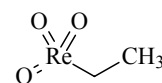


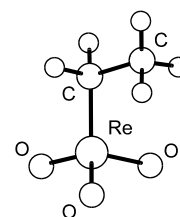
**290 C<sub>2</sub>H<sub>5</sub>O<sub>3</sub>Re**ED, vibrational spectroscopy,  
DFT calculations**Ethyltrioxorhenium**C<sub>s</sub> assumed

$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
Re–C	2.095(6)	Re–C–C	112.0(9)
C–C	1.530(16)	O=Re–C	104.6(5)
Re=O	1.711(2)		
C–H	1.106(13)		

According to the results of BPW91 calculations, it was assumed in the ED analysis that the CReO<sub>3</sub> and CH<sub>3</sub> groups have local C<sub>3v</sub> symmetry and the CH<sub>3</sub>–CH<sub>2</sub>–Re unit has staggered conformation. Though the eclipsed conformation of the CH<sub>3</sub>–CH<sub>2</sub>–Re group could not be ruled out from the ED data alone, the DFT calculations indicated that this conformation was less stable by 7.9 kJ mol<sup>–1</sup>.

The nozzle was at room temperature.

<sup>a</sup>) Twice the estimated standard errors including a systematic error.



Downs, A.J., Geisberger, M.R., Green, J.C., Greene, T.M., Haaland, A., Herrmann, W.A., Morris, L.J., Parsons, S., Scherer, W., Volden, H.V.: J. Chem. Soc., Dalton Trans. (2002) 3342.