



Crystal structure of 3-[4-(1*H*-imidazol-1-yl)phenyl]-2-(4-nitrophenyl)prop-2-ene-nitrile

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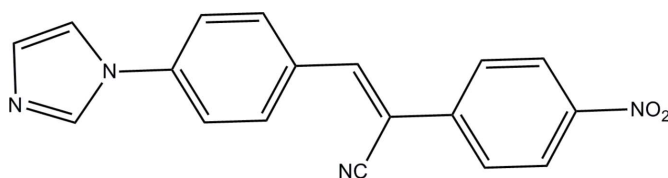
In the title compound, C₁₈H₁₂N₄O₂, which has a delocalized *D*– π –*A* electronic structure, the dihedral angles between the central benzene ring and the planes of the pendant imidazole and nitrobenzene rings are 37.65 (9) and 4.96 (7)°, respectively. In the centrosymmetric crystal structure, molecules are linked by weak C–H···O interactions, generating [001] *C*(6) chains.

Keywords: crystal structure; delocalised *D*– π –*A* electronic structure; hydrogen bonding.

CCDC reference: 1045501

1. Related literature

For chemical and photophysical background, see: Liu *et al.* (2006); Zheng *et al.* (2013). For a related structure, see: Li (2011).



2. Experimental

2.1. Crystal data

C ₁₈ H ₁₂ N ₄ O ₂	<i>V</i> = 1483.3 (6) Å ³
<i>M_r</i> = 316.32	<i>Z</i> = 4
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 7.1792 (16) Å	μ = 0.10 mm ⁻¹
<i>b</i> = 16.512 (4) Å	<i>T</i> = 296 K
<i>c</i> = 12.771 (3) Å	0.25 × 0.2 × 0.18 mm
β = 101.557 (3)°	

2.2. Data collection

Bruker SMART CCD diffractometer	10392 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	2609 independent reflections
<i>T</i> _{min} = 0.320, <i>T</i> _{max} = 0.439	2081 reflections with <i>I</i> > 2σ(<i>I</i>)
	<i>R</i> _{int} = 0.024

2.3. Refinement

<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.036	217 parameters
<i>wR</i> (<i>F</i> ²) = 0.105	H-atom parameters constrained
<i>S</i> = 1.07	$\Delta\rho_{\text{max}}$ = 0.18 e Å ⁻³
2609 reflections	$\Delta\rho_{\text{min}}$ = -0.17 e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C18–H18···O2 ⁱ	0.93	2.54	3.464 (2)	173

Symmetry code: (i) *x*, –*y* + $\frac{3}{2}$, *z* + $\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7432).

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supporting information

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Crystal structure of 3-[4-(1*H*-imidazol-1-yl)phenyl]-2-(4-nitrophenyl)prop-2-enitrile

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S1. Synthesis and crystallization

3-(4-Imidazol-1-yl-phenyl)-2-(4-nitro-phenyl)-acrylonitrile was dissolved in ethanol solvent. Then added 4-nitro-benzonitrile into the solvent. When the two compounds were mixed completely, dropwise added a few piperidine into them. About seven hours later, we could get the title compound.

S2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}$.

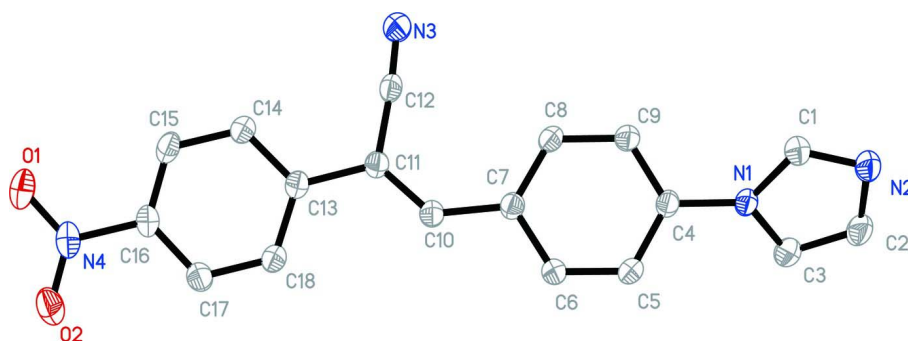


Figure 1

The molecular structure of the title molecule.

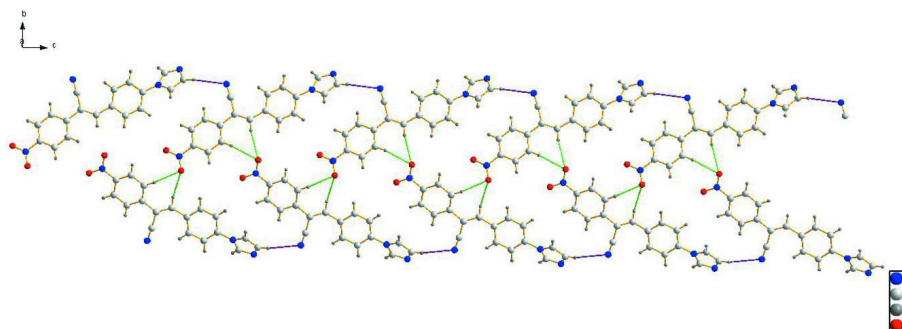


Figure 2

The extended structure of the title compound.

3-[4-(1*H*-Imidazol-1-yl)phenyl]-2-(4-nitrophenyl)prop-2-enenitrile

Crystal data

$C_{18}H_{12}N_4O_2$	$Z = 4$
$M_r = 316.32$	$F(000) = 656$
Monoclinic, $P2_1/c$	$D_x = 1.416 \text{ Mg m}^{-3}$
Hall symbol: $-P 2ybc$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.1792 (16) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 16.512 (4) \text{ \AA}$	$T = 296 \text{ K}$
$c = 12.771 (3) \text{ \AA}$	Block, red
$\beta = 101.557 (3)^\circ$	$0.25 \times 0.2 \times 0.18 \text{ mm}$
$V = 1483.3 (6) \text{ \AA}^3$	

Data collection

Bruker SMART CCD diffractometer	10392 measured reflections
Radiation source: sealed tube	2609 independent reflections
Graphite monochromator	2081 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.024$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2000)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
$T_{\text{min}} = 0.320$, $T_{\text{max}} = 0.439$	$h = -8 \rightarrow 8$
	$k = -19 \rightarrow 17$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.105$	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.2091P]$
$S = 1.07$	where $P = (F_o^2 + 2F_c^2)/3$
2609 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
217 parameters	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.33343 (18)	0.36839 (7)	0.53687 (9)	0.0409 (3)
C11	0.2512 (2)	0.49937 (9)	0.03244 (11)	0.0373 (3)
C16	0.1639 (2)	0.65848 (9)	-0.23484 (11)	0.0433 (4)
C7	0.2711 (2)	0.47837 (9)	0.23353 (10)	0.0380 (3)
C14	0.2517 (2)	0.52940 (9)	-0.15944 (11)	0.0441 (4)

H14	0.2917	0.4765	-0.1669	0.053*
C9	0.3390 (2)	0.36047 (9)	0.34742 (11)	0.0412 (4)
H9	0.3709	0.3059	0.3557	0.049*
C4	0.3103 (2)	0.40518 (9)	0.43461 (10)	0.0379 (3)
C13	0.2195 (2)	0.55534 (8)	-0.06072 (11)	0.0370 (3)
C5	0.2614 (2)	0.48643 (9)	0.42196 (11)	0.0458 (4)
H5	0.2416	0.5167	0.4802	0.055*
C10	0.2475 (2)	0.52285 (9)	0.13288 (11)	0.0404 (4)
H10	0.2257	0.5780	0.1395	0.048*
C6	0.2421 (2)	0.52205 (9)	0.32260 (11)	0.0438 (4)
H6	0.2091	0.5765	0.3147	0.053*
C8	0.3203 (2)	0.39658 (9)	0.24824 (11)	0.0421 (4)
H8	0.3408	0.3661	0.1904	0.050*
N4	0.1372 (2)	0.71310 (10)	-0.32681 (11)	0.0563 (4)
C18	0.1554 (2)	0.63447 (9)	-0.05281 (11)	0.0441 (4)
H18	0.1308	0.6527	0.0120	0.053*
C15	0.2251 (2)	0.58088 (10)	-0.24634 (11)	0.0481 (4)
H15	0.2484	0.5632	-0.3117	0.058*
O2	0.0835 (2)	0.78255 (8)	-0.31500 (10)	0.0736 (4)
O1	0.1702 (2)	0.68742 (9)	-0.41145 (10)	0.0818 (5)
C17	0.1280 (2)	0.68607 (9)	-0.13928 (12)	0.0461 (4)
H17	0.0859	0.7388	-0.1331	0.055*
N3	0.3111 (3)	0.35246 (9)	-0.02129 (11)	0.0666 (5)
C12	0.2850 (2)	0.41644 (10)	0.00623 (11)	0.0448 (4)
N2	0.4589 (2)	0.29296 (8)	0.67745 (10)	0.0579 (4)
C1	0.4684 (2)	0.31340 (9)	0.57988 (12)	0.0496 (4)
H1	0.5579	0.2926	0.5436	0.059*
C3	0.2306 (3)	0.38325 (10)	0.61467 (12)	0.0562 (5)
H3	0.1281	0.4184	0.6103	0.067*
C2	0.3083 (3)	0.33654 (10)	0.69857 (12)	0.0603 (5)
H2	0.2653	0.3342	0.7625	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0543 (8)	0.0397 (7)	0.0291 (6)	-0.0003 (6)	0.0094 (5)	0.0024 (5)
C11	0.0401 (8)	0.0386 (8)	0.0334 (7)	-0.0035 (6)	0.0078 (6)	0.0014 (6)
C16	0.0444 (9)	0.0498 (9)	0.0355 (8)	-0.0052 (7)	0.0075 (6)	0.0098 (7)
C7	0.0425 (8)	0.0386 (8)	0.0322 (7)	-0.0036 (6)	0.0062 (6)	-0.0001 (6)
C14	0.0549 (10)	0.0432 (8)	0.0363 (8)	0.0002 (7)	0.0137 (7)	-0.0001 (6)
C9	0.0526 (9)	0.0356 (8)	0.0356 (8)	-0.0009 (7)	0.0097 (7)	0.0000 (6)
C4	0.0441 (9)	0.0398 (8)	0.0295 (7)	-0.0026 (6)	0.0066 (6)	0.0015 (6)
C13	0.0376 (8)	0.0414 (8)	0.0319 (7)	-0.0054 (6)	0.0071 (6)	0.0008 (6)
C5	0.0640 (11)	0.0425 (9)	0.0312 (7)	0.0033 (7)	0.0100 (7)	-0.0040 (6)
C10	0.0490 (9)	0.0375 (8)	0.0348 (8)	-0.0009 (6)	0.0084 (6)	0.0018 (6)
C6	0.0600 (10)	0.0355 (8)	0.0354 (8)	0.0036 (7)	0.0080 (7)	0.0014 (6)
C8	0.0556 (9)	0.0402 (8)	0.0315 (7)	-0.0008 (7)	0.0116 (6)	-0.0033 (6)
N4	0.0608 (9)	0.0647 (10)	0.0443 (8)	-0.0025 (8)	0.0127 (7)	0.0175 (7)

C18	0.0555 (10)	0.0446 (9)	0.0333 (7)	-0.0009 (7)	0.0115 (7)	-0.0002 (6)
C15	0.0576 (10)	0.0577 (10)	0.0315 (8)	-0.0041 (8)	0.0152 (7)	0.0016 (7)
O2	0.0926 (11)	0.0641 (9)	0.0665 (8)	0.0148 (7)	0.0215 (7)	0.0280 (7)
O1	0.1185 (12)	0.0900 (10)	0.0419 (7)	0.0087 (9)	0.0283 (7)	0.0193 (6)
C17	0.0548 (10)	0.0412 (8)	0.0420 (8)	-0.0010 (7)	0.0085 (7)	0.0040 (6)
N3	0.1093 (14)	0.0488 (9)	0.0411 (8)	0.0102 (8)	0.0134 (8)	-0.0023 (7)
C12	0.0594 (10)	0.0468 (10)	0.0280 (7)	-0.0003 (8)	0.0081 (7)	0.0032 (6)
N2	0.0896 (11)	0.0457 (8)	0.0374 (7)	0.0032 (7)	0.0100 (7)	0.0066 (6)
C1	0.0659 (11)	0.0437 (9)	0.0390 (8)	0.0049 (8)	0.0102 (7)	0.0048 (7)
C3	0.0763 (12)	0.0558 (10)	0.0417 (9)	0.0094 (9)	0.0247 (8)	0.0039 (7)
C2	0.0971 (14)	0.0522 (10)	0.0362 (8)	-0.0022 (10)	0.0245 (9)	0.0046 (7)

Geometric parameters (Å, °)

N1—C1	1.361 (2)	C13—C18	1.395 (2)
N1—C3	1.3736 (19)	C5—C6	1.380 (2)
N1—C4	1.4197 (17)	C5—H5	0.9300
C11—C10	1.3455 (19)	C10—H10	0.9300
C11—C12	1.442 (2)	C6—H6	0.9300
C11—C13	1.4876 (19)	C8—H8	0.9300
C16—C15	1.372 (2)	N4—O1	1.2277 (18)
C16—C17	1.375 (2)	N4—O2	1.2287 (18)
C16—N4	1.4626 (19)	C18—C17	1.377 (2)
C7—C6	1.3971 (19)	C18—H18	0.9300
C7—C8	1.399 (2)	C15—H15	0.9300
C7—C10	1.4606 (18)	C17—H17	0.9300
C14—C15	1.381 (2)	N3—C12	1.141 (2)
C14—C13	1.3939 (19)	N2—C1	1.306 (2)
C14—H14	0.9300	N2—C2	1.370 (2)
C9—C8	1.3820 (19)	C1—H1	0.9300
C9—C4	1.3853 (19)	C3—C2	1.347 (2)
C9—H9	0.9300	C3—H3	0.9300
C4—C5	1.388 (2)	C2—H2	0.9300
C1—N1—C3	105.65 (12)	C5—C6—C7	121.66 (14)
C1—N1—C4	126.83 (13)	C5—C6—H6	119.2
C3—N1—C4	127.46 (13)	C7—C6—H6	119.2
C10—C11—C12	122.11 (13)	C9—C8—C7	121.00 (13)
C10—C11—C13	123.67 (13)	C9—C8—H8	119.5
C12—C11—C13	114.22 (12)	C7—C8—H8	119.5
C15—C16—C17	121.71 (13)	O1—N4—O2	123.44 (14)
C15—C16—N4	118.88 (13)	O1—N4—C16	118.48 (15)
C17—C16—N4	119.41 (15)	O2—N4—C16	118.08 (14)
C6—C7—C8	117.63 (12)	C17—C18—C13	121.15 (14)
C6—C7—C10	116.55 (13)	C17—C18—H18	119.4
C8—C7—C10	125.82 (12)	C13—C18—H18	119.4
C15—C14—C13	121.12 (14)	C16—C15—C14	118.97 (14)
C15—C14—H14	119.4	C16—C15—H15	120.5

C13—C14—H14	119.4	C14—C15—H15	120.5
C8—C9—C4	120.27 (13)	C16—C17—C18	119.00 (15)
C8—C9—H9	119.9	C16—C17—H17	120.5
C4—C9—H9	119.9	C18—C17—H17	120.5
C9—C4—C5	119.76 (13)	N3—C12—C11	175.48 (15)
C9—C4—N1	120.17 (13)	C1—N2—C2	104.24 (14)
C5—C4—N1	120.06 (12)	N2—C1—N1	112.88 (15)
C14—C13—C18	118.02 (13)	N2—C1—H1	123.6
C14—C13—C11	120.40 (13)	N1—C1—H1	123.6
C18—C13—C11	121.58 (12)	C2—C3—N1	106.02 (15)
C6—C5—C4	119.68 (13)	C2—C3—H3	127.0
C6—C5—H5	120.2	N1—C3—H3	127.0
C4—C5—H5	120.2	C3—C2—N2	111.20 (14)
C11—C10—C7	132.31 (14)	C3—C2—H2	124.4
C11—C10—H10	113.8	N2—C2—H2	124.4
C7—C10—H10	113.8		
C8—C9—C4—C5	0.4 (2)	C10—C7—C8—C9	179.97 (14)
C8—C9—C4—N1	-178.68 (13)	C15—C16—N4—O1	0.2 (2)
C1—N1—C4—C9	38.6 (2)	C17—C16—N4—O1	179.89 (15)
C3—N1—C4—C9	-144.54 (16)	C15—C16—N4—O2	-179.52 (15)
C1—N1—C4—C5	-140.54 (16)	C17—C16—N4—O2	0.2 (2)
C3—N1—C4—C5	36.3 (2)	C14—C13—C18—C17	-1.2 (2)
C15—C14—C13—C18	1.4 (2)	C11—C13—C18—C17	179.44 (14)
C15—C14—C13—C11	-179.21 (14)	C17—C16—C15—C14	-0.1 (2)
C10—C11—C13—C14	170.92 (14)	N4—C16—C15—C14	179.55 (14)
C12—C11—C13—C14	-9.6 (2)	C13—C14—C15—C16	-0.8 (2)
C10—C11—C13—C18	-9.7 (2)	C15—C16—C17—C18	0.4 (2)
C12—C11—C13—C18	169.74 (14)	N4—C16—C17—C18	-179.33 (14)
C9—C4—C5—C6	-0.2 (2)	C13—C18—C17—C16	0.3 (2)
N1—C4—C5—C6	178.97 (14)	C10—C11—C12—N3	-178 (2)
C12—C11—C10—C7	-0.7 (3)	C13—C11—C12—N3	3 (2)
C13—C11—C10—C7	178.73 (14)	C2—N2—C1—N1	0.59 (19)
C6—C7—C10—C11	-174.72 (15)	C3—N1—C1—N2	-0.18 (19)
C8—C7—C10—C11	5.5 (3)	C4—N1—C1—N2	177.24 (14)
C4—C5—C6—C7	-0.1 (2)	C1—N1—C3—C2	-0.32 (18)
C8—C7—C6—C5	0.1 (2)	C4—N1—C3—C2	-177.72 (14)
C10—C7—C6—C5	-179.70 (14)	N1—C3—C2—N2	0.7 (2)
C4—C9—C8—C7	-0.5 (2)	C1—N2—C2—C3	-0.8 (2)
C6—C7—C8—C9	0.2 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C18—H18 \cdots O2 ⁱ	0.93	2.54	3.464 (2)	173

Symmetry code: (i) *x*, -*y*+3/2, *z*+1/2.