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(*E*)-2-Cyano-3-[4-(dimethylamino)-phenyl]-*N*-phenylprop-2-enamide

Abdullah Mohamed Asiri,[a] Mehmet Akkurt,[b]* Salman A. Khan,[a] Islam Ullah Khan[c] and Muhammad Nadeem Arshad[c]

[a]Chemistry Department, Faculty of Science, King Abdul-Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, [b]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, and [c]Department of Chemistry, Government College University, Lahore, Pakistan
Correspondence e-mail: akkurt@erciyes.edu.tr

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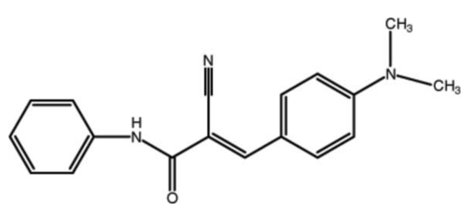
Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.060; *wR* factor = 0.165; data-to-parameter ratio = 17.2.

In the title compound, $C_{18}H_{17}N_3O$, the dihedral angle between the phenyl and benzene rings is 11.22 (14)°. Apart from the methyl H atoms, the molecule is close to planar, with a maximum deviation of 0.145 (3) Å. Intramolecular C—H⋯O and C—H⋯N interactions occur. In the crystal, inversion dimers linked by pairs of N—H⋯N hydrogen bonds occur, resulting in an $R_2^2(12)$ ring motif. Further C—H⋯N and C—H⋯O bonds generate $R_1^2(7)$ and $R_2^2(22)$ motifs and a C—H⋯π interaction also occurs.

Related literature

For background on the properties and uses of organic dyes, see: Grabowski *et al.* (2003); Guo *et al.* (2007); Kwak *et al.* (2008); Moylan *et al.* (1996). For reference structural data, see Allen *et al.* (1987). For graph-set terminology, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{17}N_3O$
M_r = 291.35
Monoclinic, $P2_1/c$
a = 12.0639 (19) Å
b = 19.983 (3) Å
c = 6.3960 (9) Å
β = 94.870 (6)°
V = 1536.3 (4) Å^3
Z = 4
Mo *K*α radiation
μ = 0.08 mm^{-1}
T = 296 K
0.44 × 0.09 × 0.07 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: none
15701 measured reflections
3484 independent reflections
1380 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.165
S = 0.97
3484 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C5—H5⋯O1	0.93	2.30	2.892 (4)	121
C12—H12⋯N2	0.93	2.61	3.445 (4)	149
N1—H1*A*⋯N2^{i}	0.86	2.50	3.245 (3)	146
C1—H1⋯N2^{i}	0.93	2.58	3.338 (4)	139
C18—H18*A*⋯O1^{ii}	0.96	2.49	3.439 (4)	169
C3—H3⋯*Cg*1^{iii}	0.93	2.66	3.514 (3)	152

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x+1, -y, -z$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$. *Cg*1 is the centroid of the C1–C6 phenyl ring.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2974).

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supplementary materials

Acta Cryst. (2009). E**65**, o1303 [**doi:10.1107/S1600536809017681**]

(*E*)-2-Cyano-3-[4-(dimethylamino)phenyl]-*N*-phenylprop-2-enamide

A. M. Asiri, M. Akkurt, S. A. Khan, I. U. Khan and M. N. Arshad

Comment

Organic dyes with donor–π-conjugation–acceptor (D–π–A) molecular structure have attracted much attention because of their inherent nonlinear optical characteristics, which are highly sensitive to changes in the external environment such as polarity and pH of media, due to their intrinsic character (*e.g.* Grabowski *et al.*, 2003). They have been intensively developed for applications using as photo-(PL) and electroluminescent (EL) materials in the fields of dye laser (Moylan *et al.*, 1996), fluorescent sonser and logic memory (Guo *et al.*, 2007), and organic light-emitting device (OLED) (Kwak *et al.*, 2008). The title compound, (I) (Fig. 1), is a representative of Push-Pull systems with dimethylamino group as a donor at one end of the conjugated system and cyano and carboonyl as acceptor at the other end.

The molecule of (I) contains a phenyl ring and a benzene ring which makes a dihedral angle of 11.22 (14)°. Except the methyl H atoms, the title molecule is almost planar, with a maximum deviation of 0.145 (3) Å for C12 and C13. The bond lengths and angles are in normal range (Allen *et al.*, 1987). The molecules of the title compound form in which two N—H···N hydrogen bonds. The N—H···N, C—H···N and C—H···O interactions generates $R_2^2(12)$, $R_1^2(7)$ and $R_2^2(22)$ motifs (Fig. 2) (Bernstein *et al.* 1995). Fig. 3 shows the molecular packing for (I) viewed down the *a* axis showing the hydrogen bonding interactions (dashed lines). Molecules form a *zigzag* pattern along the *b* axis.

The crystal structure is stabilized by intermolecular N—H···N, C—H···O and C—H···N hydrogen bonding, and C—H···π interactions (Table 1).

Experimental

N-Phenyl-2-cyanoacetamide (1.60 g, 0.010 mol) and 4-*N*,*N*-dimethylaminobenzaldehyde (1.49 g, 0.010 mol) were dissolved in 50 ml of ethanol then heated to boiling before pipyridine (0.5 ml) was added. The reaction mixture was refluxed for 7 h, cooled then the precipitate was filtered and recrystalized from ethanol to yield red prisms of (I) [yield: 90%, m.p.: 382–384 K]. IR;ν (cm^{-1}): 3348, 2941, 2890 (–C—H), 2198 (CN), 1671 (C=O), 1601 (C=C), 1580 (C=C).

Refinement

The H atoms were positioned geometrically and treated as riding, with N—H = 0.86 Å and C—H = 0.93–0.96 Å, and refined as riding with U_{iso}(H) = 1.2 or 1.5U_{eq}(parent atom).

Figures

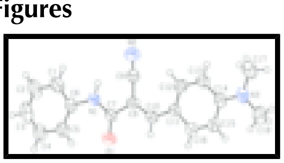


Fig. 1. The molecular structure of (I) showing displacement ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

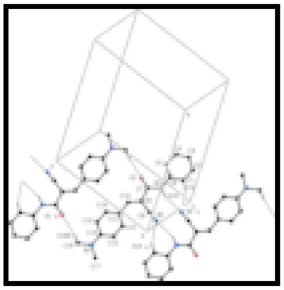


Fig. 2. View of the hydrogen bonding interactions (dashed lines) for (I). H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (*a*) 1–x, –y, 1–z; (*b*) 1–x, –y, –z].

Fig. 3. The molecular packing for (I) viewed down the *a* axis showing the hydrogen bonding interactions (dashed lines). Molecules form a *zigzag* pattern along the *b* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

(E)-2-Cyano-3-[4-(dimethylamino)phenyl]-*N*-phenylprop-2-enamide

Crystal data

$C_{18}H_{17}N_3O$	F_{000} = 616
M_r = 291.35	D_x = 1.260 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1223 reflections
a = 12.0639 (19) Å	θ = 3.4–19.8º
b = 19.983 (3) Å	μ = 0.08 mm^{-1}
c = 6.3960 (9) Å	*T* = 296 K
β = 94.870 (6)º	Prism, red
V = 1536.3 (4) Å^3	0.44 × 0.09 × 0.07 mm
Z = 4	

Data collection

Bruker Kappa APEXII CCD diffractometer	1380 reflections with $I > 2\sigma(I)$
Radiation source: sealed tube	R_{int} = 0.082
Monochromator: graphite	θ_{max} = 27.5º
T = 296 K	θ_{min} = 2.0º
φ and ω scans	*h* = −15→15
Absorption correction: none	*k* = −25→25
15701 measured reflections	*l* = −8→5
3484 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.165$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.97$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
3484 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
202 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0038 (12)
Secondary atom site location: difference Fourier map	

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 on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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	0.37797 (16)	0.07494 (10)	0.5929 (3)	0.0639 (8)
N1	0.19658 (18)	0.07922 (10)	0.6643 (3)	0.0444 (8)
N2	0.0364 (2)	−0.00214 (14)	0.2850 (4)	0.0714 (10)
N3	0.3109 (2)	−0.16820 (12)	−0.4827 (4)	0.0619 (10)
C1	0.1026 (3)	0.13303 (16)	0.9294 (5)	0.0740 (12)
C2	0.0994 (3)	0.17166 (17)	1.1086 (6)	0.0876 (17)
C3	0.1948 (4)	0.19793 (16)	1.2024 (5)	0.0757 (16)
C4	0.2923 (3)	0.18648 (16)	1.1198 (5)	0.0754 (14)
C5	0.2976 (3)	0.14743 (15)	0.9411 (5)	0.0615 (11)
C6	0.2018 (2)	0.12058 (13)	0.8457 (4)	0.0439 (10)
C7	0.2811 (2)	0.05968 (13)	0.5505 (4)	0.0425 (10)
C8	0.2467 (2)	0.01696 (13)	0.3648 (4)	0.0391 (9)
C9	0.1308 (3)	0.00579 (14)	0.3162 (4)	0.0480 (10)
C10	0.3244 (2)	−0.00906 (13)	0.2492 (4)	0.0414 (9)
C11	0.3150 (2)	−0.04902 (13)	0.0609 (4)	0.0392 (9)
C12	0.2159 (2)	−0.06559 (14)	−0.0565 (4)	0.0480 (10)
C13	0.2145 (2)	−0.10416 (14)	−0.2344 (4)	0.0488 (10)
C14	0.3122 (2)	−0.12898 (14)	−0.3082 (4)	0.0458 (10)
C15	0.4128 (2)	−0.11114 (14)	−0.1943 (4)	0.0506 (11)
C16	0.4124 (2)	−0.07274 (13)	−0.0153 (4)	0.0471 (10)
C17	0.2077 (3)	−0.18754 (16)	−0.5982 (5)	0.0770 (16)
C18	0.4122 (3)	−0.19039 (16)	−0.5680 (5)	0.0755 (15)
H1	0.03700	0.11530	0.86510	0.0890*

H1A	0.13160	0.06470	0.62090	0.0530*
H2	0.03200	0.17960	1.16470	0.1050*
H3	0.19290	0.22370	1.32310	0.0910*
H4	0.35720	0.20510	1.18370	0.0900*
H5	0.36550	0.13960	0.88690	0.0740*
H10	0.39720	0.00050	0.30000	0.0500*
H12	0.14890	−0.05000	−0.01300	0.0580*
H13	0.14660	−0.11400	−0.30780	0.0590*
H15	0.48010	−0.12540	−0.24010	0.0610*
H16	0.48010	−0.06220	0.05780	0.0570*
H17A	0.15590	−0.20220	−0.50190	0.1150*
H17B	0.22150	−0.22340	−0.69260	0.1150*
H17C	0.17720	−0.14990	−0.67680	0.1150*
H18A	0.46280	−0.15340	−0.57210	0.1130*
H18B	0.39490	−0.20720	−0.70750	0.1130*
H18C	0.44600	−0.22520	−0.48100	0.1130*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0432 (13)	0.0847 (17)	0.0632 (13)	−0.0141 (12)	0.0010 (10)	−0.0260 (12)
N1	0.0437 (14)	0.0484 (15)	0.0409 (12)	−0.0052 (12)	0.0033 (11)	−0.0120 (11)
N2	0.0486 (17)	0.106 (2)	0.0607 (16)	−0.0128 (16)	0.0113 (13)	−0.0316 (15)
N3	0.0715 (19)	0.0641 (18)	0.0502 (14)	−0.0024 (15)	0.0063 (14)	−0.0211 (13)
C1	0.075 (2)	0.073 (2)	0.079 (2)	−0.031 (2)	0.035 (2)	−0.031 (2)
C2	0.108 (3)	0.075 (3)	0.088 (3)	−0.035 (2)	0.056 (2)	−0.036 (2)
C3	0.129 (4)	0.050 (2)	0.0486 (19)	−0.003 (2)	0.010 (2)	−0.0106 (16)
C4	0.087 (3)	0.068 (2)	0.066 (2)	0.019 (2)	−0.024 (2)	−0.0251 (19)
C5	0.061 (2)	0.059 (2)	0.0608 (19)	0.0158 (17)	−0.0159 (16)	−0.0210 (17)
C6	0.060 (2)	0.0341 (16)	0.0377 (14)	0.0019 (15)	0.0046 (15)	0.0007 (13)
C7	0.0429 (18)	0.0431 (18)	0.0412 (15)	−0.0066 (15)	0.0020 (14)	−0.0047 (13)
C8	0.0359 (16)	0.0451 (18)	0.0361 (13)	−0.0036 (13)	0.0013 (12)	0.0012 (12)
C9	0.0472 (19)	0.058 (2)	0.0396 (15)	−0.0055 (16)	0.0085 (14)	−0.0122 (14)
C10	0.0401 (16)	0.0427 (17)	0.0408 (14)	−0.0019 (14)	−0.0004 (13)	0.0003 (13)
C11	0.0377 (17)	0.0409 (17)	0.0387 (14)	−0.0017 (13)	0.0018 (13)	−0.0005 (13)
C12	0.0423 (18)	0.060 (2)	0.0425 (15)	0.0023 (15)	0.0080 (13)	−0.0058 (14)
C13	0.0477 (19)	0.058 (2)	0.0399 (15)	−0.0051 (15)	−0.0006 (13)	−0.0048 (14)
C14	0.058 (2)	0.0411 (18)	0.0389 (15)	−0.0003 (15)	0.0071 (15)	−0.0008 (13)
C15	0.051 (2)	0.049 (2)	0.0526 (17)	0.0034 (15)	0.0100 (15)	−0.0066 (15)
C16	0.0447 (18)	0.0462 (19)	0.0503 (16)	0.0012 (15)	0.0037 (14)	−0.0038 (14)
C17	0.093 (3)	0.079 (3)	0.057 (2)	−0.007 (2)	−0.0048 (19)	−0.0198 (18)
C18	0.098 (3)	0.073 (3)	0.0592 (19)	0.001 (2)	0.0285 (19)	−0.0163 (17)

Geometric parameters (Å, °)

O1—C7	1.216 (3)	C12—C13	1.373 (4)
N1—C6	1.422 (3)	C13—C14	1.397 (4)
N1—C7	1.359 (3)	C14—C15	1.407 (4)
N2—C9	1.150 (4)	C15—C16	1.379 (4)

N3—C14	1.363 (4)	C1—H1	0.9300
N3—C17	1.445 (4)	C2—H2	0.9300
N3—C18	1.450 (4)	C3—H3	0.9300
N1—H1A	0.8600	C4—H4	0.9300
C1—C2	1.385 (5)	C5—H5	0.9300
C1—C6	1.375 (4)	C10—H10	0.9300
C2—C3	1.358 (6)	C12—H12	0.9300
C3—C4	1.349 (6)	C13—H13	0.9300
C4—C5	1.390 (4)	C15—H15	0.9300
C5—C6	1.370 (4)	C16—H16	0.9300
C7—C8	1.493 (4)	C17—H17A	0.9600
C8—C9	1.424 (4)	C17—H17B	0.9600
C8—C10	1.347 (4)	C17—H17C	0.9600
C10—C11	1.442 (4)	C18—H18A	0.9600
C11—C16	1.393 (3)	C18—H18B	0.9600
C11—C12	1.397 (4)	C18—H18C	0.9600

C6—N1—C7	128.4 (2)	C2—C1—H1	120.00
C14—N3—C17	121.5 (2)	C6—C1—H1	120.00
C14—N3—C18	122.2 (2)	C1—C2—H2	120.00
C17—N3—C18	116.3 (3)	C3—C2—H2	120.00
C6—N1—H1A	116.00	C2—C3—H3	120.00
C7—N1—H1A	116.00	C4—C3—H3	120.00
C2—C1—C6	120.6 (3)	C3—C4—H4	119.00
C1—C2—C3	119.9 (3)	C5—C4—H4	119.00
C2—C3—C4	119.7 (3)	C4—C5—H5	120.00
C3—C4—C5	121.3 (3)	C6—C5—H5	120.00
C4—C5—C6	119.4 (3)	C8—C10—H10	114.00
N1—C6—C5	124.7 (2)	C11—C10—H10	114.00
C1—C6—C5	119.0 (3)	C11—C12—H12	119.00
N1—C6—C1	116.3 (2)	C13—C12—H12	119.00
N1—C7—C8	114.8 (2)	C12—C13—H13	119.00
O1—C7—N1	124.0 (2)	C14—C13—H13	119.00
O1—C7—C8	121.2 (2)	C14—C15—H15	120.00
C9—C8—C10	122.4 (2)	C16—C15—H15	120.00
C7—C8—C10	119.9 (2)	C11—C16—H16	119.00
C7—C8—C9	117.7 (2)	C15—C16—H16	119.00
N2—C9—C8	177.1 (3)	N3—C17—H17A	109.00
C8—C10—C11	131.6 (2)	N3—C17—H17B	109.00
C12—C11—C16	116.1 (2)	N3—C17—H17C	109.00
C10—C11—C12	125.7 (2)	H17A—C17—H17B	109.00
C10—C11—C16	118.2 (2)	H17A—C17—H17C	109.00
C11—C12—C13	121.9 (2)	H17B—C17—H17C	110.00
C12—C13—C14	121.9 (2)	N3—C18—H18A	109.00
N3—C14—C15	121.3 (2)	N3—C18—H18B	109.00
N3—C14—C13	122.0 (2)	N3—C18—H18C	109.00
C13—C14—C15	116.8 (2)	H18A—C18—H18B	109.00
C14—C15—C16	120.5 (2)	H18A—C18—H18C	110.00
C11—C16—C15	122.9 (2)	H18B—C18—H18C	109.00

C6—N1—C7—O1	1.3 (4)	O1—C7—C8—C9	−175.1 (2)
C7—N1—C6—C1	179.4 (3)	O1—C7—C8—C10	4.5 (4)
C7—N1—C6—C5	−1.4 (4)	N1—C7—C8—C9	5.0 (3)
C6—N1—C7—C8	−178.8 (2)	C9—C8—C10—C11	2.3 (5)
C18—N3—C14—C15	−3.8 (4)	C7—C8—C10—C11	−177.2 (3)
C17—N3—C14—C13	−1.5 (4)	C8—C10—C11—C12	5.6 (5)
C18—N3—C14—C13	175.8 (3)	C8—C10—C11—C16	−175.5 (3)
C17—N3—C14—C15	179.0 (3)	C10—C11—C12—C13	−179.9 (3)
C2—C1—C6—N1	178.7 (3)	C16—C11—C12—C13	1.3 (4)
C2—C1—C6—C5	−0.6 (5)	C10—C11—C16—C15	−179.8 (2)
C6—C1—C2—C3	0.4 (5)	C12—C11—C16—C15	−0.8 (4)
C1—C2—C3—C4	0.3 (5)	C11—C12—C13—C14	−0.1 (4)
C2—C3—C4—C5	−0.8 (5)	C12—C13—C14—N3	178.9 (3)
C3—C4—C5—C6	0.7 (5)	C12—C13—C14—C15	−1.6 (4)
C4—C5—C6—N1	−179.1 (3)	N3—C14—C15—C16	−178.5 (3)
C4—C5—C6—C1	0.0 (4)	C13—C14—C15—C16	2.0 (4)
N1—C7—C8—C10	−175.5 (2)	C14—C15—C16—C11	−0.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.93	2.30	2.892 (4)	121
C12—H12···N2	0.93	2.61	3.445 (4)	149
N1—H1A···N2^{i}	0.86	2.50	3.245 (3)	146
C1—H1···N2^{i}	0.93	2.58	3.338 (4)	139
C18—H18A···O1^{ii}	0.96	2.49	3.439 (4)	169
C3—H3···Cg1^{iii}	0.93	2.66	3.514 (3)	152

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

Fig. 1

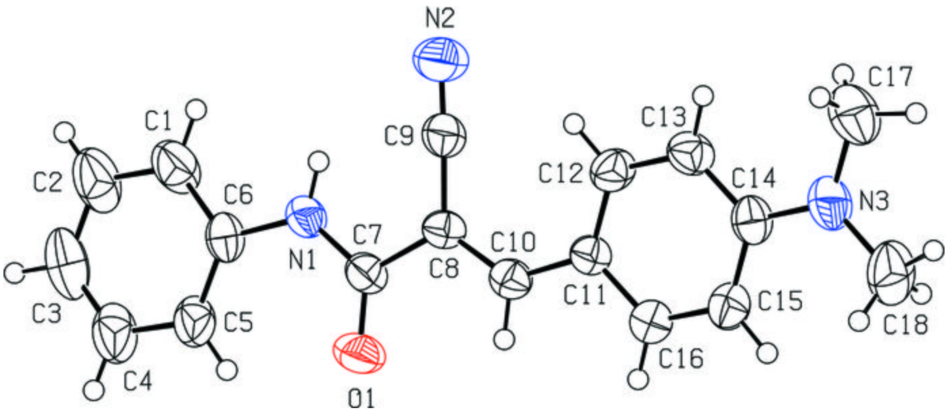
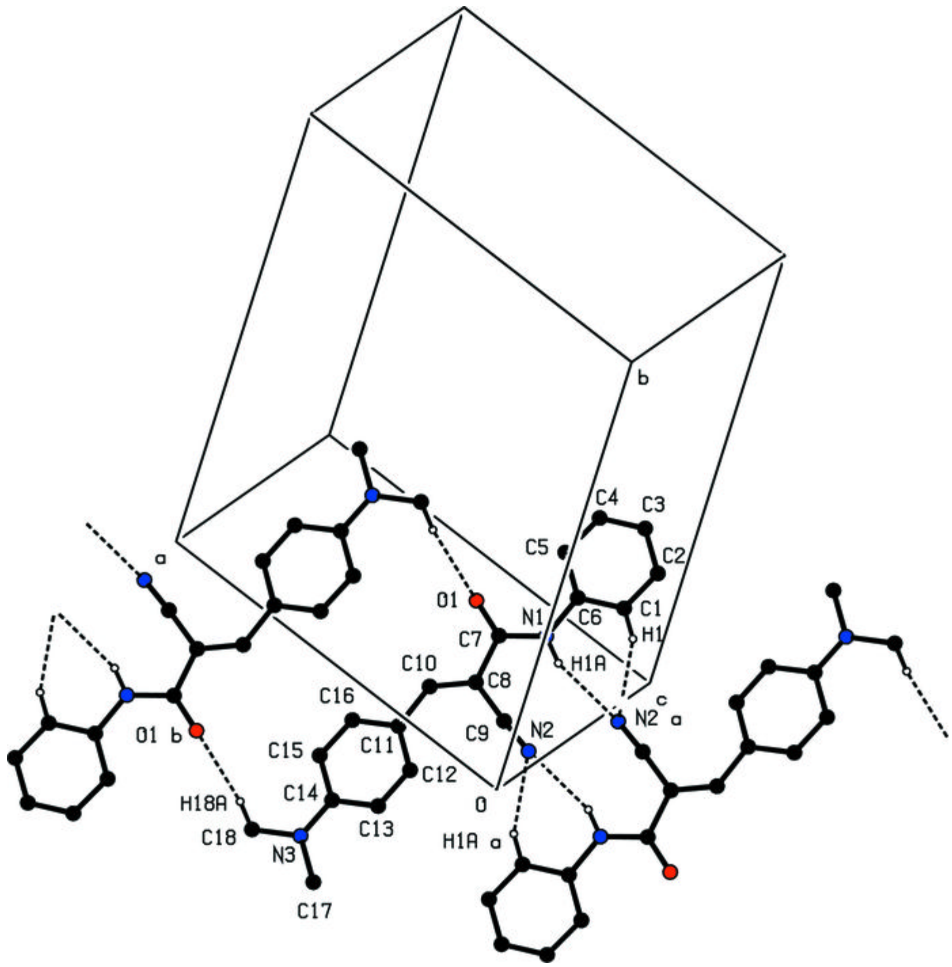

N2
C17
C1
C13
C9
C12
C2
C14
C6
N3
C7
N1
C8
C10
C11
C15
C3
C5
C18
C16
C4
O1

Fig. 2



a
C4
C3
C5
C2
O1
N1
C6
C1
H1
C7
H1A
C10
C8
C16
N2
c
a
C9
N2
O1 b
C15
C11
C12
H18A
C14
O
C18
C13
H1A a
N3
C17

Fig. 3