Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (*E*)-*N*-{(*E*)-2-[(3,5-Dimethylbiphenyl-4-yl)imino]acenaphthen-1-ylidene}-2,6-dimethyl-4-phenylaniline

**Jianchao Yuan,* Xiaoli Xie, Yufeng Liu, Chengping Miao and Jing Li**

Key Laboratory of Eco-Environment-Related Polymer Materials of the Ministry of Education, Key Laboratory of Polymer Materials of Gansu Province, College of Chemistry & Chemical Engineering, Northwest Normal University, Lanzhou 730070, People's Republic of China
Correspondence e-mail: jianchaoyuan@nwnu.edu.cn

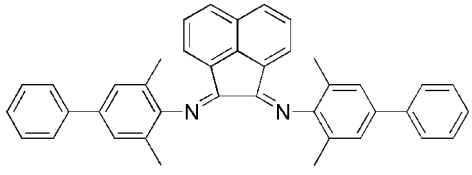
Received 14 November 2011; accepted 15 December 2011

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.059; $wR$ factor = 0.211; data-to-parameter ratio = 14.8.

The title compound, $C_{40}H_{32}N_2$, has crystallographic twofold rotation symmetry, with two C atoms lying on the axis. The dihedral angle between the two benzene rings of the 4-phenyl-2,6-dimethylphenyl group is 35.74 (17)°. The acenaphthene ring makes an angle of 76.93 (11)° with the benzene ring bonded to the N atom and an angle of 41.53 (13)° with the other benzene ring.

## Related literature

The title compound was synthesized as an $\alpha$-diimine ligand for use in $Ni^{II}$–$\alpha$-diimine olefin polymerization catalysts. For applications of metal-organic polymerization catalysts, see: Johnson *et al.* (1995); Killian *et al.* (1996); Popeney *et al.* (2005, 2010, 2011). For a related structure, see: Lohr *et al.* (2011).



## Experimental

### Crystal data

$C_{40}H_{32}N_2$
$M_r$ = 540.68
Monoclinic, $C2/c$
$a$ = 22.994 (14) Å
$b$ = 8.676 (5) Å
$c$ = 18.652 (18) Å
$\beta$ = 124.084 (4)°
$V$ = 3082 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 296 K
0.23 × 0.21 × 0.19 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
$T_{min}$ = 0.985, $T_{max}$ = 0.987
10667 measured reflections
2857 independent reflections
1596 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.211
$S$ = 1.16
2857 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); software used to prepare material for publication: *SHELXTL*.

We thank the National Natural Science Foundation of China (20964003) for funding. We also thank the Key Laboratory of Eco Environment-Related Polymer Materials of the Ministry of Education, Key Laboratory of Polymer Materials of Gansu Province (Northwest Normal University), for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2034).

## References

Bruker (2008). *SAINT* and *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, L. K., Killian, C. M. & Brookhart, M. (1995). *J. Am. Chem. Soc.* **117**, 6414–6415.
Killian, C. M., Tempel, D. J., Johnson, L. K. & Brookhart, M. (1996). *J. Am. Chem. Soc.* **118**, 11664–11665.
Lohr, T. L., Piers, W. E. & Parvez, M. (2011). *Acta Cryst.* E**67**, o2280.
Popeney, C. & Guan, Z. B. (2005). *Organometallics*, **24**, 1145–1155.
Popeney, C. S. & Guan, Z. B. (2010). *Macromolecules*, **43**, 4091–4097.
Popeney, C. S., Levins, C. M. & Guan, Z. B. (2011). *Organometallics*, **30**, 2432–2452.
Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o210 [ **doi:10.1107/S1600536811054092** ]

# (*E*)-*N*-{(*E*)-2-[(3,5-Dimethylbiphenyl-4-yl)imino]acenaphthen-1-ylidene}-2,6-dimethyl-4-phenylaniline

**J. Yuan, X. Xie, Y. Liu, C. Miao and J. Li**

## Comment

In recent years, α-diimine nickel catalysts have drawn wide-spread attention due to their high catalytic activity in ethylene polymerization (Johnson *et al.*, 1995; Killian *et al.*, 1996). It is well known that the ligand structure has significant influence on the product properties and polymerization activities (Popeney *et al.*, 2011; Popeney *et al*., 2010; Popeney *et al.*, 2005). In this study, we designed and synthesized the title compound as a bidentate ligand, and its molecular structure was characterized by X-ray diffraction.

## Experimental

Formic acid (1 ml) was added to a stirred solution of acenaphthenequinone (0.25 g, 1.37 mmol) and 4-phenyl-2,6-dimehylaniline (0.54 g, 2.74 mmol) in methanol (20 ml). The mixture was refluxed for 24 h, then cooled and the precipitate was separated by filtration. The solid was recrystallized from ethanol/dichloromethane (*v*/*v* = 8:1), washed and dried under vacuum. Yield: 0.55 g (74%). Anal. Calcd. for $C_{40}H_{32}N_2$: C, 88.85; H, 5.97; N, 5.18. Found: C, 88.91; H, 6.03; N, 5.06. Crystals suitable for X-ray structure determination were grown from a solution of the title compound in a mixture of cyclohexane/dichloromethane (1:2, *v*/*v*) by slow evaporation.

## Refinement

All hydrogen atoms were placed in calculated positions with C—H distances of 0.93 and 0.96 Å for aryl and methyl type H-atoms, respectively. They were included in the refinement in a riding model approximation. The H-atoms were assigned *U*iso = 1.2 times $U_{eq}$ of the aryl C atoms and 1.5 times $U_{eq}$ of the methyl C atoms.

## Figures

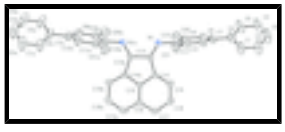


Fig. 1. Structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H-atoms have been excluded for clarity. The atom name suffix indicates symmetry code (a): –*x*, *y*, –*z* + 1/2.

### (*E*)-*N*-{(*E*)-2-[(3,5-Dimethylbiphenyl-4- yl)imino]acenaphthen-1-ylidene}-2,6-dimethyl-4-phenylaniline

*Crystal data*

| | |
|---|---|
| $C_{40}H_{32}N_2$ | $F(000)$ = 1144 |
| $M_r$ = 540.68 | $D_x$ = 1.165 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| *a* = 22.994 (14) Å | Cell parameters from 3073 reflections |

| | |
|---|---|
| $b$ = 8.676 (5) Å | θ = 2.1–25.7° |
| $c$ = 18.652 (18) Å | μ = 0.07 mm$^{-1}$ |
| β = 124.084 (4)° | $T$ = 296 K |
| $V$ = 3082 (4) Å$^3$ | Block, red |
| $Z$ = 4 | 0.23 × 0.21 × 0.19 mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 2857 independent reflections |
| Radiation source: fine-focus sealed tube | 1596 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int}$ = 0.031 |
| φ and ω scans | $\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.1° |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*) | $h$ = −27→27 |
| $T_{min}$ = 0.985, $T_{max}$ = 0.987 | $k$ = −10→10 |
| 10667 measured reflections | $l$ = −22→20 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.059 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.211 | H-atom parameters constrained |
| $S$ = 1.16 | $w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 3.4006P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2857 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 193 parameters | $\Delta\rho_{max}$ = 0.23 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.20 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.2760 (2) | 0.8437 (6) | 0.7549 (2) | 0.1024 (15) |

| | | | | |
|---|---|---|---|---|
| H1 | 0.2411 | 0.7699 | 0.7368 | 0.123* |
| C2 | 0.3295 (3) | 0.8543 (8) | 0.8419 (3) | 0.132 (2) |
| H2 | 0.3303 | 0.7877 | 0.8815 | 0.159* |
| C3 | 0.3807 (3) | 0.9614 (9) | 0.8696 (3) | 0.135 (3) |
| H3 | 0.4158 | 0.9705 | 0.9283 | 0.162* |
| C4 | 0.3807 (2) | 1.0559 (8) | 0.8112 (4) | 0.126 (2) |
| H4 | 0.4165 | 1.1278 | 0.8300 | 0.151* |
| C5 | 0.3271 (2) | 1.0452 (6) | 0.7229 (3) | 0.1089 (16) |
| H5 | 0.3277 | 1.1089 | 0.6832 | 0.131* |
| C6 | 0.27359 (18) | 0.9396 (5) | 0.6951 (2) | 0.0804 (11) |
| C7 | 0.21565 (18) | 0.9254 (4) | 0.6012 (2) | 0.0691 (9) |
| C8 | 0.22787 (19) | 0.9461 (4) | 0.5373 (2) | 0.0719 (10) |
| H8 | 0.2729 | 0.9726 | 0.5534 | 0.086* |
| C9 | 0.1758 (2) | 0.9289 (4) | 0.4504 (2) | 0.0707 (10) |
| C10 | 0.10860 (19) | 0.8859 (3) | 0.42739 (19) | 0.0639 (9) |
| C11 | 0.09402 (17) | 0.8687 (4) | 0.4894 (2) | 0.0668 (9) |
| C12 | 0.14776 (18) | 0.8885 (4) | 0.5757 (2) | 0.0720 (10) |
| H12 | 0.1382 | 0.8768 | 0.6177 | 0.086* |
| C13 | 0.02861 (17) | 0.7530 (3) | 0.29823 (18) | 0.0617 (9) |
| C14 | 0.04351 (15) | 0.5886 (3) | 0.32523 (18) | 0.0526 (8) |
| C15 | 0.0000 | 0.5015 (4) | 0.2500 | 0.0497 (10) |
| C16 | 0.0000 | 0.3396 (5) | 0.2500 | 0.0642 (12) |
| C17 | 0.0457 (2) | 0.2681 (4) | 0.3300 (2) | 0.0833 (12) |
| H17 | 0.0476 | 0.1610 | 0.3334 | 0.100* |
| C18 | 0.08782 (19) | 0.3537 (4) | 0.4034 (2) | 0.0753 (10) |
| H18 | 0.1177 | 0.3028 | 0.4555 | 0.090* |
| C19 | 0.08738 (16) | 0.5154 (3) | 0.4025 (2) | 0.0619 (9) |
| H19 | 0.1162 | 0.5712 | 0.4532 | 0.074* |
| C20 | 0.1907 (3) | 0.9524 (5) | 0.3822 (2) | 0.1042 (15) |
| H20A | 0.2376 | 0.9908 | 0.4088 | 0.156* |
| H20B | 0.1579 | 1.0253 | 0.3402 | 0.156* |
| H20C | 0.1861 | 0.8559 | 0.3542 | 0.156* |
| C21 | 0.02117 (19) | 0.8275 (5) | 0.4649 (3) | 0.0984 (14) |
| H21A | −0.0123 | 0.8974 | 0.4212 | 0.148* |
| H21B | 0.0194 | 0.8350 | 0.5151 | 0.148* |
| H21C | 0.0101 | 0.7240 | 0.4430 | 0.148* |
| N1 | 0.05454 (16) | 0.8787 (3) | 0.33777 (16) | 0.0755 (9) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.081 (3) | 0.157 (4) | 0.056 (2) | 0.001 (3) | 0.030 (2) | −0.013 (3) |
| C2 | 0.095 (3) | 0.217 (7) | 0.060 (3) | 0.012 (4) | 0.028 (3) | −0.017 (3) |
| C3 | 0.071 (3) | 0.239 (7) | 0.071 (3) | 0.023 (4) | 0.025 (3) | −0.055 (4) |
| C4 | 0.070 (3) | 0.205 (6) | 0.098 (4) | −0.027 (3) | 0.044 (3) | −0.082 (4) |
| C5 | 0.080 (3) | 0.158 (5) | 0.082 (3) | −0.031 (3) | 0.041 (2) | −0.059 (3) |
| C6 | 0.064 (2) | 0.113 (3) | 0.060 (2) | −0.005 (2) | 0.0321 (19) | −0.030 (2) |
| C7 | 0.070 (2) | 0.074 (2) | 0.054 (2) | −0.0068 (17) | 0.0291 (18) | −0.0192 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.077 (2) | 0.070 (2) | 0.063 (2) | −0.0172 (18) | 0.0356 (19) | −0.0174 (17) |
| C9 | 0.095 (3) | 0.0485 (18) | 0.058 (2) | −0.0117 (18) | 0.036 (2) | −0.0076 (15) |
| C10 | 0.084 (2) | 0.0305 (15) | 0.0465 (19) | 0.0000 (15) | 0.0174 (18) | −0.0051 (12) |
| C11 | 0.063 (2) | 0.0528 (19) | 0.060 (2) | −0.0019 (15) | 0.0198 (17) | −0.0129 (15) |
| C12 | 0.067 (2) | 0.082 (2) | 0.059 (2) | −0.0036 (18) | 0.0293 (18) | −0.0152 (17) |
| C13 | 0.080 (2) | 0.0283 (15) | 0.0504 (17) | −0.0004 (14) | 0.0208 (16) | −0.0002 (12) |
| C14 | 0.0646 (18) | 0.0322 (15) | 0.0498 (17) | 0.0021 (13) | 0.0252 (15) | 0.0007 (12) |
| C15 | 0.063 (2) | 0.0282 (19) | 0.051 (2) | 0.000 | 0.027 (2) | 0.000 |
| C16 | 0.078 (3) | 0.036 (2) | 0.064 (3) | 0.000 | 0.031 (3) | 0.000 |
| C17 | 0.102 (3) | 0.0344 (17) | 0.087 (3) | 0.0073 (17) | 0.036 (2) | 0.0108 (17) |
| C18 | 0.086 (2) | 0.050 (2) | 0.065 (2) | 0.0111 (17) | 0.0268 (19) | 0.0197 (17) |
| C19 | 0.073 (2) | 0.0420 (17) | 0.0547 (19) | 0.0052 (15) | 0.0257 (17) | 0.0054 (14) |
| C20 | 0.145 (4) | 0.091 (3) | 0.073 (3) | −0.020 (3) | 0.059 (3) | 0.001 (2) |
| C21 | 0.067 (2) | 0.105 (3) | 0.091 (3) | −0.003 (2) | 0.025 (2) | −0.028 (2) |
| N1 | 0.100 (2) | 0.0295 (13) | 0.0510 (16) | −0.0021 (13) | 0.0140 (15) | −0.0045 (11) |

*Geometric parameters (Å, °)*

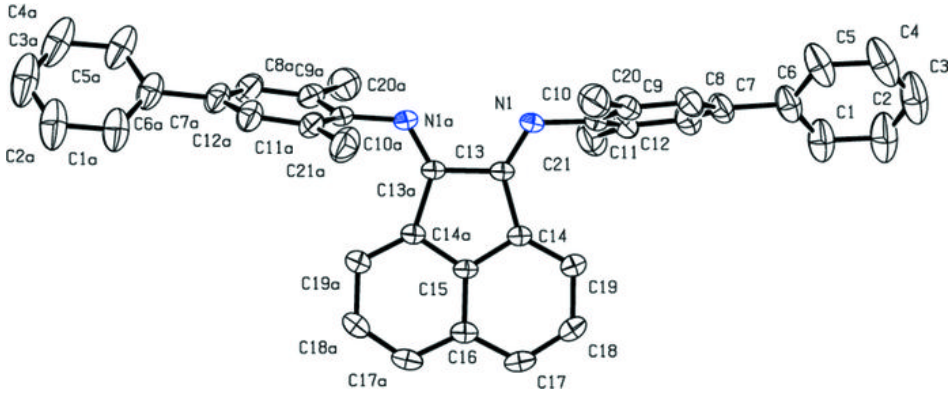
| | | | |
|---|---|---|---|
| C1—C6 | 1.368 (6) | C12—H12 | 0.9300 |
| C1—C2 | 1.386 (6) | C13—N1 | 1.263 (4) |
| C1—H1 | 0.9300 | C13—C14 | 1.487 (4) |
| C2—C3 | 1.355 (8) | C13—C13$^{i}$ | 1.522 (6) |
| C2—H2 | 0.9300 | C14—C19 | 1.368 (4) |
| C3—C4 | 1.363 (8) | C14—C15 | 1.403 (3) |
| C3—H3 | 0.9300 | C15—C14$^{i}$ | 1.403 (3) |
| C4—C5 | 1.402 (6) | C15—C16 | 1.404 (6) |
| C4—H4 | 0.9300 | C16—C17$^{i}$ | 1.400 (4) |
| C5—C6 | 1.381 (6) | C16—C17 | 1.400 (4) |
| C5—H5 | 0.9300 | C17—C18 | 1.370 (5) |
| C6—C7 | 1.497 (5) | C17—H17 | 0.9300 |
| C7—C8 | 1.381 (5) | C18—C19 | 1.403 (4) |
| C7—C12 | 1.391 (5) | C18—H18 | 0.9300 |
| C8—C9 | 1.382 (4) | C19—H19 | 0.9300 |
| C8—H8 | 0.9300 | C20—H20A | 0.9600 |
| C9—C10 | 1.404 (5) | C20—H20B | 0.9600 |
| C9—C20 | 1.504 (5) | C20—H20C | 0.9600 |
| C10—C11 | 1.381 (5) | C21—H21A | 0.9600 |
| C10—N1 | 1.419 (4) | C21—H21B | 0.9600 |
| C11—C12 | 1.385 (4) | C21—H21C | 0.9600 |
| C11—C21 | 1.512 (5) | | |
| C6—C1—C2 | 121.2 (5) | C7—C12—H12 | 119.2 |
| C6—C1—H1 | 119.4 | N1—C13—C14 | 133.3 (3) |
| C2—C1—H1 | 119.4 | N1—C13—C13$^{i}$ | 120.18 (17) |
| C3—C2—C1 | 120.3 (6) | C14—C13—C13$^{i}$ | 106.44 (15) |
| C3—C2—H2 | 119.9 | C19—C14—C15 | 119.7 (3) |
| C1—C2—H2 | 119.9 | C19—C14—C13 | 134.2 (3) |
| C2—C3—C4 | 119.8 (5) | C15—C14—C13 | 106.2 (2) |
| C2—C3—H3 | 120.1 | C14$^{i}$—C15—C14 | 114.8 (3) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 120.1 | $C14^{i}$—C15—C16 | 122.62 (17) |
| C3—C4—C5 | 120.4 (5) | C14—C15—C16 | 122.62 (17) |
| C3—C4—H4 | 119.8 | $C17^{i}$—C16—C17 | 127.3 (4) |
| C5—C4—H4 | 119.8 | $C17^{i}$—C16—C15 | 116.3 (2) |
| C6—C5—C4 | 119.8 (5) | C17—C16—C15 | 116.3 (2) |
| C6—C5—H5 | 120.1 | C18—C17—C16 | 120.8 (3) |
| C4—C5—H5 | 120.1 | C18—C17—H17 | 119.6 |
| C1—C6—C5 | 118.5 (4) | C16—C17—H17 | 119.6 |
| C1—C6—C7 | 120.4 (4) | C17—C18—C19 | 122.3 (3) |
| C5—C6—C7 | 121.1 (4) | C17—C18—H18 | 118.8 |
| C8—C7—C12 | 117.9 (3) | C19—C18—H18 | 118.8 |
| C8—C7—C6 | 121.4 (3) | C14—C19—C18 | 118.2 (3) |
| C12—C7—C6 | 120.8 (3) | C14—C19—H19 | 120.9 |
| C9—C8—C7 | 122.5 (3) | C18—C19—H19 | 120.9 |
| C9—C8—H8 | 118.7 | C9—C20—H20A | 109.5 |
| C7—C8—H8 | 118.7 | C9—C20—H20B | 109.5 |
| C8—C9—C10 | 117.9 (3) | H20A—C20—H20B | 109.5 |
| C8—C9—C20 | 121.3 (4) | C9—C20—H20C | 109.5 |
| C10—C9—C20 | 120.8 (3) | H20A—C20—H20C | 109.5 |
| C11—C10—C9 | 121.0 (3) | H20B—C20—H20C | 109.5 |
| C11—C10—N1 | 121.2 (3) | C11—C21—H21A | 109.5 |
| C9—C10—N1 | 117.3 (3) | C11—C21—H21B | 109.5 |
| C10—C11—C12 | 118.9 (3) | H21A—C21—H21B | 109.5 |
| C10—C11—C21 | 121.4 (3) | C11—C21—H21C | 109.5 |
| C12—C11—C21 | 119.7 (4) | H21A—C21—H21C | 109.5 |
| C11—C12—C7 | 121.7 (3) | H21B—C21—H21C | 109.5 |
| C11—C12—H12 | 119.2 | C13—N1—C10 | 122.7 (2) |
| C6—C1—C2—C3 | 0.3 (8) | C21—C11—C12—C7 | 179.6 (3) |
| C1—C2—C3—C4 | −2.0 (8) | C8—C7—C12—C11 | 1.7 (5) |
| C2—C3—C4—C5 | 1.5 (8) | C6—C7—C12—C11 | −177.3 (3) |
| C3—C4—C5—C6 | 0.8 (7) | N1—C13—C14—C19 | 4.2 (7) |
| C2—C1—C6—C5 | 2.0 (7) | $C13^{i}$—C13—C14—C19 | −178.1 (4) |
| C2—C1—C6—C7 | 179.5 (4) | N1—C13—C14—C15 | −176.1 (4) |
| C4—C5—C6—C1 | −2.5 (6) | $C13^{i}$—C13—C14—C15 | 1.6 (4) |
| C4—C5—C6—C7 | 180.0 (4) | C19—C14—C15—$C14^{i}$ | 179.1 (3) |
| C1—C6—C7—C8 | −142.6 (4) | C13—C14—C15—$C14^{i}$ | −0.65 (17) |
| C5—C6—C7—C8 | 34.9 (5) | C19—C14—C15—C16 | −0.9 (3) |
| C1—C6—C7—C12 | 36.4 (5) | C13—C14—C15—C16 | 179.35 (17) |
| C5—C6—C7—C12 | −146.1 (4) | $C14^{i}$—C15—C16—$C17^{i}$ | 0.5 (2) |
| C12—C7—C8—C9 | −1.1 (5) | C14—C15—C16—$C17^{i}$ | −179.5 (2) |
| C6—C7—C8—C9 | 177.9 (3) | $C14^{i}$—C15—C16—C17 | −179.5 (2) |
| C7—C8—C9—C10 | −1.3 (5) | C14—C15—C16—C17 | 0.5 (2) |
| C7—C8—C9—C20 | 179.9 (3) | $C17^{i}$—C16—C17—C18 | 179.8 (4) |
| C8—C9—C10—C11 | 3.2 (5) | C15—C16—C17—C18 | −0.2 (4) |
| C20—C9—C10—C11 | −178.0 (3) | C16—C17—C18—C19 | 0.1 (6) |
| C8—C9—C10—N1 | 175.9 (3) | C15—C14—C19—C18 | 0.8 (5) |

| | | | |
|---|---|---|---|
| C20—C9—C10—N1 | −5.3 (5) | C13—C14—C19—C18 | −179.5 (4) |
| C9—C10—C11—C12 | −2.7 (5) | C17—C18—C19—C14 | −0.5 (6) |
| N1—C10—C11—C12 | −175.1 (3) | C14—C13—N1—C10 | −1.7 (7) |
| C9—C10—C11—C21 | 177.9 (3) | $C13^{i}$—C13—N1—C10 | −179.2 (4) |
| N1—C10—C11—C21 | 5.5 (5) | C11—C10—N1—C13 | −78.7 (5) |
| C10—C11—C12—C7 | 0.2 (5) | C9—C10—N1—C13 | 108.6 (4) |

Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

**Fig. 1**


C4a
C3a
C5a
C6a
C7a
C2a
C1a
C8a
C9a
C20a
C12a
C11a
C10a
C21a
N1a
C13
C13a
C14a
C14
C19a
C15
C19
C18a
C16
C18
C17a
C17
N1
C10
C20
C9
C8
C7
C6
C5
C4
C3
C2
C1
C21
C11
C12