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# {2,2′-[Cyclohexane-1,2-diylbis(nitrilomethylidyne)]diphenolato}nickel(II)

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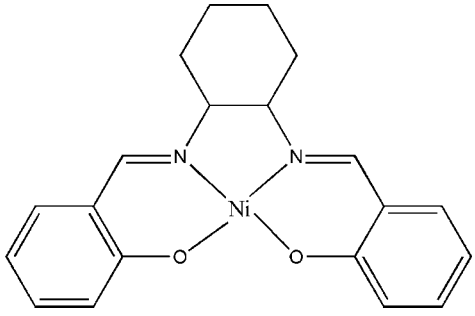
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.027; $wR$ factor = 0.069; data-to-parameter ratio = 16.2.

In the title mononuclear nickel(II) complex, [Ni($C_{20}H_{20}N_2O_2$)], the Ni atom is four-coordinated in a square-planar geometry by the four donor atoms of the Schiff base ligand. The dihedral angle between the two benzene rings is 9.4 (2)°. The cyclohexyl group adopts a *C*-form chair conformation.

## Related literature

For nickel(II) complexes in bio-inorganic chemistry and coordination chemistry, see: Angulo *et al.* (2001); Dey *et al.* (2004); Edison *et al.* (2004); Ramadevi *et al.* (2005); Suh *et al.* (1996). For puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

[Ni($C_{20}H_{20}N_2O_2$)]
$M_r$ = 379.09
Monoclinic, $P2_1/c$
$a$ = 7.6193 (8) Å
$b$ = 19.118 (2) Å
$c$ = 11.5459 (12) Å
$\beta$ = 90.907 (1)°
$V$ = 1681.6 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.17 mm$^{-1}$
$T$ = 298 K
0.30 × 0.30 × 0.28 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.721, $T_{max}$ = 0.735
9694 measured reflections
3650 independent reflections
3023 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.069
$S$ = 1.05
3650 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ni1—O1 | 1.8897 (12) | Ni1—N1 | 1.9435 (15) |
| Ni1—O2 | 1.9125 (12) | Ni1—N2 | 1.9507 (14) |
| O1—Ni1—O2 | 89.22 (5) | O1—Ni1—N2 | 177.83 (6) |
| O1—Ni1—N1 | 93.76 (5) | O2—Ni1—N2 | 92.71 (5) |
| O2—Ni1—N1 | 175.27 (6) | N1—Ni1—N2 | 84.25 (6) |

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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2125).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, m317 [ **doi:10.1107/S1600536809006084** ]

# {2,2'-[Cyclohexane-1,2-diylbis(nitrilomethylidyne)]diphenolato}nickel(II)

**C. Tang**

## Comment

Nickel(II) complexes play an important role in both bioinorganic chemistry and coordination chemistry (Suh *et al.*, 1996; Dey *et al.*, 2004; Angulo *et al.*, 2001; Ramadevi *et al.*, 2005; Edison *et al.*, 2004). As a further study of the structures of such complexes, the title mononuclear nickel(II) complex, (I), is reported in this paper.

In (I), the Ni atom is four-coordinated in a square planar geometry by the four donor atoms of the Schiff base ligand. The dihedral angle between the two benzene rings is 9.4 (2)°. The cyclohexyl group adopts C-form chair conformation with the generalized puckering coordinates; q(3)=-0.569 (1)Å, q(2)=0.009 (1)Å and φ=96.288 (1)° (Cremer & Pople, 1975) (Fig. 1).

## Experimental

Salicylaldehyde (0.2 mmol, 24.5 mg) and cyclohexyl-1,2-diamine (0.1 mmol, 11.4 mg) were dissolved in 10 ml methanol. To the mixture was added dropwise a 5 ml me thanol solution of nickel(II) nitrate hexahydrate (0.2 mmol, 58.2 mg) with stirring. The final solution was allowed to stand in air for two weeks, yielding red block-shaped crystals of (I).

## Refinement

H atoms were constrained to ideal geometries, with C—H = 0.93–0.97Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

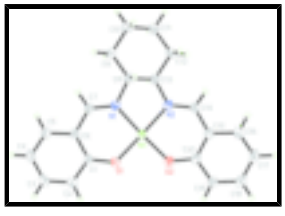

Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

## {2,2'-[Cyclohexane-1,2-diylbis(nitrilomethylidyne)]diphenolato}nickel(II)

*Crystal data*

| | |
|---|---|
| $[Ni(C_{20}H_{20}N_2O_2)]$ | $F_{000}$ = 792 |
| $M_r$ = 379.09 | $D_x$ = 1.497 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $a$ = 7.6193 (8) Å | Cell parameters from 3779 reflections |
| $b$ = 19.118 (2) Å | θ = 2.6–28.6º |

| | |
|---|---|
| $c$ = 11.5459 (12) Å | μ = 1.17 mm$^{-1}$ |
| β = 90.9070 (10)º | $T$ = 298 K |
| $V$ = 1681.6 (3) Å$^3$ | Block, red |
| $Z$ = 4 | 0.30 × 0.30 × 0.28 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3650 independent reflections |
| Radiation source: fine-focus sealed tube | 3023 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.022 |
| $T$ = 298 K | $\theta_{max}$ = 27.0º |
| ω scans | $\theta_{min}$ = 2.1º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −9→9 |
| $T_{min}$ = 0.721, $T_{max}$ = 0.735 | $k$ = −24→24 |
| 9694 measured reflections | $l$ = −14→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.027 | H-atom parameters constrained |
| $wR(F^2)$ = 0.069 | $w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.2023P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.05 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3650 reflections | $\Delta\rho_{max}$ = 0.29 e Å$^{-3}$ |
| 226 parameters | $\Delta\rho_{min}$ = −0.22 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.80232 (3) | 0.468244 (10) | 0.481224 (17) | 0.03293 (8) |

| | | | | |
|---|---|---|---|---|
| O1 | 0.86946 (19) | 0.37326 (6) | 0.49143 (10) | 0.0477 (3) |
| O2 | 0.89546 (18) | 0.48282 (6) | 0.63411 (11) | 0.0484 (3) |
| N1 | 0.6899 (2) | 0.45709 (7) | 0.33007 (12) | 0.0378 (3) |
| N2 | 0.7259 (2) | 0.56527 (7) | 0.46659 (12) | 0.0386 (3) |
| C1 | 0.8626 (2) | 0.32645 (9) | 0.40841 (15) | 0.0395 (4) |
| C2 | 0.9388 (3) | 0.26009 (9) | 0.42918 (17) | 0.0472 (5) |
| H2 | 0.9899 | 0.2508 | 0.5012 | 0.057* |
| C3 | 0.9392 (3) | 0.20924 (9) | 0.34579 (18) | 0.0500 (5) |
| H3 | 0.9903 | 0.1661 | 0.3625 | 0.060* |
| C4 | 0.8651 (3) | 0.22058 (10) | 0.23682 (18) | 0.0526 (5) |
| H4 | 0.8671 | 0.1859 | 0.1804 | 0.063* |
| C5 | 0.7887 (3) | 0.28423 (9) | 0.21422 (17) | 0.0488 (5) |
| H5 | 0.7383 | 0.2923 | 0.1415 | 0.059* |
| C6 | 0.7842 (2) | 0.33781 (9) | 0.29806 (15) | 0.0386 (4) |
| C7 | 0.6995 (2) | 0.40218 (9) | 0.26570 (15) | 0.0412 (4) |
| H7 | 0.6473 | 0.4044 | 0.1924 | 0.049* |
| C8 | 0.5917 (3) | 0.52030 (8) | 0.29253 (16) | 0.0401 (4) |
| H8 | 0.4767 | 0.5185 | 0.3292 | 0.048* |
| C9 | 0.5592 (3) | 0.52841 (9) | 0.16326 (16) | 0.0482 (5) |
| H9A | 0.4894 | 0.4895 | 0.1346 | 0.058* |
| H9B | 0.6703 | 0.5281 | 0.1233 | 0.058* |
| C10 | 0.4630 (3) | 0.59708 (10) | 0.13887 (18) | 0.0565 (5) |
| H10A | 0.4499 | 0.6032 | 0.0558 | 0.068* |
| H10B | 0.3464 | 0.5947 | 0.1712 | 0.068* |
| C11 | 0.5588 (3) | 0.65940 (10) | 0.18949 (17) | 0.0555 (5) |
| H11A | 0.4900 | 0.7013 | 0.1755 | 0.067* |
| H11B | 0.6703 | 0.6649 | 0.1512 | 0.067* |
| C12 | 0.5911 (3) | 0.65080 (9) | 0.31981 (16) | 0.0488 (5) |
| H12A | 0.6590 | 0.6901 | 0.3490 | 0.059* |
| H12B | 0.4797 | 0.6502 | 0.3594 | 0.059* |
| C13 | 0.6899 (2) | 0.58284 (9) | 0.34426 (15) | 0.0419 (4) |
| H13 | 0.8032 | 0.5860 | 0.3056 | 0.050* |
| C14 | 0.7157 (2) | 0.60977 (9) | 0.54952 (16) | 0.0423 (4) |
| H14 | 0.6733 | 0.6541 | 0.5315 | 0.051* |
| C15 | 0.7650 (2) | 0.59611 (9) | 0.66825 (15) | 0.0397 (4) |
| C16 | 0.7300 (3) | 0.64851 (10) | 0.75078 (17) | 0.0478 (5) |
| H16 | 0.6726 | 0.6890 | 0.7268 | 0.057* |
| C17 | 0.7777 (3) | 0.64176 (10) | 0.86443 (17) | 0.0551 (5) |
| H17 | 0.7512 | 0.6766 | 0.9175 | 0.066* |
| C18 | 0.8670 (3) | 0.58153 (11) | 0.89957 (17) | 0.0547 (5) |
| H18 | 0.9010 | 0.5764 | 0.9768 | 0.066* |
| C19 | 0.9054 (3) | 0.52957 (10) | 0.82153 (16) | 0.0478 (5) |
| H19 | 0.9663 | 0.4902 | 0.8469 | 0.057* |
| C20 | 0.8544 (2) | 0.53471 (8) | 0.70409 (15) | 0.0398 (4) |

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

| $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| Ni1 | 0.03599 (14) | 0.03109 (12) | 0.03155 (13) | 0.00174 (9) | −0.00469 (9) | −0.00265 (8) |
| O1 | 0.0670 (9) | 0.0363 (6) | 0.0396 (7) | 0.0052 (6) | −0.0079 (6) | −0.0018 (5) |
| O2 | 0.0549 (9) | 0.0475 (7) | 0.0424 (7) | 0.0133 (6) | −0.0129 (6) | −0.0091 (6) |
| N1 | 0.0390 (9) | 0.0359 (7) | 0.0382 (8) | −0.0005 (6) | −0.0033 (6) | −0.0002 (6) |
| N2 | 0.0408 (9) | 0.0366 (7) | 0.0383 (8) | 0.0000 (6) | −0.0041 (6) | −0.0020 (6) |
| C1 | 0.0409 (10) | 0.0362 (9) | 0.0415 (10) | −0.0038 (7) | 0.0029 (8) | 0.0004 (7) |
| C2 | 0.0541 (12) | 0.0384 (9) | 0.0491 (11) | 0.0025 (8) | −0.0001 (9) | 0.0025 (8) |
| C3 | 0.0547 (13) | 0.0345 (9) | 0.0609 (13) | 0.0020 (8) | 0.0081 (10) | 0.0003 (8) |
| C4 | 0.0640 (14) | 0.0391 (10) | 0.0548 (13) | −0.0022 (9) | 0.0059 (10) | −0.0113 (9) |
| C5 | 0.0580 (13) | 0.0442 (10) | 0.0442 (11) | −0.0040 (9) | −0.0020 (9) | −0.0057 (8) |
| C6 | 0.0406 (10) | 0.0365 (9) | 0.0388 (9) | −0.0046 (7) | 0.0013 (8) | −0.0021 (7) |
| C7 | 0.0441 (11) | 0.0425 (9) | 0.0369 (10) | −0.0049 (8) | −0.0055 (8) | −0.0036 (8) |
| C8 | 0.0400 (10) | 0.0393 (9) | 0.0410 (10) | 0.0001 (7) | −0.0040 (8) | 0.0013 (7) |
| C9 | 0.0525 (12) | 0.0489 (11) | 0.0429 (11) | 0.0013 (9) | −0.0084 (9) | −0.0008 (8) |
| C10 | 0.0652 (14) | 0.0527 (11) | 0.0511 (12) | 0.0051 (10) | −0.0157 (10) | 0.0055 (9) |
| C11 | 0.0613 (14) | 0.0498 (11) | 0.0550 (12) | 0.0024 (10) | −0.0072 (10) | 0.0114 (9) |
| C12 | 0.0562 (13) | 0.0391 (10) | 0.0507 (11) | 0.0022 (9) | −0.0070 (9) | 0.0029 (8) |
| C13 | 0.0437 (11) | 0.0412 (9) | 0.0408 (10) | −0.0031 (8) | −0.0016 (8) | 0.0030 (7) |
| C14 | 0.0443 (11) | 0.0349 (9) | 0.0476 (11) | −0.0004 (8) | −0.0023 (8) | −0.0030 (8) |
| C15 | 0.0389 (10) | 0.0396 (9) | 0.0406 (10) | −0.0043 (8) | 0.0003 (8) | −0.0051 (7) |
| C16 | 0.0510 (12) | 0.0420 (10) | 0.0506 (12) | −0.0018 (9) | 0.0021 (9) | −0.0090 (8) |
| C17 | 0.0660 (14) | 0.0536 (11) | 0.0458 (12) | −0.0066 (10) | 0.0056 (10) | −0.0159 (9) |
| C18 | 0.0616 (14) | 0.0647 (13) | 0.0377 (11) | −0.0109 (10) | −0.0017 (9) | −0.0072 (9) |
| C19 | 0.0515 (12) | 0.0506 (11) | 0.0413 (11) | −0.0033 (9) | −0.0053 (9) | −0.0010 (8) |
| C20 | 0.0376 (10) | 0.0426 (9) | 0.0391 (10) | −0.0050 (8) | −0.0010 (8) | −0.0047 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O1 | 1.8897 (12) | C9—C10 | 1.528 (2) |
| Ni1—O2 | 1.9125 (12) | C9—H9A | 0.9700 |
| Ni1—N1 | 1.9435 (15) | C9—H9B | 0.9700 |
| Ni1—N2 | 1.9507 (14) | C10—C11 | 1.510 (3) |
| O1—C1 | 1.312 (2) | C10—H10A | 0.9700 |
| O2—C20 | 1.320 (2) | C10—H10B | 0.9700 |
| N1—C7 | 1.289 (2) | C11—C12 | 1.530 (3) |
| N1—C8 | 1.483 (2) | C11—H11A | 0.9700 |
| N2—C14 | 1.284 (2) | C11—H11B | 0.9700 |
| N2—C13 | 1.473 (2) | C12—C13 | 1.526 (2) |
| C1—C2 | 1.414 (2) | C12—H12A | 0.9700 |
| C1—C6 | 1.415 (2) | C12—H12B | 0.9700 |
| C2—C3 | 1.368 (2) | C13—H13 | 0.9800 |
| C2—H2 | 0.9300 | C14—C15 | 1.439 (2) |
| C3—C4 | 1.388 (3) | C14—H14 | 0.9300 |
| C3—H3 | 0.9300 | C15—C16 | 1.411 (2) |
| C4—C5 | 1.372 (3) | C15—C20 | 1.416 (2) |
| C4—H4 | 0.9300 | C16—C17 | 1.362 (3) |
| C5—C6 | 1.410 (2) | C16—H16 | 0.9300 |
| C5—H5 | 0.9300 | C17—C18 | 1.394 (3) |
| C6—C7 | 1.437 (2) | C17—H17 | 0.9300 |

| | | | |
|---|---|---|---|
| C7—H7 | 0.9300 | C18—C19 | 1.376 (3) |
| C8—C9 | 1.517 (2) | C18—H18 | 0.9300 |
| C8—C13 | 1.527 (2) | C19—C20 | 1.408 (3) |
| C8—H8 | 0.9800 | C19—H19 | 0.9300 |
| O1—Ni1—O2 | 89.22 (5) | H9A—C9—H9B | 108.2 |
| O1—Ni1—N1 | 93.76 (5) | C11—C10—C9 | 112.26 (17) |
| O2—Ni1—N1 | 175.27 (6) | C11—C10—H10A | 109.2 |
| O1—Ni1—N2 | 177.83 (6) | C9—C10—H10A | 109.2 |
| O2—Ni1—N2 | 92.71 (5) | C11—C10—H10B | 109.2 |
| N1—Ni1—N2 | 84.25 (6) | C9—C10—H10B | 109.2 |
| C1—O1—Ni1 | 127.04 (11) | H10A—C10—H10B | 107.9 |
| C20—O2—Ni1 | 125.90 (11) | C10—C11—C12 | 111.42 (16) |
| C7—N1—C8 | 121.87 (15) | C10—C11—H11A | 109.3 |
| C7—N1—Ni1 | 125.39 (12) | C12—C11—H11A | 109.3 |
| C8—N1—Ni1 | 112.73 (10) | C10—C11—H11B | 109.3 |
| C14—N2—C13 | 123.45 (15) | C12—C11—H11B | 109.3 |
| C14—N2—Ni1 | 125.94 (13) | H11A—C11—H11B | 108.0 |
| C13—N2—Ni1 | 110.53 (10) | C13—C12—C11 | 110.17 (16) |
| O1—C1—C2 | 118.46 (16) | C13—C12—H12A | 109.6 |
| O1—C1—C6 | 124.38 (16) | C11—C12—H12A | 109.6 |
| C2—C1—C6 | 117.16 (16) | C13—C12—H12B | 109.6 |
| C3—C2—C1 | 121.58 (18) | C11—C12—H12B | 109.6 |
| C3—C2—H2 | 119.2 | H12A—C12—H12B | 108.1 |
| C1—C2—H2 | 119.2 | N2—C13—C12 | 117.09 (15) |
| C2—C3—C4 | 121.41 (18) | N2—C13—C8 | 106.20 (13) |
| C2—C3—H3 | 119.3 | C12—C13—C8 | 110.91 (15) |
| C4—C3—H3 | 119.3 | N2—C13—H13 | 107.4 |
| C5—C4—C3 | 118.45 (18) | C12—C13—H13 | 107.4 |
| C5—C4—H4 | 120.8 | C8—C13—H13 | 107.4 |
| C3—C4—H4 | 120.8 | N2—C14—C15 | 124.88 (16) |
| C4—C5—C6 | 121.89 (19) | N2—C14—H14 | 117.6 |
| C4—C5—H5 | 119.1 | C15—C14—H14 | 117.6 |
| C6—C5—H5 | 119.1 | C16—C15—C20 | 119.10 (16) |
| C5—C6—C1 | 119.49 (16) | C16—C15—C14 | 117.73 (16) |
| C5—C6—C7 | 117.35 (16) | C20—C15—C14 | 123.08 (15) |
| C1—C6—C7 | 123.16 (15) | C17—C16—C15 | 122.23 (18) |
| N1—C7—C6 | 125.24 (16) | C17—C16—H16 | 118.9 |
| N1—C7—H7 | 117.4 | C15—C16—H16 | 118.9 |
| C6—C7—H7 | 117.4 | C16—C17—C18 | 118.67 (18) |
| N1—C8—C9 | 116.41 (14) | C16—C17—H17 | 120.7 |
| N1—C8—C13 | 106.37 (14) | C18—C17—H17 | 120.7 |
| C9—C8—C13 | 112.08 (15) | C19—C18—C17 | 120.90 (19) |
| N1—C8—H8 | 107.2 | C19—C18—H18 | 119.5 |
| C9—C8—H8 | 107.2 | C17—C18—H18 | 119.5 |
| C13—C8—H8 | 107.2 | C18—C19—C20 | 121.48 (18) |
| C8—C9—C10 | 109.85 (15) | C18—C19—H19 | 119.3 |
| C8—C9—H9A | 109.7 | C20—C19—H19 | 119.3 |
| C10—C9—H9A | 109.7 | O2—C20—C19 | 118.21 (16) |
| C8—C9—H9B | 109.7 | O2—C20—C15 | 124.17 (16) |

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|---|---|---|---|
| C10—C9—H9B | 109.7 | C19—C20—C15 | 117.61 (16) |

**Fig. 1**