

The two phenyl groups are planar with the following coefficients of the plane equations (the phenyl-phenyl angle is 76°):

	C(3)–C(8) phenyl	C(9)–C(14) phenyl
A	1.118 ± 0.086	-1.147 ± 0.090
B	1.806 ± 0.138	-2.156 ± 0.165
C	2.102 ± 0.161	1.480 ± 0.114
D	-1.363 ± 0.108	-6.276 ± 0.485

The mean distances of the phenyl C atoms (distances in parentheses are for the P atom) from the plane are 0.01 (0.01 Å) for the first phenyl and 0.03 (0.11 Å) for the second phenyl.

References

- BAILEY, M. & BROWN, C. J. (1967). *Acta Cryst.* **22**, 387–391.
- BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1964). *ORFFE*. Report ORNL-TM-306. Oak Ridge National Laboratory, Tennessee.
- CHURCHILL, M. R. & KALRA, K. L. (1974). *Inorg. Chem.* **13**, 1427–1434.
- CRUICKSHANK, D. W. J., PILLING, D. E., BUJOSA, A., LOVELL, F. M. & TRUTER, M. R. (1961). *Computing Methods and the Phase Problem in X-ray Crystal Analysis*. Oxford: Pergamon Press.
- HOUSTY, J. & HOSPITAL, M. (1965). *Acta Cryst.* **18**, 693–697.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
- PAYNE, D. S., MOKUOLO, J. A. A. & SPEAKMAN, J. C. (1965). *Chem. Commun.* p. 599.
- ROBINSON, D. J. & KENNARD, C. H. L. (1970). *J. Chem. Soc. A*, pp. 1008–1012.
- RŮŽIČKOVÁ, J. & PODLAHOVÁ, J. (1978). *Coll. Czech. Chem. Commun.* To be published.
- SALES, D. L., STOKES, J. & WOODWARD, P. (1968). *J. Chem. Soc. A*, pp. 1852–1858.
- SIM, G. A., ROBERTSON, J. M. & GOODWIN, T. H. (1955). *Acta Cryst.* **8**, 157–164.
- SKLENÁŘ, I. (1973). Programs *TLS*, *ÚFPL ČSAV*, Prague.

Acta Cryst. (1979). **B35**, 330–334

The Structure of a Complex between Rubidium Thiocyanate, Water and Dibenzo- $[b,q][1,4,7,10,13,16,19,22,25,28]$ decaoxacyclotriacontane (Dibenzo-30-crown-10)

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Abstract

The crystal and molecular structure of dibenzo-30-crown-10. $\text{RbSCN} \cdot \text{H}_2\text{O}$ [$\text{Rb}(\text{C}_{28}\text{H}_{40}\text{O}_{10})\text{SCN} \cdot \text{H}_2\text{O}$, $\text{C}_{28}\text{H}_{40}\text{O}_{10}\text{Rb}^+ \cdot \text{SCN}^- \cdot \text{H}_2\text{O}$] has been determined by the heavy-atom method and refined to $R_1 = 0.046$ for 3251 observed reflexions measured with a Syntex $P2_1$ diffractometer. The cell is monoclinic, space group $P2_1/c$, with $a = 13.596$ (3), $b = 12.411$ (3), $c = 21.869$ (7) Å, $\beta = 114.36$ (2)°, $V = 3362$ (2) Å³, $Z = 4$. The macroring surrounds the Rb^+ cation. The SCN^- anions and water molecules form infinite chains and have no direct contact with the Rb^+ atom.

Introduction

One of the characteristic features of macrocyclic polyethers exists in their ability to form complexes with various inorganic cations, bound by ion-dipole interactions with electronegative O atoms in the macroring.

The structure of the title compound has been studied as part of the systematic investigation of the proper-

ties of macrocyclic polyethers containing 1,4,7,10-, 13,16-hexaoxacyclooctadecane (18-crown-6) and 1,4,7,10,13,16,19,22,25,28-decaoxacyclotriacontane (30-crown-10) (Hašek & Huml, 1975, 1976, 1978; Hašek, Hlavatá & Huml, 1977; Hlavatá, Hašek & Huml, 1978).

Experimental

The crystals (white) were prepared by Petránek & Ryba (1974). The molecular formula was confirmed by elemental analysis. All measurements were performed at room temperature.

Crystal data

$\text{C}_{28}\text{H}_{40}\text{O}_{10}\text{Rb}^+ \cdot \text{SCN}^- \cdot \text{H}_2\text{O}$, monoclinic, $P2_1/c$, $a = 13.596$ (3), $b = 12.411$ (3), $c = 21.869$ (7) Å, $\beta = 114.36$ (2)°, $V = 3362$ (2) Å³, $Z = 4$, $D_c = 1.38$, $D_m = 1.37$ Mg m⁻³ (flotation in heptane- CCl_4 solution), FW 680.1, m.p. 393–394 K, $F(000) = 1456$, $\mu(\text{Cu } K\alpha) = 3.28$ mm⁻¹.

Systematic absences (for $Ok0$: $k = 2n + 1$ and for $h0l$: $l = 2n + 1$) were determined from Weissenberg photographs and confirmed by the ψ scan with the Syntex $P2_1$ diffractometer. The unit-cell parameters (15 reflexions refined) and intensities were measured with the same four-circle diffractometer (Cu $K\alpha$, $\lambda = 1.54178$ Å, graphite monochromator in the equatorial arrangement, $\theta-2\theta$ scan). A crystal was ground to a sphere with $r = 0.15$ mm and was placed on the goniometric head in a general position. 4377 independent reflexions were measured up to $\sin \theta/\lambda = 0.56$ Å⁻¹; 3251 of these were classed as observed with $I > 4\sigma_I$, where σ_I was calculated from counting statistics.* No pronounced decrease in the intensities of reference reflexions (measured after every 30 reflexions) was observed. Correction was made for absorption in a spherical sample ($\mu r = 0.5$), but not for extinction. For the L_p correction formula and other measurement details see Hašek, Hlavatá & Huml (1977).

Structure determination and refinement

The position of the cation was determined from the sharpened Patterson map. In the following difference map, 20 ligand atoms were localized. After three cycles of block-diagonal least-squares refinement with the modified NRC 10 program (Ahmed, Hall, Pippy & Huber, 1966) all the remaining non-hydrogen atoms were found in the electron density map, except the SCN group. After several more cycles of isotropic refinement, the difference map showed only a row of overlapping maxima, 5–7 e Å⁻³ high. Thus we suppose that the SCN group is situated here, but it is disordered so that it occupies two positions in which the N and S atoms are interchangeable.

Instead of S and N, two fictitious atoms, N(40) and N(42), were involved in a further refinement with which the occupation factors were refined. We started with both occupation factors being 1.65, corresponding to an equal amount of both orientations. Although the occupation factors were further refined independently, the sum of both remained preserved, being 3.3.

Firstly the C atom from the SCN group was refined in both possible positions (there is a great difference between C–N 1.1 Å and S–C 1.6 Å) with the occupation factor 0.5, but one of the atoms slipped into an unrealistic position and its B_{iso} value increased rapidly. Therefore only one atom, labelled C(41), with the fixed occupation factor 1.0 was further refined as the C atom of the SCN group.

* Lists of structure factors and all refined coordinates and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34013 (48 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Subsequent refinement showed that this model is adequate as a rough description of the position of the SCN group in spite of the fact that it cannot give its precise atomic coordinates.

At this stage of refinement, Professor M. R. Truter drew our attention to the presence of the water of crystallization. The O of the water molecule, O(43), was placed at the highest maximum (1.0 e Å⁻³) on the difference map and the R_1 factor dropped from 0.076 to 0.046. To save computing expenses, at this stage we stopped the refinement of H(51), H(82), H(241), H(281), H(311) which have distances between their refined and ideal positions larger than 0.25 Å; they were fixed in theoretically expected positions leaving their B_{iso} unchanged. The water H atoms were calculated in the directions of the S and N atoms of neighbouring thiocyanate groups. Four subsequent refinements led to shifts of all non-hydrogen atomic parameters less than 0.15 of their e.s.d.'s.

The atomic scattering factors of C, N and O atoms were taken from *International Tables for X-ray Crystallography* (1962). The Rb atom was regarded as singly ionized in the relativistic Hartree–Fock approximation (Doyle & Turner, 1968). The scattering factors of the H atoms were taken as a spherical approximation of the bonded atom in the hydrogen molecule (Stewart, Davidson & Simpson, 1965).

The structure was refined by the least-squares method in the block-diagonal approximation [9×9 for the non-hydrogen atoms, except 10×10 for N(40) and N(42), and 4×4 for the H atoms]. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 4I[\sigma_I^2 + (0.04I)^2]^{-1}$.

At the final stage, $n = 390$ parameters were refined and all the $m = 3251$ observed reflexions were used. This led to

$$R_1 = \frac{\sum (|F_o| - |F_c|)}{\sum |F_o|} = 0.046,$$

$$RW_2 = \left[\frac{\sum w(|F_o| - |F_c|)^2}{\sum w|F_o|^2} \right]^{1/2} = 0.064,$$

$$S = \left[\frac{\sum w(|F_o| - |F_c|)^2}{(m - n)} \right]^{1/2} = 2.3.$$

Five of the highest maxima on the corresponding difference map (from 0.7 to 0.8 e Å⁻³) are near the disordered SCN group, while two maxima lie between the C(21), C(22) and C(28), O(29) atoms. The refined positional parameters of C(21) and C(22) appeared to be unrealistic (distance 1.27 Å). The difference map based on F_c calculated without C(21) and C(22) showed two appropriate maxima, but on including them in the input data, the refinement procedure failed again. Therefore in the calculation of the molecular geometry the coordinates of C(21) and C(22) from the difference map were used.

Final positional parameters and B_{eq} thermal parameters (Hamilton, 1959) of non-hydrogen atoms are given in Table 1; those of the H atoms are given in

Table 2.* Occupation factors of N(40) and N(42) were refined to 1.9 and 1.4 respectively, which gives 3:2 in favour of the SCN group orientation having the S atom on site N(40). Therefore, in the following discussion the position N(40) is labelled as S(40), although the refined coordinates of S(40), C(41) and N(42) cannot be considered as real atomic coordinates.

* See deposition footnote on p. 331.

It seems that the B_{eq} thermal parameters (Table 1) are in our case greatly influenced by effects that cannot be well approximated by harmonic thermal motion of the atoms. It is to be expected that in the case of atoms with higher B_{eq} values the real difference from the refined position may be several times larger than published e.s.d.'s (B_{eq} in the range 5.1–9.3 Å² for well determined atoms, 10–16 Å² for the more poorly localized atoms of the macroring and from 10–28 Å²

Table 1. Fractional coordinates for non-hydrogen atoms and their e.s.d.'s ($\times 10^4$) and B_{eq} (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	B_{eq}		<i>x</i>	<i>y</i>	<i>z</i>	B_{eq}
O(1)	1812 (2)	4331 (3)	4920 (2)	6.3	O(23)	1057 (3)	835 (4)	4598 (2)	9.5
C(2)	2836 (4)	4802 (4)	5324 (3)	7.4	C(24)	897 (6)	−114 (6)	4218 (5)	10.9
C(3)	3225 (4)	5375 (5)	4896 (3)	7.6	C(25)	70 (6)	59 (6)	3571 (4)	10.0
O(4)	3409 (2)	4644 (3)	4465 (2)	6.7	O(26)	465 (3)	798 (4)	3211 (2)	9.0
C(5)	3689 (5)	5201 (5)	3978 (4)	8.2	C(27)	−214 (6)	1008 (7)	2564 (4)	10.3
C(6)	3764 (4)	4446 (5)	3496 (3)	7.6	C(28)	−976 (5)	1805 (8)	2514 (4)	11.0
O(7)	2678 (2)	4094 (3)	3074 (2)	6.5	O(29)	−438 (3)	2890 (4)	2785 (2)	8.9
C(8)	2645 (5)	3538 (5)	2492 (3)	7.7	C(30)	−1135 (4)	3569 (5)	2968 (3)	8.5
C(9)	3190 (4)	2473 (5)	2646 (3)	6.6	C(31)	−1092 (4)	3331 (5)	3635 (3)	7.1
O(10)	2683 (2)	1821 (3)	2974 (2)	5.8	O(32)	−47 (2)	3653 (3)	4122 (2)	6.2
C(11)	3242 (4)	831 (4)	3252 (3)	6.1	C(33)	186 (4)	3559 (4)	4795 (3)	5.2
C(12)	4215 (3)	1013 (4)	3906 (2)	5.8	C(34)	−522 (4)	3152 (5)	5050 (3)	6.6
O(13)	3839 (2)	1385 (2)	4385 (1)	5.5	C(35)	−172 (5)	3120 (5)	5753 (3)	6.8
C(14)	4590 (3)	1608 (3)	5023 (2)	5.8	C(36)	818 (5)	3467 (5)	6173 (4)	7.9
C(15)	5701 (4)	1617 (4)	5208 (3)	7.0	C(37)	1514 (5)	3884 (5)	5900 (3)	6.9
C(16)	6374 (4)	1840 (5)	5881 (3)	8.9	C(38)	1199 (4)	3938 (4)	5219 (3)	5.9
C(17)	5970 (5)	2059 (4)	6330 (4)	9.3	Rb(39)	1821 (0)	2728 (0)	3908 (8)	5.1
C(18)	4883 (5)	2075 (4)	6150 (3)	7.9	S(40)	6584 (3)	1192 (2)	3150 (2)	10.0
C(19)	4190 (4)	1837 (4)	5493 (2)	5.9	C(41)	6479 (10)	2124 (9)	3468 (13)	23.3
O(20)	3085 (3)	1865 (3)	5296 (2)	6.6	N(42)	6224 (7)	2912 (9)	3436 (7)	28.3
C(21)*	2733 (−)	927 (−)	5541 (−)	10.6	O(43)	4155 (6)	4799 (10)	7042 (4)	23.1
C(22)*	1612 (−)	855 (−)	5348 (−)	15.6					

* The coordinates of C(21) and C(22) are taken from a difference map.

Table 2. Fractional coordinates of hydrogen atoms ($\times 10^3$) and their e.s.d.'s and B_{iso} (Å²)

The atoms marked with an asterisk are in their ideal calculated positions.

	<i>x</i>	<i>y</i>	<i>z</i>	B_{iso}		<i>x</i>	<i>y</i>	<i>z</i>	B_{iso}
H(21)	276 (3)	519 (3)	562 (2)	7.7	H(242)	174 (5)	−24 (6)	429 (4)	16.1
H(22)	324 (3)	425 (4)	555 (2)	8.0	H(251)	−61 (4)	30 (4)	360 (3)	11.5
H(31)	401 (3)	581 (4)	512 (2)	8.8	H(252)	0 (4)	−50 (5)	336 (3)	13.0
H(32)	260 (4)	593 (4)	455 (2)	9.8	H(271)	−61 (4)	29 (4)	225 (3)	10.2
H(51)*	442 (−)	558 (−)	422 (−)	10.3	H(272)	11 (6)	135 (6)	226 (4)	17.2
H(52)	312 (4)	577 (5)	376 (3)	13.3	H(281)*	−140 (−)	156 (−)	277 (−)	14.9
H(61)	432 (5)	388 (5)	375 (3)	14.2	H(282)	−150 (5)	191 (5)	214 (3)	14.1
H(62)	411 (5)	481 (5)	313 (3)	14.3	H(301)	−106 (4)	426 (4)	295 (3)	11.5
H(81)	307 (3)	403 (4)	233 (2)	9.5	H(302)	−180 (3)	349 (4)	268 (2)	8.1
H(82)*	188 (−)	345 (−)	217 (−)	12.4	H(311)*	−166 (−)	376 (−)	371 (−)	13.8
H(91)	393 (3)	248 (3)	295 (2)	6.4	H(312)	−116 (3)	245 (3)	367 (3)	7.6
H(92)	312 (3)	205 (4)	223 (2)	8.2	H(151)	602 (3)	163 (3)	483 (2)	6.7
H(111)	273 (3)	23 (4)	337 (2)	8.5	H(161)	711 (4)	184 (4)	593 (3)	10.6
H(112)	360 (3)	52 (4)	295 (2)	9.6	H(171)	643 (5)	220 (5)	679 (3)	12.8
H(121)	454 (3)	29 (3)	399 (2)	7.6	H(181)	457 (4)	217 (4)	654 (3)	11.9
H(122)	464 (2)	149 (3)	380 (2)	5.7	H(341)	−118 (3)	287 (3)	468 (2)	5.3
H(211)	306 (4)	91 (6)	599 (3)	13.1	H(351)	−61 (6)	275 (6)	591 (4)	15.3
H(212)	305 (6)	26 (7)	546 (4)	18.6	H(361)	102 (5)	334 (6)	667 (3)	14.5
H(221)	150 (7)	135 (9)	555 (5)	23.4	H(371)	218 (4)	418 (5)	614 (3)	11.5
H(222)	144 (3)	6 (4)	550 (2)	8.8	H(431)*	403 (−)	556 (−)	688 (−)	25.0
H(241)*	66 (−)	−71 (−)	443 (−)	12.5	H(432)*	487 (−)	451 (−)	737 (−)	25.0

for the disordered atoms of the SCN group and the water molecule).

Structure description and discussion

The numbering scheme and selected interatomic distances and angles are shown in Fig. 1. The macroring (Fig. 2) surrounds the Rb⁺ cation like the seam on a tennis ball [compare with dibenzo-30-crown-10. KI in Bush & Truter (1972)].

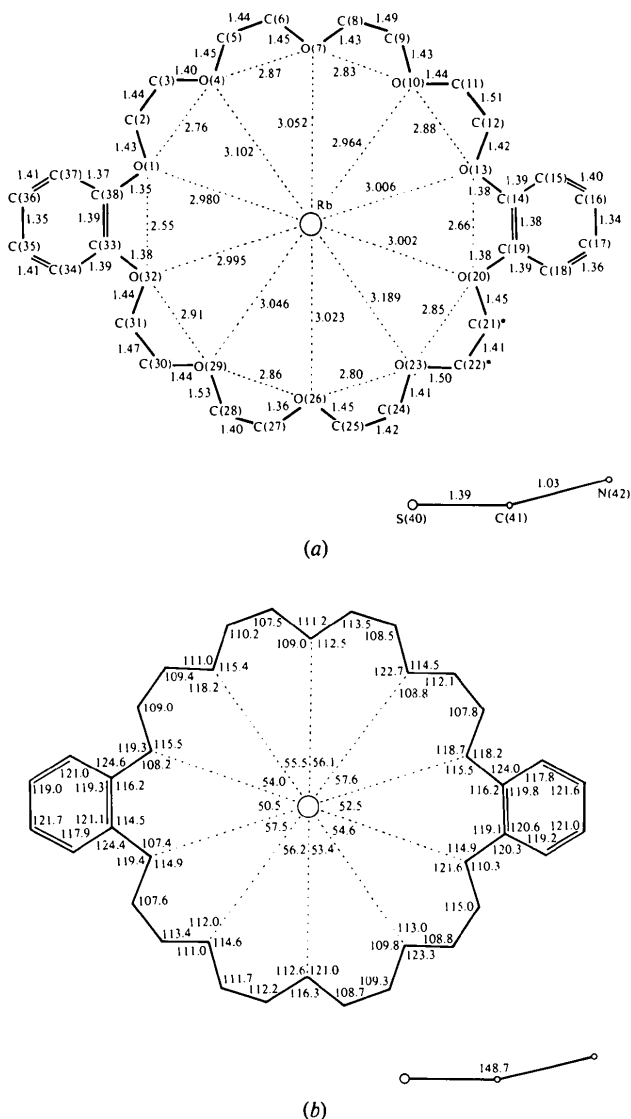


Fig. 1. The numbering scheme of dibenzo-30-crown-10.RbSCN.H₂O showing (a) bond lengths (Å) and (b) some angles (°) for non-hydrogen atoms. E.s.d.'s: Rb...O distances, 0.004 Å; adjacent O atoms in the macroring, 0.006 Å; bond distances in the macroring, 0.005–0.012 Å; angles Rb...O–C type, 0.2°; interbond angles in the macroring, 0.3–0.9°; distances between refined points in SCN group, 0.2 Å, and corresponding angle 2.0°.

The Rb⁺...O distances lie between 2.96 and 3.19 Å. Their mean value (3.04 Å) is in good agreement with the respective values in the crown-type structures, e.g. 3.02, 3.02, 3.00 Å (Dobler & Phizackerley, 1974; Hašek & Huml, 1978; Hlavatá, Hašek & Huml, 1978). In the vicinity of the phenyl groups O(1)...O(32) and O(13)...O(20) give rather short contacts (mean 2.60 Å). The distances between other neighbouring O atoms of the macroring (mean 2.84 Å) are only a little longer than the van der Waals contacts. The bond distances and angles around C(14), C(19), C(33) and C(38) are very close to values in the complexes mentioned above.

Distances C(sp³)–O are from 1.41 to 1.45, mean 1.44 Å, except two bonds, at C(27), 1.36, and at C(29), 1.53 Å. These differences are ascribed to the inaccuracy of the description of the disordered SCN group of atoms in the crystal.

Bond distances C(sp³)–C(sp³) (from 1.40 to 1.49, mean 1.45 Å) are too short for the expected single C–C bond. This effect which is observed with all crown-type structures can be partly ascribed to a specific thermal motion of atoms in the macroring, but a satisfactory explanation has not been given up to now. For a discussion see Dunitz, Dobler, Seiler & Phizackerley (1974) and Goldberg (1975).

Table 3 gives details of some weighted mean planes. Atoms C(2) and C(31) lie approximately in the plane of the neighbouring benzene ring, in accordance with structures containing benzo-1,4,7,10,14,17-hexaoxacyclooctadecane (Hašek, Hlavatá & Huml, 1977; Hlavatá, Hašek & Huml, 1978; Hašek & Huml, 1978). However, in the case of the second benzene ring, the atoms C(12) and especially C(21) exhibit large deviations from the benzene plane.

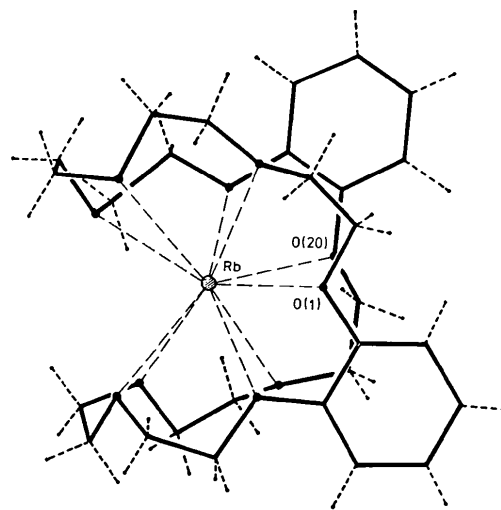


Fig. 2. The macroring of dibenzo-30-crown-10.RbSCN.H₂O around the Rb cation viewed along the line through the centres of group O(1), O(4), O(7), O(29), O(32) and group O(10), O(13), O(20), O(23), O(26).

Table 3. Angles between some weighted mean planes in dibenzo-30-crown-10.RbSCN.H₂O

Plane	Atoms defining mean plane and their deviations (Å)						χ^2
<i>a</i>	C(14)	C(15)	C(16)	C(17)	C(18)	C(19)	10.2
	0.00	0.01	-0.01	-0.01	0.01	0.00	
<i>b</i>	C(33)	C(34)	C(35)	C(36)	C(37)	C(38)	6.4
	-0.01	0.00	0.01	-0.01	0.00	0.01	
<i>c</i>	O(1)	O(4)	O(7)	O(32)			8.7
	-0.01	0.01	0.00	0.00			
<i>d</i>	O(1)	O(4)	O(7)	O(29)	O(32)		2881.4
	-0.04	-0.05	0.08	-0.15	0.10		
<i>e</i>	O(13)	O(20)	O(23)	O(26)			3994.1
	-0.10	0.22	-0.37	0.26			
<i>f</i>	O(10)	O(13)	O(20)	O(23)	O(26)		47743.5
	0.31	-0.44	0.48	-0.18	-0.19		

Some angles between planes (°): *a*-*b* 29.9, *d*-*f* 14.3, *a*-*f* 20.0, *b*-*d* 18.4, *c*-*e* 5.9.

Deviations from plane *a* (Å): C(12) -0.19, O(13) -0.01, O(20) 0.04, C(21) -1.26.

Deviations from plane *b* (Å): C(2) 0.12, O(1) 0.02, O(32) 0.01, C(31) 0.05.

The SCN anions and water molecules form infinite chains (Fig. 3). The short distance between O(43) of the water molecule and C(11) of the macroring, 3.44 (1) Å, and the angle C(11)-H(112)-O(43) of 164 (1)° indicate a weak hydrogen bond.

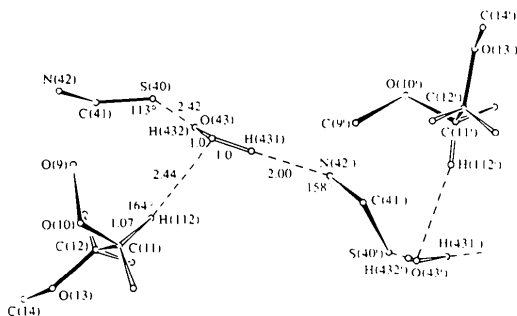


Fig. 3. The infinite chain formed by thiocyanate groups and water molecules viewed perpendicular to the plane through C(21), N(42) and O(43) atoms. Short contacts are denoted by dashed lines.

The result of the SCN group refinement may be interpreted by assuming that in this group two possible orientations prevail, arising by a rotation along the centre of gravity by approximately 120°, one of which has 60% occupation and the other 40%. This can also quantitatively explain the apparent shortening of the S-C bonds (expected value 1.62 Å) and C-N bonds (expected value 1.15 Å), as well as the apparent S-C-N angle.

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References

- AHMED, F. R., HALL, S. R., PIPPY, M. E. & HUBER, C. P. (1966). NRC Crystallographic Programs for the IBM/360 System. National Research Council, Ottawa, Canada.
- BUSH, M. A. & TRUTER, M. R. (1972). *J. Chem. Soc. Perkin Trans. 2*, pp. 345-349.
- DOBLER, M. & PHIZACKERLEY, R. P. (1974). *Acta Cryst.* **B30**, 2746-2748.
- DOYLE, P. A. & TURNER, P. S. (1968). *Acta Cryst.* **A24**, 390-397.
- DUNITZ, J. D., DOBLER, M., SEILER, P. & PHIZACKERLEY, R. P. (1974). *Acta Cryst.* **B30**, 2733-2750.
- GOLDBERG, I. (1975). *Acta Cryst.* **B31**, 754-762.
- HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609-610.
- HAŠEK, J., HLAVATÁ, D. & HUML, K. (1977). *Acta Cryst.* **B33**, 3372-3376.
- HAŠEK, J. & HUML, K. (1975). *Z. Kristallogr.* **141**, 158-159.
- HAŠEK, J. & HUML, K. (1976). *Z. Kristallogr.* **144**, 142-143.
- HAŠEK, J. & HUML, K. (1978). *Acta Cryst.* **B34**, 1812-1814.
- HLAVATÁ, D., HAŠEK, J. & HUML, K. (1978). *Acta Cryst.* **B34**, 416-420.
- International Tables for X-ray Crystallography* (1962). Vol. III, pp. 275-276. Birmingham: Kynoch Press.
- PETRÁNEK, J. & RYBA, O. (1974). *Collect. Czech. Chem. Commun.* **39**, 2033-2036.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175-3187.