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# Bis[4-(3-aminophenoxy)phenyl] ketone

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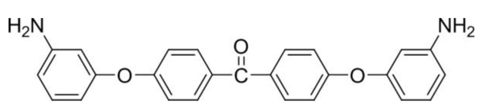
Key indicators: single-crystal X-ray study; $T$ = 292 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.053; $wR$ factor = 0.165; data-to-parameter ratio = 12.8.

In the molecule of the title compound, $C_{25}H_{20}N_2O_3$, the dihedral angles formed by adjacent benzene rings are 66.75 (8), 48.37 (8) and 71.43 (9)°. In the crystal structure, centrosymmetrically related molecules are linked into dimers by intermolecular N—H···O hydrogen bonds.

## Related literature

For the properties and synthesis of the title compound, see: Wilson *et al.* (1990); Mehdipour-Ataei & Saidi (2008). For the applications of the title compound, see: Rao & Prabhakaran (1992).



## Experimental

*Crystal data*

$C_{25}H_{20}N_2O_3$
$M_r$ = 396.43
Triclinic, $P\bar{1}$
$a$ = 7.370 (3) Å
$b$ = 11.856 (3) Å
$c$ = 12.319 (3) Å
$\alpha$ = 101.79 (4)°
$\beta$ = 95.10 (4)°
$\gamma$ = 107.86 (3)°
$V$ = 989.6 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 292 K
0.48 × 0.42 × 0.23 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3693 measured reflections
3682 independent reflections
2206 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.006
3 standard reflections every 200 reflections intensity decay: 1.5%

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.165
$S$ = 1.05
3682 reflections
288 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$N$1···O1$^{i}$ | 0.92 (4) | 2.32 (4) | 3.223 (5) | 164 (3) |

Symmetry code: (i) $-x+2, -y+2, -z+1$.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Undergraduates' Innovative Experiment Project of Sichuan University and thank Mr Zhi-Hua Mao of Sichuan University for the X-Ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2344).

## References

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# supporting information

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## Bis[4-(3-aminophenoxy)phenyl] ketone

**Yang Wang, Xin-yi Zhu, Xiao-yan Ma, Guo-wei Gao and Jian Men**

### S1. Comment

Aromatic polyimides has found useful applications in aircraft technology, space vehicles, sea transport equipment and other applications due to their excellent thermal stability, good mechanical properties, low dielectric constants and intrinsic purity (Wilson *et al.*, 1990). The title compound is an important raw material for the synthesis of aromatic polyimides, as the presence of ether and ketone groups connected by aromatic rings greatly improves the chain flexibility (Rao & Prabhakaran, 1992; Mehdipour-Ataei & Saidi, 2008). Herein, we report the synthesis and crystal structure of the title compound.

The structure of the title compound (Fig. 1) is not planar. The dihedral angle between the two central benzene rings, ring A (C7–C12) and ring B (C14–C19), is 48.37 (8)°. Ring A forms a dihedral angle of 66.75 (8)° with the C1–C6 benzene ring. The corresponding dihedral angle between ring B and the C20–C25 benzene ring is 71.43 (9)°. The plane formed by atoms C10, C14, O1 and C13, makes a dihedral angle of 22.28 (12)° and 31.23 (8)° with ring A and B, respectively. The crystal structure is stabilized by N—H···O hydrogen bonds (Table 1) linking centrosymmetrically related molecules into dimers.

### S2. Experimental

4,4′-Difluorobenzophenone (11.0 g, 0.05 mol), *m*-aminophenol (22.0 g, 0.20 mol) and anhydrous potassium carbonate (14.0 g, 0.10 mol) were dissolved in a solution of toluene (60 ml) and *N*,*N*-dimethylformamide (100 ml) in a three-necked flask. The mixture was heated to reflux and water was removed by azeotropic distillation. After complete dehydration, the mixture was poured to a large excess of ice water. Then, the precipitated solid was collected by filtration and recrystallized from ethanol to obtain a tan solid (16.5 g, 76% yield, m.p.411–413 K). Red single crystals suitable for X-ray diffraction were obtained by slow evaporation at room temperature of a toluene solution.

### S3. Refinement

H-atoms bound to nitrogen atoms were located in a difference Fourier map and refined isotropically. The remaining H atoms were positioned geometrically (C—H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

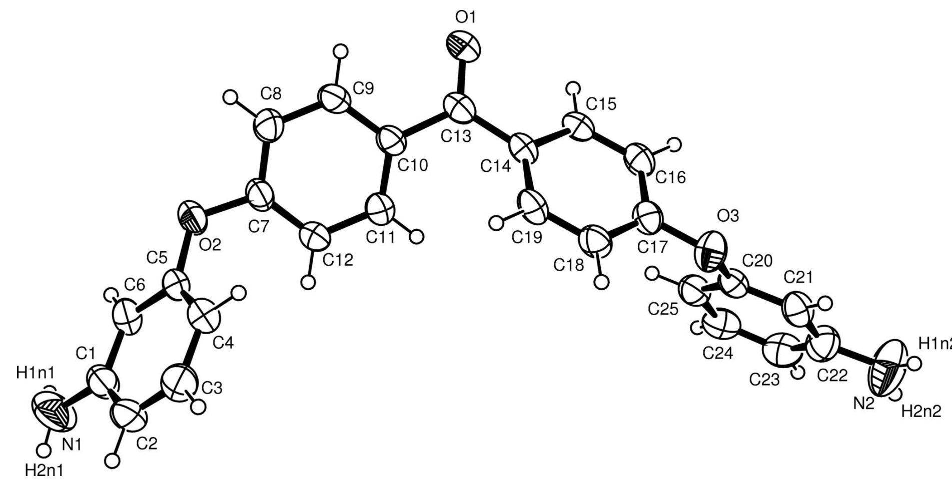


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

**Bis[4-(3-aminophenoxy)phenyl] ketone**

*Crystal data*

$C_{25}H_{20}N_2O_3$
$M_r = 396.43$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.370$ (3) Å
$b = 11.856$ (3) Å
$c = 12.319$ (3) Å
$\alpha = 101.79$ (4)°
$\beta = 95.10$ (4)°
$\gamma = 107.86$ (3)°
$V = 989.6$ (6) Å$^3$
$Z = 2$
$F(000) = 416$
$D_x = 1.330$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 23 reflections
$\theta = 5.4$–5.6°
$\mu = 0.09$ mm$^{-1}$
$T = 292$ K
Block, red
0.48 × 0.42 × 0.23 mm

*Data collection*

Enraf–Nonius CAD-4
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
3693 measured reflections
3682 independent reflections
2206 reflections with $I > 2\sigma(I)$
$R_{int} = 0.006$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.7°$
$h = -8 \rightarrow 8$
$k = -4 \rightarrow 14$
$l = -14 \rightarrow 14$
3 standard reflections every 200 reflections
intensity decay: 1.5%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.165$
$S = 1.05$
3682 reflections
288 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0943P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.027 (5)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.4068 (2) | 0.59493 (16) | 0.42259 (15) | 0.0665 (5) |
| O2 | 1.2554 (2) | 0.95837 (18) | 0.55618 (15) | 0.0746 (6) |
| O3 | 0.0557 (2) | 0.57862 (15) | 0.86702 (15) | 0.0623 (5) |
| N1 | 1.7663 (5) | 1.3024 (3) | 0.7708 (4) | 0.0988 (11) |
| H1N1 | 1.729 (5) | 1.346 (3) | 0.725 (3) | 0.116 (15)* |
| H2N1 | 1.840 (5) | 1.333 (3) | 0.828 (3) | 0.109 (15)* |
| N2 | −0.3694 (6) | 0.6550 (4) | 1.1145 (3) | 0.1179 (13) |
| H1N2 | −0.378 (6) | 0.581 (4) | 1.131 (3) | 0.119 (14)* |
| H2N2 | −0.399 (8) | 0.712 (5) | 1.153 (5) | 0.19 (3)* |
| C1 | 1.6441 (3) | 1.1849 (2) | 0.7619 (2) | 0.0591 (7) |
| C2 | 1.6600 (4) | 1.1216 (3) | 0.8431 (2) | 0.0655 (7) |
| H2 | 1.7550 | 1.1581 | 0.9064 | 0.079* |
| C3 | 1.5354 (4) | 1.0050 (3) | 0.8303 (2) | 0.0631 (7) |
| H3 | 1.5464 | 0.9638 | 0.8859 | 0.076* |
| C4 | 1.3949 (3) | 0.9477 (2) | 0.7371 (2) | 0.0544 (6) |
| H4 | 1.3115 | 0.8685 | 0.7286 | 0.065* |
| C5 | 1.3819 (3) | 1.0112 (2) | 0.6574 (2) | 0.0509 (6) |
| C6 | 1.5030 (3) | 1.1280 (2) | 0.6682 (2) | 0.0558 (7) |
| H6 | 1.4901 | 1.1689 | 0.6126 | 0.067* |
| C7 | 1.0692 (3) | 0.8848 (2) | 0.5542 (2) | 0.0518 (6) |
| C8 | 0.9903 (3) | 0.7910 (2) | 0.4600 (2) | 0.0549 (6) |
| H8 | 1.0622 | 0.7789 | 0.4031 | 0.066* |
| C9 | 0.8035 (3) | 0.7150 (2) | 0.4507 (2) | 0.0517 (6) |
| H9 | 0.7494 | 0.6512 | 0.3869 | 0.062* |
| C10 | 0.6938 (3) | 0.73176 (19) | 0.53531 (19) | 0.0450 (6) |
| C11 | 0.7750 (3) | 0.8300 (2) | 0.6275 (2) | 0.0511 (6) |
| H11 | 0.7023 | 0.8444 | 0.6834 | 0.061* |
| C12 | 0.9628 (3) | 0.9070 (2) | 0.6377 (2) | 0.0543 (6) |
| H12 | 1.0165 | 0.9728 | 0.7000 | 0.065* |
| C13 | 0.4904 (3) | 0.6501 (2) | 0.5182 (2) | 0.0505 (6) |
| C14 | 0.3844 (3) | 0.63592 (19) | 0.6137 (2) | 0.0451 (6) |
| C15 | 0.1849 (3) | 0.61103 (19) | 0.5934 (2) | 0.0475 (6) |
| H15 | 0.1256 | 0.6057 | 0.5218 | 0.057* |

| | | | | |
|---|---|---|---|---|
| C16 | 0.0742 (3) | 0.5943 (2) | 0.6765 (2) | 0.0521 (6) |
| H16 | −0.0585 | 0.5779 | 0.6615 | 0.063* |
| C17 | 0.1629 (3) | 0.6021 (2) | 0.7822 (2) | 0.0502 (6) |
| C18 | 0.3584 (3) | 0.6242 (2) | 0.8042 (2) | 0.0552 (6) |
| H18 | 0.4165 | 0.6282 | 0.8757 | 0.066* |
| C19 | 0.4680 (3) | 0.6404 (2) | 0.7205 (2) | 0.0539 (6) |
| H19 | 0.6000 | 0.6546 | 0.7356 | 0.065* |
| C20 | −0.0391 (3) | 0.6582 (2) | 0.9107 (2) | 0.0470 (6) |
| C21 | −0.1542 (3) | 0.6200 (2) | 0.9866 (2) | 0.0560 (6) |
| H21 | −0.1692 | 0.5443 | 1.0020 | 0.067* |
| C22 | −0.2484 (4) | 0.6946 (3) | 1.0405 (2) | 0.0665 (7) |
| C23 | −0.2239 (4) | 0.8067 (3) | 1.0155 (3) | 0.0705 (8) |
| H23 | −0.2847 | 0.8584 | 1.0514 | 0.085* |
| C24 | −0.1107 (4) | 0.8412 (2) | 0.9382 (2) | 0.0635 (7) |
| H24 | −0.0982 | 0.9157 | 0.9210 | 0.076* |
| C25 | −0.0142 (3) | 0.7687 (2) | 0.8849 (2) | 0.0550 (6) |
| H25 | 0.0647 | 0.7937 | 0.8334 | 0.066* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0462 (10) | 0.0733 (12) | 0.0579 (12) | 0.0017 (9) | −0.0019 (9) | 0.0004 (9) |
| O2 | 0.0424 (10) | 0.1008 (14) | 0.0539 (12) | −0.0116 (9) | 0.0015 (8) | 0.0184 (10) |
| O3 | 0.0645 (11) | 0.0627 (10) | 0.0744 (13) | 0.0286 (9) | 0.0262 (10) | 0.0307 (9) |
| N1 | 0.088 (2) | 0.0664 (18) | 0.105 (3) | −0.0097 (16) | −0.007 (2) | 0.0029 (18) |
| N2 | 0.136 (3) | 0.121 (3) | 0.142 (3) | 0.069 (3) | 0.092 (3) | 0.059 (3) |
| C1 | 0.0427 (13) | 0.0545 (15) | 0.0680 (18) | 0.0079 (12) | 0.0060 (13) | 0.0026 (13) |
| C2 | 0.0490 (15) | 0.0799 (19) | 0.0562 (17) | 0.0168 (14) | −0.0056 (13) | 0.0050 (14) |
| C3 | 0.0568 (16) | 0.0775 (18) | 0.0614 (18) | 0.0285 (14) | 0.0051 (14) | 0.0232 (15) |
| C4 | 0.0461 (13) | 0.0527 (14) | 0.0602 (16) | 0.0117 (11) | 0.0058 (12) | 0.0129 (12) |
| C5 | 0.0317 (11) | 0.0637 (15) | 0.0497 (15) | 0.0084 (11) | 0.0058 (11) | 0.0092 (12) |
| C6 | 0.0421 (13) | 0.0581 (15) | 0.0662 (17) | 0.0109 (12) | 0.0091 (12) | 0.0217 (13) |
| C7 | 0.0373 (12) | 0.0609 (15) | 0.0496 (15) | 0.0040 (11) | 0.0012 (11) | 0.0184 (12) |
| C8 | 0.0405 (13) | 0.0699 (16) | 0.0527 (16) | 0.0158 (12) | 0.0086 (11) | 0.0151 (13) |
| C9 | 0.0449 (13) | 0.0532 (14) | 0.0467 (15) | 0.0110 (11) | −0.0030 (11) | 0.0025 (11) |
| C10 | 0.0368 (12) | 0.0481 (13) | 0.0460 (14) | 0.0111 (10) | −0.0010 (10) | 0.0101 (11) |
| C11 | 0.0395 (13) | 0.0554 (14) | 0.0544 (16) | 0.0122 (11) | 0.0072 (11) | 0.0107 (12) |
| C12 | 0.0446 (14) | 0.0606 (15) | 0.0450 (14) | 0.0052 (11) | −0.0002 (11) | 0.0075 (11) |
| C13 | 0.0394 (13) | 0.0462 (13) | 0.0580 (17) | 0.0100 (11) | −0.0019 (12) | 0.0062 (12) |
| C14 | 0.0324 (11) | 0.0424 (12) | 0.0548 (15) | 0.0075 (9) | −0.0002 (10) | 0.0100 (11) |
| C15 | 0.0379 (12) | 0.0471 (13) | 0.0491 (14) | 0.0094 (10) | −0.0064 (11) | 0.0066 (11) |
| C16 | 0.0331 (12) | 0.0540 (14) | 0.0647 (17) | 0.0119 (10) | 0.0018 (12) | 0.0109 (12) |
| C17 | 0.0476 (14) | 0.0433 (12) | 0.0589 (16) | 0.0128 (10) | 0.0094 (12) | 0.0140 (11) |
| C18 | 0.0460 (14) | 0.0611 (15) | 0.0527 (16) | 0.0105 (11) | −0.0043 (12) | 0.0176 (12) |
| C19 | 0.0336 (12) | 0.0553 (14) | 0.0661 (17) | 0.0072 (10) | −0.0026 (12) | 0.0167 (12) |
| C20 | 0.0384 (12) | 0.0478 (13) | 0.0482 (14) | 0.0095 (10) | −0.0022 (11) | 0.0089 (11) |
| C21 | 0.0472 (13) | 0.0560 (15) | 0.0651 (17) | 0.0156 (12) | 0.0063 (12) | 0.0189 (13) |
| C22 | 0.0605 (17) | 0.0778 (19) | 0.0654 (19) | 0.0269 (15) | 0.0164 (14) | 0.0179 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.0716 (19) | 0.0689 (18) | 0.072 (2) | 0.0342 (15) | 0.0058 (16) | 0.0045 (15) |
| C24 | 0.0725 (18) | 0.0523 (15) | 0.0602 (18) | 0.0216 (14) | −0.0049 (14) | 0.0076 (13) |
| C25 | 0.0520 (14) | 0.0529 (14) | 0.0546 (16) | 0.0118 (12) | 0.0022 (12) | 0.0128 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C13 | 1.226 (3) | C10—C11 | 1.384 (3) |
| O2—C7 | 1.377 (3) | C10—C13 | 1.484 (3) |
| O2—C5 | 1.390 (3) | C11—C12 | 1.383 (3) |
| O3—C17 | 1.387 (3) | C11—H11 | 0.9300 |
| O3—C20 | 1.390 (3) | C12—H12 | 0.9300 |
| N1—C1 | 1.384 (4) | C13—C14 | 1.478 (3) |
| N1—H1N1 | 0.92 (4) | C14—C19 | 1.386 (3) |
| N1—H2N1 | 0.79 (4) | C14—C15 | 1.396 (3) |
| N2—C22 | 1.383 (4) | C15—C16 | 1.373 (3) |
| N2—H1N2 | 0.93 (4) | C15—H15 | 0.9300 |
| N2—H2N2 | 0.84 (5) | C16—C17 | 1.377 (3) |
| C1—C6 | 1.381 (4) | C16—H16 | 0.9300 |
| C1—C2 | 1.384 (4) | C17—C18 | 1.374 (3) |
| C2—C3 | 1.373 (4) | C18—C19 | 1.374 (3) |
| C2—H2 | 0.9300 | C18—H18 | 0.9300 |
| C3—C4 | 1.375 (4) | C19—H19 | 0.9300 |
| C3—H3 | 0.9300 | C20—C21 | 1.370 (3) |
| C4—C5 | 1.368 (3) | C20—C25 | 1.373 (3) |
| C4—H4 | 0.9300 | C21—C22 | 1.387 (4) |
| C5—C6 | 1.370 (3) | C21—H21 | 0.9300 |
| C6—H6 | 0.9300 | C22—C23 | 1.387 (4) |
| C7—C8 | 1.371 (3) | C23—C24 | 1.364 (4) |
| C7—C12 | 1.379 (3) | C23—H23 | 0.9300 |
| C8—C9 | 1.374 (3) | C24—C25 | 1.380 (4) |
| C8—H8 | 0.9300 | C24—H24 | 0.9300 |
| C9—C10 | 1.394 (3) | C25—H25 | 0.9300 |
| C9—H9 | 0.9300 | | |
| | | | |
| C7—O2—C5 | 120.22 (19) | C7—C12—H12 | 120.5 |
| C17—O3—C20 | 119.63 (18) | C11—C12—H12 | 120.5 |
| C1—N1—H1N1 | 117 (2) | O1—C13—C14 | 119.2 (2) |
| C1—N1—H2N1 | 115 (3) | O1—C13—C10 | 119.3 (2) |
| H1N1—N1—H2N1 | 124 (4) | C14—C13—C10 | 121.5 (2) |
| C22—N2—H1N2 | 118 (2) | C19—C14—C15 | 117.8 (2) |
| C22—N2—H2N2 | 112 (4) | C19—C14—C13 | 124.5 (2) |
| H1N2—N2—H2N2 | 127 (5) | C15—C14—C13 | 117.6 (2) |
| C6—C1—N1 | 119.0 (3) | C16—C15—C14 | 121.7 (2) |
| C6—C1—C2 | 118.8 (2) | C16—C15—H15 | 119.2 |
| N1—C1—C2 | 122.2 (3) | C14—C15—H15 | 119.2 |
| C3—C2—C1 | 120.1 (3) | C15—C16—C17 | 118.9 (2) |
| C3—C2—H2 | 120.0 | C15—C16—H16 | 120.6 |
| C1—C2—H2 | 120.0 | C17—C16—H16 | 120.6 |

| | | | |
|---|---|---|---|
| C2—C3—C4 | 121.5 (3) | C18—C17—C16 | 120.8 (2) |
| C2—C3—H3 | 119.2 | C18—C17—O3 | 118.1 (2) |
| C4—C3—H3 | 119.2 | C16—C17—O3 | 121.0 (2) |
| C5—C4—C3 | 117.7 (2) | C19—C18—C17 | 119.9 (2) |
| C5—C4—H4 | 121.2 | C19—C18—H18 | 120.0 |
| C3—C4—H4 | 121.2 | C17—C18—H18 | 120.0 |
| C4—C5—C6 | 122.2 (2) | C18—C19—C14 | 120.9 (2) |
| C4—C5—O2 | 122.2 (2) | C18—C19—H19 | 119.6 |
| C6—C5—O2 | 115.4 (2) | C14—C19—H19 | 119.6 |
| C5—C6—C1 | 119.8 (2) | C21—C20—C25 | 122.1 (2) |
| C5—C6—H6 | 120.1 | C21—C20—O3 | 114.4 (2) |
| C1—C6—H6 | 120.1 | C25—C20—O3 | 123.5 (2) |
| C8—C7—O2 | 115.7 (2) | C20—C21—C22 | 119.7 (2) |
| C8—C7—C12 | 121.3 (2) | C20—C21—H21 | 120.1 |
| O2—C7—C12 | 122.9 (2) | C22—C21—H21 | 120.1 |
| C7—C8—C9 | 119.2 (2) | N2—C22—C21 | 120.0 (3) |
| C7—C8—H8 | 120.4 | N2—C22—C23 | 121.2 (3) |
| C9—C8—H8 | 120.4 | C21—C22—C23 | 118.8 (3) |
| C8—C9—C10 | 121.1 (2) | C24—C23—C22 | 120.0 (3) |
| C8—C9—H9 | 119.4 | C24—C23—H23 | 120.0 |
| C10—C9—H9 | 119.4 | C22—C23—H23 | 120.0 |
| C11—C10—C9 | 118.4 (2) | C23—C24—C25 | 121.9 (2) |
| C11—C10—C13 | 122.8 (2) | C23—C24—H24 | 119.0 |
| C9—C10—C13 | 118.6 (2) | C25—C24—H24 | 119.0 |
| C12—C11—C10 | 120.9 (2) | C20—C25—C24 | 117.4 (2) |
| C12—C11—H11 | 119.5 | C20—C25—H25 | 121.3 |
| C10—C11—H11 | 119.5 | C24—C25—H25 | 121.3 |
| C7—C12—C11 | 119.0 (2) | | |

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| C6—C1—C2—C3 | −0.7 (4) | O1—C13—C14—C19 | 147.9 (2) |
| N1—C1—C2—C3 | −179.9 (3) | C10—C13—C14—C19 | −33.6 (3) |
| C1—C2—C3—C4 | 0.9 (4) | O1—C13—C14—C15 | −29.1 (3) |
| C2—C3—C4—C5 | −0.5 (4) | C10—C13—C14—C15 | 149.3 (2) |
| C3—C4—C5—C6 | −0.1 (4) | C19—C14—C15—C16 | 1.5 (3) |
| C3—C4—C5—O2 | 174.8 (2) | C13—C14—C15—C16 | 178.8 (2) |
| C7—O2—C5—C4 | 43.0 (3) | C14—C15—C16—C17 | −0.1 (3) |
| C7—O2—C5—C6 | −141.8 (2) | C15—C16—C17—C18 | −1.1 (3) |
| C4—C5—C6—C1 | 0.2 (4) | C15—C16—C17—O3 | −176.1 (2) |
| O2—C5—C6—C1 | −174.9 (2) | C20—O3—C17—C18 | 116.9 (2) |
| N1—C1—C6—C5 | 179.4 (3) | C20—O3—C17—C16 | −68.0 (3) |
| C2—C1—C6—C5 | 0.1 (4) | C16—C17—C18—C19 | 0.9 (4) |
| C5—O2—C7—C8 | −147.3 (2) | O3—C17—C18—C19 | 176.0 (2) |
| C5—O2—C7—C12 | 36.4 (4) | C17—C18—C19—C14 | 0.6 (4) |
| O2—C7—C8—C9 | −178.7 (2) | C15—C14—C19—C18 | −1.8 (3) |
| C12—C7—C8—C9 | −2.4 (4) | C13—C14—C19—C18 | −178.8 (2) |
| C7—C8—C9—C10 | 0.0 (4) | C17—O3—C20—C21 | 174.4 (2) |
| C8—C9—C10—C11 | 2.4 (3) | C17—O3—C20—C25 | −8.5 (3) |
| C8—C9—C10—C13 | 177.4 (2) | C25—C20—C21—C22 | −0.5 (4) |

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| C9—C10—C11—C12 | −2.4 (3) | O3—C20—C21—C22 | 176.6 (2) |
| C13—C10—C11—C12 | −177.1 (2) | C20—C21—C22—N2 | 178.0 (3) |
| C8—C7—C12—C11 | 2.4 (4) | C20—C21—C22—C23 | 0.3 (4) |
| O2—C7—C12—C11 | 178.4 (2) | N2—C22—C23—C24 | −177.0 (3) |
| C10—C11—C12—C7 | 0.1 (4) | C21—C22—C23—C24 | 0.8 (4) |
| C11—C10—C13—O1 | 154.3 (2) | C22—C23—C24—C25 | −1.6 (4) |
| C9—C10—C13—O1 | −20.4 (3) | C21—C20—C25—C24 | −0.2 (4) |
| C11—C10—C13—C14 | −24.2 (3) | O3—C20—C25—C24 | −177.1 (2) |
| C9—C10—C13—C14 | 161.1 (2) | C23—C24—C25—C20 | 1.3 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*1···O1$^{i}$ | 0.92 (4) | 2.32 (4) | 3.223 (5) | 164 (3) |

Symmetry code: (i) $-x+2, -y+2, -z+1$.