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# Benzil bis(ketazine)

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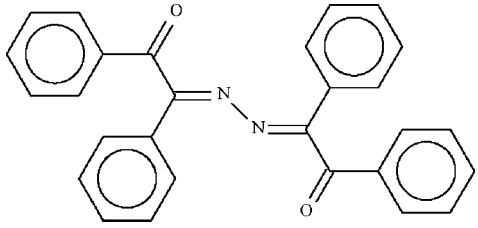
Key indicators: single-crystal X-ray study; $T$ = 140 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.040; $wR$ factor = 0.107; data-to-parameter ratio = 16.8.

The title compound (systematic name: 1,1′,2,2′-tetraphenyl-2,2′-azinodiethanone), $C_{28}H_{20}N_2O_2$, was obtained by the reaction of benzil monohydrazone with chromium(III) nitrate. The dibenzylidene hydrazine unit is nearly planar (r.m.s. deviation = 0.073 Å) and the two benzoyl units are oriented almost perpendicular to it [dihedral angle = 87.81 (2), 87.81 (2)°]. The molecules are linked into chains along the $c$ axis by C—H···O hydrogen bonds and the chains are cross-linked *via* C—H···$\pi$ interactions involving the benzoyl phenyl rings.

## Related literature

For the synthesis of title compound using copper bis(acetylacetonate) as catalyst, see: Ibata & Singh (1994); Singh (1983).




## Experimental

### Crystal data

$C_{28}H_{20}N_2O_2$
$M_r$ = 416.46
Monoclinic, $P2_1/c$
$a$ = 8.2875 (2) Å
$b$ = 22.1023 (4) Å
$c$ = 11.6602 (2) Å
$\beta$ = 97.539 (1)°
$V$ = 2117.37 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 140 K
0.30 × 0.04 × 0.03 mm

### Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: none
17323 measured reflections
4857 independent reflections
3510 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
$S$ = 1.03
4857 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O1$^{i}$ | 0.95 | 2.24 | 3.0832 (16) | 147 |
| C13—H13···$Cg1^{ii}$ | 0.95 | 2.68 | 3.5705 (16) | 157 |
| C18—H18···$Cg2^{iii}$ | 0.95 | 2.66 | 3.5304 (16) | 153 |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $x-1, y, z$. $Cg1$ and $Cg2$ are centroids of the C1–C6 and C23–C28 rings, respectively.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

The authors thank Vijaygarh Jyotish Ray College and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2835).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, o1745 [doi:10.1107/S1600536809024489]

## Benzil bis(ketazine)

**Goutam Kumar Patra, Anindita Mukherjee and Seik Weng Ng**

### S1. Experimental

Benzil monohydrazone (0.224 g, 1 mmol) was dissolved in acetonitrile (20 ml) and to this was added chromium nitrate nonahyrate (0.40 g, 1 mmol). The greenish yellowish mixture was stirred at room temperature for 6 h. Bright yellow prisms were collected in 40% yield.

### S2. Refinement

H-atoms were placed in calculated positions (C-H = 0.95 Å) and were included in the refinement in the riding model approximation, with $U_{iso}$(H) set to 1.2$U_{eq}$(C).

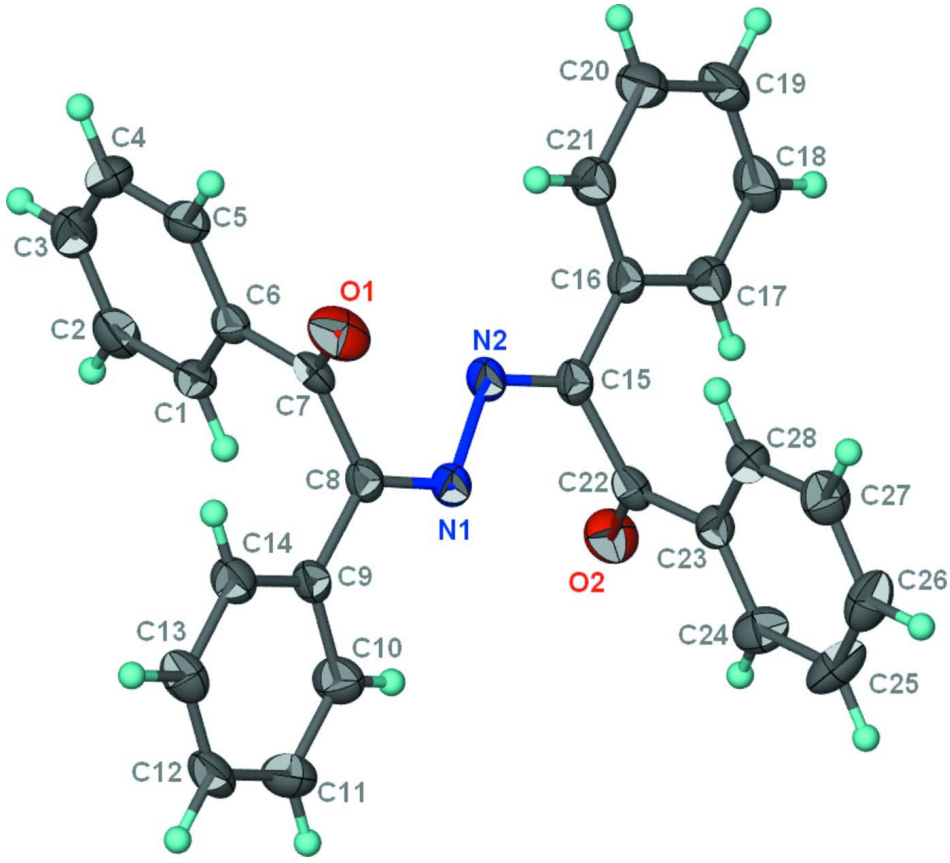


**Figure 1**

Displacement ellipsoid plot (Barbour, 2001) of $C_{28}H_{20}N_2O_2$ at the 70% probability level; H atoms are drawn as spheres of arbitrary radius.

## 1,1′,2,2′-tetraphenyl-2,2′-azinodiethanone

*Crystal data*

$C_{28}H_{20}N_2O_2$
$M_r = 416.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.2875$ (2) Å
$b = 22.1023$ (4) Å
$c = 11.6602$ (2) Å
$\beta = 97.539$ (1)°
$V = 2117.37$ (7) Å$^3$
$Z = 4$
$F(000) = 872$
$D_x = 1.306$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3878 reflections
$\theta = 2.5$–27.9°
$\mu = 0.08$ mm$^{-1}$
$T = 140$ K
Prism, yellow
0.30 × 0.04 × 0.03 mm

*Data collection*

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
17323 measured reflections
4857 independent reflections
3510 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -10 \rightarrow 10$
$k = -28 \rightarrow 27$
$l = -15 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.107$
$S = 1.03$
4857 reflections
289 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
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.4715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.37058 (13) | 0.75630 (5) | 0.13158 (8) | 0.0366 (3) |
| O2 | 0.17265 (13) | 0.56277 (5) | 0.47749 (8) | 0.0336 (3) |
| N1 | 0.34699 (13) | 0.66169 (5) | 0.33697 (11) | 0.0257 (3) |
| N2 | 0.18382 (13) | 0.66513 (5) | 0.28286 (10) | 0.0252 (3) |
| C1 | 0.27649 (16) | 0.81384 (6) | 0.40407 (11) | 0.0215 (3) |
| H1 | 0.3294 | 0.7835 | 0.4531 | 0.026* |
| C2 | 0.20231 (17) | 0.86230 (7) | 0.45113 (13) | 0.0303 (3) |
| H2 | 0.2043 | 0.8653 | 0.5326 | 0.036* |
| C3 | 0.12519 (19) | 0.90640 (7) | 0.37938 (15) | 0.0377 (4) |
| H3 | 0.0744 | 0.9397 | 0.4118 | 0.045* |
| C4 | 0.12170 (19) | 0.90223 (7) | 0.26063 (15) | 0.0370 (4) |
| H4 | 0.0678 | 0.9325 | 0.2119 | 0.044* |
| C5 | 0.19592 (17) | 0.85447 (6) | 0.21267 (13) | 0.0278 (3) |
| H5 | 0.1945 | 0.8520 | 0.1312 | 0.033* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.27335 (15) | 0.80970 (6) | 0.28467 (11) | 0.0198 (3) |
| C7 | 0.35415 (15) | 0.75841 (6) | 0.23347 (11) | 0.0219 (3) |
| C8 | 0.42829 (16) | 0.70877 (6) | 0.31371 (11) | 0.0211 (3) |
| C9 | 0.59933 (16) | 0.71554 (6) | 0.36520 (11) | 0.0211 (3) |
| C10 | 0.66251 (18) | 0.67959 (7) | 0.45829 (13) | 0.0318 (3) |
| H10 | 0.5949 | 0.6504 | 0.4881 | 0.038* |
| C11 | 0.82226 (18) | 0.68586 (7) | 0.50792 (14) | 0.0349 (4) |
| H11 | 0.8639 | 0.6612 | 0.5717 | 0.042* |
| C12 | 0.92181 (17) | 0.72815 (7) | 0.46459 (13) | 0.0296 (3) |
| H12 | 1.0319 | 0.7324 | 0.4985 | 0.036* |
| C13 | 0.86090 (17) | 0.76404 (7) | 0.37219 (13) | 0.0312 (3) |
| H13 | 0.9294 | 0.7929 | 0.3422 | 0.037* |
| C14 | 0.70016 (17) | 0.75823 (6) | 0.32287 (12) | 0.0267 (3) |
| H14 | 0.6586 | 0.7835 | 0.2599 | 0.032* |
| C15 | 0.10218 (16) | 0.61745 (6) | 0.30204 (11) | 0.0215 (3) |
| C16 | −0.06870 (16) | 0.61175 (6) | 0.24937 (11) | 0.0215 (3) |
| C17 | −0.16874 (17) | 0.56676 (6) | 0.28567 (13) | 0.0279 (3) |
| H17 | −0.1274 | 0.5398 | 0.3460 | 0.033* |
| C18 | −0.32831 (18) | 0.56134 (7) | 0.23374 (14) | 0.0327 (3) |
| H18 | −0.3961 | 0.5306 | 0.2586 | 0.039* |
| C19 | −0.38917 (17) | 0.60026 (7) | 0.14627 (13) | 0.0307 (3) |
| H19 | −0.4987 | 0.5962 | 0.1110 | 0.037* |
| C20 | −0.29147 (17) | 0.64511 (7) | 0.10965 (13) | 0.0302 (3) |
| H20 | −0.3338 | 0.6720 | 0.0495 | 0.036* |
| C21 | −0.13179 (17) | 0.65073 (6) | 0.16090 (12) | 0.0269 (3) |
| H21 | −0.0646 | 0.6815 | 0.1355 | 0.032* |
| C22 | 0.17830 (16) | 0.56479 (6) | 0.37387 (11) | 0.0222 (3) |
| C23 | 0.25313 (16) | 0.51611 (6) | 0.31005 (12) | 0.0215 (3) |
| C24 | 0.34362 (17) | 0.47038 (7) | 0.37097 (13) | 0.0299 (3) |
| H24 | 0.3554 | 0.4697 | 0.4531 | 0.036* |
| C25 | 0.4161 (2) | 0.42613 (7) | 0.31128 (15) | 0.0372 (4) |
| H25 | 0.4800 | 0.3956 | 0.3528 | 0.045* |
| C26 | 0.39637 (19) | 0.42599 (7) | 0.19180 (14) | 0.0344 (4) |
| H26 | 0.4459 | 0.3952 | 0.1516 | 0.041* |
| C27 | 0.30485 (18) | 0.47042 (7) | 0.13063 (13) | 0.0309 (3) |
| H27 | 0.2903 | 0.4700 | 0.0484 | 0.037* |
| C28 | 0.23428 (17) | 0.51564 (6) | 0.18982 (12) | 0.0242 (3) |
| H28 | 0.1725 | 0.5466 | 0.1478 | 0.029* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0392 (6) | 0.0513 (7) | 0.0191 (5) | 0.0020 (5) | 0.0023 (4) | −0.0069 (5) |
| O2 | 0.0389 (6) | 0.0379 (6) | 0.0238 (5) | 0.0007 (5) | 0.0037 (4) | −0.0048 (4) |
| N1 | 0.0177 (6) | 0.0207 (6) | 0.0374 (7) | −0.0007 (4) | −0.0007 (5) | −0.0034 (5) |
| N2 | 0.0167 (6) | 0.0214 (6) | 0.0366 (7) | −0.0006 (4) | 0.0000 (5) | −0.0056 (5) |
| C1 | 0.0188 (6) | 0.0230 (6) | 0.0220 (7) | −0.0012 (5) | −0.0003 (5) | 0.0008 (5) |
| C2 | 0.0244 (7) | 0.0341 (8) | 0.0317 (8) | −0.0013 (6) | 0.0009 (6) | −0.0103 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.0286 (8) | 0.0273 (8) | 0.0549 (11) | 0.0056 (6) | −0.0034 (7) | −0.0120 (7) |
| C4 | 0.0334 (8) | 0.0229 (7) | 0.0501 (10) | 0.0023 (6) | −0.0119 (7) | 0.0057 (7) |
| C5 | 0.0265 (7) | 0.0266 (7) | 0.0278 (7) | −0.0057 (6) | −0.0051 (6) | 0.0066 (6) |
| C6 | 0.0162 (6) | 0.0200 (6) | 0.0227 (7) | −0.0044 (5) | 0.0004 (5) | 0.0012 (5) |
| C7 | 0.0171 (6) | 0.0267 (7) | 0.0206 (6) | −0.0055 (5) | −0.0017 (5) | −0.0039 (5) |
| C8 | 0.0199 (7) | 0.0202 (6) | 0.0230 (7) | −0.0002 (5) | 0.0026 (5) | −0.0061 (5) |
| C9 | 0.0187 (6) | 0.0207 (6) | 0.0238 (7) | −0.0006 (5) | 0.0018 (5) | −0.0055 (5) |
| C10 | 0.0245 (7) | 0.0319 (8) | 0.0380 (8) | −0.0049 (6) | −0.0002 (6) | 0.0069 (6) |
| C11 | 0.0291 (8) | 0.0367 (8) | 0.0363 (8) | 0.0007 (6) | −0.0058 (7) | 0.0049 (7) |
| C12 | 0.0178 (7) | 0.0347 (8) | 0.0350 (8) | −0.0014 (6) | −0.0014 (6) | −0.0115 (6) |
| C13 | 0.0231 (7) | 0.0346 (8) | 0.0358 (8) | −0.0082 (6) | 0.0029 (6) | −0.0029 (6) |
| C14 | 0.0244 (7) | 0.0276 (7) | 0.0275 (7) | −0.0033 (6) | 0.0010 (6) | −0.0008 (6) |
| C15 | 0.0206 (7) | 0.0192 (6) | 0.0252 (7) | −0.0008 (5) | 0.0045 (5) | −0.0066 (5) |
| C16 | 0.0197 (6) | 0.0192 (6) | 0.0261 (7) | −0.0010 (5) | 0.0045 (5) | −0.0064 (5) |
| C17 | 0.0244 (7) | 0.0256 (7) | 0.0332 (8) | −0.0025 (6) | 0.0025 (6) | −0.0012 (6) |
| C18 | 0.0242 (7) | 0.0331 (8) | 0.0413 (9) | −0.0104 (6) | 0.0064 (6) | −0.0038 (7) |
| C19 | 0.0185 (7) | 0.0386 (8) | 0.0343 (8) | −0.0021 (6) | 0.0002 (6) | −0.0102 (6) |
| C20 | 0.0254 (7) | 0.0341 (8) | 0.0300 (8) | 0.0014 (6) | −0.0004 (6) | −0.0013 (6) |
| C21 | 0.0232 (7) | 0.0257 (7) | 0.0320 (8) | −0.0030 (6) | 0.0041 (6) | −0.0009 (6) |
| C22 | 0.0180 (6) | 0.0241 (7) | 0.0240 (7) | −0.0051 (5) | 0.0013 (5) | −0.0032 (5) |
| C23 | 0.0186 (6) | 0.0189 (6) | 0.0270 (7) | −0.0030 (5) | 0.0027 (5) | −0.0001 (5) |
| C24 | 0.0288 (8) | 0.0319 (8) | 0.0295 (8) | 0.0032 (6) | 0.0060 (6) | 0.0076 (6) |
| C25 | 0.0386 (9) | 0.0268 (8) | 0.0485 (10) | 0.0117 (7) | 0.0140 (8) | 0.0129 (7) |
| C26 | 0.0374 (9) | 0.0232 (7) | 0.0455 (9) | 0.0040 (6) | 0.0166 (7) | −0.0017 (6) |
| C27 | 0.0326 (8) | 0.0313 (8) | 0.0295 (8) | 0.0000 (6) | 0.0063 (6) | −0.0050 (6) |
| C28 | 0.0238 (7) | 0.0221 (7) | 0.0264 (7) | 0.0009 (5) | 0.0016 (6) | 0.0000 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.2143 (16) | C13—H13 | 0.95 |
| O2—C22 | 1.2160 (16) | C14—H14 | 0.95 |
| N1—C8 | 1.2878 (17) | C15—C16 | 1.4733 (18) |
| N1—N2 | 1.4173 (15) | C15—C22 | 1.5216 (19) |
| N2—C15 | 1.2877 (17) | C16—C21 | 1.3922 (19) |
| C1—C2 | 1.3839 (19) | C16—C17 | 1.3955 (19) |
| C1—C6 | 1.3920 (18) | C17—C18 | 1.385 (2) |
| C1—H1 | 0.95 | C17—H17 | 0.95 |
| C2—C3 | 1.385 (2) | C18—C19 | 1.378 (2) |
| C2—H2 | 0.95 | C18—H18 | 0.95 |
| C3—C4 | 1.384 (2) | C19—C20 | 1.383 (2) |
| C3—H3 | 0.95 | C19—H19 | 0.95 |
| C4—C5 | 1.377 (2) | C20—C21 | 1.384 (2) |
| C4—H4 | 0.95 | C20—H20 | 0.95 |
| C5—C6 | 1.3980 (18) | C21—H21 | 0.95 |
| C5—H5 | 0.95 | C22—C23 | 1.4890 (18) |
| C6—C7 | 1.4814 (18) | C23—C28 | 1.3902 (19) |
| C7—C8 | 1.5185 (18) | C23—C24 | 1.3959 (19) |
| C8—C9 | 1.4727 (18) | C24—C25 | 1.383 (2) |

| | | | |
|---|---|---|---|
| C9—C10 | 1.3908 (19) | C24—H24 | 0.95 |
| C9—C14 | 1.3929 (19) | C25—C26 | 1.381 (2) |
| C10—C11 | 1.380 (2) | C25—H25 | 0.95 |
| C10—H10 | 0.95 | C26—C27 | 1.381 (2) |
| C11—C12 | 1.385 (2) | C26—H26 | 0.95 |
| C11—H11 | 0.95 | C27—C28 | 1.3869 (19) |
| C12—C13 | 1.379 (2) | C27—H27 | 0.95 |
| C12—H12 | 0.95 | C28—H28 | 0.95 |
| C13—C14 | 1.386 (2) | | |

| | | | |
|---|---|---|---|
| C8—N1—N2 | 110.97 (11) | C9—C14—H14 | 119.9 |
| C15—N2—N1 | 111.78 (11) | N2—C15—C16 | 119.72 (12) |
| C2—C1—C6 | 119.77 (13) | N2—C15—C22 | 122.16 (12) |
| C2—C1—H1 | 120.1 | C16—C15—C22 | 118.06 (11) |
| C6—C1—H1 | 120.1 | C21—C16—C17 | 119.04 (12) |
| C1—C2—C3 | 119.93 (14) | C21—C16—C15 | 120.20 (12) |
| C1—C2—H2 | 120.0 | C17—C16—C15 | 120.75 (12) |
| C3—C2—H2 | 120.0 | C18—C17—C16 | 120.00 (14) |
| C4—C3—C2 | 120.32 (14) | C18—C17—H17 | 120.0 |
| C4—C3—H3 | 119.8 | C16—C17—H17 | 120.0 |
| C2—C3—H3 | 119.8 | C19—C18—C17 | 120.34 (13) |
| C5—C4—C3 | 120.37 (14) | C19—C18—H18 | 119.8 |
| C5—C4—H4 | 119.8 | C17—C18—H18 | 119.8 |
| C3—C4—H4 | 119.8 | C18—C19—C20 | 120.25 (13) |
| C4—C5—C6 | 119.54 (14) | C18—C19—H19 | 119.9 |
| C4—C5—H5 | 120.2 | C20—C19—H19 | 119.9 |
| C6—C5—H5 | 120.2 | C19—C20—C21 | 119.76 (14) |
| C1—C6—C5 | 120.06 (13) | C19—C20—H20 | 120.1 |
| C1—C6—C7 | 120.21 (12) | C21—C20—H20 | 120.1 |
| C5—C6—C7 | 119.71 (12) | C20—C21—C16 | 120.61 (13) |
| O1—C7—C6 | 122.57 (13) | C20—C21—H21 | 119.7 |
| O1—C7—C8 | 119.13 (12) | C16—C21—H21 | 119.7 |
| C6—C7—C8 | 118.18 (11) | O2—C22—C23 | 122.88 (13) |
| N1—C8—C9 | 119.89 (12) | O2—C22—C15 | 120.51 (12) |
| N1—C8—C7 | 122.21 (12) | C23—C22—C15 | 116.58 (11) |
| C9—C8—C7 | 117.89 (11) | C28—C23—C24 | 119.31 (12) |
| C10—C9—C14 | 118.78 (12) | C28—C23—C22 | 120.68 (12) |
| C10—C9—C8 | 120.25 (12) | C24—C23—C22 | 120.01 (12) |
| C14—C9—C8 | 120.96 (12) | C25—C24—C23 | 119.74 (14) |
| C11—C10—C9 | 120.80 (14) | C25—C24—H24 | 120.1 |
| C11—C10—H10 | 119.6 | C23—C24—H24 | 120.1 |
| C9—C10—H10 | 119.6 | C26—C25—C24 | 120.49 (14) |
| C10—C11—C12 | 119.94 (14) | C26—C25—H25 | 119.8 |
| C10—C11—H11 | 120.0 | C24—C25—H25 | 119.8 |
| C12—C11—H11 | 120.0 | C25—C26—C27 | 120.26 (14) |
| C13—C12—C11 | 119.90 (13) | C25—C26—H26 | 119.9 |
| C13—C12—H12 | 120.0 | C27—C26—H26 | 119.9 |
| C11—C12—H12 | 120.0 | C26—C27—C28 | 119.63 (14) |

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|---|---|---|---|
| C12—C13—C14 | 120.27 (14) | C26—C27—H27 | 120.2 |
| C12—C13—H13 | 119.9 | C28—C27—H27 | 120.2 |
| C14—C13—H13 | 119.9 | C23—C28—C27 | 120.55 (13) |
| C13—C14—C9 | 120.30 (13) | C23—C28—H28 | 119.7 |
| C13—C14—H14 | 119.9 | C27—C28—H28 | 119.7 |
| | | | |
| C8—N1—N2—C15 | 177.82 (12) | N1—N2—C15—C16 | −177.87 (11) |
| C6—C1—C2—C3 | 0.1 (2) | N1—N2—C15—C22 | −0.55 (17) |
| C1—C2—C3—C4 | 0.1 (2) | N2—C15—C16—C21 | 13.52 (19) |
| C2—C3—C4—C5 | −0.5 (2) | C22—C15—C16—C21 | −163.92 (12) |
| C3—C4—C5—C6 | 0.8 (2) | N2—C15—C16—C17 | −167.62 (13) |
| C2—C1—C6—C5 | 0.20 (19) | C22—C15—C16—C17 | 14.95 (18) |
| C2—C1—C6—C7 | 179.23 (12) | C21—C16—C17—C18 | 0.1 (2) |
| C4—C5—C6—C1 | −0.6 (2) | C15—C16—C17—C18 | −178.82 (13) |
| C4—C5—C6—C7 | −179.66 (12) | C16—C17—C18—C19 | −0.1 (2) |
| C1—C6—C7—O1 | −171.53 (13) | C17—C18—C19—C20 | −0.1 (2) |
| C5—C6—C7—O1 | 7.51 (19) | C18—C19—C20—C21 | 0.2 (2) |
| C1—C6—C7—C8 | 4.51 (18) | C19—C20—C21—C16 | −0.2 (2) |
| C5—C6—C7—C8 | −176.45 (12) | C17—C16—C21—C20 | 0.1 (2) |
| N2—N1—C8—C9 | 177.59 (11) | C15—C16—C21—C20 | 178.98 (12) |
| N2—N1—C8—C7 | −2.72 (17) | N2—C15—C22—O2 | 91.73 (16) |
| O1—C7—C8—N1 | −93.45 (16) | C16—C15—C22—O2 | −90.91 (15) |
| C6—C7—C8—N1 | 90.38 (15) | N2—C15—C22—C23 | −90.28 (15) |
| O1—C7—C8—C9 | 86.25 (15) | C16—C15—C22—C23 | 87.09 (14) |
| C6—C7—C8—C9 | −89.92 (14) | O2—C22—C23—C28 | 169.79 (13) |
| N1—C8—C9—C10 | −15.03 (19) | C15—C22—C23—C28 | −8.15 (18) |
| C7—C8—C9—C10 | 165.26 (12) | O2—C22—C23—C24 | −10.4 (2) |
| N1—C8—C9—C14 | 165.69 (13) | C15—C22—C23—C24 | 171.70 (12) |
| C7—C8—C9—C14 | −14.01 (18) | C28—C23—C24—C25 | 1.4 (2) |
| C14—C9—C10—C11 | −0.2 (2) | C22—C23—C24—C25 | −178.43 (13) |
| C8—C9—C10—C11 | −179.45 (13) | C23—C24—C25—C26 | −1.6 (2) |
| C9—C10—C11—C12 | −0.3 (2) | C24—C25—C26—C27 | 0.5 (2) |
| C10—C11—C12—C13 | 0.2 (2) | C25—C26—C27—C28 | 0.7 (2) |
| C11—C12—C13—C14 | 0.4 (2) | C24—C23—C28—C27 | −0.2 (2) |
| C12—C13—C14—C9 | −0.8 (2) | C22—C23—C28—C27 | 179.65 (13) |
| C10—C9—C14—C13 | 0.7 (2) | C26—C27—C28—C23 | −0.9 (2) |
| C8—C9—C14—C13 | −179.97 (13) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O1$^{i}$ | 0.95 | 2.24 | 3.0832 (16) | 147 |
| C13—H13···*Cg*1$^{ii}$ | 0.95 | 2.68 | 3.5705 (16) | 157 |
| C18—H18···*Cg*2$^{iii}$ | 0.95 | 2.66 | 3.5304 (16) | 153 |

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*+1, *y*, *z*; (iii) *x*−1, *y*, *z*.