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Pyrazine *N*,*N*′-dioxide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.106
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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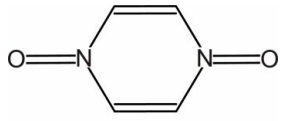
In the crystal structure of the title compound, $C_4H_4N_2O_2$, the pyrazine *N*,*N*′-dioxide molecules are located on centres of inversion. The molecules are stacked in the direction of the crystallographic *a* axis and are connected *via* C—H···O hydrogen bonding.

Comment

We are interested in the synthesis, structures and properties of coordination polymers based on transition metals and amine ligands. The synthesis of these compounds, performed at room temperature or under solvothermal conditions, leads frequently to mixtures of different compounds. For the optimization of the preparation conditions in order to obtain pure compounds, all phases obtained must be identified. This is the case, for example, if transition metal compounds are reacted with pyrazine *N*,*N*′-dioxide. In this case, we have frequently obtained mixtures of different crystals. Single-crystal structure analysis shows that one phase consists of crystals of the title compound, (I). According to a search in the Cambridge Structural Database (Allen & Kennard, 1993), the structure of (I) is unknown. We have found only one structure, that of the coordination polymer *catena*-[(μ_2-pyrazine *N*,*N*′-dioxide)diaquadibromocadmium(II)], containing pyrazine *N*,*N*′-dioxide as a ligand (Pecaut & Masse, 1995).



(I)

The crystal structure of (I) is built up of pyrazine *N*,*N*′-dioxide molecules that are located on centres of inversion. The molecules are stacked in the direction of the crystallographic *a* axis and are connected *via* C—H···O hydrogen bonding. Two molecules are connected by two co-operative C—H···O hydrogen bonds, forming dimers which are built up of eight-membered coplanar rings. These dimers are linked into chains, which extend in the direction of the crystallographic *c* axis. Each O atom acts as an acceptor for a second C—H···O hydrogen bond, which links neighbouring chains, forming a three-dimensional hydrogen-bonded network in a pseudo-hexagonal arrangement.

Experimental

The title compound was prepared by the reaction of 190.5 mg copper(I) iodide with 72.0 mg pyrazine *N*,*N*′-dioxide in 4 ml of acetonitrile in a Teflon-lined steel autoclave at 413 K under solvo-

thermal conditions. After 7 d, the reaction mixture was cooled to room temperature, filtered and the resulting precipitate washed with water. The precipitate is a mixture of several phases. The colourless blocks consist of the title compound.

Crystal data

$C_4H_4N_2O_2$	D_x = 1.594 Mg m^{-3}
M_r = 112.09	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1392 reflections
a = 3.7376 (6) Å	θ = 4–28°
b = 11.0011 (18) Å	μ = 0.13 mm^{-1}
c = 5.7184 (9) Å	T = 293 (2) K
β = 96.778 (19)°	Block, colourless
V = 233.48 (6) Å^3	0.3 × 0.2 × 0.2 mm
Z = 2	

Data collection

Stoe IPDS diffractometer	R_{int} = 0.032
φ scans	θ_{max} = 28.0°
Absorption correction: none	$h = -4 \rightarrow 4$
1450 measured reflections	$k = -14 \rightarrow 11$
551 independent reflections	$l = -7 \rightarrow 7$
427 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.0228P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.039	
$wR(F^2)$ = 0.106	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
551 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
38 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.41 (9)

Table 1
Selected geometric parameters (Å, °).

N1—O1	1.2962 (14)	N1—C1	1.3582 (17)
N1—C2	1.3526 (17)	C1—C2^{i}	1.3617 (19)
O1—N1—C2	121.08 (11)	N1—C1—C2^{i}	120.83 (13)
O1—N1—C1	120.61 (12)	N1—C2—C1^{i}	120.87 (12)
C2—N1—C1	118.30 (11)		

Symmetry code: (i) $-x, 1-y, 1-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{ii}	0.93	2.27	3.1682 (18)	162
C2—H2···O1^{iii}	0.93	2.29	3.2067 (19)	168

Symmetry codes: (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $1-x, 1-y, 2-z$.

The H atoms were positioned with idealized geometry (d_{CH}) = 0.93 Å and refined with fixed isotropic displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)], using a riding model.

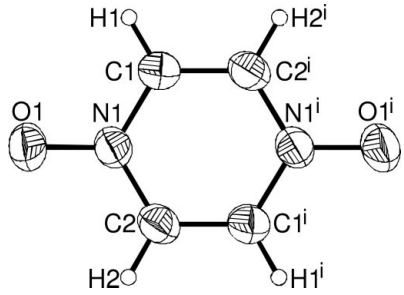


Figure 1
The crystal structure of the title compound, with atom labelling, and displacement ellipsoids drawn at the 50% probability level [symmetry code: (i) $-x, 1-y, 1-z$].

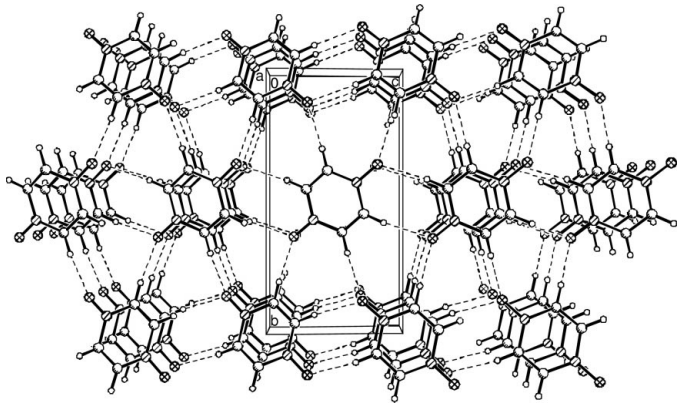


Figure 2
The crystal structure of the title compound, viewed along the crystallographic *a* axis. Hydrogen bonding is shown as dashed lines.

Data collection: *IPDS Program Package* (Stoe & Cie, 1998); cell refinement: *IPDS Program Package*; data reduction: IPDS Program Package; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXL*97.

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