Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Butylamino-6-chloro-4-(2,4,4-trimethylpentan-2-ylamino)-1,3,5-triazine

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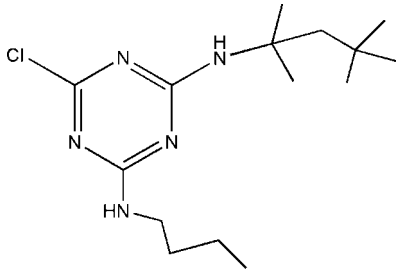
Received 22 June 2007; accepted 28 June 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.161; data-to-parameter ratio = 16.1.

The crystal structure of the title compound, $C_{15}H_{28}ClN_5$, is stabilized by intermolecular N—H···N hydrogen bonds, forming zigzag chains running along the c axis.

Related literature

For general background, see: Borzatta & Carrozza (1991). For related structures, see: Deng *et al.* (2006). For related literature, see: Kaiser & Thurston (1951).



Experimental

Crystal data

$C_{15}H_{28}ClN_5$
M_r = 313.87
Monoclinic, $C2/c$
a = 19.411 (4) Å
b = 8.2182 (17) Å
c = 23.245 (5) Å
β = 101.091 (4)°
V = 3638.9 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.963
8608 measured reflections
3213 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.161
S = 1.04
3213 reflections
200 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N1^{i}	0.77 (3)	2.31 (3)	3.079 (3)	171 (3)
N5—H5···N2^{ii}	0.83 (3)	2.34 (3)	3.151 (3)	167 (3)

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

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2407).

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 doi:10.1107/S1600536807031637

supplementary materials

Acta Cryst. (2007). E**63**, o3367 [**doi:10.1107/S1600536807031637**]

2-Butylamino-6-chloro-4-(2,4,4-trimethylpentan-2-ylamino)-1,3,5-triazine

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Comment

The title compound is an intermediate in the synthesis of hindered light stabilizers (Borzatta & Carrozza, 1991). This kind of compounds is widely used (Deng *et al.*, 2006).

The triazine ring is essentially planar. The r.m.s. deviation from the mean plane is 0.014 (3) Å.

Intermolecular N—H···N hydrogen bonds link the molecules into zigzag-like chains running along the *c* axis.

Experimental

The title compound was prepared according to the method of Kaiser & Thurston (1951). 2,4,6-Trichloro-1,3,5-triazine (40.0 g, 0.217 mol) was dissolved in toluene (120 ml) and then cooled to 278 K. With stirring, a solution of 2,4,4-trimethylpentan-2-amine (27.5 g, 0.213 mol) in toluene (50 ml) was then added dropwise to the mixture over a period of 0.5 h. A solution of Na_2CO_3 (23.02 g, 0.217 mol) in water (50 ml) was then added dropwise for 0.5 h. The mixture was stirred at 273–278 K for a further 3 h, 1-butylamine(15.5 g, 0.213 mol) and solid Na_2CO_3 (23.02 g, 0.217 mol) were added to the mixture, maintaining the temperature at 338 k for 5 h. The organic layer was washed with water and then concentrated *in vacuo*. The title compound (57.8 g) was obtained as a powder form in a yield of 86.5%. Crystals were obtained by slow evaporation of a solution of methanol.

Refinement

The coordinates of the H atoms bonded to N were refined with $U_{iso}(H) = 1.2U_{eq}(N)$. All H atoms bonded to C were positioned geometrically (C—H = 0.96–0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5_{eq}(C_{methyl})$.

Figures

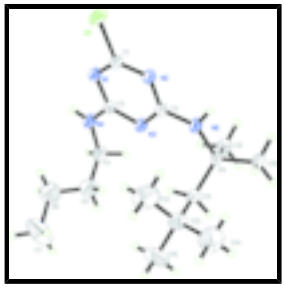

Fig. 1. A view of the molecule (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

2-Butylamino-6-chloro-4-(2,4,4-trimethylpentan-2-ylamino)-1,3,5-triazine

Crystal data

$C_{15}H_{28}ClN_5$	$D_x = 1.146$ Mg m^{-3}
$M_r = 313.87$	Melting point: 156-158 K
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 19.411$ (4) Å	Cell parameters from 2586 reflections
$b = 8.2182$ (17) Å	$\theta = 2.5$–23.1º
$c = 23.245$ (5) Å	$\mu = 0.21$ mm^{-1}
$\beta = 101.091$ (4)º	$T = 294$ (2) K
$V = 3638.9$ (13) Å^3	Block, colourless
$Z = 8$	0.22 × 0.20 × 0.18 mm
$F_{000} = 1360$	

Data collection

Bruker SMART CCD area-detector diffractometer	3213 independent reflections
Radiation source: fine-focus sealed tube	2283 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 294$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -22 \rightarrow 22$
$T_{min} = 0.955$, $T_{max} = 0.963$	$k = -9 \rightarrow 9$
8608 measured reflections	$l = -27 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.161$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 3.6231P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
3213 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
200 parameters	$\Delta\rho_{min} = -0.29$ 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}
Cl1	1.11711 (4)	−0.02496 (10)	0.15825 (3)	0.0586 (3)
N1	1.00664 (10)	0.0414 (3)	0.08007 (9)	0.0376 (5)
N2	1.00846 (10)	0.1316 (3)	0.17761 (8)	0.0375 (5)
N3	0.90867 (10)	0.1911 (3)	0.10248 (8)	0.0367 (5)
N4	0.91215 (12)	0.1087 (3)	0.00839 (9)	0.0441 (6)
H4	0.9338 (16)	0.063 (4)	−0.0112 (14)	0.053*
N5	0.91392 (11)	0.2638 (3)	0.19970 (9)	0.0406 (6)
H5	0.9351 (15)	0.245 (4)	0.2334 (13)	0.049*
C1	1.03346 (12)	0.0595 (3)	0.13587 (11)	0.0358 (6)
C2	0.94263 (12)	0.1942 (3)	0.15820 (10)	0.0338 (6)
C3	0.94272 (12)	0.1153 (3)	0.06501 (10)	0.0344 (6)
C8	0.84288 (13)	0.3361 (3)	0.19418 (11)	0.0420 (7)
C9	0.78787 (14)	0.2044 (4)	0.17388 (15)	0.0580 (8)
H9A	0.7902	0.1716	0.1347	0.087*
H9B	0.7420	0.2466	0.1746	0.087*
H9C	0.7969	0.1122	0.1996	0.087*
C10	0.83748 (17)	0.3866 (4)	0.25678 (13)	0.0659 (9)
H10A	0.8719	0.4688	0.2704	0.099*
H10B	0.8458	0.2936	0.2822	0.099*
H10C	0.7914	0.4290	0.2569	0.099*
C11	0.82914 (15)	0.4783 (3)	0.15022 (13)	0.0478 (7)
H11A	0.7811	0.5125	0.1494	0.057*
H11B	0.8299	0.4316	0.1120	0.057*
C12	0.87304 (19)	0.6361 (4)	0.15384 (16)	0.0684 (10)
C13	0.9485 (2)	0.6015 (5)	0.1488 (3)	0.124 (2)
H13A	0.9491	0.5404	0.1138	0.185*
H13B	0.9710	0.5399	0.1823	0.185*
H13C	0.9730	0.7024	0.1473	0.185*
C14	0.8716 (3)	0.7385 (5)	0.2077 (2)	0.131 (2)
H14A	0.8970	0.6839	0.2418	0.196*
H14B	0.8238	0.7545	0.2120	0.196*
H14C	0.8929	0.8421	0.2036	0.196*
C15	0.8392 (3)	0.7383 (5)	0.1007 (2)	0.1218 (18)

H15A	0.8644	0.8388	0.1007	0.183*
H15B	0.7912	0.7607	0.1029	0.183*
H15C	0.8409	0.6793	0.0654	0.183*
C4	0.84612 (15)	0.1883 (4)	−0.01574 (12)	0.0559 (8)
H4A	0.8134	0.1688	0.0102	0.067*
H4B	0.8267	0.1389	−0.0533	0.067*
C5	0.8518 (2)	0.3659 (5)	−0.02418 (16)	0.0793 (11)
H5A	0.8051	0.4089	−0.0384	0.095*
H5B	0.8694	0.4154	0.0137	0.095*
C6	0.8958 (2)	0.4149 (5)	−0.0636 (2)	0.0987 (14)
H6A	0.8782	0.3671	−0.1017	0.118*
H6B	0.9427	0.3730	−0.0496	0.118*
C7	0.8997 (3)	0.6042 (6)	−0.0704 (2)	0.149 (2)
H7A	0.9226	0.6297	−0.1023	0.223*
H7B	0.9258	0.6503	−0.0348	0.223*
H7C	0.8531	0.6485	−0.0781	0.223*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0456 (4)	0.0801 (6)	0.0485 (4)	0.0282 (4)	0.0048 (3)	−0.0040 (4)
N1	0.0381 (12)	0.0436 (13)	0.0323 (11)	0.0069 (9)	0.0096 (9)	−0.0024 (10)
N2	0.0337 (11)	0.0484 (13)	0.0314 (11)	0.0066 (9)	0.0089 (9)	−0.0011 (10)
N3	0.0357 (11)	0.0443 (12)	0.0312 (11)	0.0055 (9)	0.0089 (9)	−0.0029 (10)
N4	0.0415 (13)	0.0603 (16)	0.0312 (12)	0.0123 (11)	0.0087 (9)	−0.0062 (11)
N5	0.0383 (12)	0.0559 (14)	0.0287 (11)	0.0112 (10)	0.0092 (9)	−0.0030 (11)
C1	0.0332 (13)	0.0395 (14)	0.0359 (14)	0.0056 (11)	0.0097 (11)	0.0013 (11)
C2	0.0349 (13)	0.0365 (14)	0.0314 (13)	0.0008 (10)	0.0103 (10)	−0.0003 (11)
C3	0.0372 (13)	0.0365 (14)	0.0307 (13)	0.0010 (11)	0.0098 (10)	0.0005 (11)
C8	0.0371 (14)	0.0516 (17)	0.0409 (15)	0.0100 (12)	0.0163 (11)	−0.0002 (13)
C9	0.0413 (16)	0.0580 (19)	0.079 (2)	0.0018 (14)	0.0215 (15)	0.0076 (17)
C10	0.072 (2)	0.081 (2)	0.0524 (18)	0.0291 (18)	0.0321 (16)	0.0016 (17)
C11	0.0474 (16)	0.0467 (16)	0.0521 (17)	0.0094 (13)	0.0168 (13)	0.0014 (14)
C12	0.083 (2)	0.0458 (18)	0.084 (2)	0.0018 (17)	0.036 (2)	−0.0050 (18)
C13	0.090 (3)	0.069 (3)	0.229 (6)	−0.028 (2)	0.073 (4)	−0.005 (3)
C14	0.216 (6)	0.061 (3)	0.131 (4)	−0.027 (3)	0.071 (4)	−0.039 (3)
C15	0.180 (5)	0.061 (3)	0.132 (4)	−0.001 (3)	0.048 (4)	0.034 (3)
C4	0.0498 (17)	0.079 (2)	0.0374 (15)	0.0144 (16)	0.0053 (13)	−0.0014 (15)
C5	0.083 (3)	0.090 (3)	0.062 (2)	0.020 (2)	0.0057 (19)	0.010 (2)
C6	0.091 (3)	0.095 (3)	0.112 (3)	−0.015 (3)	0.024 (3)	−0.002 (3)
C7	0.202 (7)	0.114 (4)	0.128 (5)	−0.052 (4)	0.028 (4)	0.032 (4)

Geometric parameters (Å, °)

Cl1—C1	1.750 (2)	C12—C14	1.514 (5)
N1—C1	1.310 (3)	C12—C13	1.518 (5)
N1—C3	1.365 (3)	C12—C15	1.532 (5)
N2—C1	1.307 (3)	C13—H13A	0.9600
N2—C2	1.371 (3)	C13—H13B	0.9600

N3—C2	1.336 (3)	C13—H13C	0.9600
N3—C3	1.344 (3)	C14—H14A	0.9600
N4—C3	1.337 (3)	C14—H14B	0.9600
N4—C4	1.452 (3)	C14—H14C	0.9600
N4—H4	0.77 (3)	C15—H15A	0.9600
N5—C2	1.333 (3)	C15—H15B	0.9600
N5—C8	1.484 (3)	C15—H15C	0.9600
N5—H5	0.83 (3)	C4—C5	1.480 (5)
C8—C9	1.530 (4)	C4—H4A	0.9700
C8—C10	1.536 (4)	C4—H4B	0.9700
C8—C11	1.541 (4)	C5—C6	1.425 (5)
C9—H9A	0.9600	C5—H5A	0.9700
C9—H9B	0.9600	C5—H5B	0.9700
C9—H9C	0.9600	C6—C7	1.567 (6)
C10—H10A	0.9600	C6—H6A	0.9700
C10—H10B	0.9600	C6—H6B	0.9700
C10—H10C	0.9600	C7—H7A	0.9600
C11—C12	1.545 (4)	C7—H7B	0.9600
C11—H11A	0.9700	C7—H7C	0.9600
C11—H11B	0.9700		
C1—N1—C3	111.8 (2)	C14—C12—C11	114.4 (3)
C1—N2—C2	112.4 (2)	C13—C12—C11	111.6 (3)
C2—N3—C3	115.1 (2)	C15—C12—C11	105.6 (3)
C3—N4—C4	123.6 (2)	C12—C13—H13A	109.5
C3—N4—H4	114 (2)	C12—C13—H13B	109.5
C4—N4—H4	122 (2)	H13A—C13—H13B	109.5
C2—N5—C8	128.3 (2)	C12—C13—H13C	109.5
C2—N5—H5	114 (2)	H13A—C13—H13C	109.5
C8—N5—H5	116 (2)	H13B—C13—H13C	109.5
N2—C1—N1	130.8 (2)	C12—C14—H14A	109.5
N2—C1—Cl1	114.49 (18)	C12—C14—H14B	109.5
N1—C1—Cl1	114.74 (18)	H14A—C14—H14B	109.5
N5—C2—N3	120.8 (2)	C12—C14—H14C	109.5
N5—C2—N2	114.6 (2)	H14A—C14—H14C	109.5
N3—C2—N2	124.6 (2)	H14B—C14—H14C	109.5
N4—C3—N3	118.5 (2)	C12—C15—H15A	109.5
N4—C3—N1	116.3 (2)	C12—C15—H15B	109.5
N3—C3—N1	125.2 (2)	H15A—C15—H15B	109.5
N5—C8—C9	109.0 (2)	C12—C15—H15C	109.5
N5—C8—C10	104.9 (2)	H15A—C15—H15C	109.5
C9—C8—C10	108.2 (2)	H15B—C15—H15C	109.5
N5—C8—C11	113.6 (2)	N4—C4—C5	114.4 (3)
C9—C8—C11	108.1 (2)	N4—C4—H4A	108.7
C10—C8—C11	112.9 (2)	C5—C4—H4A	108.7
C8—C9—H9A	109.5	N4—C4—H4B	108.7
C8—C9—H9B	109.5	C5—C4—H4B	108.7
H9A—C9—H9B	109.5	H4A—C4—H4B	107.6
C8—C9—H9C	109.5	C6—C5—C4	115.6 (3)
H9A—C9—H9C	109.5	C6—C5—H5A	108.4

H9B—C9—H9C	109.5	C4—C5—H5A	108.4
C8—C10—H10A	109.5	C6—C5—H5B	108.4
C8—C10—H10B	109.5	C4—C5—H5B	108.4
H10A—C10—H10B	109.5	H5A—C5—H5B	107.4
C8—C10—H10C	109.5	C5—C6—C7	113.1 (4)
H10A—C10—H10C	109.5	C5—C6—H6A	109.0
H10B—C10—H10C	109.5	C7—C6—H6A	109.0
C8—C11—C12	125.2 (3)	C5—C6—H6B	109.0
C8—C11—H11A	106.0	C7—C6—H6B	109.0
C12—C11—H11A	106.0	H6A—C6—H6B	107.8
C8—C11—H11B	106.0	C6—C7—H7A	109.5
C12—C11—H11B	106.0	C6—C7—H7B	109.5
H11A—C11—H11B	106.3	H7A—C7—H7B	109.5
C14—C12—C13	109.9 (4)	C6—C7—H7C	109.5
C14—C12—C15	106.8 (3)	H7A—C7—H7C	109.5
C13—C12—C15	108.1 (4)	H7B—C7—H7C	109.5
C2—N2—C1—N1	1.4 (4)	C1—N1—C3—N4	177.6 (2)
C2—N2—C1—Cl1	−179.32 (17)	C1—N1—C3—N3	−3.2 (4)
C3—N1—C1—N2	1.7 (4)	C2—N5—C8—C9	60.6 (3)
C3—N1—C1—Cl1	−177.58 (17)	C2—N5—C8—C10	176.3 (3)
C8—N5—C2—N3	4.2 (4)	C2—N5—C8—C11	−60.0 (4)
C8—N5—C2—N2	−177.0 (2)	N5—C8—C11—C12	−58.3 (3)
C3—N3—C2—N5	−179.1 (2)	C9—C8—C11—C12	−179.4 (3)
C3—N3—C2—N2	2.3 (4)	C10—C8—C11—C12	61.0 (3)
C1—N2—C2—N5	177.7 (2)	C8—C11—C12—C14	−63.0 (4)
C1—N2—C2—N3	−3.6 (4)	C8—C11—C12—C13	62.5 (4)
C4—N4—C3—N3	4.2 (4)	C8—C11—C12—C15	179.8 (3)
C4—N4—C3—N1	−176.5 (3)	C3—N4—C4—C5	77.2 (4)
C2—N3—C3—N4	−179.5 (2)	N4—C4—C5—C6	61.1 (4)
C2—N3—C3—N1	1.4 (4)	C4—C5—C6—C7	−179.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N1^{i}	0.77 (3)	2.31 (3)	3.079 (3)	171 (3)
N5—H5···N2^{ii}	0.83 (3)	2.34 (3)	3.151 (3)	167 (3)

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

Fig. 1