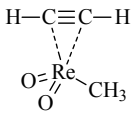
385 **$C_3H_5O_2Re$** **Acetylene(methyldioxo)rhenium** **C_s**
MW (η^2-Ethyne)methyldioxorhenium

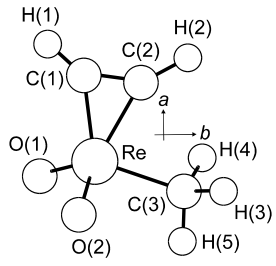


r_0	Å	θ_0	deg
Re–C(3)	2.116(2)	C(1)≡C(2)–H(2)	145.7(3)
Re–C(2)	2.067(2)	C(2)≡C(1)–H(1)	147.3(3)
Re–C(1)	2.043(2)	C(3)–Re–C(2)	81.9(2)
Re=O	1.710(1)	C(1)–Re–C(3)	118.6(1)
C(3)–H(5)	1.088 [a])	C(3)–Re=O	100.8(2)
C(3)–H(4)	1.088 [a])	O–Re=O [b])	120.9
C(2)–H(2)	1.075(3)	Re–C(3)–H(5)	108.9 [a])
C(1)–H(1)	1.072(3)	Re–C(3)–H(4)	108.9 [a])
C(1)≡C(2)	1.294(2)	Re–C(2)–H(2)	143.7(2)
		Re–C(1)–H(1)	140.1(3)
		C(1)–Re–C(2)	36.7(2)
		Re–C(1)≡C(2)–O [c])	82.1(6)

r_s	Å	θ_s	deg
Re–C(3)	2.115(19)	C(1)≡C(2)–H(2)	145.6(5) [d])
Re–C(2)	2.066(18)	C(2)≡C(1)–H(1)	147.4(5) [d])
Re–C(1)	2.041(18)	C(3)–Re–C(2)	81.7(7)
C(2)–H(2)	1.068(2)	C(1)–Re–C(3)	118.3(9)
C(1)–H(1)	1.070(3)	Re–C(2)–H(2)	143.7(5)
C(1)≡C(2)	1.289(3)	Re–C(1)–H(1)	139.9(6)
		C(1)–Re–C(2)	36.6(3)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
Re	0.0828	–0.0772	0.0
C(1)	–1.9101	–0.5274	0.0
C(2)	–1.8059	0.7624	0.0
C(3)	0.6599	1.9585	0.0
O(1)	0.7456	–0.5985	1.4881
O(2)	0.7456	–0.5985	–1.4881
H(1)	–2.5609	–1.3798	0.0
H(2)	–2.3387	1.6963	0.0
H(3)	0.2609	2.4379	–0.8914
H(4)	0.2609	2.4379	0.8914
H(5)	1.7464	2.0618	0.0

Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
Re	0.0831	0.0778	0.006i [e])
C(1)	1.9093	0.5230	0.008
C(2)	1.8045	0.7619	0.032
C(3)	0.6563	1.9578	0.051i [e])
H(1)	2.5581	1.3742	0.040i [e])
H(2)	2.3338	1.6894	0.106



[a]) Assumed.
[b]) Dependent parameter.
[c]) Dihedral angle.
[d]) Uncertainties were not estimated in the original paper.
[e]) Imaginary values, which may be set to zero.

Kukolich, S.G., Drouin, B.J., Indris, O., Dannemiller, J.J., Zoller, J.P., Herrmann, W.A.: J. Chem. Phys. **112** (2000) 7891.