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# Diethyl 4-(4-cyanophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

**Peng Zhang and Weiqun Zhu***

School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China
Correspondence e-mail: zhuwq@sdu.edu.cn

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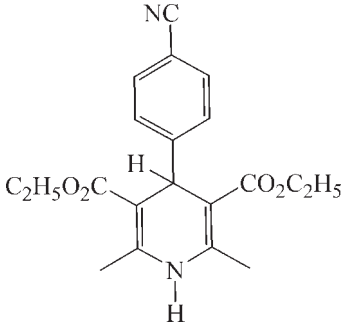
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.051; $wR$ factor = 0.162; data-to-parameter ratio = 13.2.

In the title compound, $C_{20}H_{22}N_2O_4$, the dihedral angle between the roughly planar dihydropyridine ring (r.m.s. deviation = 0.092 Å) and the benzene ring is 87.09 (6)°. One of the ethoxy side chains is disordered over two orientations in a 0.669 (14):0.331 (14) ratio. In the crystal, molecules are linked by N—H···N hydrogen bonds, generating chains.

## Related literature

For general background to dihydropyridine derivatives, see: Gaudio *et al.* (1994).




## Experimental

### Crystal data

$C_{20}H_{22}N_2O_4$
$M_r$ = 354.40
Monoclinic, $P2_1/n$
$a$ = 10.4596 (13) Å
$b$ = 9.5117 (12) Å
$c$ = 19.160 (2) Å
$\beta$ = 91.493 (1)°
$V$ = 1905.6 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.12 × 0.10 × 0.08 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.990, $T_{max}$ = 0.993
10000 measured reflections
3298 independent reflections
2408 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.162
$S$ = 1.02
3298 reflections
249 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···N1$^{i}$ | 0.86 | 2.32 | 3.098 (3) | 150 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5444).

## References

Bruker (2001). *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gaudio, A. C., Korolkovas, A. & Takahata, Y. (1994). *J. Pharm. Sci. A*, **83**, 1110–1115.
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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1424 [ **doi:10.1107/S1600536810018155** ]

# Diethyl 4-(4-cyanophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

**P. Zhang and W. Zhu**

## Comment

The synthesis of 1,4-dihydropyridine derivatives has attracted continuous research interest due to various vasodilator, anti-hypertensive, bronchodilator, heptaprotective, anti-tumor, anti-mutagenic, geroprotective and anti-diabetic agents (Gaudio *et al.*, 1994). Here, we describe the recystallization and structural characterization of the title compound.

The molecular structure is shown in Fig 1. The dihedral angle between the two rings is 87.09 (6) °. The mean devation of the dihydropyridine plane is 0.0824 Å. The intermolecular hydrogen bonding of N2—H2···N1 leads to a consolidation of the structure (Fig. 2; Table 1).

## Experimental

Diethyl 2,6-dimethyl-4-(4-cyanophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (1 mmol 0.39 g) was dissolved in 20 ml ethanol was evaporated in one open flask at room temperature. One week later, yellow blocks of (I) were obained. Anal. $C_{20}H_{22}N_2O_4$: C, 67.72; H, 5.64; N, 7.90 %. Found: C, 67.56; H, 5.46; N, 7.61 %.

## Refinement

All hydrogen atoms bound to aromatic carbon atoms were refined in calculated positions using a riding model with a C—H distance of 0.93 Å and $U_{iso}$ = 1.2$U_{eq}$(C). Hydrogen atoms attached to aromatic N atoms were refined with a N—H distance of 0.86 Å and $U_{iso}$ = 1.2$U_{eq}$(N).

## Figures

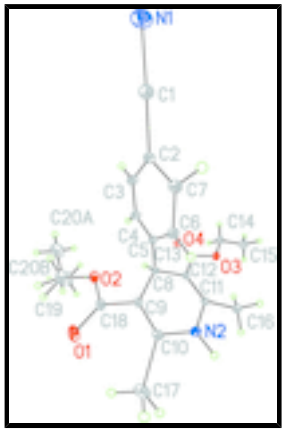


Fig. 1. The molecular structure of (I) showing displacement ellipsoids drawn at the 30% probability level.

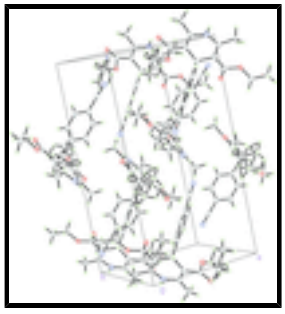

Fig. 2. The crystal packing of (I), displayed with N—H···N hydrogen bonds as dashed lines.

**Diethyl 4-(4-cyanophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate**

*Crystal data*

| | |
|---|---|
| $C_{20}H_{22}N_2O_4$ | $F(000) = 752$ |
| $M_r = 354.40$ | $D_x = 1.235$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 3532 reflections |
| $a = 10.4596$ (13) Å | $\theta = 2.4$–$25.9°$ |
| $b = 9.5117$ (12) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 19.160$ (2) Å | $T = 296$ K |
| $\beta = 91.493$ (1)° | Block, colorless |
| $V = 1905.6$ (4) Å$^3$ | 0.12 × 0.10 × 0.08 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 3298 independent reflections |
| Radiation source: fine-focus sealed tube | 2408 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.020$ |
| phi and ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2001) | $h = -12 \rightarrow 10$ |
| $T_{min} = 0.990$, $T_{max} = 0.993$ | $k = -9 \rightarrow 11$ |
| 10000 measured reflections | $l = -22 \rightarrow 22$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.051$ | H-atom parameters constrained |
| $wR(F^2) = 0.162$ | $w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 0.6251P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3298 reflections | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |

| | |
|---|---|
| 249 parameters | $\Delta\rho_{min} = -0.28$ e Å$^{-3}$ |
| 2 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: 0.012 (2) |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.5366 (2) | 0.1062 (3) | 0.32734 (12) | 0.0574 (6) | |
| C2 | 0.4507 (2) | 0.0690 (2) | 0.27004 (10) | 0.0483 (5) | |
| C3 | 0.3890 (2) | −0.0596 (3) | 0.26959 (12) | 0.0607 (6) | |
| H3 | 0.4024 | −0.1222 | 0.3063 | 0.073* | |
| C4 | 0.3078 (2) | −0.0948 (2) | 0.21466 (12) | 0.0573 (6) | |
| H4 | 0.2670 | −0.1817 | 0.2145 | 0.069* | |
| C5 | 0.28599 (19) | −0.0030 (2) | 0.15987 (10) | 0.0419 (5) | |
| C6 | 0.3497 (2) | 0.1239 (2) | 0.16056 (12) | 0.0535 (6) | |
| H6 | 0.3378 | 0.1854 | 0.1233 | 0.064* | |
| C7 | 0.4306 (2) | 0.1614 (2) | 0.21529 (12) | 0.0552 (6) | |
| H7 | 0.4713 | 0.2483 | 0.2154 | 0.066* | |
| C8 | 0.19219 (19) | −0.0393 (2) | 0.09975 (11) | 0.0444 (5) | |
| H8 | 0.1533 | −0.1305 | 0.1098 | 0.053* | |
| C9 | 0.2616 (2) | −0.0512 (2) | 0.03111 (12) | 0.0507 (6) | |
| C10 | 0.2559 (2) | 0.0529 (3) | −0.01647 (11) | 0.0528 (6) | |
| C11 | 0.08375 (19) | 0.1693 (2) | 0.04492 (10) | 0.0445 (5) | |
| C12 | 0.08624 (18) | 0.0706 (2) | 0.09551 (10) | 0.0425 (5) | |
| C13 | −0.0033 (2) | 0.0607 (2) | 0.15302 (12) | 0.0490 (5) | |
| C14 | −0.1644 (3) | 0.1750 (3) | 0.21848 (15) | 0.0738 (8) | |
| H14A | −0.1152 | 0.1750 | 0.2621 | 0.089* | |
| H14B | −0.2190 | 0.0925 | 0.2175 | 0.089* | |
| C15 | −0.2415 (3) | 0.3012 (3) | 0.2130 (2) | 0.0980 (11) | |
| H15A | −0.1871 | 0.3823 | 0.2168 | 0.147* | |
| H15B | −0.3019 | 0.3025 | 0.2498 | 0.147* | |
| H15C | −0.2864 | 0.3024 | 0.1687 | 0.147* | |
| C16 | −0.0089 (2) | 0.2888 (3) | 0.03443 (13) | 0.0586 (6) | |
| H16A | −0.0883 | 0.2659 | 0.0557 | 0.088* | |
| H16B | −0.0235 | 0.3045 | −0.0146 | 0.088* | |

| | | | | | |
|---|---|---|---|---|---|
| H16C | 0.0261 | 0.3724 | 0.0555 | 0.088* | |
| C17 | 0.3287 (3) | 0.0650 (4) | −0.08253 (13) | 0.0756 (8) | |
| H17A | 0.4001 | 0.1272 | −0.0752 | 0.113* | |
| H17B | 0.2735 | 0.1017 | −0.1190 | 0.113* | |
| H17C | 0.3592 | −0.0261 | −0.0958 | 0.113* | |
| C18 | 0.3377 (2) | −0.1776 (3) | 0.01887 (15) | 0.0676 (7) | |
| C19 | 0.3950 (6) | −0.3990 (5) | 0.0605 (3) | 0.158 (2) | |
| H19A | 0.3515 | −0.4556 | 0.0251 | 0.190* | 0.669 (14) |
| H19B | 0.4793 | −0.3765 | 0.0437 | 0.190* | 0.669 (14) |
| H19C | 0.4473 | −0.3909 | 0.0196 | 0.190* | 0.331 (14) |
| H19D | 0.4514 | −0.4147 | 0.1007 | 0.190* | 0.331 (14) |
| C20A | 0.4079 (13) | −0.4759 (9) | 0.1207 (5) | 0.185 (6) | 0.669 (14) |
| H20A | 0.4549 | −0.5603 | 0.1116 | 0.278* | 0.669 (14) |
| H20B | 0.3248 | −0.4999 | 0.1371 | 0.278* | 0.669 (14) |
| H20C | 0.4530 | −0.4213 | 0.1556 | 0.278* | 0.669 (14) |
| C20B | 0.3114 (12) | −0.5133 (12) | 0.0522 (12) | 0.141 (9) | 0.331 (14) |
| H20D | 0.3600 | −0.5980 | 0.0467 | 0.212* | 0.331 (14) |
| H20E | 0.2573 | −0.4988 | 0.0116 | 0.212* | 0.331 (14) |
| H20F | 0.2598 | −0.5213 | 0.0927 | 0.212* | 0.331 (14) |
| N1 | 0.6066 (2) | 0.1329 (3) | 0.37179 (12) | 0.0765 (7) | |
| N2 | 0.17490 (18) | 0.1647 (2) | −0.00618 (9) | 0.0534 (5) | |
| H2 | 0.1813 | 0.2363 | −0.0333 | 0.064* | |
| O1 | 0.4059 (2) | −0.2026 (3) | −0.02939 (13) | 0.1062 (8) | |
| O2 | 0.3246 (2) | −0.2705 (2) | 0.06982 (13) | 0.0967 (7) | |
| O3 | −0.07949 (16) | 0.17231 (17) | 0.16008 (9) | 0.0641 (5) | |
| O4 | −0.00600 (19) | −0.0369 (2) | 0.19268 (11) | 0.0824 (6) | |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0631 (14) | 0.0625 (15) | 0.0467 (13) | 0.0055 (12) | −0.0004 (11) | −0.0063 (11) |
| C2 | 0.0482 (12) | 0.0555 (13) | 0.0413 (11) | 0.0057 (10) | −0.0013 (9) | −0.0061 (9) |
| C3 | 0.0722 (15) | 0.0591 (15) | 0.0503 (13) | −0.0007 (12) | −0.0094 (12) | 0.0147 (11) |
| C4 | 0.0642 (14) | 0.0456 (13) | 0.0617 (14) | −0.0084 (11) | −0.0080 (11) | 0.0095 (10) |
| C5 | 0.0410 (10) | 0.0396 (11) | 0.0452 (11) | 0.0051 (9) | 0.0025 (8) | −0.0017 (8) |
| C6 | 0.0648 (14) | 0.0462 (13) | 0.0489 (12) | −0.0052 (11) | −0.0103 (11) | 0.0075 (10) |
| C7 | 0.0603 (13) | 0.0466 (12) | 0.0582 (13) | −0.0064 (11) | −0.0068 (11) | −0.0006 (10) |
| C8 | 0.0446 (11) | 0.0371 (11) | 0.0513 (12) | −0.0006 (9) | −0.0025 (9) | −0.0032 (9) |
| C9 | 0.0453 (12) | 0.0539 (13) | 0.0525 (12) | 0.0024 (10) | −0.0052 (10) | −0.0144 (10) |
| C10 | 0.0461 (12) | 0.0658 (15) | 0.0464 (12) | −0.0015 (11) | −0.0022 (9) | −0.0127 (11) |
| C11 | 0.0433 (11) | 0.0461 (12) | 0.0436 (11) | 0.0011 (9) | −0.0056 (9) | −0.0029 (9) |
| C12 | 0.0398 (11) | 0.0418 (11) | 0.0456 (11) | −0.0011 (9) | −0.0029 (9) | −0.0042 (9) |
| C13 | 0.0465 (12) | 0.0448 (12) | 0.0557 (12) | −0.0004 (10) | 0.0026 (10) | 0.0015 (10) |
| C14 | 0.0735 (17) | 0.0753 (18) | 0.0740 (17) | 0.0031 (14) | 0.0293 (14) | −0.0027 (14) |
| C15 | 0.088 (2) | 0.074 (2) | 0.135 (3) | 0.0022 (16) | 0.058 (2) | −0.0069 (19) |
| C16 | 0.0624 (14) | 0.0569 (14) | 0.0562 (13) | 0.0106 (11) | −0.0044 (11) | 0.0070 (11) |
| C17 | 0.0687 (16) | 0.106 (2) | 0.0526 (14) | 0.0028 (15) | 0.0107 (12) | −0.0091 (14) |
| C18 | 0.0628 (15) | 0.0681 (17) | 0.0715 (17) | 0.0159 (13) | −0.0080 (13) | −0.0218 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.203 (5) | 0.090 (3) | 0.183 (5) | 0.084 (4) | 0.027 (4) | −0.008 (3) |
| C20A | 0.279 (14) | 0.093 (5) | 0.186 (9) | 0.083 (7) | 0.039 (9) | 0.046 (6) |
| C20B | 0.128 (12) | 0.070 (9) | 0.23 (2) | 0.017 (7) | 0.035 (12) | 0.030 (10) |
| N1 | 0.0915 (16) | 0.0847 (16) | 0.0522 (12) | −0.0014 (13) | −0.0187 (12) | −0.0122 (11) |
| N2 | 0.0585 (11) | 0.0569 (11) | 0.0450 (10) | 0.0036 (9) | 0.0028 (8) | 0.0062 (8) |
| O1 | 0.1042 (16) | 0.1076 (18) | 0.1084 (17) | 0.0390 (14) | 0.0303 (14) | −0.0284 (14) |
| O2 | 0.1248 (18) | 0.0670 (13) | 0.0989 (16) | 0.0474 (13) | 0.0125 (13) | −0.0023 (12) |
| O3 | 0.0684 (10) | 0.0557 (10) | 0.0694 (11) | 0.0101 (8) | 0.0264 (9) | 0.0053 (8) |
| O4 | 0.0811 (13) | 0.0715 (12) | 0.0963 (14) | 0.0160 (10) | 0.0341 (11) | 0.0318 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.137 (3) | C14—H14A | 0.9700 |
| C1—C2 | 1.444 (3) | C14—H14B | 0.9700 |
| C2—C7 | 1.380 (3) | C15—H15A | 0.9600 |
| C2—C3 | 1.383 (3) | C15—H15B | 0.9600 |
| C3—C4 | 1.377 (3) | C15—H15C | 0.9600 |
| C3—H3 | 0.9300 | C16—H16A | 0.9600 |
| C4—C5 | 1.380 (3) | C16—H16B | 0.9600 |
| C4—H4 | 0.9300 | C16—H16C | 0.9600 |
| C5—C6 | 1.378 (3) | C17—H17A | 0.9600 |
| C5—C8 | 1.533 (3) | C17—H17B | 0.9600 |
| C6—C7 | 1.377 (3) | C17—H17C | 0.9600 |
| C6—H6 | 0.9300 | C18—O1 | 1.206 (3) |
| C7—H7 | 0.9300 | C18—O2 | 1.326 (4) |
| C8—C9 | 1.523 (3) | C19—C20A | 1.370 (8) |
| C8—C12 | 1.524 (3) | C19—C20B | 1.401 (9) |
| C8—H8 | 0.9800 | C19—O2 | 1.440 (4) |
| C9—C10 | 1.346 (3) | C19—H19A | 0.9700 |
| C9—C18 | 1.464 (3) | C19—H19B | 0.9700 |
| C10—N2 | 1.377 (3) | C19—H19C | 0.9700 |
| C10—C17 | 1.499 (3) | C19—H19D | 0.9700 |
| C11—C12 | 1.349 (3) | C20A—H20A | 0.9600 |
| C11—N2 | 1.385 (3) | C20A—H20B | 0.9600 |
| C11—C16 | 1.504 (3) | C20A—H20C | 0.9600 |
| C12—C13 | 1.467 (3) | C20B—H20D | 0.9600 |
| C13—O4 | 1.201 (3) | C20B—H20E | 0.9600 |
| C13—O3 | 1.336 (3) | C20B—H20F | 0.9600 |
| C14—O3 | 1.447 (3) | N2—H2 | 0.8600 |
| C14—C15 | 1.448 (4) | | |
| N1—C1—C2 | 178.1 (3) | H15B—C15—H15C | 109.5 |
| C7—C2—C3 | 119.8 (2) | C11—C16—H16A | 109.5 |
| C7—C2—C1 | 120.1 (2) | C11—C16—H16B | 109.5 |
| C3—C2—C1 | 120.1 (2) | H16A—C16—H16B | 109.5 |
| C4—C3—C2 | 119.9 (2) | C11—C16—H16C | 109.5 |
| C4—C3—H3 | 120.0 | H16A—C16—H16C | 109.5 |
| C2—C3—H3 | 120.0 | H16B—C16—H16C | 109.5 |
| C3—C4—C5 | 120.9 (2) | C10—C17—H17A | 109.5 |
| C3—C4—H4 | 119.5 | C10—C17—H17B | 109.5 |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 119.5 | H17A—C17—H17B | 109.5 |
| C6—C5—C4 | 118.5 (2) | C10—C17—H17C | 109.5 |
| C6—C5—C8 | 120.27 (18) | H17A—C17—H17C | 109.5 |
| C4—C5—C8 | 121.25 (19) | H17B—C17—H17C | 109.5 |
| C7—C6—C5 | 121.4 (2) | O1—C18—O2 | 120.5 (3) |
| C7—C6—H6 | 119.3 | O1—C18—C9 | 128.2 (3) |
| C5—C6—H6 | 119.3 | O2—C18—C9 | 111.2 (2) |
| C6—C7—C2 | 119.5 (2) | C20A—C19—C20B | 74.2 (9) |
| C6—C7—H7 | 120.3 | C20A—C19—O2 | 112.8 (5) |
| C2—C7—H7 | 120.3 | C20B—C19—O2 | 110.7 (7) |
| C9—C8—C12 | 111.57 (17) | C20A—C19—H19A | 109.0 |
| C9—C8—C5 | 110.82 (16) | O2—C19—H19A | 109.0 |
| C12—C8—C5 | 109.63 (16) | C20A—C19—H19B | 109.0 |
| C9—C8—H8 | 108.2 | C20B—C19—H19B | 134.7 |
| C12—C8—H8 | 108.2 | O2—C19—H19B | 109.0 |
| C5—C8—H8 | 108.2 | H19A—C19—H19B | 107.8 |
| C10—C9—C18 | 120.7 (2) | C20A—C19—H19C | 132.7 |
| C10—C9—C8 | 121.06 (19) | C20B—C19—H19C | 109.5 |
| C18—C9—C8 | 118.2 (2) | O2—C19—H19C | 109.5 |
| C9—C10—N2 | 119.2 (2) | H19A—C19—H19C | 75.2 |
| C9—C10—C17 | 127.9 (2) | C20B—C19—H19D | 109.5 |
| N2—C10—C17 | 112.9 (2) | O2—C19—H19D | 109.5 |
| C12—C11—N2 | 119.03 (18) | H19A—C19—H19D | 137.2 |
| C12—C11—C16 | 128.49 (19) | H19B—C19—H19D | 76.0 |
| N2—C11—C16 | 112.47 (18) | H19C—C19—H19D | 108.1 |
| C11—C12—C13 | 125.70 (19) | C19—C20A—H20A | 109.5 |
| C11—C12—C8 | 121.06 (18) | C19—C20A—H20B | 109.5 |
| C13—C12—C8 | 113.16 (18) | H20A—C20A—H20B | 109.5 |
| O4—C13—O3 | 121.7 (2) | C19—C20A—H20C | 109.5 |
| O4—C13—C12 | 123.4 (2) | H20A—C20A—H20C | 109.5 |
| O3—C13—C12 | 114.78 (19) | H20B—C20A—H20C | 109.5 |
| O3—C14—C15 | 108.1 (2) | C19—C20B—H20D | 109.5 |
| O3—C14—H14A | 110.1 | C19—C20B—H20E | 109.5 |
| C15—C14—H14A | 110.1 | H20D—C20B—H20E | 109.5 |
| O3—C14—H14B | 110.1 | C19—C20B—H20F | 109.5 |
| C15—C14—H14B | 110.1 | H20D—C20B—H20F | 109.5 |
| H14A—C14—H14B | 108.4 | H20E—C20B—H20F | 109.5 |
| C14—C15—H15A | 109.5 | C10—N2—C11 | 124.26 (19) |
| C14—C15—H15B | 109.5 | C10—N2—H2 | 117.9 |
| H15A—C15—H15B | 109.5 | C11—N2—H2 | 117.9 |
| C14—C15—H15C | 109.5 | C18—O2—C19 | 114.2 (3) |
| H15A—C15—H15C | 109.5 | C13—O3—C14 | 118.16 (19) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···N1$^{i}$ | 0.86 | 2.32 | 3.098 (3) | 150 |

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

**Fig. 1**

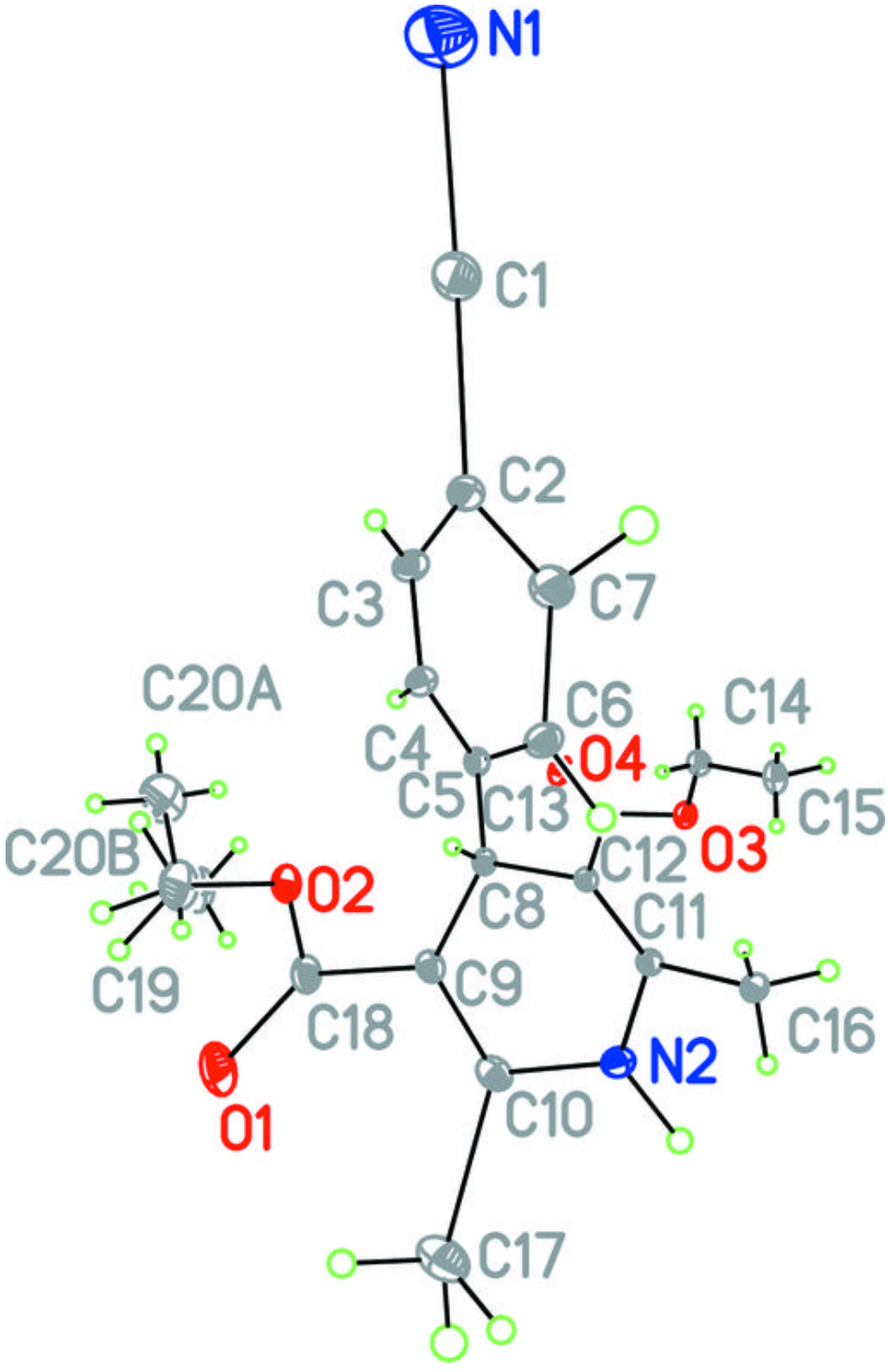
N1
C1
C2
C3
C7
C20A
C6
C14
C4
O4
C5
C13
C15
C20B
O3
C12
O2
C8
C11
C19
C9
C16
C18
N2
O1
C10
C17

**Fig. 2**