Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Ethyl-4-methylpiperidine-2,6-dione

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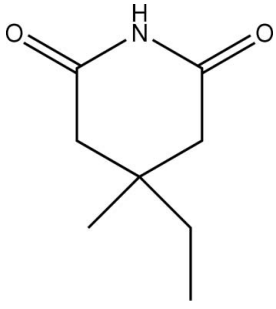
Received 12 November 2007; accepted 13 November 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.157; data-to-parameter ratio = 14.3.

The glutarimide ring of the title compound, $C_8H_{13}NO_2$, adopts an envelope conformation. The C atom opposite the ring N atom is displaced by 0.65 (4) Å from this plane. The axial methyl and the equatorial ethyl groups are in a synclinal arrangement [C—C—C—C torsion angle = −63.3 (3)°]. Two N—H···O hydrogen bonds stabilize a centrosymmetric dimer. These dimers are further connected by weak C—H···O hydrogen bonds.

Related literature

For related structures, see: Feibush *et al.* (1986); Hu *et al.* (2006).



Experimental

Crystal data

$C_8H_{13}NO_2$
M_r = 155.19
Monoclinic, $P2_1/c$
a = 11.128 (2) Å
b = 6.6820 (10) Å
c = 11.311 (2) Å
β = 98.375 (15)°
V = 832.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.54 × 0.50 × 0.24 mm

Data collection

STOE IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.945, T_{max} = 0.979
8827 measured reflections
1528 independent reflections
1130 reflections with $I > 2\sigma(I)$
R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.157
S = 1.04
1528 reflections
107 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.85 (3)	2.09 (3)	2.939 (3)	173 (3)
C3—H3A···O6^{ii}	0.99	2.57	3.272 (3)	128

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

We thank Professor Dr E. Egert for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2486).

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supplementary materials

Acta Cryst. (2007). E**63**, o4743 [**doi:10.1107/S1600536807058436**]

4-Ethyl-4-methylpiperidine-2,6-dione

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Experimental

Single crystals of title compound were obtained by recrystallization of the commercially available 4-ethyl-4-methylpiperidine-2,6-dione from methanol at room temperature.

Refinement

All H atoms were initially located by difference Fourier synthesis. Subsequently the positions of those bonded to C atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.5 U_{eq}(C_{methyl}) and 1.2 U_{eq}($C_{secondary}$)] using a riding model with methyl C—H = 0.98 and secondary C—H = 0.99 Å. The H atom bonded to N was refined isotropically.

Figures

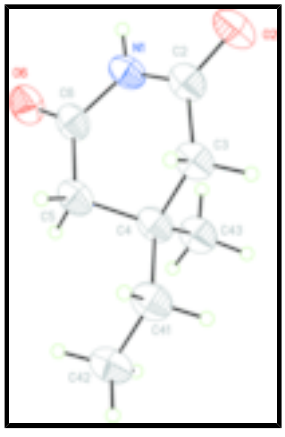

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

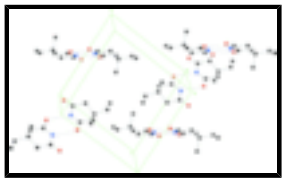

Fig. 2. Partial packing diagram of the title compound. Hydrogen bonds shown as dashed lines.

4-Ethyl-4-methylpiperidine-2,6-dione

Crystal data

$C_8H_{13}NO_2$	F_{000} = 336
M_r = 155.19	D_x = 1.239 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2ybc	Cell parameters from 13160 reflections
a = 11.128 (2) Å	θ = 3.5–25.6º
b = 6.6820 (10) Å	μ = 0.09 mm^{-1}
c = 11.311 (2) Å	T = 173 (2) K
β = 98.375 (15)º	Block, yellow
V = 832.1 (2) $Å^3$	0.54 × 0.50 × 0.24 mm
Z = 4	

Data collection

STOE IPDS II two-circle-diffractometer	1528 independent reflections
Radiation source: fine-focus sealed tube	1130 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.098
T = 173(2) K	θ_{max} = 25.5º
ω scans	θ_{min} = 3.6º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -13 \rightarrow 13$
T_{min} = 0.945, T_{max} = 0.979	$k = -8 \rightarrow 8$
8827 measured reflections	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.0909P)^2 + 0.0725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.157	$(\Delta/\sigma)_{max} < 0.001$
S = 1.04	$\Delta\rho_{max}$ = 0.33 e $Å^{-3}$
1528 reflections	$\Delta\rho_{min}$ = −0.22 e $Å^{-3}$
107 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.060 (11)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2sigma(F^2)$ is used only for calculat-

ing *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}
N1	0.94659 (18)	0.7726 (3)	0.40135 (17)	0.0354 (5)
H1	1.008 (3)	0.811 (4)	0.450 (3)	0.057 (8)*
C2	0.8476 (2)	0.8979 (3)	0.3819 (2)	0.0360 (5)
O2	0.84861 (15)	1.0581 (2)	0.43594 (16)	0.0475 (5)
C3	0.7416 (2)	0.8331 (3)	0.2919 (2)	0.0369 (6)
H3A	0.7490	0.8965	0.2142	0.044*
H3B	0.6659	0.8832	0.3178	0.044*
C4	0.73052 (19)	0.6045 (3)	0.2736 (2)	0.0342 (5)
C41	0.6354 (2)	0.5648 (3)	0.1622 (2)	0.0409 (6)
H41A	0.5561	0.6179	0.1778	0.049*
H41B	0.6592	0.6411	0.0942	0.049*
C42	0.6186 (2)	0.3456 (4)	0.1250 (2)	0.0491 (7)
H42A	0.6952	0.2929	0.1048	0.074*
H42B	0.5555	0.3354	0.0552	0.074*
H42C	0.5944	0.2680	0.1912	0.074*
C43	0.6928 (2)	0.5058 (3)	0.3847 (2)	0.0408 (6)
H43A	0.6933	0.3600	0.3754	0.061*
H43B	0.6110	0.5502	0.3946	0.061*
H43C	0.7501	0.5439	0.4553	0.061*
C5	0.8558 (2)	0.5270 (3)	0.2520 (2)	0.0384 (6)
H5A	0.8537	0.3789	0.2504	0.046*
H5B	0.8711	0.5732	0.1723	0.046*
C6	0.9598 (2)	0.5927 (3)	0.3434 (2)	0.0357 (5)
O6	1.05502 (15)	0.4985 (2)	0.36586 (16)	0.0459 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0459 (11)	0.0320 (10)	0.0272 (11)	−0.0004 (8)	0.0018 (8)	−0.0018 (8)
C2	0.0477 (12)	0.0332 (11)	0.0272 (12)	0.0010 (9)	0.0051 (9)	0.0024 (9)
O2	0.0609 (11)	0.0350 (9)	0.0441 (11)	0.0045 (7)	−0.0001 (8)	−0.0111 (7)
C3	0.0492 (13)	0.0305 (11)	0.0303 (13)	0.0008 (9)	0.0036 (9)	0.0022 (9)
C4	0.0453 (12)	0.0298 (11)	0.0271 (12)	0.0008 (9)	0.0038 (9)	0.0004 (9)
C41	0.0501 (13)	0.0408 (13)	0.0307 (13)	0.0000 (10)	0.0023 (10)	0.0014 (10)
C42	0.0582 (15)	0.0472 (14)	0.0399 (16)	−0.0070 (11)	0.0006 (11)	−0.0084 (11)
C43	0.0523 (14)	0.0369 (12)	0.0338 (13)	−0.0015 (10)	0.0082 (10)	0.0031 (9)
C5	0.0492 (13)	0.0362 (11)	0.0297 (12)	0.0010 (9)	0.0056 (9)	−0.0039 (9)
C6	0.0457 (12)	0.0373 (12)	0.0251 (12)	0.0017 (9)	0.0082 (9)	0.0002 (9)
O6	0.0509 (10)	0.0490 (10)	0.0372 (10)	0.0095 (8)	0.0042 (7)	−0.0047 (8)

Geometric parameters (Å, °)

N1—C2	1.375 (3)	C41—H41A	0.9900
N1—C6	1.388 (3)	C41—H41B	0.9900
N1—H1	0.85 (3)	C42—H42A	0.9800
C2—O2	1.232 (3)	C42—H42B	0.9800
C2—C3	1.505 (3)	C42—H42C	0.9800
C3—C4	1.544 (3)	C43—H43A	0.9800
C3—H3A	0.9900	C43—H43B	0.9800
C3—H3B	0.9900	C43—H43C	0.9800
C4—C43	1.532 (3)	C5—C6	1.501 (3)
C4—C5	1.540 (3)	C5—H5A	0.9900
C4—C41	1.545 (3)	C5—H5B	0.9900
C41—C42	1.528 (3)	C6—O6	1.227 (3)
C2—N1—C6	126.1 (2)	H41A—C41—H41B	107.5
C2—N1—H1	118 (2)	C41—C42—H42A	109.5
C6—N1—H1	116 (2)	C41—C42—H42B	109.5
O2—C2—N1	120.0 (2)	H42A—C42—H42B	109.5
O2—C2—C3	122.36 (19)	C41—C42—H42C	109.5
N1—C2—C3	117.60 (19)	H42A—C42—H42C	109.5
C2—C3—C4	114.54 (18)	H42B—C42—H42C	109.5
C2—C3—H3A	108.6	C4—C43—H43A	109.5
C4—C3—H3A	108.6	C4—C43—H43B	109.5
C2—C3—H3B	108.6	H43A—C43—H43B	109.5
C4—C3—H3B	108.6	C4—C43—H43C	109.5
H3A—C3—H3B	107.6	H43A—C43—H43C	109.5
C43—C4—C5	110.35 (18)	H43B—C43—H43C	109.5
C43—C4—C3	109.99 (19)	C6—C5—C4	114.67 (19)
C5—C4—C3	107.30 (18)	C6—C5—H5A	108.6
C43—C4—C41	111.00 (18)	C4—C5—H5A	108.6
C5—C4—C41	109.97 (18)	C6—C5—H5B	108.6
C3—C4—C41	108.14 (18)	C4—C5—H5B	108.6
C42—C41—C4	115.51 (19)	H5A—C5—H5B	107.6
C42—C41—H41A	108.4	O6—C6—N1	119.6 (2)
C4—C41—H41A	108.4	O6—C6—C5	123.3 (2)
C42—C41—H41B	108.4	N1—C6—C5	117.05 (19)
C4—C41—H41B	108.4		
C6—N1—C2—O2	−177.2 (2)	C3—C4—C41—C42	176.0 (2)
C6—N1—C2—C3	1.7 (3)	C43—C4—C5—C6	−68.7 (2)
O2—C2—C3—C4	−155.4 (2)	C3—C4—C5—C6	51.1 (2)
N1—C2—C3—C4	25.7 (3)	C41—C4—C5—C6	168.52 (19)
C2—C3—C4—C43	70.0 (2)	C2—N1—C6—O6	177.2 (2)
C2—C3—C4—C5	−50.0 (2)	C2—N1—C6—C5	−0.8 (3)
C2—C3—C4—C41	−168.61 (18)	C4—C5—C6—O6	154.5 (2)
C43—C4—C41—C42	−63.3 (3)	C4—C5—C6—N1	−27.7 (3)
C5—C4—C41—C42	59.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.85 (3)	2.09 (3)	2.939 (3)	173 (3)
C3—H3A···O6^{ii}	0.99	2.57	3.272 (3)	128

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

Fig. 1

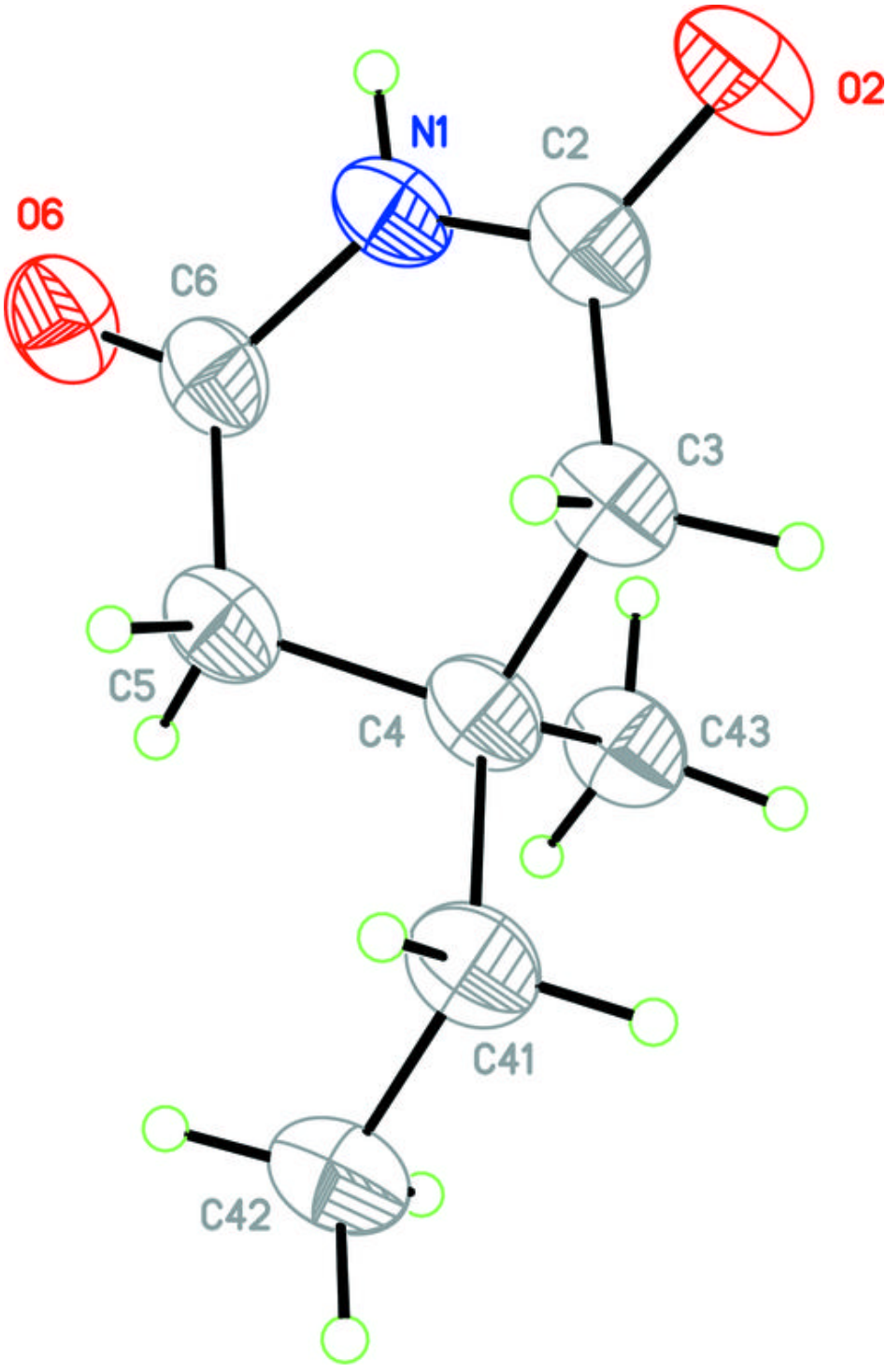
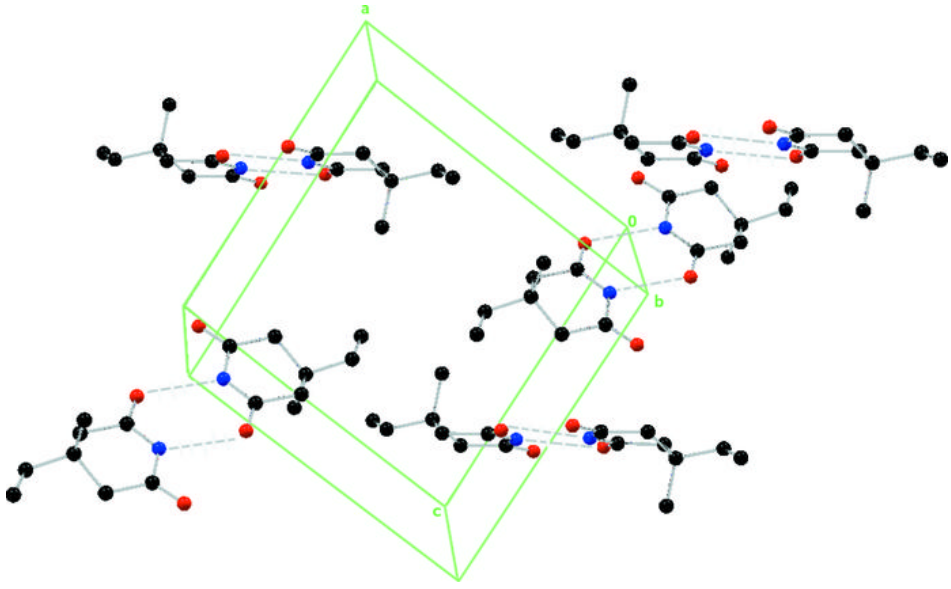
Fig. 2