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# Dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-pyridine-3,5-dicarboxylate

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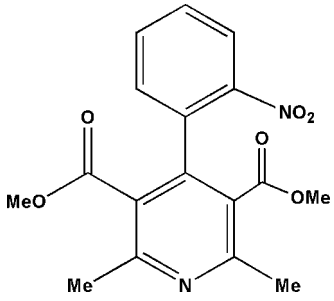
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.038; $wR$ factor = 0.097; data-to-parameter ratio = 16.7.

The title compound, $C_{17}H_{16}N_2O_6$, is a decomposition product of the hypertension drug nifedipine [systematic name: dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate]. The dihedral angle between the nitrosophenyl ring and the pyridine ring is 67.1 (5)°.

## Related literature

For the calcium antagonistic activity of compounds of the 1,4-dihydropyridine class, which inhibit the influx of $Ca^{2+}$ ions through plasma membrane channels, see: Núnez-Vergara *et al.* (1994) and for their current use in the treatment of a variety of cardiovascular disorders such as angina and hypertension, see: Triggle *et al.* (1989); Hurwitz *et al.* (1991). For general background to derivatives of the dihydropyridine calcium channel blockers nifedipine [3,5-dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate] and nisoldipine [isobutyl methyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate], see: Chen *et al.* (2010); Rowan & Holt (1996, 1997*a*,*b*); Schultheiss *et al.* (2010). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{17}H_{16}N_2O_6$
$M_r$ = 344.32
Triclinic, $P\overline{1}$
$a$ = 7.578 (4) Å
$b$ = 8.141 (4) Å
$c$ = 14.235 (9) Å
$\alpha$ = 103.32 (2)°
$\beta$ = 93.75 (5)°
$\gamma$ = 105.39 (3)°
$V$ = 816.4 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 298 K
0.20 × 0.18 × 0.12 mm

### Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.979, $T_{max}$ = 0.987
8658 measured reflections
3843 independent reflections
2247 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
$S$ = 1.03
3843 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2031).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o2820 [ **doi:10.1107/S1600536811039626** ]

# Dimethyl 2,6-dimethyl-4-(2-nitrophenyl)pyridine-3,5-dicarboxylate

**J. Zheng, X. Wang, D. Pang, Y. Sun and W. Su**

## Comment

Compounds of the 1,4-dihydropyridine class exhibit calcium antagonistic activity, as they inhibit the influx of $Ca^{2+}$ ions through plasma membrane channels (Núnez-Vergara, Sunkel & Squella, 1994). Compounds of this class are currently being used in the treatment of a variety of cardiovascular disorders, such as angina and hypertension (Triggle *et al.*, 1989; Hurwitz *et al.*, 1991). Nifedipine [dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate], is the best known member of this class. The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the nitrosophenyl ring and the pyridine ring is 67.1°.

## Experimental

The title compound was prepared by adding following steps. 1: Add 1 g nifedipine and 10 g $(NH_4)_2S_2O_8$ to the 100 ml acetone solution(50%). 2: Stir for 12 h at 30 °C.3:Regulate the solution to pH=8 with $Na_2CO_3$. The resulting solution was extracted with methylene chloride. The organic layer was dried over $MgSO_4$ and evaporated under reduced pressure. Following washing the extract with water, crystals of suitable size for single-crystal analysis were recrystallized from methanol.

## Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 A ° for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}$(H) = xUeq(C), where $x$ = 1.2 for aromatic and $x$ = 1.5 for methyl H atoms.

## Figures

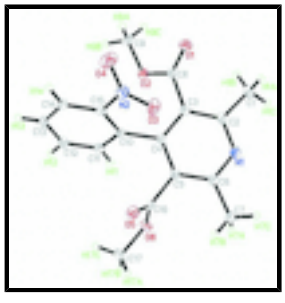


Fig. 1. [3,5-dimethyl 2,6-dimethyl-4-(2-nitrophenyl)pyridine-3,5-dicarboxylate]

## Dimethyl 2,6-dimethyl-4-(2-nitrophenyl)pyridine-3,5-dicarboxylate

*Crystal data*

| | |
|---|---|
| $C_{17}H_{16}N_2O_6$ | $Z$ = 2 |
| $M_r$ = 344.32 | $F$(000) = 360 |

| | |
|---|---|
| Triclinic, $P\bar{1}$ | $D_x$ = 1.401 Mg m$^{-3}$ |
| $a$ = 7.578 (4) Å | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $b$ = 8.141 (4) Å | Cell parameters from 2919 reflections |
| $c$ = 14.235 (9) Å | θ = 1.5–28.0° |
| α = 103.32 (2)° | μ = 0.11 mm$^{-1}$ |
| β = 93.75 (5)° | $T$ = 298 K |
| γ = 105.39 (3)° | Prism, yellow |
| $V$ = 816.4 (8) Å$^3$ | 0.20 × 0.18 × 0.12 mm |

*Data collection*

| | |
|---|---|
| Rigaku Saturn724 CCD diffractometer | 3843 independent reflections |
| Radiation source: rotating anode | 2247 reflections with $I > 2\sigma(I)$ |
| multilayer | $R_{int}$ = 0.047 |
| Detector resolution: 14.22 pixels mm$^{-1}$ | $\theta_{max}$ = 27.9°, $\theta_{min}$ = 1.5° |
| ω and φ scans | $h$ = −9→9 |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005) | $k$ = −10→10 |
| $T_{min}$ = 0.979, $T_{max}$ = 0.987 | $l$ = −18→17 |
| 8658 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.097 | H-atom parameters constrained |
| $S$ = 1.03 | $w = 1/[\sigma^2(F_o^2) + (0.028P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3843 reflections | $(\Delta/\sigma)_{max}$ = 0.001 |
| 230 parameters | $\Delta\rho_{max}$ = 0.21 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.29 e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.76803 (15) | 0.93198 (15) | 0.92024 (8) | 0.0333 (3) |
| O2 | 0.84798 (13) | 0.68996 (14) | 0.85050 (7) | 0.0240 (3) |
| O3 | 0.40716 (15) | 0.78829 (15) | 0.70787 (8) | 0.0344 (3) |
| O4 | 0.63979 (19) | 0.91761 (16) | 0.64507 (10) | 0.0520 (4) |
| O5 | 0.13443 (14) | 0.30250 (15) | 0.61801 (7) | 0.0279 (3) |
| O6 | 0.18628 (14) | 0.11367 (14) | 0.70271 (7) | 0.0259 (3) |
| N1 | 0.26875 (17) | 0.55143 (17) | 0.95102 (9) | 0.0218 (3) |
| N2 | 0.54570 (19) | 0.78817 (18) | 0.66853 (9) | 0.0283 (3) |
| C1 | 0.5124 (2) | 0.7905 (2) | 1.05399 (10) | 0.0256 (4) |
| H1A | 0.4799 | 0.8996 | 1.0549 | 0.038* |
| H1B | 0.6471 | 0.8165 | 1.0651 | 0.038* |
| H1C | 0.4582 | 0.7401 | 1.1054 | 0.038* |
| C2 | 0.4386 (2) | 0.6606 (2) | 0.95644 (10) | 0.0200 (3) |
| C3 | 0.53855 (19) | 0.65051 (19) | 0.87679 (10) | 0.0184 (3) |
| C4 | 0.45649 (19) | 0.52477 (19) | 0.78913 (10) | 0.0175 (3) |
| C5 | 0.2806 (2) | 0.4125 (2) | 0.78490 (10) | 0.0188 (3) |
| C6 | 0.1892 (2) | 0.4295 (2) | 0.86757 (11) | 0.0200 (3) |
| C7 | −0.0011 (2) | 0.3140 (2) | 0.86810 (11) | 0.0278 (4) |
| H7A | 0.0077 | 0.2160 | 0.8954 | 0.042* |
| H7B | −0.0653 | 0.2675 | 0.8013 | 0.042* |
| H7C | −0.0701 | 0.3832 | 0.9080 | 0.042* |
| C8 | 0.7278 (2) | 0.7743 (2) | 0.88633 (11) | 0.0214 (3) |
| C9 | 1.0316 (2) | 0.8018 (2) | 0.84997 (12) | 0.0297 (4) |
| H9A | 1.0228 | 0.8948 | 0.8183 | 0.045* |
| H9B | 1.1038 | 0.7310 | 0.8141 | 0.045* |
| H9C | 1.0925 | 0.8554 | 0.9171 | 0.045* |
| C10 | 0.55534 (18) | 0.50220 (19) | 0.70104 (10) | 0.0176 (3) |
| C11 | 0.6085 (2) | 0.3487 (2) | 0.67264 (10) | 0.0226 (4) |
| H11 | 0.5774 | 0.2612 | 0.7077 | 0.027* |
| C12 | 0.7059 (2) | 0.3213 (2) | 0.59432 (11) | 0.0267 (4) |
| H12 | 0.7401 | 0.2154 | 0.5759 | 0.032* |
| C13 | 0.7538 (2) | 0.4482 (2) | 0.54255 (11) | 0.0263 (4) |
| H13 | 0.8218 | 0.4296 | 0.4893 | 0.032* |
| C14 | 0.7024 (2) | 0.6014 (2) | 0.56854 (11) | 0.0237 (4) |
| H14 | 0.7342 | 0.6887 | 0.5334 | 0.028* |
| C15 | 0.60384 (19) | 0.6254 (2) | 0.64663 (10) | 0.0202 (3) |
| C16 | 0.19127 (19) | 0.2747 (2) | 0.69257 (11) | 0.0200 (3) |
| C17 | 0.1122 (2) | −0.0294 (2) | 0.61593 (12) | 0.0364 (4) |
| H17A | −0.0139 | −0.0318 | 0.5937 | 0.055* |
| H17B | 0.1105 | −0.1415 | 0.6307 | 0.055* |
| H17C | 0.1898 | −0.0116 | 0.5646 | 0.055* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0287 (7) | 0.0182 (6) | 0.0483 (8) | 0.0042 (5) | 0.0079 (5) | 0.0014 (6) |
| O2 | 0.0200 (6) | 0.0216 (6) | 0.0293 (6) | 0.0058 (5) | 0.0056 (5) | 0.0041 (5) |
| O3 | 0.0382 (7) | 0.0388 (8) | 0.0381 (7) | 0.0221 (6) | 0.0167 (6) | 0.0170 (6) |
| O4 | 0.0680 (10) | 0.0273 (8) | 0.0727 (10) | 0.0148 (7) | 0.0355 (8) | 0.0278 (8) |
| O5 | 0.0279 (6) | 0.0343 (7) | 0.0211 (6) | 0.0059 (5) | 0.0023 (5) | 0.0102 (5) |
| O6 | 0.0320 (6) | 0.0194 (6) | 0.0223 (6) | 0.0061 (5) | −0.0008 (5) | 0.0004 (5) |
| N1 | 0.0245 (7) | 0.0220 (7) | 0.0214 (7) | 0.0086 (6) | 0.0074 (5) | 0.0072 (6) |
| N2 | 0.0376 (9) | 0.0251 (8) | 0.0255 (8) | 0.0098 (7) | 0.0069 (6) | 0.0111 (7) |
| C1 | 0.0318 (9) | 0.0260 (9) | 0.0212 (8) | 0.0119 (8) | 0.0040 (7) | 0.0058 (7) |
| C2 | 0.0248 (8) | 0.0195 (8) | 0.0188 (8) | 0.0109 (7) | 0.0036 (6) | 0.0057 (7) |
| C3 | 0.0200 (8) | 0.0168 (8) | 0.0211 (8) | 0.0080 (7) | 0.0040 (6) | 0.0065 (7) |
| C4 | 0.0205 (8) | 0.0173 (8) | 0.0188 (8) | 0.0094 (7) | 0.0062 (6) | 0.0072 (7) |
| C5 | 0.0210 (8) | 0.0190 (8) | 0.0188 (8) | 0.0077 (7) | 0.0052 (6) | 0.0066 (7) |
| C6 | 0.0222 (8) | 0.0190 (8) | 0.0217 (8) | 0.0082 (7) | 0.0065 (6) | 0.0072 (7) |
| C7 | 0.0247 (9) | 0.0281 (10) | 0.0287 (9) | 0.0048 (8) | 0.0119 (7) | 0.0045 (8) |
| C8 | 0.0248 (8) | 0.0223 (9) | 0.0176 (8) | 0.0074 (7) | 0.0039 (6) | 0.0051 (7) |
| C9 | 0.0192 (8) | 0.0312 (10) | 0.0363 (10) | 0.0029 (7) | 0.0059 (7) | 0.0085 (8) |
| C10 | 0.0131 (7) | 0.0195 (8) | 0.0170 (8) | 0.0008 (6) | 0.0016 (6) | 0.0034 (6) |
| C11 | 0.0219 (8) | 0.0213 (9) | 0.0241 (9) | 0.0054 (7) | 0.0041 (7) | 0.0055 (7) |
| C12 | 0.0244 (9) | 0.0258 (9) | 0.0285 (9) | 0.0101 (8) | 0.0054 (7) | 0.0005 (8) |
| C13 | 0.0201 (8) | 0.0334 (10) | 0.0210 (9) | 0.0047 (8) | 0.0067 (6) | 0.0012 (8) |
| C14 | 0.0207 (8) | 0.0276 (9) | 0.0194 (8) | 0.0001 (7) | 0.0039 (6) | 0.0071 (7) |
| C15 | 0.0185 (8) | 0.0193 (8) | 0.0207 (8) | 0.0034 (7) | 0.0023 (6) | 0.0036 (7) |
| C16 | 0.0142 (7) | 0.0234 (9) | 0.0231 (9) | 0.0041 (7) | 0.0080 (6) | 0.0073 (7) |
| C17 | 0.0424 (11) | 0.0262 (10) | 0.0303 (10) | 0.0072 (9) | −0.0033 (8) | −0.0074 (8) |

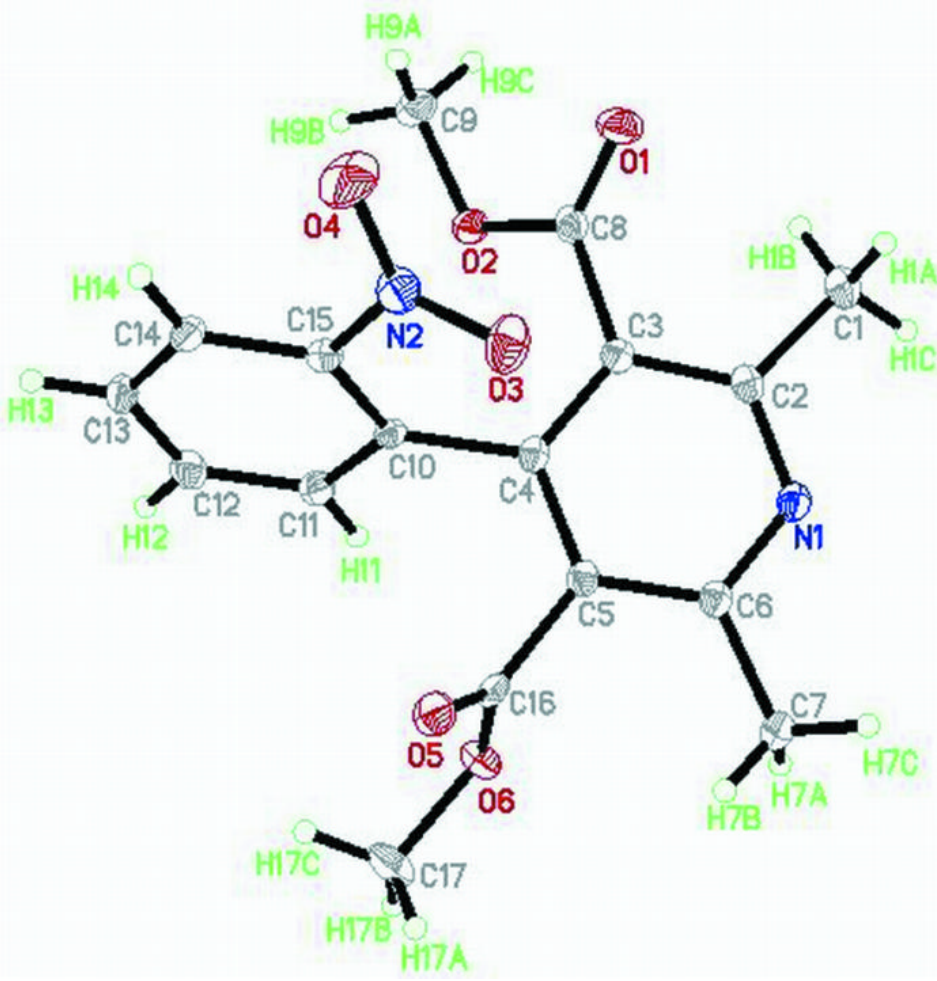
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.2086 (18) | C5—C16 | 1.498 (2) |
| O2—C8 | 1.3392 (18) | C6—C7 | 1.500 (2) |
| O2—C9 | 1.4485 (18) | C7—H7A | 0.9800 |
| O3—N2 | 1.2218 (16) | C7—H7B | 0.9800 |
| O4—N2 | 1.2349 (16) | C7—H7C | 0.9800 |
| O5—C16 | 1.2107 (18) | C9—H9A | 0.9800 |
| O6—C16 | 1.3427 (19) | C9—H9B | 0.9800 |
| O6—C17 | 1.4481 (19) | C9—H9C | 0.9800 |
| N1—C2 | 1.342 (2) | C10—C15 | 1.393 (2) |
| N1—C6 | 1.344 (2) | C10—C11 | 1.394 (2) |
| N2—C15 | 1.478 (2) | C11—C12 | 1.385 (2) |
| C1—C2 | 1.506 (2) | C11—H11 | 0.9500 |
| C1—H1A | 0.9800 | C12—C13 | 1.388 (2) |
| C1—H1B | 0.9800 | C12—H12 | 0.9500 |
| C1—H1C | 0.9800 | C13—C14 | 1.381 (2) |
| C2—C3 | 1.403 (2) | C13—H13 | 0.9500 |
| C3—C4 | 1.401 (2) | C14—C15 | 1.385 (2) |

| | | | |
|---|---|---|---|
| C3—C8 | 1.495 (2) | C14—H14 | 0.9500 |
| C4—C5 | 1.390 (2) | C17—H17A | 0.9800 |
| C4—C10 | 1.502 (2) | C17—H17B | 0.9800 |
| C5—C6 | 1.402 (2) | C17—H17C | 0.9800 |
| C8—O2—C9 | 115.40 (13) | O2—C8—C3 | 111.74 (14) |
| C16—O6—C17 | 115.28 (12) | O2—C9—H9A | 109.5 |
| C2—N1—C6 | 120.11 (13) | O2—C9—H9B | 109.5 |
| O3—N2—O4 | 123.19 (15) | H9A—C9—H9B | 109.5 |
| O3—N2—C15 | 118.96 (13) | O2—C9—H9C | 109.5 |
| O4—N2—C15 | 117.85 (14) | H9A—C9—H9C | 109.5 |
| C2—C1—H1A | 109.5 | H9B—C9—H9C | 109.5 |
| C2—C1—H1B | 109.5 | C15—C10—C11 | 116.86 (13) |
| H1A—C1—H1B | 109.5 | C15—C10—C4 | 125.17 (14) |
| C2—C1—H1C | 109.5 | C11—C10—C4 | 117.94 (13) |
| H1A—C1—H1C | 109.5 | C12—C11—C10 | 121.28 (15) |
| H1B—C1—H1C | 109.5 | C12—C11—H11 | 119.4 |
| N1—C2—C3 | 121.69 (15) | C10—C11—H11 | 119.4 |
| N1—C2—C1 | 114.91 (13) | C11—C12—C13 | 120.22 (15) |
| C3—C2—C1 | 123.39 (14) | C11—C12—H12 | 119.9 |
| C4—C3—C2 | 118.72 (14) | C13—C12—H12 | 119.9 |
| C4—C3—C8 | 121.45 (13) | C14—C13—C12 | 119.93 (14) |
| C2—C3—C8 | 119.83 (14) | C14—C13—H13 | 120.0 |
| C5—C4—C3 | 118.81 (13) | C12—C13—H13 | 120.0 |
| C5—C4—C10 | 118.94 (14) | C13—C14—C15 | 118.90 (15) |
| C3—C4—C10 | 122.20 (13) | C13—C14—H14 | 120.5 |
| C4—C5—C6 | 119.36 (14) | C15—C14—H14 | 120.5 |
| C4—C5—C16 | 119.84 (13) | C14—C15—C10 | 122.80 (15) |
| C6—C5—C16 | 120.80 (14) | C14—C15—N2 | 116.56 (14) |
| N1—C6—C5 | 121.30 (14) | C10—C15—N2 | 120.61 (13) |
| N1—C6—C7 | 116.40 (13) | O5—C16—O6 | 123.94 (15) |
| C5—C6—C7 | 122.30 (14) | O5—C16—C5 | 125.59 (15) |
| C6—C7—H7A | 109.5 | O6—C16—C5 | 110.45 (13) |
| C6—C7—H7B | 109.5 | O6—C17—H17A | 109.5 |
| H7A—C7—H7B | 109.5 | O6—C17—H17B | 109.5 |
| C6—C7—H7C | 109.5 | H17A—C17—H17B | 109.5 |
| H7A—C7—H7C | 109.5 | O6—C17—H17C | 109.5 |
| H7B—C7—H7C | 109.5 | H17A—C17—H17C | 109.5 |
| O1—C8—O2 | 123.61 (15) | H17B—C17—H17C | 109.5 |
| O1—C8—C3 | 124.63 (14) | | |
| C6—N1—C2—C3 | −0.6 (2) | C5—C4—C10—C15 | 115.28 (17) |
| C6—N1—C2—C1 | −179.75 (12) | C3—C4—C10—C15 | −67.4 (2) |
| N1—C2—C3—C4 | 1.1 (2) | C5—C4—C10—C11 | −66.86 (18) |
| C1—C2—C3—C4 | −179.85 (13) | C3—C4—C10—C11 | 110.45 (17) |
| N1—C2—C3—C8 | −179.70 (13) | C15—C10—C11—C12 | 0.4 (2) |
| C1—C2—C3—C8 | −0.7 (2) | C4—C10—C11—C12 | −177.67 (14) |
| C2—C3—C4—C5 | −1.2 (2) | C10—C11—C12—C13 | 0.4 (2) |
| C8—C3—C4—C5 | 179.60 (13) | C11—C12—C13—C14 | −0.7 (2) |
| C2—C3—C4—C10 | −178.56 (13) | C12—C13—C14—C15 | 0.2 (2) |

| | | | |
|---|---|---|---|
| C8—C3—C4—C10 | 2.3 (2) | C13—C14—C15—C10 | 0.6 (2) |
| C3—C4—C5—C6 | 0.9 (2) | C13—C14—C15—N2 | −177.47 (13) |
| C10—C4—C5—C6 | 178.33 (13) | C11—C10—C15—C14 | −0.9 (2) |
| C3—C4—C5—C16 | −178.88 (13) | C4—C10—C15—C14 | 176.99 (14) |
| C10—C4—C5—C16 | −1.5 (2) | C11—C10—C15—N2 | 177.12 (13) |
| C2—N1—C6—C5 | 0.3 (2) | C4—C10—C15—N2 | −5.0 (2) |
| C2—N1—C6—C7 | −179.65 (13) | O3—N2—C15—C14 | 152.38 (14) |
| C4—C5—C6—N1 | −0.5 (2) | O4—N2—C15—C14 | −27.0 (2) |
| C16—C5—C6—N1 | 179.35 (13) | O3—N2—C15—C10 | −25.7 (2) |
| C4—C5—C6—C7 | 179.50 (13) | O4—N2—C15—C10 | 154.89 (15) |
| C16—C5—C6—C7 | −0.7 (2) | C17—O6—C16—O5 | 1.9 (2) |
| C9—O2—C8—O1 | −3.1 (2) | C17—O6—C16—C5 | −176.59 (11) |
| C9—O2—C8—C3 | 175.45 (12) | C4—C5—C16—O5 | −70.6 (2) |
| C4—C3—C8—O1 | 131.12 (17) | C6—C5—C16—O5 | 109.63 (18) |
| C2—C3—C8—O1 | −48.0 (2) | C4—C5—C16—O6 | 107.95 (15) |
| C4—C3—C8—O2 | −47.44 (18) | C6—C5—C16—O6 | −71.86 (17) |
| C2—C3—C8—O2 | 133.40 (14) | | |

**Fig. 1**


H9A
H9C
H9B
C9
O1
O4
O2
C8
H1B
H1A
H14
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N2
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C1
H1C
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H13
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C12
C11
N1
H12
H11
C5
C6
C16
C7
O5
H7C
O6
H7A
H7B
H17C
C17
H17B
H17A