Table 2. *Geometry of the hydrogen bonds (e.s.d.'s in parentheses)*

It is assumed that e.s.d.'s for H atoms in unrefined positions are ten times those of the atoms to which are attached.

D—H···A	D—H (Å)	H···A (Å)	D···A (Å)	∠D—H···A (°)
N(1)—H(5)···Cl(1^{i})	1·00 (3)	2·61 (3)	3·263 (3)	123 (3)
N(1)—H(5)···Cl(2^{i})		2·21 (3)	3·137 (3)	153 (3)
N(3)—H(12)···Cl(2^{ii})		2·63 (3)	3·336 (3)	129 (3)
N(3)—H(12)···Cl(1^{iii})		2·77 (3)	3·368 (3)	122 (4)
N(3)—H(12)···Cl(1^{iv})	1·00 (3)	2·62 (3)	3·285 (3)	121 (3)
N(4)—H(14)···Cl(4^{v})	1·00 (3)	2·15 (3)	3·137 (3)	170 (3)
N(2)—H(7)···O	1·00 (3)	1·96 (3)	2·897 (4)	155 (4)
O—H(1*w*)···Cl(4)	0·84 (2)	2·21 (3)	2·988 (3)	156 (4)
O—H(2*w*)···Cl(4^{v})	0·81 (2)	2·29 (3)	3·012 (3)	149 (3)
C(7)—H(6)···Cl(3)	1·00 (3)	2·54 (3)	3·422 (5)	147 (4)
C(7)—H(6)···Cl(1^{i})		2·86 (4)	3·382 (5)	113 (3)
C(14)—H(13)···Cl(3^{vi})	1·00 (3)	2·63 (3)	3·550 (5)	156 (3)

Symmetry code: (i) $-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (ii) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (iii) $1+x, -\frac{1}{2}-y, \frac{1}{2}+z$; (iv) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$; (v) $x, -1+y, z$; (vi) $1-x, -1-y, 1-z$.

puckering of the aromatic rings under the influence of hydrogen bonds. Benzimidazolium cations form stacked columns extending along the *y* axis. Short van der Waals contacts within both crystallographically independent columns are shown in Fig. 2. Four cationic columns surround each polymeric chain, forming a net of hydrogen bonds. Their geometry with calculated H-atom positions is illustrated in Table 2. The H(5) atom forms inequivalent bifurcated hydrogen bonds $\mathrm{N(1)—H(5)}\begin{smallmatrix}\cdot^{\cdot^{\cdot}}\mathrm{Cl(1^{i})}\\ \cdot_{\cdot_{\cdot}}\mathrm{Cl(2^{i})}\end{smallmatrix}$ of 2·21 (3) and 2·61 (3) Å. The H(12) atom is in the field of three Cl^- ions with distances H(12)—Cl(2^{ii}) 2·63 (3), H(12)—Cl(1^{iii}) 2·77 (3) and H(12)—Cl(1^{iv}) 2·62 (3) Å. The shortest H···Cl hydrogen bond is 2·15 (3) Å. C—H···Cl hydrogen bonds of 2·54 (3), 2·63 (3) and 2·86 (4) Å were observed. Symmetry codes are given in Table 2.

In order to explain the mechanism of reversible thermochromic properties of the crystals, a study of the structure of the orange form is planned.

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Structure of Disodium Ethylenebisdithiocarbamate Hexahydrate

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Abstract. $Na_2[S_2CNH(CH_2)_2HNCS_2].6H_2O$, $M_r = 364{\cdot}4$, triclinic, $P\bar{1}$, $a = 5{\cdot}781\ (4)$, $b = 7{\cdot}237\ (7)$, $c = 10{\cdot}063\ (12)$ Å, $\alpha = 88{\cdot}50\ (9)$, $\beta = 81{\cdot}60\ (8)$, $\gamma = 74{\cdot}24\ (7)°$, $V = 400{\cdot}8\ (7)$ Å^3, $Z = 1$, $D_m = 1{\cdot}51$, $D_x = 1{\cdot}51$ Mg m^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}6$ mm^{-1}, $F(000) = 190$, $T = 295$ K, $R = 0{\cdot}038$ for 1308 observed reflections. The geometry about Na^+ is distorted octahedral, consisting of five water molecules and one S atom from the organic ligand. Four bidentate water molecules form bridging units between two Na^+ cations on both sides of the organic anion and thus form an infinite chain structure. The ethylenebisdithiocarbamate ion acts as a bidentate ligand; each S atom is an acceptor of three hydrogen bonds.

Introduction. In complexes containing the $R_2NCS_2^-$ ligand, the geometry of the $>NCS_2$ moiety is dependent on the substituents R_2 as well as the actual coordination environment. It has previously been shown that for sodium dithiocarbamates, $Na[S_2CNR_2].nH_2O$, there is a strong correlation between the ligand bite and the bulkiness of the substituents R (Ymén, 1983). Although

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Table 1. *Final atomic coordinates with e.s.d.'s in parentheses and equivalent isotropic thermal parameters*

$$U_{\text{eq}} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	U_{eq}(Å^2)
Na	−0·2642 (2)	0·4470 (2)	0·0915 (1)	0·0403 (8)
S(1)	0·0787 (1)	0·0679 (1)	0·1664 (1)	0·0329 (5)
S(2)	0·0748 (1)	0·3321 (1)	0·3929 (1)	0·0349 (5)
O(1)	−0·5087 (4)	0·2719 (3)	0·0084 (3)	0·0420 (16)
O(2)	0·0288 (4)	0·6143 (4)	0·1329 (2)	0·0443 (17)
O(3)	−0·4743 (5)	0·5376 (3)	0·3147 (3)	0·0443 (16)
N	0·2991 (4)	−0·0368 (3)	0·3781 (2)	0·0327 (15)
C(1)	0·1641 (5)	0·1097 (4)	0·3174 (3)	0·0274 (16)
C(2)	0·3804 (6)	−0·0276 (5)	0·5077 (3)	0·0348 (19)

Table 2. *Selected distances* (Å), *bond angles* (°) *and torsion angles* (°) *with e.s.d.'s in parentheses*

The coordination polyhedron			
Na—S(1)	3·066 (1)	Na—O(3)	2·407 (3)
Na—O(1)	2·382 (3)	Na—O(1$^{\text{i}}$)	2·388 (3)
Na—O(2)	2·420 (3)	Na—O(2$^{\text{ii}}$)	2·445 (2)
S(1)—Na—O(1)	89·6 (1)	O(1)—Na—O(1$^{\text{i}}$)	88·5 (1)
S(1)—Na—O(2)	89·7 (1)	O(1)—Na—O(2$^{\text{ii}}$)	83·9 (1)
S(1)—Na—O(3)	96·9 (1)	O(2)—Na—O(3)	88·7 (1)
S(1)—Na—O(1$^{\text{i}}$)	169·3 (1)	O(2)—Na—O(1$^{\text{i}}$)	90·1 (1)
S(1)—Na—O(2$^{\text{ii}}$)	85·3 (1)	O(2)—Na—O(2$^{\text{ii}}$)	85·0 (1)
O(1)—Na—O(2)	168·9 (1)	O(3)—Na—O(1$^{\text{i}}$)	93·8 (1)
O(1)—Na—O(3)	102·4 (1)	O(3)—Na—O(2$^{\text{ii}}$)	173·3 (1)
The ethylenebisdithiocarbamate ligand			
S(1)—C(1)	1·722 (3)	C(1)—N	1·328 (3)
S(2)—C(1)	1·712 (3)	C(2)—N	1·458 (4)
S(1)···S(2)	3·007 (1)	C(2)—C(2$^{\text{iii}}$)	1·527 (6)
S(1)—C(1)—S(2)	122·2 (2)	C(1)—N—C(2)	125·6 (3)
S(1)—C(1)—N	118·6 (2)	C(1)—S(1)—Na	106·3 (1)
S(2)—C(1)—N	119·2 (2)	S(1)—C(1)—N—C(2)	−178·0 (2)
N—C(2)—C(2$^{\text{iii}}$)	111·5 (3)	C(1)—N—C(2)—C(2$^{\text{iii}}$)	−87·4 (4)
The hydrogen bonds			
S(1)···O(1$^{\text{iv}}$)	3·309 (3)	S(2)···O(2)	3·273 (2)
S(1)···O(1$^{\text{v}}$)	3·329 (3)	S(2)···O(3$^{\text{v}}$)	3·327 (3)
S(1)···O(2$^{\text{vi}}$)	3·402 (3)	S(2)···O(3)	3·318 (3)
O(3)···N$^{\text{vii}}$	3·046 (3)		

O—H range: 0·727 (40) – 0·957 (31) Å.

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

the crystal structures of four Na(dtc).nH$_2$O complexes have been determined: Na[S$_2$CN(C$_2$H$_5$)$_2$].3H$_2$O (Colapietro, Domenicano & Vaciago, 1968); Na[S$_2$CN(CH$_2$)$_4$].2H$_2$O (Albertsson, Oskarsson, Stahl, Svensson & Ymén, 1980); Na[S$_2$CN(C$_3$H$_7$)$_2$].5H$_2$O (Ymén, 1983); and Na[S$_2$CN(CH$_3$)$_2$].2H$_2$O (Oskarsson & Ymén, 1983), to date no information on the bonding and structural properties is available for bisdithiocarbamate complexes, especially for those of type M_2[S$_2$CNH(CH$_2$)$_n$HNCS$_2$].nH$_2$O with central ion Li$^+$, Na$^+$, K$^+$ or NH$_4^+$. This paper reports the structure of Na$_2$[S$_2$CNH(CH$_2$)$_2$HNCS$_2$].6H$_2$O.

Experimental. The title compound was prepared by dissolving stoichiometric quantities of NH$_2$(CH$_2$)$_2$NH$_2$, CS$_2$ and NaOH in water. Crystals were obtained by addition of acetone to the solution. Recrystallization from aqueous solution gave colourless plates at 323 K. Found: N, 7·83; C, 13·24; H, 4·94%. Calc.: N, 7·69; C, 13·19; H, 4·98%. To obtain the intensity data a crystal 0·05 × 0·1 × 0·2 mm was chosen. Density measured by flotation (C$_2$H$_5$Br–CHCl$_3$). The approximate values of the lattice parameters, calculated from rotation and Weissenberg patterns, were refined on a Syntex $P2_1$ four-circle diffractometer by a least-squares procedure from ten precisely centred reflections using Mo $K\alpha$ radiation. Intensities collected in range $0 < 2\theta < 50°$ yielding 1852 independent reflections, 1308 with $I \geq 2{\cdot}00\sigma(I)$, index range h ±7, k ±9, l 0→12, were considered as observed and used in the structure solution, 118 parameters. All intensities corrected for Lorentz and polarization effects. No corrections for absorption or secondary extinction. Structure solved by heavy-atom method. H atoms located from difference Fourier synthesis. Structure refined to $R = 0{\cdot}038$ and $wR = 0{\cdot}044$ using full-matrix least squares, minimizing function $M = \sum w(|F_o| - |F_c|)^2$ with weights $w = 1{\cdot}291/[\sigma^2(F) + 0{\cdot}0006|F_o|^2]$. Positions of H atoms were refined with isotropic temperature factors. Heavier atoms refined anisotropically. Max. and min. heights in final difference Fourier synthesis 0·39 and −0·32 e Å^{-3}. $(\Delta/\sigma)_{\max} = 0{\cdot}186$. Scattering factors from *International Tables for X-ray Crystallography* (1974). All calculations carried out on a Siemens 4004/150 computer using the *NRC* crystallographic programs (Ahmed, 1970) and *SHELX76* (Sheldrick, 1976).

Discussion. The final positional parameters for the non-H atoms are given in Table 1* and selected distances and angles in Table 2. A view of the structure projected along **a** is shown in Fig. 1. The crystal structure consists of an infinite polymeric chain of Na$_2$[S$_2$CNH(CH$_2$)$_2$HNCS$_2$].6H$_2$O units connected by

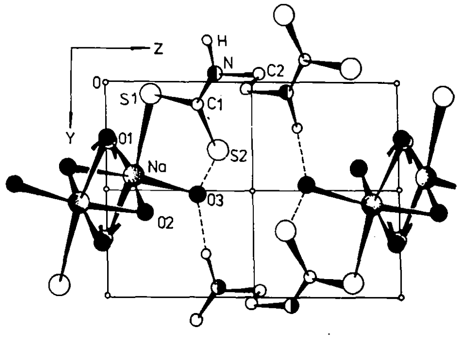

Fig. 1. View of the structure along **a**.

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[*] Lists of anisotropic thermal parameters for the non-H atoms, isotropic thermal parameters and coordinates of the H atoms, least-squares planes and deviations from them and lists of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44224 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

four water-molecule bridges at each end of the organic anion. The Na^+ ions and water molecules are situated along **a**. In addition to one S atom at 3·066 (1) Å, the Na^+ ion is coordinated by five water O atoms at distances ranging from 2·382 (3) to 2·445 (2) Å forming a distorted octahedron. The other S atom of the anion ligand is outside the sodium coordination sphere, being situated 3·801 (1) Å from the Na^+ ion, which lies close to the centre of the square plane formed by O(1), O(2), O(3), $O(2^{ii})$ (O—Na—O angles range from 83·9 to 102·4°). The deviation of the Na^+ ion from this plane is 0·028 (1) Å. Each S atom accepts three hydrogen bonds from the H_2O molecules with O···S distances in the range 3·273 (2) to 3·402 (3) Å and H···S distances from 2·40 (5) to 2·69 (4) Å. Along the **bc** diagonal the structure is held together by O(3)···H—N hydrogen bonds, 2·30 (4) Å. The geometry of the organic ligand in the title compound may be compared with the corresponding parts in $Na[S_2CH(CH_2)_4].2H_2O$ (Albertsson *et al.*, 1980; Ymén, 1982), $Na[S_2CN(CH_3)_2].2H_2O$ (Oskarsson & Ymén, 1983) and $Na[S_2CN(C_3H_7)_2].5H_2O$ (Ymén, 1983). The difference in length between the S(1)—C(1) and S(2)—C(1) bonds, $3{\cdot}3\tau$, is only possibly significant in spite of the fact that S(1) is within the sodium coordination sphere and S(2) is not. This is consistent with the ionic character of the Na—S(1) interaction. A typical feature of the compounds with ionic metal–ligand interactions is a larger ligand bite angle S—C—S (120–122°) than in the dithiocarbamates of *d*-group metals. For Na dithiocarbamates this ligand bite angle decreases very significantly as the substituents R_2 in $-S_2CNR_2$ become bulkier (Ymén, 1983). This was interpreted as the result of C—H···S intramolecular steric interactions between the substituents and the S atoms. S(1) and S(2) are pushed closer together the more bulky the substituents are. In the title compound the S(1)—C—S(2) angle [122·2 (2)°] is similar to that found in $Na[S_2CN(CH_2)_4].2H_2O$. The high degree of π conjugation in the S_2CNHC ligand fragment is reflected in the near-planarity of this fragment, the small (but significant) deviations from planarity being indicative of a small twist (2°) about the C(1)—N bond. C(2) and H(N) lie on opposite sides of the S_2CN plane at −0·037 (3) and 0·055 (7) Å, respectively.

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Structure of Polymeric Pyridinium Pentachlorodicadmate(II)*†

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Abstract. $[C_5H_6N^+.Cd_2Cl_5^-]_n$, $M_r = 482{\cdot}175n$, orthorhombic, $Pmmn$, $a = 15{\cdot}2175$ (6), $b = 3{\cdot}7897$ (2), $c = 10{\cdot}3138$ (4) Å, $V = 594{\cdot}75$ (5) Å^3, $Z = 2$, $D_x = 2{\cdot}691$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha_1) = 1{\cdot}54056$ Å, $\mu = 396{\cdot}8$ cm^{-1}, $F(000) = 448$, $T = 296$ (1) K. Final $R(F) = 0{\cdot}050$ for 626 counter data with $F_o^2 \geq 2\sigma(F_o^2)$. Cd atoms are on crystallographic mirror planes at $y = 0$ or $\frac{1}{2}$; Cl^- ions form distorted octahedra about them. These octahedra share edges in the **b** direction and corners in the **a** direction to give a two-dimensional polymeric network. The $C_5H_5NH^+$ ions are each hydrogen bonded to a neighboring Cl atom with the $N—H\cdots Cl^-$ linkages parallel to the z direction. The four independent Cd—Cl distances are 2·561 (1), 2·585 (2), 2·668 (2) and 2·723 (1) Å and Cl—Cd—Cl angles range from 83·38 (6) to 94·48 (10)° for *cis*-related Cl atoms.

Introduction. Among transition-metal–nucleotide complexes that have been structurally characterized, two of them are those with uridine monophosphate (UMP): $[Co_2(H_2O)_4(5'\text{-}UMP)_2]_n$ (Cartwright, Goodgame, Jeeves

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