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# 1,2-Diphenyl-1*H*-imidazo[4,5-*f*][1,10]-phenanthroline

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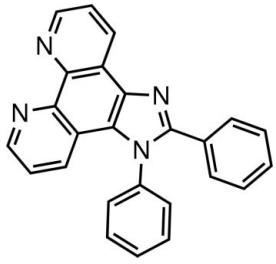
Key indicators: single-crystal X-ray study; $T$ = 170 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.042; $wR$ factor = 0.117; data-to-parameter ratio = 13.4.

In the title compound, $C_{25}H_{16}N_4$, the fused ring system is essentially planar [maximum deviation = 0.1012 (15) Å]. The imidazole ring makes dihedral angles of 77.41 (8) and 56.26 (8)° with the phenyl rings attached to nitrogen and carbon, respectively. The dihedral angle between the two phenyl rings is 65.50 (8)°. Weak C—H$\cdots\pi$ interactions are found in the crystal structure.

## Related literature

For 1,2-diphenyl-1*H*-imidazo[4,5-*f*][1,10]phenanthroline derivatives, see: Hadadzadeh *et al.* (2006). For metal complexes of the 1,10-phenanthroline-5,6-dione ligand, see: Goss & Abruna (1985).



## Experimental

### Crystal data

$C_{25}H_{16}N_4$ $M_r$ = 372.42
Triclinic, $P\overline{1}$
$a$ = 8.8693 (7) Å
$b$ = 10.0637 (6) Å
$c$ = 11.8960 (9) Å
$\alpha$ = 100.219 (6)°
$\beta$ = 110.310 (7)°
$\gamma$ = 102.475 (6)°
$V$ = 934.63 (14) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 0.63 mm$^{-1}$
$T$ = 170 K
0.43 × 0.38 × 0.26 mm

### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
$T_{min}$ = 0.965, $T_{max}$ = 1.000
5832 measured reflections
3522 independent reflections
3121 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
$S$ = 1.05
3522 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

*Cg*4 and *Cg*6 are the centroids of the C4–C6/C11/C12/C17 and C24–C29 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C15—H15$\cdots$*Cg*6$^{i}$ | 0.95 | 2.86 | 3.757 (3) | 157 |
| C25—H25$\cdots$*Cg*4$^{ii}$ | 0.95 | 2.75 | 3.4835 (16) | 135 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5009).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o989 [ **doi:10.1107/S1600536811010890** ]

# 1,2-Diphenyl-1*H*-imidazo[4,5-*f*][1,10]phenanthroline

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## Comment

1,2-diphenyl-1*H*-imidazo[4,5-*f*][1,10]phenanthroline derivatives play important roles as molecular scaffolding for supramolecular assemblies, building block for the synthesis of metallo-dendrimers, thin films of luminescent complexes and ligands for synthesis of ring opening metathesis polymerization (ROMP) (Hadadzadeh *et al.*, 2006). Metal complexes of phen-dione ligand allow for the variation and control of redox properties over a wide range as well as the fine tuning of potentials through pH changes (Goss & Abruna, 1985). Since our group doing the research in organic light emitting devices, we are interested to use the title compound as ligand for synthesizing Ir(III) complexes.

In the title compound (Fig. 1), $C_{25}H_{16}N_4$, the fused ring system is essentially planar [maximum deviation of 0.1012 (15) Å for N13]. The imidazole ring makes dihedral angles of 77.41 (8) and 56.26 (8)° with the phenyl ring (C18—C23) attached to N1 and phenyl ring (C24—C29) attached to C2 respectively. The dihedral angle between the two phenyl rings is 65.50 (8)°. Further, weak C15—H15···π interaction involving phenyl (C24—C29) ring and C25—H25···π interaction involving (C4/C5/C6/C11/C12/C17) ring are found in the crystal structure (Table 1).

## Experimental

Pure 1,10-Phenanthroline-5,6-dione (2.10 g, 10 mmol) in ethanol (10 ml), aniline (0.91 g, 10 mmol), ammonium acetate (0.77 g, 10 mmol) and benzaldehyde (1.0 g, 10 mmol) was added about 1 h by maintaining the temperature at 333 K. The reaction mixture was refluxed for 7 days and extracted with dichloromethane. The solid separated was purified by column chromatography using Benzene: Ethyl acetate as the eluent. Yield: 1.48 g (40%). Crystals suitable for X-ray diffraction studies were grown by slow solvent evaporation of a solution of the compound in dichloromethane.

## Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å; $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

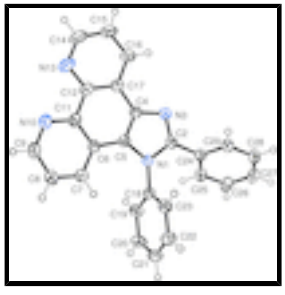

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

## 1,2-Diphenyl-1*H*-imidazo[4,5-*f*][1,10]phenanthroline

### *Crystal data*

| | |
|---|---|
| $C_{25}H_{16}N_4$ | $Z = 2$ |
| $M_r = 372.42$ | $F(000) = 388$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.323$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 579 K |
| $a = 8.8693$ (7) Å | Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å |
| $b = 10.0637$ (6) Å | Cell parameters from 3954 reflections |
| $c = 11.8960$ (9) Å | $\theta = 4.7$–$70.6°$ |
| $\alpha = 100.219$ (6)° | $\mu = 0.63$ mm$^{-1}$ |
| $\beta = 110.310$ (7)° | $T = 170$ K |
| $\gamma = 102.475$ (6)° | Block, colourless |
| $V = 934.63$ (14) Å$^3$ | 0.43 × 0.38 × 0.26 mm |

### *Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Eos Gemini diffractometer | 3522 independent reflections |
| Radiation source: Enhance (Cu) X-ray Source | 3121 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.014$ |
| Detector resolution: 16.1500 pixels mm$^{-1}$ | $\theta_{max} = 70.7°$, $\theta_{min} = 4.7°$ |
| ω scans | $h = -10 \rightarrow 10$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010) | $k = -12 \rightarrow 7$ |
| $T_{min} = 0.965$, $T_{max} = 1.000$ | $l = -13 \rightarrow 14$ |
| 5832 measured reflections | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.117$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.1268P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3522 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 262 parameters | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.17$ e Å$^{-3}$ |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.44262 (13) | 0.14038 (11) | 0.37008 (9) | 0.0404 (3) |
| N3 | 0.21256 (13) | 0.07897 (11) | 0.41050 (10) | 0.0436 (3) |
| N10 | 0.70826 (15) | 0.57164 (12) | 0.72960 (11) | 0.0510 (4) |
| N13 | 0.4425 (2) | 0.47849 (14) | 0.78916 (13) | 0.0678 (5) |
| C2 | 0.28544 (15) | 0.04678 (13) | 0.33444 (12) | 0.0414 (4) |
| C4 | 0.32764 (16) | 0.19978 (13) | 0.49979 (11) | 0.0407 (4) |
| C5 | 0.47004 (15) | 0.24080 (13) | 0.47676 (11) | 0.0394 (3) |
| C6 | 0.60568 (15) | 0.36743 (13) | 0.55079 (11) | 0.0399 (3) |
| C7 | 0.74828 (17) | 0.41987 (15) | 0.52720 (13) | 0.0503 (4) |
| C8 | 0.86537 (19) | 0.54488 (16) | 0.60380 (14) | 0.0555 (5) |
| C9 | 0.83894 (19) | 0.61654 (15) | 0.70255 (13) | 0.0546 (4) |
| C11 | 0.59107 (17) | 0.44797 (13) | 0.65524 (11) | 0.0425 (4) |
| C12 | 0.44390 (18) | 0.40051 (14) | 0.68438 (12) | 0.0462 (4) |
| C14 | 0.3052 (3) | 0.4386 (2) | 0.81063 (19) | 0.0818 (7) |
| C15 | 0.1641 (3) | 0.32423 (19) | 0.73479 (18) | 0.0710 (7) |
| C16 | 0.1669 (2) | 0.24145 (16) | 0.63142 (15) | 0.0550 (5) |
| C17 | 0.31040 (17) | 0.27871 (14) | 0.60500 (12) | 0.0436 (4) |
| C18 | 0.54455 (15) | 0.13773 (12) | 0.29871 (11) | 0.0392 (3) |
| C19 | 0.68211 (17) | 0.08736 (15) | 0.33628 (14) | 0.0511 (4) |
| C20 | 0.7747 (2) | 0.08003 (17) | 0.26423 (16) | 0.0598 (5) |
| C21 | 0.72777 (19) | 0.12065 (16) | 0.15536 (15) | 0.0584 (5) |
| C22 | 0.5928 (2) | 0.17260 (17) | 0.12019 (14) | 0.0582 (5) |
| C23 | 0.50057 (17) | 0.18306 (15) | 0.19273 (13) | 0.0487 (4) |
| C24 | 0.21038 (15) | −0.07711 (13) | 0.22359 (11) | 0.0418 (4) |
| C25 | 0.29258 (18) | −0.17796 (15) | 0.21043 (13) | 0.0515 (4) |
| C26 | 0.2173 (2) | −0.29636 (15) | 0.10929 (14) | 0.0581 (5) |
| C27 | 0.0601 (2) | −0.31457 (15) | 0.01978 (13) | 0.0578 (5) |
| C28 | −0.02154 (19) | −0.21497 (18) | 0.03113 (14) | 0.0599 (5) |
| C29 | 0.05283 (17) | −0.09633 (16) | 0.13260 (13) | 0.0526 (4) |
| H7 | 0.76323 | 0.36890 | 0.45861 | 0.0604* |
| H8 | 0.96307 | 0.58201 | 0.58965 | 0.0666* |
| H9 | 0.92067 | 0.70407 | 0.75433 | 0.0655* |
| H14 | 0.30294 | 0.49252 | 0.88384 | 0.0983* |
| H15 | 0.06790 | 0.30395 | 0.75426 | 0.0852* |

| | | | | |
|---|---|---|---|---|
| H16 | 0.07396 | 0.16076 | 0.57882 | 0.0660* |
| H19 | 0.71247 | 0.05821 | 0.41066 | 0.0613* |
| H20 | 0.87050 | 0.04707 | 0.28955 | 0.0718* |
| H21 | 0.78933 | 0.11258 | 0.10446 | 0.0701* |
| H22 | 0.56247 | 0.20157 | 0.04571 | 0.0698* |
| H23 | 0.40854 | 0.22091 | 0.16961 | 0.0584* |
| H25 | 0.40137 | −0.16534 | 0.27149 | 0.0618* |
| H26 | 0.27385 | −0.36536 | 0.10130 | 0.0697* |
| H27 | 0.00829 | −0.39617 | −0.04980 | 0.0693* |
| H28 | −0.12955 | −0.22749 | −0.03092 | 0.0718* |
| H29 | −0.00436 | −0.02771 | 0.13996 | 0.0631* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0356 (5) | 0.0448 (5) | 0.0376 (5) | 0.0087 (4) | 0.0158 (4) | 0.0053 (4) |
| N3 | 0.0372 (5) | 0.0500 (6) | 0.0417 (6) | 0.0100 (4) | 0.0173 (4) | 0.0092 (5) |
| N10 | 0.0563 (7) | 0.0464 (6) | 0.0427 (6) | 0.0103 (5) | 0.0167 (5) | 0.0069 (5) |
| N13 | 0.0882 (10) | 0.0568 (7) | 0.0632 (8) | 0.0142 (7) | 0.0476 (8) | 0.0020 (6) |
| C2 | 0.0353 (6) | 0.0468 (7) | 0.0400 (6) | 0.0102 (5) | 0.0147 (5) | 0.0106 (5) |
| C4 | 0.0393 (6) | 0.0468 (7) | 0.0387 (6) | 0.0153 (5) | 0.0172 (5) | 0.0122 (5) |
| C5 | 0.0381 (6) | 0.0456 (6) | 0.0351 (6) | 0.0145 (5) | 0.0148 (5) | 0.0098 (5) |
| C6 | 0.0379 (6) | 0.0440 (6) | 0.0367 (6) | 0.0135 (5) | 0.0129 (5) | 0.0114 (5) |
| C7 | 0.0443 (7) | 0.0549 (8) | 0.0470 (7) | 0.0086 (6) | 0.0205 (6) | 0.0060 (6) |
| C8 | 0.0461 (8) | 0.0567 (8) | 0.0549 (8) | 0.0041 (6) | 0.0197 (6) | 0.0096 (7) |
| C9 | 0.0547 (8) | 0.0477 (7) | 0.0462 (7) | 0.0039 (6) | 0.0126 (6) | 0.0066 (6) |
| C11 | 0.0478 (7) | 0.0423 (6) | 0.0361 (6) | 0.0158 (5) | 0.0139 (5) | 0.0112 (5) |
| C12 | 0.0563 (8) | 0.0456 (7) | 0.0427 (7) | 0.0198 (6) | 0.0241 (6) | 0.0122 (5) |
| C14 | 0.1087 (15) | 0.0699 (11) | 0.0839 (12) | 0.0187 (10) | 0.0718 (12) | 0.0037 (9) |
| C15 | 0.0838 (12) | 0.0683 (10) | 0.0838 (12) | 0.0221 (9) | 0.0620 (11) | 0.0180 (9) |
| C16 | 0.0581 (9) | 0.0587 (8) | 0.0605 (9) | 0.0203 (7) | 0.0360 (7) | 0.0176 (7) |
| C17 | 0.0476 (7) | 0.0483 (7) | 0.0433 (7) | 0.0203 (6) | 0.0228 (6) | 0.0160 (6) |
| C18 | 0.0362 (6) | 0.0397 (6) | 0.0395 (6) | 0.0077 (5) | 0.0179 (5) | 0.0050 (5) |
| C19 | 0.0470 (7) | 0.0592 (8) | 0.0555 (8) | 0.0211 (6) | 0.0243 (6) | 0.0219 (7) |
| C20 | 0.0510 (8) | 0.0654 (9) | 0.0765 (10) | 0.0258 (7) | 0.0356 (8) | 0.0208 (8) |
| C21 | 0.0578 (9) | 0.0624 (9) | 0.0638 (9) | 0.0141 (7) | 0.0401 (8) | 0.0112 (7) |
| C22 | 0.0611 (9) | 0.0690 (9) | 0.0492 (8) | 0.0152 (7) | 0.0288 (7) | 0.0192 (7) |
| C23 | 0.0441 (7) | 0.0563 (8) | 0.0472 (7) | 0.0166 (6) | 0.0187 (6) | 0.0155 (6) |
| C24 | 0.0388 (6) | 0.0453 (7) | 0.0379 (6) | 0.0059 (5) | 0.0165 (5) | 0.0097 (5) |
| C25 | 0.0506 (8) | 0.0487 (7) | 0.0449 (7) | 0.0138 (6) | 0.0091 (6) | 0.0105 (6) |
| C26 | 0.0726 (10) | 0.0453 (7) | 0.0491 (8) | 0.0184 (7) | 0.0167 (7) | 0.0105 (6) |
| C27 | 0.0705 (10) | 0.0473 (7) | 0.0386 (7) | 0.0035 (7) | 0.0131 (7) | 0.0068 (6) |
| C28 | 0.0460 (8) | 0.0730 (10) | 0.0430 (7) | 0.0075 (7) | 0.0072 (6) | 0.0086 (7) |
| C29 | 0.0414 (7) | 0.0639 (9) | 0.0481 (7) | 0.0149 (6) | 0.0163 (6) | 0.0094 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C2 | 1.3752 (18) | C20—C21 | 1.380 (2) |
| N1—C5 | 1.3840 (16) | C21—C22 | 1.372 (3) |

| | | | |
|---|---|---|---|
| N1—C18 | 1.4402 (18) | C22—C23 | 1.386 (2) |
| N3—C2 | 1.3168 (18) | C24—C25 | 1.389 (2) |
| N3—C4 | 1.3789 (17) | C24—C29 | 1.386 (2) |
| N10—C9 | 1.317 (2) | C25—C26 | 1.380 (2) |
| N10—C11 | 1.3506 (18) | C26—C27 | 1.379 (2) |
| N13—C12 | 1.356 (2) | C27—C28 | 1.371 (3) |
| N13—C14 | 1.323 (3) | C28—C29 | 1.383 (2) |
| C2—C24 | 1.4782 (18) | C7—H7 | 0.9500 |
| C4—C5 | 1.377 (2) | C8—H8 | 0.9500 |
| C4—C17 | 1.4330 (19) | C9—H9 | 0.9500 |
| C5—C6 | 1.4321 (18) | C14—H14 | 0.9500 |
| C6—C7 | 1.403 (2) | C15—H15 | 0.9500 |
| C6—C11 | 1.4204 (18) | C16—H16 | 0.9500 |
| C7—C8 | 1.365 (2) | C19—H19 | 0.9500 |
| C8—C9 | 1.385 (2) | C20—H20 | 0.9500 |
| C11—C12 | 1.468 (2) | C21—H21 | 0.9500 |
| C12—C17 | 1.408 (2) | C22—H22 | 0.9500 |
| C14—C15 | 1.389 (3) | C23—H23 | 0.9500 |
| C15—C16 | 1.369 (3) | C25—H25 | 0.9500 |
| C16—C17 | 1.405 (2) | C26—H26 | 0.9500 |
| C18—C19 | 1.384 (2) | C27—H27 | 0.9500 |
| C18—C23 | 1.3745 (19) | C28—H28 | 0.9500 |
| C19—C20 | 1.381 (2) | C29—H29 | 0.9500 |
| N10···N13 | 2.716 (2) | C18···H25 | 2.9500 |
| N13···C23$^{i}$ | 3.290 (2) | C18···H7 | 2.5900 |
| N13···N10 | 2.716 (2) | C19···H7 | 2.7600 |
| N3···H19$^{ii}$ | 2.7100 | C19···H25 | 2.9200 |
| N3···H16 | 2.7900 | C20···H29$^{viii}$ | 3.0900 |
| N3···H20$^{iii}$ | 2.7900 | C21···H9$^{ix}$ | 2.9300 |
| N10···H23$^{i}$ | 2.7900 | C24···H15$^{v}$ | 3.1000 |
| N10···H27$^{iv}$ | 2.9200 | C27···H21$^{x}$ | 3.0600 |
| N10···H28$^{iv}$ | 2.8500 | C27···H9$^{vi}$ | 3.0200 |
| N13···H23$^{i}$ | 2.9000 | C27···H27$^{vii}$ | 2.9500 |
| C4···C8$^{i}$ | 3.551 (2) | C28···H9$^{vi}$ | 3.0800 |
| C4···C9$^{i}$ | 3.418 (2) | C28···H15$^{v}$ | 2.9800 |
| C5···C9$^{i}$ | 3.585 (2) | C29···H15$^{v}$ | 2.8900 |
| C6···C11$^{i}$ | 3.5427 (19) | H7···C18 | 2.5900 |
| C7···C18 | 3.2173 (19) | H7···C19 | 2.7600 |
| C7···C12$^{i}$ | 3.532 (2) | H9···C27$^{iv}$ | 3.0200 |
| C7···C19 | 3.497 (2) | H9···C28$^{iv}$ | 3.0800 |
| C8···C17$^{i}$ | 3.439 (2) | H9···C21$^{ix}$ | 2.9300 |
| C8···C4$^{i}$ | 3.551 (2) | H9···H21$^{ix}$ | 2.5900 |
| C9···C4$^{i}$ | 3.418 (2) | H15···C24$^{v}$ | 3.1000 |
| C9···C27$^{iv}$ | 3.452 (2) | H15···C28$^{v}$ | 2.9800 |
| C9···C5$^{i}$ | 3.585 (2) | H15···C29$^{v}$ | 2.8900 |

| | | | |
|---|---|---|---|
| C11···C26$^{ii}$ | 3.521 (2) | H16···N3 | 2.7900 |
| C11···C6$^{i}$ | 3.5427 (19) | H19···N3$^{ii}$ | 2.7100 |
| C11···C25$^{ii}$ | 3.551 (2) | H19···C4$^{ii}$ | 2.9700 |
| C12···C7$^{i}$ | 3.532 (2) | H20···N3$^{viii}$ | 2.7900 |
| C15···C29$^{v}$ | 3.597 (3) | H20···H29$^{viii}$ | 2.4900 |
| C17···C8$^{i}$ | 3.439 (2) | H21···H29$^{viii}$ | 2.5100 |
| C18···C7 | 3.2173 (19) | H21···C27$^{x}$ | 3.0600 |
| C18···C25 | 3.211 (2) | H21···H9$^{ix}$ | 2.5900 |
| C19···C7 | 3.497 (2) | H23···N10$^{i}$ | 2.7900 |
| C19···C25 | 3.509 (2) | H23···N13$^{i}$ | 2.9000 |
| C23···C24 | 3.421 (2) | H23···H28$^{xi}$ | 2.4700 |
| C23···N13$^{i}$ | 3.290 (2) | H25···C18 | 2.9500 |
| C24···C23 | 3.421 (2) | H25···C19 | 2.9200 |
| C25···C18 | 3.211 (2) | H25···C4$^{ii}$ | 3.0700 |
| C25···C19 | 3.509 (2) | H25···C12$^{ii}$ | 3.0200 |
| C25···C11$^{ii}$ | 3.551 (2) | H25···C17$^{ii}$ | 3.0400 |
| C26···C11$^{ii}$ | 3.521 (2) | H26···C11$^{ii}$ | 3.0600 |
| C27···C9$^{vi}$ | 3.452 (2) | H26···C12$^{ii}$ | 3.0300 |
| C27···C27$^{vii}$ | 3.549 (2) | H27···N10$^{vi}$ | 2.9200 |
| C29···C15$^{v}$ | 3.597 (3) | H27···C9$^{vi}$ | 2.8500 |
| C4···H25$^{ii}$ | 3.0700 | H27···C27$^{vii}$ | 2.9500 |
| C4···H19$^{ii}$ | 2.9700 | H27···H27$^{vii}$ | 2.5800 |
| C9···H27$^{iv}$ | 2.8500 | H28···N10$^{vi}$ | 2.8500 |
| C11···H26$^{ii}$ | 3.0600 | H28···H23$^{xi}$ | 2.4700 |
| C12···H26$^{ii}$ | 3.0300 | H29···C20$^{iii}$ | 3.0900 |
| C12···H25$^{ii}$ | 3.0200 | H29···H20$^{iii}$ | 2.4900 |
| C17···H25$^{ii}$ | 3.0400 | H29···H21$^{iii}$ | 2.5100 |
| C2—N1—C5 | 106.40 (11) | C2—C24—C25 | 121.16 (12) |
| C2—N1—C18 | 124.47 (10) | C2—C24—C29 | 119.87 (13) |
| C5—N1—C18 | 128.80 (11) | C25—C24—C29 | 118.94 (13) |
| C2—N3—C4 | 104.52 (12) | C24—C25—C26 | 120.44 (14) |
| C9—N10—C11 | 117.80 (13) | C25—C26—C27 | 120.03 (16) |
| C12—N13—C14 | 116.67 (16) | C26—C27—C28 | 120.05 (14) |
| N1—C2—N3 | 112.63 (11) | C27—C28—C29 | 120.24 (15) |
| N1—C2—C24 | 122.78 (12) | C24—C29—C28 | 120.30 (15) |
| N3—C2—C24 | 124.59 (13) | C6—C7—H7 | 120.00 |
| N3—C4—C5 | 111.31 (12) | C8—C7—H7 | 120.00 |
| N3—C4—C17 | 127.30 (13) | C7—C8—H8 | 121.00 |
| C5—C4—C17 | 121.38 (12) | C9—C8—H8 | 121.00 |
| N1—C5—C4 | 105.14 (11) | N10—C9—H9 | 118.00 |
| N1—C5—C6 | 131.74 (13) | C8—C9—H9 | 118.00 |
| C4—C5—C6 | 123.04 (12) | N13—C14—H14 | 117.00 |
| C5—C6—C7 | 125.74 (12) | C15—C14—H14 | 117.00 |

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|---|---|---|---|
| C5—C6—C11 | 116.56 (13) | C14—C15—H15 | 121.00 |
| C7—C6—C11 | 117.68 (12) | C16—C15—H15 | 121.00 |
| C6—C7—C8 | 119.33 (14) | C15—C16—H16 | 121.00 |
| C7—C8—C9 | 118.70 (16) | C17—C16—H16 | 121.00 |
| N10—C9—C8 | 124.49 (14) | C18—C19—H19 | 120.00 |
| N10—C11—C6 | 121.98 (14) | C20—C19—H19 | 120.00 |
| N10—C11—C12 | 117.39 (12) | C19—C20—H20 | 120.00 |
| C6—C11—C12 | 120.61 (12) | C21—C20—H20 | 120.00 |
| N13—C12—C11 | 117.44 (13) | C20—C21—H21 | 120.00 |
| N13—C12—C17 | 122.17 (15) | C22—C21—H21 | 120.00 |
| C11—C12—C17 | 120.40 (12) | C21—C22—H22 | 120.00 |
| N13—C14—C15 | 125.3 (2) | C23—C22—H22 | 120.00 |
| C14—C15—C16 | 118.5 (2) | C18—C23—H23 | 121.00 |
| C15—C16—C17 | 118.39 (17) | C22—C23—H23 | 121.00 |
| C4—C17—C12 | 117.84 (14) | C24—C25—H25 | 120.00 |
| C4—C17—C16 | 123.29 (13) | C26—C25—H25 | 120.00 |
| C12—C17—C16 | 118.86 (13) | C25—C26—H26 | 120.00 |
| N1—C18—C19 | 119.73 (11) | C27—C26—H26 | 120.00 |
| N1—C18—C23 | 118.93 (13) | C26—C27—H27 | 120.00 |
| C19—C18—C23 | 121.33 (14) | C28—C27—H27 | 120.00 |
| C18—C19—C20 | 119.13 (14) | C27—C28—H28 | 120.00 |
| C19—C20—C21 | 119.88 (17) | C29—C28—H28 | 120.00 |
| C20—C21—C22 | 120.41 (16) | C24—C29—H29 | 120.00 |
| C21—C22—C23 | 120.35 (15) | C28—C29—H29 | 120.00 |
| C18—C23—C22 | 118.84 (15) | | |
| C5—N1—C2—N3 | −0.73 (15) | C4—C5—C6—C11 | 2.93 (19) |
| C5—N1—C2—C24 | −179.76 (12) | C5—C6—C7—C8 | 177.87 (14) |
| C18—N1—C2—N3 | −174.58 (12) | C11—C6—C7—C8 | −0.4 (2) |
| C18—N1—C2—C24 | 6.4 (2) | C5—C6—C11—N10 | −177.82 (12) |
| C2—N1—C5—C4 | 0.88 (14) | C5—C6—C11—C12 | 0.63 (19) |
| C2—N1—C5—C6 | −175.82 (14) | C7—C6—C11—N10 | 0.6 (2) |
| C18—N1—C5—C4 | 174.37 (12) | C7—C6—C11—C12 | 179.08 (13) |
| C18—N1—C5—C6 | −2.3 (2) | C6—C7—C8—C9 | −0.3 (2) |
| C2—N1—C18—C19 | −104.93 (15) | C7—C8—C9—N10 | 0.9 (2) |
| C2—N1—C18—C23 | 73.81 (17) | N10—C11—C12—N13 | −4.9 (2) |
| C5—N1—C18—C19 | 82.65 (17) | N10—C11—C12—C17 | 174.82 (13) |
| C5—N1—C18—C23 | −98.62 (16) | C6—C11—C12—N13 | 176.55 (13) |
| C4—N3—C2—N1 | 0.24 (15) | C6—C11—C12—C17 | −3.7 (2) |
| C4—N3—C2—C24 | 179.25 (12) | N13—C12—C17—C4 | −177.04 (14) |
| C2—N3—C4—C5 | 0.35 (15) | N13—C12—C17—C16 | 3.7 (2) |
| C2—N3—C4—C17 | −179.93 (14) | C11—C12—C17—C4 | 3.2 (2) |
| C11—N10—C9—C8 | −0.7 (2) | C11—C12—C17—C16 | −176.00 (14) |
| C9—N10—C11—C6 | −0.1 (2) | N13—C14—C15—C16 | 2.6 (3) |
| C9—N10—C11—C12 | −178.58 (13) | C14—C15—C16—C17 | −1.9 (3) |
| C14—N13—C12—C11 | 176.58 (15) | C15—C16—C17—C4 | 179.78 (16) |
| C14—N13—C12—C17 | −3.2 (2) | C15—C16—C17—C12 | −1.0 (2) |
| C12—N13—C14—C15 | 0.0 (3) | N1—C18—C19—C20 | 177.39 (13) |
| N1—C2—C24—C25 | 56.56 (19) | C23—C18—C19—C20 | −1.3 (2) |
| N1—C2—C24—C29 | −125.55 (15) | N1—C18—C23—C22 | −176.22 (13) |

| | | | |
|---|---|---|---|
| N3—C2—C24—C25 | −122.35 (16) | C19—C18—C23—C22 | 2.5 (2) |
| N3—C2—C24—C29 | 55.54 (19) | C18—C19—C20—C21 | −1.0 (2) |
| N3—C4—C5—N1 | −0.78 (15) | C19—C20—C21—C22 | 2.1 (3) |
| N3—C4—C5—C6 | 176.28 (12) | C20—C21—C22—C23 | −0.9 (3) |
| C17—C4—C5—N1 | 179.48 (12) | C21—C22—C23—C18 | −1.4 (2) |
| C17—C4—C5—C6 | −3.5 (2) | C2—C24—C25—C26 | 176.95 (14) |
| N3—C4—C17—C12 | −179.46 (13) | C29—C24—C25—C26 | −1.0 (2) |
| N3—C4—C17—C16 | −0.3 (2) | C2—C24—C29—C28 | −177.29 (14) |
| C5—C4—C17—C12 | 0.2 (2) | C25—C24—C29—C28 | 0.7 (2) |
| C5—C4—C17—C16 | 179.43 (14) | C24—C25—C26—C27 | 0.6 (2) |
| N1—C5—C6—C7 | 0.8 (2) | C25—C26—C27—C28 | 0.1 (3) |
| N1—C5—C6—C11 | 179.13 (13) | C26—C27—C28—C29 | −0.4 (3) |
| C4—C5—C6—C7 | −175.39 (14) | C27—C28—C29—C24 | 0.0 (2) |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*+1, *y*+1, *z*+1; (v) −*x*, −*y*, −*z*+1; (vi) *x*−1, *y*−1, *z*−1; (vii) −*x*, −*y*−1, −*z*; (viii) *x*+1, *y*, *z*; (ix) −*x*+2, −*y*+1, −*z*+1; (x) −*x*+1, −*y*, −*z*; (xi) −*x*, −*y*, −*z*.

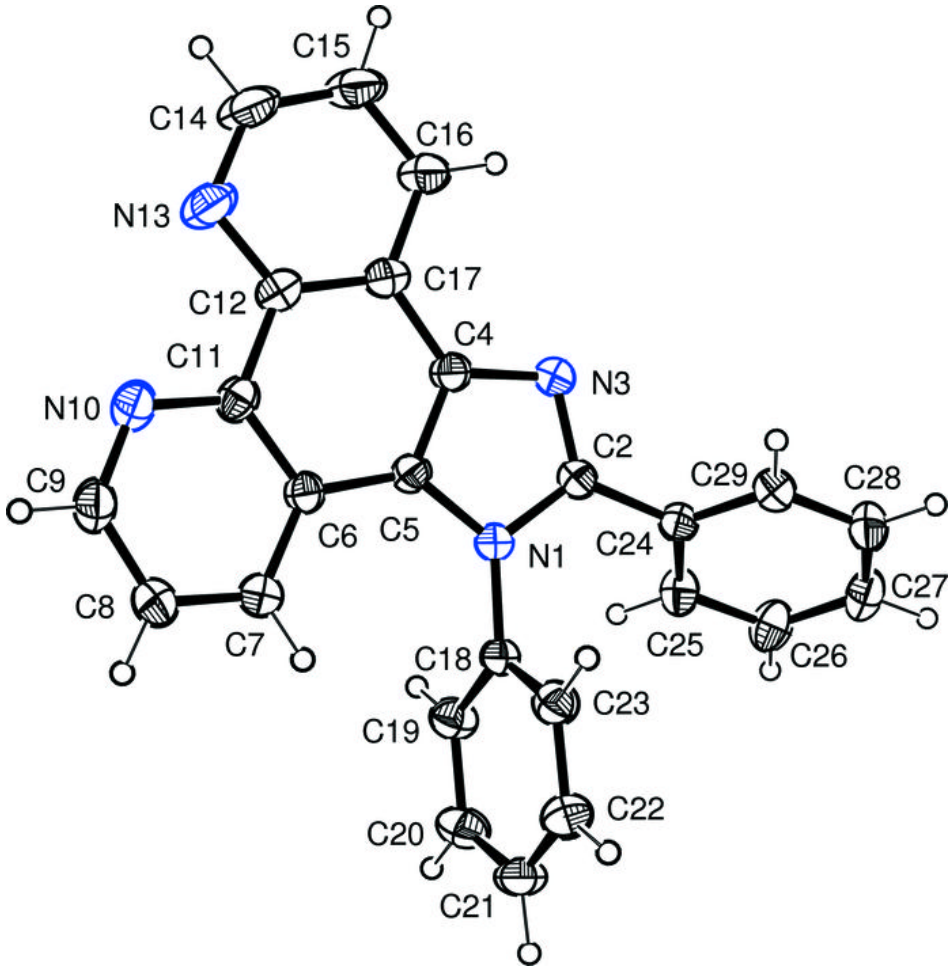
*Hydrogen-bond geometry (Å, °)*

Cg4 and Cg6 are the centroids of the C4–C6/C11/C12/C17 and C24–C29 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C15—H15···Cg6$^{v}$ | 0.95 | 2.86 | 3.757 (3) | 157 |
| C25—H25···Cg4$^{ii}$ | 0.95 | 2.75 | 3.4835 (16) | 135 |

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

**Fig. 1**


C15
C14
C16
N13
C17
C12
C4
C11
N3
N10
C2
C29
C28
C9
C6
C5
N1
C24
C27
C8
C7
C25
C26
C18
C23
C19
C22
C20
C21