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# Structural Characterization of a Basic Trinuclear Ruthenium Acetate[1]

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*The compound previously reported to be $Ru_2(O_2CCH_3)_4(PPh_3)_2$ has been characterized as $Ru_3O(O_2CCH_3)_6(PPh_3)_3$ by an X-ray structural determination. It is thus related to the known basic acetates of general formula $[M_3O(O_2CR)_6L_3]^+$, M = Cr, Mn, Fe, Ru; L = $H_2O$, $O_2CR$. There is no direct metal-metal interaction. The equilateral triangle of ruthenium atoms is bridged by the six acetate groups and the central oxygen atom, which lies essentially in the $Ru_3$ plane. One $PPh_3$ ligand is coordinated to each metal opposite the central oxygen atom. Average values of interatomic distances (and average e.s.d.'s) include: Ru–P = 2.414(7); Ru–O(central) = 1.92(2); Ru–O(acetate) = 2.06(2); C–O = 1.26(3); Ru . . . Ru = 3.329 (3); O . . . O = 2.26(2) A. The identity of the solid state and solution IR spectra indicates that the same structure is maintained in solution. The non-integral oxidation state ($2^2/_3$) for Ru and the diamagnetism of the compound can be rationalized in terms of a qualitative molecular-orbital treatment of the $Ru_3OP_3$ π-electron system.*

*The compound crystallizes in the triclinic space group $P\bar{1}$ with unit cell dimensions a = 31.372(7), b = 26.21(2), c = 9.375(8) A; α = 99.06(3), β = 84.03(2), γ = 100.51(1)°; V = 3180(30) $A^3$; $\rho_{calc}$ = 1.52(1) g/cm³ for Z = 2; $\rho_{obs}$ = 1.56(3) g/ml. The structure, excluding hydrogen atoms, was determined from the intensities of 3227 unique reflections collected with a counter diffractometer. It was solved by Patterson and difference Fourier syntheses and refined by full-matrix least-squares methods to a conventional R = 0.100 and weighted R = 0.091.*

## Introduction

The structural chemistry of transition metal carboxylates has been a subject of active interest for several years, chiefly due to the pronounced tendency of carboxylate ligands to stabilize polynuclear configurations in which the metals are brought near to or within bonding distance of each other. X-ray investigations have demonstrated that a number of carboxylate complexes are dinuclear, with the formulation $[M(O_2CR)_2L]_2$, where M = V,[3] Cr[4], Mo,[5] Re,[6] Ru,[7] Rh,[4] Cu,[8] and L = $H_2O$, Cl, NCS, $h^5$-$C_5H_5$, etc. The general structure[9] corresponding to this formulation is shown in Figure 1. In the absence of severe steric hinderance by the axial ligands L (as occurs for the case M = V, L = $h^5$-$C_5H_5$)[3], the metal-metal distances derived from the X-ray work have shown that the four bridging carboxylates provide a non-constraining framework within which the two metals are free to position themselves for a strong or weak interaction with each other,, according to their particular bonding potentialities.

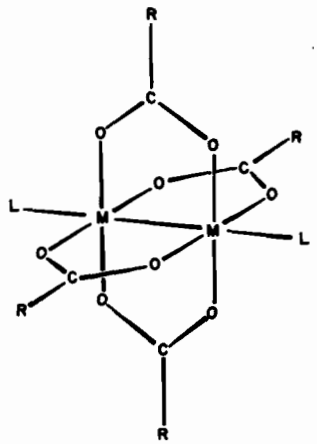


Figure 1. The general structure adopted by the compounds of formula $[M(O_2CR)_2L]_2$, M = V, Cr, Mo, Re, Ru, Rh and Cu.

With the foregoing considerations in mind, we were very interested to learn of the preparation of a compound formulated as $[Ru(O_2CCH_3)_2PPh_3]_2$,[10] since not only should an axial $PPh_3$ interact quite strongly with

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the metal, but the proposed formulation is closely related to (containing one more electron than) the known $[Ru(O_2CCH_3)_2]_2Cl$, which contains a strong metal-metal bond (Ru–Ru = 2.281(4) A) and weakly-bonded, bridging, axial chloride ions (Ru–Cl = 2.587 (5) A).[7] A significant difference in electronic structure seemed indicated by the paramagnetism (equivalent to three unpaired electrons) of the chloro species,[11] as opposed to the diamagnetism reported for the $PPh_3$ complex.[10] We decided, therefore, to determine the crystal structure of the $PPh_3$ compound in order to obtain an exact value of the Ru–Ru distance for comparison with the chloro analog. This paper reports the results of that structural investigation and related experiments. A preliminary report of this and related chemical studies has been published.[12]

## Experimental Section

*Preparation and Characterization of "$[Ru(OAc)_2PPh_3]_2$".* The compound was prepared by the literature method,[10] with the exception of the final step in which the $PPh_3$ adduct is formed from "ruthenium acetate". Here, in order to obtain crystals of the adduct suitable for X-ray investigation, it was necessary to adopt a special procedure as follows.

A solution of 0.30 g "ruthenium acetate" in 30 ml methanol was frozen by immersion in a Dewar containing liquid nitrogen. A solution of 0.75 g $PPh_3$ in 75 ml methanol, previously cooled by immersion in dry ice-acetone, was added slowly enough so that no appreciable melting took place during the addition. The Dewar was wrapped with aluminum foil and the mixture was allowed to warm to room temperature over a period of 36 hr as the liquid nitrogen evaporated. The green crystals which formed were filtered, washed with ether and pentane, and dried in vacuum over $P_4O_{10}$. *IR Spectrum* (Nujol, 4000-400 $cm^{-1}$): 3060m, 1590w, 1575w, 1540m, 1485m, 1440s, 1415s, 1345m, 1189m, 1157w, 1098m, 1072w, 1041m, 1028m, 997w, 845w, 740m, 693s, 616m, 508s, 470w $cm^{-1}$. This spectrum, not previously reported, is identical to that of an authentic sample of the compound kindly supplied by Professor G. Wilkinson. The spectrum of a freshly prepared solution ($CHCl_3$ and $CS_2$) is identical to that above. The reported diamagnetism of the compound is confirmed by the fact that a completely normal PMR spectrum was obtained (see below).

The compound appears indefinitely stable to air. It is soluble to varying degrees in almost all organic solvents and insoluble in water; the best solvents are $CHCl_3$ and $CS_2$. However, attempts to obtain good crystals using a variety of solvents and conditions were unsuccessful, necessitating the special procedure described above. The apparent reason for this was slow decomposition of the compound in solution, as revealed by changes in the PMR and electronic spectra with time. The spectral data for freshly prepared solutions were as follows: *PMR Spectrum* ($CDCl_3$, 60 MHz): 2.6 $\tau$, complex multiplet, intensity 5; 8.35 $\tau$, singlet, intensity 2. The spectrum is thus consistent with the ratio 2 $O_2CCH_3$: 1 $P(C_6H_5)_3$. *Electronic Spectrum* ($CHCl_3$, 13-38 kK): $\nu_{max}$ = 13.3 ($\varepsilon$ 4800), 25.0 (10,000), 26.3 (11,000) kK. Within a few hours after preparation of the solution, several small peaks in addition to those above became visible in the PMR spectrum, and the 26.3 kK band in the electronic spectrum decreased in intensity and moved to slightly lower energy.

*Collection and Reduction of X-ray Data.* Weissenberg (hk0, hk1) and precession, h0$\ell$, 0k$\ell$) photographs on a thin plate-like crystal using Cu K$\alpha$ radiation showed triclinic symmetry, implying space groups P1 ($C_1^1$, no. 1) or P$\bar{1}$ $C_i^1$, no. 2). The crystal was transferred to a General Electric XRD-5 manual diffractometer and aligned at $\chi$ = 90° so that c* was coincident with the $\varphi$ axis. The crystal dimensions were carefully measured and the major faces were identified from their diffraction positions and relations to each other as (100), (010), and (001). Unit cell dimensions were determined using Cu K$\alpha$ radiation ($\lambda$ = 1.5418 A) by least-squares refinement based on the accurately measured angular settings of 20 reflections; they are a = 13.372(7), b = 26.21 (2), c = 9.375(8) A, $\alpha$ = 99.06(3), $\beta$ = 84.03(2), $\gamma$ = 100.51(1)°; V = 3180(30) $A^3$. These values lead to $\rho_{calc}$ = 1.51(1) g/$cm^3$ for Z = 3, using the molecular weight for $[Ru(OAc)_2PPh_3]_2$; $\rho_{obs}$ = 1.56 (3) g/ml (flotation, aq. KI).

Intensities were measured by a scintillation counter using Ni-filtered Cu K$\alpha$ radiation a takeoff angle of 1°. The pulse-height analyzer was set to admit 92% of the Cu K$\alpha$ peak. Scans were of the $\theta$-2$\theta$ type with a scan rate of 4°/min and a fixed scan width of 2.66°. Background counts $B_1$ and $B_2$ were taken for 20 sec at each end of the scan range. The intensity, I, of each reflection was therefore taken as $I = P - B_1 - B_2$, where P is the number of counts in scanning the peak. The intensities of 3867 unique reflections within the range 2$\theta$ = 0-80° were collected. Three reflections (1$\bar{1}$0, $\bar{1}$01, and 0$\bar{1}$1) were remeasured at regular intervals throughout as a check on crystal and instrument stability. None of the three showed any systematic deviation from their original values; the maximum variation from mean intensity was 2.3%, for 1$\bar{1}$0.

Statistical analysis showed that more than 50% of the reflections had $I > 2\sigma_I$, where $\sigma_I = (P + B_1 + B_2)^{1/2}$, in every ten-degree interval of 2$\theta$ except 70-80°. Reflections with $I < 2\sigma_I$ in 2$\theta$ = 70-80° were therefore rejected, while those with $I < \sigma_I/2$ for 2$\theta$ < 70° were assigned the value $I = \sigma_I/2$. Intensities of the 3227 accepted reflections were converted to structure factor amplitudes $|F_o| = (I/Lp)^{1/2}$, where Lp = Lorentz-polarization factor, and their estimated standard deviations $\sigma_F = [4ILp]^{-1/2}[\sigma_I^2 + (0.0251)^2]^{1/2}$.

*Solution and Refinement.* Atomic scattering factors used were those of Cromer and Waber.[13] All

(11) T. A. Stephenson and G. Wilkinson, *J. Inorg. Nucl. Chem.*, *28*, 2285 (1966).
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were corrected for the real and imaginary part of anomalous dispersion using the values for $\Delta f'$ and $\Delta f''$ given by Cromer.[14]

Inspection of a three-dimensional map of the Patterson function indicated strongly that the molecular structure was not as expected. No reasonable solution could be derived in terms of dimeric $Ru_2$ units in either P1 or $P\bar{1}$. However, a completely consistent solution was obtained in $P\bar{1}$ for two trinuclear $Ru_3$ units per cell in general positions; the derived coordinates for the three unique ruthenium atoms indicated a roughly equilateral-triangular arrangement with Ru–Ru ≈ 3.3 A. Two cycles of least-squares refinement on these coordinates gave $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o| = 0.378$ and $R_2 = \Sigma w_F||F_o|-|F_c||^2/\Sigma w_F|F_o|^2 = 0.398$, where the weights were $w_F = \sigma_F^{-2}$. A difference Fourier synthesis was computed, and from it positions were derived for 53 more atoms. Two cycles of refinement gave $R_1 = 0.231$, $R_2 = 0.219$. A second difference Fourier revealed the positions of the 28 remaining atoms expected for the formulation $[Ru(OAc)_2PPh_3]_3$. Three cycles of refinement gave $R_1 = 0.145$, $R_2 = 0.106$.

The data were corrected for absorption ($\mu = 71.25$ cm$^{-1}$); calculated transmission factors ranged from 0.613 to 0.917. Two cycles of refinement using the corrected data gave $R_1 = 0.138$, $R_2 = 0.102$. Anisotropic thermal parameters were introduced for the three ruthenium and three phosphorus atoms and a cycle of refinement was carired out. At this point, several carbon atoms in four of the phenyl rings had unreasonably high temperature factors. These atoms were removed from the parameter list and carefully relocated by difference Fourier syntheses; their thermal parameters were also refined by Fourier methods. Both the positional and thermal parameters derived in this way were essentially identical to the original ones obtained from the least-squares process. It thus appears that the high thermal parameters are due to a slight disorder in the phenyl rings involved, and are not caused by misplacement of the atoms.

The strongest peak in the initial difference map used to relocate the questionable phenyl carbons was not due to one of these atoms; it was located near the center of the $Ru_3$ triangle and had intensity relative to the phenyl carbon peaks suggesting a nitrogen or oxygen atoms. Since there was no source of nitrogen in the reaction system other than the air, the atom was initially treated as an oxygen atom. Two cycles of rifinement, including this atom and the relocated phenyl carbon atoms, gave $R_1 = 0.102$, $R_2 = 0.072$. The central atom was returned with the reasonable value B= 5.2 after the first cycle and was assigned anisotropic thermal parameters in the second cycle.

An empirical weighting scheme, $\sigma = \sigma_F(0.12|F_o|)^{1/2}$, was introduced at this point to remove an observed $|F_o|$ dependence in the quantity $w_F||F_o|F_c||^2$, in accordance with Cruickshank's criterion.[15] (Inspection of the data indicated that the dependence was not the result of extinction.) Two cycles of refinement were carried out using this weighting scheme. The final $R_1$ and $R_2$ were 0.100 and 0.091, respectively. There were no significant correlations between parameters on different atoms. The e.s.d. of an observation of unit weight was 1.04, and the quantity $w_F||F_o|-|F_c||^2$ was now essentially independent of both $|F_o|$ and $\lambda^{-1}$ sin θ, indicating the correctness of the weighting scheme.

A difference Fourier synthesis was computed using the final parameters. The largest peak, in the vicinity of atom Ru(2), had a density of 1.06 electrons/A$^3$. Refinement was terminated at this point since it was felt that the information desired from the structure did not justify the expense of introducing a fully anisotropic model.

*Computer Programs.* Programs used in the structure determination include PICK2 (J. A. Ibers) for refining cell constants and generating settings for data collection; DRAB70 (B. G. De Boer) for reduction and the absorption correction; FORDAP (A. Zalkin) for Patterson and Fourier syntheses; SFIX and SIDIOT (local versions of C. T. Prewitt's SFLS-5) for full-matrix least-squares refinement based on minimization of the function $D = \Sigma w_F||F_o|-|F_c||^2$; STAN1 (B. G. De Boer) for interatomic distances and angles; MGEOM (J. S. Wood) for least-squares planes; and ORTEP (C. K. Johnson) for intermolecular contacts and diagrams.

## Results and Description of Structure

A table of the final values of $|F_c|$ and $|F_o|$ scaled to $|F_c|$ appears in the microfilm edition of this journal. Fractional coordinates and thermal parameters for the 85 unique atoms are given in Table I. Tables II-IV present data on interatomic distances, angles, and least-squares planes, respectively. Figures 2 and 3 depicit the molecular structure and illustrate the atom numbering scheme.

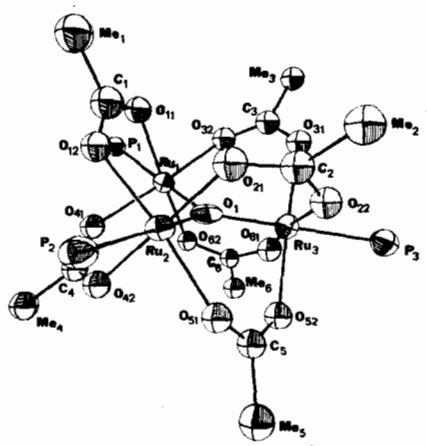


Figure 2. A "side" view of the molecular structure omitting phenyl groups. The ellipsoids enclose 30 percent probability of thermal motion.

(14) D. T. Cromer, *ibid.*, *18*, 17 (1965).

(15) D. W. J. Cruickshank in "Computing Methods in Crystallography," J. S. Rollet, Ed., Pergamon Press, New York, 1965.

**Table I.** Fractional Coordinates and Thermal Parameters.

| ATOM | X | Y | Z | B,[b] Å² |
|---|---|---|---|---|
| RU1 | 0.2702(1) | 0.30523(8) | 0.2029(2) | 3.4(1) |
| RU2 | 0.0442(1) | 0.25025(8) | 0.0868(2) | 3.9(1) |
| RU3 | 0.2234(1) | 0.17678(8) | 0.0904(2) | 3.9(1) |
| P1 | 0.3660(5) | 0.3860(3) | 0.3191(7) | 4.0(4) |
| P2 | -0.1258(5) | 0.2609(3) | 0.0465(8) | 4.8(4) |
| P3 | 0.2851(6) | 0.0949(3) | 0.0513(9) | 5.6(5) |
| O1 | 0.181(1) | 0.2423(6) | 0.119(2) | 4.8(9) |
| O11 | 0.170(1) | 0.3186(6) | 0.379(2) | 5.1(4) |
| O12 | 0.026(1) | 0.3379(6) | 0.260(2) | 4.9(4) |
| O21 | -0.022(1) | 0.1954(6) | 0.217(2) | 5.4(4) |
| O22 | 0.084(1) | 0.1358(6) | 0.147(2) | 5.3(4) |
| O31 | 0.253(1) | 0.1835(6) | 0.308(2) | 4.7(4) |
| O32 | 0.336(1) | 0.2671(6) | 0.333(2) | 5.0(4) |
| O41 | 0.224(1) | 0.3536(6) | 0.080(2) | 4.8(4) |
| O42 | 0.097(1) | 0.3046(6) | -0.049(2) | 4.7(4) |
| O51 | 0.045(1) | 0.1949(6) | -0.100(2) | 4.8(4) |
| O52 | 0.193(1) | 0.1667(6) | -0.126(2) | 5.1(4) |
| O61 | 0.369(1) | 0.2358(6) | 0.019(2) | 5.3(4) |
| O62 | 0.383(1) | 0.2934(6) | 0.037(2) | 3.8(4) |
| C1 | 0.077(2) | 0.321(1) | 0.373(3) | 6.7(8) |
| C2 | 0.004(2) | 0.153(1) | 0.214(3) | 5.2(7) |
| C3 | 0.311(2) | 0.223(1) | 0.375(3) | 5.0(7) |
| C4 | 0.163(2) | 0.345(1) | -0.025(3) | 4.7(6) |
| C5 | 0.115(2) | 0.175(1) | -0.173(3) | 4.7(6) |
| C6 | 0.411(2) | 0.250(1) | -0.013(3) | 3.6(6) |
| ME1 | 0.020(2) | 0.342(1) | 0.513(3) | 7.9(8) |
| ME2 | -0.076(2) | 0.108(1) | 0.280(3) | 5.9(7) |
| ME3 | 0.353(2) | 0.2127(9) | 0.512(3) | 4.9(6) |
| ME4 | 0.173(2) | 0.388(1) | -0.125(3) | 6.0(7) |
| ME5 | 0.097(2) | 0.158(1) | -0.333(3) | 6.8(8) |
| ME6 | 0.504(2) | 0.2533(9) | -0.119(3) | 5.2(7) |
| C11 | 0.471(2) | 0.422(1) | 0.214(3) | 4.6(6) |
| C12 | 0.545(2) | 0.3905(9) | 0.142(3) | 4.7(6) |
| C13 | 0.632(2) | 0.4161(9) | 0.068(3) | 4.3(6) |
| C14 | 0.648(2) | 0.470(1) | 0.055(3) | 6.8(8) |
| C15 | 0.574(2) | 0.496(1) | 0.131(3) | 6.1(7) |
| C16 | 0.482(2) | 0.474(1) | 0.203(3) | 5.2(7) |
| C21 | 0.426(2) | 0.3806(9) | 0.485(3) | 4.6(6) |
| C22 | 0.529(2) | 0.405(1) | 0.503(3) | 5.7(7) |
| C23 | 0.565(2) | 0.399(1) | 0.638(3) | 7.0(8) |
| C24 | 0.504(2) | 0.372(1) | 0.743(3) | 7.2(8) |
| C25 | 0.407(2) | 0.350(1) | 0.722(3) | 5.6(7) |
| C26 | 0.367(2) | 0.3519(9) | 0.587(3) | 4.5(6) |
| C31 | 0.288(2) | 0.4351(9) | 0.397(3) | 4.6(6) |
| C32 | 0.299(2) | 0.467(1) | 0.535(3) | 5.5(7) |
| C33 | 0.233(2) | 0.532(1) | 0.587(3) | 6.8(7) |
| C34 | 0.158(2) | 0.513(1) | 0.500(4) | 7.9(8) |
| C35 | 0.147(2) | 0.482(1) | 0.361(4) | 8.4(9) |
| C36 | 0.211(2) | 0.446(1) | 0.308(3) | 5.7(7) |
| C41 | -0.124(2) | 0.326(1) | -0.015(3) | 6.0(7) |
| C42 | -0.087(2) | 0.368(2) | 0.077(4) | 10(1) |
| C43 | -0.084(2) | 0.422(1) | 0.029(4) | 10(1) |
| C44 | -0.115(3) | 0.417(1) | -0.101(5) | 9(1) |
| C45 | -0.160(3) | 0.381(2) | -0.188(4) | 10(1) |
| C46 | -0.170(2) | 0.326(1) | -0.152(3) | 7.9(8) |
| C51 | -0.218(2) | 0.2630(9) | 0.196(3) | 4.4(6) |
| C52 | -0.201(2) | 0.2511(9) | 0.338(3) | 5.0(7) |
| C53 | -0.273(2) | 0.254(1) | 0.455(3) | 8.1(8) |
| C54 | -0.365(2) | 0.274(1) | 0.444(4) | 8.3(9) |
| C55 | -0.387(2) | 0.285(1) | 0.312(4) | 8.1(9) |
| C56 | -0.312(2) | 0.281(1) | 0.182(3) | 5.9(7) |
| C61 | -0.192(2) | 0.206(1) | -0.090(3) | 6.5(7) |
| C62 | -0.273(2) | 0.173(1) | -0.031(3) | 8.2(9) |
| C63 | -0.318(3) | 0.124(2) | -0.144(5) | 15(1) |
| C64 | -0.269(3) | 0.133(2) | -0.285(5) | 12(1) |
| C65 | -0.194(3) | 0.162(2) | -0.345(4) | 12(1) |
| C66 | -0.141(2) | 0.208(1) | -0.233(4) | 8.0(8) |
| C71 | 0.194(2) | 0.038(1) | 0.124(4) | 8.4(9) |
| C72 | 0.161(3) | 0.053(1) | 0.264(5) | 12(1) |
| C73 | 0.093(3) | 0.012(2) | 0.342(5) | 15(1) |
| C74 | 0.074(3) | -0.036(2) | 0.252(6) | 13(1) |
| C75 | 0.106(5) | -0.048(2) | 0.141(7) | 20(2) |
| C76 | 0.190(3) | -0.014(2) | 0.049(5) | 16(1) |
| C81 | 0.315(2) | 0.072(1) | -0.141(3) | 6.7(8) |
| C82 | 0.235(3) | 0.042(2) | -0.224(5) | 13(1) |
| C83 | 0.263(4) | 0.033(2) | -0.386(5) | 14(1) |
| C84 | 0.361(3) | 0.050(2) | -0.442(4) | 12(1) |
| C85 | 0.426(3) | 0.083(2) | -0.367(5) | 12(1) |
| C86 | 0.406(3) | 0.095(1) | -0.207(4) | 9(1) |
| C91 | 0.406(2) | 0.092(1) | 0.129(3) | 4.7(6) |
| C92 | 0.432(2) | 0.042(1) | 0.142(3) | 8.7(9) |
| C93 | 0.524(3) | 0.040(1) | 0.202(4) | 9.5(9) |
| C94 | 0.577(2) | 0.088(1) | 0.265(3) | 7.9(8) |
| C95 | 0.553(2) | 0.134(1) | 0.258(3) | 7.0(8) |
| C96 | 0.461(2) | 0.139(1) | 0.192(3) | 6.2(7) |

ANISOTROPIC THERMAL PARAMETERS,[c] Å²

| ATOM | B11 | B22 | B33 | B12 | B13 | B23 |
|---|---|---|---|---|---|---|
| RU1 | 2.9(1) | 3.7(1) | 3.5(1) | 0.34(9) | -0.7(1) | 0.5(1) |
| RU2 | 3.0(1) | 4.8(1) | 3.8(1) | 0.5(1) | -0.6(1) | 0.3(1) |
| RU3 | 3.3(1) | 3.7(1) | 4.6(1) | 0.0(1) | -0.5(1) | 0.3(1) |
| P1 | 4.8(4) | 3.5(4) | 3.8(4) | 0.3(3) | -0.4(3) | 0.7(4) |
| P2 | 4.1(4) | 6.2(5) | 4.1(4) | 1.2(4) | -0.6(3) | 0.1(4) |
| P3 | 5.5(5) | 5.7(5) | 5.6(5) | 0.1(4) | -0.8(4) | 1.2(4) |
| O1 | 4.4(9) | 6(1) | 2.7(9) | -0.4(8) | 1.3(7) | 1.1(8) |

[a] Numbers in parentheses are e.s.d.'s in the last figure quoted for all tables. [b] Effective isotropic B's are given for the anisotropically refined atoms. [c] The form of the temperature factor expression is: $\exp[-1/4(B_{11}h^2a^{*2}+B_{22}k^2b^{*2}+B_{33}l^2c^{*2}+2B_{12}hka^*b^*+2B_{13}hla^*c^*+2B_{23}klb^*c^*)]$.

The structural analysis yields the molecular formula $Ru_3O(O_2CCH_3)_6(PPh_3)_3$ for the compound rather than $Ru_2(O_2CCH_3)_4(PPh_3)_2$ as anticipated. This results in $\rho_{calc}$ = 1.52(1) g/cm$^3$ for Z = 2. The three ruthenium atoms form an almost perfect equilateral triangle around the central oxygen with the average side of length 3.33 A. The average Ru-O (central) distance is significantly shorter (0.14 A) than the average Ru-O(acetate) distance. The 0.06 A deviation of the central oxygen from the $Ru_3$ plane is at most barely significant. The four acetate oxygen atoms surrounding each ruthenium atom are essentially coplanar, and the planes are perpendicular to the $Ru_3$ unit within experimental error. Each ruthenium atom is displaced from the $O_4$ plane toward the central ovygen by about 0.1 A. The $CCO_2$ groups are all rigorously planar, but the ruthenium atoms which they bridge all lie out of these planes by 0.24-0.82 A. The orientations of the acetate planes with respect to the $Ru_3$ unit vary over a 9° range

**Table II.** Principal Bond Distances and Intramolecular Contacts [a].

| | | | |
|---|---|---|---|
| Ru(1)-P(1) | 2.425(7) | C(1)-O(11) | 1.26(3) |
| Ru(2)-P(2) | 2.416(7) | C(1)-O(12) | 1.28(4) |
| Ru(3)-P(3) | 2.400(8) | C(2)-O(21) | 1.22(3) |
| Ru(1)-O(1) | 1.95(2) | C(2)-O(22) | 1.30(3) |
| Ru(2)-O(1) | 1.94(1) | C(3)-O(31) | 1.30(3) |
| Ru(3)-O(1) | 1.87(2) | C(3)-O(32) | 1.25(3) |
| Ru(1)-O(11) | 2.04(2) | C(4)-O(41) | 1.30(3) |
| Ru(1)-O(32) | 2.05(2) | C(4)-O(42) | 1.26(3) |
| Ru(1)-O(41) | 2.05(2) | C(5)-O(51) | 1.25(3) |
| Ru(1)-O(62) | 2.08(1) | C(5)-O52 | 1.23(3) |
| Ru(2)-O(12) | 2.07(2) | C(6)-O(61) | 1.27(3) |
| Ru(2)-O(21) | 2.05(2) | C(6)-O(62) | 1.25(3) |
| Ru(2)-O(42) | 2.04(2) | C(1)-Me(1) | 1.53(4) |
| Ru(2)-O(51) | 2.09(2) | C(2)-Me(2) | 1.60(4) |
| Ru(3)-O(22) | 2.03(2) | C(3)-Me(3) | 1.53(4) |
| Ru(3)-O(31) | 2.09(2) | C(4)-Me(4) | 1.55(4) |
| Ru(3)-O(52) | 2.08(2) | C(5)-Me(5) | 1.53(4) |
| Ru(3)-O(61) | 2.04(2) | C(6)-Me(6) | 1.51(3) |
| P(1)-C(11) | 1.83(2) | Ru(1)...Ru(2) | 3.316(3) |
| P(1)-C(21) | 1.85(3) | Ru(1)...Ru(3) | 3.329(3) |
| P(1)-C(31) | 1.82(2) | Ru(2)...Ru(3) | 3.342(3) |
| P(2)-C(41) | 1.87(3) | O(11)...O(12) | 2.28(2) |
| P(2)-C(51) | 1.77(3) | O(21)...O(22) | 2.27(2) |
| P(2)-C(61) | 1.93(3) | O(31)...O(32) | 2.26(2) |
| P(3)-C(71) | 1.91(3) | O(41)...O(42) | 2.26(2) |
| P(3)-C(81) | 1.84(3) | O(51)...O(52) | 2.21(2) |
| P(3)-C(91) | 1.85(2) | O(61)...O(62) | 2.25(2) |
| Average Bond Distances and Contacts [b] | | | |
| Ru-P | 2.414(7) | C-O | 1.26(3) |
| Ru-O(central) | 1.92(2) | C-Me | 1.54(4) |
| Ru-O(acetate) | 2.06(2) | Ru...Ru | 3.329(3) |
| P-C | 1.85(3) | O...O | 2.26(2) |

[a] E.s.d.'s occuring in least significant digit in parentheses. [b] Standard deviations as well as bond lengths represent average values.

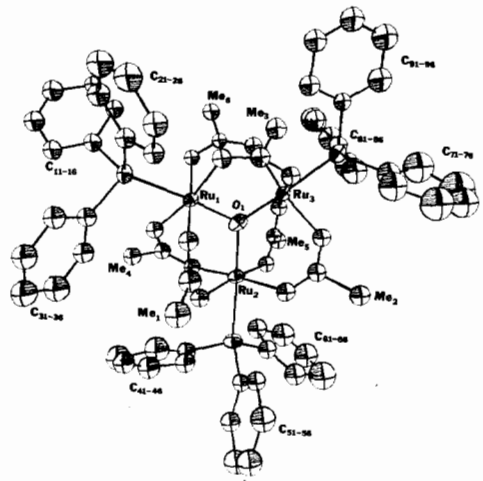

Figure 3. A "top" view of the molecular structure. The ellipsoids enclose 30 percent probability of thermal motion.

**Table III.** Principal Bond Angles [a]

| | | | | | |
|---|---|---|---|---|---|
| Ru(1)-O(1)-Ru(2) | 116.7(8) | O(42)-Ru(2)-O(12) | 91.8(6) | O(11)-C(1)-Me(1) | 117(3) |
| Ru(1)-O(1)-Ru(3) | 120.8(7) | O(12)-Ru(2)-O(51) | 171.8(6) | O(21)-C(2)-Me(2) | 118(2) |
| Ru(2)-O(1)-Ru(3) | 122.2(8) | O(21)-Ru(2)-O(42) | 175.0(7) | O(31)-C(3)-Me(3) | 115(2) |
| P(1)-Ru(1)-O(1) | 174.5(5) | O(22)-Ru(3)-O(31) | 86.8(6) | O(41)-C(4)-Me(4) | 118(2) |
| P(2)-Ru(2)-O(1) | 179.5(4) | O(31)-Ru(3)-O(61) | 95.6(7) | O(51)-C(5)-Me(5) | 114(2) |
| P(3)-Ru(3)-O(1) | 177.3(5) | O(61)-Ru(3)-O(52) | 85.4(6) | O(61)-C(6)-Me(6) | 118(2) |
| P(1)-Ru(1)-O(11) | 81.7(5) | O(52)-Ru(3)-O(22) | 92.0(6) | C(11)-P(1)-Ru(1) | 118.9(8) |
| P(1)-Ru(1)-O(32) | 86.9(5) | O(22)-Ru(3)-O(61) | 170.4(7) | C(21)-P(1)-Ru(1) | 115.6(8) |
| P(1)-Ru(1)-O(41) | 84.0(5) | O(31)-Ru(3)-O(52) | 117.6(7) | C(31)-P(1)-Ru(1) | 114.0(8) |
| P(1)-Ru(1)-O(62) | 94.6(4) | C(1)-O(11)-Ru(1) | 125(2) | C(11)-P(1)-C(21) | 103(1) |
| P(2)-Ru(2)-O(12) | 82.5(5) | C(1)-O(12)-Ru(2) | 128(2) | C(11)-P(1)-C(31) | 104(1) |
| P(2)-Ru(2)-O(21) | 87.8(5) | C(2)-O(21)-Ru(2) | 125(2) | C(21)-P(1)-C(31) | 99(1) |
| P(2)-Ru(2)-O(42) | 87.3(5) | C(2)-O(22)-Ru(3) | 130(2) | C(41)-P(2)-Ru(2) | 110.9(9) |
| P(2)-Ru(2)-O(51) | 89.5(5) | C(3)-O(31)-Ru(3) | 124(2) | C(51)-P(2)-Ru(2) | 118.2(9) |
| P(3)-Ru(3)-O(22) | 87.2(5) | C(3)-O(32)-Ru(1) | 133(2) | C(61)-P(2)-Ru(2) | 113.5(9 |
| P(3)-Ru(3)-O(31) | 87.8(5) | C(4)-O(41)-Ru(1) | 133(2) | C(41)-P(2)-C(51) | 102(1) |
| P(3)-Ru(3)-O(51) | 90.1(5) | C(4)-O(42)-Ru(2) | 127(2) | C(41)-P(2)-C(61) | 109(1) |
| P(3)-Ru(3)-O(61) | 83.6(5) | C(5)-O(51)-Ru(2) | 131(2) | C(51)-P(2)-C(61) | 103(1) |
| O(11)-Ru(1)-O(32) | 85.2(6) | C(5)-O(52)-Ru(3) | 126(2) | C(71)-P(3)-Ru(3) | 115(1) |
| O(32)-Ru(1)-O(62) | 90.9(6) | C(6)-O(61)-Ru(3) | 133(2) | C(81)-P(3)-Ru(3) | 113(1) |
| O(62)-Ru(1)-O(41) | 86.7(6) | C(6)-O(62)-Ru(1) | 126(1) | C(91)-P(3)-Ru(3) | 118.7(9) |
| O(41)-Ru(3)-O(11) | 96.6(6) | O(11)-C(1)-O(12) | 127(3) | C(71)-P(3)-C(81) | 106(1) |
| O(11)-Ru(1)-O(62) | 174.7(6) | O(21)-C(2)-O(22) | 128(2) | C(71)-P(3)-C(91) | 102(1) |
| O(32)-Ru(1)-O(41) | 170.4(6) | O(31)-C(3)-O(32) | 125(2) | C(81)-P(3)-C(91) | 101(1) |
| O(12)-Ru(2)-O(21) | 88.5(6) | O(41)-C(4)-O(42) | 124(2) | Ru(1)..Ru(2)..Ru(3) | 60.39(6) |
| O(21)-Ru(2)-O(51) | 93.3(6) | O(51)-C(5)-O(52) | 126(2) | Ru(2)..Ru(1)..Ru(3) | 60.00(6) |
| O(51)-Ru(2)-O(42) | 85.7(6) | O(61)-C(6)-O(62) | 126(2) | Ru(3)..Ru(1)..Ru(2) | 59.61(66) |

[a] E.s.d.'s occuring in least significant digit in parentheses.

**Table IV.**

Weighted Least Squares Planes [a]

| Plane | Equation | Angle with Plane 1, deg. |
|---|---|---|
| 1. Ru(1)Ru(2)Ru(3) | $-0.2668x-0.2526y+0.9301z=-1.0234$ | — |
| 2. O(11)O(32)O(41O(62) | $0.644x+0.666y+0.375z=7.896$ | 39.5(6) |
| 3. O(12)O(21)O(42)O(51) | $0.942x-0.272y+0.199z=1.070$ | 89.9(6) |
| 4. O(22)O(31)O(52)O(61) | $-0.291x+0.943y+0.161z=2.887$ | 90.6(6) |
| 5. O(11)O(12)C(1)Me(1) | $-0.244x-0.942y+0.231z=-6.751$ | 58.8(9) |
| 6. 0(21)O(22)C(2)Me(2) | $0.509x+0.073y+0.858z=2.021$ | 50.0(9) |
| 7. O(31)O(32)C(3)Me(3) | $-0.758x+0.366y+0.539z=0.211$ | 52.3(9) |
| 8. O(41)O(42)C(4)Me(4) | $-0.631x+0.981y+0.609z=2.697$ | 52.2(9) |
| 9. O(51)O(52)C(5)Me(5) | $-0.456x-0.870y+0.187z=-4.888$ | 59.0(9) |
| 10. O(61)O(62)C(6)Me(6) | $0.646x-0.114y+0.755z=2.763$ | 56.0(9) |

Distances of Atoms from Planes, [b] A

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1. | P(1), | 0.208; | P(2), | 0.067; | P(3), | 0.021; | O(1), | −0.06 | | | | |
| 2. | O(11), | −0.05; | O(32), | 0.05; | O(41), | 0.05; | O(62), | −0.04; | Ru(1), | −0.119 | | |
| 3. | O(12), | −0.03; | O(21), | 0.03; | O(42), | 0.03; | O(51), | −0.03; | Ru(2), | 0.116 | | |
| 4. | O(22), | −0.06; | O(31), | 0.06; | O(52), | 0.07; | O(61), | −0.06; | Ru(3), | 0.102 | | |
| 5. | O(11), | 0.00; | O(12), | 0.00; | C(1), | −0.00; | Me(1), | 0.00; | Ru(1), | −0.350; | Ru(2), | 0.825 |
| 6. | O(21), | −0.01; | O(22), | −0.01; | C(2), | 0.04; | Me(2), | −0.02; | Ru(2), | −0.544; | Ru(3), | 0.513 |
| 7. | O(31), | −0.00; | O(32), | −0.00; | C(3), | 0.01; | Me(3), | −0.01; | Ru(1), | 0.575; | Ru(3) | −0.588 |
| 8. | O(41), | 0.00; | O(42), | 0.00; | C(4), | −0.00; | Me(4), | 0.00; | Ru(1), | −0.503; | Ru(2), | 0.425 |
| 9. | O(51), | 0.00; | O(52), | 0.00; | C(5), | −0.02; | Me(5), | 0.01; | Ru(2), | −0.756; | Ru(3), | 0.234 |
| 10. | O(61), | 0.00; | O(62), | 0.00; | C(6), | −0.01; | Me(6), | 0.00; | Ru(1), | 0.240; | Ru(3), | −0.643 |

[a] The orthogonal coordinates (x,y,z) are directed along the crystal axes $c^* \times a$, $b$ and $c^*$, respectively, and are in Ångstroms. The weight given to each atom $i$ in forming the planes is $w_i = [a_\sigma x_i b_\sigma y_i c_\sigma z_i]^{-2/3}$. [b] Average e.s.d.'s of atomic positions are (A): Ru, 0.002; P, 0.007; O, 0.015; C, 0.03; Me, 0.03.

**Table V.** Average Interatomic Distances in Trinuclear Cr and Ru Acetates (A) [a].

| | $[Cr_3O(OAc)_6(H_2O)_3]Cl \cdot 6H_2O$ [b] | $[Ru_3O(OAc)_6(PPh_3)_3]$ [c] |
|---|---|---|
| M...M | 3.274(4) | 3.329(3) |
| M-O(central) | 1.89(1) | 1.92(2) |
| M-O(acetate) | 1.98(1) | 2.06(2) |
| M-L | 2.02(1) (L=$H_2O$) | 2.414(7) (L=$PPh_3$) |
| O...O | 2.21(2) | 2.26(2) |

[a] Average values of e.s.d.'s are also given. [b] Reference 22. [c] This work.

for the three ligands "above" the unit and over a 7° range for the three "below". On the average, the Ru-Ru separations are 1.07 A. greater than the O...O "bite" of the bridging acetates, resulting in a mean Ru-O-C angle of 128°. As discussed in the Experimental section, the unusually high thermal parameters for some of the phenyl carbon atoms are apparently due to a slight disorder. There are no intermolecular contacts significantly shorter than van der Waals radii.

## Discussion

The surprising result of the structure determination is that the substance originally thought to be $Ru_2(OAc)_4(Ph_3)_2$ is in fact $Ru_3O(OAc)_6(Ph_3)_3$, both the molecular weight and metal oxidation state differing from the anticipated result. The complete identity of the solution and solid state infrared spectra demonstrates that no change in structure occurs upon dissolution of the compound; the previously reported solution molecular weight of 960[10] (calcd. for the dinuclear formulation: 963) is erroneous. One possible reason for this error might be the slow decomposition which we have observed for the complex in solution.

Rather than belonging to the class compounds with formulation $M_2(O_2CR)_4L_2$, the complex is thus an example of the other major structural type that has been established for transition-metal carboxylates, for which the general formula is $M_3O(O_2CR)_6L_3$. Where M = $Cr^{III}$ and $Fe^{III}$, L is most commonly $H_2O$, and the complexes are thus cationic; they occur with a wide variety of counterions and varying amounts of lattice water[16]. For M = $Ru^{III}$ and $Mn^{III}$, one example each of this cationic type of complex has been reported, with the apparent formulations $[Ru_3O(OAc)_6(H_2O)_3]OAc \cdot 5H_2O$[17] and $[Mn_3O(OAc)_6]OAc \cdot HOAc$[18].

There is also a brief report of a tungsten compound which might have the trinuclear structure[19], but recent work in This Laboratory[20] indicates that the reported synthesis is not completely reproducible. The infrared and Raman spectra of the cationic complexes

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(20) F. A. Cotton and M. Jeremic, *Syn. Inorg. Metal-Org. Chem.*, *1*, 265 (1971).

Observed and Calculated Structure Factors in Units of 0.1 Electron.

| H | K | FOBS | FCAL |
|---|---|---|---|
| | **L = 0** | | |
| 0 | -1 | 58 | 75 |
| 0 | -2 | 2795 | 2856 |
| 0 | -3 | 167 | 209 |
| 0 | -4 | 588 | 507 |
| 0 | -5 | 96 | 156 |
| 0 | -6 | 244 | 191 |
| 0 | -7 | 199 | 235 |
| 0 | -8 | 271 | 337 |
| 0 | -9 | 1271 | 1333 |
| 0 | -10 | 290 | 213 |
| 0 | -11 | 322 | 256 |
| 0 | -12 | 796 | 726 |
| 0 | -13 | 106 | 85 |
| 0 | -14 | 1270 | 1337 |
| 0 | -15 | 571 | 564 |
| 0 | -16 | 861 | 886 |
| 0 | -17 | 162 | 169 |
| 0 | -18 | 726 | 698 |
| 0 | -20 | 460 | 369 |
| -1 | 0 | 654 | 621 |
| 1 | 1 | 1934 | 2046 |
| 1 | -1 | 2908 | 3013 |
| -1 | 2 | 1240 | 1285 |
| -1 | -2 | 1872 | 1906 |
| -1 | 3 | 122 | 82 |
| -1 | -3 | 403 | 395 |
| 1 | 4 | 561 | 582 |
| -1 | 4 | 1377 | 1372 |
| 1 | -5 | 231 | 215 |
| -1 | -5 | 856 | 830 |
| 1 | 6 | 386 | 407 |
| 1 | -6 | 1161 | 1132 |
| 1 | 7 | 1524 | 1442 |
| -1 | 7 | 2019 | 1983 |
| -1 | 8 | 113 | 134 |
| -1 | -8 | 146 | 101 |
| 1 | 9 | 1272 | 1328 |
| 1 | -9 | 765 | 707 |
| 1 | -10 | 1305 | 1329 |
| 1 | 10 | 384 | 303 |
| 1 | -11 | 123 | 124 |
| 1 | 11 | 193 | 216 |
| -1 | -12 | 861 | 896 |
| -1 | 12 | 674 | 721 |
| -1 | -13 | 700 | 657 |
| -1 | 13 | 206 | 207 |
| 1 | -14 | 372 | 395 |
| 1 | 14 | 1524 | 1383 |
| 1 | -15 | 762 | 744 |
| -1 | -15 | 713 | 736 |
| 1 | -16 | 160 | 118 |
| -1 | -16 | 1305 | 1351 |
| 1 | -17 | 383 | 349 |
| 1 | 17 | 314 | 266 |
| 1 | 18 | 657 | 651 |
| -1 | 18 | 133 | 49 |
| 1 | 19 | 365 | 301 |
| -1 | 19 | 136 | 160 |
| 1 | 20 | 312 | 283 |
| -1 | 21 | 315 | 103 |
| -2 | 0 | 1236 | 1321 |
| 2 | 1 | 78 | 84 |
| 2 | -1 | 554 | 623 |
| 2 | 2 | 85 | 77 |
| 2 | -2 | 896 | 965 |
| 2 | -3 | 79 | 179 |
| -2 | -3 | 854 | 961 |
| 2 | 4 | 593 | 574 |
| 2 | -4 | 711 | 764 |
| 2 | 5 | 888 | 883 |
| 2 | -5 | 256 | 186 |
| -2 | 6 | 2224 | 2191 |
| -2 | -6 | 881 | 892 |
| 2 | 7 | 716 | 754 |
| -2 | 7 | 162 | 282 |
| 2 | 8 | 1026 | 1054 |
| -2 | 8 | 2448 | 2287 |
| 2 | 9 | 164 | 72 |
| 2 | -9 | 766 | 796 |
| 2 | -10 | 774 | 777 |
| -2 | -10 | 762 | 697 |
| 2 | -11 | 1193 | 1165 |
| -2 | -11 | 161 | 34 |
| 2 | -12 | 213 | 65 |
| 2 | 12 | 140 | 197 |
| 2 | -13 | 264 | 289 |
| 2 | 13 | 674 | 695 |
| 2 | 14 | 337 | 282 |
| -2 | 14 | 165 | 185 |
| -2 | -15 | 996 | 1001 |
| -2 | 15 | 550 | 501 |
| 2 | -16 | 369 | 386 |
| 2 | 16 | 165 | 202 |
| 2 | -17 | 336 | 347 |
| 2 | 17 | 622 | 663 |
| 2 | 18 | 642 | 673 |
| -2 | 18 | 132 | 163 |
| -2 | 19 | 141 | 129 |
| -2 | -20 | 381 | 373 |
| 2 | -21 | 315 | 221 |
| 3 | 0 | 236 | 117 |
| 3 | 1 | 477 | 405 |
| 3 | -1 | 163 | 201 |
| 3 | -2 | 681 | 695 |
| -3 | -2 | 1049 | 1017 |
| 3 | -3 | 512 | 516 |
| -3 | -3 | 1163 | 1078 |
| 3 | 4 | 257 | 349 |
| -3 | 4 | 625 | 661 |
| 3 | 5 | 1160 | 1161 |
| 3 | -5 | 478 | 486 |
| 3 | 6 | 966 | 1009 |
| -3 | 6 | 854 | 893 |
| -3 | 7 | 1166 | 1234 |
| -3 | -7 | 1390 | 1425 |
| 3 | 8 | 413 | 465 |
| 3 | -8 | 453 | 440 |
| 3 | 9 | 966 | 893 |
| -3 | 9 | 1865 | 1853 |
| -3 | 10 | 654 | 639 |
| 3 | 10 | 205 | 62 |
| -3 | -11 | 473 | 492 |
| 3 | -11 | 593 | 442 |
| -3 | -12 | 105 | 149 |
| -3 | 12 | 603 | 719 |
| 3 | -13 | 144 | 166 |
| 3 | 13 | 365 | 467 |
| 3 | 14 | 557 | 519 |
| -3 | 14 | 128 | 116 |
| 3 | 15 | 129 | 106 |
| -3 | 15 | 131 | 186 |
| 3 | -16 | 784 | 736 |
| -3 | -16 | 526 | 558 |
| -3 | -17 | 227 | 204 |
| -3 | 17 | 138 | 37 |
| 3 | -18 | 653 | 644 |
| 3 | -19 | 114 | 97 |
| -3 | -19 | 381 | 263 |
| 3 | -21 | 483 | 462 |
| 4 | 0 | 683 | 678 |
| 4 | -1 | 1226 | 1206 |
| -4 | -1 | 397 | 376 |
| 4 | 2 | 291 | 281 |
| 4 | -2 | 1185 | 1161 |
| -4 | 3 | 1714 | 1703 |
| -4 | -3 | 437 | 333 |
| 4 | 4 | 366 | 411 |
| -4 | 4 | 716 | 760 |
| 4 | 5 | 725 | 734 |
| 4 | -5 | 825 | 839 |
| 4 | -6 | 337 | 293 |
| -4 | -6 | 1169 | 1186 |
| 4 | 7 | 1161 | 1111 |
| 4 | -7 | 280 | 356 |
| 4 | 8 | 568 | 625 |
| -4 | 8 | 966 | 936 |
| 4 | -9 | 202 | 134 |
| -4 | -9 | 256 | 240 |
| 4 | 10 | 355 | 321 |
| -4 | 10 | 439 | 429 |
| 4 | -11 | 323 | 375 |
| 4 | 11 | 141 | 55 |
| -4 | -12 | 640 | 877 |
| 4 | 12 | 878 | 877 |
| 4 | 13 | 168 | 73 |
| -4 | 13 | 273 | 262 |
| -4 | -14 | 690 | 696 |
| -4 | 16 | 434 | 484 |
| 4 | -15 | 805 | 836 |
| 4 | 15 | 443 | 452 |
| 4 | 16 | 179 | 168 |
| -4 | 17 | 1693 | 1002 |
| 4 | -18 | 759 | 776 |
| -4 | 19 | 737 | 695 |
| -5 | 0 | 420 | 405 |
| 5 | 1 | 1229 | 1263 |
| -5 | 1 | 1615 | 1656 |
| -5 | 2 | 437 | 324 |
| -5 | -2 | 471 | 478 |
| 5 | 3 | 438 | 438 |
| -5 | 3 | 1535 | 1539 |
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| 7 | 9 | 142 | 32 |
| 7 | -9 | 278 | 321 |
| -7 | 9 | 579 | 552 |
| -7 | -9 | 128 | 29 |
| 7 | -10 | 420 | 441 |
| -7 | 10 | 1634 | 1037 |
| -7 | -10 | 531 | 606 |
| 7 | -11 | 684 | 650 |
| -7 | -11 | 580 | 578 |
| -7 | 11 | 392 | 397 |
| 7 | -12 | 452 | 493 |
| -7 | 12 | 606 | 675 |
| 7 | -13 | 152 | 119 |
| -7 | -13 | 508 | 522 |
| -7 | 13 | 175 | 130 |
| 7 | -14 | 318 | 396 |
| -7 | 14 | 574 | 464 |
| 7 | -15 | 137 | 147 |
| -7 | 16 | 328 | 163 |
| 7 | -19 | 518 | 436 |
| 8 | 0 | 337 | 327 |
| -8 | 0 | 158 | 15 |
| 8 | 1 | 403 | 412 |
| 8 | -1 | 194 | 211 |
| -8 | 1 | 271 | 256 |
| -8 | -1 | 127 | 156 |
| 8 | 2 | 201 | 279 |
| 8 | -2 | 476 | 375 |
| -8 | 2 | 131 | 158 |
| -8 | -2 | 161 | 153 |
| 8 | 3 | 1032 | 1053 |
| 8 | -3 | 533 | 559 |
| -8 | 3 | 746 | 750 |
| -8 | -3 | 369 | 351 |
| 8 | 4 | 163 | 177 |
| 8 | -4 | 719 | 765 |
| -8 | 4 | 130 | 49 |
| -8 | -4 | 673 | 738 |
| 8 | 5 | 314 | 451 |
| 8 | -5 | 461 | 501 |
| -8 | 5 | 131 | 115 |
| 8 | 6 | 540 | 541 |
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| -8 | 6 | 442 | 474 |
| -8 | -6 | 922 | 938 |
| 8 | 7 | 143 | 19 |
| 8 | -7 | 383 | 274 |
| -8 | 7 | 955 | 934 |
| -8 | -7 | 1036 | 1116 |
| 8 | -8 | 655 | 617 |
| -8 | 8 | 285 | 278 |
| -8 | -8 | 585 | 507 |
| 8 | -9 | 348 | 111 |
| 8 | 9 | 431 | 212 |
| -8 | 9 | 984 | 992 |
| -8 | -9 | 478 | 509 |
| 8 | -10 | 123 | 53 |
| 8 | 10 | 357 | 105 |
| -8 | 10 | 353 | 226 |
| 8 | -11 | 130 | 160 |
| -8 | 11 | 435 | 487 |
| 8 | -12 | 393 | 361 |
| -8 | 12 | 307 | 181 |
| 8 | -13 | 761 | 798 |
| 8 | -14 | 137 | 91 |
| 8 | -15 | 513 | 525 |
| 9 | 0 | 135 | 13 |
| -9 | 0 | 377 | 352 |
| 9 | 1 | 136 | 173 |
| 9 | -1 | 248 | 259 |
| -9 | 1 | 466 | 391 |
| -9 | -1 | 135 | 98 |
| 9 | 2 | 442 | 351 |
| 9 | -2 | 610 | 606 |
| -9 | 2 | 351 | 378 |
| -9 | -2 | 297 | 361 |
| 9 | 3 | 149 | 42 |
| 9 | -3 | 360 | 351 |
| -9 | 3 | 136 | 23 |
| -9 | -3 | 622 | 665 |
| 9 | -4 | 1178 | 1197 |
| 9 | 4 | 385 | 363 |
| -9 | 4 | 323 | 409 |
| 9 | -5 | 565 | 574 |
| 9 | 5 | 540 | 542 |
| -9 | 5 | 143 | 234 |
| -9 | -5 | 731 | 698 |
| 9 | -6 | 1183 | 1204 |
| 9 | 6 | 310 | 200 |
| 9 | -7 | 523 | 449 |
| -9 | -7 | 606 | 578 |
| 9 | -8 | 561 | 499 |
| 9 | 8 | 356 | 357 |
| -9 | 8 | 702 | 733 |
| 9 | -7 | 134 | 128 |
| 9 | -10 | 293 | 249 |
| -9 | 10 | 449 | 611 |
| 9 | -11 | 138 | 206 |
| -9 | 11 | 346 | 297 |
| 9 | -14 | 474 | 427 |
| -10 | 1 | 691 | 629 |
| -10 | -1 | 520 | 496 |
| -10 | -2 | 377 | 308 |
| -10 | 3 | 371 | 504 |
| 10 | -3 | 637 | 653 |
| -10 | 4 | 472 | 395 |
| 10 | -5 | 1058 | 1139 |
| -10 | 5 | 645 | 555 |
| 10 | -7 | 672 | 737 |
| 10 | -8 | 335 | 32 |
| 10 | -10 | 309 | 244 |
| 10 | -12 | 546 | 612 |
| | **L = 3** | | |
| 0 | 0 | 419 | 447 |
| 0 | 1 | 820 | 911 |
| 0 | -1 | 741 | 715 |
| 0 | 2 | 389 | 394 |
| 0 | -2 | 409 | 358 |
| 0 | 3 | 814 | 681 |
| 0 | -3 | 601 | 574 |
| 0 | 4 | 647 | 637 |
| 0 | -4 | 658 | 690 |
| 0 | 5 | 334 | 264 |
| 0 | -5 | 824 | 845 |
| 0 | 6 | 801 | 793 |
| 0 | -6 | 224 | 192 |
| 0 | 7 | 757 | 709 |
| 0 | -7 | 876 | 927 |
| 0 | 8 | 425 | 414 |
| 0 | -8 | 275 | 171 |
| 0 | 9 | 597 | 631 |
| 0 | -9 | 1339 | 1302 |
| 0 | 10 | 426 | 351 |
| 0 | -10 | 681 | 732 |
| 0 | 11 | 1335 | 1337 |
| 0 | -11 | 537 | 505 |
| 0 | 12 | 457 | 463 |
| 0 | -12 | 1065 | 1041 |
| 0 | 13 | 1043 | 1050 |
| 0 | -13 | 695 | 736 |
| 0 | 14 | 141 | 114 |
| 0 | -14 | 122 | 165 |
| 0 | 15 | 541 | 595 |
| 0 | -15 | 157 | 183 |
| 0 | -16 | 444 | 419 |
| 0 | 17 | 344 | 269 |
| 0 | -17 | 289 | 179 |
| 0 | -18 | 345 | 415 |
| 0 | -20 | 378 | 273 |
| 1 | 0 | 256 | 311 |
| -1 | 0 | 589 | 566 |

| H | K | FOBS | FCAL | H | K | FOBS | FCAL |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1228 | 1230 | 3 | -6 | 231 | 115 |
| 1 | -1 | 496 | 507 | -3 | -6 | 964 | 933 |
| -1 | 1 | 109 | 158 | 3 | 7 | 303 | 82 |
| -1 | -1 | 1062 | 1517 | 3 | -7 | 670 | 656 |
| 1 | 2 | 869 | 871 | -3 | 7 | 1418 | 1444 |
| 1 | -2 | 555 | 564 | -3 | -7 | 1116 | 1141 |
| -1 | 2 | 296 | 244 | 3 | 8 | 185 | 313 |
| -1 | -2 | 334 | 359 | 3 | -8 | 114 | 62 |
| 1 | 3 | 1526 | 1494 | -3 | 8 | 1070 | 1091 |
| -1 | 3 | 222 | 244 | -3 | -8 | 374 | 400 |
| 1 | -3 | 549 | 624 | 3 | 9 | 728 | 700 |
| -1 | -3 | 1379 | 1323 | 3 | -9 | 743 | 725 |
| 1 | 4 | 581 | 571 | -3 | 9 | 747 | 762 |
| 1 | -4 | 348 | 314 | -3 | -9 | 849 | 787 |
| -1 | 4 | 265 | 350 | 3 | -10 | 571 | 522 |
| -1 | -4 | 165 | 104 | 3 | 10 | 137 | 110 |
| 1 | 5 | 1873 | 1839 | -3 | 10 | 281 | 208 |
| 1 | -5 | 163 | 191 | -3 | -10 | 330 | 323 |
| -1 | 5 | 423 | 357 | 3 | -11 | 676 | 680 |
| -1 | -5 | 966 | 923 | 3 | 11 | 567 | 599 |
| 1 | 6 | 352 | 379 | -3 | 11 | 133 | 136 |
| -1 | 6 | 457 | 449 | -3 | -11 | 1184 | 1239 |
| 1 | -6 | 281 | 274 | 3 | -12 | 524 | 598 |
| -1 | -6 | 295 | 287 | 3 | 12 | 557 | 569 |
| 1 | 7 | 1632 | 1489 | -3 | 12 | 706 | 592 |
| 1 | -7 | 706 | 722 | -3 | -12 | 263 | 338 |
| -1 | 7 | 125 | 132 | 3 | -13 | 355 | 327 |
| -1 | -7 | 118 | 284 | 3 | 13 | 496 | 446 |
| 1 | -8 | 119 | 196 | -3 | 13 | 150 | 190 |
| 1 | 8 | 138 | 133 | -3 | -13 | 545 | 531 |
| -1 | 8 | 582 | 660 | 3 | -14 | 205 | 178 |
| -1 | -8 | 325 | 314 | 3 | 14 | 367 | 400 |
| 1 | 9 | 928 | 986 | -3 | 14 | 223 | 330 |
| 1 | -9 | 1354 | 1292 | -3 | -14 | 609 | 606 |
| -1 | 9 | 593 | 493 | 3 | -15 | 163 | 116 |
| -1 | -9 | 916 | 872 | -3 | 15 | 151 | 249 |
| 1 | 10 | 346 | 405 | -3 | -15 | 300 | 339 |
| 1 | -10 | 226 | 115 | 3 | -16 | 370 | 480 |
| -1 | 10 | 352 | 304 | -3 | -16 | 489 | 478 |
| -1 | -10 | 137 | 112 | 3 | -17 | 260 | 305 |
| 1 | 11 | 233 | 114 | 3 | -18 | 594 | 621 |
| 1 | -11 | 1666 | 1668 | -3 | -18 | 437 | 430 |
| -1 | 11 | 1087 | 1072 | 3 | -19 | 553 | 470 |
| -1 | -11 | 291 | 281 | 3 | -20 | 458 | 500 |
| 1 | 12 | 775 | 787 | 3 | -21 | 682 | 626 |
| 1 | -12 | 141 | 215 | 4 | 0 | 835 | 804 |
| -1 | 12 | 1065 | 1017 | -4 | 0 | 1333 | 1334 |
| -1 | -12 | 251 | 313 | 4 | 1 | 660 | 652 |
| 1 | 13 | 208 | 65 | 4 | -1 | 686 | 656 |
| 1 | -13 | 925 | 950 | -4 | 1 | 399 | 449 |
| -1 | 13 | 862 | 849 | -4 | -1 | 271 | 307 |
| -1 | -13 | 151 | 195 | 4 | 2 | 182 | 127 |
| 1 | 14 | 682 | 685 | 4 | -2 | 1564 | 1609 |
| 1 | -14 | 152 | 72 | -4 | 2 | 668 | 621 |
| -1 | 14 | 618 | 612 | -4 | -2 | 716 | 684 |
| -1 | -14 | 122 | 197 | 4 | 3 | 801 | 747 |
| 1 | 15 | 221 | 306 | -4 | 3 | 1067 | 1054 |
| 1 | -15 | 124 | 187 | -4 | -3 | 551 | 580 |
| -1 | -15 | 819 | 847 | 4 | -3 | 372 | 194 |
| -1 | 15 | 401 | 317 | 4 | 4 | 164 | 42 |
| 1 | -16 | 403 | 471 | 4 | -4 | 1364 | 1324 |
| -1 | 16 | 333 | 215 | -4 | 4 | 121 | 314 |
| -1 | -16 | 415 | 395 | -4 | -4 | 117 | 69 |
| 1 | -17 | 126 | 146 | 4 | 5 | 458 | 516 |
| -1 | 17 | 371 | 365 | 4 | -5 | 288 | 327 |
| -1 | -17 | 860 | 842 | -4 | 5 | 435 | 507 |
| 1 | -18 | 356 | 406 | -4 | -5 | 115 | 49 |
| -1 | -18 | 335 | 355 | 4 | 6 | 125 | 43 |
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| -2 | -1 | 160 | 31 | 4 | 8 | 812 | 801 |
| 2 | 2 | 736 | 781 | -4 | 8 | 1208 | 1252 |
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| -2 | 2 | 141 | 43 | -4 | -8 | 703 | 718 |
| -2 | -2 | 1384 | 1408 | 4 | 9 | 465 | 402 |
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| -2 | 3 | 1466 | 1429 | 4 | -9 | 534 | 534 |
| 2 | -3 | 658 | 630 | -4 | -9 | 586 | 610 |
| -2 | -3 | 545 | 440 | 4 | -10 | 365 | 327 |
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| 2 | 5 | 1391 | 1324 | 4 | 11 | 863 | 803 |
| 2 | -5 | 200 | 219 | -4 | 11 | 393 | 502 |
| -2 | 5 | 1193 | 1181 | -4 | -11 | 466 | 312 |
| -2 | -5 | 175 | 270 | 4 | -12 | 475 | 402 |
| 2 | 6 | 591 | 600 | 4 | 12 | 707 | 726 |
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| -2 | -6 | 248 | 173 | -4 | -12 | 636 | 636 |
| 2 | 7 | 315 | 266 | 4 | -13 | 311 | 312 |
| 2 | -7 | 471 | 395 | 4 | 13 | 577 | 642 |
| -2 | 7 | 1603 | 1576 | -4 | 13 | 563 | 582 |
| -2 | -7 | 969 | 903 | -4 | -13 | 178 | 53 |
| 2 | 8 | 214 | 299 | 4 | -14 | 241 | 295 |
| 2 | -8 | 871 | 880 | -4 | 14 | 233 | 155 |
| -2 | 8 | 662 | 652 | -4 | -14 | 141 | 83 |
| -2 | -8 | 291 | 130 | 4 | -15 | 438 | 409 |
| 2 | 9 | 228 | 211 | -4 | 15 | 437 | 357 |
| 2 | -9 | 116 | 190 | 4 | -16 | 457 | 441 |
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| -2 | -9 | 792 | 654 | 4 | -17 | 131 | 122 |
| 2 | 10 | 233 | 53 | 4 | -18 | 399 | 419 |
| 2 | -10 | 1332 | 1304 | 4 | -20 | 859 | 795 |
| -2 | -10 | 126 | 176 | 5 | 0 | 657 | 631 |
| 2 | 11 | 240 | 194 | -5 | 0 | 650 | 853 |
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| -2 | -11 | 476 | 479 | -5 | 1 | 839 | 845 |
| 2 | 12 | 308 | 192 | -5 | -1 | 912 | 925 |
| 2 | -12 | 1456 | 1529 | 5 | 2 | 130 | 4 |
| -2 | 12 | 474 | 414 | 5 | -2 | 745 | 755 |
| -2 | -12 | 124 | 64 | -5 | 2 | 201 | 148 |
| 2 | 13 | 513 | 593 | -5 | -2 | 902 | 865 |
| 2 | -13 | 257 | 204 | 5 | 3 | 949 | 955 |
| -2 | 13 | 430 | 421 | 5 | -3 | 470 | 447 |
| -2 | -13 | 300 | 347 | -5 | 3 | 123 | 114 |
| 2 | 14 | 147 | 51 | -5 | -3 | 404 | 412 |
| 2 | -14 | 684 | 740 | 5 | 4 | 137 | 231 |
| -2 | 14 | 461 | 451 | 5 | -4 | 272 | 336 |
| -2 | -14 | 128 | 305 | -5 | 4 | 136 | 125 |
| 2 | 15 | 150 | 258 | -5 | -4 | 481 | 465 |
| 2 | -15 | 395 | 357 | 5 | 5 | 800 | 859 |
| -2 | 15 | 148 | 44 | 5 | -5 | 622 | 581 |
| -2 | -15 | 532 | 605 | -5 | 5 | 593 | 613 |
| 2 | -16 | 125 | 69 | -5 | -5 | 119 | 46 |
| -2 | -16 | 850 | 841 | 5 | 6 | 277 | 366 |
| 2 | -17 | 397 | 411 | -5 | 6 | 289 | 146 |
| -2 | -17 | 675 | 624 | 5 | -6 | 783 | 778 |
| 2 | -18 | 132 | 196 | -5 | -6 | 815 | 840 |
| -2 | -18 | 495 | 451 | 5 | 7 | 129 | 132 |
| 2 | -19 | 305 | 363 | 5 | -7 | 899 | 890 |
| 2 | -20 | 453 | 447 | -5 | 7 | 525 | 588 |
| 3 | 0 | 294 | 242 | -5 | -7 | 654 | 675 |
| -3 | 0 | 334 | 242 | 5 | 8 | 664 | 741 |
| 3 | 1 | 242 | 170 | 5 | -8 | 781 | 721 |
| 3 | -1 | 353 | 257 | -5 | 8 | 129 | 62 |
| -3 | 1 | 171 | 193 | -5 | -8 | 798 | 738 |
| -3 | -1 | 648 | 776 | -5 | -9 | 685 | 659 |
| 3 | 2 | 985 | 900 | 5 | 9 | 337 | 276 |
| 3 | -2 | [illegible] | 22 | 5 | -9 | 204 | 173 |
| -3 | 2 | 483 | 471 | -5 | 9 | 126 | 92 |
| -3 | -2 | 492 | 412 | 5 | -10 | 803 | 815 |
| 3 | 3 | 423 | 409 | -5 | 10 | 514 | 490 |
| -3 | 3 | 117 | 106 | -5 | -10 | 656 | 642 |
| -3 | -3 | 776 | 737 | 5 | -11 | 1362 | 1335 |
| 3 | -3 | 1119 | 1152 | 5 | 11 | 443 | 365 |
| 3 | 4 | 1027 | 1032 | -5 | 11 | 138 | 6 |
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| -3 | 4 | 726 | 704 | 5 | -12 | 735 | 747 |
| -3 | -4 | 117 | 98 | 5 | 12 | 1128 | 1161 |
| -3 | -5 | 628 | 629 | -5 | 12 | 615 | 630 |
| 3 | 5 | 739 | 730 | -5 | -12 | 138 | 32 |
| 3 | -5 | 2203 | 2165 | 5 | -13 | 1090 | 1192 |
| -3 | 5 | 1206 | 1256 | -5 | 13 | 359 | 224 |
| 3 | 6 | 390 | 626 | -5 | -13 | 145 | 53 |
| -3 | 6 | 671 | 656 | 5 | -14 | 616 | 584 |

containing Cr, Fe and Ru have been discussed in detail[21].

The only accurate X-ray data available for compounds of this type, other than that reported herein, are for $[Cr_3O(OAc)_6(H_2O)_3]Cl\cdot 6H_2O$[22]. Important structural parameters for the Cr and Ru compounds are compared in Table V. In both, the metal-metal separation is about 3.3 A, far too long for any significant direct interaction to take place, and the metal–O(central) distances are significantly shorter than the metal–O(acetate) distances. The overall configurations of the metals in the two compounds are quite similar allowing for a small increase in covalent radius from Cr to Ru.

A structural report for the compound $[Mn_3O(OAc)_6]OAc\cdot HOAc$ has also appeared[18]; the analysis clearly demonstrates that the basic structure is the same as that of the Cr and Ru compounds, but the accuracy of the determination is so low that no attempt to make a quantitative comparison with the other two molecules would be worthwile. The iron(III) compound $[Fe_3O(OAc)_6(H_2O)_3]Cl\cdot 6H_2O$ was reported to be isomorphous to the chromium(III) analog.[23a] Recently, a preliminary X-ray analysis of $[Fe_3O(OAc)_6(H_2O)_3]ClO_4$ confirmed the same basic structure as found for Cr.[23b]

A closer comparison with the previous work on basic carboxylates of this type suggests that the compound whose structure is reported here is somewhat unique. The $Ru_3O(OAc)_6(PPh_3)_3$ unit is neutral and the average formal oxidation state of Ru is therefore $2^2/_3$, whereas in all other examples the $M_3O(OAc)_6L_3$ unit is cationic and the metal oxidation state is three. The compound is diamagnetic whereas a system of one $Ru^{II}$ and two $Ru^{III}$ ions in which the metals are isolated from one another should have at least two unpaired electrons. The Cr and Fe compounds, on the other hand, all exhibit some paramagnetism, although the measured values are uniformly lower than expected for isolated ions; the $\chi_M(T)$ curves have been successfully fitted by a model in which partial coupling of spins occurs, probably through the central oxygen.[16]

These comparisons suggest that rather extensive electron delocalization occurs in the $Ru_3O$ system, and therefore that the electronic structure and magnetic properties are best treated from a molecular orbital viewpoint rather than using the essentially ionic model applied to the Cr and Fe systems. Such an MO treatment has in fact been briefly outlined for the anions of the type $[Ir_3N(SO_4)_6]^{4-}$,[24] which have a similar structure to the compounds under discussion, with a central nitrogen and bridging sulfates[25a] (a crystal structure of one salt has appeared).[25b] Considering the $Ru_3O$ system as a unit in the point group $D_{3h}$, with the $C_3$ axis coincident with z, we may set aside one $\sigma$ orbital on each metal of the proper symmetry for combining with an $sp^2$ oxygen orbital to form the normal $\sigma$-bond framework. Five orbitals on each metal are also used in $\sigma$-bonding to the carboxylate oxygen atoms and the phosphorus. There are then three *d*-type orbitals remaining on each metal. One of these is capable of forming a linear combination with the same type of *d* orbital on each of the other two metal atoms which will have the proper symmetry for interaction with the $p_z$ orbital on the oxygen atom, leading to one bonding and one antibonding MO. The other eight combinations of the *d*-type metal orbitals are nonbonding with respect to the metal-oxygen interaction. The resulting correlation diagram for the $Ru_3O$ $\pi$ system thus has one strongly bonding, one strongly antibonding, and eight essentially non-bonding MO's. The 16 electrons from the three metal atoms and the two electrons available from the central oxygen atom just fill all of the bonding and non-bonding orbitals, accounting nicely for both the diamagnetism of the compound and its particular stability as a 16-*d*-electron system. Some $\pi$ donation from certain of the bonding or non-bonding MO's to empty *d* orbitals on the phosphorus atoms may occur, but the effect of such donation can only be to lower the energy of these MO's, so that none of the above conclusions are affected.

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