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The Crystal and Molecular Structure of 3-(2-Diethylammoniumethoxy)-1,2-benzisothiazole Tetrachlorocobaltate

BY A. CORRADI BONAMARTINI, M. NARDELLI AND C. PALMIERI

Istituto di Chimica Generale, Università di Parma, Parma, Italy – Centro di Studio per la Strutturistica Diffrattometrica del C.N.R.

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Crystals of $(C_{13}H_{19}N_2OS)_2^+[CoCl_4]^{2-}$ are triclinic ($P\bar{1}$): $a=8{\cdot}92(2)$, $b=13{\cdot}57(2)$, $c=14{\cdot}47(1)$Å, $\alpha=88{\cdot}1(2)°$, $\beta=84{\cdot}6(2)°$, $\gamma=69{\cdot}2(3)°$, $Z=2$. The structure was solved by three-dimensional Patterson and Fourier methods and refined by least-squares calculations (final $R=8{\cdot}7\%$). The organic cation shows no coordinative interaction with metal, which forms a slightly distorted tetrahedral tetrachlorocobaltate ion [Co–Cl = 2·230(8), 2·271(3), 2·317(6), 2·245(8) Å]. Packing is mainly determined by hydrogen bonding interactions (NH···Cl = 3·13, 3·22 Å) and by the S···Cl = 3·52 Å van der Waals contact.

The crystal structure of 3-(2-diethylammoniumethoxy)-1,2-benzisothiazole tetrachlorocobaltate has been determined as part of a study concerning the compounds 3-(2-diethylammoniumethoxy)-1,2-benzisothiazole forms with transition metal halides, MCl_2 (M = Mn, Co, Cu). The corresponding Cu compound has been recently studied (Corradi Bonamartini, Nardelli, Palmieri & Pelizzi, 1971).

The compound gives blue triclinic crystals. Their crystal data, determined from rotation and Weissenberg photographs (Co $K\alpha$, $\lambda = 1{\cdot}7902$ Å), are as follows (standard deviations given in parentheses are in units of the last decimal figure):

$(C_{13}H_{19}N_2OS)_2^+[CoCl_4]^{2-}$, $M = 703{\cdot}4$,
$a = 8{\cdot}92(2)$, $b = 13{\cdot}57(2)$, $c = 14{\cdot}47(1)$ Å
$\alpha = 88{\cdot}1(2)°$, $\beta = 84{\cdot}6(2)°$, $\gamma = 69{\cdot}2(3)°$
$V = 1629$ Å^3, $Z = 2$, $D_m = 1{\cdot}44$, $D_c = 1{\cdot}43$ g.cm^{-3}
$F(000) = 730$, $\mu = 72{\cdot}8$ cm^{-1}
Space group: $P\bar{1}$ (from structure analysis).

Three-dimensional intensity data were determined photometrically on integrated Weissenberg photographs taken up to the sixth and tenth layers around the [100] and [010] axes respectively (multiple-film technique, Co $K\alpha$). No absorption correction was used since the samples were small (mean radii: 0·04 and 0·15 mm). After correction for Lorentz and polarization factors, the intensities were placed on the same relative scale following Rollett & Sparks (1960) and the absolute scale was established by Wilson's (1942) method.

The structure was solved by the heavy-atom method and refined by block-diagonal and full-matrix least squares with anisotropic thermal parameters down to $R = 9{\cdot}4\%$ for residual error index. The function minimized was: $\sum w|(F_o - F_c)|^2$ with the weighting scheme: $w = 1/(A + B|F_o|)^2$ with $A = 1{\cdot}80$, $B = 0{\cdot}15$. All the hydrogen atoms were located from a $\varrho_o - \varrho_c$ final map: a block-diagonal least-squares isotropic refinement for the hydrogen atoms reduced the R index to the final value of 8·7 %. Final coordinates with thermal parameters are listed in Tables 1 and 2. Tables of observed and calculated structure factors are available from the authors on request.

Fig. 1 shows the structure projected along [100]. It consists of discrete tetrachlorocobaltate anions and of 3-(2-diethylammoniumethoxy)-1,2-benzisothiazole cations. Bond distances and angles are quoted in Table 3.

The anion has a slightly distorted tetrahedral structure; bond distances and angles in it agree with those

Table 1. *Final atomic fractional coordinates* ($\times 10^4$), *thermal parameters* ($\times 10 \,.\, 8\pi^2$Å^2) *with e.s.d.'s*

The anisotropic temperature factors are expressed in the form:
$\exp[-\frac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^*\cos\gamma^* + 2B_{13}hla^*c^*\cos\beta^* + 2B_{23}klb^*c^*\cos\alpha^*)]$

	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Co	2380 (2)	313 (1)	2390 (1)	41 (1)	38 (1)	28 (1)	−8 (1)	1 (1)	0 (1)
Cl(1)	51 (3)	1631 (2)	2722 (2)	27 (1)	34 (1)	38 (1)	3 (1)	−5 (1)	−4 (1)
Cl(2)	3325 (3)	359 (2)	882 (1)	57 (1)	37 (1)	20 (1)	−20 (1)	7 (1)	−5 (1)
Cl(3)	4160 (3)	597 (2)	3323 (2)	23 (1)	62 (1)	25 (1)	0 (1)	−5 (1)	−8 (1)
Cl(4)	2146 (4)	−1265 (2)	2672 (2)	78 (2)	28 (1)	47 (1)	−17 (1)	17 (1)	5 (1)
S(1)	2817 (4)	6050 (2)	3093 (2)	65 (2)	48 (1)	−28 (1)	−29 (1)	−12 (1)	10 (1)
S(2)	−1367 (4)	4500 (3)	1935 (2)	57 (2)	74 (2)	26 (1)	−8 (1)	−51 (1)	13 (1)
O(1)	2101 (7)	3988 (4)	4646 (4)	41 (3)	29 (3)	21 (2)	−15 (2)	−10 (2)	2 (2)
O(2)	−4004 (9)	6329 (5)	283 (4)	54 (4)	38 (3)	28 (3)	48 (3)	−55 (3)	1 (2)
N(1)	2353 (11)	4990 (6)	3345 (5)	59 (5)	37 (4)	31 (3)	−13 (4)	−23 (3)	8 (3)
N(2)	1867 (8)	1754 (5)	5033 (5)	21 (3)	30 (3)	28 (3)	−8 (3)	3 (2)	−5 (2)
N(3)	−2793 (12)	5604 (8)	1621 (6)	57 (5)	62 (5)	26 (3)	−5 (4)	1 (3)	6 (3)
N(4)	−6312 (9)	8446 (5)	−487 (5)	32 (3)	24 (3)	36 (3)	−5 (3)	−11 (3)	−9 (3)
C(1)	3165 (10)	6252 (7)	4212 (6)	20 (4)	36 (4)	32 (4)	−3 (3)	−2 (3)	−6 (3)
C(2)	3532 (11)	7054 (7)	4603 (7)	29 (4)	27 (4)	46 (5)	−7 (3)	−8 (4)	3 (3)
C(3)	3675 (11)	7022 (7)	5533 (7)	25 (4)	29 (4)	60 (5)	−7 (3)	−6 (4)	−8 (4)
C(4)	3442 (11)	6245 (7)	6103 (6)	41 (5)	36 (4)	24 (4)	−10 (4)	2 (3)	−10 (3)
C(5)	3065 (10)	5452 (7)	5721 (6)	26 (4)	33 (4)	34 (4)	−13 (3)	2 (3)	−4 (3)
C(6)	2914 (10)	5456 (6)	4783 (5)	28 (4)	17 (3)	23 (3)	−4 (3)	−7 (3)	1 (3)
C(7)	2449 (11)	4772 (6)	4217 (6)	33 (4)	21 (3)	32 (4)	−7 (3)	−15 (3)	8 (3)
C(8)	1475 (12)	3379 (8)	4067 (7)	48 (5)	45 (5)	35 (4)	−27 (4)	−17 (4)	−1 (4)
C(9)	714 (11)	2767 (7)	4709 (6)	27 (4)	36 (4)	32 (4)	−12 (3)	−4 (3)	2 (3)
C(10)	3090 (12)	1869 (8)	5630 (7)	36 (5)	37 (5)	53 (5)	−17 (4)	−15 (4)	12 (4)
C(11)	2425 (20)	2388 (13)	6560 (8)	110 (11)	100 (9)	26 (5)	−51 (9)	−11 (6)	−10 (5)
C(12)	901 (13)	1111 (8)	5465 (8)	43 (5)	37 (5)	61 (6)	−25 (4)	1 (4)	1 (4)
C(13)	1970 (15)	1 (8)	5632 (9)	63 (7)	35 (5)	80 (7)	−30 (5)	−19 (5)	15 (5)
C(14)	−839 (12)	3981 (8)	827 (6)	39 (5)	49 (5)	25 (4)	−16 (4)	−1 (3)	16 (3)
C(15)	323 (11)	3026 (8)	514 (8)	22 (4)	37 (5)	61 (6)	−4 (4)	0 (4)	12 (4)
C(16)	465 (14)	2834 (9)	−411 (9)	39 (5)	50 (6)	59 (6)	−7 (5)	14 (5)	−8 (5)
C(17)	−550 (16)	3552 (10)	−1009 (8)	59 (7)	58 (6)	50 (6)	−2 (5)	−11 (5)	−7 (5)
C(18)	−1650 (13)	4461 (8)	−740 (7)	48 (6)	37 (5)	42 (5)	0 (4)	−3 (4)	0 (4)
C(19)	−1856 (10)	4698 (7)	241 (6)	26 (4)	37 (4)	38 (4)	−13 (3)	0 (3)	12 (3)
C(20)	−2928 (12)	5573 (8)	739 (7)	38 (5)	37 (4)	34 (4)	−6 (4)	−1 (4)	4 (3)
C(21)	−5051 (15)	7232 (9)	809 (8)	56 (6)	48 (5)	39 (5)	−3 (5)	0 (4)	−2 (4)
C(22)	−6507 (13)	7750 (8)	317 (6)	47 (5)	46 (5)	24 (4)	−5 (4)	12 (4)	8 (3)
C(23)	−7927 (13)	9066 (9)	−819 (8)	35 (5)	48 (5)	58 (6)	−4 (4)	−9 (4)	−13 (5)
C(24)	−7896 (15)	9875 (9)	−1515 (9)	54 (6)	47 (6)	59 (6)	3 (5)	−22 (5)	4 (5)
C(25)	−5103 (13)	7848 (8)	−1254 (6)	49 (5)	54 (5)	20 (4)	−21 (5)	13 (3)	−7 (3)
C(26)	−5595 (14)	7072 (10)	−1716 (9)	48 (6)	62 (7)	58 (6)	−5 (5)	−5 (5)	−35 (5)

Table 2. *Fractional coordinates* ($\times 10^3$) *and isotropic thermal parameters* ($8\pi^2$Å^2) *for hydrogen atoms*

	x/a	y/c	z/c	B		x/a	y/c	z/c	B
H(1)	360 (13)	767 (8)	423 (7)	3·7 (2·6)	H(20)	112 (14)	249 (9)	92 (8)	4·4 (2·8)
H(2)	397 (15)	760 (9)	575 (8)	5·8 (3·1)	H(21)	136 (16)	216 (10)	−65 (9)	6·5 (3·5)
H(3)	349 (13)	626 (8)	677 (7)	4·1 (2·6)	H(22)	−38 (18)	339 (11)	−164 (10)	8·8 (4·2)
H(4)	287 (13)	500 (8)	609 (7)	4·5 (2·7)	H(23)	−250 (15)	512 (10)	93 (9)	6·0 (3·3)
H(5)	63 (14)	389 (9)	366 (8)	4·9 (3·0)	H(24)	−434 (15)	776 (9)	81 (8)	5·3 (3·1)
H(6)	257 (15)	283 (9)	363 (8)	5·4 (3·1)	H(25)	−536 (16)	697 (10)	147 (9)	6·6 (3·4)
H(7)	16 (12)	326 (8)	532 (7)	3·4 (2·4)	H(26)	−742 (14)	816 (9)	77 (8)	4·7 (2·9)
H(8)	−17 (13)	262 (8)	436 (7)	3·6 (2·5)	H(27)	−688 (14)	715 (9)	10 (8)	5·0 (3·0)
H(9)	251 (11)	141 (7)	455 (6)	2·4 (2·1)	H(28)	−870 (15)	943 (10)	−27 (9)	6·5 (3·5)
H(10)	392 (15)	111 (9)	572 (8)	5·7 (3·2)	H(29)	−841 (15)	856 (9)	−105 (9)	5·9 (3·3)
H(11)	369 (12)	234 (8)	528 (7)	3·1 (2·5)	H(30)	−494 (14)	839 (9)	−177 (8)	4·6 (3·0)
H(12)	322 (18)	242 (11)	692 (10)	7·4 (4·0)	H(31)	−398 (14)	746 (9)	−97 (8)	5·0 (3·0)
H(13)	180 (16)	191 (10)	695 (9)	6·1 (3·7)	H(32)	−466 (17)	664 (11)	−224 (10)	7·7 (3·9)
H(14)	154 (19)	316 (12)	648 (11)	8·9 (4·5)	H(33)	−578 (16)	649 (10)	−121 (9)	6·2 (3·5)
H(15)	15 (16)	150 (10)	614 (9)	7·2 (3·6)	H(34)	−677 (18)	743 (11)	−204 (10)	8·0 (4·0)
H(16)	22 (16)	100 (10)	494 (9)	6·1 (3·3)	H(35)	−921 (17)	1032 (11)	−172 (10)	7·5 (3·7)
H(17)	131 (16)	−47 (10)	595 (9)	6·3 (3·5)	H(36)	−732 (16)	1042 (10)	−123 (9)	6·4 (3·4)
H(18)	283 (17)	−1 (11)	607 (10)	7·7 (3·9)	H(37)	−707 (16)	948 (10)	−198 (9)	6·0 (3·4)
H(19)	265 (19)	−32 (12)	498 (11)	9·8 (4·5)	H(38)	−590 (13)	886 (8)	−30 (8)	4·6 (2·7)

Table 3. *Bond distances and angles*

(i) In $[CoCl_4]^{2-}$.
(ii) In the organic cations.
(iii) Involving hydrogen atoms.

(i)

Co-Cl(1)	2.230(8) Å
Co-Cl(2)	2.271(3)
Co-Cl(3)	2.317(6)
Co-Cl(4)	2.245(8)

Cl(1)-Co-Cl(2)	111.5(1)°
Cl(1)-Co-Cl(3)	105.1(1)
Cl(2)-Co-Cl(3)	108.6(1)
Cl(2)-Co-Cl(4)	108.5(1)
Cl(3)-Co-Cl(4)	111.4(1)
Cl(1)-Co-Cl(4)	111.7(1)

(ii)

S(1)-C(1)	1.77(1) Å
C(1)-C(2)	1.37(1)
C(2)-C(3)	1.36(1)
C(3)-C(4)	1.38(1)
C(4)-C(5)	1.38(1)
C(5)-C(6)	1.38(1)
C(6)-C(7)	1.45(1)
C(1)-C(6)	1.38(1)
C(7)-N(1)	1.29(1)
N(1)-S(1)	1.65(1)
C(7)-O(1)	1.33(1)
O(1)-C(8)	1.47(1)
C(8)-C(9)	1.50(1)
C(9)-N(2)	1.49(1)
N(2)-C(10)	1.51(1)
C(10)-C(11)	1.51(2)
N(2)-C(12)	1.51(1)
C(12)-C(13)	1.49(2)
C(14)-C(19)	1.40(1)
C(14)-C(15)	1.40(2)
C(15)-C(16)	1.36(1)
C(16)-C(17)	1.41(2)
C(17)-C(18)	1.32(2)
C(18)-C(19)	1.45(1)
C(19)-C(20)	1.40(1)
C(20)-N(3)	1.30(1)
N(3)-S(2)	1.67(1)
S(2)-C(14)	1.73(1)
C(20)-O(2)	1.34(1)
O(2)-C(21)	1.44(1)
C(21)-C(22)	1.48(2)
C(22)-N(4)	1.51(1)
N(4)-C(23)	1.50(1)
C(23)-C(24)	1.47(2)
N(4)-C(25)	1.50(1)
C(25)-C(26)	1.48(2)

N(1)-S(1)-C(1)	94.8(4)°
S(1)-C(1)-C(2)	129.8(8)
S(1)-C(1)-C(6)	107.4(7)
C(1)-C(2)-C(3)	116.6(9)
C(2)-C(3)-C(4)	122.9(9)
C(3)-C(4)-C(5)	119.2(8)°
C(4)-C(5)-C(6)	119.6(9)
C(5)-C(6)-C(7)	131.2(8)
C(2)-C(1)-C(6)	122.7(8)
C(7)-C(6)-C(1)	109.8(7)
N(1)-C(7)-C(6)	117.7(8)
S(1)-N(1)-C(7)	110.3(7)
O(1)-C(7)-C(6)	117.1(7)
O(1)-C(7)-N(1)	125.2(8)
C(8)-O(1)-C(7)	115.4(6)
C(9)C(8)-O(1)	107.3(7)
N(2)-C(9)-C(8)	114.2(7)
C(10)-N(2)-C(9)	114.6(7)
C(11)-C(10)-N(2)	115.6(9)
C(9)-N(2)-C(12)	107.8(7)
C(13)-C(12)-N(2)	110.9(9)
C(1)-C(6)-C(5)	118.9(8)
C(10)-N(2)-C(12)	114.6(7)
S(2)-C(14)-C(19)	106.9(7)
C(14)-C(19)-C(18)	118.4(9)
C(19)-C(20)-N(3)	117.4(9)
C(20)-N(3)-S(2)	109.5(8)
N(3)-S(2)-C(14)	95.1(5)
N(3)-C(20)-O(2)	123.9(9)
C(14)-C(19)-C(20)	111.1(8)
C(15)-C(14)-S(2)	130.1(8)
C(19)-C(14)-C(15)	123.0(9)
C(14)-C(15)-C(16)	116.5(9)
C(15)-C(16)-C(17)	121.0(1.1)
C(16)-C(17)-C(18)	124.1(1.1)
C(17)-C(18)-C(19)	116.9(1.0)
C(18)-C(19)-C(20)	130.5(9)
C(19)-C(20)-O(2)	118.7(8)
C(20)-O(2)-C(21)	117.3(7)
O(2)-C(21)-C(22)	109.0(9)
C(21)-C(22)-N(4)	115.4(9)
C(22)-N(4)-C(23)	109.9(8)
C(22)-N(4)-C(25)	112.9(8)
N(4)-C(23)-C(24)	114.1(9)
N(4)-C(25)-C(26)	113.3(9)
C(23)-N(4)-C(25)	112.9(7)

(iii)

C(2)-H(1)	1.00(12) Å
C(3)-H(2)	0.98(14)
C(4)-H(3)	0.98(11)
C(5)-H(4)	0.85(12)
C(8)-H(5)	1.04(12)
C(8)-H(6)	1.20(13)
C(9)-H(7)	1.09(11)
C(9)-H(8)	1.05(11)
N(2)-H(9)	0.89(10)
C(10)-H(10)	1.05(14)
C(10)-H(11)	1.05(11)
C(11)-H(12)	0.93(16)
C(11)-H(13)	1.10(15) Å
C(11)-H(14)	1.08(17)
C(12)-H(15)	1.16(14)
C(12)-H(16)	1.07(14)
C(13)-H(17)	1.09(15)
C(13)-H(18)	1.03(12)
C(13)-H(19)	1.09(17)
C(15)-H(20)	1.03(29)
C(16)-H(21)	1.02(20)
C(17)-H(22)	0.93(16)
C(18)-H(23)	1.17(26)
C(21)-H(24)	1.11(14)
C(21)-H(25)	1.06(14)
C(22)-H(26)	1.00(12)
C(22)-H(27)	1.05(13)
C(23)-H(28)	1.02(13)
C(23)-H(29)	1.02(14)
C(25)-H(30)	1.06(13)
C(25)-H(31)	1.07(12)
C(26)-H(32)	1.09(15)
C(26)-H(33)	1.10(14)
C(26)-H(34)	1.12(13)
C(24)-H(35)	1.17(15)
C(24)-H(36)	1.15(15)
C(24)-H(37)	0.97(31)
N(4)-H(38)	0.84(12)

C(1)-C(2)-H(1)	122.7(6.6)°
C(3)-C(2)-H(1)	120.5(6.6)
C(2)-C(3)-H(2)	113.5(7.6)
C(4)-C(3)-H(2)	123.6(7.6)
C(3)-C(4)-H(3)	121.7(7.3)
C(5)-C(4)-H(3)	119.1(7.2)
C(4)-C(5)-H(4)	117.9(8.1)
C(6)-C(5)-H(4)	122.4(8.1)
O(1)-C(8)-H(5)	109.8(7.3)
O(1)-C(8)-H(6)	102.1(6.4)
C(9)-C(8)-H(5)	110.3(7.0)
C(9)-C(8)-H(6)	113.0(6.6)
H(5)-C(8)-H(6)	113.9(9.1)
N(2)-C(9)-H(7)	107.6(5.8)
N(2)-C(9)-H(8)	109.7(6.4)
C(8)-C(9)-H(7)	107.1(6.2)
C(8)-C(9)-H(8)	107.9(6.1)
H(7)-C(9)-H(8)	110.3(8.3)
C(9)-N(2)-H(9)	109.0(6.6)
C(10)-N(2)-H(9)	100.8(6.4)
C(12)-N(2)-H(9)	109.7(6.9)
N(2)-C(10)-H(10)	106.4(7.4)
N(2)-C(10)-H(11)	109.1(5.9)
C(11)-C(10)-H(10)	110.1(7.1)
C(11)-C(10)-H(11)	106.1(6.1)
H(10)-C(10)-H(11)	109.4(9.5)
C(10)-C(11)-H(13)	107.7(7.7)
C(10)-C(11)-H(14)	111.0(8.8)
C(10)-C(11)-H(12)	112.9(9.6)
H(13)-C(11)-H(14)	106.9(9.9)°
H(13)-C(11)-H(12)	107.0(9.4)
H(14)-C(11)-H(12)	111.0(9.8)
N(2)-C(12)-H(15)	111.3(7.6)
N(2)-C(12)-H(16)	106.6(7.5)
C(13)-C(12)-H(15)	111.6(7.4)
C(13)-C(12)-H(16)	100.9(7.8)
H(15)-C(12)-H(16)	115.0(9.1)
C(12)-C(13)-H(17)	112.3(7.6)
C(12)-C(13)-H(18)	110.3(8.9)
C(12)-C(13)-H(19)	108.3(9.2)
H(17)-C(15)-H(18)	107.7(9.2)
H(17)-C(13)-H(19)	113.2(9.1)
H(18)-C(13)-H(19)	104.9(9.6)
C(14)-C(15)-H(20)	125.2(9.2)
C(16)-C(15)-H(20)	118.2(9.8)
C(15)-C(16)-H(21)	116.9(2.5)
C(17)-C(16)-H(21)	122.1(2.6)
C(16)-C(17)-H(22)	117.0(9.8)
C(18)-C(17)-H(22)	118.7(9.9)
C(17)-C(18)-H(23)	128.4(7.0)
C(19)-C(18)-H(23)	114.7(7.0)
C(22)-C(21)-H(24)	109.9(2.2)
C(22)-C(21)-H(25)	110.3(7.5)
O(2)-C(21)-H(24)	104.0(2.7)
O(2)-C(21)-H(25)	108.0(8.0)
H(24)-C(21)-H(25)	115.5(9.2)
C(21)-C(22)-H(26)	109.7(6.8)
C(21)-C(22)-H(27)	106.6(6.8)
N(4)-C(22)-H(26)	110.0(7.2)
N(4)-C(22)-H(27)	111.3(6.8)
H(26)-C(22)-H(27)	103.0(9.9)
C(24)-C(23)-H(28)	108.3(8.0)
C(24)-C(23)-H(29)	111.6(7.6)
N(4)-C(23)-H(28)	108.9(7.5)
N(4)-C(23)-H(29)	109.0(7.6)
H(28)-C(23)-H(29)	104.3(8.8)
C(23)-C(24)-H(35)	108.8(7.6)
C(23)-C(24)-H(36)	109.8(7.0)
C(23)-C(24)-H(37)	103.1(5.4)
H(35)-C(24)-H(36)	113.4(9.5)
H(35)-C(24)-H(37)	119.7(9.7)
H(36)-C(24)-H(37)	101.3(9.1)
C(26)-C(25)-H(30)	107.6(6.8)
C(26)-C(25)-H(31)	109.8(7.2)
N(4)-C(25)-H(30)	109.3(6.8)
N(4)-C(25)-H(31)	108.2(6.7)
H(30)-C(25)-H(31)	108.4(9.6)
C(25)-C(26)-H(32)	110.4(8.3)
C(25)-C(26)-H(33)	110.6(7.4)
C(25)-C(26)-H(34)	113.5(8.4)
H(32)-C(26)-H(33)	107.1(9.1)
H(32)-C(26)-H(34)	109.5(9.9)
H(33)-C(26)-H(34)	105.4(9.7)
C(22)-N(4)-H(38)	107.6(8.0)
C(23)-N(4)-H(38)	109.6(8.2)
C(25)-N(4)-H(38)	103.5(7.9)

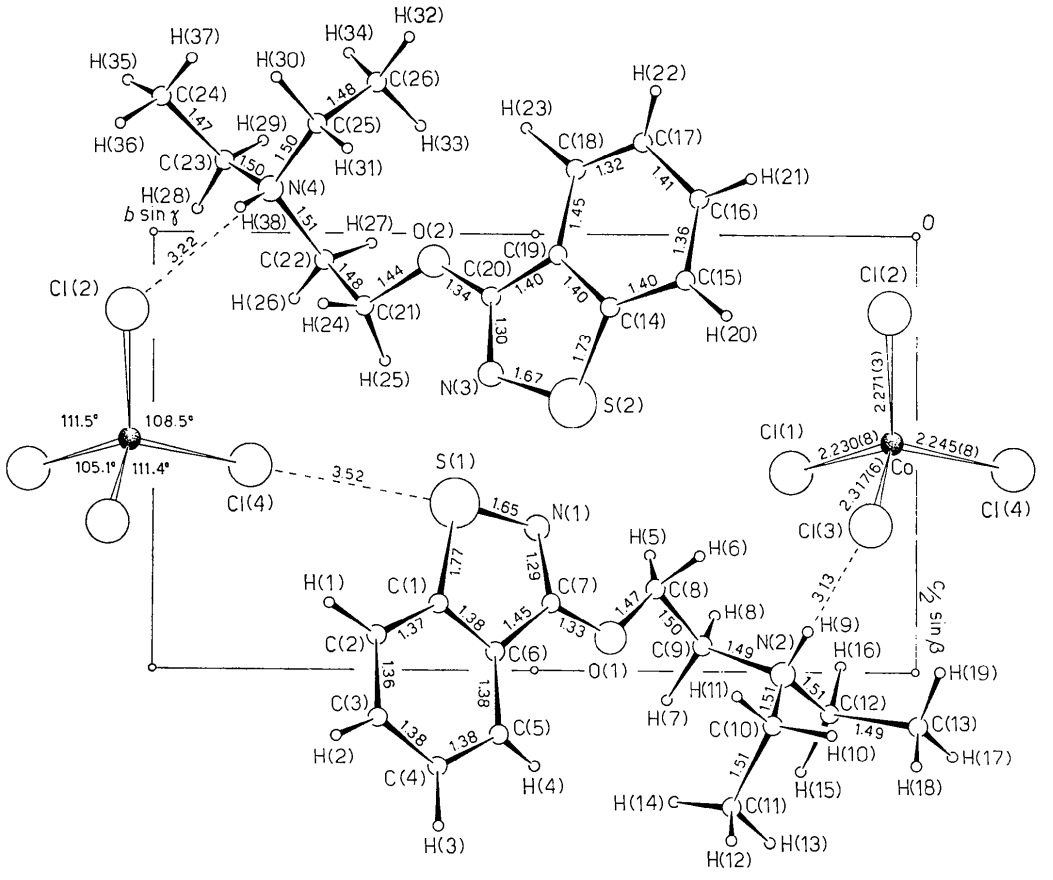

Fig. 1. Projection of $(C_{13}H_{19}N_2OS)^+_2[CoCl_4]^{2-}$ along [100].

(Co–Cl = 2·22, 2·25, 2·23, 2·23 Å; Cl–Co–Cl = 107, 107·5, 109, 117°) found in Cs_2CoCl_4 by Poray-Košic (1954). The two longest distances Co–Cl = 2·271, 2·317 Å

Table 4. *Van der Waals contacts* (*less than* 3·60 Å)

Cl(2)–C(25^{iii})	3·42 (2) Å
Cl(2)–N(4^{iii})	3·57 (1)
O(1)—C(3^{iv})	3·51 (2)
C(1)—C(9^{v})	3·45 (2)
C(1)—C(5^{iv})	3·34 (2)
C(2)—Cl(4^{ii})	3·57 (1)
C(3)—O(1^{iv})	3·51 (2)
C(3)—C(7^{iv})	3·49 (2)
C(4)—C(6^{iv})	3·41 (2)
C(4)—C(7^{iv})	3·42 (2)
C(5)—C(9^{v})	3·48 (2)
C(5)—S(2^{v})	3·57 (1)
C(5)—C(6^{iv})	3·37 (2)
C(6)—C(9^{v})	3·31 (2)
C(12)–Cl(4^{vi})	3·60 (1)
C(14)–C(18^{iii})	3·56 (2)
C(15)–C(18^{iii})	3·56 (2)
C(16)–C(20^{iii})	3·58 (2)
C(17)–N(3^{iii})	3·58 (2)
C(23)–Cl(2^{i})	3·55 (1)

i $x-1, y+1, z$
ii $x, \quad y+1, z$
iii $\bar{x}, \quad \bar{y}+1, \bar{z}$
iv $\bar{x}+1, \bar{y}+1, \bar{z}+1$
v $\bar{x}, \quad \bar{y}+1, \bar{z}+1$
vi $\bar{x}, \quad \bar{y}, \quad \bar{z}+1$

are significantly different from the other ones and correspond to Cl(2) and Cl(3) atoms respectively, which are engaged in hydrogen bonds with the ammonium nitrogens N(4) and N(3) of two independent organic cations.

The two independent 3-(2-diethylammoniumethoxy)-1,2-benzisothiazole systems are practically equal and bond distances and angles in them agree fairly well with those found in the similar $CuCl_4$ derivative.

Packing is mainly determined by the hydrogen bonding N(2)H···Cl(3) = 3·13(1)Å[∠N(2)HCl(3) = 176·5°] and N(4)H···Cl(2^{i}) = 3·22(1)Å[∠N(4)HCl(2^{i}) = 137·5°] and by the contact S(1)···Cl(4^{ii}) = 3·52 (1) Å. This contact corresponds well to the sum of the van der Waals radii (3·50 Å) calculated assuming a 1·70 Å value for the sulphur atom, and it is significantly longer than the corresponding contact (3·33 Å) found in $(C_{13}H_{19}N_2OS)^+_2[CuCl_4]^{2-}$. The other packing contacts less than 3·60 Å are given in Table 4.

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