Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Diamino-6-methyl-1,3,5-triazine ethanol solvate

Zun-Hong Xiao

School of Physics and Chemistry Science, Guizhou Normal University, Guiyang, 550001, People's Republic of China.
Correspondence e-mail: xzh729@126.com

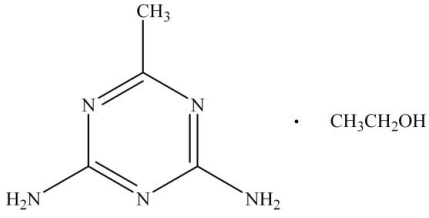
Received 23 December 2007; accepted 2 January 2008

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 14.0.

The crystal structure of the title compound, $C_4H_7N_5\cdot C_2H_6O$, is determined by extensive hydrogen bonding. A sequence of dimeric associations, formed by N—H(amino)···N(ring), connects the triazine rings into a molecular tape. Molecules are linked into a supramolecular structure by N—H···O and O—H···O hydrogen bonds. The asymmetric unit consists of two formula units.

Related literature

For general background, see: Sebenik *et al.* (1989); Tashiro & Oiwa (1981).



Experimental

Crystal data

$C_4H_7N_5\cdot C_2H_6O$
M_r = 171.21
Triclinic, $P\overline{1}$
a = 8.3860 (6) Å
b = 9.1514 (6) Å
c = 11.9104 (9) Å
α = 88.703 (1)°
β = 87.614 (2)°
γ = 76.668 (2)°
V = 888.56 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.34 × 0.26 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.985
7627 measured reflections
3111 independent reflections
2619 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
S = 1.07
3111 reflections
223 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4B···N7^{i}	0.86	2.11	2.9666 (18)	171
N5—H5D···N8^{ii}	0.86	2.19	3.0132 (19)	159
N5—H5E···O2^{iii}	0.86	2.29	3.0071 (19)	142
N10—H10A···O2^{iv}	0.86	2.10	2.9337 (18)	163
O2—H2···O1^{v}	0.82	1.90	2.7185 (18)	174

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $x, y, z+1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Nomarch Education Foundation of Guizhou, China (No. 2004–07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2061).

References

Bruker (2002). *SMART* and *SAINT*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Bruker (2005). *SADABS*. Version 1.22. Bruker AXS, Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sebenik, A., Osredkar, U. & Zigon, M. (1989). *Polym. Bull.* **22**, 155–161.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tashiro, T. & Oiwa, M. (1981). *J. Polym. Sci. Polym. Chem.* **19**, 645–654.

supporting information

Acta Cryst. (2008). E**64**, o411 [doi:10.1107/S1600536808000159]

2,4-Diamino-6-methyl-1,3,5-triazine ethanol solvate

Zun-Hong Xiao

S1. Comment

Triazine compounds are used in pharmaceutical industry as coupling agents for the synthesis of peptides and as side chain of antibiotics, as well as in formulating bactericides and fungicides. 2,4-Diamino-6-methyl-1,3,5-triazine (acetoguanamine) is used as an intermediate for pharmaceuticals and as a modifier and flexibilizer of formaldehyde resins (Sebenik *et al.*, 1989, Tashiro *et al.*, 1981).

The crystal structure of the title compound (Fig. 1) consists of triazine and solvate ethanol molecule. The amino groups are coplanar with the ring plane, the dihedral angle between the triazine ring (C2,N2,C4,N1,C3,N3) and the ring (C8,N7,C9,N8,C10,N6) is 12.73 (7)°. A lot of hydrogen bonds are observed (Table 1), each NH_2 group acts as a donor in hydrogen bond with the ring nitrogen atoms of neighboring molecules, these contacts and the cross-linking interactions stabilize the crystal packing.

S2. Experimental

2,4-diamino-6-methyl-1,3,5-triazine (0.625 g, 0.05 mol) was added to a stirred solvent of ethanol (100 ml) at 50°C for 3 h. After cooling to room temperature, the mixture was filtered. The filtrate was set aside for one week to obtain colorless crystals.

S3. Refinement

Water H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to O atoms with U_{iso}(H) = 1.2U_{eq}(O). All other H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å, N—H = 0.86 Å, and U_{iso}(H) = 1.2–1.5 U_{eq}(C,*N*).

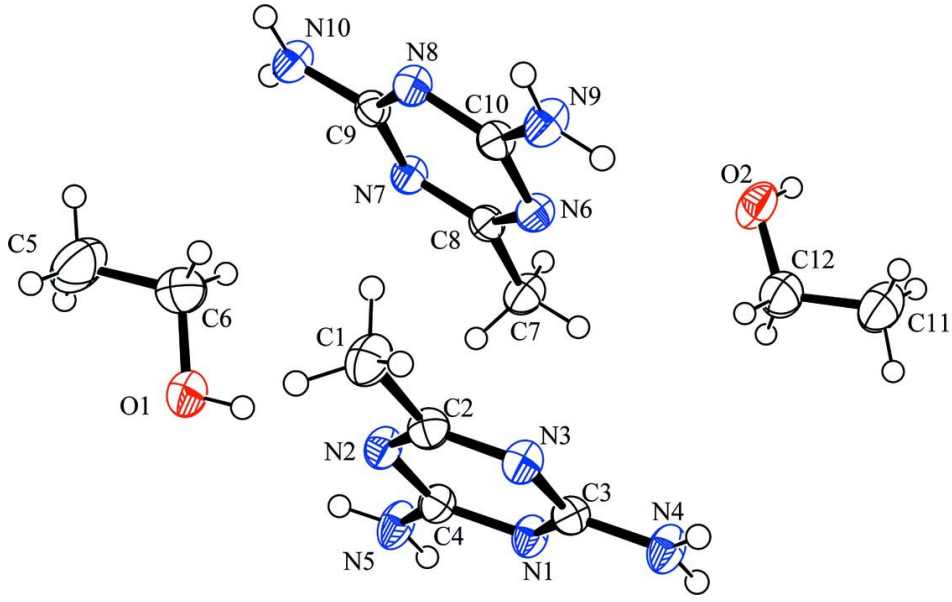


Figure 1

The molecular structure of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

2,4-Diamino-6-methyl-1,3,5-triazine ethanol solvate

Crystal data

$C_4H_7N_5·C_2H_6O$
M_r = 171.21
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.3860 (6) Å
b = 9.1514 (6) Å
c = 11.9104 (9) Å
α = 88.703 (1)°
β = 87.614 (2)°
γ = 76.668 (2)°
V = 888.56 (11) Å^3

Z = 4
F(000) = 368.0
D_x = 1.280 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3111 reflections
θ = 1.7–25.0°
μ = 0.09 mm^{-1}
T = 273 K
Block, colorless
0.34 × 0.26 × 0.21 mm

Data collection

Bruker CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.985

7627 measured reflections
3111 independent reflections
2619 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −9→9
k = −10→10
l = −12→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118

S = 1.07
3111 reflections
223 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
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.2811P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0454 (2)	0.41963 (19)	0.15635 (15)	0.0388 (4)
H1A	−0.0653	0.4778	0.1527	0.058*
H1B	0.0892	0.3946	0.0817	0.058*
H1C	0.1110	0.4770	0.1920	0.058*
C2	0.04756 (19)	0.27874 (17)	0.22268 (13)	0.0290 (4)
C3	−0.07229 (18)	0.14537 (17)	0.34835 (13)	0.0258 (3)
C4	0.18337 (18)	0.04532 (17)	0.27722 (13)	0.0268 (3)
C5	0.6644 (3)	0.2978 (3)	0.0124 (2)	0.0651 (6)
H5A	0.7394	0.2012	0.0089	0.098*
H5B	0.7212	0.3716	0.0348	0.098*
H5C	0.6200	0.3244	−0.0602	0.098*
C6	0.5286 (2)	0.2917 (2)	0.09584 (17)	0.0486 (5)
H6A	0.5730	0.2628	0.1691	0.058*
H6B	0.4548	0.3900	0.1019	0.058*
C7	0.3737 (2)	0.18852 (18)	0.49621 (15)	0.0342 (4)
H7A	0.4172	0.1132	0.4412	0.051*
H7B	0.2683	0.1765	0.5241	0.051*
H7C	0.4469	0.1780	0.5572	0.051*
C8	0.35597 (18)	0.34072 (16)	0.44340 (12)	0.0254 (3)
C9	0.47170 (18)	0.50943 (16)	0.34763 (12)	0.0244 (3)
C10	0.20147 (18)	0.56977 (16)	0.39979 (12)	0.0255 (3)
N1	0.05944 (15)	0.02890 (14)	0.34824 (11)	0.0279 (3)
N2	0.18531 (16)	0.17023 (15)	0.21443 (11)	0.0299 (3)
N3	−0.08554 (15)	0.27267 (14)	0.28518 (11)	0.0284 (3)
N4	−0.20112 (16)	0.13534 (15)	0.41484 (11)	0.0323 (3)
H4A	−0.1984	0.0563	0.4559	0.039*
H4B	−0.2871	0.2079	0.4167	0.039*
N6	0.20797 (15)	0.43256 (14)	0.44771 (11)	0.0273 (3)
N7	0.49186 (15)	0.37128 (13)	0.39648 (10)	0.0268 (3)

N8	0.32886 (15)	0.61343 (14)	0.34805 (11)	0.0274 (3)
N9	0.05530 (15)	0.66659 (15)	0.40412 (12)	0.0336 (3)
H9A	0.0442	0.7546	0.3742	0.040*
H9B	−0.0276	0.6409	0.4368	0.040*
N10	0.60412 (15)	0.54140 (15)	0.29698 (11)	0.0309 (3)
H10A	0.5979	0.6276	0.2650	0.037*
H10B	0.6959	0.4759	0.2962	0.037*
O1	0.44204 (16)	0.18580 (16)	0.06094 (10)	0.0475 (4)
H1	0.3607	0.1897	0.1024	0.071*
C11	0.0989 (3)	0.1326 (3)	0.89654 (19)	0.0599 (6)
H11A	0.1324	0.1124	0.9725	0.090*
H11B	0.0321	0.0655	0.8769	0.090*
H11C	0.0370	0.2344	0.8900	0.090*
C12	0.2460 (2)	0.1100 (2)	0.81971 (17)	0.0495 (5)
H12A	0.3036	0.0053	0.8237	0.059*
H12B	0.2103	0.1310	0.7434	0.059*
N5	0.31467 (16)	−0.06868 (15)	0.26948 (12)	0.0353 (3)
H5D	0.3180	−0.1490	0.3091	0.042*
H5E	0.3961	−0.0619	0.2249	0.042*
O2	0.35702 (16)	0.19983 (16)	0.84251 (11)	0.0461 (3)
H2	0.3769	0.1931	0.9095	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0392 (10)	0.0326 (9)	0.0423 (10)	−0.0051 (7)	0.0017 (8)	0.0095 (8)
C2	0.0299 (8)	0.0272 (8)	0.0294 (8)	−0.0059 (7)	−0.0023 (6)	0.0018 (6)
C3	0.0241 (8)	0.0242 (8)	0.0282 (8)	−0.0041 (6)	−0.0011 (6)	−0.0001 (6)
C4	0.0250 (8)	0.0267 (8)	0.0281 (8)	−0.0051 (6)	−0.0004 (6)	0.0010 (6)
C5	0.0531 (13)	0.0762 (16)	0.0747 (16)	−0.0344 (12)	0.0045 (11)	0.0046 (12)
C6	0.0485 (11)	0.0488 (11)	0.0516 (12)	−0.0174 (9)	0.0003 (9)	−0.0063 (9)
C7	0.0298 (9)	0.0250 (8)	0.0454 (10)	−0.0028 (7)	0.0032 (7)	0.0040 (7)
C8	0.0248 (8)	0.0233 (8)	0.0269 (8)	−0.0032 (6)	0.0004 (6)	−0.0019 (6)
C9	0.0251 (8)	0.0230 (7)	0.0242 (8)	−0.0037 (6)	0.0001 (6)	−0.0011 (6)
C10	0.0237 (8)	0.0244 (8)	0.0270 (8)	−0.0028 (6)	−0.0012 (6)	−0.0002 (6)
N1	0.0247 (7)	0.0251 (7)	0.0313 (7)	−0.0019 (5)	0.0038 (5)	0.0036 (5)
N2	0.0293 (7)	0.0285 (7)	0.0311 (7)	−0.0062 (6)	0.0035 (5)	0.0031 (6)
N3	0.0257 (7)	0.0258 (7)	0.0321 (7)	−0.0030 (5)	0.0003 (5)	0.0039 (5)
N4	0.0258 (7)	0.0250 (7)	0.0419 (8)	0.0007 (5)	0.0089 (6)	0.0058 (6)
N6	0.0237 (7)	0.0234 (7)	0.0334 (7)	−0.0032 (5)	0.0008 (5)	0.0007 (5)
N7	0.0241 (7)	0.0228 (7)	0.0312 (7)	−0.0013 (5)	0.0016 (5)	0.0015 (5)
N8	0.0251 (7)	0.0239 (7)	0.0309 (7)	−0.0016 (5)	0.0009 (5)	0.0026 (5)
N9	0.0223 (7)	0.0269 (7)	0.0478 (9)	0.0005 (5)	0.0038 (6)	0.0078 (6)
N10	0.0237 (7)	0.0253 (7)	0.0411 (8)	−0.0017 (5)	0.0039 (6)	0.0054 (6)
O1	0.0477 (8)	0.0614 (9)	0.0398 (7)	−0.0274 (7)	0.0112 (6)	−0.0083 (6)
C11	0.0513 (12)	0.0746 (15)	0.0606 (14)	−0.0303 (11)	0.0095 (10)	−0.0034 (11)
C12	0.0453 (11)	0.0601 (13)	0.0463 (11)	−0.0190 (10)	0.0023 (9)	−0.0044 (9)
N5	0.0260 (7)	0.0298 (7)	0.0455 (8)	0.0005 (6)	0.0105 (6)	0.0072 (6)

O2	0.0461 (8)	0.0581 (8)	0.0391 (7)	−0.0241 (6)	0.0010 (6)	0.0112 (6)

Geometric parameters (Å, º)

C1—C2	1.494 (2)	C8—N7	1.3327 (19)
C1—H1A	0.9600	C9—N10	1.3300 (19)
C1—H1B	0.9600	C9—N8	1.3471 (19)
C1—H1C	0.9600	C9—N7	1.3571 (19)
C2—N3	1.327 (2)	C10—N9	1.3364 (19)
C2—N2	1.340 (2)	C10—N8	1.3459 (19)
C3—N4	1.332 (2)	C10—N6	1.3580 (19)
C3—N1	1.3466 (19)	N4—H4A	0.8600
C3—N3	1.3576 (19)	N4—H4B	0.8600
C4—N5	1.332 (2)	N9—H9A	0.8600
C4—N1	1.346 (2)	N9—H9B	0.8600
C4—N2	1.355 (2)	N10—H10A	0.8600
C5—C6	1.490 (3)	N10—H10B	0.8600
C5—H5A	0.9600	O1—H1	0.8200
C5—H5B	0.9600	C11—C12	1.482 (3)
C5—H5C	0.9600	C11—H11A	0.9600
C6—O1	1.417 (2)	C11—H11B	0.9600
C6—H6A	0.9700	C11—H11C	0.9600
C6—H6B	0.9700	C12—O2	1.415 (2)
C7—C8	1.494 (2)	C12—H12A	0.9700
C7—H7A	0.9600	C12—H12B	0.9700
C7—H7B	0.9600	N5—H5D	0.8600
C7—H7C	0.9600	N5—H5E	0.8600
C8—N6	1.3285 (19)	O2—H2	0.8200
C2—C1—H1A	109.5	N10—C9—N7	116.38 (13)
C2—C1—H1B	109.5	N8—C9—N7	124.41 (13)
H1A—C1—H1B	109.5	N9—C10—N8	118.57 (13)
C2—C1—H1C	109.5	N9—C10—N6	116.26 (13)
H1A—C1—H1C	109.5	N8—C10—N6	125.17 (13)
H1B—C1—H1C	109.5	C4—N1—C3	114.56 (13)
N3—C2—N2	125.90 (14)	C2—N2—C4	114.89 (13)
N3—C2—C1	117.42 (14)	C2—N3—C3	114.50 (13)
N2—C2—C1	116.68 (14)	C3—N4—H4A	120.0
N4—C3—N1	117.82 (13)	C3—N4—H4B	120.0
N4—C3—N3	116.89 (13)	H4A—N4—H4B	120.0
N1—C3—N3	125.28 (13)	C8—N6—C10	114.35 (12)
N5—C4—N1	117.59 (14)	C8—N7—C9	114.99 (12)
N5—C4—N2	117.68 (13)	C10—N8—C9	114.81 (12)
N1—C4—N2	124.72 (14)	C10—N9—H9A	120.0
C6—C5—H5A	109.5	C10—N9—H9B	120.0
C6—C5—H5B	109.5	H9A—N9—H9B	120.0
H5A—C5—H5B	109.5	C9—N10—H10A	120.0
C6—C5—H5C	109.5	C9—N10—H10B	120.0

H5A—C5—H5C	109.5	H10A—N10—H10B	120.0
H5B—C5—H5C	109.5	C6—O1—H1	109.5
O1—C6—C5	109.36 (17)	C12—C11—H11A	109.5
O1—C6—H6A	109.8	C12—C11—H11B	109.5
C5—C6—H6A	109.8	H11A—C11—H11B	109.5
O1—C6—H6B	109.8	C12—C11—H11C	109.5
C5—C6—H6B	109.8	H11A—C11—H11C	109.5
H6A—C6—H6B	108.3	H11B—C11—H11C	109.5
C8—C7—H7A	109.5	O2—C12—C11	114.80 (17)
C8—C7—H7B	109.5	O2—C12—H12A	108.6
H7A—C7—H7B	109.5	C11—C12—H12A	108.6
C8—C7—H7C	109.5	O2—C12—H12B	108.6
H7A—C7—H7C	109.5	C11—C12—H12B	108.6
H7B—C7—H7C	109.5	H12A—C12—H12B	107.5
N6—C8—N7	126.22 (13)	C4—N5—H5D	120.0
N6—C8—C7	117.53 (13)	C4—N5—H5E	120.0
N7—C8—C7	116.25 (13)	H5D—N5—H5E	120.0
N10—C9—N8	119.21 (13)	C12—O2—H2	109.5

N5—C4—N1—C3	−177.19 (14)	N7—C8—N6—C10	−0.8 (2)
N2—C4—N1—C3	3.9 (2)	C7—C8—N6—C10	178.93 (13)
N4—C3—N1—C4	178.53 (14)	N9—C10—N6—C8	−178.84 (13)
N3—C3—N1—C4	−0.9 (2)	N8—C10—N6—C8	2.1 (2)
N3—C2—N2—C4	−0.2 (2)	N6—C8—N7—C9	−1.2 (2)
C1—C2—N2—C4	178.97 (14)	C7—C8—N7—C9	179.03 (13)
N5—C4—N2—C2	177.66 (14)	N10—C9—N7—C8	−177.94 (13)
N1—C4—N2—C2	−3.4 (2)	N8—C9—N7—C8	2.4 (2)
N2—C2—N3—C3	2.9 (2)	N9—C10—N8—C9	179.85 (13)
C1—C2—N3—C3	−176.34 (14)	N6—C10—N8—C9	−1.1 (2)
N4—C3—N3—C2	178.33 (14)	N10—C9—N8—C10	179.00 (13)
N1—C3—N3—C2	−2.3 (2)	N7—C9—N8—C10	−1.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*B*···N7^{i}	0.86	2.11	2.9666 (18)	171
N5—H5*D*···N8^{ii}	0.86	2.19	3.0132 (19)	159
N5—H5*E*···O2^{iii}	0.86	2.29	3.0071 (19)	142
N10—H10*A*···O2^{iv}	0.86	2.10	2.9337 (18)	163
O2—H2···O1^{v}	0.82	1.90	2.7185 (18)	174

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