Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bromidosodium(I)]-bis(*μ*-dimethyl sulfoxide-κ^2O:O)]

Tian-Jia Bu, Bao Li, Ling Ye and Li-Xin Wu*

Key Laboratory for Supramolecular Structure and Materials of the Ministry of Education, College of Chemistry, Jilin University, Changchun 130012, People's Republic of China
Correspondence e-mail: wulx@jlu.edu.cn

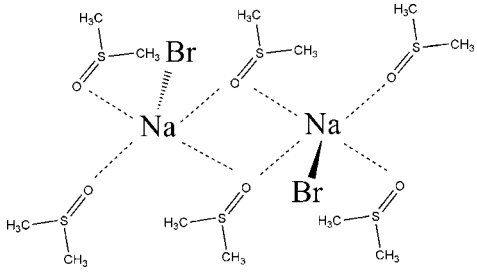
Received 28 May 2007; accepted 30 May 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(Na–O) = 0.002 Å; R factor = 0.034; wR factor = 0.072; data-to-parameter ratio = 25.3.

In the title compound, $[NaBr(C_2H_6OS)_2]_n$, each Na^I cation is coordinated by four O atoms from four dimethyl sulfoxide ligands and by one Br^- anion in a distorted pyramidal geometry. Each O atom coordinates two Na^I cations, leading to the formation of polymeric coordination chains parallel to the a axis with protruding Br^- anions and methyl groups.

Related literature

For the crystal structures of analogues of the title compound, see: Chiarella *et al.* (2006); Gao *et al.* (1993); Nieuwenhuyzen *et al.* (1993); Schrauzer *et al.* (1990). For the crystal structure of a nickel complex formed in the same synthesis as the title compound, see: Zhu *et al.* (2007).



Experimental

Crystal data

$[NaBr(C_2H_6OS)_2]$
M_r = 259.16
Monoclinic, $P2_1/c$
a = 6.433 (3) Å
b = 9.969 (4) Å
c = 16.430 (6) Å
β = 94.046 (17)°
V = 1051.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.30 mm^{-1}
T = 291 (2) K
0.21 × 0.20 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.461, T_{max} = 0.491
(expected range = 0.415–0.442)
10170 measured reflections
2401 independent reflections
1772 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.072
S = 1.04
2401 reflections
95 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Na1—Br1	2.8869 (13)	Na1—O1^{i}	2.368 (2)
Na1—O2	2.345 (2)	Na1—O2^{ii}	2.399 (2)
Na1—O1	2.365 (2)		
O2—Na1—O1	111.08 (8)	O1^{i}—Na1—O2^{ii}	161.75 (8)
O2—Na1—O1^{i}	88.73 (8)	O2—Na1—Br1	123.62 (7)
O1—Na1—O1^{i}	79.26 (8)	O1—Na1—Br1	125.28 (6)
O2—Na1—O2^{ii}	79.83 (8)	O1^{i}—Na1—Br1	99.62 (6)
O1—Na1—O2^{ii}	91.58 (8)	O2^{ii}—Na1—Br1	98.55 (6)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support from the National Natural Science Foundation of China (grant No. 20473032), PCSIRT of the Ministry of Education of China (grant No. IRT0422), the 111 project (grant No. B06009) and the Innovation Fund of Jilin University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2251).

References

Chiarella, G. M., Melgarejo, D. Y. & Koch, S. A. (2006). *J. Am. Chem. Soc.* **128**, 1416–1417.
Gao, Y., Guery, J. & Jacoboni, C. (1993). *Acta Cryst.* C**49**, 963–965.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Nieuwenhuyzen, M., Robinson, W. T. & Wilkins, C. J. (1993). *Acta Cryst.* C**49**, 1173–1175.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Schrauzer, G. N., Zhang, C. & Chadha, R. (1990). *Inorg. Chem.* **29**, 4104–4107.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zhu, T., Li, B., Yang, G.-D. & Wu, L.-X. (2007). *Acta Cryst.* E**63**, m409–m410.

 doi:10.1107/S1600536807026402

supplementary materials

Acta Cryst. (2007). E**63**, m1807 [**doi:10.1107/S1600536807026402**]

catena-Poly[[bromidosodium(I)]-bis(*μ*-dimethyl sulfoxide-κ^2O:*O*)]

T.-J. Bu, B. Li, L. Ye and L.-X. Wu

Comment

Dimethyl sulfoxide has been widely used to build up supramolecular structures (Chiarella *et al.*, 2006; Gao *et al.*, 1993; Nieuwenhuyzen *et al.*, 1993; Schrauzer *et al.*, 1990). In our attempt to synthesize nickel complex with malonic acid, we obtained two types of crystals differently coloured - green (Zhu *et al.*, 2007) and colourless. We herein report the crystal structure of the colourless one, the title compound, (I).

In the asymmetric unit of (I), there are two dimethyl sulfoxide ligands, one sodium ion and one bromide anion (Fig.1). The sodium ion is five-coordinated in a distorted pyramid by four oxygen atoms from four dimethyl sulfoxide ligands and one bromide anion (Table 1). Every oxygen atom is used as bridge unit to link sodium ions to form an infinite chain along *a* axis.

Experimental

Malonic acid and $NiBr_2{\cdot}6H_2O$ of analytical grade were used without further purification. Malonic acid (1.04 g, 10 mmol) dissolved in dimethyl sulfoxide (10 ml) and $NiBr_2{\cdot}6H_2O$ (1.64 g, 5 mmol) dissolved in water (10 ml) were mixed and the pH was adjusted to about 5 by using NaOH solution (0.1 *M*) with stirring. The mixture was heated with stirring for half an hour and then cooled to room temperature. The filtrate was allowed to stand over a night, to generate two types of block crystals, one was colourless and another one was green.

Refinement

C-bound H atoms were geonetrically positioned (C—H = 0.96 Å) and treated as riding with $U_{iso}(H) = 1.5U_{eq}(C)$.

Figures

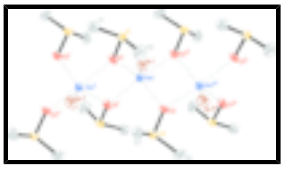


Fig. 1. Part of the structure of the title complex, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been ommited. [Symmetry codes: (i) 2 − *x*, 3/2 + *y*, 1/2 − *x*; (ii) −1 + *x*, *y*, *z*; (iii) 1 − *x*, 3/2 + *y*, 1/2 − *z*; (iv) 1 + *x*, *y*, *z*.]

catena-Poly[[bromidosodium(I)]-bis(μ-dimethyl sulfoxide-κ^2O:*O*)]

Crystal data

$[NaBr(C_2H_6OS)_2]$	F_{000} = 520
M_r = 259.16	D_x = 1.638 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7474 reflections
a = 6.433 (3) Å	θ = 6.4–55.0º
b = 9.969 (4) Å	μ = 4.30 mm^{-1}
c = 16.430 (6) Å	T = 291 (2) K
β = 94.046 (17)º	Block, colourless
V = 1051.0 (7) $Å^3$	0.21 × 0.20 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	2401 independent reflections
Radiation source: fine-focus sealed tube	1772 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 291(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -8 \rightarrow 8$
T_{min} = 0.461, T_{max} = 0.491	$k = -12 \rightarrow 12$
10170 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.072	$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 0.2048P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
2401 reflections	$\Delta\rho_{max}$ = 0.31 e $Å^{-3}$
95 parameters	$\Delta\rho_{min}$ = −0.40 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 $F^2 > \sigma(F^2)$ 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}
Br1	0.71849 (5)	0.19369 (3)	−0.13185 (2)	0.05075 (12)
C1	1.1343 (5)	0.4654 (3)	0.23986 (19)	0.0531 (8)
H3A	1.2370	0.3970	0.2335	0.080*
H3B	1.0944	0.4652	0.2951	0.080*
H3C	1.1916	0.5513	0.2275	0.080*
C2	0.7672 (6)	0.5765 (4)	0.1974 (2)	0.0704 (11)
H2A	0.8535	0.6549	0.1956	0.106*
H2B	0.7207	0.5664	0.2513	0.106*
H2C	0.6487	0.5860	0.1589	0.106*
C3	0.7631 (6)	0.8295 (3)	−0.0050 (3)	0.0635 (10)
H4A	0.6740	0.8410	0.0389	0.095*
H4B	0.8098	0.9157	−0.0224	0.095*
H4C	0.8813	0.7759	0.0132	0.095*
C4	0.4105 (6)	0.8611 (3)	−0.0979 (2)	0.0630 (10)
H1A	0.3125	0.8304	−0.1406	0.094*
H1B	0.4597	0.9487	−0.1111	0.094*
H1C	0.3437	0.8650	−0.0475	0.094*
Na1	0.74441 (16)	0.42912 (10)	−0.02932 (6)	0.0324 (2)
O2	0.5379 (3)	0.62069 (18)	−0.05373 (12)	0.0401 (5)
O1	0.9778 (3)	0.4577 (2)	0.08719 (11)	0.0397 (5)
S1	0.91242 (12)	0.43317 (7)	0.17235 (4)	0.03852 (18)
S2	0.62360 (12)	0.74854 (7)	−0.08747 (5)	0.04170 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0597 (2)	0.03973 (18)	0.0550 (2)	−0.00658 (15)	0.01907 (16)	−0.01221 (14)
C1	0.060 (2)	0.062 (2)	0.0368 (17)	−0.0069 (17)	0.0002 (16)	−0.0009 (15)
C2	0.072 (3)	0.085 (3)	0.056 (2)	0.025 (2)	0.016 (2)	−0.005 (2)
C3	0.048 (2)	0.049 (2)	0.092 (3)	−0.0068 (16)	−0.007 (2)	−0.0026 (19)
C4	0.068 (2)	0.0321 (16)	0.085 (3)	0.0036 (16)	−0.015 (2)	0.0140 (17)
Na1	0.0328 (6)	0.0304 (5)	0.0343 (6)	−0.0003 (4)	0.0049 (5)	0.0000 (4)
O2	0.0406 (11)	0.0259 (9)	0.0552 (12)	0.0003 (8)	0.0135 (10)	0.0082 (9)
O1	0.0377 (11)	0.0554 (12)	0.0268 (10)	−0.0104 (9)	0.0067 (8)	−0.0010 (9)
S1	0.0432 (4)	0.0430 (4)	0.0301 (4)	−0.0122 (3)	0.0079 (3)	−0.0019 (3)
S2	0.0504 (5)	0.0298 (4)	0.0465 (4)	−0.0020 (3)	0.0148 (4)	0.0052 (3)

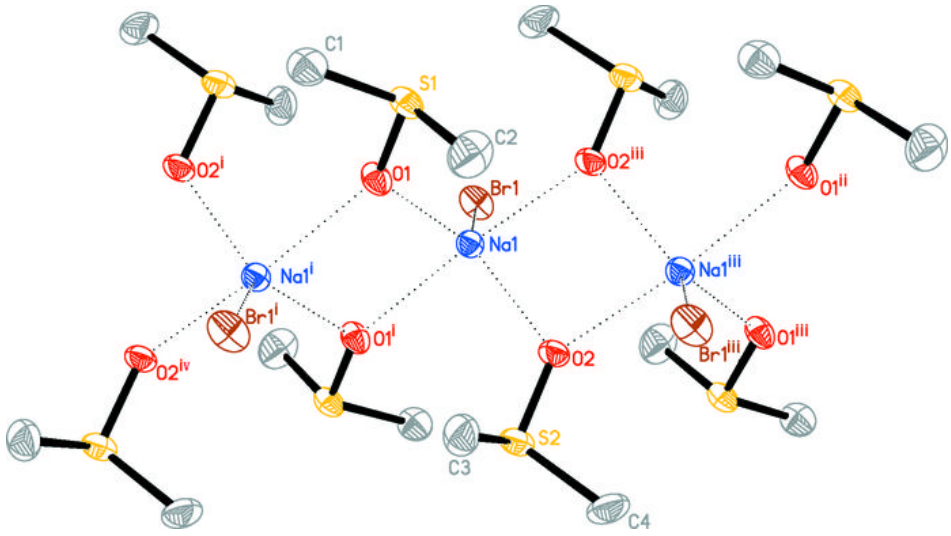
Geometric parameters (Å, °)

Na1—Br1	2.8869 (13)	C4—H1A	0.9600
C1—S1	1.774 (3)	C4—H1B	0.9600
C1—H3A	0.9600	C4—H1C	0.9600
C1—H3B	0.9600	Na1—O2	2.345 (2)
C1—H3C	0.9600	Na1—O1	2.365 (2)

C2—S1	1.772 (3)	Na1—O1^{i}	2.368 (2)
C2—H2A	0.9600	Na1—O2^{ii}	2.399 (2)
C2—H2B	0.9600	Na1—Na1^{ii}	3.639 (2)
C2—H2C	0.9600	Na1—Na1^{i}	3.646 (2)
C3—S2	1.767 (4)	O2—S2	1.5095 (19)
C3—H4A	0.9600	O2—Na1^{ii}	2.399 (2)
C3—H4B	0.9600	O1—S1	1.5093 (19)
C3—H4C	0.9600	O1—Na1^{i}	2.368 (2)
C4—S2	1.770 (3)		
S1—C1—H3A	109.5	O1^{i}—Na1—O2^{ii}	161.75 (8)
S1—C1—H3B	109.5	O2—Na1—Br1	123.62 (7)
H3A—C1—H3B	109.5	O1—Na1—Br1	125.28 (6)
S1—C1—H3C	109.5	O1^{i}—Na1—Br1	99.62 (6)
H3A—C1—H3C	109.5	O2^{ii}—Na1—Br1	98.55 (6)
H3B—C1—H3C	109.5	O2—Na1—Na1^{ii}	40.47 (5)
S1—C2—H2A	109.5	O1—Na1—Na1^{ii}	104.47 (7)
S1—C2—H2B	109.5	O1^{i}—Na1—Na1^{ii}	127.73 (7)
H2A—C2—H2B	109.5	O2^{ii}—Na1—Na1^{ii}	39.36 (5)
S1—C2—H2C	109.5	Br1—Na1—Na1^{ii}	117.05 (5)
H2A—C2—H2C	109.5	O2—Na1—Na1^{i}	102.64 (7)
H2B—C2—H2C	109.5	O1—Na1—Na1^{i}	39.66 (5)
S2—C3—H4A	109.5	O1^{i}—Na1—Na1^{i}	39.60 (5)
S2—C3—H4B	109.5	O2^{ii}—Na1—Na1^{i}	129.41 (7)
H4A—C3—H4B	109.5	Br1—Na1—Na1^{i}	118.90 (5)
S2—C3—H4C	109.5	Na1^{ii}—Na1—Na1^{i}	124.03 (6)
H4A—C3—H4C	109.5	S2—O2—Na1	122.25 (11)
H4B—C3—H4C	109.5	S2—O2—Na1^{ii}	133.96 (11)
S2—C4—H1A	109.5	Na1—O2—Na1^{ii}	100.17 (8)
S2—C4—H1B	109.5	S1—O1—Na1	121.89 (11)
H1A—C4—H1B	109.5	S1—O1—Na1^{i}	135.81 (12)
S2—C4—H1C	109.5	Na1—O1—Na1^{i}	100.74 (8)
H1A—C4—H1C	109.5	O1—S1—C2	105.70 (15)
H1B—C4—H1C	109.5	O1—S1—C1	106.60 (13)
O2—Na1—O1	111.08 (8)	C2—S1—C1	97.05 (18)
O2—Na1—O1^{i}	88.73 (8)	O2—S2—C3	106.45 (15)
O1—Na1—O1^{i}	79.26 (8)	O2—S2—C4	105.67 (15)
O2—Na1—O2^{ii}	79.83 (8)	C3—S2—C4	97.61 (18)
O1—Na1—O2^{ii}	91.58 (8)		

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

Fig. 1


C1
S1
C2
O2^{i}
O1
Br1
O2^{iii}
O1^{ii}
Na1
Na1^{i}
Na1^{iii}
Br1^{i}
Br1^{iii}
O1^{i}
O1^{iii}
O2^{iv}
O2
S2
C3
C4