Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

tert-Butyl *N*-[*N*,*N*-bis(2-chloroethyl)-sulfamoyl]-*N*-(2-chloroethyl)carbamate

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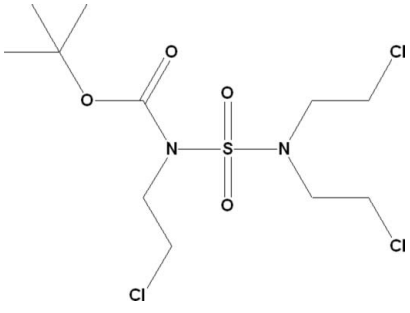
Received 17 September 2009; accepted 21 September 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.068; data-to-parameter ratio = 20.6.

The title compound, $C_{11}H_{21}Cl_3N_2O_4S$, was produced as part of a development programme of a new synthetic route to chloroethylnitrososulfamides (CENS) with three chloroethyl moieties. These compounds possess structural features that confer potential biological activity and act as alkylating agents. The packing is governed by four weak C—H···O interactions, forming an infinite three-dimensional network.

Related literature

For the potential biological activity, pharmaceutical utility and cytotoxic activity of chloroethylnitrososulfamides, see: Abdaoui *et al.* (1996, 2000); Dokhane *et al.* (2002); Galešić *et al.* (1987); Gnewuch & Sosnovsky (1997); Ishiguro *et al.* (2006); Jonnalagadda *et al.* (2007); Passagne *et al.* (2003); Seridi *et al.* (2006); Skinner & Scharts (1972); Voutsinas *et al.* (1993); Winum *et al.* (2003). For the synthetic procedure, see: Mitsunobu (1981).



Experimental

Crystal data

$C_{11}H_{21}Cl_3N_2O_4S$
M_r = 383.71
Monoclinic, $P2_1/c$
a = 9.6132 (5) Å
b = 17.1282 (9) Å
c = 10.6763 (5) Å
β = 93.868 (3)°
V = 1753.92 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 100 K
0.15 × 0.12 × 0.1 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.862, T_{max} = 0.937
17775 measured reflections
3982 independent reflections
3662 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.068
S = 1.03
3982 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O1^{i}	0.97	2.59	3.5465 (16)	167
C8—H8B···O1^{i}	0.97	2.58	3.5047 (17)	159
C9—H91···O3^{ii}	0.97	2.39	3.3156 (17)	160
C11—H11B···O2^{ii}	0.97	2.44	3.0428 (16)	120

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

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); 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).

Dr T. Roisnel is acknowledged for his assistance during the data measurement. The authors are grateful to the Université de Rennes 1 for access to the Centre de Diffractométrie X, CDIFX, available at the Laboratoire des Sciences Chimiques de Rennes. The authors are also indebted to the Université du 20 Août 1955 – Skikda (Algeria) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2489).

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supplementary materials

Acta Cryst. (2009). E**65**, o2543-o2544 [**doi:10.1107/S1600536809038185**]

tert-Butyl *N*-[*N*,*N*-bis(2-chloroethyl)sulfamoyl]-*N*-(2-chloroethyl)carbamate

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Comment

Compounds with one or more *N*-(2-chloroethyl) moieties show many pharmacological activities (Galešić *et al.*, 1987). They are cytotoxic (Ishiguro *et al.*, 2006), mutagenic (Voutsinas *et al.*, 1993), and immuno-suppressive (Skinner & Scharts, 1972). Many of them include Mechlorethamine, Chlorambucil, Melphalan,Cyclophosmamide, Ifosfamide, are used for the treatment of wide variety of cancers (Jonnalagadda *et al.*, 2007). Among others, *N*-(2-chloroethyl) nitrososulfamides (CENS) are promising antitumoral agents which have been developed as new family of alkylating agents structurally related to 2-chloroethylnitrosoureas (CENU) (Abdaoui *et al.*, 1996). A certain number of these derivatives exhibited interesting cytotoxic activity and among them, some prouved to be considerably more potent than the parent nitrosourea (Abdaoui *et al.*, 2000; Gnewuch & Sosnovsky, 1997; Passagne *et al.*, 2003; Seridi *et al.*, 2006; Winum *et al.*, 2003).

In order to extend our knowledge about such sulfamides derivatives with three *N*-(2-chloroethyl) moieties the crystal structure of the title compound is presented.

In all essential details, the molecular geometry in terms of bond distances and angles is in good agreement with related structure (Dokhane *et al.* 2002). In the molecular geometry (Fig.1), the sulfamide moiety N1—S—N2 exhibit an asymmetry of S—N bond distance, with values of 1.688 (1) and 1.615 (1) Å respectively. The molecules are linked by four C—H···O intermolecular interactions involving sulfonamide (oxygen atoms O1 and O2) and carbonyl (oxygen atom O3) functions (table 1). Thus, these interactions lead to an infinite three-dimensional network.

Experimental

The synthetic pathway used for the preparation of the title compound is outlined in Fig. 2. First the formation of *tert*-butyl*N*-(2-chloroethyl)sulfamoylcarbamate which is performed in dried dichloromethane with successive addition of tBuOH, and Chloroethylamine/TEA into CSI. After purification, the carbamate was recovered at (yield 80%). The second step is carried out according to the Mitsunobu procedure (Mitsunobu, 1981) in anhydrous THF as a solvent. The mixture of DEAD (diethyl azodicarboxylate) and *tert*-butyl*N*-(2-chloroethyl)sulfamoylcarbamate is added to a solution of excess of chloroethanol and PPh3. The product was recrystallized in pure ethanol.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined isotropically using a riding model (including free rotation about the ethanol C—C bond), with C—H = 0.97 Å (methylene) or 0.96Å (methyl) and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Figures

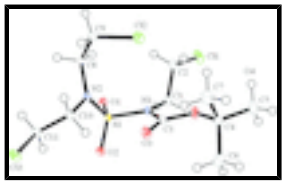


Fig. 1. (Farrugia, 1997) The molecule of the title compound in the crystal. Ellipsoids correspond to 50% probability levels and H atoms are shown as small spheres of arbitrary radii.

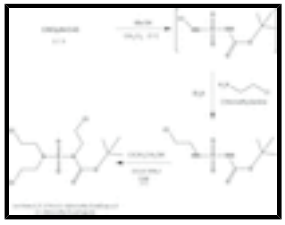


Fig. 2. Synthesis of the title compound.

tert-Butyl *N*-[*N*,*N*-bis(2-chloroethyl)sulfamoyl]- *N*-(2-chloroethyl)carbamate

Crystal data

$C_{11}H_{21}Cl_3N_2O_4S$	F_{000} = 800
M_r = 383.71	D_x = 1.453 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9788 reflections
a = 9.6132 (5) Å	θ = 2.4–27.4º
b = 17.1282 (9) Å	μ = 0.66 mm^{-1}
c = 10.6763 (5) Å	T = 100 K
β = 93.868 (3)º	Prism, colourless
V = 1753.92 (15) Å^3	0.15 × 0.12 × 0.1 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	3662 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 100 K	θ_{max} = 27.4º
CCD rotation images, thick slices scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	h = −12→11
T_{min} = 0.862, T_{max} = 0.937	k = −22→21
17775 measured reflections	l = −13→13
3982 independent reflections	

Refinement

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

$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 0.8873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3982 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
193 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.30088 (13)	−0.00247 (8)	0.74767 (12)	0.0142 (3)
H1A	0.3977	−0.0155	0.7375	0.017*
H1B	0.2483	−0.0120	0.6684	0.017*
C2	0.24504 (14)	−0.05402 (8)	0.84875 (13)	0.0166 (3)
H2A	0.1511	−0.0381	0.8649	0.020*
H2B	0.3033	−0.0489	0.9261	0.020*
C3	0.16945 (13)	0.12486 (8)	0.74993 (12)	0.0141 (3)
C4	−0.07329 (14)	0.11154 (9)	0.66503 (14)	0.0212 (3)
C5	−0.15279 (16)	0.03860 (10)	0.62057 (17)	0.0332 (4)
H5A	−0.1090	0.0162	0.5508	0.050*
H5B	−0.2473	0.0523	0.5950	0.050*
H5C	−0.1521	0.0014	0.6878	0.050*
C6	−0.05995 (16)	0.16890 (10)	0.55745 (15)	0.0281 (3)
H6A	−0.0128	0.2151	0.5885	0.042*
H6B	−0.1511	0.1825	0.5220	0.042*
H6C	−0.0075	0.1452	0.4941	0.042*
C7	−0.13690 (15)	0.14725 (10)	0.77813 (15)	0.0285 (3)
H7A	−0.1375	0.1092	0.8442	0.043*
H7B	−0.2307	0.1635	0.7550	0.043*
H7C	−0.0827	0.1916	0.8068	0.043*
C8	0.38802 (13)	0.13068 (8)	1.08849 (12)	0.0150 (3)
H8A	0.4597	0.1523	1.1468	0.018*
H8B	0.4115	0.0765	1.0741	0.018*
C9	0.24946 (14)	0.13378 (8)	1.14857 (13)	0.0184 (3)

H91	0.2239	0.1879	1.1609	0.022*
H92	0.2594	0.1090	1.2304	0.022*
C10	0.36795 (13)	0.25857 (8)	0.96777 (12)	0.0139 (3)
H10A	0.3144	0.2731	1.0379	0.017*
H10B	0.3146	0.2733	0.8910	0.017*
C11	0.50586 (14)	0.30294 (8)	0.97652 (12)	0.0158 (3)
H11A	0.5593	0.2904	0.9053	0.019*
H11B	0.5605	0.2888	1.0528	0.019*
Cl1	0.24477 (4)	−0.15386 (2)	0.79617 (4)	0.02567 (9)
Cl2	0.11302 (3)	0.08604 (2)	1.05440 (3)	0.02616 (10)
Cl3	0.46514 (4)	0.40555 (2)	0.97723 (3)	0.02271 (9)
N1	0.29004 (10)	0.08109 (6)	0.78128 (10)	0.0123 (2)
N2	0.38924 (11)	0.17329 (6)	0.96878 (9)	0.0121 (2)
O1	0.52796 (9)	0.06756 (6)	0.87615 (9)	0.01627 (19)
O2	0.46793 (9)	0.18884 (6)	0.75688 (8)	0.0161 (2)
O3	0.16339 (9)	0.19465 (6)	0.76460 (9)	0.0177 (2)
O4	0.06748 (9)	0.07794 (6)	0.70365 (9)	0.0181 (2)
S1	0.43157 (3)	0.129314 (19)	0.84310 (3)	0.01123 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0159 (6)	0.0112 (7)	0.0153 (6)	0.0002 (5)	−0.0004 (4)	−0.0037 (5)
C2	0.0169 (6)	0.0110 (7)	0.0219 (7)	−0.0006 (5)	0.0011 (5)	−0.0016 (5)
C3	0.0131 (6)	0.0153 (7)	0.0136 (6)	−0.0015 (5)	−0.0015 (4)	0.0027 (5)
C4	0.0122 (6)	0.0221 (8)	0.0283 (7)	−0.0004 (5)	−0.0076 (5)	0.0057 (6)
C5	0.0238 (8)	0.0296 (9)	0.0438 (10)	−0.0088 (6)	−0.0159 (7)	0.0055 (7)
C6	0.0227 (7)	0.0311 (9)	0.0292 (8)	−0.0003 (6)	−0.0074 (6)	0.0102 (7)
C7	0.0161 (7)	0.0343 (9)	0.0347 (9)	0.0020 (6)	0.0001 (6)	0.0067 (7)
C8	0.0183 (6)	0.0143 (7)	0.0120 (6)	−0.0011 (5)	−0.0008 (5)	0.0028 (5)
C9	0.0248 (7)	0.0161 (7)	0.0149 (6)	−0.0041 (5)	0.0052 (5)	−0.0016 (5)
C10	0.0165 (6)	0.0094 (6)	0.0158 (6)	−0.0009 (5)	0.0008 (5)	0.0000 (5)
C11	0.0197 (6)	0.0114 (7)	0.0166 (6)	−0.0031 (5)	0.0027 (5)	−0.0008 (5)
Cl1	0.02584 (18)	0.01139 (18)	0.0396 (2)	−0.00249 (13)	0.00118 (14)	−0.00252 (14)
Cl2	0.01773 (16)	0.0387 (2)	0.02252 (18)	−0.00801 (14)	0.00518 (12)	−0.00232 (15)
Cl3	0.03418 (19)	0.01075 (17)	0.02329 (18)	−0.00579 (13)	0.00268 (13)	0.00063 (12)
N1	0.0116 (5)	0.0097 (6)	0.0153 (5)	−0.0015 (4)	−0.0014 (4)	−0.0013 (4)
N2	0.0158 (5)	0.0093 (5)	0.0112 (5)	−0.0010 (4)	0.0014 (4)	−0.0002 (4)
O1	0.0130 (4)	0.0164 (5)	0.0190 (5)	0.0027 (4)	−0.0014 (3)	−0.0026 (4)
O2	0.0182 (4)	0.0162 (5)	0.0139 (4)	−0.0048 (4)	0.0031 (3)	0.0001 (4)
O3	0.0164 (4)	0.0112 (5)	0.0247 (5)	0.0001 (3)	−0.0037 (4)	0.0019 (4)
O4	0.0138 (4)	0.0142 (5)	0.0251 (5)	−0.0013 (4)	−0.0071 (4)	0.0017 (4)
S1	0.01039 (14)	0.01148 (17)	0.01178 (15)	−0.00120 (11)	0.00045 (10)	−0.00080 (11)

Geometric parameters (Å, °)

C1—N1	1.4809 (17)	C7—H7B	0.9600
C1—C2	1.5201 (18)	C7—H7C	0.9600
C1—H1A	0.9700	C8—N2	1.4725 (16)

C1—H1B	0.9700	C8—C9	1.5178 (18)
C2—Cl1	1.7997 (14)	C8—H8A	0.9700
C2—H2A	0.9700	C8—H8B	0.9700
C2—H2B	0.9700	C9—Cl2	1.7950 (14)
C3—O3	1.2074 (17)	C9—H91	0.9700
C3—O4	1.3364 (15)	C9—H92	0.9700
C3—N1	1.4020 (16)	C10—N2	1.4749 (17)
C4—O4	1.5024 (15)	C10—C11	1.5255 (17)
C4—C7	1.519 (2)	C10—H10A	0.9700
C4—C6	1.523 (2)	C10—H10B	0.9700
C4—C5	1.524 (2)	C11—Cl3	1.8007 (14)
C5—H5A	0.9600	C11—H11A	0.9700
C5—H5B	0.9600	C11—H11B	0.9700
C5—H5C	0.9600	N1—S1	1.6875 (10)
C6—H6A	0.9600	N2—S1	1.6147 (11)
C6—H6B	0.9600	O1—S1	1.4345 (10)
C6—H6C	0.9600	O2—S1	1.4326 (10)
C7—H7A	0.9600		
N1—C1—C2	110.82 (10)	H7B—C7—H7C	109.5
N1—C1—H1A	109.5	N2—C8—C9	114.08 (11)
C2—C1—H1A	109.5	N2—C8—H8A	108.7
N1—C1—H1B	109.5	C9—C8—H8A	108.7
C2—C1—H1B	109.5	N2—C8—H8B	108.7
H1A—C1—H1B	108.1	C9—C8—H8B	108.7
C1—C2—Cl1	108.88 (9)	H8A—C8—H8B	107.6
C1—C2—H2A	109.9	C8—C9—Cl2	112.10 (9)
Cl1—C2—H2A	109.9	C8—C9—H91	109.2
C1—C2—H2B	109.9	Cl2—C9—H91	109.2
Cl1—C2—H2B	109.9	C8—C9—H92	109.2
H2A—C2—H2B	108.3	Cl2—C9—H92	109.2
O3—C3—O4	127.07 (12)	H91—C9—H92	107.9
O3—C3—N1	123.01 (11)	N2—C10—C11	111.92 (10)
O4—C3—N1	109.92 (11)	N2—C10—H10A	109.2
O4—C4—C7	109.86 (11)	C11—C10—H10A	109.2
O4—C4—C6	109.51 (11)	N2—C10—H10B	109.2
C7—C4—C6	113.49 (13)	C11—C10—H10B	109.2
O4—C4—C5	101.24 (11)	H10A—C10—H10B	107.9
C7—C4—C5	110.95 (13)	C10—C11—Cl3	107.35 (9)
C6—C4—C5	111.09 (13)	C10—C11—H11A	110.2
C4—C5—H5A	109.5	Cl3—C11—H11A	110.2
C4—C5—H5B	109.5	C10—C11—H11B	110.2
H5A—C5—H5B	109.5	Cl3—C11—H11B	110.2
C4—C5—H5C	109.5	H11A—C11—H11B	108.5
H5A—C5—H5C	109.5	C3—N1—C1	121.97 (10)
H5B—C5—H5C	109.5	C3—N1—S1	117.61 (9)
C4—C6—H6A	109.5	C1—N1—S1	119.98 (8)
C4—C6—H6B	109.5	C8—N2—C10	119.21 (10)
H6A—C6—H6B	109.5	C8—N2—S1	120.48 (9)
C4—C6—H6C	109.5	C10—N2—S1	119.90 (8)

H6A—C6—H6C	109.5	C3—O4—C4	119.72 (11)
H6B—C6—H6C	109.5	O2—S1—O1	120.08 (6)
C4—C7—H7A	109.5	O2—S1—N2	106.74 (6)
C4—C7—H7B	109.5	O1—S1—N2	109.53 (6)
H7A—C7—H7B	109.5	O2—S1—N1	108.80 (5)
C4—C7—H7C	109.5	O1—S1—N1	103.05 (5)
H7A—C7—H7C	109.5	N2—S1—N1	108.16 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2B···O1^{i}	0.97	2.59	3.5465 (16)	167
C8—H8B···O1^{i}	0.97	2.58	3.5047 (17)	159
C9—H91···O3^{ii}	0.97	2.39	3.3156 (17)	160
C11—H11B···O2^{ii}	0.97	2.44	3.0428 (16)	120

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

Fig. 1

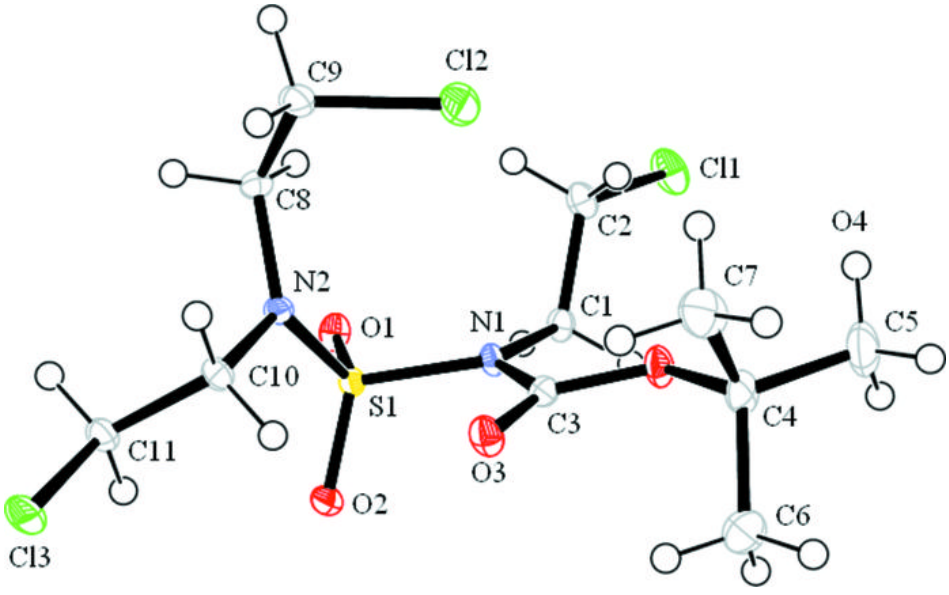
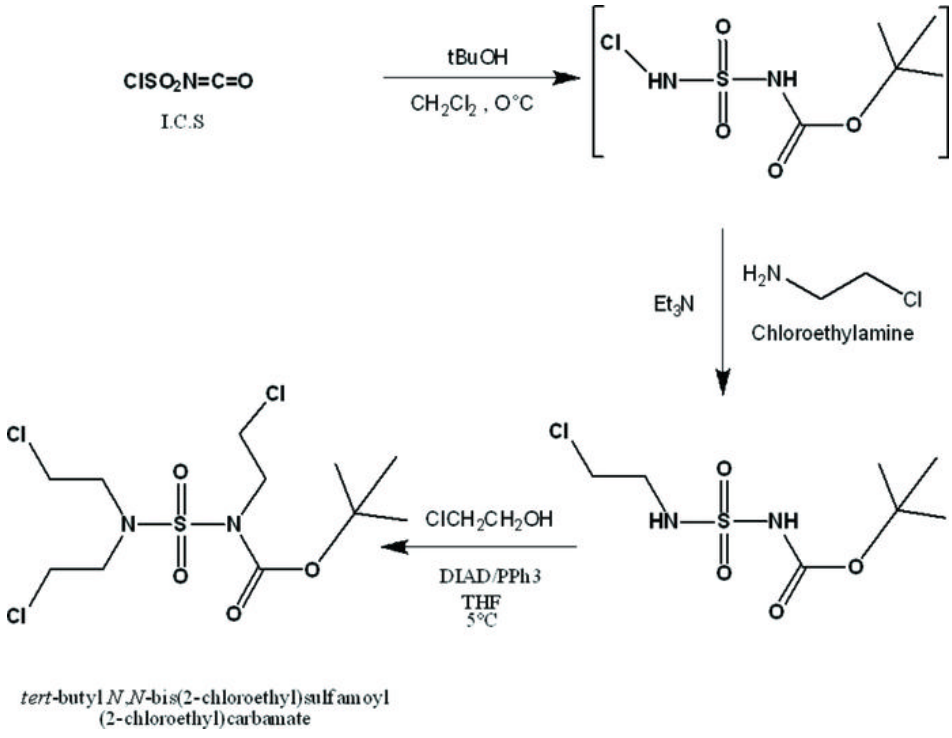


Fig. 2



tert-butyl *N*,*N*-bis(2-chloroethyl)sulfamoyl (2-chloroethyl)carbamate