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

# 2-(4-Fluorophenyl)-1,4,5-triphenyl-1*H*-imidazole

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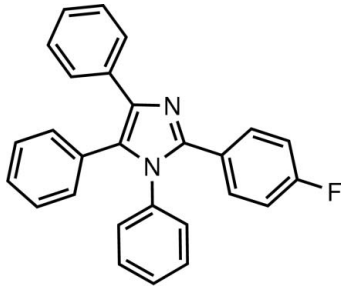
Received 26 August 2010; accepted 2 September 2010

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.049; $wR$ factor = 0.128; data-to-parameter ratio = 30.8.

In the title molecule, $C_{27}H_{19}FN_2$, the imidazole ring is essentially planar [maximum deviation = 0.004 (1) Å] and makes dihedral angles of 62.80 (6), 36.98 (6), 33.16 (6) and 46.24 (6)°, respectively, with the substituent rings in the 1-, 2-, 4- and 5-positions. No classical hydrogen bonds are observed in the crystal structure.

## Related literature

For the synthesis and pharmacological evaluation of substituted 1*H*-imidazoles, see: (Nagalakshmi, 2008). For contact allergy to imidazoles used as antimycotic agents, see: Dooms-Goossens *et al.* (1995). For related structures and applications of imidazole derivatives, see: Gayathri *et al.* (2010*a*,*b*,*c*).




## Experimental

### Crystal data

$C_{27}H_{19}FN_2$ $M_r$ = 390.44
Triclinic, $P\overline{1}$
$a$ = 10.1794 (5) Å
$b$ = 10.5239 (6) Å
$c$ = 10.6175 (6) Å
$\alpha$ = 80.750 (5)°
$\beta$ = 85.776 (4)°
$\gamma$ = 67.348 (5)°
$V$ = 1035.95 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 K
0.51 × 0.44 × 0.15 mm

### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min}$ = 0.973, $T_{max}$ = 1.000
15513 measured reflections
8350 independent reflections
3489 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.128
$S$ = 0.86
8350 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS86* (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).

JJ is thankful to the Department of Science and Technology [No. SR/S1/IC-07/2007] and the University Grants Commission (F. No. 36–21/2008 (S*R*)) for providing funds for this research. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2707).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o2519 [ **doi:10.1107/S1600536810035464** ]

# 2-(4-Fluorophenyl)-1,4,5-triphenyl-1*H*-imidazole

**P. Gayathri, A. Thiruvalluvar, N. Srinivasan, J. Jayabharathi and R. J. Butcher**

## Comment

Nagalakshmi (2008) has reported synthesis and pharmacological evaluation of 2-(4-Halo substituted phenyl)-4,5-diphenyl-1*H*-imidazoles, and Dooms-Goossens *et al.* (1995) have reported contact allergy to imidazoles used as antimycotic agents. As part of our research (Gayathri *et al.*, (2010*a*,*b*,*c*)), we have synthesized the title compound (I) and report its crystal structure here.

In (I), Fig. 1, the imidazole ring is essentially planar [maximum deviation = 0.004 (1) Å for N1]. The imidazole ring makes dihedral angles of 62.80 (6), 36.98 (6), 33.16 (6) and 46.24 (6) ° with the phenyl (C11—C16) attached to N1, fluorophenyl (C21—C26) attached to C2, and two phenyl rings (C41—C46) & (C51—C56) attached to C4 and C5, respectively. The phenyl ring at N1 makes dihedral angles of 54.26 (6), 85.21 (7) and 65.02 (6) ° with the fluorophenyl at C2, and phenyl rings attached to C4 and C5, respectively. The fluorophenyl ring makes dihedral angles of 63.01 (6) and 78.99 (6) ° with the phenyl rings at C4 and C5, respectively. Finally, the dihedral angle between the phenyl rings at C4 and C5 is 51.10 (6) °. In the crystal structure no classical hydrogen bonds are observed.

## Experimental

To benzil (3.15 g, 15 mmol) in ethanol (10 ml), aniline (1.5 g, 15 mmol), ammonium acetate (7 g, 15 mmol) and *p*-fluorobenzaldehyde (1.7 g, 15 mmol) were added over about 1 h while maintaining the temperature at 333 K. The reaction mixture was refluxed for 7 days and extracted with dichloromethane. The solid that separated was purified by column chromatography using hexane: ethyl acetate as the eluent. Yield: 3.51 g (60%).

## Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(parent atom).

## Figures

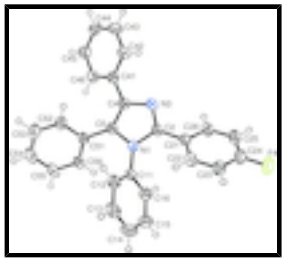

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.

### 2-(4-Fluorophenyl)-1,4,5-triphenyl-1*H*-imidazole

*Crystal data*

| | |
|---|---|
| $C_{27}H_{19}FN_2$ | $Z = 2$ |
| $M_r = 390.44$ | $F(000) = 408$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.252$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 509 K |
| $a = 10.1794$ (5) Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 10.5239$ (6) Å | Cell parameters from 3942 reflections |
| $c = 10.6175$ (6) Å | $\theta = 5.1$–$34.9°$ |
| $\alpha = 80.750$ (5)° | $\mu = 0.08$ mm$^{-1}$ |
| $\beta = 85.776$ (4)° | $T = 295$ K |
| $\gamma = 67.348$ (5)° | Plate, colourless |
| $V = 1035.95$ (11) Å$^3$ | 0.51 × 0.44 × 0.15 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur Ruby Gemini diffractometer | 8350 independent reflections |
| Radiation source: Enhance (Mo) X-ray Source | 3489 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.030$ |
| Detector resolution: 10.5081 pixels mm$^{-1}$ | $\theta_{max} = 35.0°$, $\theta_{min} = 5.1°$ |
| ω scans | $h = -15 \rightarrow 12$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | $k = -16 \rightarrow 14$ |
| $T_{min} = 0.973$, $T_{max} = 1.000$ | $l = -17 \rightarrow 16$ |
| 15513 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 |
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.128$ | H-atom parameters constrained |
| $S = 0.86$ | $w = 1/[\sigma^2(F_o^2) + (0.0586P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 8350 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 271 parameters | $\Delta\rho_{max} = 0.22$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.19$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F4 | 0.80372 (8) | 0.08837 (10) | −0.40649 (7) | 0.0903 (3) |
| N1 | 0.26200 (8) | 0.23531 (9) | −0.01235 (8) | 0.0437 (3) |
| N3 | 0.42488 (8) | 0.27540 (10) | 0.08546 (8) | 0.0497 (3) |
| C2 | 0.39877 (10) | 0.23282 (11) | −0.01679 (10) | 0.0459 (3) |
| C4 | 0.30225 (10) | 0.30605 (11) | 0.15929 (9) | 0.0455 (3) |
| C5 | 0.19960 (10) | 0.28135 (11) | 0.10135 (9) | 0.0429 (3) |
| C11 | 0.20194 (9) | 0.18684 (11) | −0.10385 (9) | 0.0439 (3) |
| C12 | 0.16843 (11) | 0.07116 (13) | −0.06763 (11) | 0.0556 (4) |
| C13 | 0.11969 (13) | 0.01955 (16) | −0.15797 (15) | 0.0743 (5) |
| C14 | 0.10664 (14) | 0.08323 (18) | −0.28296 (15) | 0.0794 (6) |
| C15 | 0.14007 (13) | 0.19852 (16) | −0.31824 (12) | 0.0715 (5) |
| C16 | 0.18572 (11) | 0.25319 (13) | −0.22810 (11) | 0.0560 (4) |
| C21 | 0.50330 (10) | 0.19099 (12) | −0.12073 (10) | 0.0477 (3) |
| C22 | 0.51945 (10) | 0.08114 (12) | −0.18562 (11) | 0.0528 (4) |
| C23 | 0.62124 (11) | 0.04652 (13) | −0.28141 (11) | 0.0590 (4) |
| C24 | 0.70603 (12) | 0.12091 (15) | −0.30998 (11) | 0.0625 (4) |
| C25 | 0.69616 (13) | 0.22763 (16) | −0.24730 (12) | 0.0694 (5) |
| C26 | 0.59330 (12) | 0.26275 (14) | −0.15231 (11) | 0.0607 (4) |
| C41 | 0.30110 (11) | 0.35537 (12) | 0.28205 (10) | 0.0468 (3) |
| C42 | 0.42822 (12) | 0.30638 (14) | 0.34878 (11) | 0.0602 (4) |
| C43 | 0.43495 (14) | 0.35356 (16) | 0.46073 (12) | 0.0713 (5) |
| C44 | 0.31579 (15) | 0.44905 (16) | 0.50961 (12) | 0.0688 (5) |
| C45 | 0.19033 (14) | 0.49726 (14) | 0.44586 (12) | 0.0654 (5) |
| C46 | 0.18239 (12) | 0.45176 (12) | 0.33263 (11) | 0.0554 (4) |
| C51 | 0.05103 (10) | 0.30008 (11) | 0.13802 (10) | 0.0438 (3) |
| C52 | 0.01739 (12) | 0.25395 (13) | 0.26117 (11) | 0.0549 (4) |
| C53 | −0.12281 (14) | 0.27662 (14) | 0.29629 (13) | 0.0693 (5) |
| C54 | −0.23054 (13) | 0.34450 (15) | 0.20932 (15) | 0.0724 (5) |
| C55 | −0.19831 (11) | 0.38917 (14) | 0.08727 (13) | 0.0638 (4) |
| C56 | −0.05946 (10) | 0.36777 (12) | 0.05109 (11) | 0.0510 (4) |
| H12 | 0.17852 | 0.02828 | 0.01676 | 0.0667* |
| H13 | 0.09574 | −0.05792 | −0.13455 | 0.0892* |
| H14 | 0.07489 | 0.04771 | −0.34393 | 0.0952* |
| H15 | 0.13200 | 0.24004 | −0.40303 | 0.0857* |

| | | | | |
|---|---|---|---|---|
| H16 | 0.20515 | 0.33333 | −0.25085 | 0.0672* |
| H22 | 0.46150 | 0.03061 | −0.16453 | 0.0633* |
| H23 | 0.63160 | −0.02634 | −0.32557 | 0.0708* |
| H25 | 0.75675 | 0.27545 | −0.26776 | 0.0832* |
| H26 | 0.58432 | 0.33573 | −0.10885 | 0.0728* |
| H42 | 0.50945 | 0.24100 | 0.31717 | 0.0722* |
| H43 | 0.52075 | 0.32058 | 0.50362 | 0.0856* |
| H44 | 0.32052 | 0.48059 | 0.58545 | 0.0825* |
| H45 | 0.10930 | 0.56144 | 0.47900 | 0.0785* |
| H46 | 0.09631 | 0.48633 | 0.29000 | 0.0664* |
| H52 | 0.08926 | 0.20754 | 0.32054 | 0.0659* |
| H53 | −0.14438 | 0.24575 | 0.37930 | 0.0831* |
| H54 | −0.32448 | 0.35981 | 0.23351 | 0.0868* |
| H55 | −0.27068 | 0.43437 | 0.02817 | 0.0766* |
| H56 | −0.03911 | 0.39881 | −0.03226 | 0.0612* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F4 | 0.0761 (5) | 0.1160 (7) | 0.0732 (5) | −0.0356 (5) | 0.0285 (4) | −0.0132 (5) |
| N1 | 0.0411 (4) | 0.0500 (5) | 0.0453 (5) | −0.0228 (4) | 0.0001 (3) | −0.0076 (4) |
| N3 | 0.0443 (4) | 0.0584 (6) | 0.0520 (5) | −0.0254 (4) | −0.0013 (4) | −0.0083 (4) |
| C2 | 0.0411 (5) | 0.0509 (7) | 0.0499 (6) | −0.0229 (5) | 0.0000 (4) | −0.0051 (5) |
| C4 | 0.0445 (5) | 0.0491 (6) | 0.0468 (6) | −0.0223 (5) | −0.0025 (4) | −0.0051 (5) |
| C5 | 0.0426 (5) | 0.0447 (6) | 0.0442 (5) | −0.0206 (4) | 0.0001 (4) | −0.0046 (5) |
| C11 | 0.0387 (5) | 0.0495 (6) | 0.0472 (6) | −0.0196 (5) | 0.0009 (4) | −0.0107 (5) |
| C12 | 0.0570 (6) | 0.0552 (7) | 0.0621 (7) | −0.0296 (6) | 0.0038 (5) | −0.0103 (6) |
| C13 | 0.0762 (8) | 0.0745 (9) | 0.0928 (11) | −0.0446 (7) | 0.0064 (7) | −0.0319 (8) |
| C14 | 0.0734 (8) | 0.0955 (12) | 0.0841 (10) | −0.0365 (8) | −0.0108 (7) | −0.0387 (9) |
| C15 | 0.0701 (8) | 0.0869 (10) | 0.0561 (8) | −0.0245 (8) | −0.0131 (6) | −0.0144 (7) |
| C16 | 0.0571 (6) | 0.0572 (7) | 0.0551 (7) | −0.0235 (6) | −0.0057 (5) | −0.0050 (5) |
| C21 | 0.0404 (5) | 0.0545 (7) | 0.0494 (6) | −0.0210 (5) | −0.0011 (4) | −0.0027 (5) |
| C22 | 0.0437 (5) | 0.0523 (7) | 0.0614 (7) | −0.0188 (5) | 0.0039 (5) | −0.0062 (5) |
| C23 | 0.0524 (6) | 0.0580 (8) | 0.0604 (7) | −0.0144 (6) | 0.0025 (5) | −0.0091 (6) |
| C24 | 0.0487 (6) | 0.0770 (9) | 0.0532 (7) | −0.0191 (6) | 0.0092 (5) | −0.0017 (6) |
| C25 | 0.0587 (7) | 0.0863 (10) | 0.0723 (8) | −0.0427 (7) | 0.0096 (6) | −0.0028 (7) |
| C26 | 0.0563 (6) | 0.0712 (8) | 0.0653 (7) | −0.0360 (6) | 0.0062 (5) | −0.0127 (6) |
| C41 | 0.0512 (6) | 0.0504 (6) | 0.0466 (6) | −0.0287 (5) | −0.0033 (4) | −0.0032 (5) |
| C42 | 0.0540 (6) | 0.0720 (9) | 0.0595 (7) | −0.0282 (6) | −0.0073 (5) | −0.0093 (6) |
| C43 | 0.0750 (8) | 0.0885 (10) | 0.0608 (8) | −0.0413 (8) | −0.0212 (6) | −0.0043 (7) |
| C44 | 0.0920 (9) | 0.0822 (10) | 0.0509 (7) | −0.0515 (8) | −0.0007 (7) | −0.0146 (7) |
| C45 | 0.0749 (8) | 0.0694 (9) | 0.0625 (7) | −0.0356 (7) | 0.0050 (6) | −0.0209 (6) |
| C46 | 0.0563 (6) | 0.0572 (7) | 0.0580 (7) | −0.0255 (6) | −0.0053 (5) | −0.0112 (6) |
| C51 | 0.0442 (5) | 0.0435 (6) | 0.0509 (6) | −0.0231 (5) | 0.0041 (4) | −0.0125 (5) |
| C52 | 0.0611 (6) | 0.0548 (7) | 0.0552 (7) | −0.0291 (6) | 0.0088 (5) | −0.0117 (5) |
| C53 | 0.0808 (9) | 0.0690 (9) | 0.0711 (8) | −0.0434 (7) | 0.0320 (7) | −0.0235 (7) |
| C54 | 0.0520 (7) | 0.0751 (9) | 0.1043 (11) | −0.0360 (7) | 0.0224 (7) | −0.0331 (8) |
| C55 | 0.0454 (6) | 0.0611 (8) | 0.0917 (9) | −0.0240 (6) | −0.0002 (6) | −0.0207 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C56 | 0.0470 (6) | 0.0503 (7) | 0.0620 (7) | −0.0247 (5) | −0.0009 (5) | −0.0095 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F4—C24 | 1.3626 (15) | C45—C46 | 1.3822 (18) |
| N1—C2 | 1.3798 (14) | C51—C52 | 1.3859 (16) |
| N1—C5 | 1.3905 (13) | C51—C56 | 1.3960 (16) |
| N1—C11 | 1.4370 (13) | C52—C53 | 1.386 (2) |
| N3—C2 | 1.3194 (14) | C53—C54 | 1.378 (2) |
| N3—C4 | 1.3798 (14) | C54—C55 | 1.367 (2) |
| C2—C21 | 1.4718 (15) | C55—C56 | 1.3779 (17) |
| C4—C5 | 1.3759 (15) | C12—H12 | 0.9300 |
| C4—C41 | 1.4761 (15) | C13—H13 | 0.9300 |
| C5—C51 | 1.4785 (16) | C14—H14 | 0.9300 |
| C11—C12 | 1.3771 (16) | C15—H15 | 0.9300 |
| C11—C16 | 1.3793 (15) | C16—H16 | 0.9300 |
| C12—C13 | 1.381 (2) | C22—H22 | 0.9300 |
| C13—C14 | 1.378 (2) | C23—H23 | 0.9300 |
| C14—C15 | 1.372 (2) | C25—H25 | 0.9300 |
| C15—C16 | 1.3825 (19) | C26—H26 | 0.9300 |
| C21—C22 | 1.3897 (16) | C42—H42 | 0.9300 |
| C21—C26 | 1.3887 (18) | C43—H43 | 0.9300 |
| C22—C23 | 1.3834 (17) | C44—H44 | 0.9300 |
| C23—C24 | 1.3621 (19) | C45—H45 | 0.9300 |
| C24—C25 | 1.363 (2) | C46—H46 | 0.9300 |
| C25—C26 | 1.3843 (19) | C52—H52 | 0.9300 |
| C41—C42 | 1.3950 (18) | C53—H53 | 0.9300 |
| C41—C46 | 1.3831 (17) | C54—H54 | 0.9300 |
| C42—C43 | 1.3755 (18) | C55—H55 | 0.9300 |
| C43—C44 | 1.374 (2) | C56—H56 | 0.9300 |
| C44—C45 | 1.365 (2) | | |
| F4···H14$^{i}$ | 2.7400 | C42···H54$^{i}$ | 2.9300 |
| F4···H53$^{ii}$ | 2.7400 | C44···H16$^{vi}$ | 2.9800 |
| N1···H22 | 2.9400 | C45···H25$^{vii}$ | 3.0000 |
| N1···H56 | 2.8800 | C46···H52 | 3.0900 |
| N3···H26 | 2.6800 | C51···H12 | 3.1000 |
| N3···H42 | 2.5900 | C51···H46 | 2.9100 |
| N3···H55$^{iii}$ | 2.9400 | C52···H46 | 2.9200 |
| C2···C22$^{iv}$ | 3.4772 (16) | C53···H44$^{viii}$ | 2.9800 |
| C4···C23$^{iv}$ | 3.5258 (17) | C53···H13$^{ix}$ | 3.0100 |
| C5···C56$^{iii}$ | 3.5569 (16) | C54···H13$^{ix}$ | 3.0100 |
| C5···C23$^{iv}$ | 3.5260 (16) | C54···H44$^{viii}$ | 2.9400 |
| C11···C56 | 3.1419 (16) | C56···H56$^{iii}$ | 2.9700 |
| C11···C22 | 3.0928 (15) | H12···C5 | 3.0300 |
| C12···C51 | 3.3300 (16) | H12···C51 | 3.1000 |
| C12···C56 | 3.4599 (17) | H13···C53$^{ix}$ | 3.0100 |
| C16···C21 | 3.2942 (17) | H13···C54$^{ix}$ | 3.0100 |

| | | | |
|---|---|---|---|
| C16···C22 | 3.2012 (17) | H14···F4$^{x}$ | 2.7400 |
| C21···C16 | 3.2942 (17) | H16···C2 | 3.0700 |
| C22···C11 | 3.0928 (15) | H16···C44$^{v}$ | 2.9800 |
| C22···C2$^{iv}$ | 3.4772 (16) | H22···N1 | 2.9400 |
| C22···C16 | 3.2012 (17) | H22···C11 | 2.6200 |
| C23···C4$^{iv}$ | 3.5258 (17) | H22···C12 | 2.9700 |
| C23···C5$^{iv}$ | 3.5260 (16) | H22···C16 | 2.9200 |
| C41···C52 | 3.4747 (18) | H22···C2$^{iv}$ | 3.0100 |
| C46···C51 | 3.4230 (16) | H23···C4$^{iv}$ | 3.0400 |
| C46···C52 | 3.3345 (18) | H25···C45$^{vii}$ | 3.0000 |
| C51···C46 | 3.4230 (16) | H26···N3 | 2.6800 |
| C51···C12 | 3.3300 (16) | H42···N3 | 2.5900 |
| C52···C46 | 3.3345 (18) | H42···H54$^{i}$ | 2.5000 |
| C52···C41 | 3.4747 (18) | H43···C24$^{vi}$ | 2.8400 |
| C56···C11 | 3.1419 (16) | H44···C53$^{viii}$ | 2.9800 |
| C56···C56$^{iii}$ | 3.4379 (16) | H44···C54$^{viii}$ | 2.9400 |
| C56···C5$^{iii}$ | 3.5569 (16) | H46···C5 | 3.0200 |
| C56···C12 | 3.4599 (17) | H46···C51 | 2.9100 |
| C2···H22$^{iv}$ | 3.0100 | H46···C52 | 2.9200 |
| C2···H16 | 3.0700 | H52···C4 | 3.0500 |
| C4···H55$^{iii}$ | 3.0300 | H52···C41 | 3.0800 |
| C4···H23$^{iv}$ | 3.0400 | H52···C46 | 3.0900 |
| C4···H52 | 3.0500 | H53···F4$^{xi}$ | 2.7400 |
| C5···H46 | 3.0200 | H54···C42$^{x}$ | 2.9300 |
| C5···H12 | 3.0300 | H54···H42$^{x}$ | 2.5000 |
| C11···H56 | 2.7600 | H55···N3$^{iii}$ | 2.9400 |
| C11···H22 | 2.6200 | H55···C4$^{iii}$ | 3.0300 |
| C12···H22 | 2.9700 | H56···N1 | 2.8800 |
| C16···H22 | 2.9200 | H56···C11 | 2.7600 |
| C16···H56 | 3.0900 | H56···C16 | 3.0900 |
| C24···H43$^{v}$ | 2.8400 | H56···C56$^{iii}$ | 2.9700 |
| C41···H52 | 3.0800 | | |
| C2—N1—C5 | 107.30 (9) | C52—C53—C54 | 120.60 (13) |
| C2—N1—C11 | 125.41 (9) | C53—C54—C55 | 119.52 (13) |
| C5—N1—C11 | 127.07 (9) | C54—C55—C56 | 120.53 (12) |
| C2—N3—C4 | 106.26 (9) | C51—C56—C55 | 120.81 (11) |
| N1—C2—N3 | 110.82 (9) | C11—C12—H12 | 120.00 |
| N1—C2—C21 | 125.85 (9) | C13—C12—H12 | 120.00 |
| N3—C2—C21 | 123.32 (10) | C12—C13—H13 | 120.00 |
| N3—C4—C5 | 110.51 (9) | C14—C13—H13 | 120.00 |
| N3—C4—C41 | 118.29 (10) | C13—C14—H14 | 120.00 |
| C5—C4—C41 | 131.20 (10) | C15—C14—H14 | 120.00 |
| N1—C5—C4 | 105.11 (9) | C14—C15—H15 | 120.00 |
| N1—C5—C51 | 122.73 (9) | C16—C15—H15 | 120.00 |

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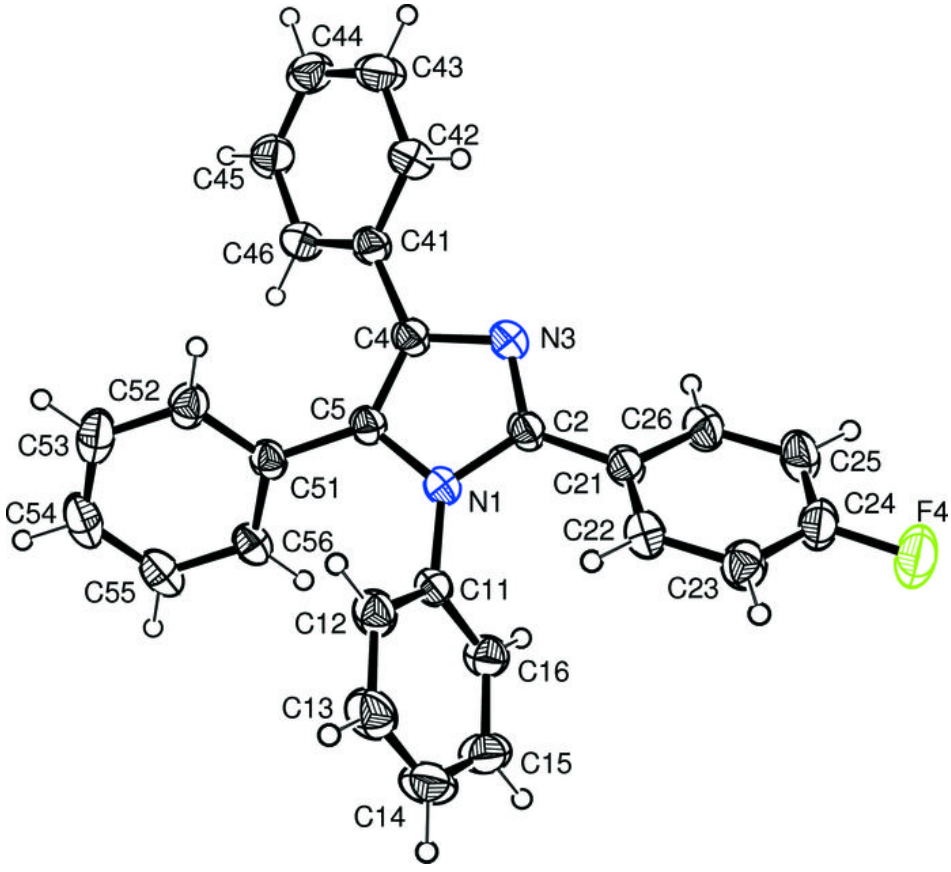
|---|---|---|---|
| C4—C5—C51 | 132.12 (9) | C11—C16—H16 | 121.00 |
| N1—C11—C12 | 119.53 (9) | C15—C16—H16 | 121.00 |
| N1—C11—C16 | 119.13 (10) | C21—C22—H22 | 120.00 |
| C12—C11—C16 | 121.26 (10) | C23—C22—H22 | 120.00 |
| C11—C12—C13 | 119.27 (11) | C22—C23—H23 | 121.00 |
| C12—C13—C14 | 119.78 (14) | C24—C23—H23 | 121.00 |
| C13—C14—C15 | 120.59 (14) | C24—C25—H25 | 121.00 |
| C14—C15—C16 | 120.18 (12) | C26—C25—H25 | 121.00 |
| C11—C16—C15 | 118.87 (12) | C21—C26—H26 | 119.00 |
| C2—C21—C22 | 123.50 (10) | C25—C26—H26 | 119.00 |
| C2—C21—C26 | 117.88 (10) | C41—C42—H42 | 120.00 |
| C22—C21—C26 | 118.59 (10) | C43—C42—H42 | 120.00 |
| C21—C22—C23 | 120.38 (11) | C42—C43—H43 | 120.00 |
| C22—C23—C24 | 118.91 (12) | C44—C43—H43 | 120.00 |
| F4—C24—C23 | 118.56 (12) | C43—C44—H44 | 120.00 |
| F4—C24—C25 | 118.58 (12) | C45—C44—H44 | 120.00 |
| C23—C24—C25 | 122.85 (12) | C44—C45—H45 | 120.00 |
| C24—C25—C26 | 118.04 (13) | C46—C45—H45 | 120.00 |
| C21—C26—C25 | 121.21 (12) | C41—C46—H46 | 120.00 |
| C4—C41—C42 | 118.31 (11) | C45—C46—H46 | 120.00 |
| C4—C41—C46 | 123.79 (11) | C51—C52—H52 | 120.00 |
| C42—C41—C46 | 117.86 (11) | C53—C52—H52 | 120.00 |
| C41—C42—C43 | 120.84 (13) | C52—C53—H53 | 120.00 |
| C42—C43—C44 | 120.44 (14) | C54—C53—H53 | 120.00 |
| C43—C44—C45 | 119.41 (13) | C53—C54—H54 | 120.00 |
| C44—C45—C46 | 120.75 (13) | C55—C54—H54 | 120.00 |
| C41—C46—C45 | 120.70 (12) | C54—C55—H55 | 120.00 |
| C5—C51—C52 | 120.62 (10) | C56—C55—H55 | 120.00 |
| C5—C51—C56 | 121.15 (9) | C51—C56—H56 | 120.00 |
| C52—C51—C56 | 118.21 (11) | C55—C56—H56 | 120.00 |
| C51—C52—C53 | 120.33 (12) | | |
| C5—N1—C2—N3 | −0.64 (12) | C16—C11—C12—C13 | 0.98 (18) |
| C5—N1—C2—C21 | −179.79 (10) | N1—C11—C16—C15 | 174.19 (11) |
| C11—N1—C2—N3 | −175.57 (9) | C12—C11—C16—C15 | −2.50 (18) |
| C11—N1—C2—C21 | 5.28 (17) | C11—C12—C13—C14 | 0.7 (2) |
| C2—N1—C5—C4 | 0.72 (11) | C12—C13—C14—C15 | −0.8 (2) |
| C2—N1—C5—C51 | 178.72 (10) | C13—C14—C15—C16 | −0.8 (2) |
| C11—N1—C5—C4 | 175.54 (10) | C14—C15—C16—C11 | 2.4 (2) |
| C11—N1—C5—C51 | −6.46 (16) | C2—C21—C22—C23 | −179.20 (11) |
| C2—N1—C11—C12 | 112.68 (12) | C26—C21—C22—C23 | −1.36 (17) |
| C2—N1—C11—C16 | −64.07 (15) | C2—C21—C26—C25 | 178.74 (12) |
| C5—N1—C11—C12 | −61.25 (15) | C22—C21—C26—C25 | 0.78 (18) |
| C5—N1—C11—C16 | 122.00 (12) | C21—C22—C23—C24 | 0.66 (18) |
| C4—N3—C2—N1 | 0.28 (12) | C22—C23—C24—F4 | −178.45 (11) |
| C4—N3—C2—C21 | 179.46 (10) | C22—C23—C24—C25 | 0.7 (2) |
| C2—N3—C4—C5 | 0.20 (12) | F4—C24—C25—C26 | 177.87 (12) |
| C2—N3—C4—C41 | 179.33 (10) | C23—C24—C25—C26 | −1.3 (2) |
| N1—C2—C21—C22 | −38.85 (17) | C24—C25—C26—C21 | 0.5 (2) |
| N1—C2—C21—C26 | 143.30 (11) | C4—C41—C42—C43 | 177.03 (12) |

| | | | |
|---|---|---|---|
| N3—C2—C21—C22 | 142.10 (12) | C46—C41—C42—C43 | −0.48 (19) |
| N3—C2—C21—C26 | −35.75 (16) | C4—C41—C46—C45 | −177.52 (12) |
| N3—C4—C5—N1 | −0.57 (12) | C42—C41—C46—C45 | −0.15 (18) |
| N3—C4—C5—C51 | −178.31 (11) | C41—C42—C43—C44 | 0.7 (2) |
| C41—C4—C5—N1 | −179.56 (11) | C42—C43—C44—C45 | −0.2 (2) |
| C41—C4—C5—C51 | 2.7 (2) | C43—C44—C45—C46 | −0.4 (2) |
| N3—C4—C41—C42 | −31.76 (15) | C44—C45—C46—C41 | 0.6 (2) |
| N3—C4—C41—C46 | 145.60 (12) | C5—C51—C52—C53 | 177.49 (11) |
| C5—C4—C41—C42 | 147.16 (13) | C56—C51—C52—C53 | −0.79 (18) |
| C5—C4—C41—C46 | −35.48 (19) | C5—C51—C56—C55 | −177.69 (11) |
| N1—C5—C51—C52 | 135.85 (11) | C52—C51—C56—C55 | 0.59 (17) |
| N1—C5—C51—C56 | −45.92 (16) | C51—C52—C53—C54 | 0.4 (2) |
| C4—C5—C51—C52 | −46.76 (18) | C52—C53—C54—C55 | 0.3 (2) |
| C4—C5—C51—C56 | 131.48 (13) | C53—C54—C55—C56 | −0.5 (2) |
| N1—C11—C12—C13 | −175.70 (11) | C54—C55—C56—C51 | 0.1 (2) |

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

**Fig. 1**


C44
C43
C42
C45
C46
C41
C4
N3
C52
C5
C2
C26
C53
C51
N1
C21
C25
C24
F4
C54
C56
C22
C55
C11
C23
C12
C16
C13
C15
C14