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1-(2-Cyanoethyl)-1*H*-imidazole-4,5-dicarbonitrile

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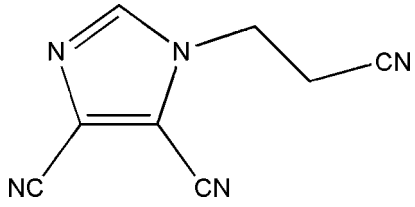
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 19.2.

In the title tricyanonitrile compound, $C_8H_5N_5$, the *N*-substituted cyanoethyl group is offset to the imidazole ring [dihedral angle = 75.41 (15)°].

Related literature

For background to the application of imidazole compounds as ligands, see: Li *et al.* (1955). For the significance of N atoms in metal complex chemistry, see: Fujita *et al.* (1994). For examples of some imidazole complexes, see: Martin & Edsall (1958).



Experimental

Crystal data

$C_8H_5N_5$ M_r = 171.17
Triclinic, $P\overline{1}$
a = 6.4831 (6) Å
b = 6.7538 (6) Å
c = 10.4040 (11) Å
α = 77.865 (9)°
β = 84.297 (8)°
γ = 74.499 (8)°
V = 428.71 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.43 × 0.25 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.973, T_{max} = 0.986
3805 measured reflections
2265 independent reflections
1439 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.124
S = 1.09
2265 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalRED* (Rigaku/MSC, 2004); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2228).

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supporting information

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1-(2-Cyanoethyl)-1*H*-imidazole-4,5-dicarbonitrile

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S1. Comment

Imidazole ligands have been used with remarkable success in coordination chemistry over past decades (Li *et al.*, 1955). Some of the reasons are for this are that the N atom plays an important role in the formation of metal complexes (Fujita *et al.*, 1994), and that imidazole complexes show conjugate acid-base properties and good complexation coordination performance in the solid state. Some examples of imidazole complexes have been reported (Martin & Edsall, 1958). Here we report on a new imidazole compound, the polycyano-substituted imidazole, the title compound $C_8H_5N_5$.

In the molecular structure of this compound (Fig. 1). The bond lengths and bond angles are within normal ranges. The *N*-bound cyanoethyl side chain is offset to the imidazole ring [torsion angles C5—N4—C4—C2 and N4—C4—C2—C1, -78.0 (2) and -61.4 (2)° respectively]. The dihedral angle between the cyanoethyl group defined by atoms N1—C1—C2—C4 and the imidazole ring is 75.41 (15)°]

S2. Experimental

A mixture of 4,5-dicyanoimidazole (1.18 g, 10 mmol) and powdered potassium hydroxide (100 mg) (as a catalyst) in acrylonitrile (20 ml) was heated at 130 °C for 3 hr in a sealed tube, after which the solution was evaporated to dryness. The crude product obtained was recrystallized twice from acetone to give a pure blue product. Yield: 89.7%. Anal: Calcd. for $C_8H_5N_5$: C, 56.1; H, 2.9; N, 40.9%: Found: C, 56.15; H, 2.96; N, 40.89%.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms [C—H = 0.93 Å (aromatic) and 0.97 Å (methylene)], with U_{iso}(H) = 1.2U_{eq}(C).

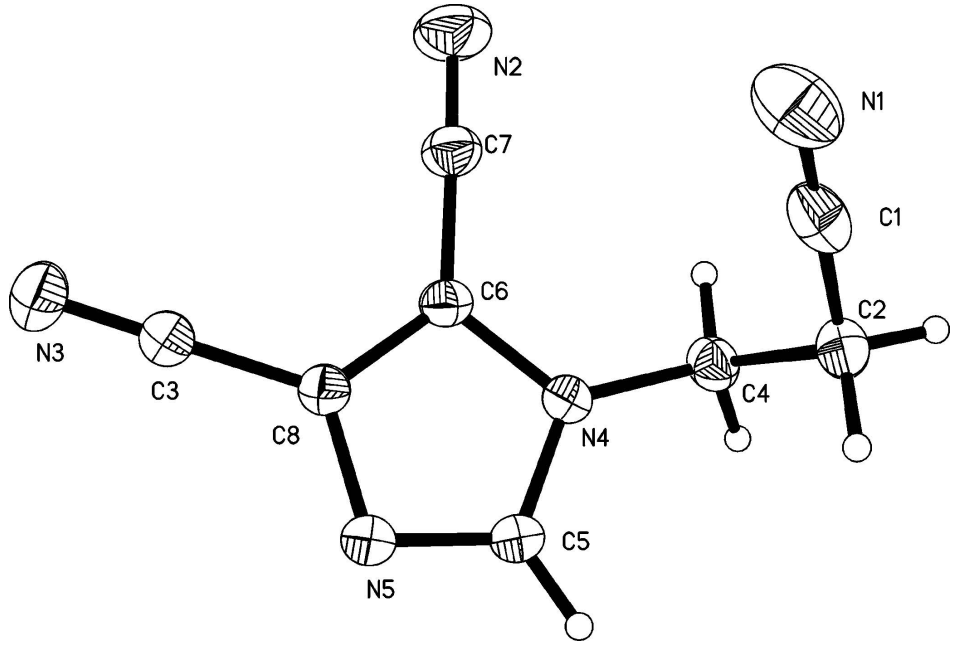

Figure 1

The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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Crystal data

$C_8H_5N_5$
$M_r = 171.17$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.4831\ (6)$ Å
$b = 6.7538\ (6)$ Å
$c = 10.4040\ (11)$ Å
$\alpha = 77.865\ (9)°$
$\beta = 84.297\ (8)°$
$\gamma = 74.499\ (8)°$
$V = 428.71\ (7)$ Å^3
$Z = 2$
$F(000) = 176$
$D_x = 1.326$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1220 reflections
$\theta = 3.2–29.0°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, blue
0.43 × 0.25 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 16.1623 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.973$, $T_{max} = 0.986$
3805 measured reflections
2265 independent reflections
1439 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 29.0°$, $\theta_{min} = 3.2°$
$h = -8\rightarrow8$
$k = -9\rightarrow9$
$l = -13\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.124$
$S = 1.09$
2265 reflections
118 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.0566P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N4	0.25841 (19)	0.19385 (19)	0.19288 (12)	0.0356 (3)
N5	0.5564 (2)	0.2497 (2)	0.08299 (14)	0.0438 (4)
C8	0.5883 (2)	0.0426 (2)	0.13842 (15)	0.0367 (4)
C7	0.3704 (3)	−0.1861 (3)	0.28068 (17)	0.0462 (4)
C6	0.4074 (2)	0.0040 (2)	0.20743 (15)	0.0353 (4)
C5	0.3567 (2)	0.3342 (2)	0.11807 (16)	0.0420 (4)
H5A	0.2902	0.4759	0.0938	0.050*
N3	0.9384 (2)	−0.2328 (3)	0.10572 (16)	0.0632 (5)
C4	0.0347 (2)	0.2341 (3)	0.24210 (16)	0.0425 (4)
H4A	−0.0060	0.1025	0.2662	0.051*
H4B	−0.0557	0.3222	0.1723	0.051*
C3	0.7842 (3)	−0.1089 (3)	0.12134 (16)	0.0430 (4)
C2	−0.0044 (3)	0.3398 (3)	0.36024 (17)	0.0502 (5)
H2A	0.0338	0.4727	0.3357	0.060*
H2B	−0.1557	0.3685	0.3862	0.060*
N2	0.3452 (3)	−0.3409 (3)	0.3388 (2)	0.0740 (6)
C1	0.1183 (3)	0.2129 (3)	0.47147 (19)	0.0534 (5)
N1	0.2152 (3)	0.1117 (3)	0.55746 (19)	0.0798 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N4	0.0358 (7)	0.0354 (7)	0.0338 (7)	−0.0091 (5)	0.0008 (5)	−0.0038 (5)
N5	0.0430 (7)	0.0361 (7)	0.0470 (8)	−0.0091 (6)	0.0055 (6)	−0.0008 (6)
C8	0.0379 (8)	0.0356 (8)	0.0347 (8)	−0.0078 (6)	−0.0010 (6)	−0.0049 (7)

C7	0.0486 (10)	0.0386 (9)	0.0500 (10)	−0.0131 (8)	−0.0032 (8)	−0.0023 (8)
C6	0.0409 (8)	0.0323 (8)	0.0324 (8)	−0.0096 (6)	−0.0032 (6)	−0.0040 (6)
C5	0.0433 (9)	0.0322 (8)	0.0452 (9)	−0.0077 (7)	0.0030 (7)	−0.0004 (7)
N3	0.0538 (9)	0.0568 (10)	0.0660 (11)	0.0044 (8)	0.0037 (8)	−0.0100 (8)
C4	0.0348 (8)	0.0482 (9)	0.0436 (10)	−0.0118 (7)	0.0015 (7)	−0.0067 (8)
C3	0.0430 (9)	0.0419 (9)	0.0407 (9)	−0.0082 (7)	0.0011 (7)	−0.0053 (7)
C2	0.0505 (10)	0.0462 (10)	0.0514 (11)	−0.0108 (8)	0.0123 (8)	−0.0124 (8)
N2	0.0836 (13)	0.0471 (10)	0.0879 (14)	−0.0269 (9)	−0.0008 (10)	0.0065 (9)
C1	0.0591 (12)	0.0660 (13)	0.0442 (11)	−0.0288 (10)	0.0112 (9)	−0.0204 (10)
N1	0.0850 (14)	0.1093 (17)	0.0516 (11)	−0.0391 (12)	−0.0047 (10)	−0.0104 (11)

Geometric parameters (Å, º)

N4—C5	1.3509 (19)	C5—H5A	0.9300
N4—C6	1.3729 (18)	N3—C3	1.142 (2)
N4—C4	1.4630 (19)	C4—C2	1.515 (2)
N5—C5	1.3172 (19)	C4—H4A	0.9700
N5—C8	1.3641 (19)	C4—H4B	0.9700
C8—C6	1.370 (2)	C2—C1	1.452 (3)
C8—C3	1.424 (2)	C2—H2A	0.9700
C7—N2	1.137 (2)	C2—H2B	0.9700
C7—C6	1.416 (2)	C1—N1	1.135 (2)
C5—N4—C6	106.18 (12)	N4—C4—C2	112.63 (13)
C5—N4—C4	126.80 (13)	N4—C4—H4A	109.1
C6—N4—C4	126.95 (13)	C2—C4—H4A	109.1
C5—N5—C8	104.35 (13)	N4—C4—H4B	109.1
N5—C8—C6	110.83 (13)	C2—C4—H4B	109.1
N5—C8—C3	122.98 (14)	H4A—C4—H4B	107.8
C6—C8—C3	126.16 (14)	N3—C3—C8	178.15 (19)
N2—C7—C6	178.5 (2)	C1—C2—C4	112.42 (15)
C8—C6—N4	105.61 (13)	C1—C2—H2A	109.1
C8—C6—C7	129.79 (15)	C4—C2—H2A	109.1
N4—C6—C7	124.59 (14)	C1—C2—H2B	109.1
N5—C5—N4	113.02 (14)	C4—C2—H2B	109.1
N5—C5—H5A	123.5	H2A—C2—H2B	107.9
N4—C5—H5A	123.5	N1—C1—C2	179.1 (2)
C5—N4—C4—C2	−78.0 (2)	C8—N5—C5—N4	0.08 (17)
C6—N4—C4—C2	105.74 (18)	C5—N5—C8—C3	178.04 (15)
C4—N4—C5—N5	−176.61 (14)	C5—N5—C8—C6	−0.40 (17)
C6—N4—C5—N5	0.25 (18)	C1—C2—C4—N4	−61.4 (2)
C4—N4—C6—C7	−3.8 (2)	N4—C6—C8—N5	0.55 (17)
C4—N4—C6—C8	176.38 (14)	N4—C6—C8—C3	−177.82 (15)
C5—N4—C6—C7	179.31 (15)	C7—C6—C8—N5	−179.22 (16)
C5—N4—C6—C8	−0.48 (16)	C7—C6—C8—C3	2.4 (3)