Materials. The purity of the arsenic pentafluoride (Ozark Mahoning) was checked by determining its ir spectrum in a 10-cm Monel gas cell with silver chloride windows. No extraneous bands were found so it was used without further purification.

Sulfuryl fluoride (Matheson of Canada Ltd.) and thionyl fluoride (Peninsular ChemResearch Inc.) showed only one line in their ^{19}F nmr spectra and were used without further purification. Anhydrous grade sulfur dioxide (Matheson of Canada Ltd.) was used without further purification. Methyl sulfuryl fluoride (Eastman Organic Chemicals) was distilled, and the middle cut was stored over molecular sieves. Sulfuryl chlorofluoride was prepared from potassium fluorosulfinate and chlorine according to Seel and Riehl.[10] In order to remove some sulfur dioxide impurity, it was condensed onto antimony pentafluoride and subsequently distilled off. Sulfur dioxide forms a much stronger complex with antimony pentafluoride than does sulfuryl chlorofluoride, and remains be-

(10) F. Seel and L. Riehl, Z. Anorg. Allg. Chem., 282, 293 (1955).

hind.[1] The gas-phase ir spectrum of the final product showed no bands due to sulfur dioxide.

Sample Preparation. Known amounts of gases were condensed into an nmr tube from a calibrated vacuum line and the tube was sealed. If one of the components was CH_3SO_2F, a known weight was added from a hypodermic syringe, prior to placing the tube on the vacuum line.

The Crystal, Molecular, and Electronic Structure of Bisacetatobis(ethylenethiourea)cobalt(II)

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Abstract: The crystal and molecular structure of bisacetatobis(ethylenethiourea)cobalt(II) [$CoS_2O_4C_{10}N_4H_{18}$] has been determined using three-dimensional X-ray data collected by counter methods. The structure has been refined by least-squares methods to a conventional R factor of 0.061 (based on anisotropic temperature factors). This complex crystallizes in the orthorhombic system in space group D_{2h}^{14}-Pbna with 4 molecules in a unit cell of dimensions $a = 12.460 \pm 0.041$, $b = 13.550 \pm 0.036$, and $c = 9.393 \pm 0.032$ Å. The geometry about the cobalt is distorted tetrahedral with two normal cobalt–sulfur, two normal cobalt–oxygen, and two long cobalt–oxygen bonds. The 80°K polarized spectrum of this compound is also presented and rationalized in terms of pseudo-tetrahedral symmetry modified by next-nearest-neighbor interactions. The room-temperature polarized spectrum of bisacetatobis(thiourea)cobalt(II) is also presented.

Although much attention has been given in recent years to the correlation of crystal field calculations with experiment,[2] to the source of intensity of spectral lines in trigonally distorted complexes,[3] and to the identification of structure types through absorption spectroscopy,[4] little has been said about systems in which the transition metal ion finds itself in an environment which deviates greatly from idealized, tetrahedral, octahedral, etc., symmetries. That this is an important problem has recently been pointed out.[5]

In a study of complexes of cobalt(II) with ethylenethiourea (etu) it was found impossible to definitely assign a structure to the complex $Co(etu)_2(CH_3COO)_2$ on the basis of its spectrum and magnetism. It was finally concluded that the acetate groups were coordinated in a bidentate fashion and that the overall geometry was octahedral.

In order to check the accuracy of this structural assignment we have completed a determination of the crystal and molecular structure of the compound in question. We have also furthered our investigations by examining the electronic structure of $Co(etu)_2(CH_3COO)_2$.

Experimental Section

Reagents. Fisher Reagent grade $Co(CH_3COO)_2 \cdot 6H_2O$ and $Zn(CH_3COO)_2 \cdot 6H_2O$ were used without further purification. Ethylenethiourea was obtained from K & K and recrystallized twice from H_2O. Reagent grade thiourea was obtained from Fisher Scientific and used as received.

Crystal Growth and Preparation. Mixed crystals of the isomorphous Zn– and Co–etu compounds suitable for optical measurements were grown from hot aqueous solution which had been acidified with a small amount of acetic acid. Single crystals of Zn-$(tu)_2(CH_3COO)_2$ containing small amounts of Co were prepared in a manner analogous to that used for the etu complex. Crystals of

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(2) J. Ferguson, Rev. Pure Appl. Chem., 14, 1 (1964), and references therein.
(3) I. M. Walker and R. L. Carlin, J. Chem. Phys., 46, 3931 (1967); R. Dingle and R. A. Palmer, Theor. Chim. Acta, 6, 249 (1966).
(4) C. K. Jorgensen, "Absorption Spectra and Chemical Bonding in Complexes," Pergamon Press, London, 1962.
(5) R. L. Carlin and S. L. Holt, Jr., Inorg. Chem., 2, 849 (1963).

pure $Co(etu)_2(CH_3COO)_2$ for X-ray use were grown in a similar fashion.

Spectral Measurements. Measurements were made on samples containing from ~2 to 100% Co(II) and ranging in diameter from 1 to 10 mm. Techniques used for measuring the low-temperature polarized spectrum have been previously described.[6–9]

On the basis of preliminary X-ray photographs taken with Cu Kα radiation the crystals were assigned to the orthorhombic system.

The cell constants and their standard deviations were determined from a least-squares refinement of the setting angles of 12 high-angle reflections which had been carefully centered on a Picker automatic four-circle diffractometer equipped with a PDP8 computer. The results of the determination of the cell dimensions, using Mo Kα_1 radiation (λ 0.70926 Å), are $a = 12.460 \pm 0.041$, $b = 13.550 \pm 0.036$, and $c = 9.393 \pm 0.032$ Å. The systematic absences observed from Weissenberg and precession photographs and later confirmed by counter data are hkl, no absence: $0kl$, $k = 2n$; $h0l$, $h + l = 2n$; $hk0$, $h = 2n$; $h00$, $h = 2n$; $0k0$, $k = 2n$; $00l$, $l = 2n$.

A density of 1.62 g/cm³ was determined by flotation in a bromobenzene–ethylene dibromide mixture. The calculated density, assuming four molecules per unit cell, is 1.59 g/cm³.

From the above data it was determined that the space group is D_{2h}^{14}-Pbna. Observation of four molecules per unit cell in space group Pbna requires that the cobalt must reside on a site of inversion symmetry or on a twofold axis.

A rhombohedral needle-shaped crystal was used for data collection. This crystal measured 0.425 × 0.175 × 0.200 mm and was mounted parallel to c, the needle axis.

Intensity data were collected with a Philips automatic integrating linear reciprocal space exploring diffractometer (Pailred) using Mo Kα (λ 0.71069) radiation. The incident beam was monochromatized by means of a graphite single crystal. The beam collimator measured 0.5 mm in diameter and the aperture of the receiving collimator was 3.5°. A takeoff angle of 3° was used. With the crystal mounted along c, data were collected in eight layers using Weissenberg geometry. Reflections, of which 2354 were independent, with 2θ less than 46.5° (Mo Kα) were scanned 1.2° (2θ) on both sides of the Bragg angle at a scanning rate of 1°/min. Background counts of 0.24 min were taken at the beginning and end of each scan. The intensities of four standard reflections were measured before and after data collection for each layer and remained essentially constant showing only deviations attributable to counting statistics.

The intensities were corrected in the usual way for Lorentz and polarization effects. Intensity measurements were not corrected for absorption effects as the linear absorption coefficient for Mo Kα was only 20.5 cm⁻¹; 2086 reflections were nonzero.

Examination of the data showed that extinction did not effect the measured intensities to any extent, therefore, no extinction correction was applied.

Solution and Refinement of the Structure

The structure was solved initially using data collected by Weissenberg techniques. Using these data the coordinates of the cobalt atom were determined from a three-dimensional Patterson function. Subsequent use of least-squares refinement and difference Fourier techniques allowed the determination of the coordinates of the ten other independent nonhydrogen atoms. When the residual had reached 17.5%[10] the data were recollected on the Pailred system. The coordinates for the 11 nonhydrogen atoms, determined from film data, were then refined by least-squares procedures using the PIB version of the least-squares program of Busing, Martin, and Levy[11] to R factor 13.5%. This value was arrived at using isotropic temperature factors and giving all ob-

Table I. Bond Distances (Å) and Bond Angles (deg) for $Co(CH_3CO_2)_2(C_3N_2H_6)_2$

Bond	Distance	Atoms	Angle
Co-S	2.328 (3)	C_E-C_D-O_B	119.3 (9)
Co-O$_A$	1.957 (7)	$H_{C_{EB}}$-C_E-$H_{C_{EC}}$	166.0 (16)
Co-O$_B$	2.928 (7)	$H_{C_{EC}}$-C_E-$H_{C_{EA}}$	82.0 (8)
S-C$_A$	1.693 (11)	$H_{C_{EA}}$-C_E-$H_{C_{EC}}$	82.0 (8)
C$_A$-N$_A$	1.305 (11)	C_D-C_E-$H_{C_{EA}}$	91.0 (8)
C$_A$-N$_B$	1.291 (12)	C_D-C_E-$H_{C_{EB}}$	125.2 (15)
N$_A$-C$_B$	1.410 (12)	C_D-C_E-$H_{C_{EC}}$	55.0 (7)
N$_B$-C$_C$	1.410 (12)	S-C_A-N_B	129.3 (8)
C$_B$-C$_C$	1.539 (13)	S-C_A-N_A	125.3 (8)
C$_D$-O$_A$	1.254 (11)	N_A-C_B-C_C	100.4 (8)
C$_D$-O$_B$	1.241 (11)	C_C-N_B-C_A	116.5 (9)
C$_D$-C$_E$	1.507 (14)	N_A-C_A-N_B	105.4 (9)
H$_{N_A}$-N$_A$	1.083 (8)	C_A-N_A-C_B	116.4 (9)
H$_{N_B}$-N$_B$	1.066 (8)	N_B-C_C-C_B	101.0 (8)
C$_B$-H$_{C_{BA}}$	0.968 (12)	H_{N_B}-N_B-C_A	112.5 (8)
C$_B$-H$_{C_{BB}}$	0.935 (12)	H_{N_B}-N_B-C_C	130.4 (9)
C$_C$-H$_{C_{CA}}$	0.950 (14)	H_{N_A}-N_A-C_A	117.1 (8)
C$_C$-H$_{C_{CB}}$	0.957 (15)	H_{N_A}-N_A-C_B	125.3 (8)
C$_E$-H$_{C_{EA}}$	1.004 (11)	$H_{C_{BA}}$-C_B-$H_{C_{BB}}$	148.4 (12)
C$_E$-H$_{C_{EB}}$	0.715 (11)	$H_{C_{BA}}$-C_B-N_A	95.2 (9)
C$_E$-H$_{C_{EC}}$	0.870 (11)	$H_{C_{BA}}$-C_B-C_C	97.3 (10)
H$_{N_B}$-O$_A$	2.668 (8)	$H_{C_{BB}}$-C_B-N_A	105.0 (10)
Atoms	**Angle**	$H_{C_{BB}}$-C_B-C_C	102.4 (10)
S-Co-O$_A$	102.8 (2)	$H_{C_{CA}}$-C_C-C_B	96.5 (10)
Co-S$_A$-C$_A$	102.5 (2)	$H_{C_{CA}}$-C_C-N_B	111.8 (12)
Co-O$_A$-C$_D$	116.4 (6)	$H_{C_{CB}}$-C_C-C_B	87.9 (10)
S$_A$-Co-S$_B$	105.9 (2)	$H_{C_{CB}}$-C_C-N_B	105.6 (11)
O$_A$-C$_D$-O$_B$	124.1 (7)	$H_{C_{CA}}$-C_C-$H_{C_{CB}}$	140.7 (12)
O$_A$-C$_D$-C$_E$	116.5 (9)	N_B-H_{N_A}-O_A	111.0 (5)

served reflections a weight of one, the unobserved reflections getting zero weight. The atomic scattering factors used for all atoms were those tabulated by Manson, et al.[12] The scattering factor for Co was corrected for the real component of anomalous dispersion.[13] Anisotropic temperature factors were then introduced and two cycles of least squares reduced the R factor to 10.7%. A difference Fourier allowed location of the nine hydrogen atoms and two additional cycles of leasts quares with these atoms included (isotropic temperature factors for hydrogens) allowed reduction of the discrepancy factor of 9.0%. At this point a weight scheme of $\sigma = \sigma Y_0$ ($Y_0 = F_o \times$ scale factor) used along with a data-rejection scheme eliminating data with F_o less than 34.0 (std dev > 1) was introduced and the final R of 6.1% was determined. A final difference Fourier showed no peak higher than 0.47 e Å⁻³.

A table of observed and final calculated structure amplitudes, multiplied by 10, has been deposited with the ASIS National Auxiliary Publications Service.[14] Bond distances and angles for $[Co(CH_3CO_2)_2(C_3N_2H_6)_2]$ are given in Table I. The positional and thermal parameters derived from the last cycle of least-squares refinement together with the associated standard deviations of these parameters, which were computed by inversion of the least-squares matrices, are presented in Table II.

(6) C. Simo and S. L. Holt, *Inorg. Chem.*, 7, 2655 (1968).
(7) E. Banks, M. Greenblatt, and S. L. Holt, *J. Chem. Phys.*, 49, 1431 (1968).
(8) J. Milstein and S. L. Holt, *Inorg. Chem.*, 8, 1021 (1969).
(9) C. Simo, E. Banks, and S. L. Holt, *ibid.*, 8, 1446 (1969).
(10) $R = \Sigma W |\Delta F| / \Sigma W |F_o|$.
(11) W. R. Busing, K. O. Martin, and H. A. Levy, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962, ORNL-TM 305.

(12) M. P. Manson, F. Herman, J. D. Lea, and S. Skillman, *Acta Crystallogr.*, 17, 1040 (1964).
(13) "International Tables for X-ray Crystallography," Vol. 3, The Kynoch Press, Birmingham, England, 1962, Table 3.3.2C.
(14) For this table, order NAPS Document No. NAPS-00829 from the ASIS National Auxiliary Publication Service, c/o CCM Information Corp., 909 3rd Ave., New York, N. Y. 10022, remitting $1.00 for microfiche or $3.00 for photocopies. Advance payment is required. Make checks or money orders payable to CCMI–NAPS.

Table II. Positional and Thermal Parameters for $(Co(CH_3CO_2)_2(C_3N_2H_6)_2)^a$

Atom	x	y	z
Cobalt	0.2457 (2)	0.2500	0.0000
Sulfur	0.1261 (2)	0.1629 (2)	0.1427 (3)
Oxygen$_A$	0.3246 (6)	0.3297 (6)	0.1386 (7)
Oxygen$_B$	0.4378 (5)	0.1281 (6)	0.0310 (7)
Nitrogen$_A$	0.1661 (6)	0.1199 (6)	0.4153 (8)
Nitrogen$_B$	0.3041 (7)	0.1199 (6)	0.2940 (8)
Carbon$_A$	0.2020 (8)	0.1335 (8)	0.2861 (10)
Carbon$_B$	0.2420 (8)	0.0910 (9)	0.5184 (10)
Carbon$_C$	0.3456 (9)	0.0980 (11)	0.4301 (10)
Carbon$_D$	0.4104 (7)	0.3676 (7)	0.0960 (11)
Carbon$_E$	0.4848 (10)	0.4067 (9)	0.2091 (10)
Hydrogen$_{N_A}$	0.0801	0.1179	0.4292
Hydrogen$_{N_B}$	0.3442	0.1381	0.1972
Hydrogen$_{C_{BA}}$	0.2301	0.0210	0.5065
Hydrogen$_{C_{BB}}$	0.2481	0.1450	0.5799
Hydrogen$_{C_{CA}}$	0.3733	0.1551	0.4758
Hydrogen$_{C_{CB}}$	0.3500	0.0277	0.4345
Hydrogen$_{C_{EA}}$	0.5300	0.4400	0.1349
Hydrogen$_{C_{EB}}$	0.4699	0.4400	0.2649
Hydrogen$_{C_{EC}}$	0.4973	0.3555	0.1559

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cobalt	0.0034 (1)	0.0033 (1)	0.0058 (2)			
Sulfur	0.0030 (2)	0.0047 (2)	0.0083 (3)	−0.0009 (2)	−0.0006 (2)	0.0020 (2)
Oxygen A	0.0031 (5)	0.0046 (6)	0.0077 (8)	−0.0009 (5)	0.0014 (5)	−0.0008 (5)
Oxygen B	0.0027 (5)	0.0053 (6)	0.0060 (10)	0.0010 (4)	0.0007 (5)	0.0000 (5)
Nitrogen A	0.0048 (7)	0.0063 (8)	0.0122 (16)	0.0002 (6)	−0.0018 (8)	0.0021 (7)
Nitrogen B	0.0076 (9)	0.0061 (8)	0.0062 (12)	−0.0002 (6)	−0.0009 (7)	0.0018 (6)
Carbon A	0.0009 (7)	0.0030 (6)	0.0071 (13)	−0.0000 (5)	0.0012 (7)	0.0011 (7)
Carbon B	0.0027 (8)	0.0080 (10)	0.0051 (12)	0.0006 (8)	−0.0005 (8)	0.0008 (8)
Carbon C	0.0063 (9)	0.0072 (13)	0.0057 (16)	−0.0015 (8)	−0.0003 (9)	0.0032 (9)
Carbon D	0.0017 (7)	0.0024 (7)	0.0071 (15)	0.0002 (5)	−0.0008 (7)	0.0002 (6)
Carbon E	0.0061 (11)	0.0068 (10)	0.0052 (13)	−0.0012 (8)	0.0027 (10)	−0.0030 (7)

^{a} The estimated standard deviations from the least-squares refinements are given in parentheses in units of the last significant figure in the parameter itself. The expression for the temperature factor is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

Description of the Structure

The molecular geometry of this compound (Figure 1) consists of a pseudo-tetrahedral array in which the four nearest neighbors of the cobalt atom, two oxygen atoms
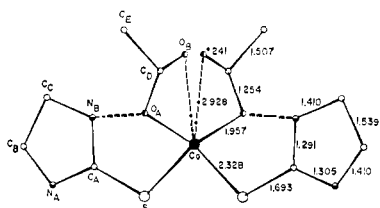

Figure 1. The molecular geometry of $Co(etu)_2(OAc)_2$.

and two sulfur atoms, are bound at 1.957 and 2.328 Å, respectively, while at 2.928 Å there are two further oxygen atoms. These atoms, as well as the carbon and nitrogen atoms, are arranged so that there exists a twofold axis of rotation parallel to the a crystallographic axis. The Co–O distance of 2.928 Å is indicative of the presence of a weak interaction. The presence of these weak bonds has, as we shall see later, a significant effect upon the electronic structure of the cobalt.

A similar metal–acetate interaction has been reported by Cavalca, et al., for $Zn[SC(NH_2)_2]_2(CH_3COO)_2$.[15]

(15) L. Cavalca, G. F. Gasparri, G. D. Andreettei, and P. Domiano, Acta Crystallogr., 22, 90 (1967).

This compound possesses four crystallographically independent oxygen atoms with metal–oxygen bond distances of 1.954, 2.891, 1.973, and 2.996 Å.

Electronic Structure of $Co(etu)_2(OAc)_2$

The spectrum of $Co(etu)_2(OAc)_2$, recorded at 80°K, is displayed in Figure 2. The band maxima are tabulated in Table III. The spectrum observed with $\vec{E}$ parallel to the unique molecular axis is labeled as z.
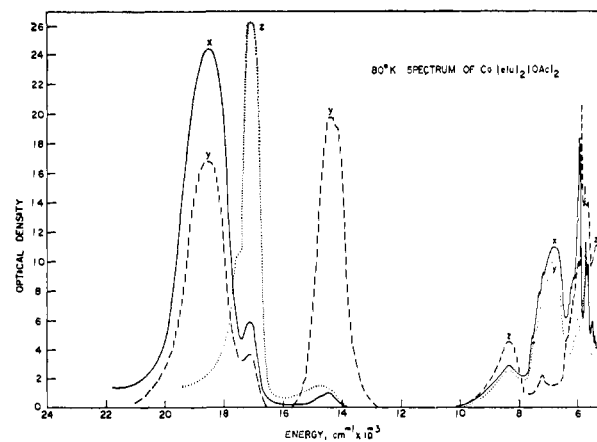

Figure 2. The 80°K spectrum of $Co(etu)_2(OAc)_2$. The letter accompanying each curve indicates the direction of the incident radiation for that particular spectrum.

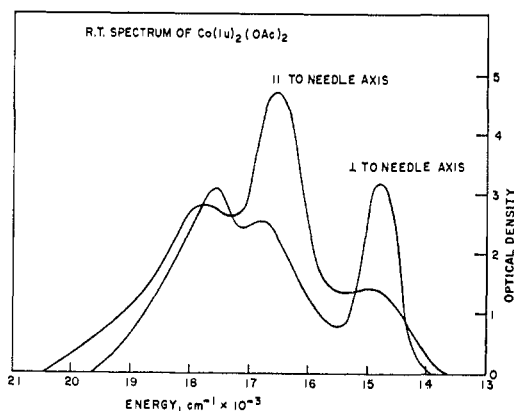Figure 3. The room-temperature spectrum of Co(tu)₂(OAc)₂.

The labels x and y are given to the spectra obtained with $\vec{E}$ parallel to c and $\vec{E}$ parallel to b. It can be seen that there are two major regions of absorption, one below 10000 cm⁻¹ and one above 12000 cm⁻¹. Although portions of the region of absorption which lie below 10000 cm⁻¹ are obviously associated with d–d transitions, there are also what appear to be ligand overtone absorptions as well. For this reason, it is necessary to ignore the details of the 7000–10000-cm⁻¹ region.

Table III. Position of Absorption Maxima in the Visible Spectrum of Co(etu)₂(OAc)₂

Energy, cm⁻¹	Polarization
18750	‖ y
18700	‖ x
17500 (sh)	‖ z
17100	‖ z
14850 (sh)	‖ y
14550 (sh)	‖ y
14400	‖ y
14150	‖ y

The geometry of the four nearest neighbors of the cobalt atom is pseudo-tetrahedral, suggesting that we may treat the electronic structure of this complex within the framework of a distorted tetrahedral model. For a tetrahedral molecule the ⁴F ground state of the Co(II) ion splits into ⁴A₂, ⁴T₂, and ⁴T₁ levels while the first excited free ion state, ⁴P, remains degenerate but transforms as ⁴T₁ in the tetrahedral group. The ordering of these levels is ⁴A₂ < ⁴T₂(F) < ⁴T₁(F) < ⁴T₁(P). The site symmetry of this complex is C₂ or considering only the four nearest neighbors to the cobalt, C₂ᵥ. Therefore, we might expect transitions to the several low-symmetry components of the ⁴T₂(F), ⁴T₁(F), and ⁴T₁(P) states. These are tabulated with their polarizations in Table III.

For most cases of tetrahedral Co(II) it is necessary to ignore the ⁴A₂ → ⁴T₂(F) transition as this occurs at such a low energy that it is masked by ligand vibrations. Here we have the case in which the ⁴A₂ → ⁴T₁(F) is also confusingly mixed with ligand vibrations. Several important conclusions can be immediately drawn, however. (1) The spectrum does not obey C₂ selection rules. If it did, all maxima which appear x should also appear y. Clearly they do not. (2) If C₂ selection

rules are not obeyed, the two maxima at ~18750 cm⁻¹ must represent two distinct transitions. (3) If conclusion 2 is valid, either the maximum at 14400 cm⁻¹ or the y-allowed component at 18750 cm⁻¹ does not have the ⁴T₁(P) as a parent state. This follows as the maximum number of low-symmetry components which any T state can exhibit is three, and in this case, T₁, there will be components x, y, and z (Table IV). It is perhaps most palatable to suggest that the 14400-cm⁻¹ absorption is a component of the ⁴T₁(F) state rather than require that the 18750-cm⁻¹ maximum be the odd absorption. This judgment is based upon the consideration that, while there is precedent[16] for a splitting of the ⁴T₁(P) to the extent of some 4000 cm⁻¹, and while this splitting might well be greater here, it would be most surprising if a component of the ⁴T₁(F) was pushed above its opposite number from the ⁴T₁(P).

Support for treatment of this system in terms of distorted tetrahedral symmetry is gained from the absorption spectrum of Co(tu)₂(OAc)₂.

Although the symmetry of the two molecules is quite different when one includes the second coordination sphere, there is a similarity in the first coordination sphere and a certain similarity between the spectra of the two compounds. The spectrum of (Co, Zn)(tu)₂(CH₃COO)₂ is shown in Figure 3. The ordering of the molecules in the crystal and the symmetry of the molecule itself preclude any detailed discussion of this spectrum. Two polarizations are included, however, as they help to clarify the spectrum.

The above arguments lead us to the conclusion that the 18700-cm⁻¹ maximum is the A₂ → B₂(P) transition, the exact assignment depending on the choice of x and y axes. This result is in contrast to the results observed for (Ph₃P)₂CoCl₂.[16] In this phosphine complex the ⁴A₂ → ⁴A₂(P) transition was found to occur in an energy range which is intermediate between the ⁴A₂ → ⁴B₁(P) and ⁴A₂ → ⁴B₂(P) transitions. This indicates, perhaps, that in Co(OAc)₂(etu)₂ the second oxygen atom from each acetate has a genuine effect upon the electronic structure of the complex even though the polarization behavior is explainable in terms of the four nearest neighbors alone.

Table IV. Correlation Table for Group Tₔ

Tₔ	C₂ᵥ	C₂
T₂	A₁ + B₁ + B₂	A + 2B
T₁	A₂ + B₁ + B₂	A + 2B

Electronic Selection Rules for C₂ᵥ and C₂ Symmetries

C₂ᵥ	C₂
A₂/A₁	A → A z
A₂ →^{y} B₁	A → B x,y
A₂ →^{x} B₂	
A₂ →^{z} A₂	

(16) C. Simo and S. L. Holt, Inorg. Chem., 7, 2655 (1968).