23 (19)
C14—C13—C12	120.8 (2)	C23—C24—C19	117.9 (2)
C14—C13—H13	119.6		
C6—C1—C2—C3	1.8 (4)	C17—C12—C13—C14	−0.2 (4)
N1—C1—C2—C3	−179.2 (2)	C12—C13—C14—C15	−0.6 (4)
C1—C2—C3—C4	−0.9 (3)	C13—C14—C15—C16	0.6 (4)
C1—C2—C3—N2	179.4 (2)	C14—C15—C16—C17	0.4 (4)
C2—C3—C4—C5	−0.3 (4)	C15—C16—C17—C18	177.7 (2)
N2—C3—C4—C5	179.4 (2)	C15—C16—C17—C12	−1.2 (4)
C3—C4—C5—C6	0.8 (4)	C11—C12—C17—C18	1.3 (3)
C3—C4—C5—N3	−178.7 (2)	C13—C12—C17—C18	−177.8 (2)
C2—C1—C6—C5	−1.3 (4)	C11—C12—C17—C16	−179.7 (2)
N1—C1—C6—C5	179.6 (2)	C13—C12—C17—C16	1.2 (3)
C4—C5—C6—C1	0.0 (4)	C16—C17—C18—C19	−179.8 (2)
N3—C5—C6—C1	179.5 (2)	C12—C17—C18—C19	−0.8 (3)
C6—C1—N1—O2	−178.3 (2)	C17—C18—C19—C20	179.7 (2)
C2—C1—N1—O2	2.6 (3)	C17—C18—C19—C24	−0.4 (3)
C6—C1—N1—O1	0.8 (3)	C18—C19—C20—C21	178.8 (2)
C2—C1—N1—O1	−178.3 (2)	C24—C19—C20—C21	−1.0 (3)
C2—C3—N2—O4	−179.7 (2)	C19—C20—C21—C22	−0.1 (4)
C4—C3—N2—O4	0.6 (3)	C20—C21—C22—C23	1.1 (4)
C2—C3—N2—O3	0.8 (3)	C21—C22—C23—C24	−0.8 (4)
C4—C3—N2—O3	−179.0 (2)	C12—C11—C24—C23	179.0 (2)
C4—C5—N3—O5	−9.2 (4)	Br1—C11—C24—C23	−1.9 (3)
C6—C5—N3—O5	171.2 (3)	C12—C11—C24—C19	−0.7 (3)
C4—C5—N3—O6	169.6 (3)	Br1—C11—C24—C19	178.46 (16)
C6—C5—N3—O6	−9.9 (4)	C22—C23—C24—C11	179.9 (2)
C24—C11—C12—C13	178.5 (2)	C22—C23—C24—C19	−0.5 (3)
Br1—C11—C12—C13	−0.6 (3)	C18—C19—C24—C11	1.2 (3)
C24—C11—C12—C17	−0.6 (3)	C20—C19—C24—C11	−179.0 (2)
Br1—C11—C12—C17	−179.70 (16)	C18—C19—C24—C23	−178.5 (2)
C11—C12—C13—C14	−179.3 (2)	C20—C19—C24—C23	1.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O6^i	0.95	2.5	3.287 (3)	140
C6—H6···O5^{ii}	0.95	2.68	3.593 (3)	162
C14—H14···O4^{iii}	0.95	2.57	3.255 (3)	129
C21—H21···O1^{iv}	0.95	2.65	3.364 (3)	132

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

1,3,5-Trinitrobenzene–2-{(E)-[4-(dimethylamino)phenyl]diazenyl}benzoic acid (1/1) (III)

Crystal data
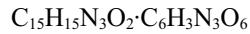
$C_{15}H_{15}N_3O_2 \cdot C_6H_3N_3O_6$	$Z = 2$
$M_r = 482.41$	$F(000) = 500$
Triclinic, $P\bar{1}$	$D_x = 1.518$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.550$ (3) Å	Cell parameters from 9824 reflections
$b = 10.437$ (3) Å	$\theta = 3.1$–28.2°
$c = 13.072$ (5) Å	$\mu = 0.12$ mm^{-1}
$\alpha = 110.689$ (10)°	$T = 173$ K
$\beta = 103.510$ (12)°	Cuboid, red
$\gamma = 90.730$ (12)°	0.29 × 0.13 × 0.12 mm
$V = 1055.2$ (7) Å^3	

Data collection

Bruker D8 Venture Photon CCD area detector diffractometer	5072 independent reflections
	3262 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.072$
ω scans	$\theta_{max} = 28.0°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
	$k = -13 \rightarrow 13$
$T_{min} = 0.9$, $T_{max} = 0.95$	$l = -17 \rightarrow 17$
39527 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.078$	
$wR(F^2) = 0.249$	$w = 1/[\sigma^2(F_o^2) + (0.1346P)^2 + 0.8758P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	
5072 reflections	$(\Delta/\sigma)_{max} < 0.001$
322 parameters	$\Delta\rho_{max} = 0.49$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.43$ e Å^{-3}
0 constraints	

Special details

Experimental. (SADABS; Sheldrick, 1996)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3627 (3)	0.4196 (3)	0.8376 (2)	0.0274 (6)
C2	0.4468 (3)	0.3469 (3)	0.7610 (2)	0.0265 (6)
H2	0.49673	0.267951	0.76649	0.032*
C3	0.4549 (3)	0.3944 (3)	0.6758 (2)	0.0266 (6)
C4	0.3817 (3)	0.5079 (3)	0.6651 (2)	0.0279 (6)
H4	0.386476	0.537651	0.605026	0.033*
C5	0.3010 (4)	0.5763 (3)	0.7456 (3)	0.0287 (6)
C6	0.2887 (3)	0.5341 (3)	0.8327 (2)	0.0284 (6)
H6	0.231723	0.582036	0.88668	0.034*
N1	0.3560 (3)	0.3737 (3)	0.9312 (2)	0.0324 (6)
N2	0.5442 (3)	0.3204 (3)	0.5938 (2)	0.0305 (6)
N3	0.2291 (3)	0.7015 (3)	0.7399 (2)	0.0367 (6)
O1	0.2796 (3)	0.4374 (3)	0.9979 (2)	0.0475 (6)
O2	0.4303 (3)	0.2766 (3)	0.93921 (19)	0.0437 (6)
O3	0.6018 (3)	0.2169 (2)	0.6015 (2)	0.0405 (6)
O4	0.5548 (3)	0.3668 (3)	0.5212 (2)	0.0435 (6)
O5	0.2266 (3)	0.7301 (3)	0.6567 (2)	0.0485 (7)
O6	0.1772 (3)	0.7707 (3)	0.8201 (2)	0.0507 (7)
C11	0.1578 (3)	0.1335 (3)	0.5551 (2)	0.0255 (6)
C12	0.1935 (4)	0.0433 (3)	0.6139 (2)	0.0272 (6)
H12A	0.258146	−0.028852	0.588579	0.033*
C13	0.1372 (3)	0.0571 (3)	0.7067 (2)	0.0278 (6)
H13	0.163717	−0.004867	0.745181	0.033*
C14	0.0402 (3)	0.1627 (3)	0.7454 (2)	0.0262 (6)
C15	−0.0005 (3)	0.2516 (3)	0.6840 (3)	0.0293 (6)
H15	−0.068293	0.32188	0.707451	0.035*
C16	0.0572 (3)	0.2365 (3)	0.5914 (3)	0.0283 (6)
H16	0.028785	0.296526	0.551294	0.034*
C17	0.0277 (4)	0.0891 (4)	0.9028 (3)	0.0388 (8)
H17A	−0.012745	−0.006156	0.852959	0.058*
H17B	−0.022233	0.116076	0.966614	0.058*
H17C	0.145383	0.096273	0.93118	0.058*
C18	−0.1074 (5)	0.2903 (4)	0.8855 (3)	0.0444 (9)
H18A	−0.116874	0.351673	0.842831	0.067*
H18B	−0.053611	0.342523	0.965088	0.067*
H18C	−0.215479	0.251383	0.87965	0.067*
C19	0.2781 (3)	0.1679 (3)	0.3235 (2)	0.0265 (6)
C20	0.3656 (4)	0.0550 (3)	0.2908 (3)	0.0336 (7)
H20	0.380119	−0.005691	0.331185	0.04*
C21	0.4310 (4)	0.0317 (3)	0.1995 (3)	0.0378 (7)
H21	0.490257	−0.045347	0.177299	0.045*
C22	0.4111 (4)	0.1198 (3)	0.1398 (3)	0.0347 (7)
H22	0.455378	0.10206	0.076507	0.042*
C23	0.3273 (4)	0.2324 (3)	0.1724 (2)	0.0315 (7)
H23	0.314185	0.292407	0.131361	0.038*

C24	0.2613 (3)	0.2597 (3)	0.2650 (2)	0.0259 (6)
C25	0.1757 (4)	0.3865 (3)	0.2948 (3)	0.0338 (7)
N11	0.2263 (3)	0.1105 (2)	0.4652 (2)	0.0280 (6)
N12	0.2057 (3)	0.1977 (3)	0.4154 (2)	0.0282 (6)
N13	−0.0133 (3)	0.1802 (3)	0.8396 (2)	0.0343 (6)
O11	0.1681 (4)	0.4628 (3)	0.2426 (2)	0.0520 (7)
O12	0.1077 (3)	0.4150 (2)	0.3810 (2)	0.0395 (6)
H12	0.130 (6)	0.347 (6)	0.413 (5)	0.096 (18)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0319 (15)	0.0312 (16)	0.0233 (14)	−0.0012 (12)	0.0082 (12)	0.0144 (12)
C2	0.0295 (15)	0.0266 (15)	0.0271 (14)	0.0022 (11)	0.0080 (12)	0.0138 (11)
C3	0.0283 (15)	0.0286 (15)	0.0275 (14)	0.0014 (11)	0.0117 (12)	0.0130 (12)
C4	0.0310 (15)	0.0302 (16)	0.0273 (14)	0.0010 (12)	0.0080 (12)	0.0162 (12)
C5	0.0340 (16)	0.0247 (15)	0.0322 (15)	0.0045 (12)	0.0108 (12)	0.0147 (12)
C6	0.0308 (15)	0.0286 (16)	0.0284 (15)	0.0018 (12)	0.0111 (12)	0.0115 (12)
N1	0.0394 (15)	0.0364 (15)	0.0263 (13)	0.0010 (11)	0.0120 (11)	0.0150 (11)
N2	0.0340 (14)	0.0340 (14)	0.0290 (13)	0.0028 (11)	0.0128 (11)	0.0151 (11)
N3	0.0400 (15)	0.0311 (15)	0.0463 (16)	0.0088 (11)	0.0155 (13)	0.0197 (12)
O1	0.0657 (17)	0.0558 (16)	0.0391 (13)	0.0174 (12)	0.0322 (12)	0.0264 (11)
O2	0.0643 (16)	0.0442 (14)	0.0379 (13)	0.0172 (12)	0.0205 (12)	0.0283 (11)
O3	0.0502 (14)	0.0396 (13)	0.0461 (14)	0.0167 (11)	0.0266 (11)	0.0232 (11)
O4	0.0583 (16)	0.0514 (15)	0.0398 (13)	0.0125 (11)	0.0292 (12)	0.0285 (11)
O5	0.0607 (16)	0.0482 (15)	0.0630 (17)	0.0212 (12)	0.0295 (13)	0.0424 (13)
O6	0.0681 (18)	0.0384 (14)	0.0545 (16)	0.0222 (12)	0.0277 (13)	0.0194 (12)
C11	0.0235 (14)	0.0251 (14)	0.0304 (15)	0.0009 (11)	0.0062 (11)	0.0138 (11)
C12	0.0304 (15)	0.0251 (15)	0.0286 (15)	0.0056 (11)	0.0074 (12)	0.0129 (11)
C13	0.0329 (16)	0.0257 (15)	0.0289 (15)	0.0065 (12)	0.0069 (12)	0.0154 (12)
C14	0.0245 (14)	0.0278 (15)	0.0284 (14)	−0.0001 (11)	0.0056 (11)	0.0134 (12)
C15	0.0269 (15)	0.0301 (16)	0.0361 (16)	0.0075 (12)	0.0095 (12)	0.0173 (13)
C16	0.0280 (15)	0.0289 (15)	0.0332 (15)	0.0029 (11)	0.0062 (12)	0.0185 (12)
C17	0.049 (2)	0.0442 (19)	0.0345 (17)	0.0110 (15)	0.0156 (15)	0.0247 (15)
C18	0.054 (2)	0.047 (2)	0.048 (2)	0.0202 (16)	0.0299 (17)	0.0257 (16)
C19	0.0272 (15)	0.0297 (15)	0.0255 (14)	0.0022 (11)	0.0074 (11)	0.0130 (11)
C20	0.0400 (18)	0.0306 (16)	0.0373 (17)	0.0089 (13)	0.0128 (14)	0.0188 (13)
C21	0.0437 (19)	0.0353 (18)	0.0395 (18)	0.0131 (14)	0.0151 (15)	0.0163 (14)
C22	0.0404 (18)	0.0392 (18)	0.0294 (15)	0.0066 (14)	0.0161 (13)	0.0135 (13)
C23	0.0387 (17)	0.0324 (17)	0.0285 (15)	0.0046 (13)	0.0106 (13)	0.0159 (12)
C24	0.0310 (15)	0.0255 (15)	0.0236 (14)	0.0031 (11)	0.0086 (11)	0.0110 (11)
C25	0.0413 (18)	0.0328 (17)	0.0356 (16)	0.0088 (13)	0.0156 (14)	0.0186 (13)
N11	0.0310 (13)	0.0289 (13)	0.0284 (12)	0.0023 (10)	0.0077 (10)	0.0155 (10)
N12	0.0303 (13)	0.0280 (13)	0.0320 (13)	0.0039 (10)	0.0104 (10)	0.0162 (10)
N13	0.0427 (15)	0.0367 (15)	0.0351 (14)	0.0125 (12)	0.0185 (12)	0.0214 (12)
O11	0.0814 (19)	0.0462 (15)	0.0579 (16)	0.0309 (13)	0.0425 (14)	0.0375 (13)
O12	0.0535 (15)	0.0356 (13)	0.0446 (14)	0.0169 (10)	0.0292 (11)	0.0218 (11)

Geometric parameters (Å, º)

C1—C6	1.374 (4)	C15—C16	1.371 (4)
C1—C2	1.382 (4)	C15—H15	0.95
C1—N1	1.476 (4)	C16—H16	0.95
C2—C3	1.384 (4)	C17—N13	1.461 (4)
C2—H2	0.95	C17—H17A	0.98
C3—C4	1.382 (4)	C17—H17B	0.98
C3—N2	1.463 (4)	C17—H17C	0.98
C4—C5	1.383 (4)	C18—N13	1.446 (4)
C4—H4	0.95	C18—H18A	0.98
C5—C6	1.383 (4)	C18—H18B	0.98
C5—N3	1.469 (4)	C18—H18C	0.98
C6—H6	0.95	C19—C20	1.396 (4)
N1—O1	1.223 (4)	C19—C24	1.412 (4)
N1—O2	1.225 (4)	C19—N12	1.418 (4)
N2—O3	1.219 (3)	C20—C21	1.380 (5)
N2—O4	1.227 (3)	C20—H20	0.95
N3—O5	1.221 (4)	C21—C22	1.390 (5)
N3—O6	1.228 (4)	C21—H21	0.95
C11—N11	1.381 (4)	C22—C23	1.374 (4)
C11—C16	1.406 (4)	C22—H22	0.95
C11—C12	1.406 (4)	C23—C24	1.395 (4)
C12—C13	1.370 (4)	C23—H23	0.95
C12—H12A	0.95	C24—C25	1.494 (4)
C13—C14	1.408 (4)	C25—O11	1.212 (4)
C13—H13	0.95	C25—O12	1.331 (4)
C14—N13	1.366 (4)	N11—N12	1.285 (3)
C14—C15	1.425 (4)	O12—H12	0.95 (6)
C6—C1—C2	123.5 (3)	C15—C16—C11	120.9 (3)
C6—C1—N1	118.4 (3)	C15—C16—H16	119.6
C2—C1—N1	118.1 (3)	C11—C16—H16	119.6
C1—C2—C3	116.9 (3)	N13—C17—H17A	109.5
C1—C2—H2	121.5	N13—C17—H17B	109.5
C3—C2—H2	121.5	H17A—C17—H17B	109.5
C4—C3—C2	122.6 (3)	N13—C17—H17C	109.5
C4—C3—N2	119.1 (2)	H17A—C17—H17C	109.5
C2—C3—N2	118.3 (3)	H17B—C17—H17C	109.5
C3—C4—C5	117.2 (3)	N13—C18—H18A	109.5
C3—C4—H4	121.4	N13—C18—H18B	109.5
C5—C4—H4	121.4	H18A—C18—H18B	109.5
C6—C5—C4	122.9 (3)	N13—C18—H18C	109.5
C6—C5—N3	118.6 (3)	H18A—C18—H18C	109.5
C4—C5—N3	118.5 (3)	H18B—C18—H18C	109.5
C1—C6—C5	116.9 (3)	C20—C19—C24	119.7 (3)
C1—C6—H6	121.6	C20—C19—N12	123.1 (3)
C5—C6—H6	121.6	C24—C19—N12	117.3 (2)

O1—N1—O2	124.0 (3)	C21—C20—C19	119.8 (3)
O1—N1—C1	117.8 (3)	C21—C20—H20	120.1
O2—N1—C1	118.2 (3)	C19—C20—H20	120.1
O3—N2—O4	124.5 (3)	C20—C21—C22	120.8 (3)
O3—N2—C3	118.1 (2)	C20—C21—H21	119.6
O4—N2—C3	117.3 (3)	C22—C21—H21	119.6
O5—N3—O6	124.7 (3)	C23—C22—C21	120.0 (3)
O5—N3—C5	117.9 (3)	C23—C22—H22	120
O6—N3—C5	117.3 (3)	C21—C22—H22	120
N11—C11—C16	126.2 (3)	C22—C23—C24	120.7 (3)
N11—C11—C12	115.5 (3)	C22—C23—H23	119.7
C16—C11—C12	118.3 (3)	C24—C23—H23	119.7
C13—C12—C11	121.6 (3)	C23—C24—C19	119.1 (3)
C13—C12—H12A	119.2	C23—C24—C25	116.4 (3)
C11—C12—H12A	119.2	C19—C24—C25	124.5 (3)
C12—C13—C14	120.3 (3)	O11—C25—O12	120.1 (3)
C12—C13—H13	119.9	O11—C25—C24	121.4 (3)
C14—C13—H13	119.9	O12—C25—C24	118.4 (3)
N13—C14—C13	121.1 (3)	N12—N11—C11	116.7 (2)
N13—C14—C15	120.6 (3)	N11—N12—C19	114.0 (2)
C13—C14—C15	118.3 (3)	C14—N13—C18	123.2 (3)
C16—C15—C14	120.6 (3)	C14—N13—C17	120.9 (3)
C16—C15—H15	119.7	C18—N13—C17	115.9 (3)
C14—C15—H15	119.7	C25—O12—H12	108 (3)
C6—C1—C2—C3	0.0 (4)	N13—C14—C15—C16	178.1 (3)
N1—C1—C2—C3	−178.3 (3)	C13—C14—C15—C16	−1.7 (4)
C1—C2—C3—C4	−0.8 (4)	C14—C15—C16—C11	−0.1 (4)
C1—C2—C3—N2	179.5 (2)	N11—C11—C16—C15	−178.3 (3)
C2—C3—C4—C5	1.5 (4)	C12—C11—C16—C15	2.1 (4)
N2—C3—C4—C5	−178.9 (3)	C24—C19—C20—C21	−1.8 (5)
C3—C4—C5—C6	−1.4 (4)	N12—C19—C20—C21	179.2 (3)
C3—C4—C5—N3	176.9 (3)	C19—C20—C21—C22	0.1 (5)
C2—C1—C6—C5	0.0 (4)	C20—C21—C22—C23	0.8 (5)
N1—C1—C6—C5	178.4 (3)	C21—C22—C23—C24	−0.1 (5)
C4—C5—C6—C1	0.7 (4)	C22—C23—C24—C19	−1.6 (4)
N3—C5—C6—C1	−177.6 (3)	C22—C23—C24—C25	178.7 (3)
C6—C1—N1—O1	2.5 (4)	C20—C19—C24—C23	2.5 (4)
C2—C1—N1—O1	−179.1 (3)	N12—C19—C24—C23	−178.5 (3)
C6—C1—N1—O2	−175.7 (3)	C20—C19—C24—C25	−177.7 (3)
C2—C1—N1—O2	2.7 (4)	N12—C19—C24—C25	1.3 (4)
C4—C3—N2—O3	−176.7 (3)	C23—C24—C25—O11	−1.7 (5)
C2—C3—N2—O3	2.9 (4)	C19—C24—C25—O11	178.5 (3)
C4—C3—N2—O4	2.8 (4)	C23—C24—C25—O12	178.5 (3)
C2—C3—N2—O4	−177.6 (3)	C19—C24—C25—O12	−1.2 (5)
C6—C5—N3—O5	−172.8 (3)	C16—C11—N11—N12	5.5 (4)
C4—C5—N3—O5	8.8 (4)	C12—C11—N11—N12	−174.9 (2)
C6—C5—N3—O6	7.8 (4)	C11—N11—N12—C19	−179.7 (2)

C4—C5—N3—O6	−170.5 (3)	C20—C19—N12—N11	−0.7 (4)
N11—C11—C12—C13	178.1 (3)	C24—C19—N12—N11	−179.7 (2)
C16—C11—C12—C13	−2.3 (4)	C13—C14—N13—C18	177.4 (3)
C11—C12—C13—C14	0.4 (4)	C15—C14—N13—C18	−2.4 (5)
C12—C13—C14—N13	−178.2 (3)	C13—C14—N13—C17	−0.4 (4)
C12—C13—C14—C15	1.6 (4)	C15—C14—N13—C17	179.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O4[i]	0.95	2.35	3.285 (4)	169
C15—H15···O11[ii]	0.95	2.34	3.254 (4)	161
C18—H18*A*···O11[ii]	0.98	2.55	3.519 (4)	170
C20—H20···O3[iii]	0.95	2.64	3.574 (4)	167
O12—H12···N12	0.95 (6)	1.70 (6)	2.577 (3)	153 (5)
C21—H21···O2[iii]	0.95	2.56	3.469 (4)	161

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

1,3,5-Trinitrobenzene–1-naphthoic acid–2-amino-5-nitropyridine (1/1/1) (IV)

Crystal data

$C_6H_3N_3O_6 \cdot C_{11}H_8O_2 \cdot C_5H_5N_3O_2$
$M_r = 524.41$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 7.5365 (15)$ Å
$b = 7.9003 (16)$ Å
$c = 19.153 (4)$ Å
$\alpha = 97.580 (7)°$
$\beta = 94.667 (6)°$
$\gamma = 99.547 (7)°$
$V = 1108.5 (4)$ Å^3

$Z = 2$
$F(000) = 540$
$D_x = 1.571$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8623 reflections
$\theta = 3.1–28.3°$
$\mu = 0.13$ mm^{-1}
$T = 173$ K
Plate, brown
$0.63 \times 0.33 \times 0.06$ mm

Data collection

Bruker D8 Venture Photon CCD area detector
    diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan
    (SADABS; Sheldrick, 1996)
$T_{min} = 0.9$, $T_{max} = 0.95$
12982 measured reflections

3988 independent reflections
3368 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.2°$
$h = −9 \rightarrow 9$
$k = −9 \rightarrow 8$
$l = −23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.072$
$wR(F^2) = 0.168$
$S = 1.22$
3988 reflections
355 parameters
0 restraints
0 constraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent
    and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 2.9593P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = −0.36$ e Å^{-3}

Special details

Experimental. (SADABS; Sheldrick, 1996)

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\mathring{A}^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3489 (5)	0.8531 (5)	0.28180 (19)	0.0286 (8)
C2	0.5027 (5)	0.7901 (5)	0.2644 (2)	0.0305 (8)
H2	0.592398	0.774878	0.299662	0.037*
C3	0.5190 (5)	0.7506 (5)	0.1933 (2)	0.0321 (9)
C4	0.3924 (5)	0.7760 (5)	0.1413 (2)	0.0337 (9)
H4	0.406294	0.747525	0.092526	0.04*
C5	0.2448 (5)	0.8441 (5)	0.1624 (2)	0.0309 (8)
C6	0.2177 (5)	0.8818 (5)	0.23294 (19)	0.0287 (8)
H6	0.113733	0.925419	0.246843	0.034*
N1	0.3220 (5)	0.8876 (4)	0.35735 (17)	0.0340 (8)
N2	0.6777 (5)	0.6813 (5)	0.1725 (2)	0.0445 (9)
N3	0.1080 (5)	0.8742 (5)	0.10842 (18)	0.0416 (9)
O1	0.1697 (4)	0.8928 (4)	0.37245 (15)	0.0441 (7)
O2	0.4547 (4)	0.9063 (5)	0.40103 (15)	0.0521 (9)
O3	0.7923 (4)	0.6648 (5)	0.2201 (2)	0.0562 (9)
O4	0.6891 (5)	0.6423 (5)	0.10927 (19)	0.0617 (10)
O5	0.1245 (5)	0.8221 (6)	0.04677 (17)	0.0680 (11)
O6	−0.0122 (4)	0.9495 (5)	0.12813 (17)	0.0520 (8)
C11	0.2801 (5)	0.3592 (5)	0.23195 (19)	0.0283 (8)
C12	0.1324 (5)	0.4164 (5)	0.2022 (2)	0.0339 (9)
H12	0.0557	0.466551	0.232661	0.041*
C13	0.0906 (6)	0.4036 (6)	0.1289 (2)	0.0413 (10)
H13	−0.013342	0.442495	0.109979	0.05*
C14	0.2039 (6)	0.3333 (6)	0.0846 (2)	0.0423 (11)
H14	0.176484	0.322585	0.034787	0.051*
C15	0.3602 (5)	0.2768 (5)	0.11240 (19)	0.0333 (9)
C16	0.4790 (6)	0.2077 (6)	0.0674 (2)	0.0427 (11)
H16	0.451417	0.196379	0.017572	0.051*
C17	0.6309 (6)	0.1573 (6)	0.0937 (2)	0.0465 (11)
H17	0.709603	0.112982	0.06254	0.056*
C18	0.6715 (5)	0.1709 (5)	0.1671 (2)	0.0370 (10)
H18	0.778609	0.136036	0.185356	0.044*
C19	0.5604 (5)	0.2332 (5)	0.2127 (2)	0.0309 (8)
H19	0.590396	0.240016	0.262266	0.037*
C20	0.3986 (5)	0.2887 (5)	0.18715 (19)	0.0296 (8)
C21	0.3071 (5)	0.3680 (5)	0.31063 (19)	0.0293 (8)
O7	0.2603 (4)	0.5052 (4)	0.34527 (15)	0.0370 (7)
O8	0.3642 (4)	0.2557 (4)	0.33988 (14)	0.0385 (7)

H5A	0.309 (7)	0.226 (7)	0.440 (3)	0.058 (15)*
H5B	0.256 (5)	0.144 (6)	0.506 (2)	0.030 (11)*
H7	0.270 (7)	0.503 (7)	0.395 (3)	0.063 (15)*
C22	0.2465 (5)	0.3802 (5)	0.51944 (18)	0.0265 (8)
C23	0.1956 (5)	0.3906 (5)	0.58930 (19)	0.0296 (8)
H23	0.183191	0.291092	0.612665	0.036*
C24	0.1651 (5)	0.5429 (5)	0.62225 (19)	0.0309 (9)
H24	0.132639	0.553261	0.669335	0.037*
C25	0.1822 (5)	0.6859 (5)	0.58541 (19)	0.0272 (8)
C26	0.2293 (5)	0.6680 (5)	0.51770 (19)	0.0295 (8)
H26	0.240027	0.766188	0.493543	0.035*
N4	0.2607 (4)	0.5197 (4)	0.48431 (15)	0.0290 (7)
N5	0.2777 (5)	0.2340 (4)	0.48463 (19)	0.0353 (8)
N6	0.1470 (4)	0.8518 (4)	0.61748 (17)	0.0325 (7)
O9	0.1578 (4)	0.9701 (4)	0.58321 (17)	0.0439 (7)
O10	0.1098 (5)	0.8655 (4)	0.67946 (15)	0.0508 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0303 (19)	0.025 (2)	0.0300 (19)	0.0012 (15)	0.0051 (15)	0.0064 (15)
C2	0.0284 (19)	0.026 (2)	0.038 (2)	0.0046 (16)	0.0043 (16)	0.0101 (16)
C3	0.0267 (19)	0.025 (2)	0.045 (2)	0.0021 (16)	0.0119 (17)	0.0048 (17)
C4	0.034 (2)	0.031 (2)	0.034 (2)	−0.0036 (17)	0.0090 (16)	0.0040 (17)
C5	0.0273 (19)	0.030 (2)	0.033 (2)	−0.0025 (16)	0.0025 (15)	0.0057 (16)
C6	0.0250 (18)	0.0252 (19)	0.036 (2)	0.0028 (15)	0.0065 (15)	0.0047 (16)
N1	0.042 (2)	0.0284 (18)	0.0328 (18)	0.0076 (15)	0.0059 (15)	0.0074 (14)
N2	0.035 (2)	0.037 (2)	0.064 (3)	0.0037 (16)	0.0163 (18)	0.0109 (19)
N3	0.037 (2)	0.050 (2)	0.034 (2)	−0.0059 (17)	0.0021 (15)	0.0095 (17)
O1	0.0461 (18)	0.052 (2)	0.0390 (16)	0.0127 (15)	0.0175 (14)	0.0090 (14)
O2	0.0512 (19)	0.069 (2)	0.0340 (16)	0.0103 (17)	−0.0051 (14)	0.0065 (15)
O3	0.0378 (18)	0.056 (2)	0.083 (3)	0.0206 (15)	0.0153 (17)	0.0201 (19)
O4	0.052 (2)	0.068 (3)	0.064 (2)	0.0079 (18)	0.0286 (17)	−0.0023 (19)
O5	0.058 (2)	0.107 (3)	0.0313 (18)	0.004 (2)	−0.0025 (15)	0.0035 (18)
O6	0.0405 (18)	0.066 (2)	0.0508 (19)	0.0108 (16)	0.0000 (15)	0.0138 (17)
C11	0.0286 (19)	0.024 (2)	0.0307 (19)	0.0004 (15)	0.0074 (15)	0.0017 (15)
C12	0.030 (2)	0.033 (2)	0.039 (2)	0.0021 (17)	0.0073 (17)	0.0092 (17)
C13	0.033 (2)	0.047 (3)	0.040 (2)	−0.0048 (19)	−0.0023 (18)	0.0105 (19)
C14	0.044 (2)	0.046 (3)	0.030 (2)	−0.006 (2)	−0.0002 (18)	0.0029 (19)
C15	0.035 (2)	0.034 (2)	0.0260 (19)	−0.0062 (17)	0.0064 (16)	−0.0008 (16)
C16	0.055 (3)	0.041 (3)	0.030 (2)	0.002 (2)	0.0142 (19)	−0.0001 (18)
C17	0.049 (3)	0.044 (3)	0.044 (2)	0.000 (2)	0.018 (2)	−0.001 (2)
C18	0.032 (2)	0.035 (2)	0.041 (2)	−0.0008 (17)	0.0113 (17)	−0.0005 (18)
C19	0.0294 (19)	0.026 (2)	0.035 (2)	0.0004 (16)	0.0047 (16)	0.0007 (16)
C20	0.032 (2)	0.025 (2)	0.0282 (19)	−0.0052 (16)	0.0064 (15)	0.0018 (15)
C21	0.0298 (19)	0.027 (2)	0.031 (2)	0.0026 (16)	0.0085 (15)	0.0050 (17)
O7	0.0569 (18)	0.0299 (16)	0.0279 (15)	0.0144 (13)	0.0103 (13)	0.0055 (12)
O8	0.0495 (17)	0.0396 (17)	0.0307 (14)	0.0163 (14)	0.0107 (12)	0.0064 (13)

C22	0.0257 (18)	0.026 (2)	0.0279 (18)	0.0047 (15)	0.0000 (14)	0.0045 (15)
C23	0.0316 (19)	0.032 (2)	0.0265 (19)	0.0071 (16)	0.0016 (15)	0.0087 (16)
C24	0.033 (2)	0.034 (2)	0.0249 (18)	0.0044 (17)	0.0033 (15)	0.0053 (16)
C25	0.0253 (18)	0.028 (2)	0.0278 (18)	0.0037 (15)	0.0020 (14)	0.0022 (15)
C26	0.033 (2)	0.023 (2)	0.032 (2)	0.0046 (16)	0.0036 (16)	0.0052 (16)
N4	0.0364 (17)	0.0246 (17)	0.0265 (16)	0.0041 (13)	0.0071 (13)	0.0043 (13)
N5	0.057 (2)	0.0199 (18)	0.0309 (18)	0.0082 (16)	0.0117 (16)	0.0045 (15)
N6	0.0298 (17)	0.0297 (19)	0.0373 (19)	0.0056 (14)	0.0041 (14)	0.0019 (15)
O9	0.0505 (18)	0.0277 (16)	0.0605 (19)	0.0122 (13)	0.0210 (15)	0.0159 (14)
O10	0.075 (2)	0.051 (2)	0.0318 (16)	0.0285 (17)	0.0119 (15)	0.0012 (14)

Geometric parameters (Å, º)

C1—C6	1.373 (5)	C15—C20	1.425 (5)
C1—C2	1.382 (5)	C16—C17	1.354 (7)
C1—N1	1.474 (5)	C16—H16	0.95
C2—C3	1.376 (5)	C17—C18	1.400 (6)
C2—H2	0.95	C17—H17	0.95
C3—C4	1.380 (6)	C18—C19	1.360 (5)
C3—N2	1.458 (5)	C18—H18	0.95
C4—C5	1.380 (6)	C19—C20	1.434 (6)
C4—H4	0.95	C19—H19	0.95
C5—C6	1.383 (5)	C21—O8	1.227 (5)
C5—N3	1.470 (5)	C21—O7	1.309 (5)
C6—H6	0.95	O7—H7	0.95 (5)
N1—O1	1.212 (4)	C22—N5	1.321 (5)
N1—O2	1.227 (4)	C22—N4	1.359 (5)
N2—O4	1.222 (5)	C22—C23	1.418 (5)
N2—O3	1.240 (5)	C23—C24	1.347 (6)
N3—O5	1.221 (5)	C23—H23	0.95
N3—O6	1.222 (5)	C24—C25	1.403 (5)
C11—C12	1.378 (5)	C24—H24	0.95
C11—C20	1.417 (5)	C25—C26	1.368 (5)
C11—C21	1.495 (5)	C25—N6	1.447 (5)
C12—C13	1.400 (6)	C26—N4	1.325 (5)
C12—H12	0.95	C26—H26	0.95
C13—C14	1.380 (6)	N5—H5A	0.90 (5)
C13—H13	0.95	N5—H5B	0.86 (4)
C14—C15	1.416 (6)	N6—O9	1.207 (4)
C14—H14	0.95	N6—O10	1.237 (4)
C15—C16	1.416 (6)		
C6—C1—C2	124.0 (3)	C17—C16—C15	121.7 (4)
C6—C1—N1	117.9 (3)	C17—C16—H16	119.2
C2—C1—N1	118.1 (3)	C15—C16—H16	119.2
C3—C2—C1	116.6 (4)	C16—C17—C18	119.7 (4)
C3—C2—H2	121.7	C16—C17—H17	120.2
C1—C2—H2	121.7	C18—C17—H17	120.2

C2—C3—C4	122.5 (4)	C19—C18—C17	121.1 (4)
C2—C3—N2	118.5 (4)	C19—C18—H18	119.4
C4—C3—N2	119.0 (4)	C17—C18—H18	119.4
C5—C4—C3	117.8 (4)	C18—C19—C20	121.0 (4)
C5—C4—H4	121.1	C18—C19—H19	119.5
C3—C4—H4	121.1	C20—C19—H19	119.5
C4—C5—C6	122.5 (4)	C11—C20—C15	118.9 (4)
C4—C5—N3	119.3 (3)	C11—C20—C19	123.7 (3)
C6—C5—N3	118.2 (4)	C15—C20—C19	117.3 (4)
C1—C6—C5	116.5 (4)	O8—C21—O7	123.2 (3)
C1—C6—H6	121.7	O8—C21—C11	123.2 (4)
C5—C6—H6	121.7	O7—C21—C11	113.5 (3)
O1—N1—O2	124.1 (3)	C21—O7—H7	112 (3)
O1—N1—C1	118.0 (3)	N5—C22—N4	116.8 (3)
O2—N1—C1	117.9 (3)	N5—C22—C23	121.9 (4)
O4—N2—O3	124.1 (4)	N4—C22—C23	121.3 (3)
O4—N2—C3	118.1 (4)	C24—C23—C22	119.4 (4)
O3—N2—C3	117.8 (4)	C24—C23—H23	120.3
O5—N3—O6	124.9 (4)	C22—C23—H23	120.3
O5—N3—C5	116.9 (4)	C23—C24—C25	118.4 (3)
O6—N3—C5	118.1 (3)	C23—C24—H24	120.8
C12—C11—C20	119.2 (3)	C25—C24—H24	120.8
C12—C11—C21	118.9 (3)	C26—C25—C24	119.7 (4)
C20—C11—C21	121.9 (3)	C26—C25—N6	119.4 (3)
C11—C12—C13	122.8 (4)	C24—C25—N6	120.9 (3)
C11—C12—H12	118.6	N4—C26—C25	122.9 (4)
C13—C12—H12	118.6	N4—C26—H26	118.5
C14—C13—C12	118.5 (4)	C25—C26—H26	118.5
C14—C13—H13	120.7	C26—N4—C22	118.2 (3)
C12—C13—H13	120.7	C22—N5—H5A	123 (3)
C13—C14—C15	121.1 (4)	C22—N5—H5B	116 (3)
C13—C14—H14	119.5	H5A—N5—H5B	121 (4)
C15—C14—H14	119.5	O9—N6—O10	123.2 (3)
C14—C15—C16	121.4 (4)	O9—N6—C25	118.9 (3)
C14—C15—C20	119.4 (4)	O10—N6—C25	117.9 (3)
C16—C15—C20	119.1 (4)		
C6—C1—C2—C3	−1.8 (6)	C15—C16—C17—C18	1.0 (7)
N1—C1—C2—C3	176.7 (3)	C16—C17—C18—C19	0.3 (7)
C1—C2—C3—C4	1.7 (6)	C17—C18—C19—C20	−0.6 (6)
C1—C2—C3—N2	−179.1 (3)	C12—C11—C20—C15	−0.8 (5)
C2—C3—C4—C5	0.2 (6)	C21—C11—C20—C15	177.1 (3)
N2—C3—C4—C5	−179.1 (3)	C12—C11—C20—C19	177.0 (4)
C3—C4—C5—C6	−2.1 (6)	C21—C11—C20—C19	−5.1 (5)
C3—C4—C5—N3	179.5 (3)	C14—C15—C20—C11	−0.8 (5)
C2—C1—C6—C5	0.1 (6)	C16—C15—C20—C11	179.5 (3)
N1—C1—C6—C5	−178.4 (3)	C14—C15—C20—C19	−178.8 (4)
C4—C5—C6—C1	1.9 (5)	C16—C15—C20—C19	1.6 (5)

N3—C5—C6—C1	−179.6 (3)	C18—C19—C20—C11	−178.2 (4)
C6—C1—N1—O1	19.8 (5)	C18—C19—C20—C15	−0.3 (5)
C2—C1—N1—O1	−158.8 (4)	C12—C11—C21—O8	142.1 (4)
C6—C1—N1—O2	−161.4 (4)	C20—C11—C21—O8	−35.8 (5)
C2—C1—N1—O2	20.0 (5)	C12—C11—C21—O7	−36.5 (5)
C2—C3—N2—O4	178.1 (4)	C20—C11—C21—O7	145.6 (3)
C4—C3—N2—O4	−2.6 (5)	N5—C22—C23—C24	−179.8 (4)
C2—C3—N2—O3	−1.5 (5)	N4—C22—C23—C24	−1.7 (5)
C4—C3—N2—O3	177.8 (4)	C22—C23—C24—C25	1.0 (5)
C4—C5—N3—O5	6.4 (5)	C23—C24—C25—C26	−0.1 (5)
C6—C5—N3—O5	−172.1 (4)	C23—C24—C25—N6	178.6 (3)
C4—C5—N3—O6	−173.2 (4)	C24—C25—C26—N4	−0.1 (6)
C6—C5—N3—O6	8.3 (5)	N6—C25—C26—N4	−178.8 (3)
C20—C11—C12—C13	1.8 (6)	C25—C26—N4—C22	−0.5 (5)
C21—C11—C12—C13	−176.1 (4)	N5—C22—N4—C26	179.7 (3)
C11—C12—C13—C14	−1.0 (6)	C23—C22—N4—C26	1.5 (5)
C12—C13—C14—C15	−0.7 (6)	C26—C25—N6—O9	1.0 (5)
C13—C14—C15—C16	−178.7 (4)	C24—C25—N6—O9	−177.7 (3)
C13—C14—C15—C20	1.6 (6)	C26—C25—N6—O10	−178.0 (3)
C14—C15—C16—C17	178.4 (4)	C24—C25—N6—O10	3.4 (5)
C20—C15—C16—C17	−1.9 (6)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N5—H5A⋯O8	0.90 (5)	2.03 (5)	2.919 (5)	168 (5)
N5—H5B⋯O9[i]	0.86 (4)	2.24 (4)	3.069 (5)	161 (4)
O7—H7⋯N4	0.95 (5)	1.71 (5)	2.650 (4)	171 (5)
C23—H23⋯O9[i]	0.95	2.5	3.272 (5)	139
C26—H26⋯O1	0.95	2.69	3.530 (5)	147
C26—H26⋯O2	0.95	2.72	3.477 (5)	138

Symmetry code: (i) $x, y−1, z$.