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# (*E*)-*N*,*N*-Diethyl-3-hydroxy-3,5-diphenylpent-4-enamide

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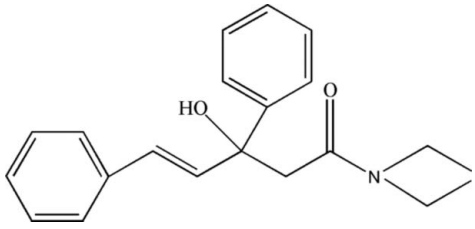
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.054; $wR$ factor = 0.202; data-to-parameter ratio = 14.9.

The title compound, $C_{21}H_{25}NO_2$, was synthesized by a Reformatsky-type reaction. In the molecule, the dihedral angle between the two phenyl rings is 66.1 (1)° and the crystal packing exhibits no classical hydrogen bonds.

## Related literature

For related literature, see: Ocamp & Doliber (2004).




## Experimental

### Crystal data

$C_{21}H_{25}NO_2$
$M_r$ = 323.42
Orthorhombic, *Pbca*
$a$ = 10.156 (3) Å
$b$ = 10.339 (4) Å
$c$ = 35.621 (12) Å
$V$ = 3741 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 294 (2) K
0.22 × 0.20 × 0.16 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.984, $T_{max}$ = 0.988
11761 measured reflections
3271 independent reflections
1480 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.202
$S$ = 1.03
3271 reflections
220 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997; data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2270).

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# supplementary materials

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# (*E*)-*N*,*N*-Diethyl-3-hydroxy-3,5-diphenylpent-4-enamide

**Z.-F. Yu, Y.-G. Li, J. Li and Z.-M. Zhao**

## Comment

The Reformatsky reaction provides a good strategy of carbon-carbon bond formation (Ocamp & Doliber, 2004). In our study on the Reformatsky-type reaction of α-bromoacetamide with α,β-unsaturated ketone, we found that the most attractive feature of the reaction is its chemoselectivity, and a new compound, (I), has been synthesized by reaction of 1,3-diphenyl-propenone with *N*,*N*-diethyl-2-bromoacetamide. The structure determination of compound (I) was undertaken and the results are presented here.

The bond distances and angles are in good agreement with those respective normal values. In compound (I), the dihedral angle between the two phenyl rings is 113.9 (1)°, and the carbon-carbon double bond adopts E-configuration, which is also confirmed by the respective coupling constant (J = 16 Hz) in the $^1$H NMR spectroscopy of compound (I). The torsion angle of C6—C7—C8 —C9 is -179.3 (3) °, which indicates that they are approximately coplannar. The bond distance of C17—N1 [1.334 (4) Å] is significantly shorter than those of C18—N1 [1.482 (4) Å] and C20—N1 [1.487 (5) Å] because of *p*-π conjugation.

## Experimental

To a solution of 1,3-diphenyl-propenone (1 mmol) in dichloromethane (5 ml), *N*,*N*-diethyl-2-bromoacetamide (2 mmol), zinc powder (3 mmol) and a trace amount of iodine were added to the mixture in order. The reaction mixture was refluxed with stirring for 5 h and then quenched with a saturated solution of ammonium chloride (8 ml). The mixture was filtered and extracted with dichloromethane, dried over magnesium sulfate. After evaporation of the solvent, a white solid was obtained (0.236 g, yield 73%) by column chromatography (silica gel/petroleum ether-ethyl acetate = 7/3, v/v). The colorless single crystals of compound was obtained through the evaporation of ethyl acetate-petroleum ether. Spectroscopic analysis: IR (KBr, νcm$^{-1}$):3293, 1613; $^1$H NMR ($CDCl_3$, δ, p.p.m.): 7.54-7.18 (m, 10H), 6.82 (s, 1H), 6.67 (d, 1H), 6.47 (d, 1H), 3.29 ( m , 4H), 2.99 (d, 1H), 2.90 (d, 1H), 1.16 (t, 3H), 0.98 (t, 3H).

## Refinement

All carbon H atoms were positioned geometrically and refined as riding (C—H = 0.93 - 0.97 Å). For the CH and $CH_2$ groups, $U_{iso}$(H) values were set equal to 1.2$U_{eq}$(C) and for the methyl groups, they were set equal to 1.5$U_{eq}$(C). Atom H1 was refined with O1—H1 = 0.82 Å and $U_{iso}$(H) = 1.5$U_{eq}$(O).

## Figures

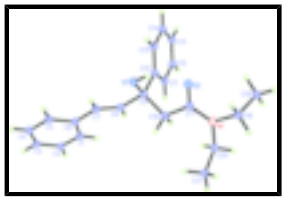


Fig. 1. View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

## (*E*)—*N*,*N*-Diethyl-3-hydroxy-3,5-diphenylpent-4-enamide

*Crystal data*

| | |
|---|---|
| $C_{21}H_{25}NO_2$ | $D_x$ = 1.149 Mg m$^{-3}$ |
| $M_r$ = 323.42 | Melting point: 318 K |
| Orthorhombic, *Pbca* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 1542 reflections |
| *a* = 10.156 (3) Å | θ = 2.3–20.5º |
| *b* = 10.339 (4) Å | μ = 0.07 mm$^{-1}$ |
| *c* = 35.621 (12) Å | *T* = 294 (2) K |
| *V* = 3741 (2) Å$^3$ | Needle, colourless |
| *Z* = 8 | 0.22 × 0.20 × 0.16 mm |
| $F_{000}$ = 1392 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3271 independent reflections |
| Radiation source: fine-focus sealed tube | 1480 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.060 |
| *T* = 294(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 1.1º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −11→11 |
| $T_{min}$ = 0.984, $T_{max}$ = 0.988 | *k* = −12→5 |
| 11761 measured reflections | *l* = −42→34 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.054 | $w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.1641P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.202 | $(\Delta/\sigma)_{max} < 0.001$ |
| *S* = 1.03 | $\Delta\rho_{max}$ = 0.14 e Å$^{-3}$ |

3271 reflections
220 parameters
12 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Extinction correction: none

*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 $F^2 > 2\text{sigma}(F^2)$ 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 | −0.0108 (2) | 0.4384 (2) | 0.34952 (6) | 0.0708 (7) |
| H1 | −0.0179 | 0.4120 | 0.3279 | 0.106* |
| O2 | 0.0823 (3) | 0.2997 (3) | 0.29268 (6) | 0.0793 (8) |
| N1 | 0.2939 (3) | 0.2396 (3) | 0.29241 (7) | 0.0690 (9) |
| C1 | 0.1788 (4) | 0.5408 (4) | 0.48042 (10) | 0.0810 (12) |
| H1A | 0.2237 | 0.4649 | 0.4747 | 0.097* |
| C2 | 0.2020 (4) | 0.6018 (5) | 0.51398 (11) | 0.0945 (14) |
| H2 | 0.2622 | 0.5666 | 0.5308 | 0.113* |
| C3 | 0.1385 (5) | 0.7126 (5) | 0.52296 (12) | 0.0944 (14) |
| H3 | 0.1554 | 0.7532 | 0.5458 | 0.113* |
| C4 | 0.0503 (5) | 0.7645 (4) | 0.49870 (13) | 0.0993 (15) |
| H4 | 0.0064 | 0.8406 | 0.5048 | 0.119* |
| C5 | 0.0261 (4) | 0.7036 (4) | 0.46502 (10) | 0.0831 (12) |
| H5 | −0.0348 | 0.7394 | 0.4485 | 0.100* |
| C6 | 0.0898 (3) | 0.5906 (3) | 0.45503 (8) | 0.0592 (9) |
| C7 | 0.0603 (3) | 0.5289 (4) | 0.41901 (8) | 0.0621 (9) |
| H7 | 0.0076 | 0.5752 | 0.4024 | 0.074* |
| C8 | 0.1004 (3) | 0.4155 (4) | 0.40781 (8) | 0.0586 (9) |
| H8 | 0.1524 | 0.3686 | 0.4244 | 0.070* |
| C9 | 0.0707 (3) | 0.3528 (3) | 0.37033 (8) | 0.0546 (9) |
| C10 | 0.0025 (3) | 0.2238 (3) | 0.37714 (8) | 0.0536 (9) |
| C11 | 0.0664 (4) | 0.1252 (4) | 0.39667 (10) | 0.0740 (11) |
| H11 | 0.1530 | 0.1382 | 0.4043 | 0.089* |
| C12 | 0.0074 (6) | 0.0114 (5) | 0.40498 (12) | 0.0988 (14) |
| H12 | 0.0531 | −0.0519 | 0.4182 | 0.119* |
| C13 | −0.1177 (7) | −0.0099 (5) | 0.39410 (13) | 0.1073 (17) |
| H13 | −0.1579 | −0.0882 | 0.3999 | 0.129* |

| | | | | |
|---|---|---|---|---|
| C14 | −0.1873 (4) | 0.0831 (6) | 0.37449 (12) | 0.0945 (15) |
| H14 | −0.2736 | 0.0679 | 0.3670 | 0.113* |
| C15 | −0.1249 (4) | 0.2011 (4) | 0.36615 (9) | 0.0746 (11) |
| H15 | −0.1707 | 0.2645 | 0.3530 | 0.089* |
| C16 | 0.2026 (3) | 0.3355 (4) | 0.34956 (8) | 0.0631 (10) |
| H16A | 0.2484 | 0.4178 | 0.3492 | 0.076* |
| H16B | 0.2566 | 0.2747 | 0.3634 | 0.076* |
| C17 | 0.1878 (4) | 0.2876 (3) | 0.30959 (9) | 0.0565 (9) |
| C18 | 0.2871 (4) | 0.2085 (4) | 0.25183 (9) | 0.0767 (11) |
| H18A | 0.2266 | 0.2676 | 0.2396 | 0.092* |
| H18B | 0.3733 | 0.2203 | 0.2407 | 0.092* |
| C19 | 0.2427 (5) | 0.0740 (4) | 0.24549 (13) | 0.1223 (17) |
| H19A | 0.3028 | 0.0152 | 0.2574 | 0.183* |
| H19B | 0.2400 | 0.0567 | 0.2190 | 0.183* |
| H19C | 0.1563 | 0.0627 | 0.2560 | 0.183* |
| C20 | 0.4265 (5) | 0.2287 (5) | 0.30977 (11) | 0.1050 (17) |
| H20A | 0.4744 | 0.1586 | 0.2979 | 0.126* |
| H20B | 0.4170 | 0.2078 | 0.3362 | 0.126* |
| C21 | 0.5042 (5) | 0.3523 (7) | 0.30588 (13) | 0.133 (2) |
| H21A | 0.5124 | 0.3741 | 0.2798 | 0.199* |
| H21B | 0.5902 | 0.3406 | 0.3165 | 0.199* |
| H21C | 0.4595 | 0.4208 | 0.3188 | 0.199* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0724 (17) | 0.0813 (17) | 0.0586 (13) | 0.0152 (13) | −0.0094 (13) | −0.0002 (12) |
| O2 | 0.0540 (16) | 0.129 (2) | 0.0554 (13) | −0.0034 (15) | −0.0014 (12) | −0.0159 (14) |
| N1 | 0.065 (2) | 0.088 (2) | 0.0539 (16) | 0.0176 (17) | 0.0032 (16) | −0.0027 (14) |
| C1 | 0.083 (3) | 0.098 (3) | 0.062 (2) | 0.011 (2) | −0.008 (2) | −0.019 (2) |
| C2 | 0.098 (4) | 0.124 (4) | 0.062 (2) | 0.000 (3) | −0.009 (2) | −0.020 (3) |
| C3 | 0.103 (4) | 0.114 (4) | 0.067 (3) | −0.033 (3) | 0.016 (3) | −0.028 (3) |
| C4 | 0.124 (4) | 0.079 (3) | 0.095 (3) | −0.002 (3) | 0.008 (3) | −0.030 (3) |
| C5 | 0.102 (3) | 0.073 (3) | 0.075 (2) | 0.002 (2) | −0.005 (2) | −0.010 (2) |
| C6 | 0.061 (2) | 0.066 (2) | 0.0509 (18) | −0.0086 (19) | 0.0087 (18) | −0.0026 (17) |
| C7 | 0.062 (2) | 0.070 (3) | 0.0534 (19) | −0.003 (2) | −0.0007 (17) | 0.0001 (18) |
| C8 | 0.054 (2) | 0.073 (3) | 0.0491 (18) | −0.0012 (19) | 0.0007 (15) | −0.0031 (17) |
| C9 | 0.0411 (19) | 0.075 (2) | 0.0479 (17) | 0.0050 (18) | −0.0027 (15) | −0.0011 (16) |
| C10 | 0.045 (2) | 0.072 (2) | 0.0440 (16) | −0.0017 (19) | 0.0070 (16) | −0.0115 (17) |
| C11 | 0.072 (3) | 0.080 (3) | 0.070 (2) | −0.008 (2) | 0.001 (2) | −0.002 (2) |
| C12 | 0.121 (4) | 0.092 (4) | 0.083 (3) | −0.014 (3) | 0.001 (3) | −0.002 (3) |
| C13 | 0.153 (6) | 0.101 (4) | 0.067 (3) | −0.036 (4) | 0.029 (3) | −0.006 (3) |
| C14 | 0.070 (3) | 0.135 (4) | 0.078 (3) | −0.044 (3) | 0.019 (2) | −0.036 (3) |
| C15 | 0.054 (2) | 0.107 (3) | 0.063 (2) | −0.004 (2) | 0.0058 (19) | −0.017 (2) |
| C16 | 0.050 (2) | 0.087 (3) | 0.0518 (18) | −0.0079 (19) | 0.0039 (16) | −0.0057 (17) |
| C17 | 0.049 (2) | 0.068 (2) | 0.0527 (19) | −0.0041 (19) | 0.0037 (18) | 0.0024 (17) |
| C18 | 0.082 (3) | 0.086 (3) | 0.062 (2) | 0.011 (2) | 0.009 (2) | −0.002 (2) |
| C19 | 0.182 (5) | 0.084 (3) | 0.101 (3) | 0.009 (3) | −0.002 (3) | −0.015 (3) |

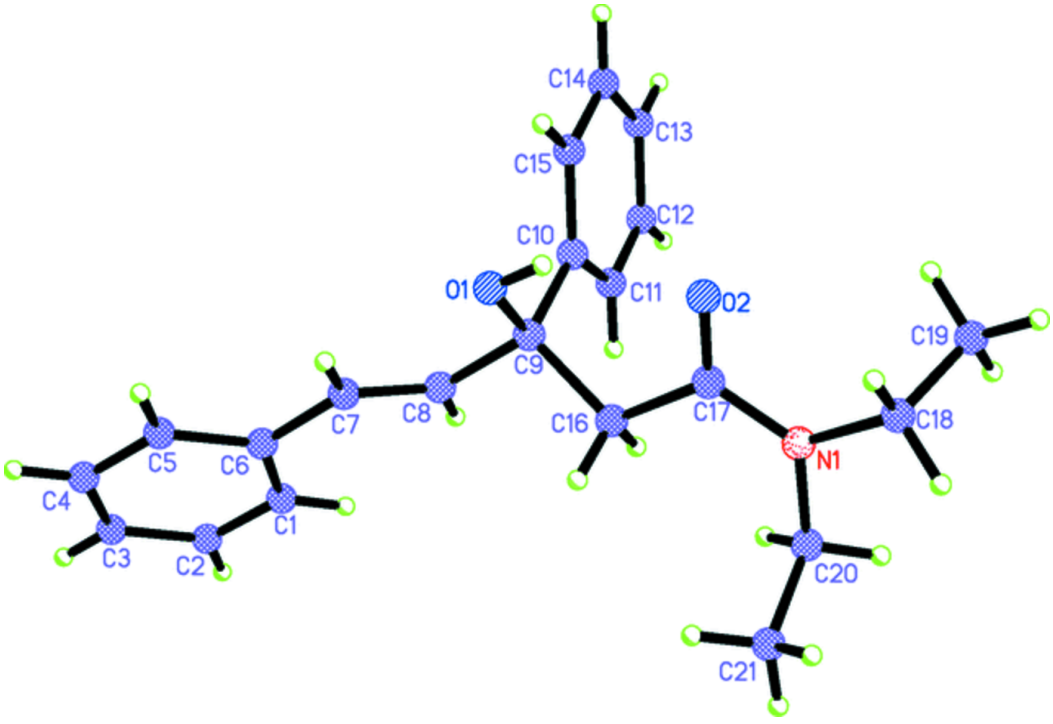
| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.099 (4) | 0.151 (5) | 0.065 (2) | 0.061 (4) | 0.006 (3) | 0.000 (3) |
| C21 | 0.080 (3) | 0.210 (6) | 0.108 (3) | −0.008 (4) | −0.001 (3) | −0.037 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C9 | 1.421 (4) | C10—C11 | 1.395 (5) |
| O1—H1 | 0.8200 | C11—C12 | 1.353 (6) |
| O2—C17 | 1.235 (4) | C11—H11 | 0.9300 |
| N1—C17 | 1.334 (4) | C12—C13 | 1.347 (6) |
| N1—C18 | 1.482 (4) | C12—H12 | 0.9300 |
| N1—C20 | 1.487 (5) | C13—C14 | 1.382 (6) |
| C1—C2 | 1.372 (5) | C13—H13 | 0.9300 |
| C1—C6 | 1.378 (5) | C14—C15 | 1.406 (6) |
| C1—H1A | 0.9300 | C14—H14 | 0.9300 |
| C2—C3 | 1.353 (6) | C15—H15 | 0.9300 |
| C2—H2 | 0.9300 | C16—C17 | 1.515 (4) |
| C3—C4 | 1.356 (6) | C16—H16A | 0.9700 |
| C3—H3 | 0.9300 | C16—H16B | 0.9700 |
| C4—C5 | 1.377 (5) | C18—C19 | 1.480 (5) |
| C4—H4 | 0.9300 | C18—H18A | 0.9700 |
| C5—C6 | 1.382 (5) | C18—H18B | 0.9700 |
| C5—H5 | 0.9300 | C19—H19A | 0.9600 |
| C6—C7 | 1.464 (4) | C19—H19B | 0.9600 |
| C7—C8 | 1.303 (4) | C19—H19C | 0.9600 |
| C7—H7 | 0.9300 | C20—C21 | 1.508 (7) |
| C8—C9 | 1.515 (4) | C20—H20A | 0.9700 |
| C8—H8 | 0.9300 | C20—H20B | 0.9700 |
| C9—C10 | 1.521 (5) | C21—H21A | 0.9600 |
| C9—C16 | 1.540 (4) | C21—H21B | 0.9600 |
| C10—C15 | 1.373 (5) | C21—H21C | 0.9600 |
| C9—O1—H1 | 109.5 | C12—C13—C14 | 120.9 (5) |
| C17—N1—C18 | 119.3 (3) | C12—C13—H13 | 119.5 |
| C17—N1—C20 | 124.7 (3) | C14—C13—H13 | 119.5 |
| C18—N1—C20 | 115.6 (3) | C13—C14—C15 | 118.7 (4) |
| C2—C1—C6 | 120.8 (4) | C13—C14—H14 | 120.7 |
| C2—C1—H1A | 119.6 | C15—C14—H14 | 120.7 |
| C6—C1—H1A | 119.6 | C10—C15—C14 | 120.9 (4) |
| C3—C2—C1 | 120.9 (4) | C10—C15—H15 | 119.6 |
| C3—C2—H2 | 119.6 | C14—C15—H15 | 119.6 |
| C1—C2—H2 | 119.6 | C17—C16—C9 | 113.8 (3) |
| C2—C3—C4 | 120.0 (4) | C17—C16—H16A | 108.8 |
| C2—C3—H3 | 120.0 | C9—C16—H16A | 108.8 |
| C4—C3—H3 | 120.0 | C17—C16—H16B | 108.8 |
| C3—C4—C5 | 119.5 (4) | C9—C16—H16B | 108.8 |
| C3—C4—H4 | 120.2 | H16A—C16—H16B | 107.7 |
| C5—C4—H4 | 120.2 | O2—C17—N1 | 120.9 (3) |
| C4—C5—C6 | 121.8 (4) | O2—C17—C16 | 120.7 (3) |
| C4—C5—H5 | 119.1 | N1—C17—C16 | 118.2 (3) |
| C6—C5—H5 | 119.1 | C19—C18—N1 | 111.6 (3) |

| | | | |
|---|---|---|---|
| C1—C6—C5 | 117.0 (3) | C19—C18—H18A | 109.3 |
| C1—C6—C7 | 123.1 (3) | N1—C18—H18A | 109.3 |
| C5—C6—C7 | 119.9 (3) | C19—C18—H18B | 109.3 |
| C8—C7—C6 | 126.6 (3) | N1—C18—H18B | 109.3 |
| C8—C7—H7 | 116.7 | H18A—C18—H18B | 108.0 |
| C6—C7—H7 | 116.7 | C18—C19—H19A | 109.5 |
| C7—C8—C9 | 126.4 (3) | C18—C19—H19B | 109.5 |
| C7—C8—H8 | 116.8 | H19A—C19—H19B | 109.5 |
| C9—C8—H8 | 116.8 | C18—C19—H19C | 109.5 |
| O1—C9—C8 | 108.0 (3) | H19A—C19—H19C | 109.5 |
| O1—C9—C10 | 111.3 (3) | H19B—C19—H19C | 109.5 |
| C8—C9—C10 | 109.0 (2) | N1—C20—C21 | 111.8 (4) |
| O1—C9—C16 | 109.2 (2) | N1—C20—H20A | 109.3 |
| C8—C9—C16 | 107.4 (2) | C21—C20—H20A | 109.3 |
| C10—C9—C16 | 111.8 (3) | N1—C20—H20B | 109.3 |
| C15—C10—C11 | 117.1 (4) | C21—C20—H20B | 109.3 |
| C15—C10—C9 | 122.3 (3) | H20A—C20—H20B | 107.9 |
| C11—C10—C9 | 120.6 (3) | C20—C21—H21A | 109.5 |
| C12—C11—C10 | 122.6 (4) | C20—C21—H21B | 109.5 |
| C12—C11—H11 | 118.7 | H21A—C21—H21B | 109.5 |
| C10—C11—H11 | 118.7 | C20—C21—H21C | 109.5 |
| C13—C12—C11 | 119.8 (5) | H21A—C21—H21C | 109.5 |
| C13—C12—H12 | 120.1 | H21B—C21—H21C | 109.5 |
| C11—C12—H12 | 120.1 | | |
| C6—C1—C2—C3 | −0.2 (6) | C9—C10—C11—C12 | 176.7 (3) |
| C1—C2—C3—C4 | 0.2 (7) | C10—C11—C12—C13 | 0.3 (6) |
| C2—C3—C4—C5 | 0.0 (7) | C11—C12—C13—C14 | 0.0 (6) |
| C3—C4—C5—C6 | −0.3 (7) | C12—C13—C14—C15 | −0.2 (6) |
| C2—C1—C6—C5 | 0.0 (5) | C11—C10—C15—C14 | 0.1 (5) |
| C2—C1—C6—C7 | −179.4 (3) | C9—C10—C15—C14 | −176.8 (3) |
| C4—C5—C6—C1 | 0.3 (6) | C13—C14—C15—C10 | 0.1 (5) |
| C4—C5—C6—C7 | 179.7 (4) | O1—C9—C16—C17 | −56.6 (4) |
| C1—C6—C7—C8 | 8.0 (6) | C8—C9—C16—C17 | −173.4 (3) |
| C5—C6—C7—C8 | −171.4 (4) | C10—C9—C16—C17 | 67.0 (4) |
| C6—C7—C8—C9 | −179.3 (3) | C18—N1—C17—O2 | 4.0 (5) |
| C7—C8—C9—O1 | −0.9 (5) | C20—N1—C17—O2 | 176.3 (4) |
| C7—C8—C9—C10 | −122.0 (4) | C18—N1—C17—C16 | −171.8 (3) |
| C7—C8—C9—C16 | 116.7 (4) | C20—N1—C17—C16 | 0.5 (5) |
| O1—C9—C10—C15 | −4.0 (4) | C9—C16—C17—O2 | 20.4 (5) |
| C8—C9—C10—C15 | 115.1 (3) | C9—C16—C17—N1 | −163.8 (3) |
| C16—C9—C10—C15 | −126.3 (3) | C17—N1—C18—C19 | −89.5 (4) |
| O1—C9—C10—C11 | 179.2 (3) | C20—N1—C18—C19 | 97.5 (4) |
| C8—C9—C10—C11 | −61.8 (4) | C17—N1—C20—C21 | −85.4 (4) |
| C16—C9—C10—C11 | 56.8 (4) | C18—N1—C20—C21 | 87.2 (4) |
| C15—C10—C11—C12 | −0.3 (5) | | |

**Fig. 1**


C14
C13
C15
C12
C10
O1
C11
O2
C19
C9
C7
C8
C16
C17
C18
C5
C6
N1
C4
C1
C3
C2
C20
C21