Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,2-Diisobutyrylhydrazine

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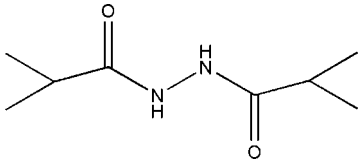
Received 30 August 2007; accepted 11 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.076; wR factor = 0.236; data-to-parameter ratio = 16.0.

The title molecule, $C_8H_{16}N_2O_2$, possesses a crystallographically imposed center of symmetry. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into ribbons extended along the a axis.

Related literature

For the crystal structure of 1,2-dibenzoylhydrazine, see: Shanmuga Sundara Raj *et al.* (2000).



Experimental

Crystal data

$C_8H_{16}N_2O_2$
M_r = 172.23
Monoclinic, $P2_1/n$
a = 4.7758 (8) Å
b = 10.9093 (13) Å
c = 9.9204 (12) Å
β = 91.0240 (10)°
V = 516.78 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.37 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.971, T_{max} = 0.988
2549 measured reflections
914 independent reflections
557 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.236
S = 0.99
914 reflections
57 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.02	2.858 (3)	164

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the support of the National Natural Science Foundation of Liaocheng University (grant No. X051040).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2297).

References

Shanmuga Sundara Raj, S., Yamin, B. M., Boshaala, A. M. A., Tarafder, M. T. H., Crouse, K. A. & Fun, H.-K. (2000). *Acta Cryst.* C**56**, 1011–1012.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

  doi:10.1107/S1600536807044406

supplementary materials

Acta Cryst. (2007). E**63**, o4068 [**doi:10.1107/S1600536807044406**]

1,2-Diisobutyrylhydrazine

K.-Z. Li, Y. Wang, R.-S. Li, D.-Q. Wang and Z.-H. Lu

Comment

In this paper,we present a title compound, 1,2-Diisobutyrylhydrazine,(I), synthesized through the substituted reaction of iso-butyryl chloride with hydrazine hydrate under mild conditions.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in 1,2-dibenzoylhydrazine (Shanmuga Sundara Raj *et al.*, 2000).

In the crystal, the molecules lies on inversion centers. There exist typical intermolecular N—H···O hydrogen bonds (Table 1), which link the molecules into ribbons extended along the *a* axis.

Experimental

A mixture of iso-butyryl chloride (2 mmol) and hydrazine hydrate (1.00 mmol) was well stirred at room temperature for 20 minutes. The crude compound was purified by recrystallization from ethanol. Elemental analysis: calculated for $C_8H_{16}N_2O_2$: C 55.79, H 9.36, N 16.27%; found: C 55.73, H 9.42, N 16.35%.

Refinement

All H atoms were placed in idealized positions (C—H 0.96–0.98 Å, N—H 0.86 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2–1.5 U_{eq}(parent atom).

Figures

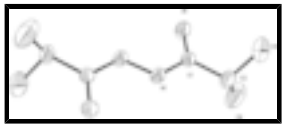


Fig. 1. The molecular structure of (I) with atomic numbering and displacement ellipsoids drawn at the 30% probability level. The unlabelled atoms are related with the labelled ones by symmetry operation (1 − *x*, −*y*, 2 − *z*). Hydrogen atoms are omitted for clarity.

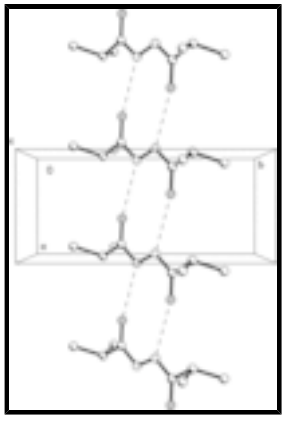


Fig. 2. A portion of the crystal packing of (I) showing the ribbon of hydrogen-bonded (dashed lines) molecules.

1,2-Diisobutyrylhydrazine

Crystal data

$C_8H_{16}N_2O_2$	F_{000} = 188
M_r = 172.23	D_x = 1.107 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 4.7758 (8) Å	Cell parameters from 540 reflections
b = 10.9093 (13) Å	θ = 2.8–22.2º
c = 9.9204 (12) Å	μ = 0.08 mm^{-1}
β = 91.0240 (10)º	T = 298 (2) K
V = 516.78 (12) Å^3	Block, colourless
Z = 2	0.37 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	914 independent reflections
Radiation source: fine-focus sealed tube	557 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.065
T = 298(2) K	θ_{max} = 25.0º
phi and ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −5→5
T_{min} = 0.971, T_{max} = 0.988	k = −12→12
2549 measured reflections	l = −11→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H-atom parameters constrained
$wR(F^2)$ = 0.236	$w = 1/[\sigma^2(F_o^2) + (0.1473P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001
914 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
57 parameters	$\Delta\rho_{min}$ = −0.24 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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.5501 (5)	0.0388 (2)	0.9509 (2)	0.0516 (8)
H1	0.7270	0.0428	0.9368	0.062*
O1	0.1184 (4)	0.10264 (19)	0.8985 (2)	0.0655 (9)
C1	0.3724 (6)	0.1075 (2)	0.8781 (3)	0.0465 (8)
C2	0.4985 (7)	0.1882 (3)	0.7727 (3)	0.0651 (11)
H2	0.7029	0.1858	0.7827	0.078*
C3	0.4004 (12)	0.3177 (4)	0.7895 (5)	0.1089 (17)
H3A	0.2018	0.3217	0.7733	0.163*
H3B	0.4938	0.3696	0.7264	0.163*
H3C	0.4428	0.3449	0.8796	0.163*
C4	0.4179 (13)	0.1435 (5)	0.6365 (4)	0.124 (2)
H4A	0.4935	0.0630	0.6233	0.186*
H4B	0.4904	0.1982	0.5699	0.186*
H4C	0.2174	0.1404	0.6281	0.186*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0353 (13)	0.0611 (17)	0.0587 (16)	0.0001 (11)	0.0101 (10)	0.0209 (12)
O1	0.0347 (12)	0.0771 (16)	0.0851 (18)	0.0045 (10)	0.0088 (10)	0.0328 (13)
C1	0.0349 (15)	0.0500 (16)	0.0547 (17)	0.0014 (12)	0.0048 (12)	0.0114 (14)
C2	0.050 (2)	0.075 (2)	0.071 (2)	0.0024 (16)	0.0088 (16)	0.0320 (19)
C3	0.138 (4)	0.075 (3)	0.115 (3)	−0.003 (3)	0.030 (3)	0.036 (3)
C4	0.172 (5)	0.121 (4)	0.080 (3)	−0.025 (4)	0.038 (3)	0.016 (3)

Geometric parameters (Å, °)

N1—C1	1.335 (3)	C2—H2	0.9800
N1—N1^{i}	1.382 (4)	C3—H3A	0.9600
N1—H1	0.8600	C3—H3B	0.9600
O1—C1	1.235 (3)	C3—H3C	0.9600
C1—C2	1.501 (4)	C4—H4A	0.9600
C2—C4	1.480 (5)	C4—H4B	0.9600
C2—C3	1.499 (5)	C4—H4C	0.9600
C1—N1—N1^{i}	120.0 (3)	C2—C3—H3A	109.5
C1—N1—H1	120.0	C2—C3—H3B	109.5
N1^{i}—N1—H1	120.0	H3A—C3—H3B	109.5

O1—C1—N1	120.3 (3)	C2—C3—H3C	109.5
O1—C1—C2	123.2 (2)	H3A—C3—H3C	109.5
N1—C1—C2	116.6 (3)	H3B—C3—H3C	109.5
C4—C2—C3	109.6 (4)	C2—C4—H4A	109.5
C4—C2—C1	110.0 (3)	C2—C4—H4B	109.5
C3—C2—C1	110.2 (3)	H4A—C4—H4B	109.5
C4—C2—H2	109.0	C2—C4—H4C	109.5
C3—C2—H2	109.0	H4A—C4—H4C	109.5
C1—C2—H2	109.0	H4B—C4—H4C	109.5

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{ii}	0.86	2.02	2.858 (3)	164

Symmetry codes: (ii) *x*+1, *y*, *z*.

Fig. 1

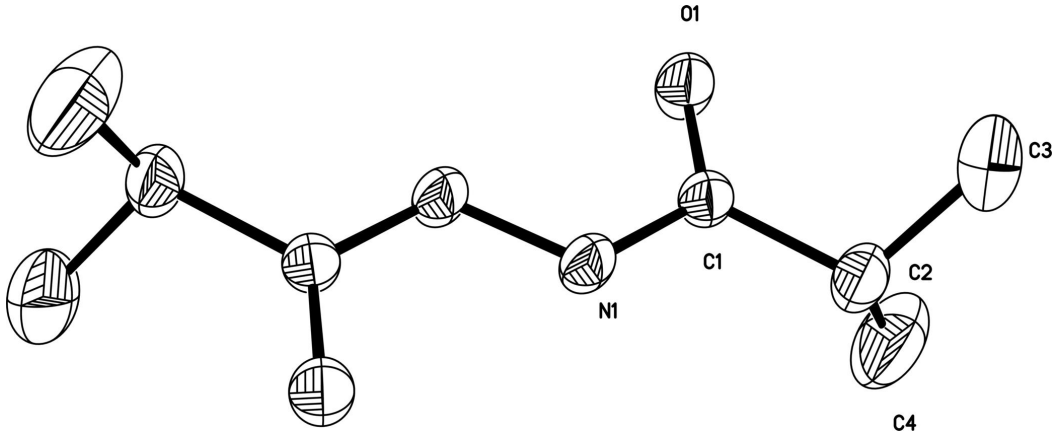


Fig. 2