Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 3,3-Dinitroazetidinium 2-hydroxybenzoate

**Rong Gao,[a] Biao Yan,[b,c]* Tao Mai,[c] Ying Hu[c] and Yu-Lei Guan[c]**

[a]Department of Chemistry, School of Pharmacy, Fourth Military Medical University, Xi'an 710032 Shaanxi, People's Republic of China, [b]School of Chemistry and Chemical Engineering, Yulin University, Yulin 719000 Shaanxi, People's Republic of China, and [c]School of Chemical Engineering, Northwest University, Xi'an 710069 Shaanxi, People's Republic of China
Correspondence e-mail: donghuhai@qq.com

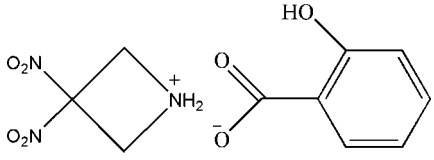
Received 26 October 2010; accepted 27 October 2010

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.040; $wR$ factor = 0.128; data-to-parameter ratio = 12.1.

In the title *gem*-dinitroazetidinium 2-hydroxybenzoate salt, $C_3H_6N_3O_4^+\cdot C_7H_5O_3^-$, the azetidine ring is virtually planar, with a mean deviation from the plane of 0.0242 Å. The dihedral angle between the two nitro groups is 87.5 (1)°.

## Related literature

For related literature on 1,3,3-trinitroazetidine and compounds prepared from its derivative 3,3-dinitroazetidine, see: Archibald *et al.* (1990); Gao *et al.* (2009); Hiskey *et al.* (1992); Ma, Yan, Li, Guan *et al.* (2009); Ma, Yan, Li, Song & Hu (2009); Ma, Yan, Song *et al.* (2009); Ma *et al.* (2010); Yan *et al.* (2009, 2010).




## Experimental

### Crystal data

$C_3H_6N_3O_4^+\cdot C_7H_5O_3^-$
$M_r$ = 285.22
Monoclinic, $P2_1/n$
$a$ = 11.174 (3) Å
$b$ = 7.013 (2) Å
$c$ = 16.661 (5) Å
$\beta$ = 105.960 (5)°
$V$ = 1255.3 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K
0.36 × 0.26 × 0.19 mm

### Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min}$ = 0.955, $T_{max}$ = 0.976
6012 measured reflections
2222 independent reflections
1504 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.128
$S$ = 0.99
2222 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$C$···O6 | 0.90 | 2.38 | 2.922 (2) | 118 |
| N1—H1$C$···O7 | 0.90 | 1.81 | 2.708 (2) | 179 |
| N1—H1$D$···O7$^{i}$ | 0.90 | 1.96 | 2.720 (2) | 141 |

Symmetry code: (i) $-x+1, -y+2, -z$.

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We thank the National Natural Science Foundation of China (grant No. 21073141), the Natural Science Foundation of Shaanxi Province (grant No. 2009JQ2002) and NWU Graduate Experimental Research Funds (grant No. 09YSY23) for generously supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5053).

## References

Archibald, T. G., Gilardi, R., Baum, K. & George, C. (1990). *J. Org. Chem.* **55**, 2920–2924.
Bruker (2003). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, R., Ma, H. X., Yan, B., Song, J. R. & Wang, Y. H. (2009). *Chem. J. Chin. Univ.* **30**, 577–582.
Hiskey, M. A., Coburn, M. D., Mitchell, M. A. & Benicewicz, B. C. (1992). *J. Heterocycl. Chem.* **29**, 1855–1856.
Ma, H. X., Yan, B., Li, Z. N., Guan, Y. L., Song, J. R., Xu, K. Z. & Hu, R. Z. (2009). *J. Hazard. Mater.* **169**, 1068–1073.
Ma, H. X., Yan, B., Li, J. F., Ren, Y. H., Chen, Y. S., Zhao, F. Q., Song, J. R. & Hu, R. Z. (2010). *J. Mol. Struct.* **981**, 103–110.
Ma, H. X., Yan, B., Li, Z. N., Song, J. R. & Hu, R. Z. (2009). *J. Therm. Anal. Calorim.* **95**, 437–444.
Ma, H. X., Yan, B., Song, J. R., Lü, X. Q. & Wang, L. J. (2009). *Chem. J. Chin. Univ.* **30**, 371–381.
Sheldrick, G. M. (2000). *SADABS* . University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yan, B., Ma, H.-X., Hu, Y., Guan, Y.-L. & Song, J.-R. (2009). *Acta Cryst.* E**65**, o3215.
Yan, B., Ma, H.-X., Li, J.-F., Guan, Y.-L. & Song, J.-R. (2010). *Acta Cryst.* E**66**, o57.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o3036 [ **doi:10.1107/S1600536810043825** ]

# 3,3-Dinitroazetidinium 2-hydroxybenzoate

**R. Gao, B. Yan, T. Mai, Y. Hu and Y.-L. Guan**

## Comment

Dinitro- and trinitro-derivatives of azetidine are of interest because they contain strained ring systems. This makes them good candidates for energetic materials (propellants or explosives). Azetidine-based explosives, such as 1,3,3-trinitroazetidine (TNAZ) (Archibald *et al.*, 1990) demonstrate excellent performance partly because of the high strain associated with the four-membered ring. As one of the important derivates of TNAZ, 3,3-dinitroazetidine (DNAZ) (Hiskey *et al.*, 1992;)can prepare a variety of solid energetic materials with high oxygen-balance (Ma, Yan, Li, Guan *et al.*, 2009; Gao *et al.*, 2009; Ma, Yan, Li, Song & Hu, 2009; Ma, Yan, Song *et al.*, 2009; Yan *et al.*, 2009; Yan *et al.*, 2010; Ma *et al.*, 2010). This paper reports synthesis and crystal structure of the title DNAZ salt.

## Experimental

A solution of DNAZ (0.30 g, 2.04 mmol), salicylic acid (0.28 ml, 2.04 mmol) in trichloromethane (15.0 ml) was stirred for 2 h. The reaction mixture was concentrated *in vacuo*, then a white solid began to precipitate. The solid product was washed with ethanol and purified by recrystallization from trichloromethane to give the pure colorless compound in 90.5% yield. The title compound (43 mg,0.15 mmol) was dissolved in chloroform (15 ml). Colorless crystals were isolated after several days. Elemental analysis calculated for $C_{10}H_{11}N_3O_7$: C 42.11, N 14.73, H 3.89%; found: C 47.44, N 14.80, H 3.89%. IR (KBr, $cm^{-1}$): 3060.25, 1647.33, 1579.29, 1298.39, 1485.78, 1454.23, 706.64.

## Refinement

H atoms were placed at calculated idealized positions and refined using a riding model, with C—H distances in the range 0.93–0.97 Å, N—H distances 0.90 Å and O—H distances 0.82 Å.

## Figures

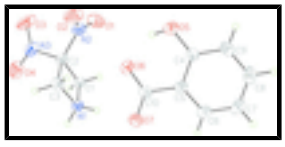


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are drawn as spheres of arbitrary radius.

## 3,3-Dinitroazetidinium 2-hydroxybenzoate

*Crystal data*

| | |
|---|---|
| $C_3H_6N_3O_4^+\cdot C_7H_5O_3^-$ | $F(000) = 592$ |
| $M_r = 285.22$ | $D_x = 1.509$ Mg $m^{-3}$ |
| Monoclinic, $P2_1/n$ | Melting point: 379.4 K |

| | |
|---|---|
| Hall symbol: -P2yn | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 11.174$ (3) Å | Cell parameters from 1275 reflections |
| $b = 7.013$ (2) Å | $\theta = 2.5–21.9°$ |
| $c = 16.661$ (5) Å | $\mu = 0.13$ mm$^{-1}$ |
| $\beta = 105.960$ (5)° | $T = 296$ K |
| $V = 1255.3$ (6) Å$^3$ | Block, colorless |
| $Z = 4$ | 0.36 × 0.26 × 0.19 mm |

*Data collection*

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 2222 independent reflections |
| Radiation source: fine-focus sealed tube | 1504 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.027$ |
| phi and ω scans | $\theta_{max} = 25.1°$, $\theta_{min} = 2.0°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000) | $h = -12\rightarrow13$ |
| $T_{min} = 0.955$, $T_{max} = 0.976$ | $k = -8\rightarrow8$ |
| 6012 measured reflections | $l = -18\rightarrow19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | H-atom parameters constrained |
| $wR(F^2) = 0.128$ | $w = 1/[\sigma^2(F_o^2) + (0.0797P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.99$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 2222 reflections | $\Delta\rho_{max} = 0.34$ e Å$^{-3}$ |
| 183 parameters | $\Delta\rho_{min} = -0.17$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.008 (2) |

*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 $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O7 | 0.58576 (13) | 0.7941 (2) | 0.06388 (8) | 0.0563 (4) |
| O6 | 0.46538 (12) | 0.5959 (2) | 0.10843 (9) | 0.0629 (4) |
| O5 | 0.53637 (13) | 0.2679 (2) | 0.15624 (10) | 0.0619 (4) |
| H5 | 0.4878 | 0.3566 | 0.1405 | 0.093* |
| C4 | 0.67334 (16) | 0.4982 (3) | 0.12215 (10) | 0.0380 (5) |
| N1 | 0.36966 (14) | 0.9772 (2) | 0.05657 (9) | 0.0447 (4) |
| H1D | 0.3660 | 1.0893 | 0.0297 | 0.054* |
| H1C | 0.4417 | 0.9169 | 0.0593 | 0.054* |
| C5 | 0.65122 (17) | 0.3202 (3) | 0.15274 (11) | 0.0407 (5) |
| N3 | 0.10748 (16) | 0.9419 (3) | 0.10825 (12) | 0.0580 (5) |
| C10 | 0.56810 (18) | 0.6383 (3) | 0.09534 (11) | 0.0439 (5) |
| C3 | 0.34209 (17) | 0.9937 (3) | 0.13919 (11) | 0.0471 (5) |
| H3B | 0.3181 | 1.1211 | 0.1514 | 0.056* |
| H3A | 0.4075 | 0.9437 | 0.1854 | 0.056* |
| C2 | 0.23289 (16) | 0.8586 (3) | 0.10855 (11) | 0.0412 (5) |
| C6 | 0.7486 (2) | 0.1923 (3) | 0.18100 (11) | 0.0511 (5) |
| H6 | 0.7340 | 0.0722 | 0.2000 | 0.061* |
| C1 | 0.25748 (18) | 0.8552 (3) | 0.02338 (11) | 0.0479 (5) |
| H1A | 0.2765 | 0.7293 | 0.0061 | 0.057* |
| H1B | 0.1928 | 0.9160 | −0.0201 | 0.057* |
| C9 | 0.79343 (18) | 0.5449 (3) | 0.12150 (12) | 0.0501 (5) |
| H9 | 0.8089 | 0.6630 | 0.1010 | 0.060* |
| N2 | 0.24179 (17) | 0.6717 (3) | 0.15310 (13) | 0.0585 (5) |
| O4 | 0.08623 (14) | 1.0972 (3) | 0.07553 (11) | 0.0771 (5) |
| C7 | 0.8681 (2) | 0.2457 (4) | 0.18067 (12) | 0.0595 (6) |
| H7 | 0.9340 | 0.1620 | 0.2011 | 0.071* |
| O3 | 0.03912 (17) | 0.8537 (3) | 0.13847 (15) | 0.0995 (7) |
| C8 | 0.89002 (19) | 0.4198 (4) | 0.15066 (13) | 0.0594 (6) |
| H8 | 0.9703 | 0.4534 | 0.1500 | 0.071* |
| O1 | 0.19839 (17) | 0.5345 (3) | 0.11130 (12) | 0.0861 (6) |
| O2 | 0.29006 (19) | 0.6747 (3) | 0.22818 (11) | 0.0891 (6) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O7 | 0.0650 (10) | 0.0485 (9) | 0.0622 (9) | 0.0038 (7) | 0.0288 (7) | 0.0121 (7) |
| O6 | 0.0415 (8) | 0.0663 (11) | 0.0854 (11) | 0.0040 (7) | 0.0248 (7) | 0.0167 (8) |
| O5 | 0.0492 (9) | 0.0573 (10) | 0.0826 (11) | −0.0109 (7) | 0.0237 (8) | 0.0107 (8) |
| C4 | 0.0390 (10) | 0.0420 (11) | 0.0340 (9) | −0.0047 (8) | 0.0115 (7) | −0.0025 (8) |
| N1 | 0.0432 (9) | 0.0451 (10) | 0.0531 (9) | 0.0044 (7) | 0.0256 (7) | 0.0105 (7) |
| C5 | 0.0418 (11) | 0.0429 (11) | 0.0363 (9) | −0.0046 (9) | 0.0087 (8) | −0.0011 (8) |
| N3 | 0.0432 (10) | 0.0605 (13) | 0.0751 (12) | −0.0041 (9) | 0.0245 (9) | −0.0147 (10) |
| C10 | 0.0500 (12) | 0.0425 (12) | 0.0400 (10) | −0.0027 (9) | 0.0140 (9) | 0.0011 (9) |
| C3 | 0.0407 (11) | 0.0577 (13) | 0.0467 (10) | −0.0116 (9) | 0.0185 (8) | −0.0046 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0330 (9) | 0.0492 (12) | 0.0447 (10) | −0.0038 (8) | 0.0162 (8) | −0.0006 (9) |
| C6 | 0.0633 (14) | 0.0489 (12) | 0.0395 (10) | 0.0057 (10) | 0.0116 (9) | 0.0042 (9) |
| C1 | 0.0484 (11) | 0.0557 (13) | 0.0401 (10) | 0.0045 (10) | 0.0131 (8) | −0.0021 (9) |
| C9 | 0.0450 (11) | 0.0535 (13) | 0.0546 (12) | −0.0094 (10) | 0.0183 (9) | −0.0029 (10) |
| N2 | 0.0551 (11) | 0.0572 (13) | 0.0725 (13) | −0.0050 (9) | 0.0333 (10) | 0.0088 (10) |
| O4 | 0.0646 (11) | 0.0716 (12) | 0.0967 (13) | 0.0169 (9) | 0.0250 (9) | −0.0032 (10) |
| C7 | 0.0537 (14) | 0.0751 (17) | 0.0443 (11) | 0.0211 (12) | 0.0041 (10) | −0.0059 (11) |
| O3 | 0.0672 (11) | 0.0869 (14) | 0.173 (2) | −0.0139 (10) | 0.0806 (13) | −0.0085 (13) |
| C8 | 0.0367 (11) | 0.0786 (17) | 0.0633 (13) | −0.0060 (11) | 0.0147 (10) | −0.0108 (12) |
| O1 | 0.0896 (13) | 0.0543 (11) | 0.1241 (16) | −0.0227 (9) | 0.0458 (11) | −0.0050 (10) |
| O2 | 0.1054 (14) | 0.1075 (15) | 0.0614 (11) | 0.0001 (11) | 0.0347 (10) | 0.0311 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O7—C10 | 1.251 (2) | C3—H3B | 0.9700 |
| O6—C10 | 1.261 (2) | C3—H3A | 0.9700 |
| O5—C5 | 1.351 (2) | C2—N2 | 1.496 (3) |
| O5—H5 | 0.8200 | C2—C1 | 1.518 (3) |
| C4—C9 | 1.384 (3) | C6—C7 | 1.388 (3) |
| C4—C5 | 1.396 (2) | C6—H6 | 0.9300 |
| C4—C10 | 1.503 (3) | C1—H1A | 0.9700 |
| N1—C1 | 1.493 (2) | C1—H1B | 0.9700 |
| N1—C3 | 1.495 (2) | C9—C8 | 1.372 (3) |
| N1—H1D | 0.9000 | C9—H9 | 0.9300 |
| N1—H1C | 0.9000 | N2—O1 | 1.208 (2) |
| C5—C6 | 1.389 (3) | N2—O2 | 1.219 (2) |
| N3—O3 | 1.196 (2) | C7—C8 | 1.367 (3) |
| N3—O4 | 1.212 (2) | C7—H7 | 0.9300 |
| N3—C2 | 1.517 (2) | C8—H8 | 0.9300 |
| C3—C2 | 1.518 (3) | | |
| C5—O5—H5 | 109.5 | N2—C2—C1 | 116.46 (16) |
| C9—C4—C5 | 118.95 (17) | N3—C2—C1 | 114.04 (15) |
| C9—C4—C10 | 121.59 (17) | N2—C2—C3 | 116.25 (16) |
| C5—C4—C10 | 119.37 (16) | N3—C2—C3 | 114.66 (16) |
| C1—N1—C3 | 91.18 (13) | C1—C2—C3 | 89.36 (14) |
| C1—N1—H1D | 113.4 | C7—C6—C5 | 119.3 (2) |
| C3—N1—H1D | 113.4 | C7—C6—H6 | 120.3 |
| C1—N1—H1C | 113.4 | C5—C6—H6 | 120.3 |
| C3—N1—H1C | 113.4 | N1—C1—C2 | 89.66 (13) |
| H1D—N1—H1C | 110.7 | N1—C1—H1A | 113.7 |
| O5—C5—C6 | 118.36 (17) | C2—C1—H1A | 113.7 |
| O5—C5—C4 | 121.62 (16) | N1—C1—H1B | 113.7 |
| C6—C5—C4 | 120.02 (17) | C2—C1—H1B | 113.7 |
| O3—N3—O4 | 125.8 (2) | H1A—C1—H1B | 110.9 |
| O3—N3—C2 | 119.7 (2) | C8—C9—C4 | 121.03 (19) |
| O4—N3—C2 | 114.47 (17) | C8—C9—H9 | 119.5 |
| O7—C10—O6 | 122.29 (18) | C4—C9—H9 | 119.5 |
| O7—C10—C4 | 119.66 (17) | O1—N2—O2 | 126.9 (2) |
| O6—C10—C4 | 118.00 (17) | O1—N2—C2 | 116.75 (19) |

| | | | |
|---|---|---|---|
| N1—C3—C2 | 89.56 (14) | O2—N2—C2 | 116.36 (19) |
| N1—C3—H3B | 113.7 | C8—C7—C6 | 120.8 (2) |
| C2—C3—H3B | 113.7 | C8—C7—H7 | 119.6 |
| N1—C3—H3A | 113.7 | C6—C7—H7 | 119.6 |
| C2—C3—H3A | 113.7 | C7—C8—C9 | 119.87 (19) |
| H3B—C3—H3A | 111.0 | C7—C8—H8 | 120.1 |
| N2—C2—N3 | 105.92 (15) | C9—C8—H8 | 120.1 |
| C9—C4—C5—O5 | 178.87 (17) | O5—C5—C6—C7 | −177.77 (16) |
| C10—C4—C5—O5 | 2.3 (2) | C4—C5—C6—C7 | 1.8 (3) |
| C9—C4—C5—C6 | −0.7 (3) | C3—N1—C1—C2 | −3.71 (15) |
| C10—C4—C5—C6 | −177.31 (16) | N2—C2—C1—N1 | −115.59 (16) |
| C9—C4—C10—O7 | 7.2 (3) | N3—C2—C1—N1 | 120.51 (16) |
| C5—C4—C10—O7 | −176.32 (16) | C3—C2—C1—N1 | 3.65 (14) |
| C9—C4—C10—O6 | −170.31 (17) | C5—C4—C9—C8 | −0.3 (3) |
| C5—C4—C10—O6 | 6.2 (2) | C10—C4—C9—C8 | 176.18 (17) |
| C1—N1—C3—C2 | 3.71 (14) | N3—C2—N2—O1 | 87.1 (2) |
| O3—N3—C2—N2 | −1.8 (2) | C1—C2—N2—O1 | −40.8 (2) |
| O4—N3—C2—N2 | 178.59 (17) | C3—C2—N2—O1 | −144.22 (18) |
| O3—N3—C2—C1 | 127.6 (2) | N3—C2—N2—O2 | −91.5 (2) |
| O4—N3—C2—C1 | −52.0 (2) | C1—C2—N2—O2 | 140.53 (18) |
| O3—N3—C2—C3 | −131.4 (2) | C3—C2—N2—O2 | 37.1 (2) |
| O4—N3—C2—C3 | 49.0 (2) | C5—C6—C7—C8 | −1.9 (3) |
| N1—C3—C2—N2 | 115.79 (17) | C6—C7—C8—C9 | 0.9 (3) |
| N1—C3—C2—N3 | −119.95 (17) | C4—C9—C8—C7 | 0.2 (3) |
| N1—C3—C2—C1 | −3.65 (14) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1C···O6 | 0.90 | 2.38 | 2.922 (2) | 118 |
| N1—H1C···O7 | 0.90 | 1.81 | 2.708 (2) | 179 |
| N1—H1D···O7$^{i}$ | 0.90 | 1.96 | 2.720 (2) | 141 |

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

**Fig. 1**