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# 1,5-Dimethyl-2-nitroimino-1,3,5-triazinane

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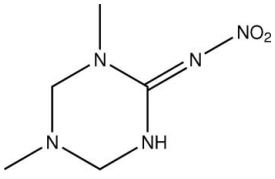
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(N–C) = 0.005 Å; $R$ factor = 0.073; $wR$ factor = 0.194; data-to-parameter ratio = 13.2.

The asymmetric unit of the title compound, $C_5H_{11}N_5O_2$, contains two independent molecules. The two triazine rings adopt envelope conformations. Intramolecular C—H···N and N—H···O hydrogen bonds result in the formation of two five- and two six-membered rings which are nearly planar; in addition, they are also nearly coplanar. In the crystal structure, intermolecular N—H···N, C—H···N and C—H···O hydrogen bonds link the molecules.

## Related literature

For general background, see: Wakita *et al.* (2003). For related literature, see: Shiokawa *et al.* (1991).




## Experimental

### Crystal data

$C_5H_{11}N_5O_2$
$M_r$ = 173.19
Monoclinic, $P2_1/n$
$a$ = 6.6490 (13) Å
$b$ = 30.103 (6) Å
$c$ = 8.2940 (17) Å
$\beta$ = 104.19 (3)°
$V$ = 1609.4 (6) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 294 (2) K
0.30 × 0.10 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.967, $T_{max}$ = 0.989
3126 measured reflections
2873 independent reflections
1979 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
3 standard reflections
frequency: 120 min
intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.194
$S$ = 1.00
2873 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···O1 | 0.86 | 1.94 | 2.549 (5) | 126 |
| N7—H7$A$···O3 | 0.86 | 1.99 | 2.583 (5) | 126 |
| N7—H7$A$···N3$^{i}$ | 0.86 | 2.57 | 3.210 (5) | 132 |
| C1—H1$C$···O3$^{ii}$ | 0.96 | 2.54 | 3.309 (6) | 137 |
| C2—H2$B$···N4 | 0.96 | 2.24 | 2.699 (6) | 108 |
| C4—H4$B$···O4$^{iii}$ | 0.97 | 2.50 | 3.411 (6) | 156 |
| C4—H4$C$···O3$^{ii}$ | 0.97 | 2.49 | 3.251 (6) | 136 |
| C7—H7$B$···N9 | 0.96 | 2.21 | 2.670 (5) | 108 |
| C7—H7$B$···O4$^{iv}$ | 0.96 | 2.59 | 3.317 (6) | 133 |
| C8—H8$B$···O3$^{iii}$ | 0.97 | 2.56 | 3.420 (5) | 148 |
| C9—H9$C$···O1$^{v}$ | 0.97 | 2.59 | 3.359 (6) | 137 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2491).

## References

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# supporting information

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## 1,5-Dimethyl-2-nitroimino-1,3,5-triazinane

**Cong Zhao, Wen-ge Yang, Yong-hong Hu, Lei Shen and Xiu-tao Lu**

### S1. Comment

Nitroguanidine derivatives have a high insecticidal activity and a wide spectrum (Wakita *et al.*, 2003). As part of our ongoing studies in this area, we report herein the crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) contains two independent molecules, in which the bond lengths and angles are generally within normal ranges. Rings A (N1-N3/C3-C5) and B (N6-N8/C8-C10) have envelope conformations, with N3 and N6 atoms displaced by -0.652 (2) and -0.645 (3) Å, respectively, from the plane of the other rings atoms. The intramolecular C-H···N and N-H···O hydrogen bonds (Table 1) result in the formation of nearly planar two five- and two six-membered rings: C (N1/N4/C2/C3/H2B), D (O1/N2/N4/N5/C3/H2A) and E (N8/N9/C7/C10/H7B), F (O3/N7/N9/N10/C10/H7A). The dihedral angles between the rings are C/D = 1.63 (3)° and E/F = 3.43 (3)°. So, rings C, D and E, F are nearly coplanar.

In the crystal structure, intermolecular N-H···N, C-H···N and C-H···O hydrogen bonds (Table 1) link the molecules, in which they may be effective in the stabilization of the structure.

### S2. Experimental

The title compound was synthesized according to the literature method (Shiokawa *et al.*, 1991). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

### S3. Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH) and C-H = 0.97 and 0.96 Å for methylene and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}$(H) = x$U_{eq}$(C,N), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

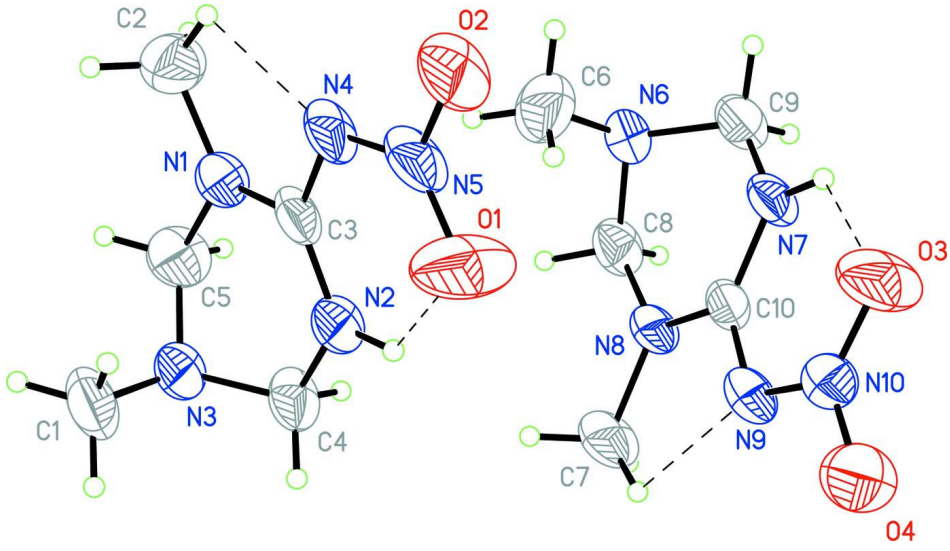


**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

### 1,5-Dimethyl-2-nitroimino-1,3,5-triazinane

*Crystal data*

$C_5H_{11}N_5O_2$
$M_r = 173.19$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 6.6490\ (13)$ Å
$b = 30.103\ (6)$ Å
$c = 8.2940\ (17)$ Å
$\beta = 104.19\ (3)°$
$V = 1609.4\ (6)$ Å$^3$
$Z = 8$
$F(000) = 736$
$D_x = 1.430$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 0.11$ mm$^{-1}$
$T = 294$ K
Block, colorless
0.30 × 0.10 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.967$, $T_{max} = 0.989$
3126 measured reflections
2873 independent reflections
1979 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.2°$, $\theta_{min} = 1.4°$
$h = -7\rightarrow7$
$k = 0\rightarrow36$
$l = 0\rightarrow9$
3 standard reflections every 120 min
intensity decay: none

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.072$
$wR(F^2) = 0.194$
$S = 1.00$
2873 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 4P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*Special details*

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

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.4157 (7) | 0.16494 (15) | 0.6298 (4) | 0.0982 (15) |
| O2 | 0.2294 (5) | 0.22215 (11) | 0.5490 (4) | 0.0699 (10) |
| N1 | 0.3763 (5) | 0.19429 (11) | 1.0927 (4) | 0.0447 (8) |
| N2 | 0.4955 (5) | 0.14315 (11) | 0.9359 (4) | 0.0466 (8) |
| H2A | 0.5027 | 0.1334 | 0.8400 | 0.056* |
| N3 | 0.6537 (5) | 0.14525 (12) | 1.2299 (4) | 0.0501 (9) |
| N4 | 0.3096 (5) | 0.20872 (11) | 0.8150 (4) | 0.0469 (8) |
| N5 | 0.3202 (5) | 0.19792 (13) | 0.6628 (4) | 0.0549 (10) |
| C1 | 0.8312 (7) | 0.17403 (17) | 1.2213 (7) | 0.0731 (15) |
| H1A | 0.8666 | 0.1925 | 1.3184 | 0.110* |
| H1B | 0.7939 | 0.1924 | 1.1238 | 0.110* |
| H1C | 0.9481 | 0.1559 | 1.2160 | 0.110* |
| C2 | 0.2708 (8) | 0.23592 (15) | 1.1160 (6) | 0.0616 (12) |
| H2B | 0.2130 | 0.2493 | 1.0097 | 0.092* |
| H2C | 0.3688 | 0.2559 | 1.1835 | 0.092* |
| H2D | 0.1617 | 0.2297 | 1.1701 | 0.092* |
| C3 | 0.3970 (6) | 0.18117 (13) | 0.9446 (5) | 0.0442 (9) |
| C4 | 0.5922 (7) | 0.11728 (14) | 1.0841 (5) | 0.0500 (10) |
| H4B | 0.4951 | 0.0950 | 1.1029 | 0.060* |
| H4C | 0.7132 | 0.1020 | 1.0657 | 0.060* |
| C5 | 0.4757 (8) | 0.16943 (17) | 1.2470 (5) | 0.0621 (13) |
| H5A | 0.5162 | 0.1902 | 1.3387 | 0.075* |
| H5B | 0.3757 | 0.1489 | 1.2734 | 0.075* |
| O3 | 0.0455 (5) | 0.07427 (13) | 0.2450 (4) | 0.0804 (12) |
| O4 | 0.3371 (5) | 0.04202 (11) | 0.2690 (4) | 0.0640 (9) |
| N6 | −0.1841 (5) | 0.09106 (11) | 0.7596 (4) | 0.0466 (8) |
| N7 | −0.1239 (4) | 0.07164 (11) | 0.4938 (4) | 0.0421 (8) |
| H7A | −0.1508 | 0.0788 | 0.3904 | 0.051* |
| N8 | 0.0994 (5) | 0.04358 (11) | 0.7263 (4) | 0.0429 (8) |
| N9 | 0.2160 (5) | 0.04411 (11) | 0.4922 (4) | 0.0424 (8) |

| | | | | |
|---|---|---|---|---|
| N10 | 0.1942 (5) | 0.05374 (11) | 0.3332 (4) | 0.0426 (8) |
| C6 | −0.0729 (8) | 0.13372 (16) | 0.7715 (7) | 0.0729 (15) |
| H6A | −0.0136 | 0.1407 | 0.8863 | 0.109* |
| H6B | −0.1680 | 0.1567 | 0.7221 | 0.109* |
| H6C | 0.0355 | 0.1316 | 0.7138 | 0.109* |
| C7 | 0.2916 (7) | 0.02129 (16) | 0.8125 (5) | 0.0579 (12) |
| H7B | 0.3745 | 0.0154 | 0.7351 | 0.087* |
| H7C | 0.2587 | −0.0062 | 0.8589 | 0.087* |
| H7D | 0.3674 | 0.0401 | 0.9001 | 0.087* |
| C8 | −0.0443 (6) | 0.05545 (15) | 0.8268 (5) | 0.0486 (10) |
| H8A | −0.1253 | 0.0294 | 0.8391 | 0.058* |
| H8B | 0.0352 | 0.0639 | 0.9369 | 0.058* |
| C9 | −0.2774 (6) | 0.07940 (15) | 0.5863 (5) | 0.0481 (10) |
| H9B | −0.3612 | 0.0529 | 0.5830 | 0.058* |
| H9C | −0.3682 | 0.1033 | 0.5342 | 0.058* |
| C10 | 0.0585 (5) | 0.05359 (12) | 0.5651 (4) | 0.0371 (8) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.131 (3) | 0.121 (3) | 0.0415 (19) | 0.080 (3) | 0.019 (2) | 0.023 (2) |
| O2 | 0.085 (2) | 0.070 (2) | 0.0385 (16) | 0.0103 (18) | −0.0163 (15) | 0.0154 (15) |
| N1 | 0.0489 (19) | 0.050 (2) | 0.0296 (16) | 0.0062 (15) | −0.0016 (14) | 0.0029 (14) |
| N2 | 0.053 (2) | 0.050 (2) | 0.0286 (16) | 0.0079 (16) | −0.0075 (14) | 0.0035 (14) |
| N3 | 0.054 (2) | 0.054 (2) | 0.0308 (17) | 0.0081 (17) | −0.0110 (14) | 0.0006 (15) |
| N4 | 0.050 (2) | 0.051 (2) | 0.0281 (17) | −0.0018 (16) | −0.0123 (14) | 0.0093 (14) |
| N5 | 0.049 (2) | 0.059 (2) | 0.043 (2) | 0.0020 (18) | −0.0152 (16) | 0.0148 (18) |
| C1 | 0.056 (3) | 0.058 (3) | 0.082 (4) | −0.009 (2) | −0.026 (3) | −0.001 (3) |
| C2 | 0.068 (3) | 0.058 (3) | 0.055 (3) | 0.011 (2) | 0.007 (2) | 0.002 (2) |
| C3 | 0.039 (2) | 0.043 (2) | 0.039 (2) | −0.0049 (17) | −0.0137 (16) | 0.0054 (17) |
| C4 | 0.059 (3) | 0.044 (2) | 0.036 (2) | −0.0027 (19) | −0.0087 (18) | 0.0081 (18) |
| C5 | 0.075 (3) | 0.070 (3) | 0.033 (2) | 0.017 (3) | −0.004 (2) | 0.010 (2) |
| O3 | 0.080 (2) | 0.117 (3) | 0.0414 (17) | 0.052 (2) | 0.0087 (16) | 0.0229 (18) |
| O4 | 0.0575 (19) | 0.079 (2) | 0.0566 (19) | 0.0107 (17) | 0.0153 (15) | 0.0055 (16) |
| N6 | 0.0420 (18) | 0.051 (2) | 0.0409 (18) | −0.0008 (15) | −0.0012 (14) | −0.0055 (16) |
| N7 | 0.0349 (17) | 0.059 (2) | 0.0275 (16) | 0.0067 (15) | −0.0026 (13) | 0.0045 (14) |
| N8 | 0.0411 (18) | 0.053 (2) | 0.0274 (16) | 0.0113 (15) | −0.0043 (13) | 0.0025 (14) |
| N9 | 0.0380 (17) | 0.050 (2) | 0.0326 (17) | 0.0027 (14) | −0.0036 (13) | 0.0066 (14) |
| N10 | 0.0430 (18) | 0.045 (2) | 0.0373 (17) | 0.0064 (15) | 0.0054 (14) | 0.0010 (14) |
| C6 | 0.065 (3) | 0.057 (3) | 0.094 (4) | −0.012 (2) | 0.015 (3) | −0.022 (3) |
| C7 | 0.054 (3) | 0.072 (3) | 0.038 (2) | 0.016 (2) | −0.0067 (19) | 0.012 (2) |
| C8 | 0.050 (2) | 0.061 (3) | 0.031 (2) | 0.001 (2) | 0.0023 (17) | 0.0038 (18) |
| C9 | 0.036 (2) | 0.064 (3) | 0.040 (2) | 0.0028 (19) | 0.0014 (16) | 0.0006 (19) |
| C10 | 0.0341 (19) | 0.035 (2) | 0.0353 (19) | −0.0013 (15) | −0.0040 (15) | −0.0016 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—N5 | 1.245 (5) | O3—N10 | 1.241 (4) |
| O2—N5 | 1.228 (4) | O4—N10 | 1.249 (4) |
| N1—C3 | 1.329 (5) | N6—C8 | 1.439 (5) |
| N1—C2 | 1.472 (5) | N6—C9 | 1.461 (5) |
| N1—C5 | 1.490 (5) | N6—C6 | 1.473 (6) |
| N2—C3 | 1.329 (5) | N7—C10 | 1.328 (4) |
| N2—C4 | 1.464 (5) | N7—C9 | 1.438 (5) |
| N2—H2A | 0.8600 | N7—H7A | 0.8600 |
| N3—C5 | 1.426 (6) | N8—C10 | 1.332 (5) |
| N3—C4 | 1.448 (5) | N8—C8 | 1.458 (5) |
| N3—C1 | 1.480 (6) | N8—C7 | 1.465 (5) |
| N4—N5 | 1.322 (5) | N9—N10 | 1.323 (4) |
| N4—C3 | 1.369 (5) | N9—C10 | 1.362 (5) |
| C1—H1A | 0.9600 | C6—H6A | 0.9600 |
| C1—H1B | 0.9600 | C6—H6B | 0.9600 |
| C1—H1C | 0.9600 | C6—H6C | 0.9600 |
| C2—H2B | 0.9600 | C7—H7B | 0.9600 |
| C2—H2C | 0.9600 | C7—H7C | 0.9600 |
| C2—H2D | 0.9600 | C7—H7D | 0.9600 |
| C4—H4B | 0.9700 | C8—H8A | 0.9700 |
| C4—H4C | 0.9700 | C8—H8B | 0.9700 |
| C5—H5A | 0.9700 | C9—H9B | 0.9700 |
| C5—H5B | 0.9700 | C9—H9C | 0.9700 |
| | | | |
| C3—N1—C2 | 122.4 (3) | C8—N6—C9 | 106.3 (3) |
| C3—N1—C5 | 121.3 (3) | C8—N6—C6 | 110.9 (3) |
| C2—N1—C5 | 116.1 (3) | C9—N6—C6 | 111.1 (4) |
| C3—N2—C4 | 122.3 (3) | C10—N7—C9 | 121.2 (3) |
| C3—N2—H2A | 118.9 | C10—N7—H7A | 119.4 |
| C4—N2—H2A | 118.9 | C9—N7—H7A | 119.4 |
| C5—N3—C4 | 108.0 (3) | C10—N8—C8 | 121.2 (3) |
| C5—N3—C1 | 113.4 (4) | C10—N8—C7 | 122.2 (3) |
| C4—N3—C1 | 111.4 (4) | C8—N8—C7 | 116.6 (3) |
| N5—N4—C3 | 119.3 (4) | N10—N9—C10 | 119.2 (3) |
| O2—N5—O1 | 119.1 (4) | O3—N10—O4 | 118.0 (3) |
| O2—N5—N4 | 117.2 (4) | O3—N10—N9 | 125.0 (3) |
| O1—N5—N4 | 123.7 (3) | O4—N10—N9 | 117.0 (3) |
| N3—C1—H1A | 109.5 | N6—C6—H6A | 109.5 |
| N3—C1—H1B | 109.5 | N6—C6—H6B | 109.5 |
| H1A—C1—H1B | 109.5 | H6A—C6—H6B | 109.5 |
| N3—C1—H1C | 109.5 | N6—C6—H6C | 109.5 |
| H1A—C1—H1C | 109.5 | H6A—C6—H6C | 109.5 |
| H1B—C1—H1C | 109.5 | H6B—C6—H6C | 109.5 |
| N1—C2—H2B | 109.5 | N8—C7—H7B | 109.5 |
| N1—C2—H2C | 109.5 | N8—C7—H7C | 109.5 |
| H2B—C2—H2C | 109.5 | H7B—C7—H7C | 109.5 |

| | | | |
|---|---|---|---|
| N1—C2—H2D | 109.5 | N8—C7—H7D | 109.5 |
| H2B—C2—H2D | 109.5 | H7B—C7—H7D | 109.5 |
| H2C—C2—H2D | 109.5 | H7C—C7—H7D | 109.5 |
| N1—C3—N2 | 118.0 (3) | N6—C8—N8 | 114.4 (3) |
| N1—C3—N4 | 115.2 (4) | N6—C8—H8A | 108.7 |
| N2—C3—N4 | 126.8 (4) | N8—C8—H8A | 108.7 |
| N3—C4—N2 | 111.6 (3) | N6—C8—H8B | 108.7 |
| N3—C4—H4B | 109.3 | N8—C8—H8B | 108.7 |
| N2—C4—H4B | 109.3 | H8A—C8—H8B | 107.6 |
| N3—C4—H4C | 109.3 | N7—C9—N6 | 112.2 (3) |
| N2—C4—H4C | 109.3 | N7—C9—H9B | 109.2 |
| H4B—C4—H4C | 108.0 | N6—C9—H9B | 109.2 |
| N3—C5—N1 | 112.0 (4) | N7—C9—H9C | 109.2 |
| N3—C5—H5A | 109.2 | N6—C9—H9C | 109.2 |
| N1—C5—H5A | 109.2 | H9B—C9—H9C | 107.9 |
| N3—C5—H5B | 109.2 | N7—C10—N8 | 118.6 (3) |
| N1—C5—H5B | 109.2 | N7—C10—N9 | 127.3 (3) |
| H5A—C5—H5B | 107.9 | N8—C10—N9 | 114.1 (3) |
| | | | |
| C3—N4—N5—O2 | 175.8 (4) | C10—N9—N10—O3 | 5.9 (6) |
| C3—N4—N5—O1 | −4.1 (6) | C10—N9—N10—O4 | −175.7 (3) |
| C2—N1—C3—N2 | 179.7 (4) | C9—N6—C8—N8 | 50.4 (4) |
| C5—N1—C3—N2 | 5.2 (6) | C6—N6—C8—N8 | −70.5 (5) |
| C2—N1—C3—N4 | −1.2 (6) | C10—N8—C8—N6 | −21.6 (5) |
| C5—N1—C3—N4 | −175.7 (4) | C7—N8—C8—N6 | 156.9 (4) |
| C4—N2—C3—N1 | −4.1 (6) | C10—N7—C9—N6 | 33.9 (5) |
| C4—N2—C3—N4 | 176.9 (4) | C8—N6—C9—N7 | −56.1 (4) |
| N5—N4—C3—N1 | −179.0 (3) | C6—N6—C9—N7 | 64.7 (5) |
| N5—N4—C3—N2 | 0.0 (6) | C9—N7—C10—N8 | −1.5 (5) |
| C5—N3—C4—N2 | 55.1 (5) | C9—N7—C10—N9 | 179.4 (4) |
| C1—N3—C4—N2 | −70.1 (4) | C8—N8—C10—N7 | −5.1 (5) |
| C3—N2—C4—N3 | −27.1 (5) | C7—N8—C10—N7 | 176.4 (4) |
| C4—N3—C5—N1 | −54.2 (5) | C8—N8—C10—N9 | 174.1 (3) |
| C1—N3—C5—N1 | 69.8 (5) | C7—N8—C10—N9 | −4.3 (5) |
| C3—N1—C5—N3 | 25.4 (6) | N10—N9—C10—N7 | 0.9 (6) |
| C2—N1—C5—N3 | −149.4 (4) | N10—N9—C10—N8 | −178.3 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O1 | 0.86 | 1.94 | 2.549 (5) | 126 |
| N7—H7*A*···O3 | 0.86 | 1.99 | 2.583 (5) | 126 |
| N7—H7*A*···N3$^{i}$ | 0.86 | 2.57 | 3.210 (5) | 132 |
| C1—H1*C*···O3$^{ii}$ | 0.96 | 2.54 | 3.309 (6) | 137 |
| C2—H2*B*···N4 | 0.96 | 2.24 | 2.699 (6) | 108 |
| C4—H4*B*···O4$^{iii}$ | 0.97 | 2.50 | 3.411 (6) | 156 |
| C4—H4*C*···O3$^{ii}$ | 0.97 | 2.49 | 3.251 (6) | 136 |
| C7—H7*B*···N9 | 0.96 | 2.21 | 2.670 (5) | 108 |

| | | | | |
|---|---|---|---|---|
| C7—H7*B*···O4$^{iv}$ | 0.96 | 2.59 | 3.317 (6) | 133 |
| C8—H8*B*···O3$^{iii}$ | 0.97 | 2.56 | 3.420 (5) | 148 |
| C9—H9*C*···O1$^{v}$ | 0.97 | 2.59 | 3.359 (6) | 137 |

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