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3-Nitrophenol–1,3,5-triazine-2,4,6-triamine (2/1)

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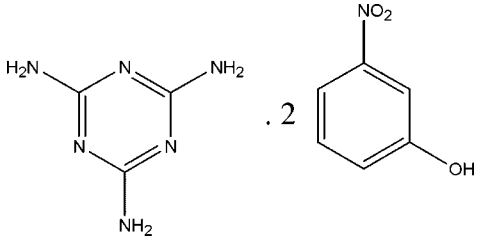
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.119; data-to-parameter ratio = 15.1.

The asymmetric unit of the title compound, $C_3H_6N_6\cdot 2C_6H_5NO_3$, contains one melamine and two 3-nitrophenol molecules. The mean planes of the 3-nitrophenol molecules are almost orthogonal to the plane of melamine, making dihedral angles of 82.77 (4) and 88.36 (5)°. In the crystal, molecules are linked *via* O—H···N, N—H···N and N—H···O hydrogen bonds, forming a three-dimensional network. The crystal also features weak C—H···π and π–π interactions [centroid–centroid distance = 3.9823 (9) Å].

Related literature

For general background to melamine derivatives, see: Desiraju *et al.* (1990); Krische & Lehn (2000). For related structures, see: Kanagathara *et al.* (2012); Wang *et al.* (2007).



Experimental

Crystal data

$C_3H_6N_6\cdot 2C_6H_5NO_3$
M_r = 404.36
Orthorhombic, *Pbca*
a = 15.5150 (6) Å
b = 12.9137 (6) Å
c = 17.8323 (6) Å
V = 3572.8 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.28 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.977
19568 measured reflections
4447 independent reflections
3352 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.03
4447 reflections
295 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*3 is the centroid of the melamine triamine ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3^{i}	0.84 (1)	1.86 (1)	2.6907 (14)	176 (2)
O4—H4A···N2^{ii}	0.83 (1)	1.87 (1)	2.6876 (14)	170 (2)
N5—H5A···N4^{iii}	0.89 (1)	2.17 (1)	3.0594 (18)	178 (17)
N5—H5B···O1^{iv}	0.87 (1)	2.25 (1)	2.9613 (16)	138 (15)
N7—H7A···O1^{v}	0.88 (1)	2.32 (1)	3.1600 (17)	159 (14)
N7—H7B···O4^{vi}	0.88 (1)	2.13 (1)	2.9180 (16)	149 (15)
C6—H6···*Cg*3^{vii}	0.93	2.95	3.7504 (18)	145

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors wish to acknowledge the SAIF, IIT Madras (India), for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2476).

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supporting information

Acta Cryst. (2013). E**69**, o827 [doi:10.1107/S1600536813011148]

3-Nitrophenol–1,3,5-triazine-2,4,6-triamine (2/1)

V. Sangeetha, N. Kanagathara, G. Chakkaravarthi, M.K. Marchewka and G. Anbalagan

S1. Comment

Melamine (1,3,5-triazine-2,4,6-triamine) and its derivatives can develop well defined non-covalent supramolecular nanoarchitectures *via* multiple hydrogen bonds by self-assembly of components containing complementary arrays of hydrogen-bonding sites (Desiraju, 1990; Krische & Lehn, 2000). The geometric parameters of the title compound (Fig. 1) are comparable to those reported for similar structures (Kanagathara *et al.*, 2012; Wang *et al.*, 2007). The mean planes of the two nitrophenol molecules (C1···C6) and (C10···C15) are almost orthogonal to the melamine (N2/C7/N4/C9/N3/C8) molecule, with dihedral angles of 82.77 (4) and 88.36 (5)°, respectively.

The crystal packing of the title compound is influenced by intermolecular O—H···N, N—H···N and N—H···O hydrogen bonds, as well as weak C—H···π (Table 1 and Fig. 2) and π–π interactions: *Cg*1···*Cg*2 (x, 1/2-y, 3/2+z) distance of 3.9823 (9) Å; *Cg*2···*Cg*1 (-1/2+x, 1/2-y, 1-z) distance of 3.9823 (9) Å; *Cg*1···*Cg*2 (-x, 1-y, 1-z) distance of 4.2397 (9) Å; *Cg*3···*Cg*1 (1/2-x, 1/2+y, z) distance of 5.0406 (8) Å; where *Cg*1, *Cg*2 and *Cg*3 are the centroids of the rings C1···C6, C10···C15, and N2/C7/N4/C9/N3/C8, respectively.

S2. Experimental

Melamine (1.261 g, 10 mmol) was dissolved in 200 ml of hot distilled water. 3-Nitrophenol (1.391 g, 10 mmol) was dissolved in 100 ml of distilled water, separately. The 3-nitrophenol solution was added gently to the hot solution of melamine, and the mixture stirred well for nearly five hours to get an homogeneous solution. Water was then allowed to evaporate. Within few days, tiny transparent, yellowish crystals were formed.

S3. Refinement

H atoms of aromatic CH groups were positioned geometrically and refined using a riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms bound to O and N atoms were found in a difference map and refined isotropically, with distances restrained to N—H = 0.88 (1) Å and O—H = 0.82 (1) Å (Sheldrick, 2008).

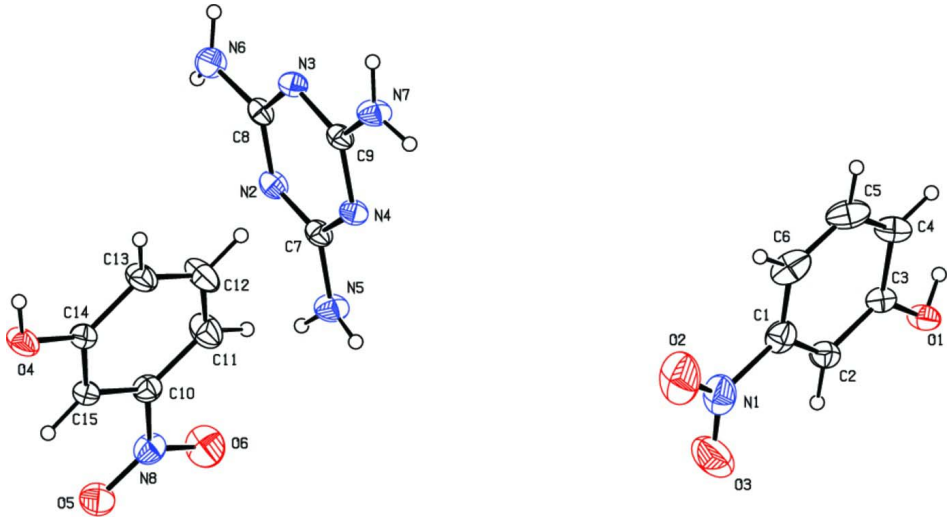

Figure 1

The molecular structure of the title compound, with 30% probability displacement ellipsoids for non-H atoms.

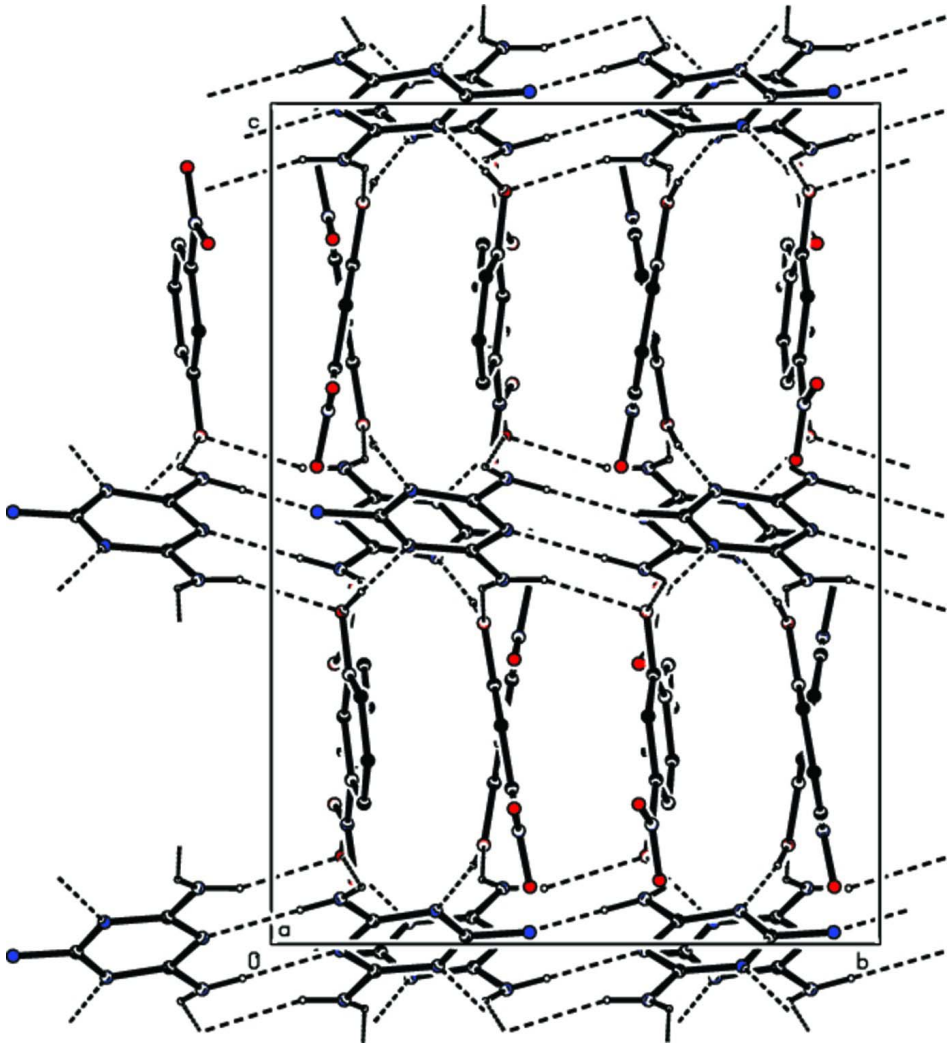

Figure 2

The packing of the title compound viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_3H_6N_6{\cdot}2C_6H_5NO_3$
M_r = 404.36
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 15.5150 (6) Å
b = 12.9137 (6) Å
c = 17.8323 (6) Å
V = 3572.8 (2) Å^3
Z = 8

F(000) = 1680
D_x = 1.503 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 4327 reflections
θ = 2.3–28.3°
μ = 0.12 mm^{-1}
T = 295 K
Block, yellow
0.28 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.977
19568 measured reflections
4447 independent reflections
3352 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.3°, θ_{min} = 2.3°
h = −20→13
k = −17→7
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.03
4447 reflections
295 parameters
8 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.7906P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0028 (5)

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.20295 (11)	0.13223 (11)	0.30457 (8)	0.0472 (4)
C2	0.18602 (9)	0.11918 (10)	0.22906 (8)	0.0406 (3)
H2	0.1305	0.1048	0.2123	0.049*
C3	0.25379 (9)	0.12802 (10)	0.17907 (8)	0.0365 (3)
C4	0.33676 (9)	0.14713 (12)	0.20566 (9)	0.0475 (4)
H4	0.3826	0.1521	0.1723	0.057*
C5	0.35064 (12)	0.15871 (14)	0.28162 (10)	0.0597 (5)
H5	0.4062	0.1712	0.2989	0.072*
C6	0.28408 (13)	0.15216 (13)	0.33219 (9)	0.0586 (5)
H6	0.2935	0.1609	0.3833	0.070*
C7	0.01234 (8)	0.66741 (10)	0.47227 (7)	0.0337 (3)
C8	0.08123 (8)	0.82016 (10)	0.49038 (7)	0.0337 (3)
C9	0.14073 (8)	0.67001 (10)	0.53192 (7)	0.0322 (3)
C10	−0.15540 (9)	0.60489 (10)	0.68536 (8)	0.0383 (3)
C11	−0.07322 (10)	0.59736 (15)	0.65597 (9)	0.0546 (4)
H11	−0.0643	0.5851	0.6052	0.066*
C12	−0.00506 (10)	0.60861 (16)	0.70459 (10)	0.0595 (5)
H12	0.0510	0.6040	0.6864	0.071*
C13	−0.01848 (9)	0.62665 (13)	0.78025 (9)	0.0464 (4)
H13	0.0283	0.6340	0.8124	0.056*
C14	−0.10170 (8)	0.63378 (10)	0.80810 (8)	0.0365 (3)
C15	−0.17126 (8)	0.62232 (10)	0.76020 (8)	0.0369 (3)
H15	−0.2274	0.6263	0.7782	0.044*

N1	0.13017 (13)	0.12490 (12)	0.35762 (9)	0.0659 (4)
N2	0.01376 (7)	0.77043 (9)	0.46051 (6)	0.0361 (3)
N3	0.14703 (7)	0.77395 (8)	0.52606 (6)	0.0354 (2)
N4	0.07430 (6)	0.61329 (8)	0.50739 (6)	0.0345 (3)
N5	−0.05479 (8)	0.61359 (11)	0.44621 (8)	0.0461 (3)
N6	0.08276 (9)	0.92415 (10)	0.48582 (8)	0.0457 (3)
N7	0.20470 (8)	0.61983 (10)	0.56654 (8)	0.0445 (3)
N8	−0.22955 (8)	0.59341 (10)	0.63461 (7)	0.0459 (3)
O1	0.23651 (6)	0.11610 (8)	0.10455 (6)	0.0433 (3)
O2	0.14494 (13)	0.13811 (14)	0.42402 (8)	0.1006 (6)
O3	0.05950 (11)	0.10386 (16)	0.33363 (10)	0.0968 (5)
O4	−0.11865 (7)	0.65065 (10)	0.88192 (6)	0.0537 (3)
O5	−0.30194 (7)	0.60094 (10)	0.66114 (7)	0.0583 (3)
O6	−0.21580 (9)	0.57499 (12)	0.56836 (6)	0.0716 (4)
H1	0.2744 (10)	0.1481 (14)	0.0807 (10)	0.068 (6)*
H4A	−0.0754 (9)	0.6682 (15)	0.9062 (9)	0.064 (6)*
H6A	0.0446 (9)	0.9511 (14)	0.4564 (9)	0.065 (5)*
H6B	0.1328 (8)	0.9538 (13)	0.4931 (10)	0.061 (5)*
H7A	0.2051 (10)	0.5516 (7)	0.5665 (9)	0.048 (4)*
H7B	0.2525 (8)	0.6534 (12)	0.5769 (9)	0.050 (5)*
H5A	−0.0593 (11)	0.5475 (8)	0.4593 (10)	0.061 (5)*
H5B	−0.1003 (8)	0.6483 (13)	0.4321 (10)	0.058 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0631 (10)	0.0362 (7)	0.0423 (8)	−0.0015 (7)	0.0035 (7)	0.0051 (6)
C2	0.0372 (7)	0.0385 (7)	0.0461 (7)	−0.0032 (6)	−0.0005 (6)	0.0041 (6)
C3	0.0350 (7)	0.0346 (6)	0.0398 (7)	−0.0048 (5)	−0.0051 (5)	0.0045 (5)
C4	0.0369 (8)	0.0514 (8)	0.0542 (8)	−0.0108 (6)	−0.0080 (7)	0.0107 (7)
C5	0.0587 (10)	0.0596 (10)	0.0608 (10)	−0.0195 (8)	−0.0260 (9)	0.0123 (8)
C6	0.0849 (13)	0.0476 (9)	0.0433 (8)	−0.0136 (8)	−0.0168 (9)	0.0063 (7)
C7	0.0258 (6)	0.0459 (7)	0.0293 (6)	0.0013 (5)	−0.0018 (5)	0.0003 (5)
C8	0.0298 (6)	0.0419 (7)	0.0295 (6)	0.0021 (5)	0.0051 (5)	0.0018 (5)
C9	0.0252 (6)	0.0416 (7)	0.0300 (6)	0.0001 (5)	−0.0010 (5)	0.0011 (5)
C10	0.0370 (7)	0.0373 (6)	0.0405 (7)	−0.0007 (5)	−0.0052 (6)	0.0000 (5)
C11	0.0469 (9)	0.0779 (11)	0.0391 (7)	0.0020 (8)	0.0061 (7)	−0.0013 (7)
C12	0.0330 (8)	0.0935 (13)	0.0520 (9)	0.0002 (8)	0.0107 (7)	−0.0027 (9)
C13	0.0281 (7)	0.0632 (9)	0.0479 (8)	−0.0024 (6)	−0.0015 (6)	−0.0034 (7)
C14	0.0300 (7)	0.0396 (6)	0.0399 (7)	−0.0037 (5)	0.0012 (5)	−0.0049 (5)
C15	0.0271 (6)	0.0389 (6)	0.0447 (7)	−0.0028 (5)	0.0000 (5)	−0.0056 (5)
N1	0.0904 (13)	0.0530 (8)	0.0543 (9)	0.0022 (8)	0.0230 (9)	0.0047 (7)
N2	0.0293 (6)	0.0447 (6)	0.0342 (5)	0.0039 (5)	−0.0022 (4)	0.0046 (4)
N3	0.0287 (5)	0.0406 (6)	0.0370 (6)	−0.0036 (4)	−0.0031 (4)	0.0018 (4)
N4	0.0259 (5)	0.0399 (6)	0.0377 (6)	0.0000 (4)	−0.0052 (4)	0.0012 (4)
N5	0.0306 (6)	0.0515 (7)	0.0561 (7)	−0.0013 (6)	−0.0156 (6)	0.0033 (6)
N6	0.0431 (8)	0.0406 (6)	0.0535 (7)	0.0022 (6)	0.0009 (6)	0.0055 (5)
N7	0.0294 (6)	0.0457 (7)	0.0585 (8)	−0.0017 (5)	−0.0150 (6)	0.0062 (6)

N8	0.0481 (8)	0.0436 (6)	0.0460 (7)	0.0003 (6)	−0.0104 (6)	−0.0007 (5)
O1	0.0350 (5)	0.0563 (6)	0.0386 (5)	−0.0122 (5)	−0.0010 (4)	0.0022 (4)
O2	0.1446 (16)	0.1092 (13)	0.0480 (8)	0.0043 (11)	0.0257 (9)	−0.0016 (8)
O3	0.0729 (10)	0.1297 (15)	0.0876 (11)	−0.0121 (10)	0.0340 (9)	−0.0054 (10)
O4	0.0298 (5)	0.0893 (8)	0.0421 (6)	−0.0117 (5)	0.0014 (4)	−0.0207 (5)
O5	0.0396 (6)	0.0704 (8)	0.0648 (7)	0.0011 (5)	−0.0132 (5)	−0.0101 (6)
O6	0.0719 (9)	0.1012 (10)	0.0417 (6)	0.0024 (8)	−0.0125 (6)	−0.0077 (6)

Geometric parameters (Å, º)

C1—C6	1.376 (2)	C10—N8	1.4712 (18)
C1—C2	1.382 (2)	C11—C12	1.375 (2)
C1—N1	1.476 (2)	C11—H11	0.9300
C2—C3	1.383 (2)	C12—C13	1.385 (2)
C2—H2	0.9300	C12—H12	0.9300
C3—O1	1.3644 (16)	C13—C14	1.3865 (19)
C3—C4	1.3938 (19)	C13—H13	0.9300
C4—C5	1.380 (2)	C14—O4	1.3599 (16)
C4—H4	0.9300	C14—C15	1.3842 (18)
C5—C6	1.374 (3)	C15—H15	0.9300
C5—H5	0.9300	N1—O3	1.208 (2)
C6—H6	0.9300	N1—O2	1.218 (2)
C7—N5	1.3356 (17)	N5—H5A	0.888 (9)
C7—N4	1.3434 (16)	N5—H5B	0.874 (9)
C7—N2	1.3469 (18)	N6—H6A	0.863 (9)
C8—N2	1.3385 (16)	N6—H6B	0.875 (9)
C8—N3	1.3429 (16)	N7—H7A	0.881 (9)
C8—N6	1.3456 (19)	N7—H7B	0.878 (9)
C9—N7	1.3364 (17)	N8—O5	1.2226 (16)
C9—N4	1.3380 (16)	N8—O6	1.2238 (17)
C9—N3	1.3498 (17)	O1—H1	0.835 (9)
C10—C15	1.3756 (19)	O4—H4A	0.830 (9)
C10—C11	1.382 (2)		
C6—C1—C2	123.05 (15)	C11—C12—C13	121.09 (14)
C6—C1—N1	118.84 (15)	C11—C12—H12	119.5
C2—C1—N1	118.10 (15)	C13—C12—H12	119.5
C1—C2—C3	118.25 (14)	C12—C13—C14	120.01 (14)
C1—C2—H2	120.9	C12—C13—H13	120.0
C3—C2—H2	120.9	C14—C13—H13	120.0
O1—C3—C2	117.97 (12)	O4—C14—C15	117.63 (12)
O1—C3—C4	122.19 (13)	O4—C14—C13	122.51 (12)
C2—C3—C4	119.83 (13)	C15—C14—C13	119.86 (13)
C5—C4—C3	119.82 (15)	C10—C15—C14	118.47 (12)
C5—C4—H4	120.1	C10—C15—H15	120.8
C3—C4—H4	120.1	C14—C15—H15	120.8
C6—C5—C4	121.37 (15)	O3—N1—O2	123.13 (18)
C6—C5—H5	119.3	O3—N1—C1	118.81 (16)

C4—C5—H5	119.3	O2—N1—C1	118.04 (19)
C5—C6—C1	117.66 (15)	C8—N2—C7	115.13 (11)
C5—C6—H6	121.2	C8—N3—C9	115.05 (11)
C1—C6—H6	121.2	C9—N4—C7	114.76 (11)
N5—C7—N4	116.71 (12)	C7—N5—H5A	118.0 (12)
N5—C7—N2	118.20 (12)	C7—N5—H5B	117.7 (12)
N4—C7—N2	125.08 (11)	H5A—N5—H5B	120.4 (17)
N2—C8—N3	124.74 (12)	C8—N6—H6A	115.2 (13)
N2—C8—N6	117.95 (12)	C8—N6—H6B	116.3 (12)
N3—C8—N6	117.30 (12)	H6A—N6—H6B	121.5 (19)
N7—C9—N4	117.24 (12)	C9—N7—H7A	119.3 (11)
N7—C9—N3	117.65 (12)	C9—N7—H7B	119.0 (11)
N4—C9—N3	125.09 (11)	H7A—N7—H7B	119.2 (15)
C15—C10—C11	122.99 (13)	O5—N8—O6	123.30 (13)
C15—C10—N8	118.25 (12)	O5—N8—C10	118.19 (12)
C11—C10—N8	118.76 (13)	O6—N8—C10	118.50 (13)
C12—C11—C10	117.58 (14)	C3—O1—H1	107.5 (14)
C12—C11—H11	121.2	C14—O4—H4A	113.1 (13)
C10—C11—H11	121.2		

C6—C1—C2—C3	−0.9 (2)	C6—C1—N1—O3	−177.46 (17)
N1—C1—C2—C3	178.75 (12)	C2—C1—N1—O3	2.9 (2)
C1—C2—C3—O1	−179.35 (12)	C6—C1—N1—O2	0.8 (2)
C1—C2—C3—C4	1.5 (2)	C2—C1—N1—O2	−178.81 (16)
O1—C3—C4—C5	179.91 (14)	N3—C8—N2—C7	3.86 (18)
C2—C3—C4—C5	−1.0 (2)	N6—C8—N2—C7	−174.73 (12)
C3—C4—C5—C6	−0.2 (3)	N5—C7—N2—C8	177.70 (12)
C4—C5—C6—C1	0.8 (3)	N4—C7—N2—C8	−3.47 (18)
C2—C1—C6—C5	−0.3 (2)	N2—C8—N3—C9	−1.28 (18)
N1—C1—C6—C5	−179.92 (14)	N6—C8—N3—C9	177.32 (12)
C15—C10—C11—C12	−0.4 (3)	N7—C9—N3—C8	179.61 (12)
N8—C10—C11—C12	179.86 (15)	N4—C9—N3—C8	−2.16 (18)
C10—C11—C12—C13	0.1 (3)	N7—C9—N4—C7	−179.26 (12)
C11—C12—C13—C14	−0.1 (3)	N3—C9—N4—C7	2.50 (18)
C12—C13—C14—O4	179.52 (15)	N5—C7—N4—C9	179.35 (12)
C12—C13—C14—C15	0.3 (2)	N2—C7—N4—C9	0.50 (18)
C11—C10—C15—C14	0.6 (2)	C15—C10—N8—O5	0.72 (19)
N8—C10—C15—C14	−179.63 (12)	C11—C10—N8—O5	−179.50 (14)
O4—C14—C15—C10	−179.81 (12)	C15—C10—N8—O6	−177.97 (14)
C13—C14—C15—C10	−0.6 (2)	C11—C10—N8—O6	1.8 (2)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the melamine triamine ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3^{i}	0.84 (1)	1.86 (1)	2.6907 (14)	176 (2)
O4—H4*A*···N2^{ii}	0.83 (1)	1.87 (1)	2.6876 (14)	170 (2)
N5—H5*A*···N4^{iii}	0.89 (1)	2.17 (1)	3.0594 (18)	178 (17)

N5—H5*B*···O1^{iv}	0.87 (1)	2.25 (1)	2.9613 (16)	138 (15)
N7—H7*A*···O1^{v}	0.88 (1)	2.32 (1)	3.1600 (17)	159 (14)
N7—H7*B*···O4^{vi}	0.88 (1)	2.13 (1)	2.9180 (16)	149 (15)
C6—H6···*Cg*3^{vii}	0.93	2.95	3.7504 (18)	145

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