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# (*E*)-1-[4-(Dimethylamino)benzylidene]-semicarbazide–acetic acid (1/2)

**Zu-Pei Liang,[a]* Jian Li,[a] Hong-Liang Wang[b] and Yun-Chen Zhang[a]**

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and [b]Weifang Examination Center of Boiler and Pressure Vessels, Weifang 261057, People's Republic of China
Correspondence e-mail: zupeiliang@yahoo.com.cn

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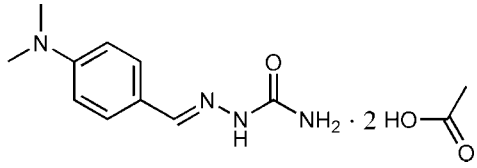
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.062; $wR$ factor = 0.202; data-to-parameter ratio = 13.6.

In the crystal structure of the title compound, $C_{10}H_{16}N_4O\cdot 2C_2H_4O_2$, the molecules interact by way of O—H···O and N—H···O hydrogen bonds, resulting in [010] chains built up from the 1-[4-(dimethylamino)benzylidene]semicarbazide molecule and one of the acetic acid molecules. The other acetic acid molecule forms isolated centrosymmetric dimers.

## Related literature

For a related structure, see Tai *et al.* (2007).



## Experimental

### *Crystal data*

$C_{10}H_{14}N_4O\cdot 2C_2H_4O_2$
$M_r$ = 326.36
Triclinic, $P\overline{1}$
$a$ = 7.2931 (2) Å
$b$ = 10.7952 (8) Å
$c$ = 12.2472 (7) Å
$\alpha$ = 71.422 (17)°
$\beta$ = 80.020 (4)°
$\gamma$ = 73.947 (4)°
$V$ = 874.49 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 294 (2) K
0.16 × 0.14 × 0.12 mm

### *Data collection*

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.985, $T_{max}$ = 0.989
4441 measured reflections
3064 independent reflections
1351 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.202
$S$ = 1.01
3064 reflections
225 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O2$^{i}$ | 0.85 | 1.82 | 2.658 (6) | 170 |
| O5—H5$A$···O1$^{ii}$ | 0.82 | 1.78 | 2.579 (4) | 166 |
| N4—H4$A$···O4$^{iii}$ | 0.87 (4) | 2.48 (4) | 3.164 (6) | 135 (3) |
| N3—H3$A$···O1$^{iv}$ | 0.897 (10) | 2.017 (11) | 2.913 (5) | 178 (4) |
| N4—H4$B$···O4$^{v}$ | 0.91 (6) | 2.16 (6) | 3.051 (6) | 166 (5) |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2411).

## References

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tai, X.-S., Hao, M.-Y., Yin, J. & Liang, Z.-P. (2007). *Acta Cryst.* E**63**, o1725–o1726.

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o2978 [ **doi:10.1107/S1600536807024956** ]

# (*E*)-1-[4-(Dimethylamino)benzylidene]semicarbazide-acetic acid (1/2)

**Z.-P. Liang, J. Li, H.-L. Wang and Y.-C. Zhang**

## Comment

Their preparation, properties and applications od Schiff bases are important in the development of coordination chemistry. The asymmetric unit of the title compound, (I), contains one (*E*)-1-(4-(dimethylamino)benzylidene)semicarbazide molecule and two acetic acid molecules (Fig. 1). The bond lengths and angles of the Schiff base in (I) agree with those in the related (*E*)-1-(4-hydroxybenzylidene)semicarbazide hemihydrate (Tai *et al.*, 2007). The main molecule in (I) is essentially planar, with a maximum deviation from the mean plane for the non-hydrogen atoms of 0.042 (2) Å. The crystal structure of (I) is stabilized by O—H···O and N—H···O hydrogen bonds (Fig. 2 and Table 1), to result in a chains built up from the $C_{10}H_{16}N_40$ molecule and the C13-containing acetic acid molecule. Conversely, the C11 acetic acid molecule forms isolated inversion dimers.

## Experimental

A mixture of 4-(dimethylamino)benzaldehyde (0.01 mol) and semicarbazide hydrochloride (0.01 mol) in ethanol (10 ml) was refluxed for 1 h. After cooling, filtration and drying, the compound (*E*)-1-(4-(dimethylamino)benzylidene)semicarbazide was obtained. 10 mg of this compound was dissolved in acetic acid (8 ml), and the solution was then allowed to evaporate at room temperature; light yellow blocks of (I) were formed after 12 d.

## Refinement

The N-bound H atoms were located in a difference map and their positions and $U_{iso}$ values were freely refined.

The O-bound H atoms were located in a difference map and refined as riding in their as-found relative positions with $U_{iso}(H) = 1.5U_{eq}(O)$.

The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

## Figures

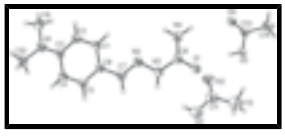

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids (arbitrary spheres for the H atoms).

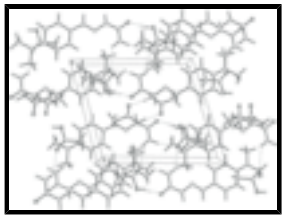

Fig. 2. The crystal packing of (I), viewed along *a* axis. Hydrogen bonds are indicated by dashed lines.

**(*E*)-1-[4-(Dimethylamino)benzylidene]semicarbazide–acetic acid (1/2)**

*Crystal data*

| | |
|---|---|
| $C_{10}H_{14}N_4O\cdot 2C_2H_4O_2$ | $Z = 2$ |
| $M_r = 326.36$ | $F_{000} = 348$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.239$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 7.2931$ (2) Å | Cell parameters from 886 reflections |
| $b = 10.7952$ (8) Å | $\theta = 2.9$–$23.5^\circ$ |
| $c = 12.2472$ (7) Å | $\mu = 0.10$ mm$^{-1}$ |
| $\alpha = 71.422$ (17)° | $T = 294$ (2) K |
| $\beta = 80.020$ (4)° | Block, light yellow |
| $\gamma = 73.947$ (4)° | 0.16 × 0.14 × 0.12 mm |
| $V = 874.49$ (12) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 3064 independent reflections |
| Radiation source: fine-focus sealed tube | 1351 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.040$ |
| $T = 294$(2) K | $\theta_{max} = 25.0^\circ$ |
| φ and ω scans | $\theta_{min} = 1.8^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 1997) | $h = -8\rightarrow 7$ |
| $T_{min} = 0.985$, $T_{max} = 0.989$ | $k = -12\rightarrow 12$ |
| 4441 measured reflections | $l = -14\rightarrow 6$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.202$ | $w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 0.1483P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} = 0.005$ |

| | |
|---|---|
| 3064 reflections | $\Delta\rho_{max}$ = 0.19 e Å$^{-3}$ |
| 225 parameters | $\Delta\rho_{min}$ = −0.21 e Å$^{-3}$ |
| 1 restraint | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.0214 (4) | 0.6237 (2) | 0.5764 (2) | 0.0645 (9) |
| N1 | 0.3989 (6) | 0.9089 (3) | −0.2633 (3) | 0.0756 (12) |
| N2 | 0.1380 (5) | 0.7164 (3) | 0.2810 (3) | 0.0543 (9) |
| N3 | 0.0888 (5) | 0.6399 (3) | 0.3916 (3) | 0.0609 (10) |
| N4 | 0.0405 (6) | 0.8213 (4) | 0.4616 (4) | 0.0686 (12) |
| C1 | 0.2324 (6) | 0.8560 (4) | 0.0449 (3) | 0.0593 (12) |
| H1 | 0.1941 | 0.9067 | 0.0972 | 0.071* |
| C2 | 0.2830 (6) | 0.9184 (4) | −0.0688 (3) | 0.0621 (13) |
| H2 | 0.2769 | 1.0101 | −0.0915 | 0.074* |
| C3 | 0.3434 (6) | 0.8470 (4) | −0.1512 (3) | 0.0540 (11) |
| C4 | 0.3461 (6) | 0.7089 (4) | −0.1113 (3) | 0.0549 (12) |
| H4 | 0.3838 | 0.6576 | −0.1631 | 0.066* |
| C5 | 0.2941 (6) | 0.6479 (3) | 0.0034 (3) | 0.0526 (11) |
| H5 | 0.2977 | 0.5565 | 0.0268 | 0.063* |
| C6 | 0.2366 (5) | 0.7196 (3) | 0.0842 (3) | 0.0470 (10) |
| C7 | 0.1849 (6) | 0.6532 (4) | 0.2048 (3) | 0.0537 (11) |
| H7 | 0.1862 | 0.5622 | 0.2267 | 0.064* |
| C8 | 0.0324 (6) | 0.6951 (4) | 0.4796 (3) | 0.0520 (11) |
| C9 | 0.3996 (8) | 1.0509 (4) | −0.3013 (4) | 0.0873 (17) |
| H9A | 0.2720 | 1.1034 | −0.2895 | 0.131* |
| H9B | 0.4438 | 1.0761 | −0.3820 | 0.131* |
| H9C | 0.4833 | 1.0670 | −0.2575 | 0.131* |
| C10 | 0.4361 (8) | 0.8414 (5) | −0.3535 (4) | 0.0910 (17) |
| H10A | 0.5516 | 0.7714 | −0.3415 | 0.137* |
| H10B | 0.4506 | 0.9053 | −0.4278 | 0.137* |
| H10C | 0.3308 | 0.8030 | −0.3508 | 0.137* |
| O2 | 0.4506 (5) | 0.5408 (3) | 0.6268 (3) | 0.0902 (12) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.4009 (5) | 0.3657 (3) | 0.5886 (3) | 0.0960 (12) |
| H3 | 0.4495 | 0.4040 | 0.5221 | 0.115* |
| C11 | 0.3914 (7) | 0.4363 (5) | 0.6571 (5) | 0.0765 (14) |
| C12 | 0.3084 (8) | 0.3842 (5) | 0.7785 (5) | 0.0920 (16) |
| H12A | 0.4089 | 0.3254 | 0.8251 | 0.138* |
| H12B | 0.2162 | 0.3355 | 0.7789 | 0.138* |
| H12C | 0.2468 | 0.4583 | 0.8096 | 0.138* |
| O4 | 0.9048 (5) | 0.8908 (3) | 0.6896 (3) | 0.0806 (10) |
| O5 | 0.8966 (5) | 0.6762 (3) | 0.7728 (2) | 0.0788 (10) |
| H5A | 0.9164 | 0.6733 | 0.7056 | 0.118* |
| C13 | 0.8785 (6) | 0.8016 (4) | 0.7749 (4) | 0.0606 (12) |
| C14 | 0.8229 (7) | 0.8142 (5) | 0.8945 (4) | 0.0776 (15) |
| H14A | 0.9334 | 0.8155 | 0.9264 | 0.116* |
| H14B | 0.7724 | 0.7390 | 0.9418 | 0.116* |
| H14C | 0.7270 | 0.8961 | 0.8924 | 0.116* |
| H4A | 0.070 (5) | 0.872 (3) | 0.393 (3) | 0.046 (11)* |
| H3A | 0.070 (5) | 0.558 (2) | 0.400 (3) | 0.070 (13)* |
| H4B | 0.000 (8) | 0.857 (6) | 0.523 (5) | 0.14 (2)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.102 (2) | 0.0522 (15) | 0.0443 (17) | −0.0302 (15) | 0.0101 (16) | −0.0185 (13) |
| N1 | 0.121 (4) | 0.064 (2) | 0.047 (2) | −0.036 (2) | 0.012 (2) | −0.0201 (18) |
| N2 | 0.068 (2) | 0.0523 (18) | 0.047 (2) | −0.0230 (17) | 0.0054 (18) | −0.0180 (17) |
| N3 | 0.091 (3) | 0.0506 (19) | 0.047 (2) | −0.0283 (19) | 0.0085 (19) | −0.0198 (17) |
| N4 | 0.109 (4) | 0.054 (2) | 0.046 (2) | −0.033 (2) | 0.002 (2) | −0.012 (2) |
| C1 | 0.080 (3) | 0.047 (2) | 0.053 (3) | −0.014 (2) | 0.005 (2) | −0.023 (2) |
| C2 | 0.089 (4) | 0.044 (2) | 0.056 (3) | −0.022 (2) | 0.009 (3) | −0.019 (2) |
| C3 | 0.066 (3) | 0.054 (2) | 0.044 (2) | −0.018 (2) | 0.002 (2) | −0.0173 (19) |
| C4 | 0.073 (3) | 0.047 (2) | 0.049 (2) | −0.015 (2) | 0.003 (2) | −0.0227 (19) |
| C5 | 0.066 (3) | 0.0389 (19) | 0.053 (3) | −0.0144 (19) | −0.001 (2) | −0.0133 (18) |
| C6 | 0.051 (3) | 0.047 (2) | 0.043 (2) | −0.0113 (19) | 0.000 (2) | −0.0166 (18) |
| C7 | 0.061 (3) | 0.046 (2) | 0.056 (3) | −0.017 (2) | 0.001 (2) | −0.017 (2) |
| C8 | 0.066 (3) | 0.045 (2) | 0.048 (3) | −0.018 (2) | −0.002 (2) | −0.014 (2) |
| C9 | 0.129 (5) | 0.066 (3) | 0.057 (3) | −0.032 (3) | 0.011 (3) | −0.006 (2) |
| C10 | 0.135 (5) | 0.102 (4) | 0.049 (3) | −0.047 (3) | 0.013 (3) | −0.035 (3) |
| O2 | 0.106 (3) | 0.067 (2) | 0.113 (3) | −0.038 (2) | −0.008 (2) | −0.0342 (19) |
| O3 | 0.125 (3) | 0.074 (2) | 0.104 (3) | −0.041 (2) | −0.011 (2) | −0.030 (2) |
| C11 | 0.067 (4) | 0.068 (3) | 0.098 (4) | −0.010 (3) | −0.020 (3) | −0.026 (3) |
| C12 | 0.085 (4) | 0.095 (4) | 0.101 (4) | −0.026 (3) | −0.011 (3) | −0.031 (3) |
| O4 | 0.116 (3) | 0.0558 (18) | 0.075 (2) | −0.0313 (18) | 0.005 (2) | −0.0225 (16) |
| O5 | 0.130 (3) | 0.0568 (17) | 0.0556 (19) | −0.0280 (17) | 0.006 (2) | −0.0264 (15) |
| C13 | 0.067 (3) | 0.055 (2) | 0.067 (3) | −0.017 (2) | −0.002 (3) | −0.027 (2) |
| C14 | 0.095 (4) | 0.085 (3) | 0.072 (3) | −0.029 (3) | 0.002 (3) | −0.047 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.256 (4) | C7—H7 | 0.9300 |

| | | | |
|---|---|---|---|
| N1—C3 | 1.367 (5) | C9—H9A | 0.9600 |
| N1—C9 | 1.454 (5) | C9—H9B | 0.9600 |
| N1—C10 | 1.458 (5) | C9—H9C | 0.9600 |
| N2—C7 | 1.273 (4) | C10—H10A | 0.9600 |
| N2—N3 | 1.388 (4) | C10—H10B | 0.9600 |
| N3—C8 | 1.344 (5) | C10—H10C | 0.9600 |
| N3—H3A | 0.897 (10) | O2—C11 | 1.243 (5) |
| N4—C8 | 1.325 (5) | O3—C11 | 1.284 (5) |
| N4—H4A | 0.87 (4) | O3—H3 | 0.8522 |
| N4—H4B | 0.91 (6) | C11—C12 | 1.496 (7) |
| C1—C2 | 1.375 (5) | C12—H12A | 0.9600 |
| C1—C6 | 1.389 (5) | C12—H12B | 0.9600 |
| C1—H1 | 0.9300 | C12—H12C | 0.9600 |
| C2—C3 | 1.401 (5) | O4—C13 | 1.203 (5) |
| C2—H2 | 0.9300 | O5—C13 | 1.331 (5) |
| C3—C4 | 1.409 (5) | O5—H5A | 0.8200 |
| C4—C5 | 1.384 (5) | C13—C14 | 1.490 (6) |
| C4—H4 | 0.9300 | C14—H14A | 0.9600 |
| C5—C6 | 1.386 (5) | C14—H14B | 0.9600 |
| C5—H5 | 0.9300 | C14—H14C | 0.9600 |
| C6—C7 | 1.455 (5) | | |
| ?···? | ? | | |
| C3—N1—C9 | 121.4 (3) | N4—C8—N3 | 118.8 (4) |
| C3—N1—C10 | 121.8 (4) | N1—C9—H9A | 109.5 |
| C9—N1—C10 | 116.4 (4) | N1—C9—H9B | 109.5 |
| C7—N2—N3 | 114.9 (3) | H9A—C9—H9B | 109.5 |
| C8—N3—N2 | 120.9 (3) | N1—C9—H9C | 109.5 |
| C8—N3—H3A | 119 (3) | H9A—C9—H9C | 109.5 |
| N2—N3—H3A | 119 (3) | H9B—C9—H9C | 109.5 |
| C8—N4—H4A | 122 (2) | N1—C10—H10A | 109.5 |
| C8—N4—H4B | 117 (4) | N1—C10—H10B | 109.5 |
| H4A—N4—H4B | 121 (4) | H10A—C10—H10B | 109.5 |
| C2—C1—C6 | 122.1 (3) | N1—C10—H10C | 109.5 |
| C2—C1—H1 | 118.9 | H10A—C10—H10C | 109.5 |
| C6—C1—H1 | 118.9 | H10B—C10—H10C | 109.5 |
| C1—C2—C3 | 121.6 (4) | C11—O3—H3 | 108.8 |
| C1—C2—H2 | 119.2 | O2—C11—O3 | 122.9 (5) |
| C3—C2—H2 | 119.2 | O2—C11—C12 | 120.9 (5) |
| N1—C3—C2 | 121.2 (4) | O3—C11—C12 | 116.3 (5) |
| N1—C3—C4 | 122.6 (3) | C11—C12—H12A | 109.5 |
| C2—C3—C4 | 116.2 (4) | C11—C12—H12B | 109.5 |
| C5—C4—C3 | 121.4 (3) | H12A—C12—H12B | 109.5 |
| C5—C4—H4 | 119.3 | C11—C12—H12C | 109.5 |
| C3—C4—H4 | 119.3 | H12A—C12—H12C | 109.5 |
| C4—C5—C6 | 121.7 (3) | H12B—C12—H12C | 109.5 |
| C4—C5—H5 | 119.2 | C13—O5—H5A | 109.5 |
| C6—C5—H5 | 119.2 | O4—C13—O5 | 122.9 (4) |
| C5—C6—C1 | 117.0 (3) | O4—C13—C14 | 125.9 (4) |

| | | | |
|---|---|---|---|
| C5—C6—C7 | 120.8 (3) | O5—C13—C14 | 111.2 (4) |
| C1—C6—C7 | 122.2 (3) | C13—C14—H14A | 109.5 |
| N2—C7—C6 | 121.7 (3) | C13—C14—H14B | 109.5 |
| N2—C7—H7 | 119.1 | H14A—C14—H14B | 109.5 |
| C6—C7—H7 | 119.1 | C13—C14—H14C | 109.5 |
| O1—C8—N4 | 122.7 (3) | H14A—C14—H14C | 109.5 |
| O1—C8—N3 | 118.5 (3) | H14B—C14—H14C | 109.5 |
| C7—N2—N3—C8 | −178.5 (4) | C3—C4—C5—C6 | 0.1 (7) |
| C6—C1—C2—C3 | −0.6 (7) | C4—C5—C6—C1 | 0.4 (6) |
| C9—N1—C3—C2 | 0.7 (7) | C4—C5—C6—C7 | −179.1 (4) |
| C10—N1—C3—C2 | −171.2 (4) | C2—C1—C6—C5 | −0.1 (6) |
| C9—N1—C3—C4 | −178.3 (4) | C2—C1—C6—C7 | 179.4 (4) |
| C10—N1—C3—C4 | 9.8 (7) | N3—N2—C7—C6 | 178.7 (4) |
| C1—C2—C3—N1 | −178.0 (4) | C5—C6—C7—N2 | 177.6 (4) |
| C1—C2—C3—C4 | 1.0 (7) | C1—C6—C7—N2 | −1.9 (6) |
| N1—C3—C4—C5 | 178.3 (4) | N2—N3—C8—O1 | 175.8 (4) |
| C2—C3—C4—C5 | −0.8 (6) | N2—N3—C8—N4 | −5.9 (6) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3···O2$^{i}$ | 0.85 | 1.82 | 2.658 (6) | 170 |
| O5—H5A···O1$^{ii}$ | 0.82 | 1.78 | 2.579 (4) | 166 |
| N4—H4A···O4$^{iii}$ | 0.87 (4) | 2.48 (4) | 3.164 (6) | 135 (3) |
| N3—H3A···O1$^{iv}$ | 0.897 (10) | 2.017 (11) | 2.913 (5) | 178 (4) |
| N4—H4B···O4$^{v}$ | 0.91 (6) | 2.16 (6) | 3.051 (6) | 166 (5) |

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

**Fig. 1**

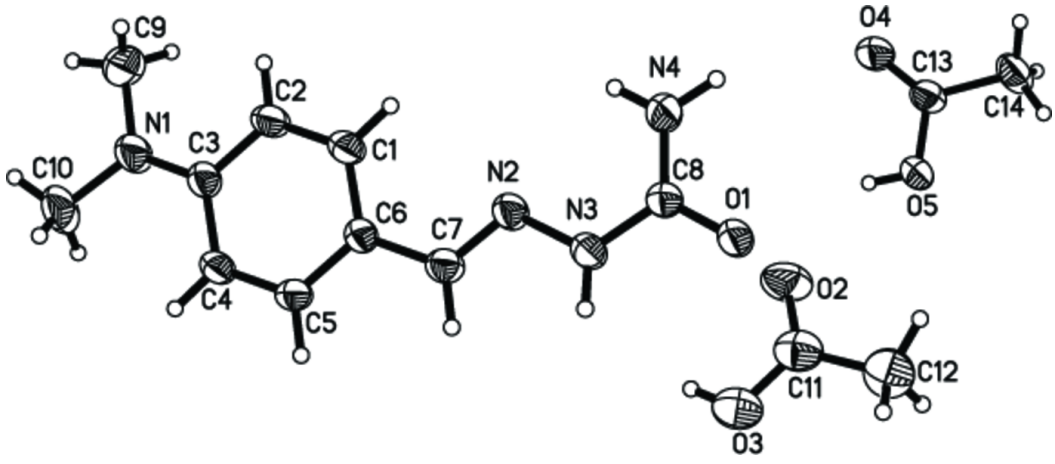
C9
N1
C10
C3
C2
C1
C6
C7
N2
N3
N4
C8
O1
C4
C5
O2
C11
C12
O3
O4
C13
C14
O5

**Fig. 2**