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# 2-Amino-4-(2,4-dichlorophenyl)-6-(naphthalen-1-yl)nicotinonitrile

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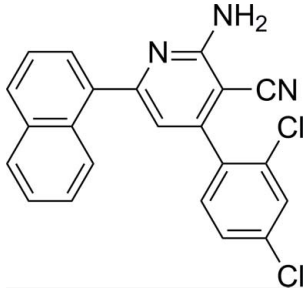
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.048; $wR$ factor = 0.146; data-to-parameter ratio = 13.7.

In the crystal structure of the title compound, $C_{22}H_{13}Cl_2N_3$, the molecules are connected *via* intermolecular C—H···N and N—H···N hydrogen bonds, forming a three-dimensional network. The dihedral angles between naphthyl ring system and the pyridyl and benzene rings are 55.04 (7) and 75.87 (7)°, respectively, whereas the pyridyl and benzene rings are oriented at a dihedral angle of 59.56 (8)°.

## Related literature

For the synthetic procedure, see: Mantri *et al.* (2008). For the use of the title compound in the preparation of medicines, see: Mkhalid *et al.* (2006). For general background to this type of compound, see: Moreau & Huber (1999).




## Experimental

### Crystal data

$C_{22}H_{13}Cl_2N_3$
$M_r$ = 390.25
Triclinic, $P\overline{1}$
$a$ = 9.5020 (19) Å
$b$ = 10.054 (2) Å
$c$ = 10.735 (2) Å
$\alpha$ = 72.78 (3)°
$\beta$ = 89.17 (3)°
$\gamma$ = 74.81 (3)°
$V$ = 943.1 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 293 K
0.30 × 0.10 × 0.10 mm

### Data collection

Entaf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.901, $T_{max}$ = 0.965
3686 measured reflections
3463 independent reflections
2648 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.146
$S$ = 1.00
3463 reflections
252 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···N1$^{i}$ | 0.85 (3) | 2.19 (3) | 3.034 (3) | 176 (2) |
| C4—H4$A$···N3$^{ii}$ | 0.93 | 2.62 | 3.488 (4) | 155 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: BQ2258).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o71 [ **doi:10.1107/S1600536810050609** ]

# 2-Amino-4-(2,4-dichlorophenyl)-6-(naphthalen-1-yl)nicotinonitrile

**Y.-F. Ye, H.-Q. Wang and Z.-Q. Feng**

## Comment

The title compound, $C_{22}H_{13}Cl_2N_3$,(I), contains amino group, which can react with different groups to prepare various function organic compounds. It is a kind of aromatic organic intermediate which can be used for many fields such as medicine (Mantri *et al.*, 2008). The molecular structure of (I) is shown in Fig. 1. In (I), the naphthyl and the two rings, pyridyl and phenyl are oriented with different dihedral angles; 55.04 (7) ° between naphthyl and pyridyl, 75.87 (7) ° between naphthyl and phenyl and 59.56 (8) ° between pyridyl and phenyl. In the crystal structure of the title compound, the molecules were connected together *via* N—H···N and C—H···N intermolecular hydrogen bonds to form a three dimensional network, which seems to be very effective in the stabilization of the crystal structure.

## Experimental

The title compound, (I) was prepared by the literature method (Mantri *et al.*, 2008). Crystals suitable for X-ray analysis were obtained by dissolving (I) (0.5 g) in methanol (20 ml) and evaporating the solvent slowly at room temperature for about 5 d.

## Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93 Å for aromatic H and 0.86 Å for N—H, respectively. The $U_{iso}$(H) = $xU_{eq}$(C), where $x$ = 1.2 for aromatic H, and $x$ = 1.5 for other H.

## Figures

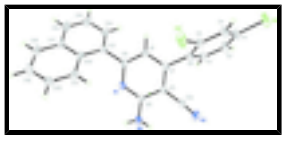


Fig. 1. The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

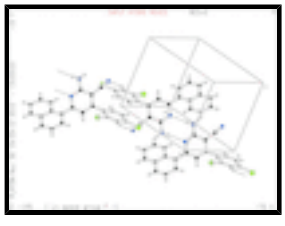


Fig. 2. A packing diagram for (I). C—H···N and N—H···N hydrogen bonds are shown by dashed lines.

## 2-Amino-4-(2,4-dichlorophenyl)-6-(naphthalen-1-yl)nicotinonitrile

*Crystal data*

| | |
|---|---|
| $C_{22}H_{13}Cl_2N_3$ | $Z$ = 2 |
| $M_r$ = 390.25 | $F$(000) = 400 |

| | |
|---|---|
| Triclinic, $P\bar{1}$ | $D_x = 1.374$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.5020$ (19) Å | Cell parameters from 25 reflections |
| $b = 10.054$ (2) Å | $\theta = 10$–$14°$ |
| $c = 10.735$ (2) Å | $\mu = 0.36$ mm$^{-1}$ |
| $\alpha = 72.78$ (3)° | $T = 293$ K |
| $\beta = 89.17$ (3)° | Block, colourless |
| $\gamma = 74.81$ (3)° | 0.30 × 0.10 × 0.10 mm |
| $V = 943.1$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Entaf–Nonius CAD-4 diffractometer | 2648 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.014$ |
| graphite | $\theta_{max} = 25.4°$, $\theta_{min} = 2.0°$ |
| ω/2θ scans | $h = 0 \rightarrow 11$ |
| Absorption correction: ψ scan (North *et al.*, 1968) | $k = -11 \rightarrow 12$ |
| $T_{min} = 0.901$, $T_{max} = 0.965$ | $l = -12 \rightarrow 12$ |
| 3686 measured reflections | 3 standard reflections every 200 reflections |
| 3463 independent reflections | intensity decay: 1% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.146$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + ]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3463 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 252 parameters | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | −0.37446 (8) | 0.08316 (9) | 0.92700 (9) | 0.0687 (3) |
| N1 | 0.36411 (19) | 0.4640 (2) | 0.89712 (17) | 0.0331 (4) |
| C1 | −0.0992 (3) | 0.2943 (3) | 0.9925 (3) | 0.0425 (6) |
| H1B | −0.0942 | 0.3531 | 1.0439 | 0.051* |
| Cl2 | 0.13996 (8) | 0.12749 (9) | 0.73801 (8) | 0.0635 (3) |
| N2 | 0.4248 (2) | 0.3529 (3) | 1.1161 (2) | 0.0414 (5) |
| H2A | 0.480 (3) | 0.408 (3) | 1.110 (2) | 0.044 (7)* |
| H2B | 0.398 (3) | 0.313 (3) | 1.193 (3) | 0.053 (8)* |
| C2 | −0.2176 (3) | 0.2375 (3) | 0.9987 (3) | 0.0477 (6) |
| H2C | −0.2919 | 0.2580 | 1.0532 | 0.057* |
| C3 | −0.2235 (3) | 0.1508 (3) | 0.9234 (3) | 0.0442 (6) |
| N3 | 0.1702 (3) | 0.1711 (3) | 1.2494 (2) | 0.0542 (6) |
| C4 | −0.1143 (3) | 0.1165 (3) | 0.8436 (2) | 0.0426 (6) |
| H4A | −0.1192 | 0.0557 | 0.7942 | 0.051* |
| C5 | 0.0034 (3) | 0.1752 (3) | 0.8384 (2) | 0.0390 (6) |
| C6 | 0.0130 (2) | 0.2659 (2) | 0.9114 (2) | 0.0350 (5) |
| C7 | 0.1356 (2) | 0.3340 (2) | 0.9053 (2) | 0.0347 (5) |
| C8 | 0.1657 (3) | 0.4256 (3) | 0.7898 (2) | 0.0394 (6) |
| H8A | 0.1114 | 0.4431 | 0.7125 | 0.047* |
| C9 | 0.2771 (2) | 0.4911 (2) | 0.7898 (2) | 0.0353 (5) |
| C10 | 0.3364 (2) | 0.3766 (2) | 1.0103 (2) | 0.0315 (5) |
| C11 | 0.2194 (2) | 0.3119 (2) | 1.0184 (2) | 0.0327 (5) |
| C12 | 0.1897 (2) | 0.2309 (3) | 1.1454 (2) | 0.0372 (5) |
| C13 | 0.3005 (2) | 0.6054 (3) | 0.6730 (2) | 0.0364 (5) |
| C14 | 0.1836 (3) | 0.7200 (3) | 0.6165 (3) | 0.0528 (7) |
| H14A | 0.0907 | 0.7181 | 0.6441 | 0.063* |
| C15 | 0.2017 (4) | 0.8417 (3) | 0.5168 (3) | 0.0660 (9) |
| H15A | 0.1209 | 0.9184 | 0.4783 | 0.079* |
| C16 | 0.3370 (3) | 0.8461 (3) | 0.4774 (3) | 0.0615 (8) |
| H16A | 0.3486 | 0.9278 | 0.4140 | 0.074* |
| C17 | 0.4602 (3) | 0.7293 (3) | 0.5308 (2) | 0.0459 (6) |
| C18 | 0.6025 (3) | 0.7317 (4) | 0.4896 (3) | 0.0615 (8) |
| H18A | 0.6156 | 0.8140 | 0.4280 | 0.074* |
| C19 | 0.7199 (3) | 0.6162 (4) | 0.5385 (3) | 0.0623 (8) |
| H19A | 0.8128 | 0.6208 | 0.5126 | 0.075* |
| C20 | 0.7004 (3) | 0.4907 (3) | 0.6275 (3) | 0.0520 (7) |
| H20A | 0.7801 | 0.4101 | 0.6576 | 0.062* |
| C21 | 0.5663 (3) | 0.4846 (3) | 0.6708 (2) | 0.0411 (6) |
| H21A | 0.5561 | 0.3999 | 0.7306 | 0.049* |
| C22 | 0.4431 (3) | 0.6037 (3) | 0.6270 (2) | 0.0355 (5) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0450 (4) | 0.0707 (5) | 0.1083 (7) | −0.0386 (4) | 0.0167 (4) | −0.0338 (5) |
| N1 | 0.0318 (10) | 0.0407 (11) | 0.0316 (10) | −0.0177 (8) | 0.0053 (8) | −0.0112 (8) |
| C1 | 0.0358 (13) | 0.0445 (14) | 0.0554 (15) | −0.0182 (11) | 0.0083 (11) | −0.0211 (12) |
| Cl2 | 0.0653 (5) | 0.0837 (5) | 0.0692 (5) | −0.0447 (4) | 0.0347 (4) | −0.0439 (4) |
| N2 | 0.0432 (12) | 0.0565 (14) | 0.0308 (11) | −0.0301 (11) | 0.0007 (9) | −0.0078 (10) |
| C2 | 0.0350 (13) | 0.0484 (15) | 0.0667 (17) | −0.0175 (11) | 0.0154 (12) | −0.0227 (13) |
| C3 | 0.0327 (13) | 0.0409 (14) | 0.0607 (16) | −0.0206 (11) | 0.0027 (11) | −0.0083 (12) |
| N3 | 0.0611 (15) | 0.0587 (14) | 0.0428 (13) | −0.0297 (12) | 0.0063 (11) | −0.0038 (11) |
| C4 | 0.0444 (14) | 0.0422 (14) | 0.0486 (14) | −0.0229 (12) | 0.0031 (11) | −0.0148 (11) |
| C5 | 0.0370 (13) | 0.0454 (14) | 0.0371 (12) | −0.0202 (11) | 0.0064 (10) | −0.0083 (11) |
| C6 | 0.0315 (12) | 0.0369 (12) | 0.0376 (12) | −0.0161 (10) | −0.0002 (10) | −0.0068 (10) |
| C7 | 0.0308 (11) | 0.0372 (12) | 0.0412 (13) | −0.0154 (10) | 0.0055 (10) | −0.0141 (10) |
| C8 | 0.0367 (13) | 0.0532 (15) | 0.0345 (12) | −0.0242 (11) | 0.0004 (10) | −0.0117 (11) |
| C9 | 0.0351 (12) | 0.0412 (13) | 0.0338 (12) | −0.0166 (10) | 0.0067 (10) | −0.0124 (10) |
| C10 | 0.0307 (11) | 0.0338 (12) | 0.0339 (12) | −0.0131 (9) | 0.0056 (9) | −0.0122 (9) |
| C11 | 0.0314 (11) | 0.0344 (12) | 0.0359 (12) | −0.0149 (9) | 0.0062 (9) | −0.0110 (10) |
| C12 | 0.0361 (12) | 0.0378 (13) | 0.0418 (14) | −0.0186 (10) | 0.0031 (10) | −0.0106 (11) |
| C13 | 0.0376 (13) | 0.0434 (13) | 0.0310 (12) | −0.0179 (11) | 0.0030 (10) | −0.0092 (10) |
| C14 | 0.0411 (15) | 0.0617 (18) | 0.0483 (15) | −0.0126 (13) | 0.0071 (12) | −0.0071 (13) |
| C15 | 0.0593 (19) | 0.0566 (18) | 0.0579 (18) | −0.0013 (15) | 0.0045 (15) | 0.0059 (14) |
| C16 | 0.0656 (19) | 0.0498 (17) | 0.0534 (17) | −0.0141 (15) | 0.0135 (14) | 0.0057 (13) |
| C17 | 0.0513 (15) | 0.0503 (15) | 0.0363 (13) | −0.0222 (13) | 0.0078 (11) | −0.0062 (11) |
| C18 | 0.065 (2) | 0.069 (2) | 0.0523 (16) | −0.0370 (17) | 0.0211 (14) | −0.0053 (15) |
| C19 | 0.0465 (16) | 0.088 (2) | 0.0569 (18) | −0.0307 (17) | 0.0174 (14) | −0.0192 (16) |
| C20 | 0.0407 (14) | 0.0675 (18) | 0.0458 (15) | −0.0114 (13) | 0.0085 (12) | −0.0174 (14) |
| C21 | 0.0445 (14) | 0.0472 (14) | 0.0315 (12) | −0.0153 (12) | 0.0056 (10) | −0.0094 (11) |
| C22 | 0.0396 (13) | 0.0437 (13) | 0.0290 (11) | −0.0191 (11) | 0.0039 (9) | −0.0125 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.736 (2) | C9—C13 | 1.488 (3) |
| N1—C10 | 1.341 (3) | C10—C11 | 1.417 (3) |
| N1—C9 | 1.345 (3) | C11—C12 | 1.434 (3) |
| C1—C2 | 1.382 (3) | C13—C14 | 1.365 (4) |
| C1—C6 | 1.392 (3) | C13—C22 | 1.432 (3) |
| C1—H1B | 0.9300 | C14—C15 | 1.414 (4) |
| Cl2—C5 | 1.736 (2) | C14—H14A | 0.9300 |
| N2—C10 | 1.347 (3) | C15—C16 | 1.356 (4) |
| N2—H2A | 0.84 (3) | C15—H15A | 0.9300 |
| N2—H2B | 0.86 (3) | C16—C17 | 1.406 (4) |
| C2—C3 | 1.365 (4) | C16—H16A | 0.9300 |
| C2—H2C | 0.9300 | C17—C18 | 1.421 (4) |
| C3—C4 | 1.376 (3) | C17—C22 | 1.421 (3) |
| N3—C12 | 1.139 (3) | C18—C19 | 1.358 (4) |
| C4—C5 | 1.388 (3) | C18—H18A | 0.9300 |

| | | | |
|---|---|---|---|
| C4—H4A | 0.9300 | C19—C20 | 1.394 (4) |
| C5—C6 | 1.387 (3) | C19—H19A | 0.9300 |
| C6—C7 | 1.490 (3) | C20—C21 | 1.360 (4) |
| C7—C8 | 1.386 (3) | C20—H20A | 0.9300 |
| C7—C11 | 1.390 (3) | C21—C22 | 1.405 (3) |
| C8—C9 | 1.384 (3) | C21—H21A | 0.9300 |
| C8—H8A | 0.9300 | | |
| C10—N1—C9 | 118.57 (19) | C7—C11—C10 | 119.3 (2) |
| C2—C1—C6 | 121.8 (2) | C7—C11—C12 | 123.0 (2) |
| C2—C1—H1B | 119.1 | C10—C11—C12 | 117.6 (2) |
| C6—C1—H1B | 119.1 | N3—C12—C11 | 175.9 (3) |
| C10—N2—H2A | 117.4 (17) | C14—C13—C22 | 120.1 (2) |
| C10—N2—H2B | 118.6 (19) | C14—C13—C9 | 118.0 (2) |
| H2A—N2—H2B | 118 (2) | C22—C13—C9 | 121.7 (2) |
| C3—C2—C1 | 118.7 (2) | C13—C14—C15 | 121.0 (3) |
| C3—C2—H2C | 120.7 | C13—C14—H14A | 119.5 |
| C1—C2—H2C | 120.7 | C15—C14—H14A | 119.5 |
| C2—C3—C4 | 122.0 (2) | C16—C15—C14 | 119.8 (3) |
| C2—C3—Cl1 | 119.0 (2) | C16—C15—H15A | 120.1 |
| C4—C3—Cl1 | 118.96 (19) | C14—C15—H15A | 120.1 |
| C3—C4—C5 | 118.3 (2) | C15—C16—C17 | 121.2 (3) |
| C3—C4—H4A | 120.8 | C15—C16—H16A | 119.4 |
| C5—C4—H4A | 120.8 | C17—C16—H16A | 119.4 |
| C6—C5—C4 | 121.7 (2) | C16—C17—C18 | 121.9 (3) |
| C6—C5—Cl2 | 121.38 (17) | C16—C17—C22 | 119.7 (2) |
| C4—C5—Cl2 | 116.88 (19) | C18—C17—C22 | 118.4 (2) |
| C5—C6—C1 | 117.4 (2) | C19—C18—C17 | 121.3 (3) |
| C5—C6—C7 | 123.1 (2) | C19—C18—H18A | 119.3 |
| C1—C6—C7 | 119.5 (2) | C17—C18—H18A | 119.3 |
| C8—C7—C11 | 118.0 (2) | C18—C19—C20 | 119.6 (3) |
| C8—C7—C6 | 121.8 (2) | C18—C19—H19A | 120.2 |
| C11—C7—C6 | 120.2 (2) | C20—C19—H19A | 120.2 |
| C9—C8—C7 | 119.8 (2) | C21—C20—C19 | 120.8 (3) |
| C9—C8—H8A | 120.1 | C21—C20—H20A | 119.6 |
| C7—C8—H8A | 120.1 | C19—C20—H20A | 119.6 |
| N1—C9—C8 | 122.7 (2) | C20—C21—C22 | 121.4 (2) |
| N1—C9—C13 | 115.38 (19) | C20—C21—H21A | 119.3 |
| C8—C9—C13 | 121.8 (2) | C22—C21—H21A | 119.3 |
| N1—C10—N2 | 117.0 (2) | C21—C22—C17 | 118.2 (2) |
| N1—C10—C11 | 121.53 (19) | C21—C22—C13 | 123.8 (2) |
| N2—C10—C11 | 121.4 (2) | C17—C22—C13 | 118.0 (2) |
| C6—C1—C2—C3 | 0.3 (4) | N2—C10—C11—C7 | −176.9 (2) |
| C1—C2—C3—C4 | 1.1 (4) | N1—C10—C11—C12 | −174.4 (2) |
| C1—C2—C3—Cl1 | −178.1 (2) | N2—C10—C11—C12 | 5.6 (3) |
| C2—C3—C4—C5 | −1.3 (4) | C7—C11—C12—N3 | −155 (4) |
| Cl1—C3—C4—C5 | 177.91 (18) | C10—C11—C12—N3 | 22 (4) |
| C3—C4—C5—C6 | 0.1 (4) | N1—C9—C13—C14 | −123.8 (2) |
| C3—C4—C5—Cl2 | 179.22 (19) | C8—C9—C13—C14 | 51.5 (3) |

| | | | |
|---|---|---|---|
| C4—C5—C6—C1 | 1.2 (4) | N1—C9—C13—C22 | 50.6 (3) |
| Cl2—C5—C6—C1 | −177.86 (18) | C8—C9—C13—C22 | −134.1 (2) |
| C4—C5—C6—C7 | −178.2 (2) | C22—C13—C14—C15 | −3.2 (4) |
| Cl2—C5—C6—C7 | 2.7 (3) | C9—C13—C14—C15 | 171.4 (3) |
| C2—C1—C6—C5 | −1.4 (4) | C13—C14—C15—C16 | −0.9 (5) |
| C2—C1—C6—C7 | 178.0 (2) | C14—C15—C16—C17 | 2.3 (5) |
| C5—C6—C7—C8 | 59.9 (3) | C15—C16—C17—C18 | 179.4 (3) |
| C1—C6—C7—C8 | −119.5 (3) | C15—C16—C17—C22 | 0.4 (5) |
| C5—C6—C7—C11 | −123.1 (3) | C16—C17—C18—C19 | −177.6 (3) |
| C1—C6—C7—C11 | 57.5 (3) | C22—C17—C18—C19 | 1.3 (4) |
| C11—C7—C8—C9 | 0.3 (4) | C17—C18—C19—C20 | 2.2 (5) |
| C6—C7—C8—C9 | 177.4 (2) | C18—C19—C20—C21 | −3.1 (4) |
| C10—N1—C9—C8 | −4.0 (3) | C19—C20—C21—C22 | 0.4 (4) |
| C10—N1—C9—C13 | 171.27 (19) | C20—C21—C22—C17 | 3.1 (4) |
| C7—C8—C9—N1 | 3.5 (4) | C20—C21—C22—C13 | −177.5 (2) |
| C7—C8—C9—C13 | −171.4 (2) | C16—C17—C22—C21 | 175.1 (2) |
| C9—N1—C10—N2 | −179.4 (2) | C18—C17—C22—C21 | −3.9 (4) |
| C9—N1—C10—C11 | 0.7 (3) | C16—C17—C22—C13 | −4.4 (4) |
| C8—C7—C11—C10 | −3.4 (3) | C18—C17—C22—C13 | 176.7 (2) |
| C6—C7—C11—C10 | 179.4 (2) | C14—C13—C22—C21 | −173.7 (2) |
| C8—C7—C11—C12 | 173.9 (2) | C9—C13—C22—C21 | 12.0 (3) |
| C6—C7—C11—C12 | −3.3 (3) | C14—C13—C22—C17 | 5.7 (3) |
| N1—C10—C11—C7 | 3.1 (3) | C9—C13—C22—C17 | −168.6 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2A···N1$^{i}$ | 0.85 (3) | 2.19 (3) | 3.034 (3) | 176 (2) |
| C4—H4A···N3$^{ii}$ | 0.93 | 2.62 | 3.488 (4) | 155 |

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

**Fig. 1**

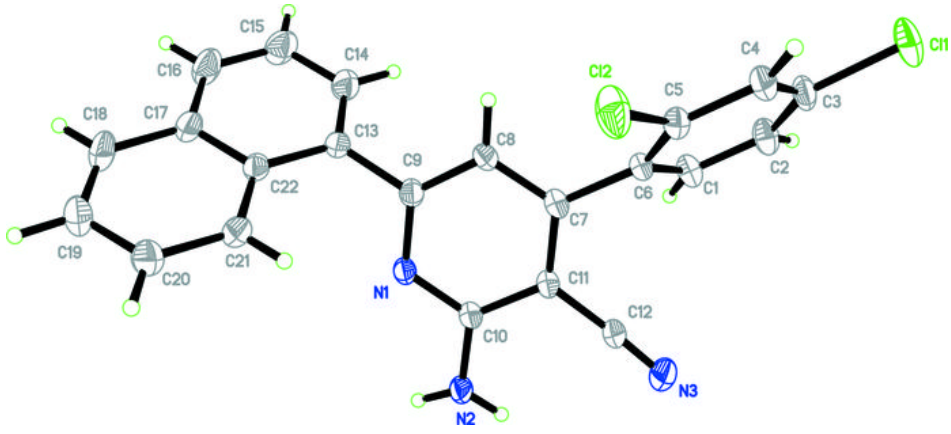
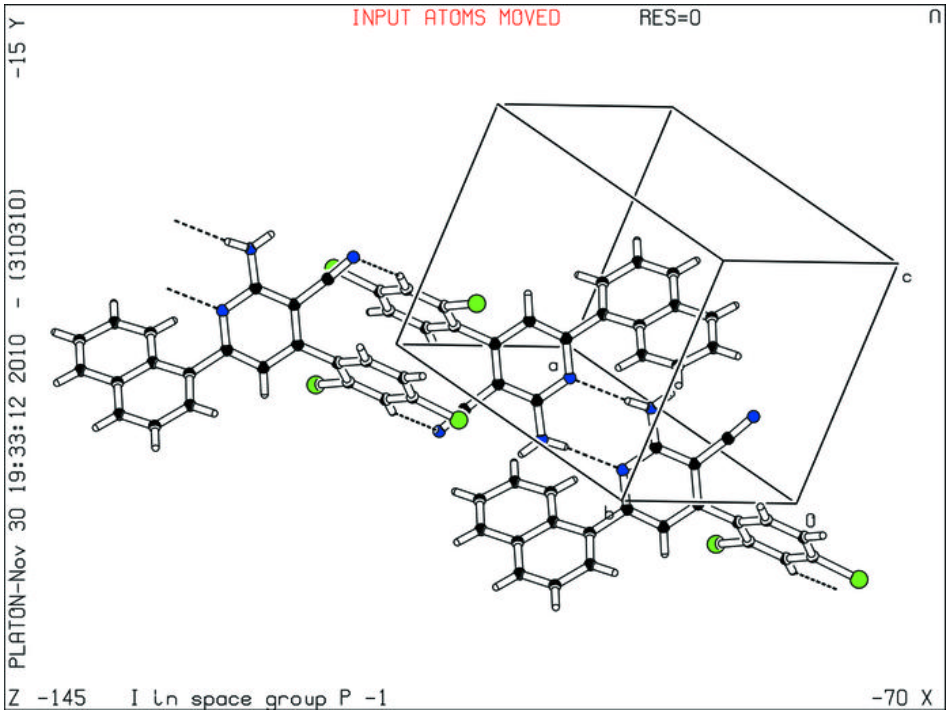

C15
C16
C14
C18
C17
C13
C22
C9
C8
C19
C20
C21
N1
C10
N2
C7
C11
C12
N3
C6
C1
C5
Cl2
C4
C3
C2
Cl1

**Fig. 2**


INPUT ATOMS MOVED
RES=0
PLATON-Nov 30 19:33:12 2010 - (310310)
-15 Y
Z -145
I ln space group P -1
-70 X
c
a
b
0