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## Structure Reports

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

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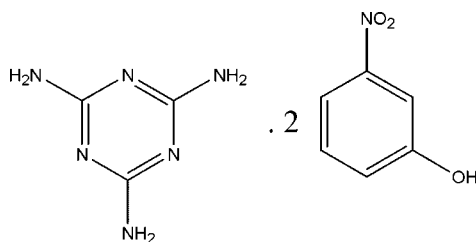
Received 29 March 2013; accepted 24 April 2013

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.119; data-to-parameter ratio = 15.1.

The asymmetric unit of the title compound,  $\text{C}_3\text{H}_6\text{N}_6 \cdot 2\text{C}_6\text{H}_5\text{NO}_3$ , 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... $\pi$  and  $\pi$ – $\pi$  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

 $\text{C}_3\text{H}_6\text{N}_6 \cdot 2\text{C}_6\text{H}_5\text{NO}_3$ 
 $M_r = 404.36$ 

 Orthorhombic, *Pbca*
 $a = 15.5150$  (6) Å  
 $b = 12.9137$  (6) Å  
 $c = 17.8323$  (6) Å  
 $V = 3572.8$  (2) Å<sup>3</sup>
 $Z = 8$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.12$  mm<sup>−1</sup>
 $T = 295$  K

 $0.28 \times 0.24 \times 0.20$  mm

### Data collection

 Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.967$ ,  $T_{\text{max}} = 0.977$ 

 19568 measured reflections  
 4447 independent reflections  
 3352 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$ 

### 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

 $\Delta\rho_{\text{max}} = 0.24$  e Å<sup>−3</sup>
 $\Delta\rho_{\text{min}} = -0.20$  e Å<sup>−3</sup>

## Table 1

Hydrogen-bond geometry (Å, °).

 $Cg3$  is the centroid of the melamine triazine ring.

| <i>D</i> –H... <i>A</i>            | <i>D</i> –H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> –H... <i>A</i> |
|------------------------------------|-------------|---------------|-----------------------|-------------------------|
| O1–H1...N3 <sup>i</sup>            | 0.84 (1)    | 1.86 (1)      | 2.6907 (14)           | 176 (2)                 |
| O4–H4A...N2 <sup>ii</sup>          | 0.83 (1)    | 1.87 (1)      | 2.6876 (14)           | 170 (2)                 |
| N5–H5A...N4 <sup>iii</sup>         | 0.89 (1)    | 2.17 (1)      | 3.0594 (18)           | 178 (17)                |
| N5–H5B...O1 <sup>iv</sup>          | 0.87 (1)    | 2.25 (1)      | 2.9613 (16)           | 138 (15)                |
| N7–H7A...O1 <sup>v</sup>           | 0.88 (1)    | 2.32 (1)      | 3.1600 (17)           | 159 (14)                |
| N7–H7B...O4 <sup>vi</sup>          | 0.88 (1)    | 2.13 (1)      | 2.9180 (16)           | 149 (15)                |
| C6–H6... <i>Cg3</i> <sup>vii</sup> | 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

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### 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.

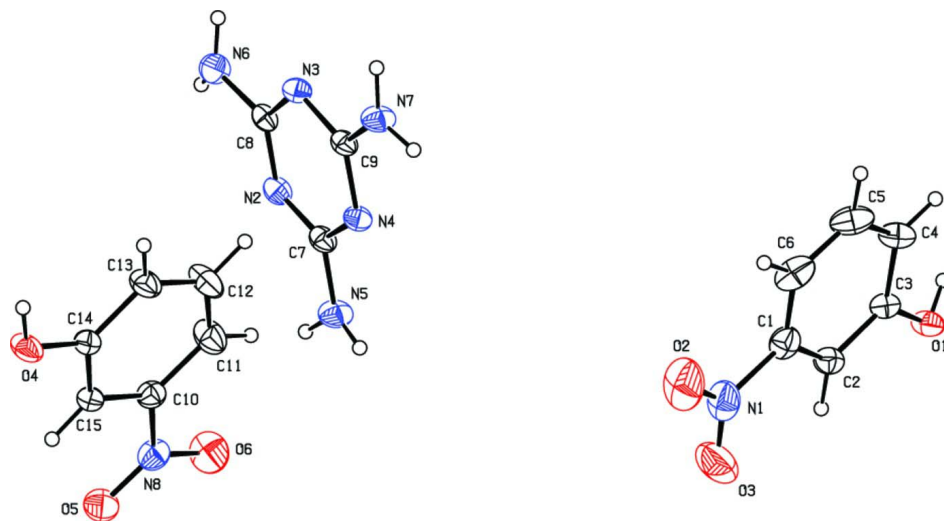
The crystal packing of the title compound is influenced by intermolecular O—H···N, N—H···N and N—H···O hydrogen bonds, as well as weak C—H··· $\pi$  (Table 1 and Fig. 2) and  $\pi$ – $\pi$  interactions: Cg1···Cg2 ( $x, 1/2-y, 3/2+z$ ) distance of 3.9823 (9) Å; Cg2···Cg1 ( $-1/2+x, 1/2-y, 1-z$ ) distance of 3.9823 (9) Å; Cg1···Cg2 ( $-x, 1-y, 1-z$ ) distance of 4.2397 (9) Å; Cg3···Cg1 ( $1/2-x, 1/2+y, z$ ) distance of 5.0406 (8) Å; where Cg1, Cg2 and Cg3 are the centroids of the rings C1···C6, C10···C15, and N2/C7/N4/C9/N3/C8, respectively.

#### S2. Experimental

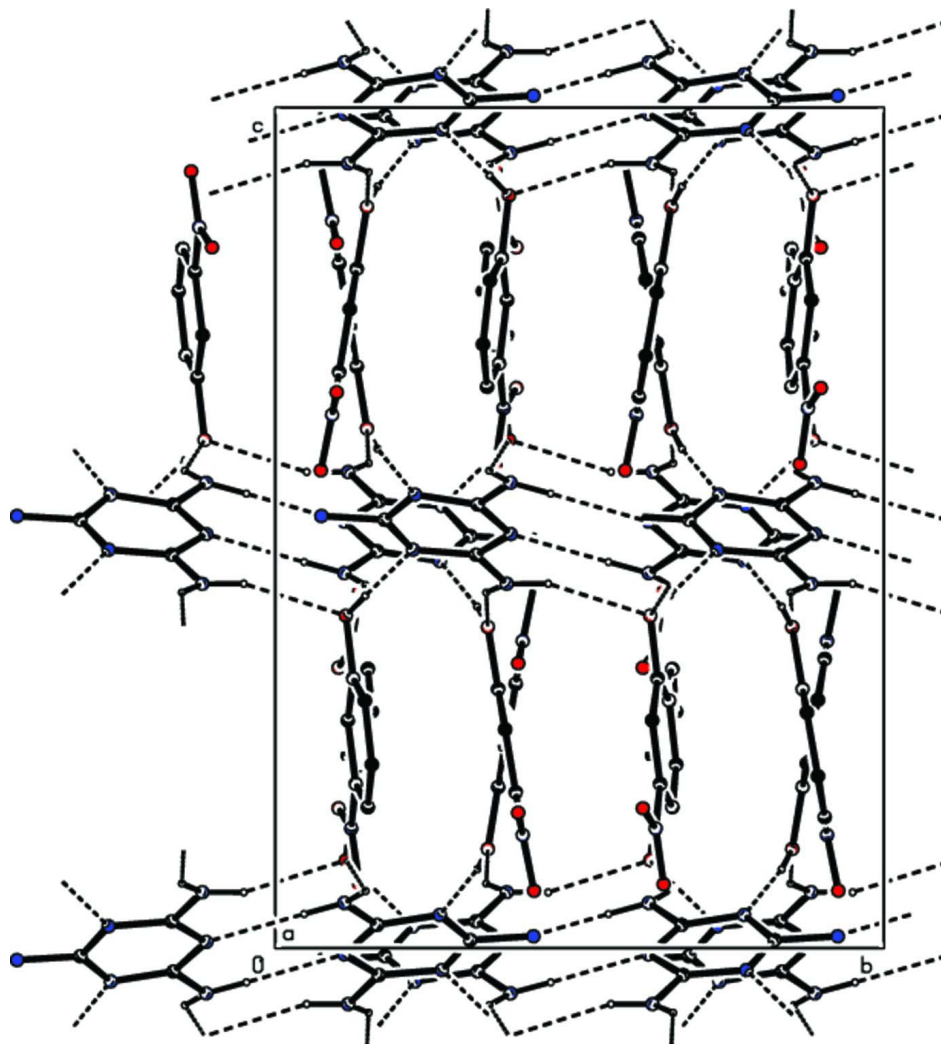
Melamine (1.261 g, 10 mmol) was dissolved in 200 ml of hot distilled water. 3-Nitrophenol (1.391 g, 10 mmol) was dissolved in 100 ml of distilled water, separately. The 3-nitrophenol solution was added gently to the hot solution of melamine, and the mixture stirred well for nearly five hours to get an 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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . 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

$a = 15.5150 (6) \text{ \AA}$

$b = 12.9137 (6) \text{ \AA}$

$c = 17.8323 (6) \text{ \AA}$

$V = 3572.8 (2) \text{ \AA}^3$

$Z = 8$

$F(000) = 1680$

$D_x = 1.503 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4327 reflections

$\theta = 2.3\text{--}28.3^\circ$

$\mu = 0.12 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Block, yellow

$0.28 \times 0.24 \times 0.20 \text{ mm}$

Data collection

Bruker Kappa APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  and  $\varphi$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\max} = 28.3^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -20 \rightarrow 13$   
 $k = -17 \rightarrow 7$   
 $l = -23 \rightarrow 23$

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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: SHELXL97 (Sheldrick,  
 2008),  $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0028 (5)

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

|     | <i>x</i>      | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| 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 (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| 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, °)*

|          |             |             |             |
|----------|-------------|-------------|-------------|
| 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 ( $\text{\AA}$ ,  $^\circ$ )

Cg3 is the centroid of the melamine triamine ring.

| <i>D</i> —H $\cdots$ <i>A</i>     | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O1—H1 $\cdots$ N3 <sup>i</sup>    | 0.84 (1)    | 1.86 (1)            | 2.6907 (14)                | 176 (2)                       |
| O4—H4A $\cdots$ N2 <sup>ii</sup>  | 0.83 (1)    | 1.87 (1)            | 2.6876 (14)                | 170 (2)                       |
| N5—H5A $\cdots$ N4 <sup>iii</sup> | 0.89 (1)    | 2.17 (1)            | 3.0594 (18)                | 178 (17)                      |



|                            |          |          |             |          |
|----------------------------|----------|----------|-------------|----------|
| N5—H5B···O1 <sup>iv</sup>  | 0.87 (1) | 2.25 (1) | 2.9613 (16) | 138 (15) |
| N7—H7A···O1 <sup>v</sup>   | 0.88 (1) | 2.32 (1) | 3.1600 (17) | 159 (14) |
| N7—H7B···O4 <sup>vi</sup>  | 0.88 (1) | 2.13 (1) | 2.9180 (16) | 149 (15) |
| C6—H6···Cg3 <sup>vii</sup> | 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)  $-x+1/2, y-1/2, z$ .