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3-Methyl-1-propargylquinoxalin-2(1*H*)-one

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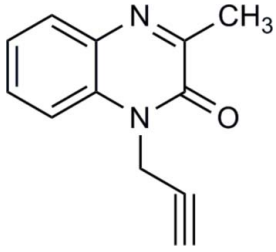
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 14.9.

The ten-membered fused ring of the title compound, $C_{12}H_{10}N_2O$, is essentially planar in the two independent molecules of the asymmetric unit (r.m.s. deviations = 0.012 and 0.015 Å).

Related literature

For the crystal structure of 1-ethyl-3-methylquinoxalin-2(1*H*)-one, see: Benzeid *et al.* (2008). For the synthesis of the reactant 3-methyl-1*H*-quinoxalin-2-one, see: Nikolaenko & Munro (2004).



Experimental

Crystal data

$C_{12}H_{10}N_2O$
M_r = 198.22
Monoclinic, $P2_1/n$
a = 21.124 (1) Å
b = 4.3709 (2) Å
c = 22.246 (1) Å
β = 105.354 (6)°
V = 1980.7 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 180 K
0.20 × 0.15 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.985, T_{max} = 0.991
14275 measured reflections
4058 independent reflections
2428 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 0.97
4058 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2590).

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supporting information

Acta Cryst. (2009). E**65**, o2196 [doi:10.1107/S1600536809032498]

3-Methyl-1-propargylquinoxalin-2(1*H*)-one

Hanane Benzeid, Youssef Ramli, Laure Vendier, El Mokhtar Essassi and Seik Weng Ng

S1. Experimental

To a solution of 3-methylquinoxalin-2(1*H*)-one (Nikolaenko & Munro *et al.*, 2004) (1 g, 6.22 mmol) in DMF (20 ml) was added propargyl bromide (0.82 ml, 6.22 mmol), potassium carbonate (1 g, 7.46 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide. The mixture was stirred at room temperature for 24 h. The solution was filtered and the solvent removed under reduced pressure. The residue was recrystallized from ethanol to afford 3-methyl-1-(propargyl)quinoxalin-2(1*H*)-one as colorless crystals.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C).

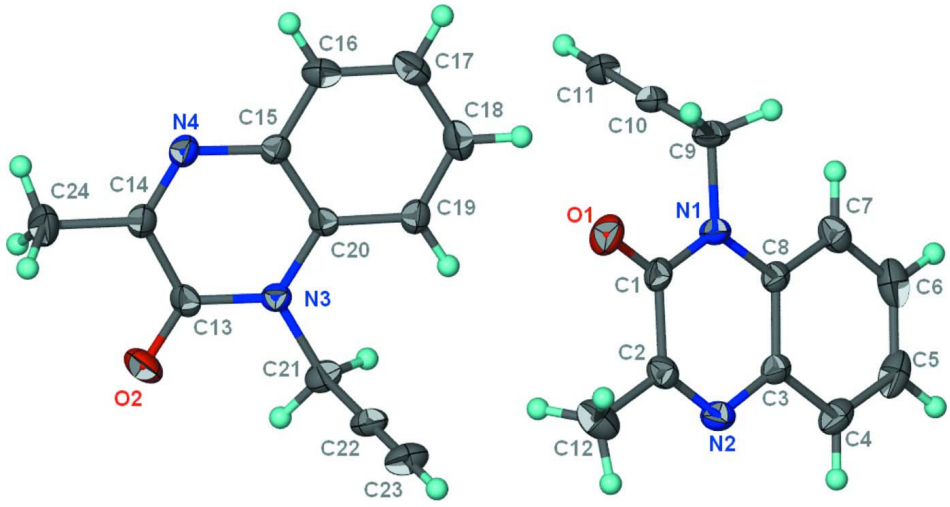

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_{12}H_{10}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

3-Methyl-1-propargylquinoxalin-2(1*H*)-one

Crystal data

$C_{12}H_{10}N_2O$
M_r = 198.22
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 21.124 (1) Å
b = 4.3709 (2) Å
c = 22.246 (1) Å
β = 105.354 (6)°
V = 1980.7 (2) Å^3
Z = 8

$F(000) = 832$
$D_x = 1.329$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5089 reflections
$\theta = 2.7$–$32.2°$
$\mu = 0.09$ mm^{-1}
$T = 180$ K
Parallelepiped, yellow
0.20 × 0.15 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min} = 0.985$, $T_{max} = 0.991$
14275 measured reflections
4058 independent reflections
2428 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.8°$
$h = -22 \rightarrow 26$
$k = -5 \rightarrow 5$
$l = -26 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.102$
$S = 0.97$
4058 reflections
273 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
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.30129 (6)	0.4482 (3)	0.53550 (5)	0.0423 (3)
O2	0.53899 (5)	0.4210 (3)	0.84138 (5)	0.0423 (3)
N1	0.24291 (6)	0.1336 (3)	0.46002 (5)	0.0259 (3)
N2	0.36089 (6)	−0.0417 (3)	0.43668 (6)	0.0301 (3)
N3	0.45992 (6)	0.5883 (3)	0.75752 (6)	0.0248 (3)
N4	0.40956 (6)	0.9390 (3)	0.83838 (6)	0.0299 (3)
C1	0.30011 (8)	0.2584 (4)	0.49493 (7)	0.0284 (4)
C2	0.36032 (8)	0.1492 (4)	0.48043 (7)	0.0299 (4)
C3	0.30152 (8)	−0.1552 (4)	0.40141 (7)	0.0265 (4)
C4	0.30203 (9)	−0.3586 (4)	0.35363 (7)	0.0359 (4)
H4	0.3427	−0.4141	0.3460	0.043*
C5	0.24506 (10)	−0.4804 (4)	0.31742 (8)	0.0438 (5)
H5	0.2459	−0.6193	0.2848	0.053*
C6	0.18630 (10)	−0.3990 (4)	0.32887 (8)	0.0441 (5)
H6	0.1466	−0.4833	0.3038	0.053*
C7	0.18398 (8)	−0.1987 (4)	0.37573 (8)	0.0342 (4)
H7	0.1430	−0.1453	0.3830	0.041*
C8	0.24165 (8)	−0.0749 (3)	0.41244 (7)	0.0250 (4)
C9	0.18204 (8)	0.2356 (4)	0.47433 (8)	0.0324 (4)
H9A	0.1884	0.4460	0.4914	0.039*
H9B	0.1462	0.2416	0.4353	0.039*

C10	0.16261 (7)	0.0368 (4)	0.51906 (7)	0.0285 (4)
C11	0.14630 (8)	−0.1151 (4)	0.55593 (8)	0.0356 (4)
H11	0.1331	−0.2379	0.5857	0.043*
C12	0.42291 (8)	0.2734 (5)	0.52009 (9)	0.0484 (5)
H12A	0.4594	0.2039	0.5040	0.073*
H12B	0.4294	0.2006	0.5630	0.073*
H12C	0.4212	0.4974	0.5194	0.073*
C13	0.49034 (7)	0.5800 (4)	0.81993 (7)	0.0284 (4)
C14	0.46119 (8)	0.7751 (4)	0.85929 (7)	0.0304 (4)
C15	0.37878 (7)	0.9314 (4)	0.77527 (7)	0.0248 (4)
C16	0.32214 (7)	1.1033 (4)	0.75256 (8)	0.0329 (4)
H16	0.3056	1.2241	0.7805	0.039*
C17	0.29004 (8)	1.1009 (4)	0.69069 (8)	0.0365 (4)
H17	0.2514	1.2194	0.6756	0.044*
C18	0.31410 (8)	0.9248 (4)	0.64995 (8)	0.0351 (4)
H18	0.2914	0.9213	0.6070	0.042*
C19	0.37008 (8)	0.7558 (4)	0.67064 (7)	0.0294 (4)
H19	0.3863	0.6373	0.6422	0.035*
C20	0.40306 (7)	0.7585 (3)	0.73351 (7)	0.0227 (3)
C21	0.48885 (8)	0.4108 (4)	0.71564 (7)	0.0323 (4)
H21A	0.5219	0.2677	0.7405	0.039*
H21B	0.4541	0.2881	0.6872	0.039*
C22	0.52007 (8)	0.6082 (4)	0.67891 (8)	0.0326 (4)
C23	0.54466 (9)	0.7662 (5)	0.64907 (8)	0.0429 (5)
H23	0.5646	0.8945	0.6248	0.051*
C24	0.49583 (9)	0.7818 (5)	0.92679 (8)	0.0503 (5)
H24A	0.5381	0.8860	0.9328	0.075*
H24B	0.5032	0.5719	0.9426	0.075*
H24C	0.4690	0.8918	0.9495	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0525 (8)	0.0439 (7)	0.0306 (7)	0.0029 (6)	0.0113 (6)	−0.0077 (6)
O2	0.0237 (6)	0.0535 (8)	0.0453 (7)	0.0048 (6)	0.0016 (5)	0.0074 (7)
N1	0.0248 (7)	0.0277 (7)	0.0275 (7)	0.0052 (6)	0.0108 (6)	0.0035 (6)
N2	0.0285 (8)	0.0303 (7)	0.0341 (8)	0.0050 (7)	0.0130 (6)	0.0079 (7)
N3	0.0218 (7)	0.0273 (7)	0.0259 (7)	−0.0017 (6)	0.0076 (6)	−0.0022 (6)
N4	0.0257 (8)	0.0407 (8)	0.0237 (7)	−0.0059 (7)	0.0074 (6)	−0.0041 (7)
C1	0.0349 (10)	0.0295 (9)	0.0216 (9)	0.0026 (8)	0.0089 (7)	0.0055 (8)
C2	0.0287 (9)	0.0295 (9)	0.0304 (9)	0.0024 (8)	0.0056 (7)	0.0078 (8)
C3	0.0319 (9)	0.0251 (8)	0.0248 (9)	0.0068 (8)	0.0118 (7)	0.0082 (7)
C4	0.0519 (12)	0.0287 (9)	0.0323 (10)	0.0102 (9)	0.0202 (9)	0.0063 (8)
C5	0.0722 (15)	0.0324 (10)	0.0271 (10)	0.0005 (10)	0.0133 (10)	−0.0017 (8)
C6	0.0542 (13)	0.0368 (11)	0.0324 (10)	−0.0058 (10)	−0.0041 (9)	0.0046 (9)
C7	0.0323 (10)	0.0330 (10)	0.0341 (10)	0.0008 (8)	0.0035 (8)	0.0089 (8)
C8	0.0309 (9)	0.0223 (8)	0.0228 (8)	0.0040 (8)	0.0089 (7)	0.0061 (7)
C9	0.0301 (9)	0.0324 (9)	0.0394 (10)	0.0100 (8)	0.0173 (8)	0.0052 (8)

C10	0.0227 (8)	0.0355 (9)	0.0285 (9)	0.0043 (8)	0.0086 (7)	−0.0034 (8)
C11	0.0274 (9)	0.0492 (11)	0.0323 (10)	0.0023 (9)	0.0115 (8)	0.0025 (9)
C12	0.0335 (11)	0.0510 (12)	0.0554 (12)	−0.0012 (10)	0.0023 (9)	0.0028 (10)
C13	0.0192 (8)	0.0364 (10)	0.0276 (9)	−0.0079 (8)	0.0028 (7)	0.0023 (8)
C14	0.0250 (9)	0.0424 (10)	0.0236 (9)	−0.0082 (8)	0.0064 (7)	−0.0001 (8)
C15	0.0211 (8)	0.0293 (8)	0.0251 (9)	−0.0075 (7)	0.0083 (7)	−0.0020 (7)
C16	0.0255 (9)	0.0325 (10)	0.0429 (11)	−0.0003 (8)	0.0130 (8)	−0.0012 (9)
C17	0.0232 (9)	0.0396 (11)	0.0440 (11)	0.0002 (8)	0.0041 (8)	0.0103 (9)
C18	0.0316 (10)	0.0416 (10)	0.0286 (9)	−0.0087 (9)	0.0017 (8)	0.0076 (9)
C19	0.0289 (9)	0.0354 (9)	0.0237 (9)	−0.0068 (8)	0.0067 (7)	−0.0012 (8)
C20	0.0177 (8)	0.0248 (8)	0.0253 (8)	−0.0055 (7)	0.0052 (6)	0.0010 (7)
C21	0.0355 (9)	0.0298 (9)	0.0347 (9)	0.0001 (8)	0.0144 (8)	−0.0050 (8)
C22	0.0273 (9)	0.0364 (10)	0.0374 (10)	0.0010 (8)	0.0144 (8)	−0.0074 (8)
C23	0.0389 (11)	0.0477 (11)	0.0493 (11)	0.0020 (9)	0.0244 (9)	−0.0007 (10)
C24	0.0372 (11)	0.0816 (15)	0.0279 (10)	−0.0060 (11)	0.0014 (8)	−0.0031 (10)

Geometric parameters (Å, º)

O1—C1	1.2213 (18)	C9—H9B	0.9900
O2—C13	1.2277 (18)	C10—C11	1.176 (2)
N1—C1	1.365 (2)	C11—H11	0.9500
N1—C8	1.3917 (19)	C12—H12A	0.9800
N1—C9	1.4732 (19)	C12—H12B	0.9800
N2—C2	1.285 (2)	C12—H12C	0.9800
N2—C3	1.383 (2)	C13—C14	1.469 (2)
N3—C13	1.3673 (19)	C14—C24	1.486 (2)
N3—C20	1.3934 (19)	C15—C16	1.390 (2)
N3—C21	1.4643 (19)	C15—C20	1.396 (2)
N4—C14	1.285 (2)	C16—C17	1.364 (2)
N4—C15	1.3826 (18)	C16—H16	0.9500
C1—C2	1.472 (2)	C17—C18	1.384 (2)
C2—C12	1.484 (2)	C17—H17	0.9500
C3—C4	1.388 (2)	C18—C19	1.367 (2)
C3—C8	1.395 (2)	C18—H18	0.9500
C4—C5	1.367 (2)	C19—C20	1.388 (2)
C4—H4	0.9500	C19—H19	0.9500
C5—C6	1.378 (3)	C21—C22	1.460 (2)
C5—H5	0.9500	C21—H21A	0.9900
C6—C7	1.372 (2)	C21—H21B	0.9900
C6—H6	0.9500	C22—C23	1.171 (2)
C7—C8	1.385 (2)	C23—H23	0.9500
C7—H7	0.9500	C24—H24A	0.9800
C9—C10	1.459 (2)	C24—H24B	0.9800
C9—H9A	0.9900	C24—H24C	0.9800
C1—N1—C8	122.01 (13)	H12A—C12—H12B	109.5
C1—N1—C9	116.60 (13)	C2—C12—H12C	109.5
C8—N1—C9	121.38 (13)	H12A—C12—H12C	109.5

C2—N2—C3	118.28 (14)	H12B—C12—H12C	109.5
C13—N3—C20	121.95 (13)	O2—C13—N3	121.98 (15)
C13—N3—C21	117.96 (13)	O2—C13—C14	122.47 (15)
C20—N3—C21	120.10 (13)	N3—C13—C14	115.55 (14)
C14—N4—C15	118.69 (14)	N4—C14—C13	123.89 (15)
O1—C1—N1	122.25 (15)	N4—C14—C24	119.90 (16)
O1—C1—C2	122.16 (16)	C13—C14—C24	116.20 (15)
N1—C1—C2	115.59 (14)	N4—C15—C16	118.96 (14)
N2—C2—C1	123.96 (15)	N4—C15—C20	122.13 (14)
N2—C2—C12	120.14 (15)	C16—C15—C20	118.91 (14)
C1—C2—C12	115.90 (15)	C17—C16—C15	120.85 (16)
N2—C3—C4	118.32 (15)	C17—C16—H16	119.6
N2—C3—C8	122.53 (14)	C15—C16—H16	119.6
C4—C3—C8	119.15 (16)	C16—C17—C18	119.63 (16)
C5—C4—C3	121.12 (17)	C16—C17—H17	120.2
C5—C4—H4	119.4	C18—C17—H17	120.2
C3—C4—H4	119.4	C19—C18—C17	120.99 (16)
C4—C5—C6	119.08 (17)	C19—C18—H18	119.5
C4—C5—H5	120.5	C17—C18—H18	119.5
C6—C5—H5	120.5	C18—C19—C20	119.59 (16)
C7—C6—C5	121.35 (17)	C18—C19—H19	120.2
C7—C6—H6	119.3	C20—C19—H19	120.2
C5—C6—H6	119.3	C19—C20—N3	122.26 (14)
C6—C7—C8	119.64 (17)	C19—C20—C15	120.01 (14)
C6—C7—H7	120.2	N3—C20—C15	117.72 (13)
C8—C7—H7	120.2	C22—C21—N3	111.69 (13)
C7—C8—N1	122.76 (14)	C22—C21—H21A	109.3
C7—C8—C3	119.66 (15)	N3—C21—H21A	109.3
N1—C8—C3	117.57 (14)	C22—C21—H21B	109.3
C10—C9—N1	112.71 (13)	N3—C21—H21B	109.3
C10—C9—H9A	109.1	H21A—C21—H21B	107.9
N1—C9—H9A	109.1	C23—C22—C21	179.5 (2)
C10—C9—H9B	109.1	C22—C23—H23	180.0
N1—C9—H9B	109.1	C14—C24—H24A	109.5
H9A—C9—H9B	107.8	C14—C24—H24B	109.5
C11—C10—C9	177.82 (17)	H24A—C24—H24B	109.5
C10—C11—H11	180.0	C14—C24—H24C	109.5
C2—C12—H12A	109.5	H24A—C24—H24C	109.5
C2—C12—H12B	109.5	H24B—C24—H24C	109.5

C8—N1—C1—O1	177.78 (14)	C20—N3—C13—O2	177.17 (14)
C9—N1—C1—O1	−1.0 (2)	C21—N3—C13—O2	−2.8 (2)
C8—N1—C1—C2	−2.2 (2)	C20—N3—C13—C14	−3.2 (2)
C9—N1—C1—C2	179.07 (12)	C21—N3—C13—C14	176.86 (13)
C3—N2—C2—C1	−0.8 (2)	C15—N4—C14—C13	0.6 (2)
C3—N2—C2—C12	179.06 (15)	C15—N4—C14—C24	179.19 (15)
O1—C1—C2—N2	−177.42 (15)	O2—C13—C14—N4	−178.51 (16)
N1—C1—C2—N2	2.6 (2)	N3—C13—C14—N4	1.9 (2)

O1—C1—C2—C12	2.7 (2)	O2—C13—C14—C24	2.9 (2)
N1—C1—C2—C12	−177.34 (14)	N3—C13—C14—C24	−176.77 (15)
C2—N2—C3—C4	179.21 (13)	C14—N4—C15—C16	178.69 (15)
C2—N2—C3—C8	−1.3 (2)	C14—N4—C15—C20	−1.9 (2)
N2—C3—C4—C5	179.55 (15)	N4—C15—C16—C17	−179.62 (15)
C8—C3—C4—C5	0.0 (2)	C20—C15—C16—C17	0.9 (2)
C3—C4—C5—C6	−0.1 (2)	C15—C16—C17—C18	0.1 (3)
C4—C5—C6—C7	0.0 (3)	C16—C17—C18—C19	−0.8 (3)
C5—C6—C7—C8	0.0 (2)	C17—C18—C19—C20	0.6 (2)
C6—C7—C8—N1	178.84 (14)	C18—C19—C20—N3	179.23 (14)
C6—C7—C8—C3	0.0 (2)	C18—C19—C20—C15	0.4 (2)
C1—N1—C8—C7	−178.59 (15)	C13—N3—C20—C19	−176.69 (14)
C9—N1—C8—C7	0.1 (2)	C21—N3—C20—C19	3.2 (2)
C1—N1—C8—C3	0.3 (2)	C13—N3—C20—C15	2.1 (2)
C9—N1—C8—C3	178.99 (13)	C21—N3—C20—C15	−177.94 (13)
N2—C3—C8—C7	−179.48 (14)	N4—C15—C20—C19	179.38 (14)
C4—C3—C8—C7	0.0 (2)	C16—C15—C20—C19	−1.2 (2)
N2—C3—C8—N1	1.6 (2)	N4—C15—C20—N3	0.5 (2)
C4—C3—C8—N1	−178.93 (13)	C16—C15—C20—N3	180.00 (14)
C1—N1—C9—C10	−93.04 (17)	C13—N3—C21—C22	−107.74 (16)
C8—N1—C9—C10	88.22 (17)	C20—N3—C21—C22	72.32 (18)