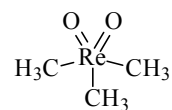


454 **C₃H₉O₂Re**
ED, NMR, IR, DFT
calculations

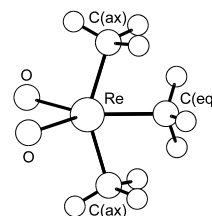
TrimethyldioxorheniumC_s assumed

r_a	Å ^{a)}	θ_a	deg ^{a)}
Re–C(eq)	2.199(22)	C(eq)–Re–C(ax)	73.5(11)
Re–C(ax)	2.122(6)	C(eq)–Re=O	118.5(10)
Re=O	1.703(3)	C(ax)–Re–C(ax)	146.9(22)
C–H	1.115(9)	O=Re=O	123.0(20)
		Re–C–H	106.5(13)

The C₃ReO₂ frame was assumed to have C_{2v} symmetry. Local C_{3v} symmetry was assumed for the methyl groups; the axial groups were assumed to have staggered conformation, while the equatorial methyl group was fixed in the position with one C–H bond in the equatorial plane according to the results of BPW91/I calculations.

The nozzle was at room temperature.

^{a)} Three times the estimated standard errors including a systematic error.



Haaland, A., Scherer, W., Volden, H.V., Verne, H.P., Gropen, O., McGrady, G.S., Downs, A.J. Dierker, G., Herrmann, W.A., Roesky, P.W., Geisberger, M.R.: *Organometallics* **19** (2000) 22.