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2,3-Bis(pyrazin-2-yloxyimino)butane

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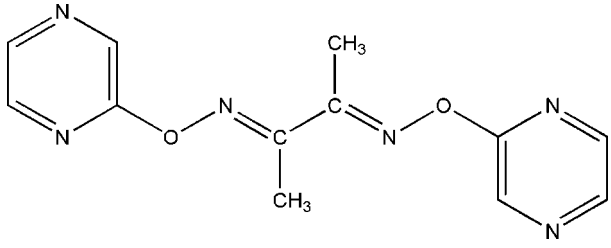
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.142; data-to-parameter ratio = 14.9.

The title molecule, $C_{12}H_{12}N_6O_2$, lies on a crystallographic inversion center with all non-H atoms essentially coplanar.

Related literature

For a related structure, see: Chen & Yang (2008).



Experimental

Crystal data

$C_{12}H_{12}N_6O_2$
M_r = 272.28
Monoclinic, $P2_1/n$
a = 4.7396 (15) Å
b = 17.141 (5) Å
c = 7.911 (3) Å
β = 98.065 (5)°
V = 636.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.43 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.994
3621 measured reflections
1368 independent reflections
872 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.142
S = 1.03
1368 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2694).

References

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Chen, J. N. & Yang, L. Y. (2008). *Acta Cryst.* E**64**, o1862.
Sheldrick, G. M. (1996). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1994 [doi:10.1107/S1600536808029991]

2,3-Bis(pyrazin-2-yloxyimino)butane

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S1. Comment

We are interested in the design and synthesis of muliti-dentate ligands containing pyrazinyl and butane-2,3-dione dioxime and hence we have previously synthesized (2E,3E)-3-(pyrazin-2-yloxyimino)butane-2-one oxime (Chen *et al.*, 2008) and now we report herein homologous title compound (I).

Fig. 1 shows the molecular structure with an inversion centre located in the middle of the C1-C1^{i} bond [symmetry code: (i) -x+1, -y+1, -z]. All of the non-hydrogen atoms define a plane within 0.0652 Å with a maximum deviation of 0.1212 (16) Å for atom C4.

S2. Experimental

A powder of the title compound (0.0473 g, 0.174 mmol) was dissolved into a mixture of solvents containing 20 ml dichloromethane and 10 ml methanol. The colorless single crystals were obtained after the solution was allowed to stand at room temperature for two days.

S3. Refinement

All H atoms were placed in calculated positions and refined as riding with C—H = 0.96 Å, U_{iso} = 1.5U_{eq}(C) for methyl group and C—H = 0.93 Å, U_{iso} = 1.2U_{eq}(C) for pyrazinyl H atoms.

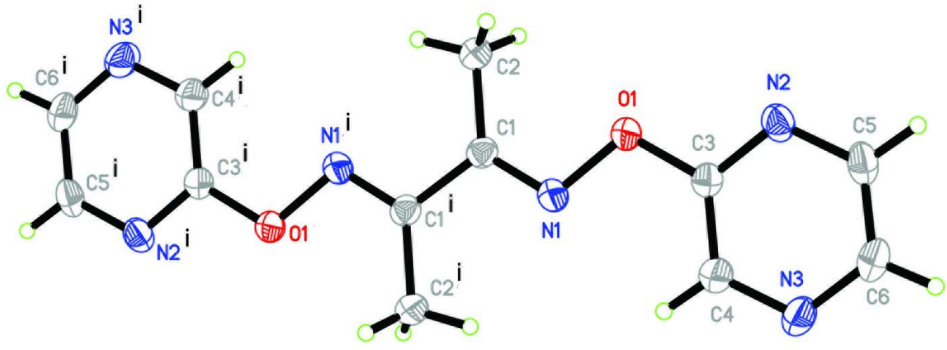

Figure 1

Molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code: (i) -x+1, -y+1, -z].

2,3-Bis(pyrazin-2-yloxyimino)butane

Crystal data

$C_{12}H_{12}N_6O_2$
M_r = 272.28
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 4.7396 (15) Å
b = 17.141 (5) Å

c = 7.911 (3) Å
β = 98.065 (5)°
V = 636.3 (4) Å^3
Z = 2
F(000) = 284
D_x = 1.421 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 556 reflections
θ = 2.4–20.6°
μ = 0.10 mm^{-1}
T = 298 K
Needle, colorless
0.43 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.994

3621 measured reflections
1368 independent reflections
872 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.0°, θ_{min} = 2.4°
h = −6→5
k = −21→17
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.142
S = 1.03
1368 reflections
92 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
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.0016P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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}
C1	0.4107 (4)	0.53547 (11)	−0.0115 (3)	0.0380 (5)
C2	0.4063 (5)	0.58565 (13)	−0.1667 (3)	0.0555 (7)
H2A	0.2172	0.5864	−0.2290	0.083*
H2B	0.5364	0.5650	−0.2380	0.083*
H2C	0.4623	0.6378	−0.1326	0.083*
C3	−0.0460 (5)	0.63257 (12)	0.2132 (3)	0.0378 (5)
C4	−0.0315 (5)	0.58891 (14)	0.3610 (3)	0.0493 (6)
H4	0.0872	0.5455	0.3752	0.059*
C5	−0.3601 (5)	0.71330 (13)	0.3082 (3)	0.0507 (7)
H5	−0.4777	0.7569	0.2942	0.061*

C6	−0.3497 (5)	0.67050 (14)	0.4551 (3)	0.0550 (7)
H6	−0.4610	0.6856	0.5373	0.066*
N1	0.2691 (4)	0.54817 (9)	0.1113 (2)	0.0413 (5)
N2	−0.2076 (4)	0.69473 (10)	0.1842 (2)	0.0473 (5)
N3	−0.1848 (5)	0.60809 (12)	0.4829 (3)	0.0585 (6)
O1	0.1028 (3)	0.61679 (8)	0.07990 (19)	0.0447 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0409 (14)	0.0379 (12)	0.0351 (12)	−0.0026 (9)	0.0053 (10)	−0.0015 (9)
C2	0.0700 (18)	0.0561 (15)	0.0443 (14)	0.0184 (13)	0.0213 (12)	0.0095 (11)
C3	0.0357 (13)	0.0368 (12)	0.0416 (13)	−0.0028 (10)	0.0084 (10)	−0.0026 (9)
C4	0.0509 (16)	0.0531 (14)	0.0453 (14)	0.0092 (11)	0.0116 (11)	0.0036 (11)
C5	0.0495 (15)	0.0371 (13)	0.0691 (18)	0.0028 (11)	0.0208 (13)	−0.0080 (11)
C6	0.0572 (17)	0.0602 (16)	0.0514 (16)	0.0023 (13)	0.0209 (12)	−0.0122 (12)
N1	0.0429 (12)	0.0382 (10)	0.0439 (11)	0.0056 (8)	0.0100 (9)	0.0015 (8)
N2	0.0504 (13)	0.0348 (11)	0.0594 (13)	0.0017 (9)	0.0176 (10)	0.0011 (8)
N3	0.0575 (14)	0.0742 (14)	0.0477 (13)	0.0163 (12)	0.0207 (10)	0.0036 (10)
O1	0.0499 (10)	0.0432 (9)	0.0441 (9)	0.0108 (7)	0.0175 (7)	0.0044 (6)

Geometric parameters (Å, º)

C1—N1	1.275 (3)	C4—N3	1.328 (3)
C1—C1^{i}	1.478 (4)	C4—H4	0.9300
C1—C2	1.496 (3)	C5—N2	1.336 (3)
C2—H2A	0.9600	C5—C6	1.369 (3)
C2—H2B	0.9600	C5—H5	0.9300
C2—H2C	0.9600	C6—N3	1.325 (3)
C3—N2	1.314 (3)	C6—H6	0.9300
C3—O1	1.376 (3)	N1—O1	1.418 (2)
C3—C4	1.381 (3)		
N1—C1—C1^{i}	113.6 (2)	N3—C4—H4	119.6
N1—C1—C2	125.36 (19)	C3—C4—H4	119.6
C1^{i}—C1—C2	121.1 (2)	N2—C5—C6	122.5 (2)
C1—C2—H2A	109.5	N2—C5—H5	118.8
C1—C2—H2B	109.5	C6—C5—H5	118.8
H2A—C2—H2B	109.5	N3—C6—C5	121.6 (2)
C1—C2—H2C	109.5	N3—C6—H6	119.2
H2A—C2—H2C	109.5	C5—C6—H6	119.2
H2B—C2—H2C	109.5	C1—N1—O1	110.30 (17)
N2—C3—O1	112.01 (18)	C3—N2—C5	115.3 (2)
N2—C3—C4	123.1 (2)	C6—N3—C4	116.7 (2)
O1—C3—C4	124.90 (19)	C3—O1—N1	111.15 (15)
N3—C4—C3	120.9 (2)		
N2—C3—C4—N3	0.3 (4)	C6—C5—N2—C3	−0.2 (3)

O1—C3—C4—N3	−179.5 (2)	C5—C6—N3—C4	−0.3 (4)
N2—C5—C6—N3	0.5 (4)	C3—C4—N3—C6	0.0 (3)
C1^{i}—C1—N1—O1	−179.78 (19)	N2—C3—O1—N1	−178.19 (15)
C2—C1—N1—O1	0.5 (3)	C4—C3—O1—N1	1.6 (3)
O1—C3—N2—C5	179.60 (18)	C1—N1—O1—C3	−178.45 (17)
C4—C3—N2—C5	−0.2 (3)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.