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# 4-(4-Nitrostyryl)-*N*,*N*-diphenylaniline

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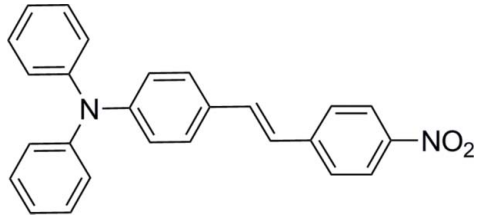
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.057; $wR$ factor = 0.185; data-to-parameter ratio = 13.3.

In the triarylamine group of the title compound, $C_{26}H_{20}N_2O_2$, the N atom adopts an approximately trigonal–planar geometry, lying 0.046 (5) Å from the plane $P$ defined by its three neighbouring C atoms; the benzene and two terminal phenyl rings are twisted by 37.4 (1), 31.4 (1) and 47.8 (1)°, respectively from plane $P$. In the *trans*-stilbene fragment, the two benzene rings form a dihedral angle of 31.3 (1)°. In the crystal, weak intermolecular C—H···O interactions link the molecules into ribbons in [100].

## Related literature

For a related structure, see: Yang *et al.* (2003). For background to push–pull chromophores, see: Marder *et al.* (1991); Reinhardt *et al.* (1998).




## Experimental

### Crystal data

$C_{26}H_{20}N_2O_2$
$M_r$ = 392.44
Monoclinic, $P2_1/c$
$a$ = 8.4884 (3) Å
$b$ = 8.9834 (3) Å
$c$ = 27.0880 (8) Å
$\beta$ = 96.500 (2)°
$V$ = 2052.31 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 K
0.30 × 0.20 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.976, $T_{max}$ = 0.984
7675 measured reflections
3606 independent reflections
2213 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.185
$S$ = 1.04
3606 reflections
272 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C15—H15···O1$^{i}$ | 0.93 | 2.58 | 3.481 (4) | 162 |
| C12—H12···O2$^{ii}$ | 0.93 | 2.56 | 3.308 (4) | 138 |

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $-x+1, -y+1, -z+2$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: CV5302).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1933 [doi:10.1107/S1600536812023719]

## 4-(4-Nitrostyryl)-*N*,*N*-diphenylaniline

**Zhi-Wen Zhang, Yan-Qiu Liu, Yu-Chao Zhu and Jie-Ying Wu**

### Comment

Push-pull chromophores are characterized by the conjugated linkage of an electron-donating group (D) and an electron-accepting group (A). Such molecules are potentially useful for nonlinear optical applications and many D-$\pi$-A type chromophores have been reported (Marder *et al.*, 1991; Reinhardt *et al.*, 1998). As a part of an ongoing study of such type chromophores, here we report the crystal structure of the title compound, (I).

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in the related 4-(4-methoxy-styryl)-N,N-diphenylaniline (Yang *et al.*, 2003). The C = C double bond ( = 1.276 (4) Å) in the molecule adopts a trans-configuration. The dihedral angle between the benzene ring of the triarylamine group and another benzene ring linked by double bond is 31.34 (13) °. In the crystal, weak intermolecular C—H···O interactions (Table 1) link the molecules into ribbons in [100].

### Experimental

2.73 g (10 mmol) of diethyl(4-nitrophenyl)methylphosphonate were put into a dry mortar, then 2.24 g (20 mmol) t-BuOK were placed into powder, a modicum of 18-crown-6 and 2.72 g (10 mmol) 4-(diphenylamino)benzaldehyde were adde and vigorously grinded. The mixture was monitored by TLC. After completion of the reaction the mixture was dissolved in 150 ml $CH_2Cl_2$ and washed with Di-water, the organic layer separated and dried over $MgSO_4$,filterd and solvent removed *in vacuo*. The product was recrystallized from anhydrous ethanol, to give 2.12 g red acicular crystal. Yield, 54.1%. 1H NMR: (400 Hz, $CDCl_3$), d(p.p.m.): 8.20(d, 2H, J = 8.4 Hz) 7.60(d, 2H, J=8.8 Hz) 7.40(d, 2H, J=8.8 Hz) 7.30–7.26(m, 4H) 7.19(s, 1H) 7.13(d, 4H, J=8.0) 7.09–7.03(m, 4H) 6.99(s, 1H) 13 C NMR (125 MHz, $CDCl_3$) d (p.p.m.) 148.7, 147.8, 147.4, 146.5, 145.0, 144.5, 133.5, 133.0, 130.0 129.7, 129.5, 129.4, 128.2, 126.7, 126.5, 125.1, 124.8, 124.3, 123.8 123.6, 122.8, 122.3. IR (KBr, $cm^{-1}$): 3029 1585 1514 1485 1335 1283 1175 1111 970 841 758 694. MS: m/*z* (%) = 504.20 (100)

### Refinement

All hydrogen atoms were placed in geometrically idealized positions (C—H = 0.93 Å), and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

### Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Sheldrick, 2008).

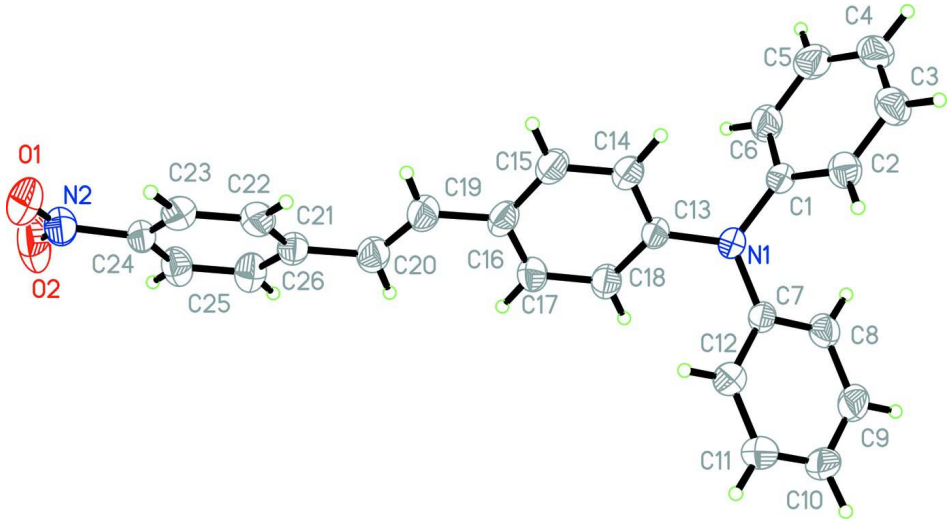


**Figure 1**

The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids.

**4-(4-Nitrostyryl)-*N*,*N*-diphenylaniline**

*Crystal data*

$C_{26}H_{20}N_2O_2$
$M_r = 392.44$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.4884$ (3) Å
$b = 8.9834$ (3) Å
$c = 27.0880$ (8) Å
$\beta = 96.500$ (2)°
$V = 2052.31$ (12) Å$^3$
$Z = 4$
$F(000) = 824$
$D_x = 1.270$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1419 reflections
$\theta = 2.4$–$21.1°$
$\mu = 0.08$ mm$^{-1}$
$T = 298$ K
Red, block
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.976$, $T_{max} = 0.984$
7675 measured reflections
3606 independent reflections
2213 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 10$
$k = -10 \rightarrow 7$
$l = -32 \rightarrow 32$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.185$
$S = 1.04$
3606 reflections
272 parameters
7 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
$w = 1/[\sigma^2(F_o^2) + (0.0857P)^2 + 0.4264P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

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

Extinction coefficient: 0.0070 (17)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.1022 (4) | 0.1217 (4) | 1.06736 (14) | 0.1466 (14) |
| O2 | 0.2236 (5) | −0.0213 (4) | 1.02338 (11) | 0.1424 (13) |
| N1 | 0.4781 (2) | 1.2271 (2) | 0.81947 (8) | 0.0608 (6) |
| N2 | 0.1826 (4) | 0.1004 (4) | 1.03580 (13) | 0.0983 (10) |
| C1 | 0.3616 (3) | 1.3187 (3) | 0.78910 (9) | 0.0553 (7) |
| C2 | 0.3483 (3) | 1.4677 (3) | 0.79922 (10) | 0.0654 (7) |
| H2 | 0.4128 | 1.5106 | 0.8254 | 0.078* |
| C3 | 0.2364 (4) | 1.5551 (4) | 0.76972 (13) | 0.0805 (9) |
| H3 | 0.2289 | 1.6559 | 0.7770 | 0.097* |
| C4 | 0.1355 (4) | 1.4960 (5) | 0.72958 (14) | 0.0883 (10) |
| H4 | 0.0631 | 1.5566 | 0.7107 | 0.106* |
| C5 | 0.1463 (4) | 1.3478 (4) | 0.71906 (13) | 0.0938 (11) |
| H5 | 0.0806 | 1.3053 | 0.6930 | 0.113* |
| C6 | 0.2598 (4) | 1.2596 (3) | 0.74862 (11) | 0.0808 (9) |
| H6 | 0.2677 | 1.1590 | 0.7411 | 0.097* |
| C7 | 0.6385 (3) | 1.2784 (3) | 0.83323 (9) | 0.0520 (6) |
| C8 | 0.7061 (3) | 1.3620 (3) | 0.80040 (11) | 0.0685 (8) |
| H8 | 0.6519 | 1.3862 | 0.7697 | 0.082* |
| C9 | 0.8628 (4) | 1.4119 (3) | 0.81420 (15) | 0.0855 (10) |
| H9 | 0.9097 | 1.4701 | 0.7915 | 0.103* |
| C10 | 0.9527 (4) | 1.3801 (3) | 0.85959 (15) | 0.0848 (10) |
| H10 | 1.0551 | 1.4169 | 0.8667 | 0.102* |
| C11 | 0.8878 (4) | 1.2964 (3) | 0.89204 (12) | 0.0769 (8) |
| H11 | 0.9441 | 1.2712 | 0.9224 | 0.092* |
| C12 | 0.7319 (3) | 1.2467 (3) | 0.87945 (10) | 0.0638 (7) |
| H12 | 0.6861 | 1.1894 | 0.9026 | 0.077* |
| C13 | 0.4293 (3) | 1.0942 (3) | 0.83959 (9) | 0.0550 (7) |
| C14 | 0.2812 (3) | 1.0854 (3) | 0.85408 (10) | 0.0634 (7) |
| H14 | 0.2101 | 1.1638 | 0.8479 | 0.076* |
| C15 | 0.2386 (4) | 0.9612 (3) | 0.87764 (11) | 0.0701 (8) |
| H15 | 0.1375 | 0.9567 | 0.8877 | 0.084* |
| C16 | 0.3393 (3) | 0.8402 (3) | 0.88742 (10) | 0.0664 (7) |
| C17 | 0.4834 (3) | 0.8447 (3) | 0.87023 (11) | 0.0679 (7) |
| H17 | 0.5512 | 0.7634 | 0.8746 | 0.081* |

| | | | | |
|---|---|---|---|---|
| C18 | 0.5286 (3) | 0.9702 (3) | 0.84636 (11) | 0.0667 (7) |
| H18 | 0.6272 | 0.9725 | 0.8345 | 0.080* |
| C19 | 0.2936 (4) | 0.7155 (3) | 0.91720 (11) | 0.0761 (8) |
| H19 | 0.1950 | 0.7239 | 0.9288 | 0.091* |
| C20 | 0.3702 (4) | 0.5964 (3) | 0.92954 (11) | 0.0729 (8) |
| H20 | 0.4687 | 0.5873 | 0.9180 | 0.088* |
| C21 | 0.3225 (3) | 0.4725 (3) | 0.95959 (10) | 0.0640 (7) |
| C22 | 0.2273 (3) | 0.4916 (3) | 0.99516 (12) | 0.0730 (8) |
| H22 | 0.1908 | 0.5861 | 1.0021 | 0.088* |
| C23 | 0.1839 (3) | 0.3702 (4) | 1.02138 (12) | 0.0793 (9) |
| H23 | 0.1189 | 0.3830 | 1.0465 | 0.095* |
| C24 | 0.2349 (3) | 0.2320 (3) | 1.01095 (11) | 0.0691 (8) |
| C25 | 0.3328 (4) | 0.2112 (3) | 0.97748 (11) | 0.0768 (9) |
| H25 | 0.3709 | 0.1169 | 0.9711 | 0.092* |
| C26 | 0.3760 (4) | 0.3325 (3) | 0.95259 (11) | 0.0752 (8) |
| H26 | 0.4469 | 0.3190 | 0.9292 | 0.090* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.102 (2) | 0.178 (3) | 0.165 (3) | −0.0168 (19) | 0.041 (2) | 0.086 (2) |
| O2 | 0.225 (4) | 0.0826 (19) | 0.114 (2) | −0.039 (2) | −0.005 (2) | 0.0338 (17) |
| N1 | 0.0531 (13) | 0.0507 (13) | 0.0774 (15) | −0.0088 (10) | 0.0022 (11) | 0.0142 (11) |
| N2 | 0.093 (2) | 0.103 (3) | 0.093 (2) | −0.029 (2) | −0.0151 (18) | 0.038 (2) |
| C1 | 0.0514 (15) | 0.0541 (16) | 0.0602 (15) | −0.0067 (12) | 0.0048 (12) | 0.0089 (12) |
| C2 | 0.0701 (18) | 0.0632 (19) | 0.0639 (17) | 0.0010 (14) | 0.0119 (14) | 0.0016 (14) |
| C3 | 0.077 (2) | 0.076 (2) | 0.093 (2) | 0.0177 (17) | 0.0258 (19) | 0.0167 (18) |
| C4 | 0.0605 (19) | 0.107 (3) | 0.098 (3) | 0.0091 (18) | 0.0143 (18) | 0.046 (2) |
| C5 | 0.079 (2) | 0.110 (3) | 0.086 (2) | −0.025 (2) | −0.0210 (18) | 0.025 (2) |
| C6 | 0.089 (2) | 0.0646 (19) | 0.084 (2) | −0.0166 (16) | −0.0122 (18) | 0.0074 (16) |
| C7 | 0.0505 (14) | 0.0440 (14) | 0.0622 (15) | −0.0018 (11) | 0.0101 (12) | 0.0037 (12) |
| C8 | 0.0616 (17) | 0.0667 (18) | 0.0794 (19) | 0.0054 (14) | 0.0177 (15) | 0.0196 (15) |
| C9 | 0.0581 (18) | 0.072 (2) | 0.131 (3) | −0.0009 (15) | 0.031 (2) | 0.0299 (19) |
| C10 | 0.0476 (17) | 0.069 (2) | 0.136 (3) | −0.0007 (15) | 0.0042 (19) | 0.010 (2) |
| C11 | 0.0645 (19) | 0.076 (2) | 0.086 (2) | −0.0012 (16) | −0.0068 (16) | 0.0027 (17) |
| C12 | 0.0594 (16) | 0.0646 (17) | 0.0673 (17) | −0.0032 (13) | 0.0075 (13) | 0.0034 (13) |
| C13 | 0.0568 (16) | 0.0473 (15) | 0.0599 (15) | −0.0101 (12) | 0.0029 (12) | 0.0041 (11) |
| C14 | 0.0604 (17) | 0.0576 (17) | 0.0724 (18) | −0.0102 (13) | 0.0086 (14) | 0.0010 (13) |
| C15 | 0.0655 (18) | 0.0692 (19) | 0.0760 (19) | −0.0166 (15) | 0.0093 (15) | 0.0024 (15) |
| C16 | 0.0727 (16) | 0.0654 (16) | 0.0598 (16) | −0.0262 (15) | 0.0022 (13) | 0.0002 (12) |
| C17 | 0.0739 (17) | 0.0495 (16) | 0.0790 (19) | −0.0023 (13) | 0.0024 (14) | 0.0040 (13) |
| C18 | 0.0679 (18) | 0.0557 (17) | 0.0778 (18) | −0.0030 (14) | 0.0136 (14) | 0.0061 (14) |
| C19 | 0.078 (2) | 0.0675 (16) | 0.080 (2) | −0.0169 (13) | −0.0011 (15) | 0.0085 (14) |
| C20 | 0.081 (2) | 0.0664 (16) | 0.0682 (18) | −0.0164 (13) | −0.0052 (15) | 0.0025 (13) |
| C21 | 0.0659 (17) | 0.0672 (17) | 0.0566 (16) | −0.0140 (14) | −0.0033 (14) | 0.0054 (12) |
| C22 | 0.0665 (18) | 0.0613 (18) | 0.089 (2) | 0.0021 (14) | −0.0002 (16) | 0.0082 (16) |
| C23 | 0.0585 (18) | 0.094 (3) | 0.085 (2) | −0.0007 (17) | 0.0104 (16) | 0.0212 (19) |
| C24 | 0.0645 (18) | 0.072 (2) | 0.0670 (18) | −0.0163 (16) | −0.0075 (15) | 0.0249 (15) |
| C25 | 0.103 (2) | 0.0576 (18) | 0.0674 (18) | −0.0071 (16) | −0.0012 (18) | 0.0044 (15) |
| C26 | 0.095 (2) | 0.068 (2) | 0.0633 (17) | −0.0131 (17) | 0.0124 (16) | −0.0006 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—N2 | 1.168 (4) | C12—H12 | 0.9300 |
| O2—N2 | 1.207 (4) | C13—C14 | 1.361 (4) |
| N1—C13 | 1.395 (3) | C13—C18 | 1.397 (4) |
| N1—C7 | 1.445 (3) | C14—C15 | 1.355 (4) |
| N1—C1 | 1.465 (3) | C14—H14 | 0.9300 |
| N2—C24 | 1.454 (4) | C15—C16 | 1.390 (4) |
| C1—C2 | 1.373 (4) | C15—H15 | 0.9300 |
| C1—C6 | 1.420 (4) | C16—C17 | 1.358 (4) |
| C2—C3 | 1.409 (4) | C16—C19 | 1.458 (4) |
| C2—H2 | 0.9300 | C17—C18 | 1.375 (4) |
| C3—C4 | 1.410 (5) | C17—H17 | 0.9300 |
| C3—H3 | 0.9300 | C18—H18 | 0.9300 |
| C4—C5 | 1.367 (5) | C19—C20 | 1.276 (4) |
| C4—H4 | 0.9300 | C19—H19 | 0.9300 |
| C5—C6 | 1.422 (4) | C20—C21 | 1.463 (4) |
| C5—H5 | 0.9300 | C20—H20 | 0.9300 |
| C6—H6 | 0.9300 | C21—C22 | 1.337 (4) |
| C7—C8 | 1.342 (3) | C21—C26 | 1.358 (4) |
| C7—C12 | 1.433 (4) | C22—C23 | 1.374 (4) |
| C8—C9 | 1.413 (4) | C22—H22 | 0.9300 |
| C8—H8 | 0.9300 | C23—C24 | 1.356 (4) |
| C9—C10 | 1.401 (5) | C23—H23 | 0.9300 |
| C9—H9 | 0.9300 | C24—C25 | 1.310 (4) |
| C10—C11 | 1.323 (4) | C25—C26 | 1.354 (4) |
| C10—H10 | 0.9300 | C25—H25 | 0.9300 |
| C11—C12 | 1.402 (4) | C26—H26 | 0.9300 |
| C11—H11 | 0.9300 | | |
| | | | |
| C13—N1—C7 | 119.0 (2) | C14—C13—N1 | 119.2 (2) |
| C13—N1—C1 | 119.2 (2) | C14—C13—C18 | 118.6 (2) |
| C7—N1—C1 | 121.44 (19) | N1—C13—C18 | 122.2 (2) |
| O1—N2—O2 | 124.3 (4) | C15—C14—C13 | 119.2 (3) |
| O1—N2—C24 | 116.1 (4) | C15—C14—H14 | 120.4 |
| O2—N2—C24 | 119.6 (4) | C13—C14—H14 | 120.4 |
| C2—C1—C6 | 117.5 (3) | C14—C15—C16 | 122.9 (3) |
| C2—C1—N1 | 120.0 (2) | C14—C15—H15 | 118.6 |
| C6—C1—N1 | 122.5 (2) | C16—C15—H15 | 118.6 |
| C1—C2—C3 | 119.7 (3) | C17—C16—C15 | 118.0 (3) |
| C1—C2—H2 | 120.1 | C17—C16—C19 | 121.3 (3) |
| C3—C2—H2 | 120.1 | C15—C16—C19 | 120.6 (3) |
| C2—C3—C4 | 122.6 (3) | C16—C17—C18 | 119.7 (3) |
| C2—C3—H3 | 118.7 | C16—C17—H17 | 120.1 |
| C4—C3—H3 | 118.7 | C18—C17—H17 | 120.1 |
| C5—C4—C3 | 118.6 (3) | C17—C18—C13 | 121.3 (3) |
| C5—C4—H4 | 120.7 | C17—C18—H18 | 119.4 |
| C3—C4—H4 | 120.7 | C13—C18—H18 | 119.4 |
| C4—C5—C6 | 118.8 (3) | C20—C19—C16 | 129.0 (3) |
| C4—C5—H5 | 120.6 | C20—C19—H19 | 115.5 |

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| C6—C5—H5 | 120.6 | C16—C19—H19 | 115.5 |
| C1—C6—C5 | 122.7 (3) | C19—C20—C21 | 128.2 (3) |
| C1—C6—H6 | 118.6 | C19—C20—H20 | 115.9 |
| C5—C6—H6 | 118.6 | C21—C20—H20 | 115.9 |
| C8—C7—C12 | 117.0 (2) | C22—C21—C26 | 117.3 (3) |
| C8—C7—N1 | 118.0 (2) | C22—C21—C20 | 122.1 (3) |
| C12—C7—N1 | 125.0 (2) | C26—C21—C20 | 120.6 (3) |
| C7—C8—C9 | 117.6 (3) | C21—C22—C23 | 119.4 (3) |
| C7—C8—H8 | 121.2 | C21—C22—H22 | 120.3 |
| C9—C8—H8 | 121.2 | C23—C22—H22 | 120.3 |
| C10—C9—C8 | 124.7 (3) | C24—C23—C22 | 120.6 (3) |
| C10—C9—H9 | 117.6 | C24—C23—H23 | 119.7 |
| C8—C9—H9 | 117.6 | C22—C23—H23 | 119.7 |
| C11—C10—C9 | 118.2 (3) | C25—C24—C23 | 121.2 (3) |
| C11—C10—H10 | 120.9 | C25—C24—N2 | 117.1 (3) |
| C9—C10—H10 | 120.9 | C23—C24—N2 | 121.8 (3) |
| C10—C11—C12 | 118.2 (3) | C24—C25—C26 | 117.3 (3) |
| C10—C11—H11 | 120.9 | C24—C25—H25 | 121.4 |
| C12—C11—H11 | 120.9 | C26—C25—H25 | 121.4 |
| C11—C12—C7 | 124.3 (3) | C25—C26—C21 | 124.2 (3) |
| C11—C12—H12 | 117.9 | C25—C26—H26 | 117.9 |
| C7—C12—H12 | 117.9 | C21—C26—H26 | 117.9 |

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| C13—N1—C1—C2 | 129.1 (3) | C18—C13—C14—C15 | 4.5 (4) |
| C7—N1—C1—C2 | −44.5 (3) | C13—C14—C15—C16 | −0.7 (4) |
| C13—N1—C1—C6 | −51.1 (3) | C14—C15—C16—C17 | −3.4 (4) |
| C7—N1—C1—C6 | 135.3 (3) | C14—C15—C16—C19 | 173.8 (3) |
| C6—C1—C2—C3 | 0.0 (4) | C15—C16—C17—C18 | 3.5 (4) |
| N1—C1—C2—C3 | 179.7 (2) | C19—C16—C17—C18 | −173.8 (3) |
| C1—C2—C3—C4 | 0.1 (4) | C16—C17—C18—C13 | 0.4 (4) |
| C2—C3—C4—C5 | 0.3 (5) | C14—C13—C18—C17 | −4.5 (4) |
| C3—C4—C5—C6 | −0.6 (5) | N1—C13—C18—C17 | 174.2 (2) |
| C2—C1—C6—C5 | −0.4 (4) | C17—C16—C19—C20 | −3.1 (5) |
| N1—C1—C6—C5 | 179.9 (3) | C15—C16—C19—C20 | 179.7 (3) |
| C4—C5—C6—C1 | 0.7 (5) | C16—C19—C20—C21 | 179.8 (3) |
| C13—N1—C7—C8 | 151.6 (2) | C19—C20—C21—C22 | −29.6 (5) |
| C1—N1—C7—C8 | −34.8 (3) | C19—C20—C21—C26 | 151.3 (3) |
| C13—N1—C7—C12 | −28.3 (4) | C26—C21—C22—C23 | −2.3 (4) |
| C1—N1—C7—C12 | 145.3 (2) | C20—C21—C22—C23 | 178.6 (3) |
| C12—C7—C8—C9 | −0.2 (4) | C21—C22—C23—C24 | −0.9 (4) |
| N1—C7—C8—C9 | 179.9 (2) | C22—C23—C24—C25 | 3.4 (5) |
| C7—C8—C9—C10 | 0.2 (5) | C22—C23—C24—N2 | −175.9 (3) |
| C8—C9—C10—C11 | 0.6 (5) | O1—N2—C24—C25 | 176.1 (3) |
| C9—C10—C11—C12 | −1.2 (5) | O2—N2—C24—C25 | −3.6 (5) |
| C10—C11—C12—C7 | 1.1 (4) | O1—N2—C24—C23 | −4.6 (5) |
| C8—C7—C12—C11 | −0.4 (4) | O2—N2—C24—C23 | 175.7 (3) |
| N1—C7—C12—C11 | 179.5 (2) | C23—C24—C25—C26 | −2.3 (5) |
| C7—N1—C13—C14 | 139.6 (3) | N2—C24—C25—C26 | 177.0 (3) |
| C1—N1—C13—C14 | −34.2 (3) | C24—C25—C26—C21 | −1.2 (5) |

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| C7—N1—C13—C18 | −39.1 (4) | C22—C21—C26—C25 | 3.5 (4) |
| C1—N1—C13—C18 | 147.1 (3) | C20—C21—C26—C25 | −177.4 (3) |
| N1—C13—C14—C15 | −174.2 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C15—H15···O1$^{i}$ | 0.93 | 2.58 | 3.481 (4) | 162 |
| C12—H12···O2$^{ii}$ | 0.93 | 2.56 | 3.308 (4) | 138 |

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