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5-Methyl-2-phenyl-2H-pyrazol-3-ol

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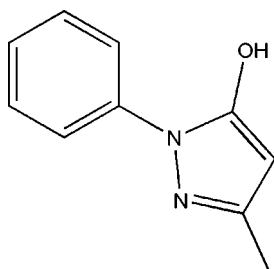
Received 28 August 2008; accepted 6 September 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 16.1.

The title compound, $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}$, known as Edaravone (MCI-186), was crystallized from methanol. The two independent molecules in the asymmetric unit are linked through an $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond. One molecule adopts a ketone form, while the other adopts an enol form. In the crystal structure, molecules are linked through intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming chains running along the b axis.

Related literature

For background to the compound, see: Watanabe *et al.* (1994); The Edaravone Acute Infarction Study Group (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}$

$M_r = 174.20$

Monoclinic, $P2_1/c$
 $a = 10.336$ (2) Å
 $b = 11.154$ (2) Å
 $c = 15.863$ (3) Å
 $\beta = 95.157$ (3)°
 $V = 1821.4$ (6) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 298$ (2) K
 $0.23 \times 0.23 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.981$, $T_{\max} = 0.983$

10551 measured reflections
 3923 independent reflections
 2894 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.106$
 $S = 1.04$
 3923 reflections
 243 parameters
 2 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-----------|-------------|-------------|---------------|
| $\text{N2}-\text{H2A}\cdots\text{N4}^i$ | 0.907 (9) | 1.904 (10) | 2.7999 (17) | 169.4 (17) |
| $\text{O2}-\text{H2B}\cdots\text{O1}$ | 0.870 (9) | 1.618 (10) | 2.4813 (15) | 170.9 (19) |

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2259).

References

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supplementary materials

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5-Methyl-2-phenyl-2*H*-pyrazol-3-ol

Q. Wang, Y. Zhang, R. Wang, Y.-L. Yang and F. Zhi

Comment

Edaravone (5-methyl-2-phenyl-2*H*-pyrazol-3-ol, MCI-186) is a free-radical scavenger that was approved by the Ministry of Health, Labor, and Welfare of Japan in 2001, and is now widely used for the treatment of acute cerebral infarction (Watanabe *et al.*, 1994; The Edaravone Acute Infarction Study Group, 2003). We report in this paper the crystal structure of the compound, (I).

The compound consists of two independent molecules (Fig. 1), which are linked through an intramolecular O2—H2B···O1 hydrogen bond (Table 1). One molecule adopts a ketone form, while the other adopts an enol form. In the ketone molecule, the dihedral angle between the C1—C6 benzene ring and the N1/N2/C9/C8/C7 ring is 22.9 (2)°. In the enol molecule, the dihedral angle between the C11—C16 benzene ring and the N3/N4/C19/C18/C17 ring is 34.3 (2)°. In the compound, all the bond lengths are within normal ranges (Allen *et al.*, 1987). The bond length of C17—O2 [1.325 (2) Å] is longer than that of C7—O1 [1.260 (2) Å], which is caused by the enol form.

In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains running along the *b* axis (Fig. 2).

Experimental

The crystal of the compound was recrystallized by edaravone in methanol.

Refinement

H2A and H2B were located in a difference Fourier map and refined isotropically, with N—H and O—H distances restrained to 0.90 (1) and 0.85 (1) Å, and with $U_{\text{iso}}(\text{H})$ set to 0.08 Å². Other H atoms were constrained to idealized geometries, with C—H = 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H})$ set to 1.2 $U_{\text{eq}}(\text{C})$ and 1.5 $U_{\text{eq}}(\text{methyl C})$.

Figures

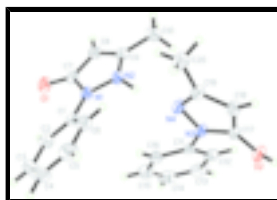


Fig. 1. The structure of (I) at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

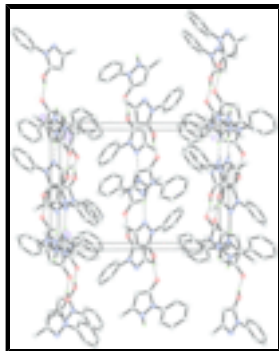


Fig. 2. Molecular packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

5-Methyl-2-phenyl-2*H*-pyrazol-3-ol

Crystal data

$C_{10}H_{10}N_2O$

$M_r = 174.20$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.336$ (2) Å

$b = 11.154$ (2) Å

$c = 15.863$ (3) Å

$\beta = 95.157$ (3)°

$V = 1821.4$ (6) Å³

$Z = 8$

$F_{000} = 736$

$D_x = 1.271$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3931 reflections

$\theta = 2.3$ – 29.0 °

$\mu = 0.09$ mm⁻¹

$T = 298$ (2) K

Block, colorless

$0.23 \times 0.23 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

ω scan

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.981$, $T_{\max} = 0.983$

10551 measured reflections

3923 independent reflections

2894 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 27.0$ °

$\theta_{\min} = 2.2$ °

$h = -13 \rightarrow 11$

$k = -13 \rightarrow 14$

$l = -20 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.106$

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

$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.3053P]$

| | |
|--|--|
| $S = 1.04$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3923 reflections | $(\Delta/\sigma)_{\max} < 0.001$ |
| 243 parameters | $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$ |
| 2 restraints | $\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: SHELXL, $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ Extinction coefficient: 0.0087 (12) |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|---------------|----------------------------------|
| O1 | 0.76081 (11) | 0.23408 (9) | 0.09473 (8) | 0.0652 (3) |
| O2 | 0.63865 (11) | 0.42520 (9) | 0.07652 (7) | 0.0577 (3) |
| N1 | 0.80235 (11) | 0.03414 (9) | 0.07061 (8) | 0.0469 (3) |
| N2 | 0.76341 (13) | -0.04917 (10) | 0.00921 (8) | 0.0516 (3) |
| N3 | 0.69321 (11) | 0.62596 (9) | 0.06745 (7) | 0.0418 (3) |
| N4 | 0.76998 (12) | 0.70070 (10) | 0.02382 (8) | 0.0490 (3) |
| C1 | 0.91015 (13) | 0.01075 (12) | 0.12978 (9) | 0.0457 (3) |
| C2 | 0.92942 (16) | 0.07840 (15) | 0.20276 (10) | 0.0603 (4) |
| H2 | 0.8722 | 0.1399 | 0.2131 | 0.072* |
| C3 | 1.03427 (19) | 0.05375 (19) | 0.26009 (12) | 0.0768 (5) |
| H3 | 1.0481 | 0.0997 | 0.3090 | 0.092* |
| C4 | 1.1181 (2) | -0.0372 (2) | 0.24600 (13) | 0.0814 (6) |
| H4 | 1.1881 | -0.0536 | 0.2853 | 0.098* |
| C5 | 1.09872 (17) | -0.10395 (18) | 0.17403 (14) | 0.0755 (5) |
| H5 | 1.1557 | -0.1661 | 0.1647 | 0.091* |
| C6 | 0.99550 (15) | -0.08041 (15) | 0.11475 (11) | 0.0597 (4) |
| H6 | 0.9837 | -0.1255 | 0.0653 | 0.072* |
| C7 | 0.73814 (14) | 0.14046 (12) | 0.05144 (10) | 0.0486 (4) |
| C8 | 0.65398 (16) | 0.11675 (14) | -0.02083 (10) | 0.0566 (4) |
| H8 | 0.5970 | 0.1713 | -0.0486 | 0.068* |
| C9 | 0.66976 (15) | 0.00076 (14) | -0.04331 (10) | 0.0536 (4) |
| C10 | 0.6047 (2) | -0.07170 (17) | -0.11335 (11) | 0.0760 (5) |
| H10A | 0.6586 | -0.0744 | -0.1596 | 0.114* |
| H10B | 0.5227 | -0.0359 | -0.1321 | 0.114* |

supplementary materials

| | | | | |
|------|--------------|--------------|---------------|------------|
| H10C | 0.5908 | -0.1517 | -0.0937 | 0.114* |
| C11 | 0.61818 (14) | 0.67394 (12) | 0.12999 (8) | 0.0441 (3) |
| C12 | 0.49765 (15) | 0.62664 (14) | 0.14196 (10) | 0.0545 (4) |
| H12 | 0.4655 | 0.5611 | 0.1104 | 0.065* |
| C13 | 0.42556 (18) | 0.67832 (19) | 0.20167 (12) | 0.0755 (6) |
| H13 | 0.3450 | 0.6462 | 0.2108 | 0.091* |
| C14 | 0.4708 (2) | 0.7760 (2) | 0.24752 (12) | 0.0860 (7) |
| H14 | 0.4205 | 0.8110 | 0.2866 | 0.103* |
| C15 | 0.5904 (2) | 0.82150 (17) | 0.23553 (11) | 0.0799 (6) |
| H15 | 0.6213 | 0.8876 | 0.2669 | 0.096* |
| C16 | 0.66614 (18) | 0.77067 (13) | 0.17737 (10) | 0.0584 (4) |
| H16 | 0.7482 | 0.8012 | 0.1703 | 0.070* |
| C17 | 0.70530 (13) | 0.51085 (11) | 0.04194 (9) | 0.0430 (3) |
| C18 | 0.79096 (15) | 0.51055 (13) | -0.01882 (10) | 0.0526 (4) |
| H18 | 0.8190 | 0.4445 | -0.0479 | 0.063* |
| C19 | 0.82756 (15) | 0.62954 (13) | -0.02813 (10) | 0.0510 (4) |
| C20 | 0.91583 (19) | 0.68181 (17) | -0.08846 (13) | 0.0794 (6) |
| H20A | 0.9060 | 0.7674 | -0.0900 | 0.119* |
| H20B | 0.8938 | 0.6496 | -0.1440 | 0.119* |
| H20C | 1.0042 | 0.6619 | -0.0700 | 0.119* |
| H2A | 0.7692 (17) | -0.1287 (9) | 0.0208 (11) | 0.080* |
| H2B | 0.6823 (16) | 0.3585 (12) | 0.0773 (12) | 0.080* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|-------------|
| O1 | 0.0757 (7) | 0.0322 (5) | 0.0864 (8) | 0.0043 (5) | -0.0001 (6) | -0.0043 (5) |
| O2 | 0.0673 (7) | 0.0311 (5) | 0.0772 (7) | 0.0007 (5) | 0.0205 (6) | 0.0059 (5) |
| N1 | 0.0531 (7) | 0.0283 (6) | 0.0577 (7) | 0.0011 (5) | -0.0031 (6) | 0.0011 (5) |
| N2 | 0.0640 (8) | 0.0310 (6) | 0.0581 (7) | 0.0018 (5) | -0.0030 (6) | 0.0012 (5) |
| N3 | 0.0493 (6) | 0.0298 (6) | 0.0476 (6) | 0.0024 (5) | 0.0114 (5) | 0.0017 (5) |
| N4 | 0.0588 (8) | 0.0324 (6) | 0.0582 (7) | -0.0021 (5) | 0.0185 (6) | 0.0015 (5) |
| C1 | 0.0456 (8) | 0.0362 (7) | 0.0551 (8) | -0.0040 (6) | 0.0031 (6) | 0.0098 (6) |
| C2 | 0.0646 (10) | 0.0555 (10) | 0.0603 (10) | -0.0023 (8) | 0.0035 (8) | 0.0003 (8) |
| C3 | 0.0793 (13) | 0.0876 (14) | 0.0607 (11) | -0.0113 (11) | -0.0084 (9) | 0.0024 (10) |
| C4 | 0.0653 (12) | 0.1020 (16) | 0.0736 (12) | -0.0004 (11) | -0.0122 (10) | 0.0206 (12) |
| C5 | 0.0569 (10) | 0.0769 (12) | 0.0919 (14) | 0.0161 (9) | 0.0016 (10) | 0.0187 (11) |
| C6 | 0.0567 (9) | 0.0531 (9) | 0.0687 (10) | 0.0082 (7) | 0.0024 (8) | 0.0050 (8) |
| C7 | 0.0513 (8) | 0.0310 (7) | 0.0640 (9) | 0.0023 (6) | 0.0082 (7) | 0.0075 (7) |
| C8 | 0.0597 (9) | 0.0453 (9) | 0.0635 (10) | 0.0101 (7) | -0.0019 (8) | 0.0127 (7) |
| C9 | 0.0599 (9) | 0.0477 (9) | 0.0523 (8) | 0.0013 (7) | -0.0006 (7) | 0.0069 (7) |
| C10 | 0.0886 (13) | 0.0739 (12) | 0.0622 (10) | -0.0045 (10) | -0.0120 (9) | -0.0032 (9) |
| C11 | 0.0544 (8) | 0.0339 (7) | 0.0447 (7) | 0.0122 (6) | 0.0093 (6) | 0.0067 (6) |
| C12 | 0.0524 (9) | 0.0531 (9) | 0.0586 (9) | 0.0130 (7) | 0.0090 (7) | 0.0135 (7) |
| C13 | 0.0686 (11) | 0.0872 (14) | 0.0749 (12) | 0.0326 (10) | 0.0304 (9) | 0.0286 (11) |
| C14 | 0.1171 (18) | 0.0853 (15) | 0.0612 (11) | 0.0533 (13) | 0.0383 (12) | 0.0143 (11) |
| C15 | 0.1298 (18) | 0.0540 (11) | 0.0579 (10) | 0.0258 (11) | 0.0198 (11) | -0.0063 (8) |
| C16 | 0.0812 (11) | 0.0414 (8) | 0.0537 (9) | 0.0066 (8) | 0.0121 (8) | -0.0019 (7) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|-------------|
| C17 | 0.0495 (8) | 0.0285 (6) | 0.0511 (7) | 0.0027 (6) | 0.0048 (6) | 0.0015 (6) |
| C18 | 0.0622 (9) | 0.0379 (8) | 0.0597 (9) | 0.0065 (7) | 0.0166 (7) | -0.0068 (7) |
| C19 | 0.0538 (8) | 0.0432 (8) | 0.0580 (9) | 0.0022 (6) | 0.0163 (7) | -0.0002 (7) |
| C20 | 0.0868 (13) | 0.0683 (12) | 0.0901 (13) | -0.0032 (10) | 0.0467 (11) | 0.0008 (10) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|---------------|-------------|
| O1—C7 | 1.260 (2) | C8—C9 | 1.356 (2) |
| O2—C17 | 1.325 (2) | C8—H8 | 0.9300 |
| O2—H2B | 0.870 (9) | C9—C10 | 1.485 (2) |
| N1—C7 | 1.379 (2) | C10—H10A | 0.9600 |
| N1—N2 | 1.380 (2) | C10—H10B | 0.9600 |
| N1—C1 | 1.415 (2) | C10—H10C | 0.9600 |
| N2—C9 | 1.340 (2) | C11—C16 | 1.381 (2) |
| N2—H2A | 0.907 (9) | C11—C12 | 1.382 (2) |
| N3—C17 | 1.355 (2) | C12—C13 | 1.383 (2) |
| N3—N4 | 1.379 (2) | C12—H12 | 0.9300 |
| N3—C11 | 1.418 (2) | C13—C14 | 1.369 (3) |
| N4—C19 | 1.323 (2) | C13—H13 | 0.9300 |
| C1—C6 | 1.381 (2) | C14—C15 | 1.365 (3) |
| C1—C2 | 1.381 (2) | C14—H14 | 0.9300 |
| C2—C3 | 1.378 (2) | C15—C16 | 1.384 (2) |
| C2—H2 | 0.9300 | C15—H15 | 0.9300 |
| C3—C4 | 1.366 (3) | C16—H16 | 0.9300 |
| C3—H3 | 0.9300 | C17—C18 | 1.366 (2) |
| C4—C5 | 1.362 (3) | C18—C19 | 1.392 (2) |
| C4—H4 | 0.9300 | C18—H18 | 0.9300 |
| C5—C6 | 1.383 (2) | C19—C20 | 1.498 (2) |
| C5—H5 | 0.9300 | C20—H20A | 0.9600 |
| C6—H6 | 0.9300 | C20—H20B | 0.9600 |
| C7—C8 | 1.400 (2) | C20—H20C | 0.9600 |
| C17—O2—H2B | 109.5 (13) | C9—C10—H10B | 109.5 |
| C7—N1—N2 | 108.62 (11) | H10A—C10—H10B | 109.5 |
| C7—N1—C1 | 129.74 (12) | C9—C10—H10C | 109.5 |
| N2—N1—C1 | 120.42 (11) | H10A—C10—H10C | 109.5 |
| C9—N2—N1 | 107.91 (11) | H10B—C10—H10C | 109.5 |
| C9—N2—H2A | 124.3 (11) | C16—C11—C12 | 120.50 (14) |
| N1—N2—H2A | 120.4 (12) | C16—C11—N3 | 118.91 (13) |
| C17—N3—N4 | 110.49 (11) | C12—C11—N3 | 120.57 (13) |
| C17—N3—C11 | 129.60 (11) | C11—C12—C13 | 118.88 (17) |
| N4—N3—C11 | 119.90 (10) | C11—C12—H12 | 120.6 |
| C19—N4—N3 | 105.14 (11) | C13—C12—H12 | 120.6 |
| C6—C1—C2 | 120.05 (14) | C14—C13—C12 | 121.09 (19) |
| C6—C1—N1 | 119.90 (13) | C14—C13—H13 | 119.5 |
| C2—C1—N1 | 120.05 (13) | C12—C13—H13 | 119.5 |
| C3—C2—C1 | 119.32 (17) | C15—C14—C13 | 119.52 (17) |
| C3—C2—H2 | 120.3 | C15—C14—H14 | 120.2 |
| C1—C2—H2 | 120.3 | C13—C14—H14 | 120.2 |
| C4—C3—C2 | 120.86 (18) | C14—C15—C16 | 120.93 (19) |

supplementary materials

| | | | |
|-------------|-------------|---------------|-------------|
| C4—C3—H3 | 119.6 | C14—C15—H15 | 119.5 |
| C2—C3—H3 | 119.6 | C16—C15—H15 | 119.5 |
| C5—C4—C3 | 119.69 (17) | C11—C16—C15 | 119.06 (18) |
| C5—C4—H4 | 120.2 | C11—C16—H16 | 120.5 |
| C3—C4—H4 | 120.2 | C15—C16—H16 | 120.5 |
| C4—C5—C6 | 120.84 (18) | O2—C17—N3 | 119.60 (12) |
| C4—C5—H5 | 119.6 | O2—C17—C18 | 133.19 (13) |
| C6—C5—H5 | 119.6 | N3—C17—C18 | 107.21 (12) |
| C1—C6—C5 | 119.23 (17) | C17—C18—C19 | 105.80 (12) |
| C1—C6—H6 | 120.4 | C17—C18—H18 | 127.1 |
| C5—C6—H6 | 120.4 | C19—C18—H18 | 127.1 |
| O1—C7—N1 | 122.01 (13) | N4—C19—C18 | 111.36 (13) |
| O1—C7—C8 | 132.37 (13) | N4—C19—C20 | 119.87 (13) |
| N1—C7—C8 | 105.62 (12) | C18—C19—C20 | 128.74 (14) |
| C9—C8—C7 | 108.35 (13) | C19—C20—H20A | 109.5 |
| C9—C8—H8 | 125.8 | C19—C20—H20B | 109.5 |
| C7—C8—H8 | 125.8 | H20A—C20—H20B | 109.5 |
| N2—C9—C8 | 109.29 (14) | C19—C20—H20C | 109.5 |
| N2—C9—C10 | 119.47 (14) | H20A—C20—H20C | 109.5 |
| C8—C9—C10 | 131.23 (15) | H20B—C20—H20C | 109.5 |
| C9—C10—H10A | 109.5 | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|-----------|-------------|-------------|---------------|
| N2—H2A \cdots N4 ⁱ | 0.907 (9) | 1.904 (10) | 2.7999 (17) | 169.4 (17) |
| O2—H2B \cdots O1 | 0.870 (9) | 1.618 (10) | 2.4813 (15) | 170.9 (19) |

Symmetry codes: (i) $x, y-1, z$.

Fig. 1

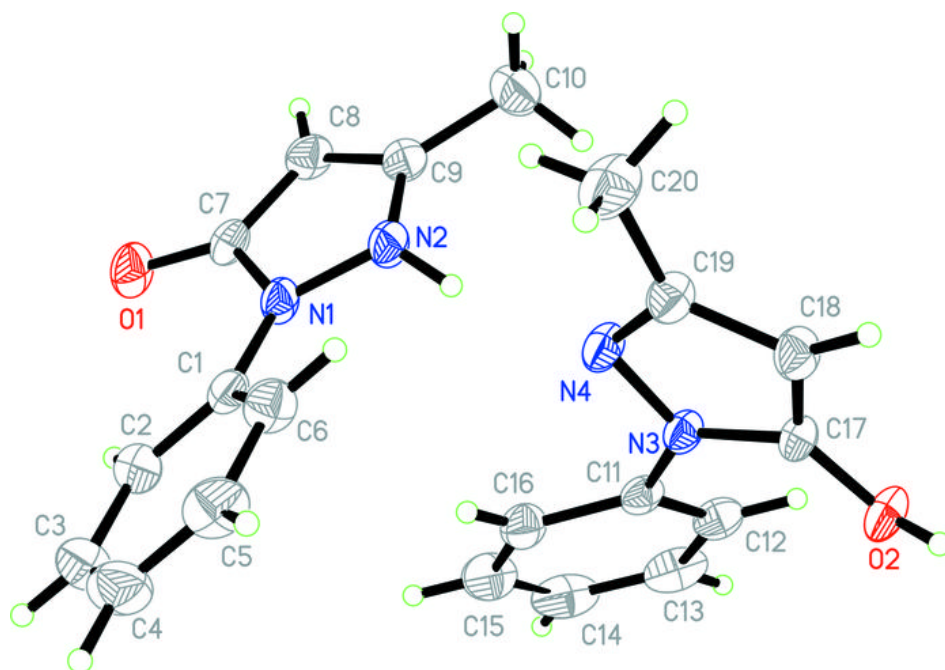


Fig. 2

