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# 1,1′-[4-(4-Methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-diyl]diethanone

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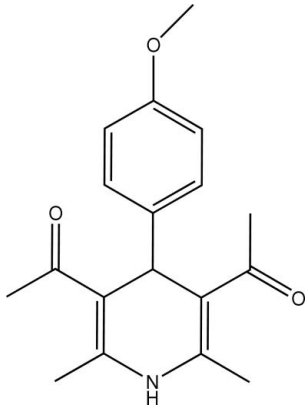
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.047; $wR$ factor = 0.148; data-to-parameter ratio = 19.5.

In the title compound, $C_{18}H_{21}NO_3$, which belongs to the family of calcium channel blockers, the dihydropyridine ring assumes a flattened boat conformation. The two carbonyl units adopt a synperiplanar conformation with respect to the double bonds in the dihydropyridine ring. The methoxyphenyl ring is almost perpendicular to the prydine ring [dihedral angle = 89.01 (7)°]. In the crystal, the molecules are connected by intermolecular N—H···O hydrogen bonds.

## Related literature

For general background, see: Ganjali *et al.* (2007); Xia *et al.* (2005). For hybridization, see: Beddoes *et al.*(1986). For ring conformational analysis, see: Cremer & Pople (1975); Nardelli (1983).




## Experimental

### Crystal data

$C_{18}H_{21}NO_3$ $M_r$ = 299.36
Orthorhombic, *Pbca*
$a$ = 12.0781 (3) Å
$b$ = 8.9650 (2) Å
$c$ = 29.3755 (8) Å
$V$ = 3180.78 (14) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.25 × 0.20 × 0.20 mm

### Data collection

Bruker Kappa APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min}$ = 0.979, $T_{max}$ = 0.983
36021 measured reflections
4055 independent reflections
2828 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
$S$ = 1.05
4055 reflections
208 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.869 (19) | 2.03 (2) | 2.8961 (19) | 173.1 (18) |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

MT thanks Dr Babu Varghese, SAIF, IIT-Madras, Chennai, India, for his help with the data collection. VV thanks the DST-India for funding the project under the Fast-Track Proposal scheme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5060).

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# supporting information

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## 1,1′-[4-(4-Methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-diyl]diethanone

**M. Thenmozhi, T. Kavitha, B. Palakshi Reddy, V. Vijayakumar and M. N. Ponnuswamy**

### S1. Comment

1,4-Dihydropyridine compounds are the important class of calcium channel blockers and as such commercialized in, for instance nifedipine, amlodipine or nimodipine (Xia *et al.*, 2005). Pyridine derivatives can be used as a suitable neutral ionophore for preparing an Er(III) membrane sensor with high selectivity, which are utilized for direct monitoring of Er(III) in binary mixtures and indirect determination of fluoride ions in mouth wash preparations (Ganjali *et al.*, 2007).

The ORTEP plot of the molecule is shown in Fig. 1. The pyridine ring assumes a flattened boat conformation with puckering parameters (Cremer & Pople, 1975) $q_2$= 0.2975 (16)Å, $q_3$ = -0.0900 (16)Å, $\varphi$ = 355.2 (3)° and asymmetry parameters (Nardelli, 1983) $\Delta_s$(N1,C4) = 3.26 (16)°. The methyl groups attached at C2 and C6 positions of the pyridine ring adopt equatorial orientation as can be seen from the torsion angles [C7-C2-N1-C6=]-165.71 (15)° and [C19-C6-N1-C2 =]164.36 (15)°. Both the carboxylate groups at 3$^{rd}$ and 5$^{th}$ positions in the pyridine ring, have synperiplanar(sp) conformation with respect to the double bonds in the dihydropyridine ring which are evident from the torsion angles [C2-C3-C8-O1=]-6.3 (3)°) and [C6-C5-C17-O3=]-17.3 (3)°. The methoxyphenyl ring is almost perpendicular to the best plane of the prydine ring as can be seen from the dihedral angle of 89.01 (7)°. The sum of the bond angles around atom N1[357.06°] of the pyridine ring is in accordance with sp$^2$ hybridization (Beddoes *et al.*, 1986).

Atom N1(x,y,z) of the pyridine ring donates a proton to atom O1(-1/2+x,y,1/2-z), leading to a zig-zag chain running along the *a* - axis (Fig. 2).

### S2. Experimental

Dimethyl-4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate was prepared by heating the mixture of 4-methoxybenzaldehyde (10 mmol), methylacetoacetate (20 mmol) and ammonium acetate (10 mmol) at 80ºC for 2 hours and 45 min (monitored by TLC). After completion of the reaction, the mixture was cooled to room temperature and kept for 3 days to get the solid product. The obtained solid was washed with diethyl ether and collected separately. The purity of the crude product was checked through TLC and recrystallized using acetone and ether.

### S3. Refinement

H atoms were positioned geometrically (C-H = 0.93-0.98Å) and allowed to ride on their parent atoms, with Uiso(H) = 1.5Ueq(C) for methyl H and 1.2Ueq(C) for other H atoms.The components of the anisotropic displacement parameters of C5 and C6 in the direction of the bond between them were restrained to be equal within an effective standard deviation of 0.001.

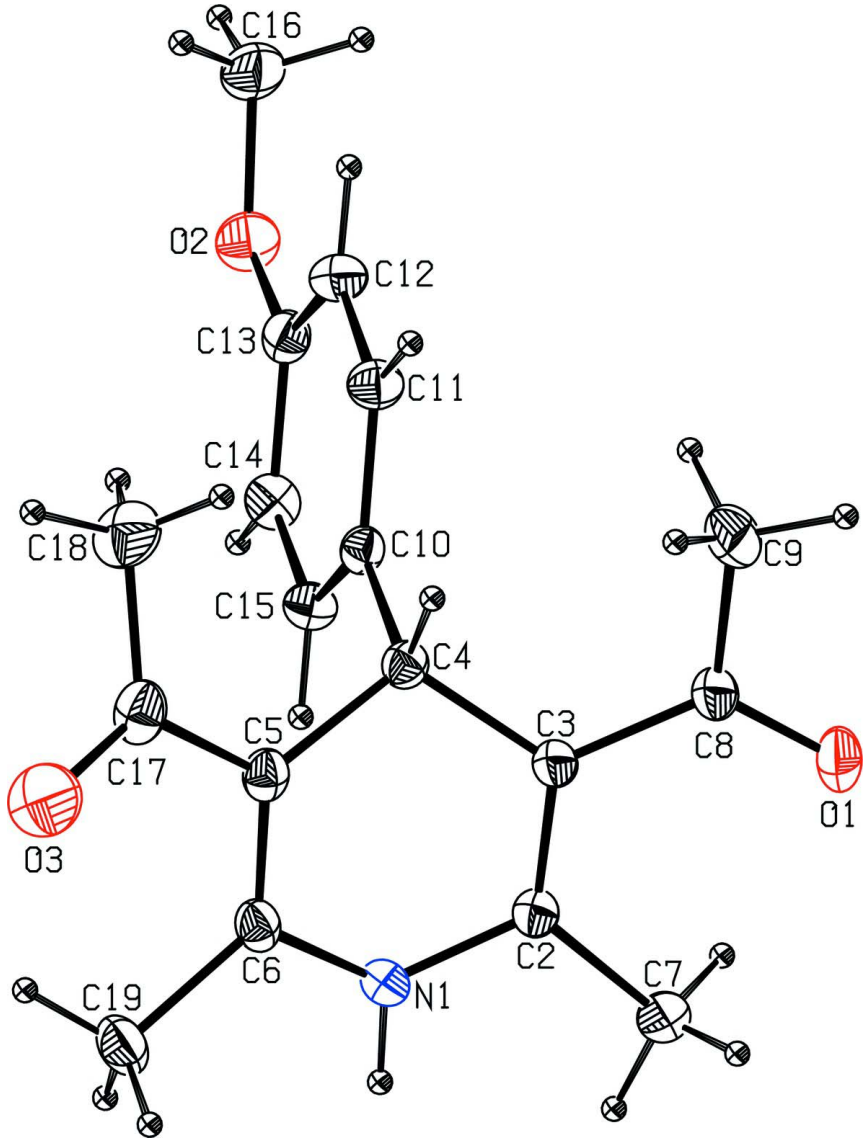


**Figure 1**

Perpective view of the molecule, showing 30% probability displacement ellipsoids.

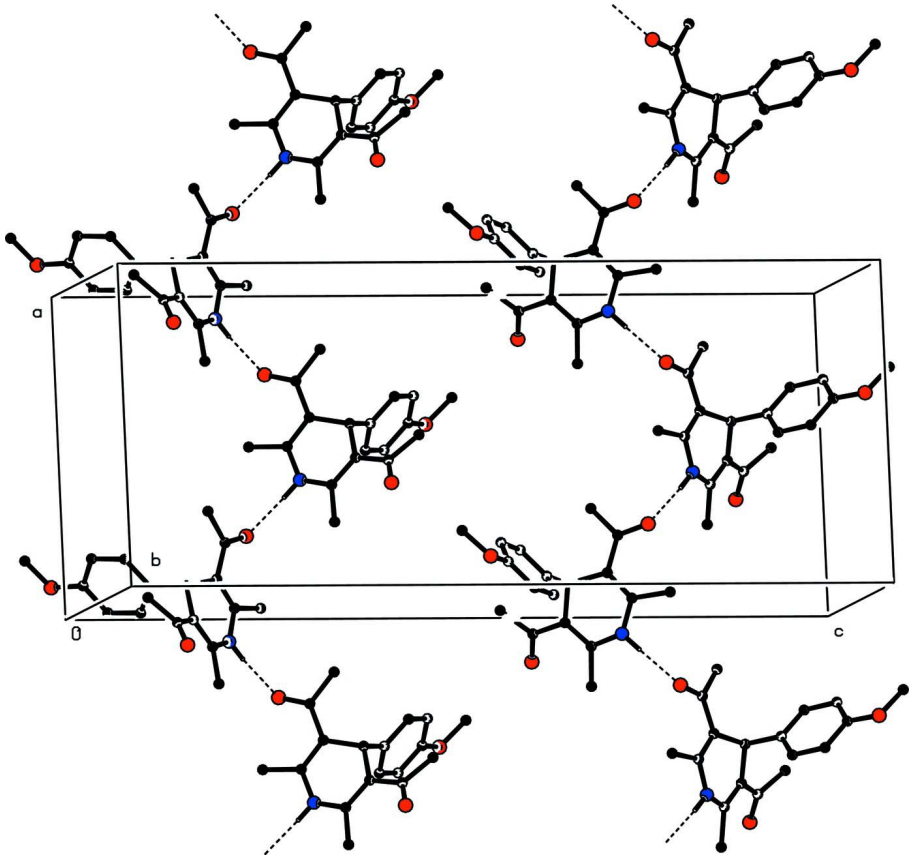


**Figure 2**

Crystal packing of the molecules viewed down *a* axis.

**1,1′-[4-(4-Methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-diyl]diethanone**

*Crystal data*

$C_{18}H_{21}NO_3$
$M_r = 299.36$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.0781\ (3)$ Å
$b = 8.9650\ (2)$ Å
$c = 29.3755\ (8)$ Å
$V = 3180.78\ (14)$ Å$^3$
$Z = 8$
$F(000) = 1280$
$D_x = 1.250$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4055 reflections
$\theta = 1.4$–$28.6°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ K
Block, light yellow
0.25 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.979$, $T_{max} = 0.983$
36021 measured reflections
4055 independent reflections
2828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 28.6°$, $\theta_{min} = 1.4°$
$h = -16 \rightarrow 14$
$k = -12 \rightarrow 10$
$l = -37 \rightarrow 39$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.148$
$S = 1.05$
4055 reflections
208 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
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
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 1.0129P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ e Å$^{-3}$

*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 $F^2 > 2$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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | 0.52089 (13) | 0.12861 (18) | 0.28911 (5) | 0.0418 (4) |
| C3 | 0.60545 (12) | 0.18029 (17) | 0.31531 (5) | 0.0392 (3) |
| C4 | 0.57919 (12) | 0.24866 (17) | 0.36162 (5) | 0.0378 (3) |
| H4 | 0.6343 | 0.3265 | 0.3675 | 0.045* |
| C5 | 0.46584 (13) | 0.32299 (17) | 0.36102 (5) | 0.0409 (3) |
| C6 | 0.38706 (12) | 0.27123 (18) | 0.33254 (5) | 0.0422 (3) |
| C7 | 0.52978 (15) | 0.0360 (2) | 0.24679 (6) | 0.0595 (5) |
| H7A | 0.5613 | 0.0949 | 0.2228 | 0.089* |
| H7B | 0.4574 | 0.0025 | 0.2379 | 0.089* |
| H7C | 0.5763 | −0.0487 | 0.2526 | 0.089* |
| C8 | 0.72005 (13) | 0.1649 (2) | 0.30089 (6) | 0.0487 (4) |
| C9 | 0.81050 (15) | 0.2381 (3) | 0.32811 (8) | 0.0741 (6) |
| H9A | 0.8186 | 0.1875 | 0.3567 | 0.111* |
| H9B | 0.7918 | 0.3407 | 0.3334 | 0.111* |
| H9C | 0.8789 | 0.2327 | 0.3115 | 0.111* |
| C10 | 0.59067 (12) | 0.13184 (16) | 0.39902 (5) | 0.0368 (3) |
| C11 | 0.67301 (14) | 0.14207 (18) | 0.43151 (5) | 0.0460 (4) |
| H11 | 0.7216 | 0.2225 | 0.4304 | 0.055* |
| C12 | 0.68580 (14) | 0.03681 (19) | 0.46561 (5) | 0.0486 (4) |
| H12 | 0.7423 | 0.0467 | 0.4869 | 0.058* |
| C13 | 0.61449 (13) | −0.08222 (17) | 0.46774 (5) | 0.0438 (4) |
| C14 | 0.53161 (14) | −0.09579 (19) | 0.43563 (6) | 0.0478 (4) |
| H14 | 0.4833 | −0.1765 | 0.4368 | 0.057* |
| C15 | 0.52023 (13) | 0.00946 (17) | 0.40189 (5) | 0.0434 (4) |

| | | | | |
|---|---|---|---|---|
| H15 | 0.4641 | −0.0015 | 0.3805 | 0.052* |
| C16 | 0.70171 (18) | −0.1747 (2) | 0.53459 (6) | 0.0664 (5) |
| H16A | 0.7741 | −0.1742 | 0.5211 | 0.100* |
| H16B | 0.6964 | −0.2558 | 0.5558 | 0.100* |
| H16C | 0.6895 | −0.0822 | 0.5502 | 0.100* |
| C17 | 0.44451 (17) | 0.44728 (19) | 0.39277 (6) | 0.0547 (5) |
| C18 | 0.5199 (2) | 0.4709 (2) | 0.43225 (7) | 0.0728 (6) |
| H18A | 0.4905 | 0.5480 | 0.4514 | 0.109* |
| H18B | 0.5918 | 0.5000 | 0.4214 | 0.109* |
| H18C | 0.5261 | 0.3800 | 0.4493 | 0.109* |
| C19 | 0.26738 (14) | 0.3160 (2) | 0.33045 (7) | 0.0589 (5) |
| H19A | 0.2469 | 0.3640 | 0.3584 | 0.088* |
| H19B | 0.2224 | 0.2289 | 0.3261 | 0.088* |
| H19C | 0.2564 | 0.3837 | 0.3055 | 0.088* |
| N1 | 0.41402 (11) | 0.16250 (16) | 0.30102 (5) | 0.0441 (3) |
| O1 | 0.74715 (11) | 0.09406 (19) | 0.26662 (4) | 0.0754 (5) |
| O2 | 0.62054 (12) | −0.19260 (14) | 0.49995 (4) | 0.0596 (4) |
| O3 | 0.36634 (16) | 0.5314 (2) | 0.38831 (6) | 0.1011 (6) |
| H1 | 0.3631 (16) | 0.135 (2) | 0.2819 (6) | 0.057 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.0386 (8) | 0.0492 (9) | 0.0374 (7) | 0.0028 (7) | 0.0024 (6) | 0.0020 (6) |
| C3 | 0.0345 (7) | 0.0462 (8) | 0.0370 (7) | 0.0005 (6) | 0.0022 (6) | 0.0023 (6) |
| C4 | 0.0386 (7) | 0.0384 (8) | 0.0364 (7) | −0.0017 (6) | 0.0021 (6) | 0.0010 (6) |
| C5 | 0.0446 (8) | 0.0388 (8) | 0.0393 (7) | 0.0045 (6) | 0.0071 (6) | 0.0067 (6) |
| C6 | 0.0384 (7) | 0.0456 (9) | 0.0426 (8) | 0.0069 (6) | 0.0071 (6) | 0.0113 (6) |
| C7 | 0.0497 (10) | 0.0809 (13) | 0.0479 (9) | 0.0060 (9) | −0.0051 (8) | −0.0174 (9) |
| C8 | 0.0378 (8) | 0.0648 (11) | 0.0435 (8) | −0.0005 (7) | 0.0069 (7) | 0.0053 (8) |
| C9 | 0.0388 (9) | 0.1061 (17) | 0.0773 (13) | −0.0135 (11) | 0.0059 (9) | −0.0123 (13) |
| C10 | 0.0387 (8) | 0.0364 (7) | 0.0351 (7) | 0.0025 (6) | 0.0030 (6) | −0.0027 (6) |
| C11 | 0.0473 (9) | 0.0436 (8) | 0.0470 (9) | −0.0054 (7) | −0.0054 (7) | 0.0002 (7) |
| C12 | 0.0517 (9) | 0.0502 (9) | 0.0440 (8) | 0.0015 (8) | −0.0097 (7) | 0.0014 (7) |
| C13 | 0.0490 (9) | 0.0414 (8) | 0.0410 (8) | 0.0093 (7) | 0.0043 (7) | 0.0038 (7) |
| C14 | 0.0475 (9) | 0.0407 (8) | 0.0552 (9) | −0.0036 (7) | 0.0007 (7) | 0.0042 (7) |
| C15 | 0.0416 (8) | 0.0432 (8) | 0.0454 (8) | −0.0025 (7) | −0.0051 (6) | 0.0006 (7) |
| C16 | 0.0765 (13) | 0.0739 (13) | 0.0488 (10) | 0.0138 (11) | −0.0043 (9) | 0.0162 (9) |
| C17 | 0.0683 (12) | 0.0430 (9) | 0.0529 (10) | 0.0123 (8) | 0.0117 (8) | 0.0041 (7) |
| C18 | 0.0929 (16) | 0.0552 (11) | 0.0704 (13) | 0.0078 (11) | −0.0053 (11) | −0.0226 (10) |
| C19 | 0.0413 (9) | 0.0695 (12) | 0.0660 (11) | 0.0145 (8) | 0.0062 (8) | 0.0108 (9) |
| N1 | 0.0335 (7) | 0.0551 (8) | 0.0438 (7) | 0.0018 (6) | −0.0028 (6) | −0.0005 (6) |
| O1 | 0.0454 (7) | 0.1195 (12) | 0.0613 (8) | −0.0014 (8) | 0.0170 (6) | −0.0231 (8) |
| O2 | 0.0696 (8) | 0.0534 (7) | 0.0559 (7) | 0.0045 (6) | −0.0023 (6) | 0.0167 (6) |
| O3 | 0.1203 (14) | 0.0915 (12) | 0.0916 (12) | 0.0615 (11) | −0.0129 (10) | −0.0239 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C2—C3 | 1.360 (2) | C11—C12 | 1.385 (2) |
| C2—N1 | 1.3715 (19) | C11—H11 | 0.9300 |
| C2—C7 | 1.499 (2) | C12—C13 | 1.373 (2) |
| C3—C8 | 1.454 (2) | C12—H12 | 0.9300 |
| C3—C4 | 1.526 (2) | C13—O2 | 1.3711 (19) |
| C4—C5 | 1.523 (2) | C13—C14 | 1.381 (2) |
| C4—C10 | 1.524 (2) | C14—C15 | 1.375 (2) |
| C4—H4 | 0.9800 | C14—H14 | 0.9300 |
| C5—C6 | 1.349 (2) | C15—H15 | 0.9300 |
| C5—C17 | 1.476 (2) | C16—O2 | 1.422 (2) |
| C6—N1 | 1.383 (2) | C16—H16A | 0.9600 |
| C6—C19 | 1.502 (2) | C16—H16B | 0.9600 |
| C7—H7A | 0.9600 | C16—H16C | 0.9600 |
| C7—H7B | 0.9600 | C17—O3 | 1.216 (2) |
| C7—H7C | 0.9600 | C17—C18 | 1.490 (3) |
| C8—O1 | 1.234 (2) | C18—H18A | 0.9600 |
| C8—C9 | 1.504 (3) | C18—H18B | 0.9600 |
| C9—H9A | 0.9600 | C18—H18C | 0.9600 |
| C9—H9B | 0.9600 | C19—H19A | 0.9600 |
| C9—H9C | 0.9600 | C19—H19B | 0.9600 |
| C10—C11 | 1.381 (2) | C19—H19C | 0.9600 |
| C10—C15 | 1.391 (2) | N1—H1 | 0.869 (19) |
| | | | |
| C3—C2—N1 | 119.13 (14) | C12—C11—H11 | 118.8 |
| C3—C2—C7 | 127.17 (14) | C13—C12—C11 | 119.51 (15) |
| N1—C2—C7 | 113.69 (14) | C13—C12—H12 | 120.2 |
| C2—C3—C8 | 121.17 (14) | C11—C12—H12 | 120.2 |
| C2—C3—C4 | 119.04 (13) | O2—C13—C12 | 123.99 (15) |
| C8—C3—C4 | 119.72 (13) | O2—C13—C14 | 116.52 (15) |
| C5—C4—C10 | 113.01 (12) | C12—C13—C14 | 119.49 (15) |
| C5—C4—C3 | 110.63 (12) | C15—C14—C13 | 120.29 (15) |
| C10—C4—C3 | 110.35 (12) | C15—C14—H14 | 119.9 |
| C5—C4—H4 | 107.5 | C13—C14—H14 | 119.9 |
| C10—C4—H4 | 107.5 | C14—C15—C10 | 121.58 (14) |
| C3—C4—H4 | 107.5 | C14—C15—H15 | 119.2 |
| C6—C5—C17 | 121.90 (15) | C10—C15—H15 | 119.2 |
| C6—C5—C4 | 119.39 (14) | O2—C16—H16A | 109.5 |
| C17—C5—C4 | 118.68 (15) | O2—C16—H16B | 109.5 |
| C5—C6—N1 | 119.43 (14) | H16A—C16—H16B | 109.5 |
| C5—C6—C19 | 127.76 (16) | O2—C16—H16C | 109.5 |
| N1—C6—C19 | 112.80 (15) | H16A—C16—H16C | 109.5 |
| C2—C7—H7A | 109.5 | H16B—C16—H16C | 109.5 |
| C2—C7—H7B | 109.5 | O3—C17—C5 | 122.42 (18) |
| H7A—C7—H7B | 109.5 | O3—C17—C18 | 118.06 (17) |
| C2—C7—H7C | 109.5 | C5—C17—C18 | 119.51 (16) |
| H7A—C7—H7C | 109.5 | C17—C18—H18A | 109.5 |

| | | | |
|---|---|---|---|
| H7B—C7—H7C | 109.5 | C17—C18—H18B | 109.5 |
| O1—C8—C3 | 122.60 (16) | H18A—C18—H18B | 109.5 |
| O1—C8—C9 | 117.72 (15) | C17—C18—H18C | 109.5 |
| C3—C8—C9 | 119.67 (15) | H18A—C18—H18C | 109.5 |
| C8—C9—H9A | 109.5 | H18B—C18—H18C | 109.5 |
| C8—C9—H9B | 109.5 | C6—C19—H19A | 109.5 |
| H9A—C9—H9B | 109.5 | C6—C19—H19B | 109.5 |
| C8—C9—H9C | 109.5 | H19A—C19—H19B | 109.5 |
| H9A—C9—H9C | 109.5 | C6—C19—H19C | 109.5 |
| H9B—C9—H9C | 109.5 | H19A—C19—H19C | 109.5 |
| C11—C10—C15 | 116.79 (14) | H19B—C19—H19C | 109.5 |
| C11—C10—C4 | 121.19 (13) | C2—N1—C6 | 123.26 (14) |
| C15—C10—C4 | 122.01 (13) | C2—N1—H1 | 116.0 (13) |
| C10—C11—C12 | 122.34 (15) | C6—N1—H1 | 117.8 (13) |
| C10—C11—H11 | 118.8 | C13—O2—C16 | 116.70 (14) |

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| N1—C2—C3—C8 | −171.57 (15) | C5—C4—C10—C15 | 58.19 (18) |
| C7—C2—C3—C8 | 8.0 (3) | C3—C4—C10—C15 | −66.27 (18) |
| N1—C2—C3—C4 | 11.4 (2) | C15—C10—C11—C12 | −0.2 (2) |
| C7—C2—C3—C4 | −169.03 (16) | C4—C10—C11—C12 | −179.46 (15) |
| C2—C3—C4—C5 | −30.7 (2) | C10—C11—C12—C13 | −0.3 (3) |
| C8—C3—C4—C5 | 152.27 (14) | C11—C12—C13—O2 | 179.63 (15) |
| C2—C3—C4—C10 | 95.13 (17) | C11—C12—C13—C14 | 0.5 (2) |
| C8—C3—C4—C10 | −81.92 (18) | O2—C13—C14—C15 | −179.49 (15) |
| C10—C4—C5—C6 | −95.93 (16) | C12—C13—C14—C15 | −0.3 (2) |
| C3—C4—C5—C6 | 28.38 (19) | C13—C14—C15—C10 | −0.2 (2) |
| C10—C4—C5—C17 | 82.28 (17) | C11—C10—C15—C14 | 0.4 (2) |
| C3—C4—C5—C17 | −153.41 (14) | C4—C10—C15—C14 | 179.66 (14) |
| C17—C5—C6—N1 | 174.94 (14) | C6—C5—C17—O3 | −17.3 (3) |
| C4—C5—C6—N1 | −6.9 (2) | C4—C5—C17—O3 | 164.55 (19) |
| C17—C5—C6—C19 | −5.9 (3) | C6—C5—C17—C18 | 161.94 (18) |
| C4—C5—C6—C19 | 172.25 (15) | C4—C5—C17—C18 | −16.2 (2) |
| C2—C3—C8—O1 | −6.3 (3) | C3—C2—N1—C6 | 13.9 (2) |
| C4—C3—C8—O1 | 170.70 (16) | C7—C2—N1—C6 | −165.71 (15) |
| C2—C3—C8—C9 | 173.28 (18) | C5—C6—N1—C2 | −16.4 (2) |
| C4—C3—C8—C9 | −9.7 (2) | C19—C6—N1—C2 | 164.36 (15) |
| C5—C4—C10—C11 | −122.56 (16) | C12—C13—O2—C16 | 4.3 (2) |
| C3—C4—C10—C11 | 112.98 (16) | C14—C13—O2—C16 | −176.55 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.869 (19) | 2.03 (2) | 2.8961 (19) | 173.1 (18) |

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