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# *catena*-Bis(benzenesulfonato)bis(ethanol)cobalt(II): Preparation, Properties and Crystal Structure

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## Abstract

Bis(benzenesulfonato)bis(ethanol)cobalt(II), $Co(BS)_2(EtOH)_2$, was crystallized from a solution of anhydrous bis(benzenesulfonato)cobalt(II), $Co(BS)_2$, in absolute ethanol. The compound crystallizes in the monoclinic space group $P2_1/c$ with $a$ = 10.313(2), $b$ = 20.114(5), $c$ = 10.835(5) Å, $\beta$ = 118.33(2)°, $Z$ = 4. The structure was determined from 5764 observed reflections and refined to $R$ = 0.076. The Co atoms show a distorted octahedral coordination, being bonded to four oxygen atoms of four different $BS^-$ anions and to two oxygen atoms of EtOH. Each $BS^-$ anion bridges two Co atoms. Hydrogen bonds between the OH groups of EtOH and the uncoordinated oxygen of the $BS^-$ anions are formed.

IR and electronic spectral data and magnetic moments of $Co(BS)_2(EtOH)_2$ were studied and compared with those of related compounds.

## Introduction

Within a general study on metal arylsulfonates this work deals with the preparation, properties and crystal structure of the polymeric compound $[Co(BS)_2(EtOH)_2]_n$, (BS = benzenesulfonate). Only the anhydrous cobalt(II) sulfonates, $Co(RSO_3)_2$, (R = $CF_3$, $CH_3$, $p$-$CH_3$-$C_6H_4$, $C_6H_5$, F) have been previously described [1–3]. The magnetic and spectral (electronic and IR) properties of these compounds lead to the conclusion that the metal ions are in an octahedral environment of oxygen atoms, each sulfonate anion being three-coordinate.

Similar studies on $Co(RSO)_3)_2\cdot 6H_2O$ compounds (R = $C_6H_5$, $p$-$CH_3$-$C_6H_4$), together with the crystal structure determination, have demonstrated that these compounds must be formulated as $[Co(H_2O)_6](RSO_3)_2$ salts [4].

## Experimental

### *Preparation of Co(BS)₂(EtOH)₂ (1)*

Anhydrous $Co(BS)_2$ was prepared by dehydration of $Co(BS)_2\cdot 6H_2O$ [4] for 72 h at 190 °C. A concentrated solution of the mauve powder so obtained in absolute ethanol was evaporated under vacuum in a desiccator over $CaCl_2$. Wine-red crystals of $Co(BS)_2(EtOH)_2$ were obtained. *Anal.* Found: C, 41.01; H, 4.63; Co, 12.50; $BS^-$, 67.65. Calc. for $C_{16}H_{22}CoO_8S_2$: C, 41.29, H, 4.76; Co, 12.66; $BS^-$, 67.57%. Co was determined by complexometry with EDTA and murexide as indicator. $BS^-$ was determined as HBS with NaOH after running of an aqueous solution of the substance through an acid resin column.

Magnetic susceptibilities were determined using a conventional Faraday system for low temperatures. Infrared spectra in Nujol mulls were recorded on a FT Nicolet 60SX spectrophotometer. Electronic spectra were obtained on a powdered sample (diffuse reflectance) using a Kontron UVIKON 820 spectrophotometer.

Thermal analysis data were obtained with a Dupont 951 Thermobalance at 10 °C/min.

### *Crystal Structure Determination of Co(BS)₂(EtOH)₂*

#### *Crystal data*

$C_{16}H_{22}CoO_8S_2$, $M$ = 465.398, monoclinic, space group $P2_1/c$, $a$ = 10.313(2), $b$ = 20.114(5), $c$ = 10.835(5) Å, $\beta$ = 118.33(2)°, $V$ = 1978 Å$^3$ (by least-squares refinement on diffractometer angles for 25 automatically centred reflections, ($\lambda$(Mo K$\alpha$) = 0.71069 Å), $Z$ = 4, $D_x$ = 1.563 g/cm$^3$. Crystal dimensions (distances to faces from centre); 0.020 × 0.052 × 0.101 mm, $\mu$(Mo K$\alpha$) = 11.054 cm$^{-1}$.

#### *Data collection and processing*

ENRAF NONIUS-CAD4 diffractometer, $\omega/2\theta$ mode with $\omega$ scan width = 1.10 + 0.34 tan $\theta$, speed

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20/6 deg/min, graphite-monochromated Mo K$\alpha$ radiation; 5764 observed reflections (merging $R = 0.01$), giving 2753 observed reflections for $2 < \theta < 30°$ with $I > 2\sigma(I)$. Two standard reflections measured every 90 min. No decomposition detected during processing; Lorentz and polarization corrections were applied but no correction for absorption was made. Atomic scattering factors and dispersion coefficients taken from International Tables for X-ray Crystallography (1974).

### *Structure analysis and refinement*

Co atoms, from Patterson method, are in special positions on inversion centers (0 ½ 0, ½ ½ 0), Wyckoff notations *c* and *d*. The remaining atoms were found by Fourier syntheses and difference Fourier synthesis and refined with isotropic and anisotropic thermal parameters to a minimum value of $w^2$ with $w = 1$. (A weighting scheme $w = 1/\sigma_1^2\sigma_2^2$, $\sigma_1 = f(F_o)$, $\sigma_2 = f(\sin\theta/\lambda)$, gave no trends in $F_o$ and $\sin\theta/\lambda$). Hydrogen atoms, clearly revealed in a difference synthesis after refinement of the other atoms, were included in the refinement with an isotropic temperature factor equivalent to the thermal parameters of atoms which are fused. The final value of $R$ was 0.076 and $R_w = (\Sigma w^2/\Sigma w F_o^2)^{1/2} = 0.081$.

Final difference Fourier map had no significant peaks. Computations were made by programs PESOS [5], XRAY76 [6], PARST [7] on a VAX11/750 computer.

Atomic coordinates are given in Table I, bond lengths and angles in Table II.

TABLE Ia. Atomic Parameters for Non-hydrogen Atoms[a]

| Atom | $x/a$ | $y/b$ | $z/c$ | $U_{eq}$ |
|---|---|---|---|---|
| Co1 | 1.0000(0) | 0.5000(0) | 0.0000(0) | 28(1) |
| Co2 | 0.5000(0) | 0.5000(0) | 0.0000(0) | 24(1) |
| S1 | 0.7849(2) | 0.4061(1) | 0.0819(2) | 23(1) |
| S2 | 0.3045(2) | 0.4080(1) | 0.1048(3) | 34(1) |
| O11 | 0.8912(6) | 0.4591(3) | 0.1079(7) | 28(3) |
| O12 | 0.6608(7) | 0.4294(3) | 0.1025(7) | 37(3) |
| O13 | 0.7418(7) | 0.3726(3) | −0.0496(7) | 35(3) |
| O21 | 0.3958(8) | 0.4657(3) | 0.1178(7) | 37(3) |
| O22 | 0.1625(7) | 0.4259(4) | 0.0925(8) | 49(3) |
| O23 | 0.2876(9) | 0.3628(4) | −0.0073(8) | 52(4) |
| O1 | 0.8782(9) | 0.4397(4) | −0.1686(9) | 49(4) |
| O2 | 0.3890(9) | 0.4318(4) | −0.1561(8) | 45(3) |
| C11 | 0.8744(8) | 0.3464(4) | 0.2174(9) | 26(3) |
| C12 | 0.8076(10) | 0.3236(5) | 0.2916(11) | 38(4) |
| C13 | 0.8762(13) | 0.2722(6) | 0.3879(12) | 52(5) |
| C14 | 1.0085(13) | 0.2464(5) | 0.4079(12) | 51(5) |
| C15 | 1.0731(11) | 0.2702(5) | 0.3329(11) | 44(4) |
| C16 | 1.0073(11) | 0.3209(4) | 0.2360(10) | 33(4) |
| C21 | 0.3965(0) | 0.3642(0) | 0.2643(0) | 44(0) |
| C22 | 0.4246(0) | 0.2958(0) | 0.2569(0) | 75(0) |
| C23 | 0.5033(0) | 0.2634(0) | 0.3915(0) | 118(0) |
| C24 | 0.5461(0) | 0.2981(0) | 0.5142(0) | 163(0) |
| C25 | 0.5141(0) | 0.3633(0) | 0.5157(0) | 124(0) |
| C26 | 0.4386(0) | 0.3984(0) | 0.3877(0) | 75(0) |
| C1 | 0.0859(14) | 0.5878(7) | 0.2692(13) | 56(5) |
| C2 | 0.1415(22) | 0.5429(10) | 0.3926(18) | 84(9) |
| C3 | 0.7082(19) | 0.5537(7) | 0.2991(14) | 74(7) |
| C4 | 0.7752(19) | 0.6146(10) | 0.3817(19) | 84(9) |

[a] Coordinates and thermal parameters as: $U_{eq} = (1/3)\Sigma(U_{ij} a_i^* a_j^* a_i a_j \cos(a_i, a_j)) \times 10^3$.

TABLE Ib. Thermal Parametrs for Non-hydrogen Atoms[a]

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 21(1) | 30(1) | 34(1) | 2(1) | 13(1) | 10(1) |
| Co2 | 22(1) | 21(1) | 35(1) | 0(1) | 16(1) | 3(1) |
| S1 | 21(1) | 21(1) | 30(1) | 0(1) | 15(1) | 5(1) |
| S2 | 25(1) | 30(1) | 47(1) | 2(1) | 18(1) | 11(1) |
| O11 | 20(3) | 28(3) | 41(4) | −2(2) | 19(3) | 5(3) |
| O12 | 25(3) | 35(4) | 55(4) | 10(3) | 24(3) | 10(3) |
| O13 | 32(3) | 38(4) | 36(3) | −7(3) | 17(3) | 1(3) |
| O21 | 43(4) | 27(4) | 49(4) | −4(3) | 28(3) | 3(3) |
| O22 | 31(3) | 52(5) | 75(5) | 18(3) | 34(4) | 43(4) |
| O23 | 61(5) | 39(4) | 62(5) | −13(4) | 33(4) | 1(4) |
| O1 | 52(5) | 59(5) | 49(4) | −21(4) | 35(4) | −5(4) |
| O2 | 45(4) | 39(4) | 41(4) | −11(3) | 13(3) | −4(3) |
| C11 | 22(4) | 21(4) | 34(4) | 1(3) | 12(3) | −4(3) |
| C12 | 35(5) | 42(5) | 47(5) | 10(4) | 28(4) | 18(4) |
| C13 | 66(7) | 50(6) | 51(6) | 4(5) | 37(6) | 31(5) |
| C14 | 62(7) | 35(6) | 58(7) | 17(5) | 31(6) | 21(5) |
| C15 | 40(5) | 45(6) | 49(6) | 15(5) | 24(5) | 12(5) |
| C16 | 43(5) | 26(4) | 40(5) | 7(4) | 26(4) | 5(4) |
| C21 | 27(0) | 47(0) | 63(0) | 14(0) | 26(0) | 33(0) |
| C22 | 54(0) | 54(0) | 134(0) | 13(0) | 59(0) | 46(0) |
| C23 | 61(0) | 87(0) | 189(0) | 24(0) | 45(0) | 102(0) |
| C24 | 56(0) | 261(0) | 157(0) | 34(0) | 39(0) | 172(0) |
| C25 | 82(0) | 200(0) | 76(0) | 2(0) | 25(0) | 76(0) |
| C26 | 59(0) | 97(0) | 66(0) | 4(0) | 28(0) | 26(0) |
| C1 | 60(7) | 64(8) | 49(6) | −8(7) | 32(6) | −9(6) |
| C2 | 83(11) | 111(14) | 60(9) | 28(11) | 36(9) | 22(9) |
| C3 | 97(12) | 58(8) | 45(7) | −16(8) | 14(7) | −10(6) |
| C4 | 72(11) | 92(13) | 72(10) | −23(10) | 21(9) | −21(9) |

[a] Thermal parameters as $\exp(-2p_i^2 \Sigma(U_{ij} a_i^* a_j^* h_i h_j)) \times 10^3$.

TABLE Ic. Atomic Parameters for Hydrogen Atoms[a]

| Atom | $x/a$ | $y/b$ | $z/c$ | $U$ |
|---|---|---|---|---|
| H1 | 0.831(15) | 0.416(7) | −0.155(15) | 49(0) |
| H2 | 0.348(15) | 0.405(7) | −0.132(14) | 40(0) |
| H121 | 0.715(13) | 0.333(6) | 0.287(13) | 40(0) |
| H131 | 0.853(14) | 0.267(7) | 0.435(14) | 50(0) |
| H141 | 1.053(14) | 0.214(7) | 0.468(14) | 45(0) |
| H151 | 1.162(14) | 0.263(6) | 0.348(13) | 41(0) |

*(continued)*

TABLE Ic. *(continued)*

| Atom | $x/a$ | $y/b$ | $z/c$ | $U$ |
|---|---|---|---|---|
| H161 | 1.051(13) | 0.342(6) | 0.187(12) | 35(0) |
| H221 | 0.412(0) | 0.251(0) | 0.186(0) | 80(0) |
| H231 | 0.536(0) | 0.188(0) | 0.389(0) | 80(0) |
| H241 | 0.600(0) | 0.256(0) | 0.581(0) | 100(0) |
| H251 | 0.523(0) | 0.409(0) | 0.586(0) | 110(0) |
| H261 | 0.406(0) | 0.474(0) | 0.392(0) | 70(0) |
| H11 | 0.002(16) | 0.605(7) | 0.254(16) | 55(0) |
| H12 | 0.139(15) | 0.624(7) | 0.306(14) | 55(0) |
| H21 | 0.116(21) | 0.566(9) | 0.458(17) | 70(0) |
| H22 | 0.255(17) | 0.541(8) | 0.432(16) | 70(0) |
| H23 | 0.051(18) | 0.554(9) | 0.391(19) | 70(0) |
| H31 | 0.814(16) | 0.528(7) | 0.313(15) | 60(0) |
| H32 | 0.673(17) | 0.524(8) | 0.346(16) | 60(0) |
| H41 | 0.685(18) | 0.631(9) | 0.378(18) | 70(0) |
| H42 | 0.843(17) | 0.596(8) | 0.473(17) | 70(0) |
| H43 | 0.836(11) | 0.631(5) | 0.365(10) | 0(0) |

[a]Coordinates and thermal parameters as $\exp(-8p_i^2 U(\sin\theta/\lambda)^2) \times 10^3$.

## Results and Discussion

The crystallization of $Co(BS)_2(EtOH)_2$ (**1**) is possible only from absolute ethanol solutions of anhydrous $Co(BS)_2$. From solutions of $Co(BS)_2 \cdot 6H_2O$ in absolute ethanol only the starting compound can be crystallized. The wine-red crystals of $Co(BS)_2(EtOH)_2$ are instable to air moisture and are transformed slowly into $Co(BS)_2 \cdot 6H_2O$.

The thermogravimetric curve of **1** (20–300 °C) shows a single step between 70 and 150 °C and the weight-loss corresponds to two ethanol molecules, the residue being identified as the anhydrous salt $Co(BS)_2$.

Table III gives the electronic spectral data (diffuse reflectance) of **1** together with those of the related compounds $Co(BS)_2$, $Co(BS)_2 \cdot 6H_2O$ and $[Co(EtOH)_6(NO_3)_2]$ [8]. The *Dq* value for **1** is

TABLE II. Bond Distances and Angles for Non-hydrogen Atoms

| | | | |
|---|---|---|---|
| Bond distances (Å) | | | |
| Co1–O11 | 2.132(8) | Co2–O21 | 2.135(9) |
| Co1–O1 | 2.049(8) | Co2–O2 | 2.056(8) |
| Co1–O22 | 2.108(7) | Co2–O12 | 2.062(6) |
| S1–O11 | 1.458(7) | S2–O21 | 1.459(8) |
| S1–O12 | 1.476(9) | S2–O22 | 1.451(9) |
| S1–O13 | 1.442(7) | S2–C22 | 1.451(9) |
| O1–C1 | 1.42(2) | O2–C3 | 1.42(1) |
| C1–C2 | 1.48(2) | C3–C4 | 1.48(2) |
| C11–C12 | 1.36(2) | C21–C22 | 1.42(1) |
| C11–C16 | 1.38(1) | C21–C26 | 1.38(1) |
| C12–C13 | 1.39(2) | C22–C23 | 1.44(1) |
| C13–C14 | 1.37(2) | C23–C24 | 1.38(1) |
| C14–C15 | 1.36(2) | C24–C25 | 1.35(1) |
| C15–C16 | 1.39(1) | C25–C26 | 1.42(1) |
| Bond angles (°) | | | |
| O11–Co1–O1 | 90.0(4) | O21–Co2–O2 | 92.1(3) |
| O11–Co1–O22 | 88.4(3) | O21–Co2–O12 | 87.7(3) |
| O1–Co1–O22 | 91.1(3) | O2–Co2–O12 | 88.6(3) |
| O13–S1–C11 | 107.2(4) | O23–S2–O21 | 107.5(3) |
| O12–S1–C11 | 103.7(4) | O22–S2–O21 | 105.3(4) |
| O12–S1–O13 | 114.5(4) | O22–S2–O23 | 111.2(5) |
| O11–S1–C11 | 106.6(4) | O21–S2–C21 | 106.3(3) |
| O11–S1–O12 | 112.6(4) | O21–S2–O23 | 113.1(5) |
| O11–S1–O13 | 111.5(4) | O21–S2–O22 | 112.9(5) |
| S1–C11–C16 | 117.4(7) | S2–C21–C26 | 118.5(1) |
| S1–C11–C12 | 120.3(8) | S2–C21–C22 | 117.4(2) |
| C12–C11–C16 | 122.1(9) | C22–C21–C26 | 124.1(1) |
| C11–C12–C13 | 117.6(1) | C21–C22–C23 | 114.4(2) |
| C12–C13–C14 | 121.4(1) | C22–C23–C24 | 121.1(1) |
| C13–C14–C15 | 119.7(2) | C23–C24–C25 | 122.3(1) |
| C14–C15–C16 | 120.8(1) | C24–C25–C26 | 119.7(1) |
| C11–C16–C15 | 118.5(1) | C21–C26–C25 | 118.4(1) |
| O1–C1–C2 | 109.1(13) | O2–C3–C4 | 111.8(13) |

| | O–H | O---O | O---H | O–H–O |
|---|---|---|---|---|
| Hydrogen bonds | | | | |
| O1–H1--O13 ($x,y,z$) | 0.77(17) | 2.68(1) | 2.02(19) | 144(15) |
| O2–H2--O23 ($x,y,z$) | 0.75(18) | 2.69(1) | 1.94(18) | 173(16) |

TABLE III. Electronic Spectra (Diffuse Reflectance) of $Co(BS)_2(EtOH)_2$ and Related Compounds

| Compound | Observed transitions ($\nu_{max}$ (cm$^{-1}$)) | | *Dq* (cm$^{-1}$) | *B* (cm$^{-1}$) |
|---|---|---|---|---|
| | $^4A_{2g} \leftarrow {}^4T_{1g}$ ($\nu_2$) | $^4T_{1g}(P) \leftarrow {}^4T_{1g}$ ($\nu_3$) | | |
| $Co(BS)_2(EtOH)_2$ | 15038w | 18939s, 20202sh, 21505sh | 816 | 859 |
| $Co(BS)_2$ | 13423w | 18519s, 20833sh | 712 | 890 |
| $[Co(H_2O)_6](BS)_2$ | 16393sh | 20000s, 21739sh, 25126sh | 862 | 907 |
| $[Co(EtOH)_5](NO_3)_2$ [8] | 18000w | 21200sh, 19800s, | 959 | 834 |

TABLE IV. Principal IR Frequencies ($\nu_{max}$ (cm$^{-1}$)) of $Co(BS)_2(EtOH)_2$ and Related Compounds

| Compound | EtOH and $H_2O$ | | $R-SO_3^-$ | | | | |
|---|---|---|---|---|---|---|---|
| | $\nu$(OH) | $\delta$(OH) | $\nu_{as}$ | $\nu_{sym}$ | $\delta_{as}$ | $\delta_{sym}$ | $\nu_{CS}$ |
| $Co(BS)_2(EtOH)_2$ | 3992vs<br>3200vs | 1649m<br>1604m | 1194vs<br>1159vs | 1129vs | 560vs<br>570vs | 494m | 675sh |
| $Co(BS)_2$ | | | 1184vs | 1135vs | 574vs | 492w | 672sh |
| $[Co(H_2O)_6](BS)_2$ | 3402vs<br>3273sh | 1674m<br>1648m | 1190vs | 1127vs | 576vs | 484w | 675w |

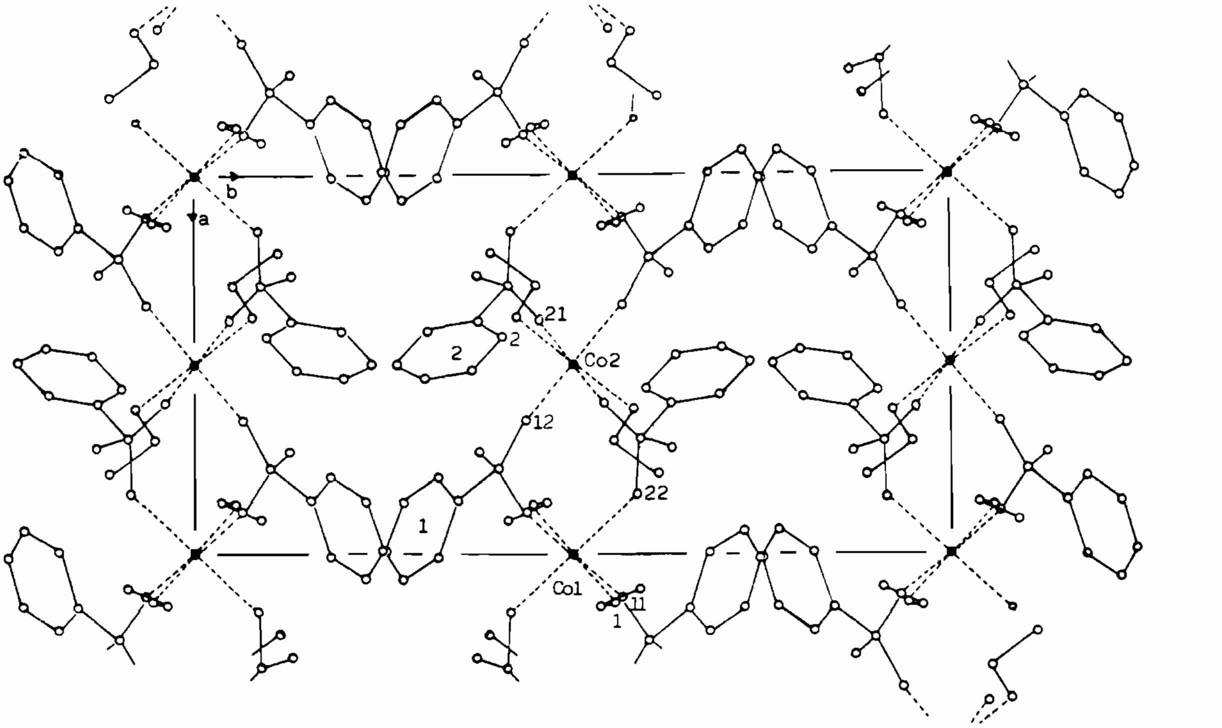

Fig 1. Projection of the crystal structure of $[CoS_2O_8C_{16}H_{22}]_2$ on to (001) plane, showing the $CoO_6$ coordination polyhedron by dotted lines.

intermediate between those of $Co(BS)_2$ and $[Co(EtOH)_6]^{2+}$, as corresponding to its composition. It is to be noted that the most intense visible band ($\nu_3$) is broad and shows one or two shoulders on the higher frequency side in all these compounds, as occurs frequently in the spectra of octahedral cobalt(II) complexes. This fact can be due to spin-orbit coupling, low symmetry components of the ligand field or transitions to doublets.

The magnetic moment of 1 at room-temperature (4.72 BM, 294 K) is characteristic also of the low-field octahedral cobalt(II) complexes and, as occurs also frequently, in this case diminishes considerably with temperature (4.49 BM at 206 K; 4.46 BM at 151 K and 4.23 BM at 77 K), as a consequence of the splitting of the ground term $^4T_{1g}$.

Table IV shows the principal infrared frequencies observed in the spectra of 1, $Co(BS)_2$ and $Co(BS)_2 \cdot 6H_2O$. It is to be noted that the vibrations corresponding to the $C_{3v}$ degenerated species of the $PhSO_3^-$ group in the spectra of $Co(BS)_2$ and $Co(BS)_2 \cdot 6H_2O$, $\nu_{as}(SO_3)$ and $\delta_{as}(SO_3)$, appear split in the case of 1. This fact indicates a more asymmetrical coordination of the $PhSO_3^-$ group through one or two oxygen atoms. Only this last possibility is consistent with the stoichiometry of 1, but the bridging or chelating nature of the bidentate $PhSO_3^-$ ligands cannot be deduced from the IR data.

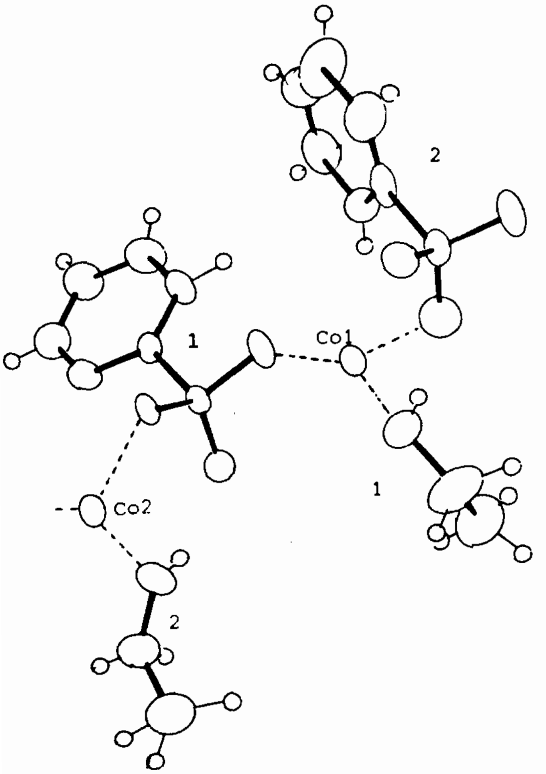

Fig. 2. View of the two independent groups of the asymmetric unit of the structure, showing the bridging nature of the bidentate $PhSO_3^-$ ligands.

### *Description of the Crystal Structure of* $Co(BS)_2(EtOH)_2$

The structure of 1 represented in Fig. 1, consists of polymeric chains of Co atoms (lying on two crystallographically independent inversion centers) connected by two benzenesulfonate ions acting as bridges through two oxygen atoms (Fig. 2). Each Co atom, bonded to four oxygen atoms from four benzenesulfonate ligands, completes its octahedral coordination through two oxygen atoms from ethanol molecules. The Co–O bond distances in the two distorted, but very similar, independent octahedrons are in the first:

Co(1)–O(11) = 2.132(8) Å
Co(1)–O(22) = 2.108(7) Å
Co(1)–O(1) = 2.049(8) Å

and in the second octahedron:

Co(2)–O(12) = 2.062(6) Å
Co(2)–O(21) = 2.135(9) Å
Co(2)–O(2) = 2.056(8) Å

The packing of the chains is determined by hydrogen bonds, which the hydroxy groups of the ethanol molecules form with the oxygen atoms of the benzenesulfonate ions not involved in the coordination of the Co atoms.

The structural data show clearly that the splitting of the degenerate vibrations $\nu_{as}$ and $\delta_{as}$ of the $PhSO_3^-$ group observed in the IR spectrum is due to its bidentate bridging behaviour. The electronic spectrum and magnetic moment correspond also to an octahedral coordination of six oxygen atoms, four belonging to four different sulfonate groups and the other two to the ethanol molecules in *trans* positions. The similarity with the electronic spectra and magnetic properties of the anhydrous sulfonates and those of the hexahydrate [1, 4] can be due to a similar environment of oxygen atoms of the $RSO^-$, EtOH and $H_2O$ ligands and to the similar position of these in the spectrochemical series.

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