Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Sodium 2-mercaptoethanesulfonate (mesna)

Massimo Bambagiotti-Alberti,[a] Bruno Bruni,[b] Massimo Di Vaira[b]* and Valerio Giannellini[a]

[a]Dipartimento di Scienze Farmaceutiche, Universitá di Firenze, Via U. Schiff 6, I-50019 Sesto Fiorentino, Firenze, Italy, and [b]Dipartimento di Chimica, Universitá di Firenze, Via della Lastruccia 3, I-50019 Sesto Fiorentino, Firenze, Italy
Correspondence e-mail: massimo.divaira@unifi.it

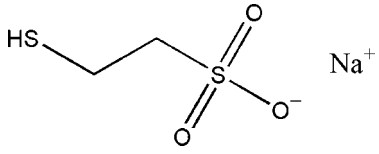
Received 19 May 2007; accepted 25 May 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.093; data-to-parameter ratio = 13.6.

The crystal structure of the title compound, $Na^+\cdot C_2H_5O_3S_2^-$, commonly known as mesna, has triple-layer sheets normal to the c axis, where the external layers of each set are formed by the anions which coordinate, through their sulfonate O atoms, the cations in the inner layer. The contacts between the outer sides of different sheets involve thiol S and methylene C atoms.

Related literature

For related literature, see: Bradley *et al.* (2007); Goren *et al.* (1998); Shaw & Graham (1987).



Experimental

Crystal data

$Na^+\cdot C_2H_5O_3S_2^-$
M_r = 164.17
Orthorhombic, *Pbca*
a = 6.1458 (3) Å
b = 8.2749 (4) Å
c = 24.2995 (11) Å
V = 1235.77 (10) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 7.88 mm^{-1}
T = 173 (2) K
0.70 × 0.20 × 0.02 mm

Data collection

Oxford Diffraction Xcalibur PX Ultra CCD diffractometer
Absorption correction: multi-scan (*ABSPACK* in *CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.154, T_{max} = 1.000 (expected range = 0.132–0.854)
7907 measured reflections
1211 independent reflections
1132 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.093
S = 1.12
1211 reflections
89 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
S1—H1*S*···O1	1.25 (3)	2.36 (3)	3.342 (1)	133 (2)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support from the Italian Ministero dell'Istruzione, dell'Universitá e della Ricerca.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2014).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bradley, L. U., Freeman, D. J., Spence, J. D. & House, A. A. (2007). *Am. J. Kidney Dis.* **49**, 109–117.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Goren, M. P., Hsu, L. C. & Li, J. T. (1998). *Cancer Res.* **58**, 4358–4362.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.29.2. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Shaw, I. C. & Graham, M. I. (1987). *Cancer Treat. Rev.* **14**, 67–86.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

  doi:10.1107/S1600536807025688

supplementary materials

Acta Cryst. (2007). E**63**, o1796 [**doi:10.1107/S1600536807025688**]

Sodium 2-mercaptoethanesulfonate (mesna)

M. Bambagiotti-Alberti, B. Bruni, M. Di Vaira and V. Giannellini

Comment

The title compound Mesna, (I), is a drug used therapeutically to reduce the incidence of haemorrhagic cystitis and haematuria in patients receiving cancer chemotherapy (Shaw & Graham, 1987; Goren *et al.*, 1998; Bradley *et al.*, 2007). It is rapidly oxidized to its major metabolite, mesna disulfide (dimesna).

In the anion (Fig. 1) the S1—H1S bond almost eclipses the S2—O1 bond, forming a sort of six-membered ring with a long O1···H1S 2.36 (3) Å contact distance. The structure presents alternating layers of anions and cations parallel to the *ab* face, grouped in sets of three. The two outer layers of each set are formed by anions, oriented with their sulfonate sides toward the inner layer, formed by the cations (Fig. 2). The outer sides of each three-layer sheet are occupied by methylene carbons and thiol sulfur atoms. The shortest contacts between thiol sulfur atoms are 4.476 (1) Å (intralayer) and 4.058 (1) Å (interlayer). The shortest contacts between thiol sulfurs and carbon atoms of vicinal sheets are 3.799 (2) Å. The Na^+ ion is in an irregular environment of six oxygen atoms from five different anions. Five Na—O distances are in the range 2.315 (2)–2.452 (2) Å; the sixth one, formed by an oxygen of the unique chelating sulfonate group in the Na^+ coordination sphere, is longer: 2.743 (2) Å. The oxygen atoms differ in their coordination modes: O1 bridges between two cations, O2 is bound to three, whereas O3 only to one.

Experimental

Samples of the compound, in microcrystalline form, were kindly provided by SIMS (SIMS srl, Reggello Firenze, Italy). Crystals suitable for X-ray diffraction were obtained by slow evaporation from water-methanol solutions, under a nitrogen atmosphere.

Refinement

The positional parameters of hydrogen atoms were refined, with U(H) = 1.2U_{eq}(C) and U(H) = 1.5U_{eq}(S). Ranges of bond distances involving refined hydrogen atoms: C—H 0.95–1.04 Å.

Figures

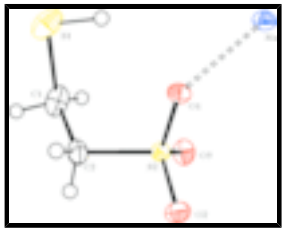


Fig. 1. A view of the asymmetric unit in (I). Displacement ellipsoids are drawn at the 30% probability level.

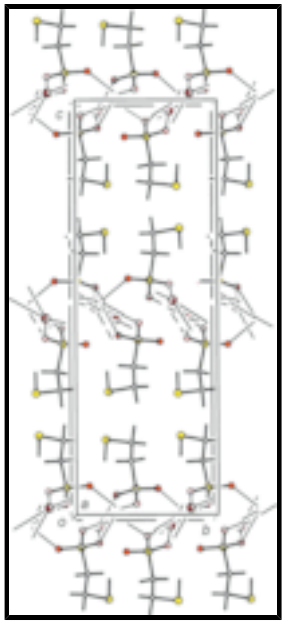


Fig. 2. The crystal packing of (I), viewed along the *a* axis.

Sodium 2-mercaptoethanesulfonate

Crystal data

$Na^+ \cdot C_2H_5O_3S_2^-$	F_{000} = 672
M_r = 164.17	D_x = 1.765 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *Kα* radiation λ = 1.54180 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 4481 reflections
a = 6.1458 (3) Å	θ = 9.0–65.0º
b = 8.2749 (4) Å	μ = 7.88 mm^{-1}
c = 24.2995 (11) Å	*T* = 173 (2) K
V = 1235.77 (10) Å^3	Thin plate, colourless
Z = 8	0.70 × 0.20 × 0.02 mm

Data collection

Oxford Diffraction Xcalibur PX Ultra CCD diffractometer	1211 independent reflections
Radiation source: fine-focus sealed tube	1132 reflections with $I > 2\sigma(I)$
Monochromator: Oxford Diffraction, Enhance ULTRA assembly	R_{int} = 0.050
T = 173(2) K	θ_{max} = 72.2º
ω scans	θ_{min} = 3.6º
Absorption correction: multi-scan (ABSPACK in CrysAlis RED; Oxford Diffraction, 2006)	*h* = −6→7
T_{min} = 0.154, T_{max} = 1.000	*k* = −9→10
7907 measured reflections	*l* = −29→29

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.093$

$S = 1.12$

1211 reflections

89 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.6874P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.58$ e Å^{-3}

$\Delta\rho_{min} = -0.43$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0007 (2)

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}
S1	−0.11102 (11)	0.24713 (8)	0.69546 (2)	0.0427 (2)
H1S	−0.182 (6)	0.253 (4)	0.6475 (12)	0.064*
C1	0.0621 (4)	0.0714 (3)	0.68613 (8)	0.0327 (5)
H11	0.142 (4)	0.057 (3)	0.7234 (11)	0.039*
H12	−0.029 (5)	−0.023 (4)	0.6839 (11)	0.039*
C2	0.2284 (3)	0.0829 (2)	0.63964 (7)	0.0231 (4)
H21	0.293 (4)	0.187 (3)	0.6382 (9)	0.028*
H22	0.340 (4)	0.001 (3)	0.6436 (9)	0.028*
S2	0.11652 (7)	0.04671 (5)	0.573398 (17)	0.01618 (19)
O1	−0.0356 (2)	0.17785 (15)	0.56133 (5)	0.0215 (3)
O2	0.3006 (2)	0.05000 (15)	0.53498 (5)	0.0238 (3)
O3	0.0128 (2)	−0.11106 (16)	0.57597 (5)	0.0253 (3)
Na	−0.37169 (11)	0.18754 (9)	0.51844 (3)	0.0202 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0508 (4)	0.0445 (4)	0.0328 (4)	−0.0012 (3)	0.0161 (2)	−0.0068 (2)
C1	0.0492 (13)	0.0256 (10)	0.0234 (10)	−0.0089 (10)	0.0006 (9)	0.0017 (8)
C2	0.0275 (10)	0.0185 (9)	0.0234 (8)	−0.0007 (8)	−0.0069 (7)	0.0003 (7)
S2	0.0168 (3)	0.0124 (3)	0.0193 (3)	0.00017 (14)	−0.00088 (14)	−0.00126 (14)
O1	0.0214 (7)	0.0186 (7)	0.0244 (6)	0.0060 (5)	−0.0020 (5)	0.0005 (5)
O2	0.0196 (7)	0.0233 (7)	0.0285 (7)	−0.0013 (5)	0.0044 (5)	−0.0059 (5)
O3	0.0318 (8)	0.0156 (7)	0.0285 (7)	−0.0066 (6)	−0.0043 (5)	−0.0003 (5)
Na	0.0177 (4)	0.0170 (4)	0.0259 (4)	0.0018 (3)	−0.0004 (2)	−0.0019 (3)

Geometric parameters (Å, °)

S1—C1	1.816 (3)	O2—Na^{iii}	2.3482 (15)
S1—H1S	1.25 (3)	O2—Na^{ii}	2.3958 (14)
C1—C2	1.526 (3)	O2—Na^{i}	2.7428 (15)
C1—H11	1.04 (3)	O3—Na^{iv}	2.3418 (14)
C1—H12	0.96 (3)	Na—O3^{v}	2.3418 (14)
C2—S2	1.7759 (18)	Na—O2^{vi}	2.3482 (15)
C2—H21	0.95 (3)	Na—O2^{ii}	2.3958 (14)
C2—H22	0.97 (3)	Na—O1^{vii}	2.4522 (15)
S2—O3	1.4542 (14)	Na—O2^{vii}	2.7428 (15)
S2—O1	1.4620 (13)	Na—S2^{vii}	3.1339 (8)
S2—O2	1.4669 (13)	Na—S2^{ii}	3.3462 (8)
S2—Na^{i}	3.1339 (8)	Na—Na^{i}	3.3637 (6)
S2—Na^{ii}	3.3462 (8)	Na—Na^{vii}	3.3637 (6)
O1—Na	2.3150 (15)	Na—Na^{viii}	3.5949 (14)
O1—Na^{i}	2.4522 (15)		
C1—S1—H1S	97.0 (16)	O2^{ii}—Na—O1^{vii}	91.11 (5)
C2—C1—S1	115.73 (15)	O1—Na—O2^{vii}	84.04 (5)
C2—C1—H11	109.7 (15)	O3^{v}—Na—O2^{vii}	82.06 (5)
S1—C1—H11	104.9 (15)	O2^{vi}—Na—O2^{vii}	142.74 (5)
C2—C1—H12	113.5 (17)	O2^{ii}—Na—O2^{vii}	108.83 (5)
S1—C1—H12	108.5 (17)	O1^{vii}—Na—O2^{vii}	54.88 (4)
H11—C1—H12	103 (2)	O1—Na—S2^{vii}	111.44 (4)
C1—C2—S2	113.64 (15)	O3^{v}—Na—S2^{vii}	85.25 (4)
C1—C2—H21	111.5 (15)	O2^{vi}—Na—S2^{vii}	116.24 (4)
S2—C2—H21	106.4 (14)	O2^{ii}—Na—S2^{vii}	101.19 (4)
C1—C2—H22	110.8 (14)	O1^{vii}—Na—S2^{vii}	26.98 (3)
S2—C2—H22	104.1 (14)	O2^{vii}—Na—S2^{vii}	27.90 (3)
H21—C2—H22	110 (2)	O1—Na—S2^{ii}	82.07 (4)

O3—S2—O1	113.24 (8)	$O3^{v}$—Na—$S2^{ii}$	169.72 (4)
O3—S2—O2	112.46 (8)	$O2^{vi}$—Na—$S2^{ii}$	103.61 (4)
O1—S2—O2	110.59 (8)	$O2^{ii}$—Na—$S2^{ii}$	22.76 (3)
O3—S2—C2	106.39 (9)	$O1^{vii}$—Na—$S2^{ii}$	85.90 (4)
O1—S2—C2	107.70 (9)	$O2^{vii}$—Na—$S2^{ii}$	87.83 (3)
O2—S2—C2	105.98 (9)	$S2^{vii}$—Na—$S2^{ii}$	86.70 (2)
O3—S2—Na^{i}	132.13 (6)	O1—Na—Na^{i}	46.80 (3)
O1—S2—Na^{i}	49.55 (5)	$O3^{v}$—Na—Na^{i}	106.18 (5)
O2—S2—Na^{i}	61.05 (5)	$O2^{vi}$—Na—Na^{i}	168.01 (5)
C2—S2—Na^{i}	121.20 (7)	$O2^{ii}$—Na—Na^{i}	86.62 (4)
O3—S2—Na^{ii}	73.39 (6)	$O1^{vii}$—Na—Na^{i}	91.44 (5)
O1—S2—Na^{ii}	126.58 (6)	$O2^{vii}$—Na—Na^{i}	43.77 (3)
O2—S2—Na^{ii}	39.19 (5)	$S2^{vii}$—Na—Na^{i}	67.40 (3)
C2—S2—Na^{ii}	121.40 (7)	$S2^{ii}$—Na—Na^{i}	64.67 (2)
Na^{i}—S2—Na^{ii}	85.45 (2)	O1—Na—Na^{vii}	161.03 (5)
S2—O1—Na	133.36 (8)	$O3^{v}$—Na—Na^{vii}	66.55 (4)
S2—O1—Na^{i}	103.47 (7)	$O2^{vi}$—Na—Na^{vii}	53.91 (3)
Na—O1—Na^{i}	89.71 (4)	$O2^{ii}$—Na—Na^{vii}	105.93 (5)
S2—O2—Na^{iii}	141.20 (8)	$O1^{vii}$—Na—Na^{vii}	43.49 (4)
S2—O2—Na^{ii}	118.05 (7)	$O2^{vii}$—Na—Na^{vii}	89.03 (4)
Na^{iii}—O2—Na^{ii}	98.53 (5)	$S2^{vii}$—Na—Na^{vii}	64.75 (3)
S2—O2—Na^{i}	91.05 (6)	$S2^{ii}$—Na—Na^{vii}	115.37 (3)
Na^{iii}—O2—Na^{i}	82.32 (4)	Na^{i}—Na—Na^{vii}	132.00 (5)
Na^{ii}—O2—Na^{i}	117.62 (6)	O1—Na—Na^{viii}	118.28 (5)
S2—O3—Na^{iv}	140.85 (8)	$O3^{v}$—Na—Na^{viii}	126.93 (5)
O1—Na—$O3^{v}$	94.95 (5)	$O2^{vi}$—Na—Na^{viii}	41.23 (3)
O1—Na—$O2^{vi}$	132.19 (6)	$O2^{ii}$—Na—Na^{viii}	40.24 (4)
$O3^{v}$—Na—$O2^{vi}$	85.71 (5)	$O1^{vii}$—Na—Na^{viii}	90.85 (4)
O1—Na—$O2^{ii}$	93.02 (5)	$O2^{vii}$—Na—Na^{viii}	137.31 (4)
$O3^{v}$—Na—$O2^{ii}$	167.14 (6)	$S2^{vii}$—Na—Na^{viii}	114.72 (3)
$O2^{vi}$—Na—$O2^{ii}$	81.47 (5)	$S2^{ii}$—Na—Na^{viii}	62.56 (2)
O1—Na—$O1^{vii}$	137.58 (5)	Na^{i}—Na—Na^{viii}	126.85 (4)
$O3^{v}$—Na—$O1^{vii}$	89.80 (5)	Na^{vii}—Na—Na^{viii}	78.35 (2)
$O2^{vi}$—Na—$O1^{vii}$	90.17 (5)		
S1—C1—C2—S2	−79.35 (18)	C2—S2—O2—Na^{i}	−117.22 (7)
C1—C2—S2—O3	−55.72 (17)	Na^{ii}—S2—O2—Na^{i}	122.36 (9)
C1—C2—S2—O1	66.00 (16)	O1—S2—O3—Na^{iv}	76.61 (15)
C1—C2—S2—O2	−175.62 (14)	O2—S2—O3—Na^{iv}	−49.67 (16)
C1—C2—S2—Na^{i}	118.91 (14)	C2—S2—O3—Na^{iv}	−165.28 (13)
C1—C2—S2—Na^{ii}	−135.95 (13)	Na^{i}—S2—O3—Na^{iv}	20.92 (19)

O3—S2—O1—Na	−23.73 (13)	Na^{ii}—S2—O3—Na^{iv}	−46.67 (12)
O2—S2—O1—Na	103.54 (11)	S2—O1—Na—$O3^{v}$	144.00 (11)
C2—S2—O1—Na	−141.08 (11)	Na^{i}—O1—Na—$O3^{v}$	−107.60 (5)
Na^{i}—S2—O1—Na	102.65 (11)	S2—O1—Na—$O2^{vi}$	55.32 (14)
Na^{ii}—S2—O1—Na	62.33 (13)	Na^{i}—O1—Na—$O2^{vi}$	163.72 (7)
O3—S2—O1—Na^{i}	−126.38 (7)	S2—O1—Na—$O2^{ii}$	−25.90 (11)
O2—S2—O1—Na^{i}	0.89 (9)	Na^{i}—O1—Na—$O2^{ii}$	82.50 (5)
C2—S2—O1—Na^{i}	116.27 (8)	S2—O1—Na—$O1^{vii}$	−120.86 (11)
Na^{ii}—S2—O1—Na^{i}	−40.32 (9)	Na^{i}—O1—Na—$O1^{vii}$	−12.46 (4)
O3—S2—O2—Na^{iii}	−154.07 (12)	S2—O1—Na—$O2^{vii}$	−134.53 (11)
O1—S2—O2—Na^{iii}	78.23 (14)	Na^{i}—O1—Na—$O2^{vii}$	−26.13 (4)
C2—S2—O2—Na^{iii}	−38.21 (15)	S2—O1—Na—$S2^{vii}$	−129.17 (10)
Na^{i}—S2—O2—Na^{iii}	79.01 (12)	Na^{i}—O1—Na—$S2^{vii}$	−20.77 (4)
Na^{ii}—S2—O2—Na^{iii}	−158.63 (18)	S2—O1—Na—$S2^{ii}$	−45.90 (10)
O3—S2—O2—Na^{ii}	4.56 (11)	Na^{i}—O1—Na—$S2^{ii}$	62.50 (3)
O1—S2—O2—Na^{ii}	−123.14 (8)	S2—O1—Na—Na^{i}	−108.40 (12)
C2—S2—O2—Na^{ii}	120.42 (9)	S2—O1—Na—Na^{vii}	156.33 (12)
Na^{i}—S2—O2—Na^{ii}	−122.36 (9)	Na^{i}—O1—Na—Na^{vii}	−95.27 (16)
O3—S2—O2—Na^{i}	126.92 (7)	S2—O1—Na—Na^{viii}	7.00 (13)
O1—S2—O2—Na^{i}	−0.78 (8)	Na^{i}—O1—Na—Na^{viii}	115.40 (5)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) −*x*, −*y*, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*−1/2, *y*−1/2, *z*; (v) −*x*−1/2, *y*+1/2, *z*; (vi) *x*−1, *y*, *z*; (vii) *x*−1/2, −*y*+1/2, −*z*+1; (viii) −*x*−1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
S1—H1S···O1	1.25 (3)	2.36 (3)	3.342 (1)	133 (2)

Fig. 1

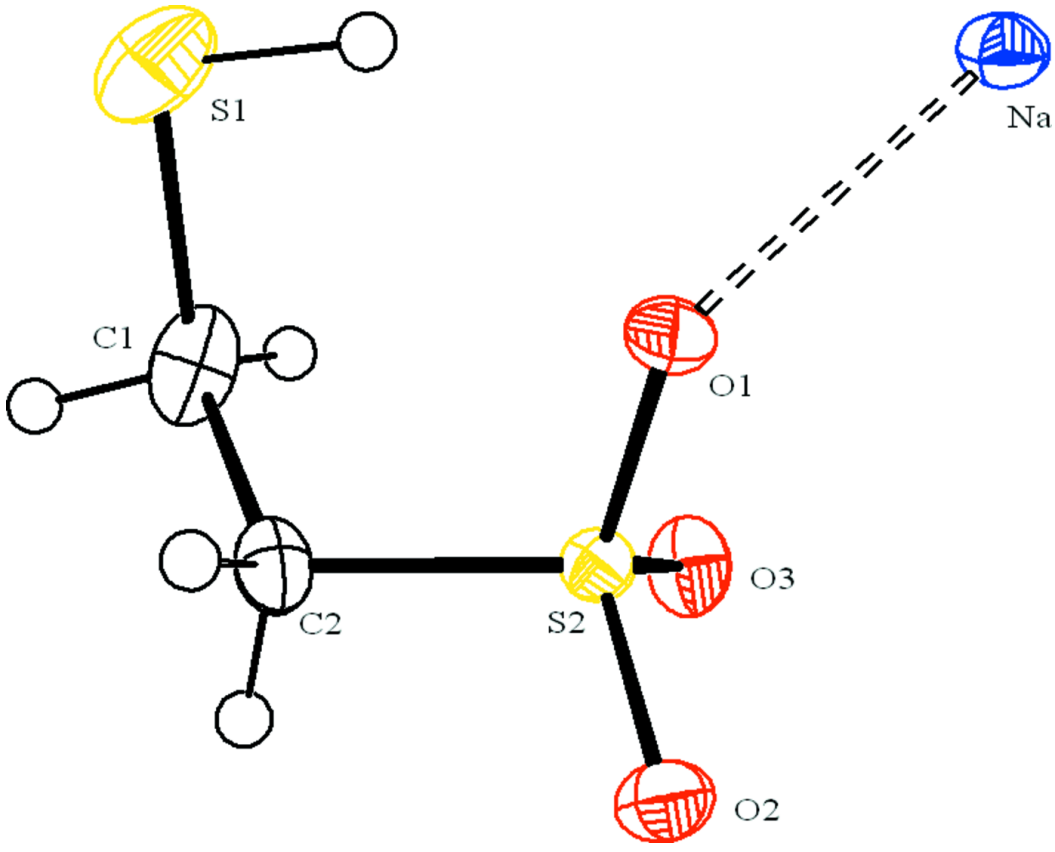


Fig. 2