

499  
MW $C_4H_2O_4Ru$ 

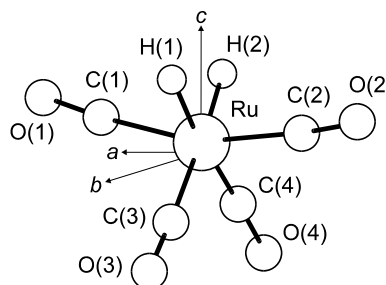
Tetracarbonyldihydorruthenium

 $C_{2v}$   
 $H_2Ru(CO)_4$ 

$r_0$	Å	$\theta_0$	deg
Ru–H	1.710(23)	H–Ru–H	87.4(24)
Ru–C(1)	1.952(21)	C(3)–Ru–C(4)	101.4(15)
Ru–C(3)	1.974(28)	C(1)–Ru–C(2)	160.6(43)
C(1)≡O(1)	1.130 <sup>a)</sup>	Ru–C(3)≡O(3)	180 <sup>a)</sup>
C(3)≡O(3)	1.143 <sup>a)</sup>	Ru–C(1)≡O(1)	172.6(76) <sup>b)</sup>

$r_s$	Å	$\theta_s$	deg <sup>c)</sup>
Ru–H	1.715(4)	H–Ru–H	86.5(20)
Ru–C(1)	1.943(17)	C(3)–Ru–C(4)	99.7(15)
Ru–C(3)	1.979(30)	C(1)–Ru–C(2)	159.7(40)

Atom	$a_0$ [Å]	$b_0$ [Å]	$c_0$ [Å]
C(1)	1.924	0.0	0.615
C(2)	–1.924	0.0	0.615
O(1)	3.004	0.0	0.948
O(2)	–3.004	0.0	0.948
C(3)	0.0	1.528	–0.965
C(4)	0.0	–1.528	–0.965
O(3)	0.0	2.413	–1.689
O(4)	0.0	–2.413	–1.689
H(1)	0.0	1.182	1.521
H(2)	0.0	–1.182	1.521
Ru	0.0	0.0	0.285



The results of the microwave data and theoretical calculations both indicate  $C_{2v}$  molecular symmetry, and show that the H atoms are separated by *ca.* 2.36 Å. These results indicate that this complex is clearly a “classical dihydride” rather than an  $\eta^2$ -bonded, “dihydrogen” complex. Fairly large deuterium isotope effects were observed for the Ru–H bond and H–Ru–H angle. The  $r_0$ , Ru–D bond lengths were observed to be 0.03(2) Å shorter than the  $r_0$ , Ru–H bond lengths. The D–Ru–D angle is 1.1° smaller than the H–Ru–H angle indicating that the anharmonicity effects are comparable for the bond lengths and for the interbond angle.

<sup>a)</sup> Assumed.

<sup>b)</sup> The *axial* carbonyl groups are bent slightly toward the hydrogen atoms.

<sup>c)</sup> Uncertainties were not estimated in the original paper.

Lavaty, T.G., Wikrent, P., Drouin, B.J., Kukolich, S.G.: J. Chem. Phys. **109** (1998) 9473.