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2-Methoxy-2-methylimidazolidine-4,5-dione

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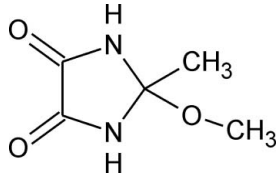
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.062; wR factor = 0.146; data-to-parameter ratio = 16.3.

The asymmetric unit of the title compound, $C_5H_8N_2O_3$, contains two molecules. The crystal structure features N—H···O=C hydrogen bonds.

Related literature

For related literature, see: Fryer *et al.* (1977); Latypov *et al.* (1998, 1999); Stasko *et al.* (2002).



Experimental

Crystal data

$C_5H_8N_2O_3$
M_r = 144.13
Monoclinic, $P2_1/c$
a = 12.4940 (6) Å
b = 6.1930 (4) Å
c = 16.8170 (9) Å
β = 95.054 (4)°
V = 1296.16 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 150 (1) K
0.49 × 0.19 × 0.15 mm

Data collection

Bruke–Nonius KappaCCD area-detector diffractometer
Absorption correction: Gaussian integration (Coppens, 1970)
T_{min} = 0.964, T_{max} = 0.989
12836 measured reflections
2951 independent reflections
2060 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.146
S = 1.12
2951 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O5^{i}	0.86	2.12	2.892 (3)	149
N1—H1···O4^{i}	0.86	2.00	2.817 (3)	159
N3—H3···O2^{ii}	0.86	2.18	2.894 (3)	140
N3—H3···O1^{ii}	0.86	2.64	3.246 (3)	129
N2—H2···O1^{iii}	0.86	2.02	2.878 (3)	175

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

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: CF2150).

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supplementary materials

Acta Cryst. (2007). E**63**, o4704 [**doi:10.1107/S160053680705708X**]

2-Methoxy-2-methylimidazolidine-4,5-dione

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Comment

2-Methoxy-2-methylimidazolidine-4,5-dione is the only known example of 2-alkoxy-2-alkylimidazolidine-4,5-diones. It is an intermediate of the synthesis of the low-sensitivity energetic material 2,2-dinitroethene-1,1-diamine (Latypov *et al.*, 1999).

The title compound (I) has been obtained as colourless crystals from a saturated methanol solution.

Two independent molecules which are positioned with an interplanar (ring to ring) angle of 88.49 (10)° are found in the asymmetric unit. The five-membered rings are formed (see Figure 1) by two N(H)—C=O fragments and one *ipso* carbon connected to both methoxy and methyl groups. The structure of similar cyclic compounds were determined previously (Stasko *et al.*, 2002; Fryer *et al.*, 1977). In both cases, a spiro derivative of imidazoline-4,5-dione (II) and benzodiazepine-1,2-dione (III) reveals very similar interatomic distances and bonding angles to those found in the title compound.

The C—O distances found in (I) [1.217 (3), 1.216 (3), 1.220 (3), and 1.216 (3) Å] are typical for double bonds between these elements. All N—H groups are bonded to C=O fragments in a similar manner to that usually found in peptides. The distances [1.531 (3)Å and 1.528 (3) Å] between the carbon atoms of C=O fragments are a little longer than found in the comparable compounds (II) and (III). All remaining interatomic distances and bonding angles are in line with those found for (II) and (III) previously.

Compound (I) forms an extensive three-dimensional network through the N—H···O=C hydrogen bonding (see Figure 2).

Experimental

Compound (I) was prepared according to a reported method (Latypov *et al.*, 1998). Elemental analysis and spectroscopic data (NMR and IR) were identical to data given in the literature (Latypov *et al.*, 1998). Crystals suitable for X-ray crystallographic analysis were obtained *via* solvent evaporation (methanol).

Refinement

All H atoms were positioned geometrically and refined as riding on their parent C or N atoms, with N—H = 0.86 Å, U_{iso}(H) = 1.2U_{eq}(C); C—H = 0.96 Å, U_{iso}(H) = 1.5U$_{e.g}$(C).

Figures

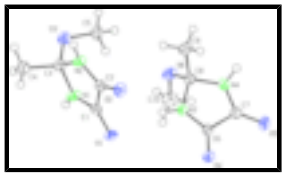

Fig. 1. Perspective view of the two independent molecules of (I) in the asymmetric unit, with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

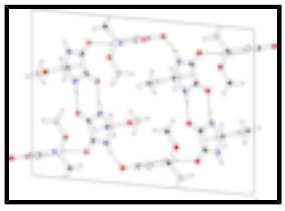

Fig. 2. View of the hydrogen bonding (dashed lines) in (I).

2-Methoxy-2-methylimidazolidine-4,5-dione

Crystal data

$C_5H_8N_2O_3$	F_{000} = 608
M_r = 144.13	D_x = 1.477 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 13590 reflections
a = 12.4940 (6) Å	θ = 1–27.5º
b = 6.1930 (4) Å	μ = 0.12 mm^{-1}
c = 16.8170 (9) Å	T = 150 (1) K
β = 95.054 (4)º	Block, colourless
V = 1296.16 (13) Å^3	0.49 × 0.19 × 0.15 mm
Z = 8	

Data collection

Bruke–Nonius KappaCCD area-detector diffractometer	2951 independent reflections
Monochromator: graphite	2060 reflections with $I > 2\sigma(I)$
Detector resolution: 9.091 pixels mm^{-1}	R_{int} = 0.068
T = 150(1) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: integration Gaussian integration (Coppens, 1970)	h = −16→16
T_{min} = 0.964, T_{max} = 0.989	k = −7→8
12836 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.063$	H-atom parameters constrained
$wR(F^2) = 0.146$	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 1.5623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
2951 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
181 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
O1	0.12247 (15)	0.6735 (3)	−0.00306 (11)	0.0255 (4)
O4	0.82756 (14)	0.1748 (3)	0.25416 (10)	0.0241 (4)
O5	0.60291 (15)	0.1821 (3)	0.29300 (11)	0.0284 (5)
O6	0.63045 (16)	0.5268 (3)	0.06070 (11)	0.0302 (5)
N1	0.15534 (18)	0.4369 (3)	0.10251 (13)	0.0246 (5)
H1	0.1729	0.5280	0.1400	0.030*
O3	0.24709 (15)	0.1223 (3)	0.15056 (11)	0.0289 (5)
O2	0.09293 (15)	0.2734 (3)	−0.09169 (10)	0.0259 (4)
C6	0.75687 (19)	0.2888 (4)	0.22195 (14)	0.0186 (5)
N3	0.76312 (17)	0.4351 (3)	0.16439 (12)	0.0210 (5)
H3	0.8214	0.4606	0.1424	0.025*
N2	0.12607 (17)	0.1272 (3)	0.03429 (12)	0.0228 (5)
H2	0.1210	−0.0076	0.0222	0.027*
N4	0.59112 (17)	0.4362 (4)	0.19236 (13)	0.0240 (5)
H4	0.5233	0.4619	0.1903	0.029*
C1	0.13122 (19)	0.4949 (4)	0.02705 (15)	0.0187 (5)
C7	0.6399 (2)	0.2909 (4)	0.24181 (14)	0.0196 (5)
C8	0.6631 (2)	0.5476 (4)	0.14202 (15)	0.0224 (6)
C3	0.1494 (2)	0.2047 (4)	0.11601 (15)	0.0235 (6)
C2	0.11345 (19)	0.2841 (4)	−0.01977 (14)	0.0188 (5)
C9	0.6684 (2)	0.7859 (4)	0.15861 (17)	0.0294 (6)
H9A	0.6906	0.8093	0.2141	0.044*
H9B	0.5988	0.8489	0.1459	0.044*
H9C	0.7193	0.8517	0.1265	0.044*

C4	0.0641 (2)	0.1466 (5)	0.17123 (16)	0.0287 (6)
H4A	−0.0043	0.2008	0.1494	0.043*
H4B	0.0822	0.2099	0.2228	0.043*
H4C	0.0603	−0.0075	0.1764	0.043*
C10	0.6166 (2)	0.3104 (5)	0.03054 (16)	0.0331 (7)
H10A	0.5943	0.3151	−0.0255	0.050*
H10B	0.5629	0.2378	0.0581	0.050*
H10C	0.6835	0.2337	0.0389	0.050*
C5	0.3385 (2)	0.1707 (5)	0.10905 (16)	0.0301 (6)
H5A	0.4013	0.1081	0.1369	0.045*
H5B	0.3472	0.3245	0.1062	0.045*
H5C	0.3286	0.1123	0.0560	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0335 (10)	0.0138 (9)	0.0294 (10)	0.0033 (8)	0.0036 (8)	0.0033 (8)
O4	0.0245 (9)	0.0237 (10)	0.0241 (9)	0.0044 (8)	0.0018 (7)	0.0062 (8)
O5	0.0292 (10)	0.0268 (11)	0.0304 (10)	−0.0065 (9)	0.0093 (8)	0.0040 (8)
O6	0.0388 (11)	0.0277 (11)	0.0228 (10)	0.0054 (9)	−0.0053 (8)	0.0022 (8)
N1	0.0380 (13)	0.0143 (11)	0.0203 (11)	0.0007 (10)	−0.0046 (9)	−0.0039 (9)
O3	0.0262 (10)	0.0329 (11)	0.0274 (10)	0.0030 (9)	0.0012 (8)	0.0079 (8)
O2	0.0316 (10)	0.0275 (11)	0.0183 (9)	−0.0044 (8)	−0.0003 (7)	−0.0014 (8)
C6	0.0218 (12)	0.0174 (13)	0.0167 (11)	−0.0003 (11)	0.0031 (9)	−0.0007 (10)
N3	0.0191 (10)	0.0229 (12)	0.0217 (11)	0.0021 (9)	0.0056 (8)	0.0043 (9)
N2	0.0316 (12)	0.0116 (11)	0.0244 (11)	0.0003 (9)	−0.0020 (9)	−0.0028 (9)
N4	0.0170 (10)	0.0280 (13)	0.0273 (11)	0.0017 (9)	0.0040 (9)	0.0014 (10)
C1	0.0176 (12)	0.0162 (13)	0.0226 (13)	0.0015 (10)	0.0033 (10)	−0.0016 (10)
C7	0.0225 (12)	0.0165 (13)	0.0200 (12)	−0.0023 (10)	0.0026 (10)	−0.0037 (10)
C8	0.0240 (13)	0.0228 (14)	0.0203 (13)	0.0040 (11)	0.0008 (10)	0.0025 (10)
C3	0.0265 (13)	0.0201 (14)	0.0230 (13)	0.0018 (11)	−0.0032 (10)	0.0010 (10)
C2	0.0163 (11)	0.0173 (13)	0.0229 (12)	−0.0001 (10)	0.0015 (9)	−0.0023 (10)
C9	0.0371 (15)	0.0200 (15)	0.0311 (14)	0.0044 (12)	0.0015 (12)	0.0017 (11)
C4	0.0226 (13)	0.0323 (16)	0.0311 (15)	0.0002 (12)	0.0017 (11)	0.0064 (12)
C10	0.0396 (16)	0.0318 (17)	0.0265 (14)	−0.0011 (14)	−0.0046 (12)	−0.0058 (12)
C5	0.0240 (13)	0.0352 (17)	0.0318 (14)	0.0002 (12)	0.0064 (11)	0.0088 (13)

Geometric parameters (Å, °)

O1—C1	1.217 (3)	N4—C7	1.335 (3)
O4—C6	1.220 (3)	N4—C8	1.461 (3)
O5—C7	1.216 (3)	N4—H4	0.8599
O6—C8	1.398 (3)	C1—C2	1.531 (3)
O6—C10	1.438 (3)	C8—C9	1.502 (4)
N1—C1	1.328 (3)	C3—C4	1.517 (4)
N1—C3	1.459 (3)	C9—H9A	0.960
N1—H1	0.860	C9—H9B	0.960
O3—C3	1.401 (3)	C9—H9C	0.960
O3—C5	1.422 (3)	C4—H4A	0.960

O2—C2	1.216 (3)	C4—H4B	0.960
C6—N3	1.333 (3)	C4—H4C	0.960
C6—C7	1.528 (3)	C10—H10A	0.960
N3—C8	1.452 (3)	C10—H10B	0.960
N3—H3	0.860	C10—H10C	0.960
N2—C2	1.330 (3)	C5—H5A	0.960
N2—C3	1.461 (3)	C5—H5B	0.960
N2—H2	0.8599	C5—H5C	0.960
C8—O6—C10	116.5 (2)	N1—C3—N2	100.73 (19)
C1—N1—C3	113.9 (2)	O3—C3—C4	107.1 (2)
C1—N1—H1	123.0	N1—C3—C4	112.1 (2)
C3—N1—H1	123.1	N2—C3—C4	113.9 (2)
C3—O3—C5	115.3 (2)	O2—C2—N2	129.9 (2)
O4—C6—N3	129.0 (2)	O2—C2—C1	124.5 (2)
O4—C6—C7	125.3 (2)	N2—C2—C1	105.6 (2)
N3—C6—C7	105.7 (2)	C8—C9—H9A	109.5
C6—N3—C8	114.2 (2)	C8—C9—H9B	109.5
C6—N3—H3	122.9	H9A—C9—H9B	109.5
C8—N3—H3	122.9	C8—C9—H9C	109.5
C2—N2—C3	113.9 (2)	H9A—C9—H9C	109.5
C2—N2—H2	123.1	H9B—C9—H9C	109.5
C3—N2—H2	123.1	C3—C4—H4A	109.5
C7—N4—C8	114.1 (2)	C3—C4—H4B	109.5
C7—N4—H4	122.9	H4A—C4—H4B	109.5
C8—N4—H4	122.9	C3—C4—H4C	109.5
O1—C1—N1	130.4 (2)	H4A—C4—H4C	109.5
O1—C1—C2	123.9 (2)	H4B—C4—H4C	109.5
N1—C1—C2	105.7 (2)	O6—C10—H10A	109.5
O5—C7—N4	129.3 (2)	O6—C10—H10B	109.5
O5—C7—C6	125.5 (2)	H10A—C10—H10B	109.5
N4—C7—C6	105.2 (2)	O6—C10—H10C	109.5
O6—C8—N3	112.3 (2)	H10A—C10—H10C	109.5
O6—C8—N4	112.5 (2)	H10B—C10—H10C	109.5
N3—C8—N4	100.5 (2)	O3—C5—H5A	109.5
O6—C8—C9	106.1 (2)	O3—C5—H5B	109.5
N3—C8—C9	113.6 (2)	H5A—C5—H5B	109.5
N4—C8—C9	112.1 (2)	O3—C5—H5C	109.5
O3—C3—N1	111.7 (2)	H5A—C5—H5C	109.5
O3—C3—N2	111.4 (2)	H5B—C5—H5C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O5^{i}	0.86	2.12	2.892 (3)	149
N1—H1···O4^{i}	0.86	2.00	2.817 (3)	159
N3—H3···O2^{ii}	0.86	2.18	2.894 (3)	140
N3—H3···O1^{ii}	0.86	2.64	3.246 (3)	129
N2—H2···O1^{iii}	0.86	2.02	2.878 (3)	175

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*, *y*−1, *z*.

Fig. 1

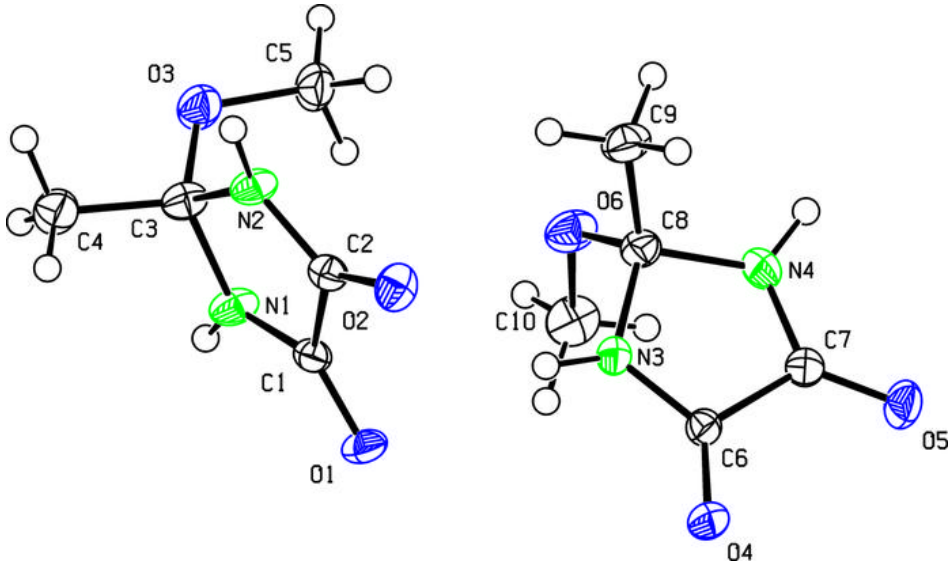

Fig. 2