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# 4,4′-Dimethoxy-2,2′-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenol

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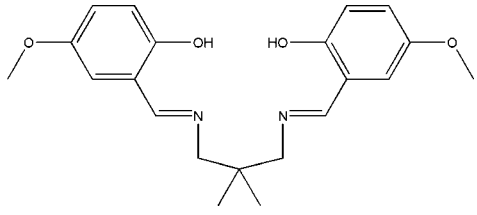
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.031; $wR$ factor = 0.058; data-to-parameter ratio = 13.7.

In the title compound, $C_{21}H_{26}N_2O_4$, the dihedral angle between the substituted benzene rings is 30.47 (15) °. Two strong intramolecular O—H···N hydrogen bonds generate two $S$(6) ring motifs.

## Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Kargar *et al.* (2009, 2010).




## Experimental

### Crystal data

$C_{21}H_{26}N_2O_4$
$M_r$ = 370.44
Monoclinic, $P2_1/c$
$a$ = 10.660 (2) Å
$b$ = 21.742 (4) Å
$c$ = 9.2767 (19) Å
$\beta$ = 108.03 (3)°
$V$ = 2044.5 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 K
0.23 × 0.15 × 0.08 mm

### Data collection

Stoe IPDS 2T Image Plate diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Blessing, 1995)
$T_{min}$ = 0.965, $T_{max}$ = 1.000
7094 measured reflections
3375 independent reflections
967 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.058
$S$ = 0.57
3375 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.11 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.81 | 1.88 | 2.593 (3) | 147 |
| O2—H2···N2 | 0.83 | 1.90 | 2.604 (3) | 143 |

Data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2716).

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# supporting information

*Acta Cryst.* (2011). E**67**, o614 [doi:10.1107/S1600536811004776]

## 4,4′-Dimethoxy-2,2′-[2,2-dimethylpropane-1,3-diylbis(nitrilomethanylylidene)]diphenol

**Hadi Kargar, Reza Kia, Elham Pahlavani and Muhammad Nawaz Tahir**

### S1. Comment

Schiff base ligands are one of the most prevalent systems in coordination chemistry. As part of a general study of potentially tetradenate Schiff bases (Kargar *et al.*, 2009; Kargar *et al.* 2010), we have determined the crystal structure of the title compound.

The asymmetric unit of the title compound, Fig. 1, comprises a potentially tetradenate Schiff base ligand. The bond lengths are comparable to previously reported structures (Kargar *et al.*, 2009, Kargar *et al.*, 2010). The dihedral angle between the two benzene rings is 30.47 (15) °. Strong intramolecular O—H···N hydrogen bonds (Table 1) generate two *S(6)* ring motifs (Bernstein *et al.*, 1995).

### S2. Experimental

The title compound was synthesized by adding 5-methoxy-salicylaldehyde (4 mmol) to a solution of 2,2-dimethyl-1,3-propanediamine (2 mmol) in ethanol (20 ml). The mixture was refluxed with stirring for 30 min. The resultant yellow solution was filtered. Yellow crystals were obtained by slow evaporation of its ethanol solution at room temperature over several days.

### S3. Refinement

H atoms of the hydroxy groups were located in a difference Fourier map and constrained at those positions with $U_{iso}$(H) = 1.5 $U_{eq}$(O), see Table 1 for distances. The remaining H atoms were positioned geometrically with C—H = 0.93–0.97 Å and included in a riding model approximation with $U_{iso}$ (H) = 1.2 or 1.5 $U_{eq}$ (C). A rotating group model was used only for the methyl groups of the methoxy substituents.

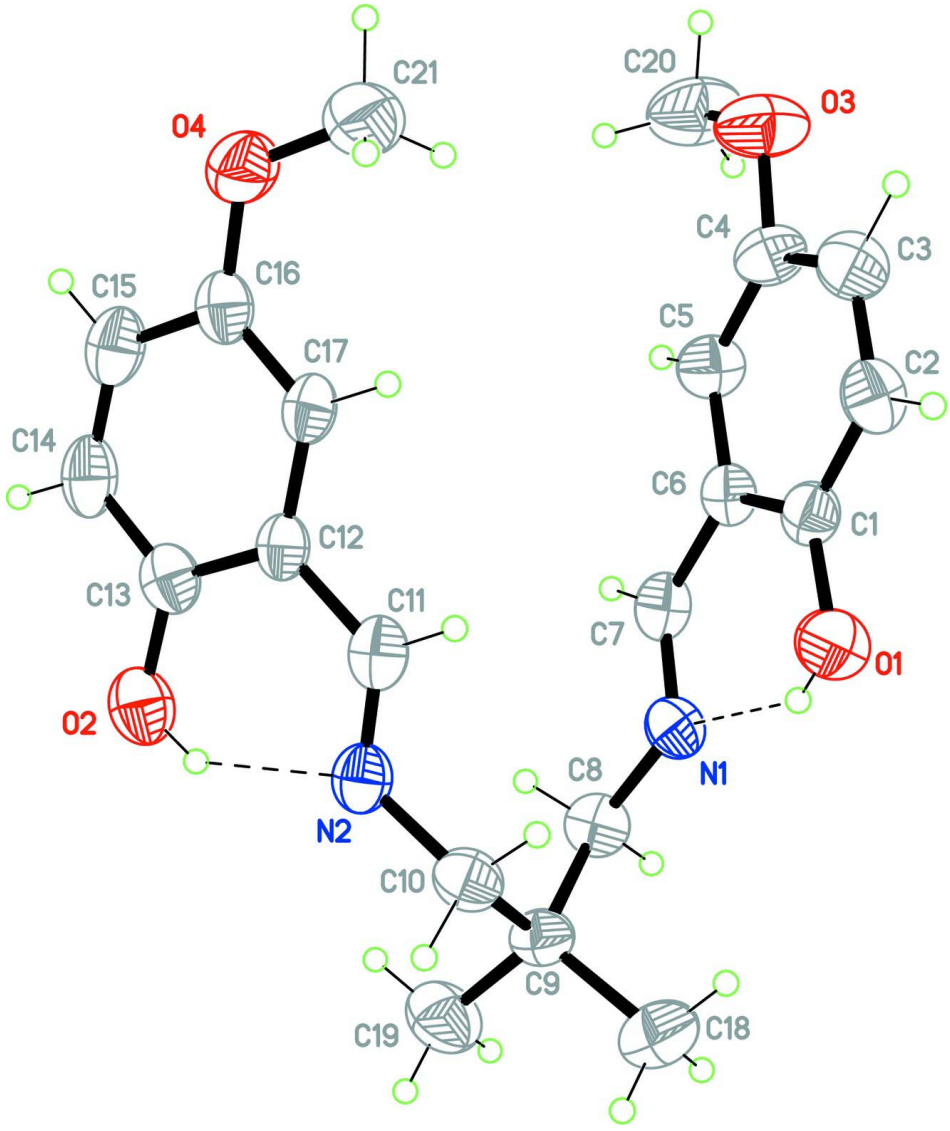


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are drawn as dashed lines.

### 4,4′-Dimethoxy-2,2′-[2,2-dimethylpropane-1,3- diylbis(nitrilomethanylylidene)]diphenol

*Crystal data*

$C_{21}H_{26}N_2O_4$
$M_r = 370.44$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.660\ (2)$ Å
$b = 21.742\ (4)$ Å
$c = 9.2767\ (19)$ Å
$\beta = 108.03\ (3)°$
$V = 2044.5\ (7)$ Å$^3$
$Z = 4$

$F(000) = 792$
$D_x = 1.204$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3220 reflections
$\theta = 2.0–24.2°$
$\mu = 0.08$ mm$^{-1}$
$T = 296$ K
Plate, yellow
0.23 × 0.15 × 0.08 mm

*Data collection*

Stoe IPDS 2T Image Plate diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.15 mm pixels $mm^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*MULABS* in *PLATON*; Blessing, 1995)
$T_{min}$ = 0.965, $T_{max}$ = 1.000
7094 measured reflections
3375 independent reflections
967 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.0°
$h$ = −12→12
$k$ = −22→25
$l$ = −11→10

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.058
$S$ = 0.57
3375 reflections
246 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0172P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.11 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.05846 (17) | 0.01529 (7) | 0.75824 (19) | 0.0807 (6) |
| H1 | −0.0997 | 0.0250 | 0.6727 | 0.121* |
| O2 | −0.1706 (2) | 0.31943 (8) | 0.4769 (2) | 0.0874 (6) |
| H2 | −0.2189 | 0.2892 | 0.4703 | 0.131* |
| O3 | 0.4634 (2) | 0.07957 (10) | 0.8988 (2) | 0.1064 (8) |
| O4 | 0.3081 (2) | 0.30533 (10) | 0.9255 (3) | 0.0936 (7) |
| N1 | −0.1073 (3) | 0.07562 (9) | 0.5057 (3) | 0.0629 (7) |
| N2 | −0.2263 (3) | 0.21006 (10) | 0.5539 (3) | 0.0662 (7) |
| C1 | 0.0688 (3) | 0.03241 (12) | 0.7858 (4) | 0.0601 (8) |
| C2 | 0.1605 (3) | 0.01492 (12) | 0.9224 (3) | 0.0685 (8) |
| H2A | 0.1336 | −0.0083 | 0.9917 | 0.082* |
| C3 | 0.2893 (3) | 0.03161 (12) | 0.9549 (3) | 0.0750 (9) |
| H3A | 0.3502 | 0.0195 | 1.0460 | 0.090* |
| C4 | 0.3300 (3) | 0.06678 (14) | 0.8524 (4) | 0.0720 (9) |
| C5 | 0.2413 (3) | 0.08523 (12) | 0.7179 (3) | 0.0705 (9) |
| H5A | 0.2691 | 0.1088 | 0.6498 | 0.085* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.1091 (3) | 0.06829 (11) | 0.6844 (3) | 0.0557 (8) |
| C7 | 0.0141 (3) | 0.08981 (11) | 0.5447 (3) | 0.0621 (8) |
| H7A | 0.0435 | 0.1151 | 0.4811 | 0.075* |
| C8 | −0.1960 (3) | 0.10405 (11) | 0.3705 (3) | 0.0689 (8) |
| H8A | −0.2106 | 0.0760 | 0.2856 | 0.083* |
| H8B | −0.1554 | 0.1410 | 0.3468 | 0.083* |
| C9 | −0.3286 (3) | 0.12057 (12) | 0.3915 (3) | 0.0647 (8) |
| C10 | −0.3096 (2) | 0.15556 (12) | 0.5410 (3) | 0.0686 (8) |
| H10A | −0.3951 | 0.1680 | 0.5473 | 0.082* |
| H10B | −0.2698 | 0.1282 | 0.6255 | 0.082* |
| C11 | −0.1179 (3) | 0.21062 (13) | 0.6614 (3) | 0.0647 (9) |
| H11A | −0.0969 | 0.1777 | 0.7287 | 0.078* |
| C12 | −0.0261 (3) | 0.26170 (13) | 0.6810 (3) | 0.0550 (8) |
| C13 | −0.0544 (3) | 0.31384 (15) | 0.5877 (3) | 0.0673 (9) |
| C14 | 0.0387 (4) | 0.36057 (13) | 0.6113 (4) | 0.0794 (11) |
| H14A | 0.0205 | 0.3954 | 0.5500 | 0.095* |
| C15 | 0.1556 (4) | 0.35591 (14) | 0.7224 (4) | 0.0804 (10) |
| H15A | 0.2167 | 0.3876 | 0.7359 | 0.096* |
| C16 | 0.1861 (4) | 0.30500 (14) | 0.8166 (4) | 0.0677 (9) |
| C17 | 0.0946 (3) | 0.25820 (12) | 0.7948 (3) | 0.0628 (8) |
| H17A | 0.1140 | 0.2238 | 0.8573 | 0.075* |
| C18 | −0.4084 (2) | 0.06177 (12) | 0.3967 (3) | 0.0982 (10) |
| H18A | −0.3598 | 0.0366 | 0.4803 | 0.147* |
| H18B | −0.4234 | 0.0393 | 0.3038 | 0.147* |
| H18C | −0.4916 | 0.0729 | 0.4092 | 0.147* |
| C19 | −0.4063 (3) | 0.16042 (12) | 0.2556 (3) | 0.0975 (10) |
| H19A | −0.3572 | 0.1971 | 0.2522 | 0.146* |
| H19B | −0.4901 | 0.1713 | 0.2666 | 0.146* |
| H19C | −0.4199 | 0.1376 | 0.1634 | 0.146* |
| C20 | 0.5161 (3) | 0.11165 (14) | 0.7998 (4) | 0.1184 (13) |
| H20A | 0.6098 | 0.1155 | 0.8448 | 0.178* |
| H20B | 0.4771 | 0.1518 | 0.7810 | 0.178* |
| H20C | 0.4974 | 0.0896 | 0.7059 | 0.178* |
| C21 | 0.3454 (3) | 0.25225 (13) | 1.0160 (3) | 0.1204 (13) |
| H21A | 0.4318 | 0.2581 | 1.0868 | 0.181* |
| H21B | 0.3463 | 0.2175 | 0.9525 | 0.181* |
| H21C | 0.2834 | 0.2450 | 1.0703 | 0.181* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0710 (15) | 0.0916 (13) | 0.0825 (14) | −0.0025 (12) | 0.0279 (14) | 0.0249 (11) |
| O2 | 0.1028 (17) | 0.0767 (14) | 0.0822 (16) | 0.0121 (13) | 0.0279 (14) | 0.0188 (12) |
| O3 | 0.0738 (17) | 0.154 (2) | 0.0852 (18) | −0.0283 (16) | 0.0154 (16) | 0.0102 (14) |
| O4 | 0.0945 (18) | 0.0784 (16) | 0.0994 (19) | −0.0159 (14) | 0.0174 (16) | 0.0104 (14) |
| N1 | 0.0633 (17) | 0.0646 (15) | 0.0623 (18) | 0.0079 (15) | 0.0216 (16) | 0.0016 (13) |
| N2 | 0.078 (2) | 0.0597 (16) | 0.0666 (19) | 0.0014 (16) | 0.0305 (16) | −0.0021 (14) |
| C1 | 0.060 (2) | 0.0550 (19) | 0.070 (2) | 0.0004 (17) | 0.027 (2) | −0.0008 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.081 (2) | 0.070 (2) | 0.062 (2) | 0.006 (2) | 0.034 (2) | 0.0144 (17) |
| C3 | 0.076 (3) | 0.085 (2) | 0.063 (2) | 0.003 (2) | 0.021 (2) | 0.0031 (18) |
| C4 | 0.061 (2) | 0.084 (2) | 0.073 (3) | −0.015 (2) | 0.024 (2) | −0.007 (2) |
| C5 | 0.069 (2) | 0.082 (2) | 0.064 (2) | −0.0074 (19) | 0.025 (2) | 0.0053 (18) |
| C6 | 0.062 (2) | 0.0521 (18) | 0.059 (2) | 0.0031 (17) | 0.027 (2) | 0.0024 (16) |
| C7 | 0.079 (2) | 0.0551 (19) | 0.063 (2) | −0.0008 (19) | 0.036 (2) | 0.0015 (16) |
| C8 | 0.072 (2) | 0.077 (2) | 0.060 (2) | 0.0013 (18) | 0.025 (2) | −0.0030 (17) |
| C9 | 0.058 (2) | 0.0713 (19) | 0.061 (2) | −0.0044 (18) | 0.0138 (19) | −0.0057 (17) |
| C10 | 0.058 (2) | 0.082 (2) | 0.071 (2) | 0.0058 (18) | 0.0274 (18) | −0.0003 (17) |
| C11 | 0.086 (3) | 0.058 (2) | 0.062 (2) | 0.003 (2) | 0.039 (2) | −0.0006 (17) |
| C12 | 0.071 (2) | 0.0477 (18) | 0.053 (2) | 0.0033 (18) | 0.0293 (19) | −0.0010 (17) |
| C13 | 0.080 (3) | 0.067 (2) | 0.061 (2) | 0.012 (2) | 0.031 (2) | 0.001 (2) |
| C14 | 0.112 (3) | 0.051 (2) | 0.089 (3) | 0.004 (2) | 0.050 (3) | 0.017 (2) |
| C15 | 0.105 (3) | 0.057 (2) | 0.092 (3) | −0.007 (2) | 0.048 (3) | 0.002 (2) |
| C16 | 0.086 (3) | 0.057 (2) | 0.066 (2) | 0.007 (2) | 0.032 (2) | 0.0060 (19) |
| C17 | 0.082 (2) | 0.0454 (19) | 0.065 (2) | −0.0025 (19) | 0.029 (2) | 0.0042 (16) |
| C18 | 0.085 (2) | 0.099 (2) | 0.102 (3) | −0.023 (2) | 0.017 (2) | −0.015 (2) |
| C19 | 0.093 (2) | 0.108 (2) | 0.078 (2) | 0.017 (2) | 0.006 (2) | 0.012 (2) |
| C20 | 0.082 (3) | 0.161 (3) | 0.113 (3) | −0.043 (2) | 0.032 (2) | 0.014 (2) |
| C21 | 0.114 (3) | 0.098 (3) | 0.119 (3) | −0.014 (2) | −0.008 (2) | 0.028 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.353 (3) | C9—C19 | 1.543 (3) |
| O1—H1 | 0.8074 | C9—C18 | 1.544 (3) |
| O2—C13 | 1.348 (3) | C10—H10A | 0.9700 |
| O2—H2 | 0.8251 | C10—H10B | 0.9700 |
| O3—C4 | 1.381 (3) | C11—C12 | 1.454 (3) |
| O3—C20 | 1.402 (3) | C11—H11A | 0.9300 |
| O4—C16 | 1.377 (3) | C12—C17 | 1.391 (3) |
| O4—C21 | 1.410 (3) | C12—C13 | 1.401 (3) |
| N1—C7 | 1.269 (3) | C13—C14 | 1.390 (3) |
| N1—C8 | 1.455 (3) | C14—C15 | 1.353 (4) |
| N2—C11 | 1.272 (3) | C14—H14A | 0.9300 |
| N2—C10 | 1.463 (3) | C15—C16 | 1.385 (3) |
| C1—C6 | 1.389 (3) | C15—H15A | 0.9300 |
| C1—C2 | 1.392 (3) | C16—C17 | 1.380 (3) |
| C2—C3 | 1.360 (3) | C17—H17A | 0.9300 |
| C2—H2A | 0.9300 | C18—H18A | 0.9600 |
| C3—C4 | 1.390 (3) | C18—H18B | 0.9600 |
| C3—H3A | 0.9300 | C18—H18C | 0.9600 |
| C4—C5 | 1.371 (3) | C19—H19A | 0.9600 |
| C5—C6 | 1.395 (3) | C19—H19B | 0.9600 |
| C5—H5A | 0.9300 | C19—H19C | 0.9600 |
| C6—C7 | 1.453 (3) | C20—H20A | 0.9600 |
| C7—H7A | 0.9300 | C20—H20B | 0.9600 |
| C8—C9 | 1.528 (3) | C20—H20C | 0.9600 |
| C8—H8A | 0.9700 | C21—H21A | 0.9600 |

| | | | |
|---|---|---|---|
| C8—H8B | 0.9700 | C21—H21B | 0.9600 |
| C9—C10 | 1.539 (3) | C21—H21C | 0.9600 |
| | | | |
| C1—O1—H1 | 108.8 | N2—C11—C12 | 121.2 (3) |
| C13—O2—H2 | 112.9 | N2—C11—H11A | 119.4 |
| C4—O3—C20 | 118.6 (3) | C12—C11—H11A | 119.4 |
| C16—O4—C21 | 117.4 (2) | C17—C12—C13 | 119.0 (3) |
| C7—N1—C8 | 118.4 (2) | C17—C12—C11 | 118.8 (3) |
| C11—N2—C10 | 116.9 (3) | C13—C12—C11 | 122.2 (3) |
| O1—C1—C6 | 121.9 (3) | O2—C13—C14 | 119.8 (3) |
| O1—C1—C2 | 118.5 (3) | O2—C13—C12 | 121.0 (3) |
| C6—C1—C2 | 119.5 (3) | C14—C13—C12 | 119.2 (3) |
| C3—C2—C1 | 120.3 (3) | C15—C14—C13 | 120.6 (3) |
| C3—C2—H2A | 119.8 | C15—C14—H14A | 119.7 |
| C1—C2—H2A | 119.8 | C13—C14—H14A | 119.7 |
| C2—C3—C4 | 120.1 (3) | C14—C15—C16 | 121.5 (3) |
| C2—C3—H3A | 119.9 | C14—C15—H15A | 119.3 |
| C4—C3—H3A | 119.9 | C16—C15—H15A | 119.3 |
| C5—C4—O3 | 125.3 (3) | O4—C16—C17 | 125.1 (3) |
| C5—C4—C3 | 120.7 (3) | O4—C16—C15 | 116.3 (3) |
| O3—C4—C3 | 114.0 (3) | C17—C16—C15 | 118.6 (3) |
| C4—C5—C6 | 119.3 (3) | C16—C17—C12 | 121.1 (3) |
| C4—C5—H5A | 120.3 | C16—C17—H17A | 119.4 |
| C6—C5—H5A | 120.3 | C12—C17—H17A | 119.4 |
| C1—C6—C5 | 120.0 (3) | C9—C18—H18A | 109.5 |
| C1—C6—C7 | 120.5 (3) | C9—C18—H18B | 109.5 |
| C5—C6—C7 | 119.4 (3) | H18A—C18—H18B | 109.5 |
| N1—C7—C6 | 123.0 (3) | C9—C18—H18C | 109.5 |
| N1—C7—H7A | 118.5 | H18A—C18—H18C | 109.5 |
| C6—C7—H7A | 118.5 | H18B—C18—H18C | 109.5 |
| N1—C8—C9 | 111.7 (2) | C9—C19—H19A | 109.5 |
| N1—C8—H8A | 109.3 | C9—C19—H19B | 109.5 |
| C9—C8—H8A | 109.3 | H19A—C19—H19B | 109.5 |
| N1—C8—H8B | 109.3 | C9—C19—H19C | 109.5 |
| C9—C8—H8B | 109.3 | H19A—C19—H19C | 109.5 |
| H8A—C8—H8B | 107.9 | H19B—C19—H19C | 109.5 |
| C8—C9—C10 | 111.2 (2) | O3—C20—H20A | 109.5 |
| C8—C9—C19 | 108.1 (2) | O3—C20—H20B | 109.5 |
| C10—C9—C19 | 110.3 (2) | H20A—C20—H20B | 109.5 |
| C8—C9—C18 | 110.4 (2) | O3—C20—H20C | 109.5 |
| C10—C9—C18 | 107.6 (2) | H20A—C20—H20C | 109.5 |
| C19—C9—C18 | 109.2 (2) | H20B—C20—H20C | 109.5 |
| N2—C10—C9 | 112.4 (2) | O4—C21—H21A | 109.5 |
| N2—C10—H10A | 109.1 | O4—C21—H21B | 109.5 |
| C9—C10—H10A | 109.1 | H21A—C21—H21B | 109.5 |
| N2—C10—H10B | 109.1 | O4—C21—H21C | 109.5 |
| C9—C10—H10B | 109.1 | H21A—C21—H21C | 109.5 |
| H10A—C10—H10B | 107.9 | H21B—C21—H21C | 109.5 |

| | | | |
|---|---|---|---|
| O1—C1—C2—C3 | −179.5 (2) | C11—N2—C10—C9 | −116.9 (3) |
| C6—C1—C2—C3 | −1.5 (4) | C8—C9—C10—N2 | 54.6 (3) |
| C1—C2—C3—C4 | 0.6 (4) | C19—C9—C10—N2 | −65.3 (3) |
| C20—O3—C4—C5 | −2.9 (4) | C18—C9—C10—N2 | 175.7 (2) |
| C20—O3—C4—C3 | 176.3 (3) | C10—N2—C11—C12 | 177.96 (19) |
| C2—C3—C4—C5 | 0.2 (4) | N2—C11—C12—C17 | −176.1 (3) |
| C2—C3—C4—O3 | −179.0 (3) | N2—C11—C12—C13 | 3.0 (4) |
| O3—C4—C5—C6 | 179.1 (3) | C17—C12—C13—O2 | −179.4 (2) |
| C3—C4—C5—C6 | −0.1 (4) | C11—C12—C13—O2 | 1.5 (4) |
| O1—C1—C6—C5 | 179.6 (2) | C17—C12—C13—C14 | 0.1 (3) |
| C2—C1—C6—C5 | 1.7 (4) | C11—C12—C13—C14 | −179.0 (2) |
| O1—C1—C6—C7 | 1.1 (4) | O2—C13—C14—C15 | 179.7 (3) |
| C2—C1—C6—C7 | −176.8 (2) | C12—C13—C14—C15 | 0.2 (4) |
| C4—C5—C6—C1 | −0.9 (4) | C13—C14—C15—C16 | −0.4 (5) |
| C4—C5—C6—C7 | 177.6 (3) | C21—O4—C16—C17 | 3.8 (4) |
| C8—N1—C7—C6 | 174.6 (2) | C21—O4—C16—C15 | −175.7 (2) |
| C1—C6—C7—N1 | −2.5 (4) | C14—C15—C16—O4 | 179.9 (3) |
| C5—C6—C7—N1 | 179.0 (3) | C14—C15—C16—C17 | 0.3 (4) |
| C7—N1—C8—C9 | −140.7 (2) | O4—C16—C17—C12 | −179.6 (2) |
| N1—C8—C9—C10 | 48.8 (3) | C15—C16—C17—C12 | −0.1 (4) |
| N1—C8—C9—C19 | 170.1 (2) | C13—C12—C17—C16 | −0.1 (4) |
| N1—C8—C9—C18 | −70.5 (3) | C11—C12—C17—C16 | 179.0 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.81 | 1.88 | 2.593 (3) | 147 |
| O2—H2···N2 | 0.83 | 1.90 | 2.604 (3) | 143 |