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# SYNTHESES AND STRUCTURAL STUDIES ON TWO CYCLORUTHENAPENTADIENYL COMPLEXES: $|(CO)_3RuC_4(CH_2OH)_4|Ru(CO)_3 \cdot H_2O AND$ $|(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2|Ru(CO)_3$

#### ANNE ASTIER, JEAN-CLAUDE DARAN, YVES JEANNIN and CATHERINE RIGAULT

Laboratoire de Chimie des Métaux de Transition, E.R.A. 608, Université Pierre et Marie Curie, 4, Place Jussieu – 75230 Paris Cedex 05 (France)

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## Summary

Syntheses and single-crystal X-ray diffraction studies have been completed on two cycloruthenapentadienyl (CO)<sub>6</sub>Ru<sub>2</sub>L<sub>2</sub> derivatives, with L = CH<sub>2</sub>OHC = CCH<sub>2</sub>OH and C<sub>2</sub>H<sub>5</sub>C=CCH<sub>2</sub>CH<sub>2</sub>OH respectively. Crystal data are as follows: for [(CO)<sub>3</sub>RuC<sub>4</sub>(CH<sub>2</sub>OH)<sub>4</sub>]Ru(CO)<sub>3</sub>·H<sub>2</sub>O, P2<sub>1</sub>/c, a 13.72(1), b 9.501(4), c 14.86(1) Å,  $\beta$  101.10(6)°,  $R_w = 0.052$  for 1911 reflections; for [(CO)<sub>3</sub>RuC<sub>4</sub>-(CH<sub>2</sub>CH<sub>2</sub>OH)<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>]Ru(CO)<sub>3</sub>, P2<sub>1</sub>/c, a 9.191(3), b 16.732(4), c 14.903(3) Å,  $\beta$ 113.61(4)°,  $R_w = 0.042$  for 2865 reflections. Both compounds are built up from binuclear units, each unit being regarded as a Ru(CO)<sub>3</sub> fragment  $\pi$ -bonded to a cycloruthenapentadienyl ring. The molecular parameters are compared with those of known cyclometallapentadienyl complexes of transition metals. The presence of a semi-bridging CO group is discussed.

## Introduction

The inhibition of corrosion of a metal surface by organic substances can be accounted for the building of a barrier between the metal surface and the corrosive solution. This barrier contains inhibitor molecules as revealed by radioactive measurements; those molecules are assumed to be attached to the metal surface by coordinative bonds, since most organic inhibitors are potential ligands.

The direct methods of surface structural determinations are at present unable to define fully and unambiguously this superficial complex. The study of the stereochemical action of organic inhibitors can be approached through X-ray diffraction, provided a crystal of a compound simulating a protected surface can be prepared. This might lead to the knowledge of the chemical bonds between the metal and the inhibitor, and of the stereochemistry of the whole system. Starting from metal carbonyl clusters, which can be considered to a first approximation as models for a metallic surface since they contain metal-metal bonds, with metal in a low oxidation state, we previously reported the reaction of mercaptobenzothiazole and mercaptoethanoic acid on dodecacarbonyltriruthenium and the structure of two compounds [1]. We describe here the reaction of some acetylenic alcohols on the same cluster, acetylenic alcohols having been widely used for more than thirty years as corrosion inhibitors. The 2-butyn-1,4-diol and the 3-hexyn-1-ol react with  $Ru_3(CO)_{12}$  to give dimeric species of formula  $Ru_2(CO)_6L_2$  containing a cycloruthenapentadienyl ring. Several transition metal complexes containing such cyclometallapentadienyl ligand moieties are known. Typical compounds are binuclear complexes of iron [2,7], rhodium [8], osmium [9], tungsten [10], iridium [11] chromium [12] and the heterobinuclear tungsten-cobalt complex [13]. However although the occurrence of such ruthenium dimeric species was mentioned by Aime and Deeming [14], no crystallographic studies have been published for ruthenium derivatives.

## **Experimental section**

#### Syntheses

Reaction of  $CH_2OHC = CCH_2OH$  on  $Ru_3(CO)_{12}$ . 2-Butyn-1,4-diol (0.4 g) in 15 ml ethanol is added to a solution of  $Ru_3(CO)_{12}$  (0.2 g) in 75 ml toluene at 60°C under dry nitrogen. After 4 h the solution is cooled to 20°C, then 15 ml of water is added, giving two phases. Pale yellow crystals of  $[(CO)_3RuC_4(CH_2OH)_4]Ru(CO)_3 \cdot H_2O$  (1), suitable for X-ray analysis, are obtained by keeping the toluene phase at  $-15^{\circ}C$  for two weeks. The yield is about 1% based on the ruthenium carbonyl. The aqueous phase contains water, ethanol and excess butyne.

Reaction of  $C_2H_5C=CCH_2CH_2OH$  on  $Ru_3(CO)_{12}$ . A solution of  $Ru_3(CO)_{12}$  (0.5 g) and the 3-hexyn-1-ol (0.4 ml) in a mixture of 75 ml hexane and 15 ml ethanol was heated under reflux under N<sub>2</sub> for 24 h. After cooling, chromatography of the solution (TLC, SiO<sub>2</sub>; eluent: light petroleum/acetaldehyde) gave [(CO)<sub>3</sub>RuC<sub>4</sub>-(C<sub>2</sub>H<sub>4</sub>OH)<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>]Ru(CO)<sub>3</sub> (II) (ca. 0.090 g, 18%) as brown air stable crystals; two others products were separated as brown yellow powders but not characterized.

## Infrared

Infrared spectra (KBr pellets) were recorded on Perkin-Elmer 597 spectrophotometer (Table 1).

## X-ray study

After survey photography by the precession technique, a selected crystal of each compound was set up on a laboratory-made automatic three circle diffractometer. In each case, cell dimensions and orientation matrices were obtained by least square analysis from the setting angles of 9 reflections chosen from various regions of reciprocal space ( $22^{\circ} < 2\theta < 34^{\circ}$ ). The scintillation counter was fitted with a pulse-height analyser tuned to accept 90% of the Mo- $K_{\alpha}$  peak. A take off angle of 3° was used.

Crystal data and data collection parameters are listed in Table 2. The intensities of two standard reflections 2 0 0, 0 1 1 for compound I and 0 10 0.5 5 0 for compound II, were measured every 100 reflections; no significant fluctuations were observed. If the counting rate exceeded 7000 counts sec<sup>-1</sup>, counting loss was taken

TABLE 1

## SPECTRAL DATA

Compound	ν(CO) (cm <sup>-1</sup> )	$\nu(Ru-C)$ (cm <sup>-1</sup> )	Reference
$\operatorname{Ru}_2(\operatorname{CO})_6\operatorname{C}_4(\operatorname{CH}_2\operatorname{OH})_4\cdot\operatorname{H}_2\operatorname{O}$	2090s, 2060vs, 2015vs, 1990sh, 1970sh	560s, 540vs	this work
$Ru_{2}(CO)_{6}C_{4}(CH_{2}CH_{2}OH)_{2}(C_{2}H_{5})_{2}$	2080s, 2045vs, 2010vs, 1975vs	560s, 540vs	this work
$\operatorname{Ru}_2(\operatorname{CO})_6 \operatorname{C}_4(\operatorname{CH}_2\operatorname{OH})_4$	2085m, 2054vs, 2009vs, 1994sh	-	[15]
$\operatorname{Ru}_{2}(\operatorname{CO})_{6}\operatorname{C}_{4}\operatorname{H}_{2}\operatorname{C}(\operatorname{CH}_{3})_{2}\operatorname{OH}_{2}$	2086m, 2054vs, 2015vs, 1992sh	~~	[14]

into account. The data were corrected for Lorentz and polarisation effects. In view of the low absorption coefficients, no absorption corrections were applied. Each structure factor was assigned a standard deviation  $\sigma = (F\Delta I)/2I$  where I was the integrated intensity and  $\Delta I$  the error. Reflections with  $F < 3\sigma$  were considered as unobserved and excluded from calculations.

Computations were performed using standard programs [16] on the CII IRIS 80 computer. Scattering factors were taken from International Tables for X-ray Crys-

## TABLE 2

EXPERIMENTAL DATA F	FOR THE X-RAY	' DIFFRACTION	STUDIES
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Compound	$[(CO)_3 RuC_4 (CH_2 OH)_4]$ -	$[(CO)_{3}Ru(C_{4}(C_{2}H_{4}OH)_{2}(C_{2}H_{5})_{2}]^{-}$
	$Ru(CO)_3 \cdot H_2O(1)$	$Ru(CO)_3$ (II)
Cryst. system	monoclinic	monoclinic
Space group	$P2_1/c$	P21/c
a, (Å)	13.72(1)	9.191(3)
b, (Å)	9.501(4)	16.732(4)
c, (Å)	14.86(1)	14.903(3)
β, (°)	101.10(6)	113.61(4)
$V, (A^3)$	1901(3)	2100(1)
Z	4	4
Mol. wt.	560.1	566.1
$\rho$ (calcd.), (g cm <sup>-3</sup> )	1.96	1.79
$\mu$ (cm <sup>-1</sup> )	16.1	13.6
<i>T</i> , (°C)	22	24
Diffractometer	Laboratory made automatic	
	three circle diffractometer	
Radiation	Mo- $K_{\alpha}$ ( $\lambda$ 0.71069 Å)	
Monochromator	graphite monochromator set	
	in front of the counter	
Reflections measd.	$+h, +k, \pm 1$	$+h, +k, \pm 1$
$2\theta$ range, (°)	3.0-50.0	3.0-50.0
Scan type	coupled $\theta(cryst)-2\theta(counter)$	
Scan speed, deg min <sup><math>-1</math></sup>	1.5	1.5
Scan range, deg	$1.0 + 0.345 \tan\theta$	$1.10 + 0.345 \tan\theta$
bkgd	stationary-crystal, stationary	
	counter at beginning and end	
	of scan, each for one-fourth of	
	the time taken for the scan	
Reflections colld	3348 independent	3700 independent

TABLE 3

FRACTIONAL ATOMIC COORDINATES OF COMPOUNDS I AND II (with e.s.d.'s in parentheses)

$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	Atom	x/a	y/b	z/¢	
Ru(1)0.21329(8)0.3314(1)0.4442(8)Ru(2)0.18924(8)0.6181(1)0.4470(8)C(1)0.2765(9)0.476(2)0.3712(9)C(2)0.3448(9)0.577(1)0.4209(8)C(3)0.264(9)0.4737(1)0.5449(8)C(4)0.2814(9)0.4737(1)0.5449(8)C(5)0.266(1)0.468(2)0.6447(9)C(7)0.411(1)0.669(2)0.376(1)C(8)0.415(1)0.677(1)0.580(1)O(5)0.336(1)0.378(1)0.2392(9)O(6)0.3544(8)0.389(1)0.6948(7)O(7)0.921(8)0.816(1)0.31912(8)O(8)0.3875(8)0.814(1)0.5698(8)O-0.5039(7)0.496(1)0.1872(6)C(11)0.132(1)0.239(2)0.339(1)O(12)0.387(8)0.814(1)0.5698(8)O-0.5039(7)0.496(1)0.1872(6)C(11)0.132(1)0.239(2)0.339(1)O(12)0.335(1)0.234(2)0.530(1)O(13)0.138(1)0.234(2)0.530(1)O(13)0.138(1)0.234(2)0.300(1)C(21)0.161(1)0.737(2)0.534(1)O(23)-0.0169(8)0.498(1)0.3839(8)I(CO) <sub>2</sub> RU <sub>4</sub> (CH <sub>2</sub> CH <sub>2</sub> OH) <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> ]Ru(CO) <sub>1</sub> (1)0.186(2)O(23)-0.0169(8)0.498(1)0.3839(8)I(23)0.036(1)0.530(2)0.466(5)O(24)0.2364(9)0.237(3)0.0834(4)<	$[(CO)_3 RuC_4]$	$(CH_2OH)_4]Ru(CO)_3 \cdot H_2$	O (I)		
Ru(2) $0.18924(8)$ $0.6181(1)$ $0.44270(8)$ C(1) $0.2765(9)$ $0.476(2)$ $0.3712(9)$ C(2) $0.3448(9)$ $0.577(1)$ $0.4209(8)$ C(3) $0.2464(9)$ $0.575(1)$ $0.517(1)$ C(4) $0.2814(9)$ $0.473(1)$ $0.5449(8)$ C(5) $0.266(1)$ $0.468(2)$ $0.2645(9)$ C(6) $0.273(1)$ $0.468(2)$ $0.4747(1)$ C(7) $0.411(1)$ $0.669(2)$ $0.376(1)$ C(8) $0.415(1)$ $0.670(1)$ $0.580(1)$ C(7) $0.334(1)$ $0.378(1)$ $0.2392(9)$ O(6) $0.3544(8)$ $0.389(1)$ $0.6948(7)$ O(7) $0.3921(8)$ $0.816(1)$ $0.912(8)$ O(8) $0.3875(8)$ $0.814(1)$ $0.5698(8)$ O $-0.5039(7)$ $0.496(1)$ $0.1872(6)$ C(11) $0.132(1)$ $0.2392(2)$ $0.339(1)$ O(11) $0.085(1)$ $0.187(1)$ $0.279(1)$ C(12) $0.3826(9)$ $0.121(1)$ $0.475(1)$ O(12) $0.3826(9)$ $0.121(1)$ $0.475(1)$ O(13) $0.0930(9)$ $0.179(1)$ $0.5714(9)$ O(21) $0.148(1)$ $0.854(2)$ $0.300(1)$ C(22) $0.151(1)$ $0.739(2)$ $0.352(1)$ O(21) $0.148(1)$ $0.854(2)$ $0.300(1)$ C(22) $0.129(1)$ $0.818(2)$ $0.300(1)$ C(23) $0.063(1)$ $0.1259(3)$ $0.14662(4)$ Ru(2) $0.23017(6)$ $0.1292(13)$ $0.0683(4)$ C(23) <td>Ru(1)</td> <td>0.21329(8)</td> <td>0.3314(1)</td> <td>0.44624(8)</td> <td></td>	Ru(1)	0.21329(8)	0.3314(1)	0.44624(8)	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Ru(2)	0.18924(8)	0.6181(1)	0.44270(8)	
$\begin{array}{cccc} (2) & 0.3448(9) & 0.577(1) & 0.4209(8) \\ (23) & 0.3464(9) & 0.575(1) & 0.517(1) \\ (24) & 0.2814(9) & 0.473(1) & 0.5449(8) \\ (25) & 0.266(1) & 0.468(2) & 0.6447(9) \\ (27) & 0.411(1) & 0.669(2) & 0.376(1) \\ (28) & 0.415(1) & 0.670(1) & 0.380(1) \\ (28) & 0.415(1) & 0.670(1) & 0.380(1) \\ (28) & 0.336(1) & 0.378(1) & 0.2392(9) \\ (26) & 0.334(18) & 0.389(1) & 0.6448(7) \\ (27) & 0.3921(8) & 0.816(1) & 0.3912(8) \\ (28) & 0.3157(8) & 0.816(1) & 0.3912(8) \\ (28) & 0.3157(8) & 0.816(1) & 0.3912(8) \\ (211) & 0.132(1) & 0.239(2) & 0.339(1) \\ (211) & 0.0132(1) & 0.239(2) & 0.339(1) \\ (212) & 0.319(1) & 0.199(2) & 0.462(1) \\ (212) & 0.319(1) & 0.199(2) & 0.462(1) \\ (213) & 0.138(1) & 0.234(2) & 0.330(1) \\ (213) & 0.138(1) & 0.234(2) & 0.330(1) \\ (213) & 0.138(1) & 0.234(2) & 0.330(1) \\ (222) & 0.151(1) & 0.757(2) & 0.352(1) \\ (211) & 0.161(1) & 0.757(2) & 0.352(1) \\ (211) & 0.161(1) & 0.757(2) & 0.352(1) \\ (212) & 0.151(1) & 0.739(2) & 0.534(1) \\ (222) & 0.151(1) & 0.739(2) & 0.534(1) \\ (223) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_3)_2]Ru(CO)_3(1) \\ (23) & -0.0169(8) & 0.498(1) & 0.2339(8) \\ [(C1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ (21) & 0.3661(8) & 0.1859(4) & 0.2230(4) \\ (21) & 0.3661(8) & 0.1859(4) & 0.2230(4) \\ (21) & 0.3661(8) & 0.1383(4) & 0.2244(5) \\ (23) & 0.063(1) & 0.530(2) & 0.408(1) \\ (23) & -0.0169(8) & 0.498(1) & 0.2339(8) \\ [(C1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ (21) & 0.3661(8) & 0.1397(3) & 0.6834(4) \\ (21) & 0.363(4) & 0.056(4) & 0.2900(5) \\ (26) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ (27) & 0.055(1) & 0.3204(4) & 0.0186(5) \\ (26) & 0.0381(7) & 0.0197(5) & 0.1768(5) \\ (21) & -0.029(18) & 0.2573(4) & 0.00887(7) \\ (21) & -0.0251(18) & 0.2573(4) & 0.0087(7) \\ (21) & -0.0251(18) & 0.2573(4) & 0.0087(7) \\ (21) & -0.0251(18) & 0.2573(4) & 0.0048(5) \\ (211) & -0.0124(8) & 0.0417(5) & 0.1768(5) \\ (212) & -0.029(18) & 0.2277(4) & 0.238(8) \\ (213) & -0.194(1) & 0.3162(6) & 0.0385(6) \\ (214) & 0.5410(9) & 0.1748(5) & 0.02926(6) \\ (214) & 0.5410(9) & 0.1748(5) & 0.02926(6$	C(1)	0.2765(9)	0.476(2)	0.3712(9)	
C(3) $0.3464(9)$ $0.575(1)$ $0.517(1)$ C(4) $0.2814(9)$ $0.473(1)$ $0.5449(8)$ C(5) $0.266(1)$ $0.468(2)$ $0.2645(9)$ C(7) $0.411(1)$ $0.669(2)$ $0.376(1)$ C(8) $0.415(1)$ $0.670(1)$ $0.880(1)$ O(5) $0.336(1)$ $0.378(1)$ $0.2382(9)$ O(6) $0.3544(8)$ $0.389(1)$ $0.6948(7)$ O(7) $0.3921(8)$ $0.816(1)$ $0.3912(8)$ O(8) $0.3875(8)$ $0.814(1)$ $0.598(8)$ O $-0.5039(7)$ $0.496(1)$ $0.1872(6)$ C(11) $0.132(1)$ $0.239(2)$ $0.339(1)$ O(11) $0.085(1)$ $0.187(1)$ $0.797(1)$ C(12) $0.3826(9)$ $0.121(1)$ $0.475(1)$ O(13) $0.1390(9)$ $0.179(1)$ $0.5714(9)$ C(14) $0.161(1)$ $0.767(2)$ $0.350(1)$ O(21) $0.148(1)$ $0.854(2)$ $0.300(1)$ C(22) $0.151(1)$ $0.739(2)$ $0.534(1)$ O(23) $-0.0169(8)$ $0.498(1)$ $0.3839(8)$ I(CO) <sub>3</sub> RuC <sub>4</sub> (CH <sub>2</sub> CH <sub>2</sub> OH <sub>2</sub> OH <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> ]Ru(CO) <sub>3</sub> (11) $U$ Ru(1) $0.01265(6)$ $0.16290(3)$ $0.14662(4)$ Ru(2) $0.23017(6)$ $0.13927(3)$ $0.06834(4)$ C(3) $0.3042(9)$ $0.2521(4)$ $0.188(5)$ C(3) $0.3042(9)$ $0.25217(4)$ $0.188(5)$ C(3) $0.3042(9)$ $0.25217(4)$ $0.1086(5)$ C(4) $0.1373(8)$ $0.2227(4)$ $0.1086(5)$ <tr< td=""><td>C(2)</td><td>0.3448(9)</td><td>0.577(1)</td><td>0.4209(8)</td><td></td></tr<>	C(2)	0.3448(9)	0.577(1)	0.4209(8)	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(3)	0.3464(9)	0.575(1)	0.517(1)	
C(5) $0.266(1)$ $0.468(2)$ $0.2643(9)$ C(6) $0.273(1)$ $0.468(2)$ $0.6447(9)$ C(7) $0.411(1)$ $0.669(2)$ $0.376(1)$ C(8) $0.415(1)$ $0.670(1)$ $0.580(1)$ C(7) $0.334(1)$ $0.378(1)$ $0.2392(9)$ O(6) $0.334(8)$ $0.389(1)$ $0.6948(7)$ O(7) $0.3921(8)$ $0.816(1)$ $0.3912(8)$ O(8) $0.3875(8)$ $0.814(1)$ $0.5698(8)$ O $-0.5039(7)$ $0.496(1)$ $0.1372(6)$ C(11) $0.132(1)$ $0.239(2)$ $0.339(1)$ O(11) $0.085(1)$ $0.187(1)$ $0.279(1)$ C(12) $0.319(1)$ $0.199(2)$ $0.462(1)$ O(12) $0.3826(9)$ $0.121(1)$ $0.475(1)$ O(13) $0.0930(9)$ $0.179(1)$ $0.5714(9)$ C(21) $0.161(1)$ $0.767(2)$ $0.352(1)$ O(13) $0.0930(9)$ $0.179(1)$ $0.5714(9)$ C(21) $0.161(1)$ $0.739(2)$ $0.534(1)$ O(22) $0.151(1)$ $0.739(2)$ $0.534(1)$ O(23) $-0.0169(8)$ $0.498(1)$ $0.3839(8)$ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_3)_2]Ru(CO)_3(11) $1.4662(4)$ Ru(2) $0.2307(6)$ $0.13927(3)$ $0.0683(4)$ C(1) $0.2487(7)$ $0.1281(4)$ $0.2230(4)$ C(21) $0.3661(8)$ $0.1839(4)$ $0.2244(5)$ C(3) $0.3061(8)$ $0.2527(4)$ $0.14662(4)$ Ru(2) $0.2307(6)$ $0.3387(5)$ $0.668(5)$ C	C(4)	0.2814(9)	0.473(1)	0.5449(8)	
$\begin{array}{ccccc} C(6) & 0.273(1) & 0.468(2) & 0.6447(9) \\ C(7) & 0.411(1) & 0.669(2) & 0.376(1) \\ O(5) & 0.336(1) & 0.378(1) & 0.2392(9) \\ O(6) & 0.3544(8) & 0.389(1) & 0.6948(7) \\ O(7) & 0.392(18) & 0.816(1) & 0.3912(8) \\ O(8) & 0.3875(8) & 0.814(1) & 0.5698(8) \\ O & -0.5039(7) & 0.496(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.382(69) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(21) & 0.085(2) & 0.179(1) & 0.5714(9) \\ C(21) & 0.188(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.129(1) & 0.810(2) & 0.533(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ C(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ C(1) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3641(8) & 0.189(4) & 0.2230(4) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(5) & 0.2961(8) & 0.0525(7) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(7) & 0.055(1) & 0.3227(4) & 0.1086(5) \\ C(1) & -0.024(8) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(1) & -0.024(8) & 0.043(4) & 0.1846(5) \\ C(1) & -0.024(8) & 0.06735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(1) & -0.024(8) & 0.0671(5) & 0.1708(5) \\ C(11) & -0.024(8) & 0.0671(5) & 0.1708(5) \\ C(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.192(18) & 0.2573(4) & 0.3081(5) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2924(8) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.434(2) & 0.377(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.43(2) & 0.377(7) & 0.2548(8) \\$	C(5)	0.266(1)	0.468(2)	0.2645(9)	
$\begin{array}{ccccc} C(7) & 0.411(1) & 0.669(2) & 0.376(1) \\ C(8) & 0.415(1) & 0.670(1) & 0.580(1) \\ O(5) & 0.336(1) & 0.378(1) & 0.2392(9) \\ O(6) & 0.3544(8) & 0.389(1) & 0.6948(7) \\ O(7) & 0.3921(8) & 0.816(1) & 0.3912(8) \\ O(8) & 0.3875(8) & 0.814(1) & 0.5098(8) \\ O & -0.5039(7) & 0.496(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.157(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_{3}(2H_{3})_{2}]Ru(CO)_{3}(11) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.036(1) & 0.535(2) & 0.08834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1616(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0352(5) & 0.0887(7) \\ C(6) & 0.2844(9) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0990(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.108(5) \\ C(5) & 0.2961(8) & 0.0617(5) & 0.1708(5) \\ C(1) & -0.0251(8) & 0.257(4) & 0.0198(5) \\ C(1) & -0.0251(8) & 0.257(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ C(12) & -0.0051(1) & 0.1282(7) & -0.0034(6) \\ C(13) & -0.3153(8) & 0.2277(4) & 0.2348(8) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.0495(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.0495(6) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.435(7) & 0.797(7) & 27943(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0$	C(6)	0.273(1)	0.468(2)	0.6447(9)	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(7)	0.411(1)	0.669(2)	0.376(1)	
$\begin{array}{cccc} O(5) & 0.336(1) & 0.378(1) & 0.2392(9) \\ O(6) & 0.3544(8) & 0.389(1) & 0.6948(7) \\ O(7) & 0.3921(8) & 0.816(1) & 0.3192(8) \\ O(8) & 0.3875(8) & 0.814(1) & 0.5698(8) \\ O & -0.5039(7) & 0.496(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.757(2) & 0.352(1) \\ O(21) & 0.161(1) & 0.757(2) & 0.352(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ I(CO_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(21) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.0942(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.096(4) & 0.2900(5) \\ C(6) & 0.3381(7) & 0.090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.1243(8) & 0.0066(4) & 0.2900(5) \\ C(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.227(4) & 0.2479(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0938(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0938(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0938(5) \\ C(14) & 0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.415(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.6447(2) & 0.3797(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(7) & 0.3162(6) & 0.1556(7) \\ C(17) & 0$	C(8)	0.415(1)	0.670(1)	0.580(1)	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(5)	0.336(1)	0.378(1)	0.2392(9)	
$\begin{array}{ccccc} Q(7) & 0.3921(8) & 0.816(1) & 0.3912(8) \\ Q(8) & 0.3875(8) & 0.814(1) & 0.5098(8) \\ Q(8) & 0.3875(8) & 0.814(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ Q(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ Q(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ Q(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.129(1) & 0.810(2) & 0.538(1) \\ Q(22) & 0.129(1) & 0.810(2) & 0.538(1) \\ Q(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_{3}RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3 & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2230(4) \\ C(2) & 0.361(8) & 0.0566(4) & 0.2900(5) \\ C(4) & 0.3373(8) & 0.2527(4) & 0.168(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(5) & 0.2961(8) & 0.0438(4) & 0.043(5) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(3) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.092(48) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.1243(8) & 0.043(4) & 0.1846(5) \\ C(11) & -0.1243(8) & 0.043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2277(4) & 0.2479(5) \\ O(11) & -0.1243(8) & 0.043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2277(4) & 0.2479(5) \\ O(11) & -0.1243(8) & 0.043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2277(4) & 0.2479(5) \\ O(12) & -0.0251(8) & 0.2573(4) & 0.0481(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1329(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.043(2) & 0.3797(7) & 0.254$	O(6)	0.3544(8)	0.389(1)	0.6948(7)	
$\begin{array}{ccccc} O(8) & 0.3875(8) & 0.814(1) & 0.5698(8) \\ O & -0.5039(7) & 0.496(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.151(1) & 0.739(2) & 0.587(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.587(1) \\ O(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3(1) \\ Ru(1) & 0.02487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.0342(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.296(18) & 0.090(4) & 0.44536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(6) & 0.384(7) & 0.090(4) & 0.44536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(6) & 0.381(7) & 0.090(4) & 0.44536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0198(5) \\ C(11) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.02926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.443(2) & 0.3792(7) & 0.2592(1) \\ C(12) &$	O(7)	0.3921(8)	0.816(1)	0.3912(8)	
$\begin{array}{cccccc} & -0.5039(T) & 0.496(1) & 0.1872(6) \\ C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.834(2) & 0.300(1) \\ C(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.129(1) & 0.810(2) & 0.587(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_3)_2]Ru(CO)_3 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(11) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(22) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.296(18) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.381(7) & 0.0090(4) & 0.4356(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.025(18) & 0.0434(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.1243(8) & 0.0434(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(11) & -0.1243(8) & 0.0434(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(11) & -0.1243(8) & 0.0434(4) & 0.1846(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.02926(6) \\ C(15) & 0.641(1) & 0.1329(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(12) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(15) & 0.641(1) & 0.1329(7) & 0.259(1) \\ C(12) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(12) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(12) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(12) & 0.043(2) & 0.3797(7) & 0.2548(8) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C(15) & 0.641(1) & 0.3162(6) & 0.1556(7) \\ C($	0(8)	0.3875(8)	0.814(1)	0.5698(8)	
$\begin{array}{ccccc} C(11) & 0.132(1) & 0.239(2) & 0.339(1) \\ O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.884(2) & 0.300(1) \\ C(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.151(1) & 0.810(2) & 0.587(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_3)_2]Ru(CO)_1 (1) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1088(5) \\ C(5) & 0.2961(8) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.384(4) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0018(5) \\ C(5) & 0.0921(8) & 0.0434(4) & 0.0198(5) \\ C(6) & 0.0381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3207(4) & 0.2497(5) \\ O(11) & -0.1243(8) & 0.0434(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ C(11) & -0.0251(8) & 0.2273(4) & 0.3081(5) \\ C(11) & -0.0251(8) & 0.2273(4) & 0.3081(5) \\ C(12) & -0.0099(9) & 0.227(4) & 0.2497(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0251(8) & 0.2273(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.02926(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0043(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.22548(8) \\ C(16) & 0.444(2) & 0.1373(6) \\ C(16) & 0.443(2) & 0.379(7) & 0.22548(8) \\ C(16) & 0.444(2) & 0.379(7) & 0.22548(8) \\ C(16) & 0.444(2) & 0.379(7) & 0.2294(1) \\ \end{array}$	0	-0.5039(7)	0.496(1)	0.1872(6)	
$\begin{array}{cccccc} O(11) & 0.085(1) & 0.187(1) & 0.279(1) \\ C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.151(1) & 0.739(2) & 0.537(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_5RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_1 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(11) & -0.019(1) & 0.1322(7) & 0.2248(8) \\ C(11) & -0.019(1) & 0.1239(7) & 0.2248(8) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3120(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3129(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3129(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3129(7) & 0.25$	can	0.132(1)	0.239(2)	0.339(1)	
$\begin{array}{cccccc} C(12) & 0.319(1) & 0.199(2) & 0.462(1) \\ O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.129(1) & 0.810(2) & 0.587(1) \\ O(22) & 0.129(1) & 0.810(2) & 0.587(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_{3}RuC_{4}(CH_{2}CH_{2}OH)_{2}(C_{2}H_{5})_{2}]Ru(CO)_{3}(11) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2577(4) & 0.108(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0018(5) \\ C(6) & 0.381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0018(5) \\ C(6) & 0.381(7) & 0.0090(4) & 0.0453(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0018(5) \\ C(6) & 0.381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0041(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.0248(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.0251(8) & 0.2277(4) & 0.249(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.0251(8) & 0.227(4) & 0.249(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(11) & -0.0251(8) & 0.227(4) & 0.3081(5) \\ C(12) & -0.0251(8) & 0.227(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.22548(8) \\ C(16) & 0.414(1) & 0.3120(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(2) & 0.379(7) & 0.2248(8) \\ C(16) & 0.414(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(2) & 0.379(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(2) & 0.379(7) & 0.2548(8) \\ C(16) & 0.414(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(2) & 0.379(7$	oan	0.085(1)	0.187(1)	0.279(1)	
$\begin{array}{ccccccc} O(12) & 0.3826(9) & 0.121(1) & 0.475(1) \\ C(13) & 0.138(1) & 0.234(2) & 0.530(1) \\ O(13) & 0.0930(9) & 0.179(1) & 0.5714(9) \\ C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.129(1) & 0.810(2) & 0.587(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.0444(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1798(5) \\ O(11) & -0.024(8) & 0.0434(4) & 0.198(5) \\ C(11) & -0.024(8) & 0.0434(4) & 0.198(5) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.198(5) & 0.093(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.444(2) & 0.1397(7) & 0.2548(8) \\ C(16) & 0.444(2) & 0.3797(7) & 0.2791(1) \\ \end{array}$	C(12)	0.319(1)	0.199(2)	0.462(1)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0(12)	0.3826(9)	0.121(1)	0.475(1)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(13)	0,138(1)	0.234(2)	0.530(1)	
$\begin{array}{cccccc} C(21) & 0.161(1) & 0.767(2) & 0.352(1) \\ O(21) & 0.148(1) & 0.854(2) & 0.300(1) \\ C(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.129(1) & 0.810(2) & 0.5387(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ \hline \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3(1) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.2844(9) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(11) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.443(2) & 0.372(7) & 0.274(1) \\ C(20) & 0.729(7) & 0.274(1) \\ C(21) & 0.043(2) $	0(13)	0.0930(9)	0.179(1)	0.5714(9)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(21)	0,161(1)	0.767(2)	0.352(1)	
$\begin{array}{cccccc} C(22) & 0.151(1) & 0.739(2) & 0.534(1) \\ O(22) & 0.129(1) & 0.810(2) & 0.587(1) \\ C(23) & 0.063(1) & 0.530(2) & 0.408(1) \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ \hline \\ [(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.2844(9) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1329(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(12) & -0.0092(7) & 0.2927(1) \\ 0.2598(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(12) & -0.0092(9) & 0.2197(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(12) & -0.0291(8) & 0.2199(7) & 0.2991(8) \\ C(12) & 0.043(2) & 0.3192(7) & 0.2991(8) \\ C(13) & -0.443(2) & 0.3192(7) & 0.2991(8) \\ C(13) & -0.443(2) & 0.3192(7) & 0.2991(8) \\ C(14) & 0.443(2) & 0.3162(6) \\ C(15) & 0.443(2) & 0.3192(7) & 0.2991(8) \\ C(15) & 0.443(2) & 0.3162(6) \\ C(15) & 0.443(2) & 0.3162$	O(21)	0.148(1)	0.854(2)	0,300(1)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(22)	0.151(1)	0.739(2)	0.534(1)	
$\begin{array}{ccccc} (223) & 0.063(1) & 0.530(2) & 0.408(1) \\ (0(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ [(CO)_3 RuC_4 (CH_2 CH_2 OH)_2 (C_2 H_5)_2] Ru(CO)_3 (II) \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ C(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ C(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ C(3) & 0.3042(9) & 0.2519(4) & 0.1618(5) \\ C(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ C(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ C(6) & 0.2844(9) & 0.0735(5) & 0.3857(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ C(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ C(8) & -0.010(1) & 0.3825(5) & 0.0887(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2248(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.155(7) \\ \end{array}$	0(22)	0.129(1)	0.810(2)	0.587(1)	
$\begin{array}{ccccc} O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ \hline \\ O(23) & -0.0169(8) & 0.498(1) & 0.3839(8) \\ \hline \\ O(2)_{3} RuC_{4}(CH_{2}CH_{2}OH)_{2}(C_{2}H_{5})_{2}]Ru(CO)_{3} (II) \\ \hline \\ Ru(1) & 0.01265(6) & 0.16290(3) & 0.14662(4) \\ Ru(2) & 0.23017(6) & 0.13927(3) & 0.06834(4) \\ O(1) & 0.2487(7) & 0.1281(4) & 0.2230(4) \\ O(2) & 0.3661(8) & 0.1839(4) & 0.2244(5) \\ O(2) & 0.3661(8) & 0.2529(4) & 0.1618(5) \\ O(4) & 0.1373(8) & 0.2527(4) & 0.1086(5) \\ O(5) & 0.2961(8) & 0.0566(4) & 0.2900(5) \\ O(6) & 0.3381(7) & 0.0090(4) & 0.4536(4) \\ O(7) & 0.055(1) & 0.3204(4) & 0.0401(5) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ O(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.0251(8) & 0.2207(4) & 0.2479(5) \\ O(12) & -0.0099(9) & 0.2207(4) & 0.3081(5) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ O(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ O(15) & 0.641(1) & 0.1239(7) & 0.2294(1) \\ O(15) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ O(17) & 0.434(2) & 0.3792(7) & 0.2294(1) \\ O(2990(5) & 0.299(1) \\ O(11) & 0.2290(5) & 0.299(1) \\ O(12) & 0.0251(8) & 0.2100(5) & -0.0034(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ O(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ O(15) & 0.641(1) & 0.1239(7) & 0.2294(1) \\ O(15) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ O(17) & 0.434(2) & 0.3792(7) & 0.2294(1) \\ O(290(5) & 0.029(1) \\ O(290(5) & 0.292(1) \\ O$	C(23)	0.063(1)	0.530(2)	0.408(1)	
	O(23)	-0.0169(8)	0.498(1)	0.3839(8)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$[(CO)_3 RuC_4]$	(CH <sub>2</sub> CH <sub>2</sub> OH),(C <sub>2</sub> H <sub>2</sub> ),	Ru(CO) <sub>3</sub> (II)		
Ru(2) $0.01265(6)$ $0.0290(3)$ $0.0402(4)$ $Ru(2)$ $0.23017(6)$ $0.13927(3)$ $0.06834(4)$ $C(1)$ $0.2487(7)$ $0.1281(4)$ $0.2230(4)$ $C(2)$ $0.3661(8)$ $0.1839(4)$ $0.2244(5)$ $C(3)$ $0.3042(9)$ $0.2519(4)$ $0.1618(5)$ $C(4)$ $0.1373(8)$ $0.2527(4)$ $0.1086(5)$ $C(5)$ $0.2961(8)$ $0.0566(4)$ $0.2900(5)$ $C(6)$ $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $-0.0034(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1728(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $O(15)$ $0.441(2)$ $0.3792(7)$ $0.2594(1)$	D.(1)	0.01265(6)	0.1600(2)	0 14662(4)	
K(2) $0.25017(0)$ $0.13921(3)$ $0.00034(4)$ $C(1)$ $0.2487(7)$ $0.1281(4)$ $0.2230(4)$ $C(2)$ $0.3661(8)$ $0.1839(4)$ $0.2244(5)$ $C(3)$ $0.3042(9)$ $0.2519(4)$ $0.1618(5)$ $C(4)$ $0.1373(8)$ $0.2527(4)$ $0.1086(5)$ $C(5)$ $0.2961(8)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $0.0495(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$	Ru(7)	0.01203(0)	0.10290(3)	0.06834(4)	
C(1) $0.2481(7)$ $0.1281(4)$ $0.2230(4)$ C(2) $0.3661(8)$ $0.1839(4)$ $0.2244(5)$ C(3) $0.3042(9)$ $0.2519(4)$ $0.1618(5)$ C(4) $0.1373(8)$ $0.2527(4)$ $0.1086(5)$ C(5) $0.2961(8)$ $0.0566(4)$ $0.2900(5)$ C(6) $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ O(6) $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ C(7) $0.055(1)$ $0.3204(4)$ $0.0401(5)$ C(8) $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ O(8) $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ C(11) $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ O(11) $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ C(12) $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ O(12) $-0.251(8)$ $0.2573(4)$ $0.3081(5)$ C(13) $-0.1947(9)$ $0.1948(5)$ $0.0495(6)$ O(13) $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ C(14) $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ C(15) $0.641(1)$ $0.2139(7)$ $0.2548(8)$ C(16) $0.416(1)$ $0.3162(6)$ $0.155(7)$	C(1)	0.23017(0)	0.13927(3)	0.00834(47	
C(2) $0.3661(8)$ $0.1859(4)$ $0.2244(5)$ $C(3)$ $0.3042(9)$ $0.2519(4)$ $0.1618(5)$ $C(4)$ $0.1373(8)$ $0.2527(4)$ $0.1086(5)$ $C(5)$ $0.2961(8)$ $0.0566(4)$ $0.2900(5)$ $C(6)$ $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $0.0495(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$	C(1)	0.2467(7)	0.1201(4)	0.2250(4)	
C(3) $0.3042(7)$ $0.2517(4)$ $0.1016(5)$ $C(4)$ $0.1373(8)$ $0.2527(4)$ $0.1086(5)$ $C(5)$ $0.2961(8)$ $0.0566(4)$ $0.2900(5)$ $C(6)$ $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $-0.0934(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$	C(2)	0.3001(8)	0.1637(4)	0.2244(0)	
C(4) $0.133(8)$ $0.2327(4)$ $0.1030(5)$ $C(5)$ $0.2961(8)$ $0.0566(4)$ $0.2900(5)$ $C(6)$ $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4436(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $0.0495(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$	C(3)	0.1373(8)	0.2313(4)	0.1086(5)	
C(3) $0.2901(3)$ $0.0306(4)$ $0.2900(5)$ $C(6)$ $0.2844(9)$ $0.0735(5)$ $0.3857(5)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $-0.0934(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3792(7)$ $0.229(1)$	C(4)	0.2575(8)	0.2527(4)	0.2000(5)	
C(6) $0.2844(9)$ $0.073(3)$ $0.383(3)$ $O(6)$ $0.3381(7)$ $0.0090(4)$ $0.4536(4)$ $C(7)$ $0.055(1)$ $0.3204(4)$ $0.0401(5)$ $C(8)$ $-0.010(1)$ $0.3825(5)$ $0.0887(7)$ $O(8)$ $-0.0924(8)$ $0.4444(4)$ $0.0198(5)$ $C(11)$ $-0.0744(8)$ $0.0617(5)$ $0.1708(5)$ $O(11)$ $-0.1243(8)$ $0.0043(4)$ $0.1846(5)$ $C(12)$ $-0.0099(9)$ $0.2207(4)$ $0.2479(5)$ $O(12)$ $-0.0251(8)$ $0.2573(4)$ $0.3081(5)$ $C(13)$ $-0.1947(9)$ $0.1948(5)$ $-0.093(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3722(7)$ $0.229(1)$	C(5)	0.2201(0)	0.0500(4)	0.2950(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0(6)	0.3381(7)	0.0733(3)	0.3837(3)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(0)	0.3381(7)	0.0090(4)	0.4330(4)	
$\begin{array}{cccc} C(3) & -0.010(1) & 0.3822(3) & 0.0083(7) \\ O(8) & -0.0924(8) & 0.4444(4) & 0.0198(5) \\ C(11) & -0.0744(8) & 0.0617(5) & 0.1708(5) \\ O(11) & -0.1243(8) & 0.0043(4) & 0.1846(5) \\ C(12) & -0.0099(9) & 0.2207(4) & 0.2479(5) \\ O(12) & -0.0251(8) & 0.2573(4) & 0.3081(5) \\ C(13) & -0.1947(9) & 0.1948(5) & 0.0495(6) \\ O(13) & -0.3153(8) & 0.2140(5) & -0.0034(6) \\ C(14) & 0.5410(9) & 0.1748(5) & 0.2926(6) \\ C(15) & 0.641(1) & 0.1239(7) & 0.2548(8) \\ C(16) & 0.416(1) & 0.3162(6) & 0.1556(7) \\ C(17) & 0.443(2) & 0.3792(7) & 0.229(1) \\ \end{array}$	C(n)		0.3204(4)	0.0907(7)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		-0.0024(8)	0.3625(3) 0.4444(4)	0.0108(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1)	-0.0744(8)	0.4444(4)	0.1708(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(11)	-0.0744(8)	0.0017(3)	0.1708(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(12)		0.0045(4)	0.2479(5)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(12)		0.2207(4)	0.2477(3)	
O(13) $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $O(13)$ $-0.3153(8)$ $0.2140(5)$ $-0.0034(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3792(7)$ $0.299(1)$	C(13)	- 0.0251(0)	0.2373(4) D 1948(5)	0.0001(0)	
C(15) $-0.5155(6)$ $0.2140(5)$ $-0.0054(6)$ $C(14)$ $0.5410(9)$ $0.1748(5)$ $0.2926(6)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3792(7)$ $0.299(1)$	0(13)		0.1740(3)	0.0470(0) 	
C(17) $0.540(7)$ $0.1740(3)$ $0.2520(7)$ $C(15)$ $0.641(1)$ $0.1239(7)$ $0.2548(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3792(7)$ $0.294(1)$	C(14)	0.5100	0.2140(3)	0.0004(0)	
C(15) $0.047(1)$ $0.1259(7)$ $0.2348(8)$ $C(16)$ $0.416(1)$ $0.3162(6)$ $0.1556(7)$ $C(17)$ $0.443(2)$ $0.3792(7)$ $0.299(1)$	C(15)	0.5410(7)	0.1/40(2)	0.2720(07	
C(17) = 0.43(7) = 0.3102(0) = 0.1350(7) C(17) = 0.443(7) = 0.3797(7) = 0.739(1)	C(16)	0.041(1)	0.1439(7)	0.2540(0)	
	C(17)	0.410(1)	0.3702(0)	0.1000(7)	

		) <b>r</b>	,	
Atom	x/a	у/Б	z/c	
C(21)	0.331(1)	0.0389(5)	0.0688(6)	
O(21)	0.3921(9)	-0.0189(4)	0.0664(5)	
C(22)	0.2973(9)	0.1797(5)	-0.0283(5)	
O(22)	0.3355(8)	0.2045(5)	-0.0864(5)	
C(23)	0.0254(9)	0.1061(4)	-0.0241(6)	
O(23)	-0.0832(7)	0.0849(4)	-0.0882(4)	

TABLE 3 (continued)

### TABLE 4

ANISOTROPIC THERMAL PARAMETERS OF COMPOUNDS I AND II (with e.s.d.'s in parentheses)

They enter the expression for the structure factor in the form:  $\exp[-0.25(B_{11}h^2a^{\star 2} + B_{22}k^2b^{\star 2} + B_{33}l^2c^{\star 2} + 2B_{12}hka^{\star}b^{\star} + 2B_{13}hla^{\star}c^{\star} + 2B_{23}klb^{\star}c^{\star})]$ 

Atom	B <sub>11</sub>	B <sub>22</sub>	B <sub>33</sub>	B <sub>12</sub>	B <sub>13</sub>	B <sub>23</sub>
[(CO) <sub>3</sub> R	uC <sub>4</sub> (CH <sub>2</sub> OH) <sub>4</sub> ]	$Ru(CO)_3 \cdot H_2O$	(I)			
Ru(1)	3.17(5)	2.02(4)	3.51(6)	-0.30(4)	0.11(4)	-0.07(4)
Ru(2)	2.79(4)	2.19(5)	2.91(5)	0.15(3)	0.14(3)	0.13(4)
C(1)	3.0(5)	3.4(5)	4.3(6)	-0.1(5)	0.9(5)	0.5(6)
C(2)	3.7(6)	3.2(5)	2.2(5)	0.2(4)	0.0(4)	0.5(4)
C(3)	3.2(5)	1.6(4)	4.4(7)	0.5(4)	-0.3(5)	0.2(4)
C(4)	2.0(6)	2.5(4)	2.7(5)	-0.0(5)	-0.4(4)	-0.4(5)
C(5)	5.2(8)	4.9(7)	4.0(6)	-0.8(7)	1.2(6)	0.4(7)
C(6)	4.9(8)	4.3(7)	3.7(6)	0.4(6)	-0.4(5)	0.2(6)
C(7)	4.9(7)	3.7(6)	7.1(10)	-1.1(6)	2.1(7)	-0.7(7)
C(8)	4.7(6)	2.1(5)	5.2(7)	-0.9(5)	-0.2(5)	-0.8(5)
O(5)	9.7(8)	4.3(5)	7.1(7)	-0.1(6)	5.0(6)	- 1.5(5)
O(6)	6.6(5)	3.7(4)	4.4(5)	0.2(5)	-0.6(4)	1.2(4)
O(7)	5.9(5)	3.4(4)	6.6(6)	-0.1(4)	1.4(5)	0.2(4)
O(8)	6.2(5)	2.9(4)	5.5(5)	-0.3(4)	0.2(4)	-0.4(4)
0	4.7(4)	2.6(5)	5.3(4)	0.5(3)	0.2(4)	0.3(4)
C(11)	5.5(8)	3.5(7)	5.7(10)	- 1.2(6)	0.6(7)	- 1.7(7)
O(11)	10.6(9)	5.2(6)	6.1(7)	- 1.2(7)	- 1.6(7)	- 1.0(6)
C(12)	5.5(8)	2.9(7)	4.4(7)	-0.4(6)	0.5(6)	-0.2(5)
O(12)	6.7(6)	3.9(5)	9.3(8)	1.9(5)	-0.2(6)	-0.0(6)
C(13)	3.9(7)	2.1(6)	6.6(10)	-0.9(5)	0.0(7)	-0.1(6)
O(13)	6.2(6)	5.9(6)	6.1(7)	-2.4(5)	1.5(5)	1.8(6)
C(21)	4.0(7)	4.1(7)	7.1(10)	1.0(6)	1.3(7)	2.4(7)
O(21)	9.3(9)	5.9(8)	9.7(10)	1.8(7)	1.7(7)	4.1(7)
C(22)	4.2(7)	4.0(8)	5.9(10)	1.5(6)	-0.2(7)	-0.4(7)
O(22)	9.8(9)	6.0(8)	6.4(8)	1.9(7)	1.0(7)	-2.6(7)
C(23)	4.2(7)	3.7(6)	4.4(7)	-0.4(6)	0.0(6)	0.6(6)
O(23)	3.7(5)	5.3(7)	7.1(6)	0.2(4)	-0.5(4)	0.2(5)
[(CO) <sub>3</sub> R	uC <sub>4</sub> (CH <sub>2</sub> CH <sub>2</sub> C	$(C_2H_5)_2]R_1$	u(CO) <sub>3</sub> (II)			
Ru(1)	3.08(2)	2.99(2)	2.55(2)	0.14(2)	1.18(2)	0.08(2)
Ru(2)	3.60(2)	3.08(2)	2,55(2)	0.20(2)	1.54(2)	-0.01(2)
C(1)	3.2(2)	3.3(3)	2.4(2)	0.0(2)	1.3(2)	-0.2(2)
C(2)	3.5(3)	3.8(3)	3.0(3)	-0.2(2)	1.4(2)	-0.1(2)

Atom	B <sub>11</sub>	<b>B</b> <sub>22</sub>	B <sub>33</sub>	B <sub>12</sub>	B <sub>13</sub>	B <sub>23</sub>
C(3)	5.6(4)	3.0(3)	3.3(3)	-0.5(2)	2.2(3)	-0.1(2)
C(4)	4.5(3)	2.8(3)	2.9(2)	0.3(2)	1.0(2)	0.0(2)
C(5)	3.7(3)	3.0(3)	3.4(3)	0.3(2)	1.3(2)	0.1(2)
C(6)	4.7(3)	4.5(3)	3.3(3)	0.3(3)	1.6(3)	0.6(3)
O(6)	5.5(3)	6.7(3)	4.6(3)	0.5(2)	1.6(2)	2.6(2)
C(7)	6.0(4)	3.4(3)	3.0(3)	0.9(3)	2.7(3)	0.7(2)
C(8)	7.3(5)	4.3(4)	6.0(4)	1.9(3)	3.8(4)	0.8(3)
O(8)	7.8(4)	4.4(3)	8.0(4)	2.5(2)	3.9(3)	1.8(3)
C(11)	3.8(3)	4.2(3)	3.6(3)	-0.4(3)	1.5(2)	-0.4(2)
0(11)	6.8(3)	4.9(3)	7.0(4)	-1.2(2)	4.4(3)	0.1(3)
C(12)	4.1(3)	4.4(3)	3.7(3)	-0.3(2)	1.8(2)	- 0.2(3)
O(12)	7.8(4)	7.3(3)	5.2(3)	-0.1(3)	3.7(3)	- 1.5(3)
C(13)	3.8(3)	5.5(4)	3.9(3)	0.7(3)	1.1(3)	0.6(3)
O(13)	4.7(3)	10.4(5)	6.0(4)	1.7(3)	-0.2(3)	2.5(4)
C(14)	3,7(3)	4.8(4)	4.7(3)	-0.3(3)	1.2(3)	0.2(3)
C(15)	3.5(3)	8.5(6)	7.1(5)	-0.4(4)	2.4(3)	-0.6(4)
C(16)	5.2(4)	5.0(5)	6.7(5)	-1.2(3)	2.6(4)	1.6(4)
C(17)	11.1(9)	6.4(6)	9.6(8)	-4.6(6)	4.3(7)	- 2.2(5)
C(21)	5.9(4)	3.9(3)	3.9(3)	1.4(3)	2.1(3)	0.1(3)
O(21)	9.1(4)	4.7(3)	6.7(3)	2.4(3)	3.4(3)	0.1(2)
C(22)	4.7(3)	4.8(3)	2.6(3)	-0.1(3)	1.5(2)	0.2(2)
O(22)	7.0(3)	10.1(5)	5.4(3)	0.0(3)	3.9(3)	1.0(3)
C(23)	4.6(4)	3.6(3)	4.6(4)	-0.4(3)	2.4(3)	-0.5(3)
O(23)	5.6(3)	6.9(3)	4,6(3)	-1.7(2)	1.7(2)	-1.9(2)

TABLE 4 (continued)

## TABLE 5

INTERATOMIC DISTANCES OF COMPOUNDS I AND II (Å) (with e.s.d.'s in parentheses)

	I	II		1	11
Ru(1)-C(1)	2.06(3)	2.089(6)	Ru(2)-Ru(1)	2.743(3)	2.717(1)
Ru(1)-C(2)	2.08(3)	2.101(6)	Ru(2)-C(1)	2.21(3)	2.250(6)
Ru(1)-C(11)	1.97(3)	1.967(8)	Ru(2)-C(2)	2.25(2)	2.281(6)
Ru(1)-C(12)	1.90(3)	1.874(7)	Ru(2)-C(3)	2.27(3)	2.279(7)
Ru(1)-C(13)	2.00(3)	1.950(7)	Ru(2)-C(4)	2.25(3)	2.259(6)
$Ru(1) \cdots C(23)$	2.76(2)	2.762(7)	Ru(2)-C(21)	1.93(3)	1.918(7)
C(11)-O(11)	1.11(2)	1.118(9)	Ru(2)-C(22)	1.92(3)	1.904(7)
C(12)-O(12)	1.13(2)	1.140(9)	Ru(2)-C(23)	1.90(2)	1.916(8)
C(13)-O(13)	1.08(2)	1.119(9)	C(21)-O(21)	1.13(2)	1.125(9)
C(1)-C(2)	1.44(3)	1.420(9)	C(22)-O(22)	1.12(2)	1.135(9)
C(2) - C(3)	1.42(2)	1.44(1)	C(23)-O(23)	1.13(2)	1.128(9)
C(3)-C(4)	1.43(2)	1.42(1)			
Compound I			Compound II		
C(1)-C(5)	1.57(2)		C(1) - C(5)	1.506(9)	
C(5)-O(5)	1.38(2)		C(5)-C(6)	1.50(1)	
C(2)-C(6)	1.50(3)		C(6)O(6)	1,426(9)	
C(6)-O(6)	1.49(2)		C(4)-C(7)	1.508(9)	
C(3) - C(7)	1.50(3)		C(7) - C(8)	1.52(1)	
C(7)-O(7)	1.41(2)		C(8)-O(8)	1.44(1)	
C(4)-C(8)	1.51(2)		C(2)-C(14)	1.53(1)	
C(8)-O(8)	1.44(2)		C(14)-C(15)	1.52(1)	
			C(3)-C(16)	1.51(1)	
			C(16)-C(17)	1.47(2)	

TABLE 6

BOND ANGLES (°) OF COMPOUNDS I AND II (with e.s.d.'s in parentheses)

4-3-4	I	II		I	11
C(1) - Ru(1) - C(4)	76.8(6)	77.7(2)	C(21) - Ru(2) - C(22)	90,3(8)	90.6(3)
C(1)-Ru(1)-C(11)	95.3(8)	94.0(3)	C(21)-Ru(2)-C(23)	95(1)	94.9(3)
C(1)-Ru(1)-C(12)	97(1)	97.5(3)	C(22) - Ru(2) - C(23)	95(1)	94.7(3)
C(1)-Ru(1)-C(13)	165.9(7)	166.8(3)	C(21) - Ru(2) - C(1)	99.7(8)	94.9(3)
C(1)-Ru(1)-C(23)	79.1(9)	89.3(2)	C(21)-Ru(2)-C(2)	96(1)	102.5(3)
C(4)-Ru(1)-C(12)	96(1)	95.5(3)	C(21)-Ru(2)-C(3)	121(1)	134.1(3)
C(4)-Ru(1)-C(13)	94.3(6)	94.6(3)	C(21)-Ru(2)-C(4)	158.0(6)	165.7(3)
C(4)-Ru(1)-C(11)	165.9(7)	166.3(3)	C(21)-Ru(2)-Ru(1)	138.1(9)	124.4(2)
C(4)-Ru(1)-C(23)	85(1)	76.6(2)	C(22) - Ru(2) - C(1)	161.9(7)	152.9(3)
C(11)-Ru(1)-C(12)	96(1)	96.4(3)	C(22)-Ru(2)-C(2)	127(1)	116.4(3)
C(11)-Ru(1)-C(13)	91.0(7)	91.3(3)	C(22)-Ru(2)-C(3)	97(1)	93.5(3)
C(11)-Ru(1)-C(23)	82(1)	92.5(3)	C(22)-Ru(2)-C(4)	94.9(7)	100.0(3)
C(12)-Ru(1)-C(13)	95(1)	93.8(3)	C(23)-Ru(2)-C(1)	99(1)	111.2(3)
C(12)-Ru(1)-C(23)	175.0(6)	168,3(3)	C(23)-Ru(2)-C(2)	136.2(8)	143.8(3)
C(13)-Ru(1)-C(23)	89(1)	78.4(3)	C(23)-Ru(2)-C(3)	141.4(7)	130.2(3)
			C(23)-Ru(2)-C(4)	106(1)	93.9(3)
			C(23)-Ru(2)-Ru(1)	70.4(7)	70.8(2)
			C(22)-Ru(2)-Ru(1)	129(1)	142.2(9)
Ru(1)-C(11)-O(11)	180(2)	180(2)	Ru(2)-C(21)-O(21)	177(2)	177.5(7)
Ru(1)-C(12)-O(12)	177(2)	178.4(7)	Ru(2)-C(22)-O(22)	179(2)	179.1(7)
Ru(1)-C(13)-O(13)	176(2)	177.3(8)	Ru(2)-C(23)-O(23)	169(1)	169.0(6)
Compound I			Compound II		
Ru(1)-C(1)-C(2)	117.8(9)		Ru(1)-C(1)-C(2)	116.2(4)	
Ru(1)-C(1)-C(5)	123(1)		Ru(1)-C(1)-C(5)	123.0(4)	
C(2)-C(1)-C(5)	118(2)		C(2)-C(1)-C(5)	119.7(5)	
C(1)-C(2)-C(3)	113(2)		C(1)-C(2)-C(3)	114.2(6)	
C(1)-C(2)-C(6)	128(1)		C(1)-C(2)-C(14)	122.4(6)	
C(3)-C(2)-C(6)	124(2)		C(3)-C(2)-C(14)	123.2(6)	
C(2)-C(3)-C(4)	114(2)		C(2)-C(3)-C(4)	115.4(6)	
C(2)-C(3)-C(7)	120(2)		C(2)-C(3)-C(16)	120.0(7)	
C(4)-C(3)-C(7)	126(1)		C(4)-C(3)-C(16)	124.5(7)	
C(3)-C(4)-Ru(1)	117(1)		C(3)-C(4)-Ru(1)	115.3(4)	
C(3)-C(4)-C(8)	118(2)		C(3)-C(4)-C(7)	121.4(6)	
Ru(1)-C(4)-C(8)	124(1)		Ru(1)-C(4)-C(7)	122.7(5)	
C(1)-C(5)-O(5)	112(2)		C(1)-C(5)-C(6)	111.7(5)	
C(2)-C(6)-O(6)	110(1)		C(5)-C(6)-O(6)	113.4(6)	
C(3)-C(7)-O(7)	113(1)		C(4)-C(7)-C(8)	112.1(6)	
C(4)-C(8)-O(8)	109(2)		C(7)-C(8)-O(8)	110.2(7)	
			C(2)-C(14)-C(15)	116.3(7)	
			C(3)-C(16)-C(17)	112.4(8)	

tallography [17] including  $\Delta f'$  and  $\Delta f''$  for ruthenium atoms. The agreement factors were defined in the usual way as  $R = \Sigma(|F_0 - F_c|)/\Sigma|F_0|$  and  $R_w = \langle \Sigma(w|F_0 - F_c|)^2/\Sigma(w|F_0|)^2 \rangle^{1/2}$ .

In all least squares refinements the quantity minimized was  $\Sigma(w|F_0 - F_c|)^2$  and the full matrix was inverted. A weighting scheme based on counting statistics,  $w = \Delta I/2F$  was used in least squares refinement.

Both structures were solved by heavy-atom techniques. Ru atoms were unambigu-

tions of planes through selected groups of atoms $\begin{array}{c} \text{fints} \\ \text{nound} I & 2 \text{ C(1), C(2), C(3), C(4)} & 0.72118 \times & -0.68265 \text{ y} & 0.11786  \\ 3 \text{ Ru(1), Ru(2), C(1), C(3), C(4)} & 0.85339 \times & -0.93051  & -0.93265  \\ 3 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.18539 \times & -0.4004  & -0.75133  \\ 3 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.15339 \times & -0.4004  & -0.75133  \\ 3 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.15444 \times & -0.75848  & -0.68365  \\ 4 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.15444 \times & -0.75848  \\ 4 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.15444 \times & -0.75848  \\ 4 \text{ Ru(1), Ru(2), C(12), C(12)} & 0.15444 \times & -0.75848  \\ 1 & 0.00 & 892  \\ 0 \text{ outd} I & 1 & 0.00 & 892  \\ 1 & 0.00 & 892  \\ 0 \text{ outd} I & 1 & 0.00 & 892  \\ 1 & 0.00 & 892  \\ 0 \text{ outd} I & 1 & 0.00 & 892  \\ 1 & 0.00 & 802  \\ 0 \text{ outd} I & 1 & 0.00 & 892  \\ 1 & 0.00 & 0.000 & C(7) & 0.008  \\ 0  & 0.003  \\ 0  & 0  & 0.003  \\ 0  & 0  & 0.003  \\ 0  & 0  & 0  & 0.003  \\ 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0  & 0 $	rallel to $y \times z$ )	, y ани 2 тори (	CSCIII ANU	nic coordinate	s in A with r	espect to orth	ogonal cry	stal axial sy	stem defin	ed as follows	t y is para	llel to b; z is	parallel to	$b \times a$ : x
nd //         Plane         Plane           and //         2 C(1), C(2), C(3), C(12) $0.32733 \times -0.54329 \times 0.11786$ $3 Ru(1), Ru(2), C(12)$ $0.32733 \times -0.54329 \times 0.13488$ $3 Ru(1), Ru(2), C(12)$ $0.32733 \times -0.54329 \times 0.01348$ $3 Ru(1), Ru(2), C(12)$ $0.43232 \times -0.49004 \times -0.98263$ $3 Ru(1), Ru(2), C(12)$ $0.13544 \times -0.5548 \times 0.055115$ $3 Ru(1), Ru(2), C(12)$ $0.15444 \times -0.55848 \times 0.534139$ $0.633131$ $0.633131$ $1 Ru(1), Ru(2), C(12)$ $0.15444 \times -0.55848 \times 0.534139$ $0.633131$ $0.78213 \times -0.5848 \times 0.534139$ $0.633131$ $0.633131$ $1 Ru(1), Ru(2), C(12)$ $0.15444 \times -0.55848 \times 0.534139$ $0.633131$ $0.78213 \times -0.5848 \times 0.534139$ $0.633131$ $0.78213 \times 0.54139 \times 0.55848$ $0.11 Ru(2), C(12)$ $0.1344 \times -0.55848$ $0.11 Ru(2), C(12)$ $0.023 \times 0.5418$ $0.11 Ru(2), C(12)$ $0.023 \times 0.5418$ $0.033 \times 0.5484 \times 0.5188 \times 0.55848$ $0.6331313$ $0.041 Ru(2) Ru(2) Ru(2) Ru(2) Ru(2) Ru(2) Ru(2)$ $0.732 \times 0.5211644$ $0.033 \times 0.5184 \times 0.513 \times 0.513 \times 0.5444$ $0.633 - 0.52184$	ons of plane	s through sele	ected grou	tps of atoms										
and $I = 2 \text{ C(I)}, \text{C(Z)}, \text{C(A)} = 0.72118 \times -0.68255 \text{ y} = 0.11786$ $3 \text{ Ru(I)}, \text{C(I)}, \text{C(I)}, \text{C(I)} = 0.12303 \times -0.3459 \text{ y} = 0.13486$ $4 \text{ Ru(I)}, \text{Ru(Z)}, \text{C(I)}, \text{C(I)} = 0.12303 \times -0.3509 \times 0.054159 \text{ y} = -0.75115$ $3 \text{ Ru(I)}, \text{C(I)}, \text{C(I)}, \text{C(I)} = 0.123509 \times 0.054159 \text{ y} = -0.75115$ $3 \text{ Ru(I)}, \text{Ru(Z)}, \text{C(I)}, \text{C(I)} = 0.12509 \times 0.15444 \times -0.75848 \text{ y} = 0.63313$ ; $2 \text{ C(I)}, \text{C(I)}, \text{C(I)}, \text{C(I)} = 0.12544 \times -0.75848 \text{ y} = 0.63313$ ; 2  Ru(I), Ru(Z), C(I), C(I) = 0.0325  y = 0.75115 4  Ru(I), Ru(Z), C(I), C(I) = 0.0325  y = 0.75415 2  Plane = 2 = 3 1  I = 10.0 = 89.2 1  I = 10.0 = 89.2 1  I = 10.0 = 89.2 1  I = 2  O -0.038  C(I) = 0.008  C(I) = 0.034 1  I = 2  O -0.038  C(I) = 0.008  C(I) = 0.034 1  I = 2  O -0.038  C(I) = 0.008  C(I) = 0.003 1  I = 2  O -0.038  C(I) = 2.798  C(I) = -0.003  C(I) = 0.012 1  Ru(I) = -0.008  C(I) = -0.008  C(I) = -2.798  C(I) = -2.142  C(I) = -2.008  C(I) = -2.798  C(I) = -2.798  C(I) = -2.798  C(I) = -0.000  C(I) = -0.000  C(I) = -2.798		Plane												
$ \begin{array}{ccccccc} & 0.82733 & -0.82739 & -0.114862 & 0.00551 & -0.93265 & -0.9326 & -0.$	I pu	2 C(I).	C(2), C(3,	), C(4)		0.72118 x		-0.68265	2	0.11786	ta	0.474	40	
dII         4 Ru(1), Ru(2), C(12), O(12)         0.18539 x         0.00051 y         -0.92055 y         -0.93265 y         -0.93064 y         -0.75115 y         -0.35313 x         -0.93064 y         -0.75115 y         -0.93265 y         -0.93064 y         -0.75115 y         -0.93731 x         -0.93731 x         -0.93641 x         -0.75348 y         0.65313 x         -0.63313 x		3 Ku(1).		4)		0.82733 x		-0.54529	~	0.13486	ы	-0.525	56	
ord II         2 C(1), C(2), C(3), C(4) $0.44232.x$ $-0.2600.y$ $-0.75348.y$ $-0.375115$ 7 ku(1), Ru(2), C(12), O(12)         0.15444.x $-0.75848.y$ $0.53313.$ 7 ku(1), Ru(2), C(12), O(12)         0.15444.x $-0.75848.y$ $0.65313.$ 7 between selected pairs of planes         2         3 $0.15444.x$ $-0.75848.y$ $0.65313.$ 7 between selected pairs of planes         2         3 $0.15444.x$ $-0.75848.y$ $0.65313.$ 7 between selected pairs of planes         2         3 $0.15444.x$ $-0.75848.y$ $0.65313.$ 7 between selected pairs of planes         2         3 $0.1544.x$ $-0.75848.y$ $0.65313.$ 7 between selected atoms from planes         87.6         89.0         87.6 $0.2000.$ $0.1001.$ $0.633.$ 7 c(1)         2         92.0         87.6 $0.001.$ $0.633.$ $0.6033.$ 8 u(1)         0         8         0.0001. $0.73.$ $0.003.$ $0.633.$ $0.003.$ 9 at (1)         2         87.6 $0.0001.$ $0.003.$ $0.0$		4 Ru(1),	i, Ru(2), C	2(12), O(12)		0.18539 x		0.00551	54	-0.98265	14	6.064	17	
$ \begin{array}{ccccccc} 3 \ Ru(1), C(1), C(4) & -0.29509 \times & 0.54150 y & 0.73871; \\ 4 \ Ru(1), Ru(2), C(12), O(12) & 0.15444 \times & -0.75848 y & 0.65313; \\ 4 \ Ru(1), Ru(2), C(12), O(12) & 0.15444 \times & -0.75848 y & 0.65313; \\ 7 \ between selected pairs of planes \\ md I & 1 & 0.0 & 89.2 \\ md I & 1 & 0.0 & 89.2 \\ 2 & 39.0 \\ md II & 1 & 9.2 & 92.0 \\ 2 & 87.6 \\ es (\dot{A}) of selected atoms from planes \\ \hline md I & 1 & 0.003 & C(2) & 0.001 & C(3) & -0.003 \\ 1 & 1 & 0.003 & C(2) & 0.000 & C(7) & 0.003 \\ 3 & Ru(1) & -0.007 & Ru(2) & 0.000 & C(7) & 0.003 \\ 3 & Ru(1) & -0.007 & Ru(2) & 0.000 & C(7) & 0.003 & C(6) & -2.798 \\ \hline md II & 1 & C(1) & -0.007 & Ru(2) & 0.000 & C(7) & 0.003 & C(6) & -2.798 \\ \hline md II & 1 & C(1) & -0.007 & Ru(2) & 0.000 & C(7) & 0.003 & C(6) & -2.798 \\ \hline md II & 1 & C(1) & -0.004 & Ru(2) & -0.000 & C(7) & 0.003 & C(10) & 0.003 \\ \hline md II & 1 & C(1) & -0.004 & C(12) & 0.013 & O(12) & -0.012 \\ \hline md II & 1 & C(1) & -0.004 & C(12) & 0.013 & O(12) & -2.78 \\ \hline md II & 1 & C(1) & -0.004 & Ru(2) & -0.000 & C(12) & 0.013 & O(12) & -2.78 \\ \hline md II & 1 & C(1) & -0.004 & Ru(2) & -0.004 & C(14) & -0.003 & C(16) & 0.005 \\ \hline md II & 1 & C(11) & -3.43 & C(13) & -1.455 & O(11) & 2.149 & O(13) & -2.181 \\ \hline mu(1) & -0.004 & Ru(2) & -0.004 & C(12) & 0.013 & O(12) & -2.78 & C(6) & -2.798 & C(6) & -2.798 & C(7) & -2.798 & C(7) & -2.788 & C(7) & -$	II pu	2 C(1), i	C(2), C(3)	), C(4).		0.44232 x		- 0.49004	2	- 0.75115	N	2.914	66	
$\begin{array}{c ccccc} 4 \ Ru(1), Ru(2), C(12), O(12) & 0.15444  x & -0.75848  y & 0.63313 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$		3 Ru(1),	<ul> <li>C(1), C(-</li> </ul>	4)		-0.29509 x		0.54150	-	0.78721	•1	-3.275	95	
(*) between selected pairs of planes md I Plane 2 3 md I 1 100 89.2 md II 1 9.2 92.0 md II 1 9.2 92.0 md II 1 9.2 92.0 md II 1 0.003 C(2) 0.001 C(3) -0.005 C(4) 0.003 md II 1 C(1) -0.003 C(2) 0.000 C(7) 0.080 C(7) 0.043 md II 1 C(1) -0.007 Ru(2) -0.000 C(7) 0.080 C(7) 0.043 md II 1 C(1) -0.007 Ru(2) -0.000 C(12) 0.019 O(13) -2.798 C(2) 0.000 C(2) 0.000 C(10) 2.019 O(13) -2.798 md II 1 C(1) -0.000 C(2) 0.000 C(10) 2.0019 O(13) -2.798 md II 1 C(1) -0.000 C(2) 0.000 C(10) 2.0019 O(13) -2.778 md II 1 C(1) -0.000 C(2) 0.000 C(10) 2.0019 O(13) -2.778 md II 1 C(1) -0.000 C(2) 0.000 C(10) 2.013 O(13) -2.778 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) -0.000 C(2) 0.000 C(12) 0.013 C(16) 0.005 md II 1 C(1) 1.421 C(2) 1.423 C(13) 1.277 C(2) 1.874		4 Ru(1).	, Ru(2), C	3(12), O(12)		0.15444 x		- 0.75848	5	0.63313	11	0.912	54	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	(°) between	selected pair:	s of plane	s										
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		Plane		2	~~									
and II         2         89.0           and II         1         9.2         92.0 $2$ 87.6         87.6         92.0 $3$ $87.6$ $87.6$ $87.6$ $1$ 1 $-0.003$ $-0.003$ $-0.003$ $1$ $1$ $-0.003$ $-0.003$ $-0.003$ $1$ $1$ $-0.003$ $-0.018$ $-0.012$ $1$ $C(5)$ $-0.010$ $-0.019$ $-0.012$ $3$ $Ru(1)$ $-0.003$ $C(2)$ $0.010$ $-0.012$ $3$ $Ru(1)$ $-0.003$ $C(2)$ $0.000$ $C(12)$ $-0.012$ $3$ $Ru(1)$ $-0.003$ $C(2)$ $0.000$ $C(12)$ $-0.012$ $1$ $Ru(1)$ $-0.003$ $C(2)$ $-0.019$ $-0.012$ $-2.798$ $nd$ II $1$ $C(1)$ $-0.004$ $C(1)$ $-2.272$ $1$ $Ru(1)$ $-0.006$ $C(2)$ $-0.001$ $-2.272$ <t< td=""><td>I pu</td><td>I</td><td></td><td>10.0</td><td>89.2</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>	I pu	I		10.0	89.2									
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The form planes from planes from planes from planes from planes and I lane $C(1) = -0.003$ $C(2) = 0.001$ $C(3) = -0.005$ $C(4) = 0.003$ $C(5) = -0.012$ $C(5) = -0.012$ $C(5) = -0.012$ $C(6) = -0.020$ $C(7) = 0.012$ $C(8) = 0.043$ $C(1) = 0.012$ $C(1) = 0.012$ $C(2) = 0.012$ $C(1) = 0.012$ $C(2) = 0.012$ $C(1) = 0.012$ $C(2) = 0.012$ $C(1) = 0.012$ $C(2) = 0.012$ $C(2) = 0.012$ $C(2) = 0.012$ $C(2) = 0.012$ $C(1) = 0.012$ $C(2) = 0.001$ $C(1) = 2.181$ $C(2) = 0.000$ $C(2) = 0.001$ $C(1) = 2.021$ $O(2) = 2.272$ $O(1) = 0.000$ $C(2) = 0.000$ $C(2) = 0.000$ $C(2) = 0.000$ $C(2) = 0.000$ $C(1) = 0.000$ $C(2) = 0.000$ $C(1) = 0.003$ $C(2) = 0.000$ $C(2) = 0.000$ $C(2) = 0.000$ $C(2) = 0.000$ $C(2) = 0.003$ $C(1) = 0.003$ $C(1) = 0.003$ $C(2) = 0.003$ $C(1) = 0.003$ $C(1) = 0.003$ $C(2) = 0.003$	II pu			9.2	92.0 87 (									
Les (Å) of selected atoms from planes $md I = \begin{bmatrix} P ane \\ C(5) & -0.018 \\ C(5) & -0.018 \\ C(5) & -0.018 \\ C(5) & -0.018 \\ C(6) & -0.080 \\ C(7) & 0.080 \\ C(7) & 0.080 \\ C(8) & 0.043 \\ C(8) & 0.043 \\ C(8) & 0.043 \\ C(12) & 0.019 \\ C(12) & 0.019 \\ C(12) & -0.012 \\ C(12) & -0.012 \\ C(12) & -0.012 \\ C(13) & -1.455 \\ C(11) & 1.374 \\ C(13) & -1.455 \\ C(11) & 1.374 \\ C(13) & -1.455 \\ C(11) & 2.181 \\ C(22) & -1.442 \\ C(21) & 1.279 \\ C(22) & -1.442 \\ C(21) & -0.000 \\ C(2) & 0.000 \\ C(2) & -0.004 \\ C(14) & -0.003 \\ C(12) & -0.000 \\ C(12) & -0.003 \\ C(12) & -0.000 \\ C(12) & -0.003 \\ C(12) & -0.003 \\ C(13) & -1.453 \\ C(11) & 2.167 \\ C(21) & 1.421 \\ C(22) & -1.166 \\ C(21) & -2.752 \\ C(22) & -1.166 \\ C(22) & $		7			87.6									
md I         Plane $mdI$ 1         C(1) $-0.003$ C(2) $0.001$ C(3) $-0.005$ C(4) $0.003$ 3         Ru(1) $-0.007$ Ru(2) $0.0000$ C(12) $0.012$ $-0.012$ 3         Ru(1) $-0.007$ Ru(2) $0.0000$ C(12) $0.012$ $-0.012$ 7         C(2) $0.0100$ C(12) $0.019$ O(12) $-0.012$ 7         C(21) $1.374$ C(13) $-1.455$ O(11) $2.149$ O(13) $-2.778$ 7         C(21) $1.374$ C(13) $-1.442$ $0.221$ $-2.798$ 7         C(21) $1.374$ C(13) $-1.442$ $0.221$ $-2.798$ 7         C(21) $-0.000$ C(22) $-1.442$ $0.221$ $-2.772$ 7         C(1) $-0.000$ C(12) $-0.001$ $(74)$ $-0.000$ 7         C(1) $-0.000$ C(11) $-0.0001$ $(14)$	es (A) of se	lected atoms	from plar	les										
$ \begin{array}{llllllllllllllllllllllllllllllllllll$		Plane												
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	I pu	-	C(1)	-0.003	C(2)	0.001	C(3)	- 0.005	C(4)	0.003	Ru(1)	0.282	Ru(2)	- 1.814
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		3	Ru(1)	- 0.007	Ru(2)	0.0000	C(12)	0.019	0(12)	- 0.012	COD	- 1.276	C(4)	- 1.292
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			C(2)	0.717	C(3)	-0.710	C(5)	2.836	C(6)	- 2.798	C(7)	1.556	C(8)	1,461
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			C(11)	1.374	C(13)	- 1,455	0(11)0	2.149	0(13)	-2.181				
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$			C(21)	1.279	C(22)	1.442	0(21)	2.021	O(22)	- 2.272	C(23)	0.183	O(23)	0.343
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	II pu		C(I)	-0.000	C(2)	0.000	C(3)	-0.001	(.(4)	-0.000	Ru(1)	-0.260	Ru(2)	1.827
I Ru(1) -0.004 Ru(2) -0.000 C(12) 0.013 O(12) -0.009 C(2) 0.083 C(3) -0.602 C(5) 2.854 C(7) -2.765 C(11) 1.343 C(13) -1.453 O(11) 2.107 O(13) -2.277 C(21) 1.421 C(22) -1.166 O(21) 2.222 O(22) 1.874			C(5)	-0.086	C(7)	-0.004	C(14)	- 0.093	C(16)	0.005				
C(2) 0.083 C(3) -0.602 C(5) 2.854 C(7) -2.765 C(11) 1.343 C(13) -1.453 O(11) 2.107 O(13) -2.277 C(21) 1.421 C(22) -1.166 O(21) 2.222 O(22) 1.874			Ru(1)	-0.004	Ru(2)	- 0.000	C(12)	0.013	0(12)	-0.009	C(1)	1.363	C(4)	- 1.261
C(11) 1.343 C(13) -1.453 O(11) 2.107 O(13) -2.277 C(21) 1.421 C(22) -1.166 O(21) 2.222 O(22) 1.874			C(2)	0.083	C(3)	- 0.602	C(5)	2.854	C(7)	- 2.765	C(14)	1.722	C(16)	- 1.308
C(21) [.42] $C(22) -1.166$ $O(21)$ 2.222 $O(22)$ ].874			C(11)	1.343	C(13)	- 1.453	0(11)	2.107	O(13)	- 2.277				
			C(21)	1.421	C(22)	- 1.166	0(21)	2.222	O(22)	1.874	C(23)	-0.584	O(23)	- 0.965

TABLE 7. LEAST-SQUARES PLANES IN THE FORM Ax + By + Cz - D = 0

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ously revealed by Patterson functions. The subsequent  $F_0$  syntheses showed the position of all non-hydrogen atoms. Refinement of their coordinates using full-matrix least-squares procedure with isotropic temperature factors, then anisotropic, gave convergence at R = 0.058 (I) and R = 0.049 (II). H atoms were then included as a fixed contribution at their calculated idealized positions (C-H 1.0 Å). They were assigned isotropic thermal parameters 1.0 Å<sup>2</sup> higher than those of the C atoms to which they are attached. Final least-squares refinements led to the agreement factors of R = 0.056 and  $R_w = 0.052$  and a GOF = 1.16(No = 1911, Nv = 244) for compound I, and R = 0.044 and  $R_w = 0.042$ , and a GOF = 2.03(No = 2865, Nv = 254) for compound II. The goodness of fit (GOF) is defined as  $\Sigma(w|F_0 - F_c|)^2/(No - Nv)$ .

Atomic coordinates and thermal parameters are given in Tables 3 and 4, bond lengths and angles with e.s.d.'s calculated from the full variance-covariance matrix and including contribution due to errors in the unit cell parameters, in Tables 5 and 6, and details of important molecular planes in Table 7. Tables of calculated and observed structure factors may be obtained from the authors.

## **Results and discussion**

Both crystals are built up from binuclear units as shown in Figures 1 and 2; in addition, the asymmetric unit of compound I contains a water molecule. Each binuclear unit can be regarded as a Ru(CO)<sub>3</sub> fragment (this Ru referred as Ru(2))  $\pi$ -bonded to a cycloruthenapentadienyl ring. The ruthenium (referred as Ru(1)) engaged in the ring also is  $\sigma$ -bonded to three CO groups. The Ru<sub>2</sub>C<sub>4</sub> fragment of each molecule (i.e. the RuC<sub>4</sub> ring and the Ru(2)) is similar to those found in the metallocycle complexes shown in Table 8.

The butadiene chain is essentially planar with equal C-C distances within the experimental deviation |1.43(1) Å|; this corresponds with delocalized electrons as found in other diene complexes, but the delocalization in this case seems to be fairly complete, since the central and terminal C-C bond lengths are equal.

Among all the known metallocycles, only  $Cr_2(CO)(\eta-C_5H_5)_2(C_6H_5)_2C_4H_2$  [12] has been regarded as containing C(1) and C(4) bridging carbene-type bonds with identical C(1)-Cr(1), C(1)-Cr(2), Cr(1)-C(4) and Cr(2)-C(4) bond lengths of 2.02 Å. In the other compounds the M(1)-C(1) and M(1)-C(4) linkages have just been defined as single bonds. However in our compounds these lengths correspond rather to lengths appropriate to metal-stabilized carbenes in which the metal-carbon bond is close to a double bond. From Table 9, it appears that the metal-carbon bond length in all the metallocycles is just as close to a double bond. In this respect the following typical single bond values are relevant:

 $Fe-CH_3-2.079(5)-Fe(CO)_2(CH_3NC)(CH_3(PPh_3)_2)$  [23];  $W-CH_2C(CH_3)_3-2.258(8)-W(CCMe_3)(CHCMe_3)(CH_2CMe_3)(dmpe)$  [24].

 $\pi$ -Bonding between Ru(1)-C(1) and Ru(1)-C(4) implies ruthenium  $t_{2g}$  orbitals. If z is the Ru(1)-C(12) axis, those  $t_{2g}$  orbitals do not lie in the Ru(1)-C(23) plane. Indeed Ru(1)-C(11) and Ru(1)-C(13) where C(11) and C(13) are carbonyl in *trans* positions with respect to C(1) and C(4), are longer than the Ru(1)-C(12) bond, suggesting again that a part of the electron density of this orbital is used for  $\pi$ -bonds with the ring. These  $\pi$ -bonds bring the Ru(1) C<sub>4</sub> fragment close to planarity. The Ru(1) atom is only slightly lifted above the perfect plane defined by the butadiene fragment, by 0.28 and 0.26 Å for compounds I and II, respectively (Table 7). It is

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STRUCTURAL PARAMETERS FOR Ru<sub>2</sub>C<sub>4</sub> FRAGMENT IN COMPOUNDS I AND II AND RELATED PARAMETERS IN SOME CYCLOMETALLAPEN. TADIENE COMPLEXES

	And the state of t		A TATAL AND A TATAL AND AND A DESCRIPTION OF A DATA AND A	A MANAGE A MANAGE AND A MANAGE AND A MANAGEMENT OF A MANAGEMENT OF A MANAGEMENT OF A MANAGEMENT OF A MANAGEMENT			
Compound	Reference	$M(1)-C(\sigma)$	$M(2)-C(\pi)$ (terminal)	$M(2)-C(\pi)$ (central)	C-C (terminal)	C-C (central)	M(1)-M(2)
(CO) <sub>6</sub> Ru <sub>2</sub> (C <sub>4</sub> (CH <sub>2</sub> OH) <sub>4</sub> )·H <sub>2</sub> O	а	2.07(4)	2.23(6)	2.26(5)	1.44(2)	1,42(2)	2.743(3)
$(CO)_{6}Ru_{2}(C_{4}(C_{2}H_{4}OH)_{2}(C_{2}H_{5})_{2})$	11	2.095(8)	2.25(1)	2.28(1)	1,42(1)	1.44(1)	2.717(1)
(CO) <sub>6</sub> Fe <sub>2</sub> (C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> )	[3]	1.95(1)	2.12(1)	2.15(1)	1.42(2)	1.43(1)	2.493
(CO) <sub>6</sub> Fe <sub>2</sub> ((CH <sub>3</sub> ) <sub>3</sub> SiOC) <sub>4</sub>	[4]	1.92(2)	2.13(2)	2.19(2)	t	i.	2.500(3)
$(CO)_6 Fe_2(C_{12}H_{16})$	[2]	1.96(2)	2.07(2)	2.18(2)	1,41(2)	1.43(2)	2.462(3)
$(CO)_{6}Fe_{2}(C_{4}(C, H_{5})_{4})$	[9]	1.97(1)	2.10(1)	2.14(1)	l		2.505(1)
(CO) <sub>5</sub> Fe <sub>2</sub> PPh <sub>3</sub> ((C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> )	[2]	(1)66'1	2.12(2)	2.15(2)	1.43(2)	1.43(1)	2.515(2)
(CO) <sub>k</sub> W <sub>2</sub> (C <sub>9</sub> H <sub>14</sub> )	[01]	2.17(3)	2.36(3)	2.35(3)	1.42(3)	1.48(3)	2.900(2)
(CO) <sub>4</sub> 1r <sub>2</sub> PPh <sub>3</sub> (C <sub>4</sub> (C <sub>2</sub> H <sub>5</sub> CO) <sub>4</sub> )	[11]	2.071(8)	2.23(2)	2.27(4)	1.435(4)	1.43(1)	2.737(1)
( <i>n</i> -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> COCr <sub>2</sub> (C <sub>4</sub> (C,H <sub>5</sub> ) <sub>2</sub> H <sub>2</sub> )	[12]	2.028(7)	2.022(7)	2.23(1)	1.42(1)	1.428(11)	2.377(2)
{( <i>n</i> -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> (CO) <sub>2</sub> W(C <sub>4</sub> H <sub>4</sub> )}Co(CO) <sub>2</sub>	113	2.13(1)	2.03(1)	2.12(1)	1.43(1)	1.42(1)	2.664(1)
er verste Anton Varianova e a sene a sene a sene a sene a vers e vers e vers a vers e vers e vers e vers e vers	Are a chaffe and a second dependence of the statement of the second s	and the second	eren mennemen alementeralen ate annual adalah. Adelah dia majuri mujuka da	and a second			And the second se

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# TABLE 9

COMPARISON OF METAL-CARBON BOND LENGTHS (A) IN METAL-STABILIZED CARBENES AND IN CYCLOMETALLAPENTADIENYL COM-PLEXES

	Carbene)	M-C	Metallocycle complexes	Reference	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	(18) (18) (10) (20) (21) (22)	2.07(3) 2.095(6) 1.97(1) 1.96(2) 2.16(2)	Ru 2(CO) <sub>6</sub> C4(CH 2OH) <sub>4</sub> . H 2O Ru 2(CO) <sub>6</sub> C4(CH 2CH 2OH) <sub>2</sub> Et 2 F2(CO) <sub>6</sub> (C, H 5, I <sub>4</sub> C4 F2(CO) <sub>6</sub> C 12 H 16 W3(CO) <sub>6</sub> C 12 H 16 W3(CO) <sub>5</sub> C 4 H 14	This work This work [6] [10]	



Fig. 1. The [(CO)<sub>3</sub>RuC<sub>4</sub>(CH<sub>2</sub>OH)<sub>4</sub>]Ru(CO)<sub>3</sub> molecule. Ellipsoids of 50% probability are shown.



Fig. 2. The  $[(CO)_3RuC_4(CH_2CH_2OH)_2(C_2H_5)_2]Ru(CO)_3$  molecule. Ellipsoids of 50% probability are shown.

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noteworthy that a cyclodimethylsilapentadienyl ring is known to act as a ligand to Ru [25]. In such a case, Si cannot give such  $\pi$ -bonds and indeed it lies 0.72 Å above the butadiene plane. Thus electron delocalization is assumed for all the bonds of that cycloruthenapentadiene ring.

Besides the C(1) and C(4) atoms, Ru(1) is also bonded to three CO groups with a square pyramidal coordination: the C(1), C(4), C(11) and C(13) atoms define the basal plane, and C(12) is in the apical position. The three CO ligands bonded to Ru(1) and the two  $\sigma$ -bonds make it a sixteen electron atom (neglecting the metal-metal bond). A 18 electrons configuration is achieved through the formation of a metal-metal donor-acceptor Ru(2)  $\rightarrow$  Ru(1) bond; such bonding causes a build up of electron density on Ru(1). Cotton [26] considers that this charge build up is relieved by the formation of a weak bond to the C(23) carbon atom which lies below Ru(1). This would explain why the Ru(2)–C(23)–O line is bent; such a CO ligand is called "semi-bridging" [27]. This point will be discussed later on.

We now consider the coordination around Ru(2). It is strikingly similar to that described for the mononuclear compounds  $[Fe(CO)_3(1,4-diphenylbutadiene)]$  [28] and for  $[Fe(CO)_3(butadiene)]$  [29]. This Ru(2) atoms (or Fe(2) in similar complexes) receives three doublets from the three CO ligands and two doublets from the substituted butadiene group, and thus is a 18 electron atom. Ru(2) has a square pyramidal environment with two carbonyl groups and the midpoint of C(1)-C(2) and C(4)-C(3) on the base vertices, and one CO group (C(23)-O(23)) on the apex. This CO group lies nearly in the symmetry plane of the butadiene fragment; the angle between this Ru-C-O line and the normal to the mean plane of the butadiene fragment can be compared to the corresponding angle observed in  $[Fe(CO)_3(butadiene)]$  complexes and cycloferrapentadienyl complexes.

		M(2)-C(23)	Reference
[Fe(CO) <sub>3</sub> (1,4-diphenylbutadiene)]	100°(2)	1.782(5)	[28]
[Fe(CO) <sub>3</sub> (butadiene)]	99°(1)	1.74(4)	[29]
$[Fe_2(CO)_6 (C_4(C_6H_5)_4)]$	105°(2)	1.784(5)	[6]
$[Ru_2(CO)_6(C_4(CH_2OH)_4)]$	125°(2)	1.90(2)	this work
$[Ru_2(CO)_6(C_4(CH_2CH_2OH)_2(C_2H_5)_2)]$	109°(1)	1.916(8)	this work

Thus it seems that the Ru-Ru bond does not strongly influence the overall geometry of Ru(2)(CO)<sub>3</sub> with respect to the butadiene fragment. Futhermore, the metal-CO distance is not noticeably changed, as is evident from the table above. If the Ru(2)-C(23) is regarded as the z axis for this ruthenium, then the  $d_{xz}$  and  $d_{yz}$  orbitals of Ru(2) may be involved in  $\pi$ -bonding with the ligands, C(23)-O included. It thus appears that this CO has no  $\pi^*$  orbitals in the plane Ru(1)-Ru(2)-C(23). Furthermore, this carbonyl group is geometrically *trans* to C(12)-O attached to Ru(1), but the Ru(1)-C(12) distance is normal, suggesting that no significant interaction between Ru(1) and C(23) occurs through the Ru(1)  $d_{z^2}$  orbital used for the Ru(1)-C(12) bond.

The Ru-Ru bond has now to be discussed. From the way in which the two squares pyramids are arranged, it appears that there is no direct metal-metal overlap. The  $d_{z^2}$  orbital of Ru(1) is mainly engaged in the Ru(1)-C(12)-O bond and its extension down Ru(1) in the Ru(1)-Ru(2)-C(23) plane is very probably quite low. Moreover Ru(2) has no orbitals extending in the Ru(1)-Ru(2)-C(23) plane, as



Fig. 3. Scheme of possible overlaps between: (a) the  $d_{xz}$  and  $d_{yz}$  orbitals of Ru(1) and the ring; (b) the  $d_{xz}$  and  $d_{yz}$  orbitals of Ru(1) and Ru(2).

pointed out earlier, except the one already used to make the Ru(2)-C(23) bond. How then does the Ru-Ru overlap occur? In the light of what has been said about the various  $\pi$  orbitals in which  $t_{2g}$  ruthenium orbitals are involved, it appears that an overlap of those orbitals is possible. The  $d_{xz}$  orbital of Ru(1) extends down (Fig. 3) into the C(13)-Ru(1)-C(12)-C(1) plane; the  $d_{xz}$  orbital of Ru(2) extends into the C(22)-Ru(2)-C(23) plane. These two planes intersects along the dotted line, and so these two orbitals may overlap. The same situation occurs for  $d_{yz}$  orbitals. This would be the interaction through which Ru(2) gives electrons to Ru(1). Then, due to the  $\pi$  bonding between the  $d_{xz}$  and  $d_{yz}$  of Ru(1) and the ring, and the bonds between that ring and Ru(2), the charge release might occur quite easily following the path Ru(2)  $\rightarrow$  Ru(1)  $\rightarrow$  ring  $\pi$ -electrons  $\rightarrow$  Ru(2). Thus the semi-bridging CO is not necessarily involved in that charge release to the extent as suggested by Cotton.

The last question to be discussed is why the Ru(2)-C(23)-O linkage is bent. Two point may be considered. First, there is quite a lot of steric crowding around this C(23)-O bond, the Ru(1)-C(23) distance is only 2.73 Å and there may be some repulsion between the  $\pi$ -CO electron density and the  $d_{z^2}$  part of Ru(1) which lies below Ru(1), trans to C(12)-O. The second point is the nonsymmetrical influence of the  $d_{xz}$  and  $d_{yz}$  orbitals of Ru(1) on C(23)-O(23), thus several kinds of overlaps occur together:  $d_{xz}$  and  $d_{yz}$  of Ru(1) with  $d_{xz}$  and  $d_{yz}$  of Ru(2);  $d_{xz}$  and  $d_{yz}$  of Ru(1) with  $p_z$  of C(1) and C(4); and  $d_{xz}$  and  $d_{yz}$  of Ru(2) with some parts of the C(23)-O  $\pi$ orbitals. It is noteworthy that this last overlap does not occur in the Ru(1)-Ru(2)-C(23) plane, and thus must be quite weak. In this respect we note that Fig. 4 shows that C(23)-O line does not go exactly through Ru(1) in projection, suggesting that the steric hindrance may dominate.

This scheme would be valid for all the described cases of iron and ruthenium. However an interesting case is that of the tungsten-metallocycle  $[(CO)_4-W(C_9H_{14})W(CO)_4]$  [10]. In this case each tungsten is bonded to four carbonyl



Fig. 4. Projection of the  $Ru_2C_4(CO)_6$  (a) and  $W_2C_4(CO)_8$  (b) onto the butadiene fragment.

groups. One of them is involved in a cyclotungstapentadiene ring which is  $\pi$ -bonded to the second one. Electron counting again suggest that the tungsten of the ring receives an electron pair from the other metal centre. However there is no semibridging CO. It is relevant to note that in  $(\eta$ -C<sub>5</sub>H<sub>5</sub>)W(CO)<sub>3</sub>Cl compound [30], one CO group and the chlorine atom *trans* to it lie in the symmetry plane as shown on Fig. 5. If a similar disposition had been retained in the cyclotungstapentadiene complexe, the semi-bridging would have occurred. However, since this is not observed for the ditungsten complex, we feel that what has been described as a semi-bridging CO group is not essential to the stability of the molecule. The steric crowding would thus be the predominant influence on the bending of the Ru(2)-C(23)-O(23) linkage.



Fig. 5. (n-C<sub>5</sub>H<sub>5</sub>)W(CO)<sub>3</sub>Cl molecule projected onto the cyclopentadienyl plane.

Another interesting feacture of the ruthenium compounds is the geometry of the lateral chains. In compound I four hydroxymethyl groups are attached to the carbon atoms of the cycloruthenapentadienyl ring, whereas in compound II there are two hydroxyethyl groups and two ethyl groups in an arrangement such that the two ethyl groups are adjacent. The carbon atoms attached to the ring are essentially coplanar with the ring, showing that there is no distortion from  $sp^2$  hybridization for the four carbon atoms of that ring. The lateral chains show some peculiarities. If the molecule is orientated in such a way that Ru(2) is below the metallaring, then in the butyne diol complexes I the oxygen atoms of the alcohol functions attached to C(1) and C(4) atoms are above the ring, while the two other oxygen atoms are below it. In the hexynol compound II, the  $CH_2OH$  groups are attached to C(1) and C(4) and are also above the ring. The reason for such a disposition might lie in the fact that if the OH or CH<sub>2</sub>OH groups were below the plane, the alcoholic H atoms would be brought too close to the C(22)-O(22) and C(21)-O(21) carbonyl groups. The chair conformation of the OH groups in the butyne diol complexe minimizes repulsion between them. In the hexynol complexe II the methyl carbons of the ethyl groups are arranged in such a way that they point away from each other; one is above the butadiene plane and the other is below it; this arrangement, quite different from that in the butyne diol compound, might be attributable to the fact that  $CH_3$  is bulkier than OH.

Although some intermolecular oxygen contacts (2.70 Å mean value) might suggest hydrogen bonds, infrared spectra indicate no significant changes in the OH stretching frequency. Moreover, in our experience when hydrogen atoms are engaged in hydrogen bonding they are often easier to locate, probably because their temperature fator is somewhat lowered; in fact the hydrogen atoms attached to oxygen could not be located.

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