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SUPPORTING INFORMATION

Synthesis, characterization and application of organorhenium(VII) trioxides in metathesis reactions and epoxidation catalysis

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1. IR spectra

[4-(trifluoromethyl)phenyl]trioxorhenium(VII) ***1b***

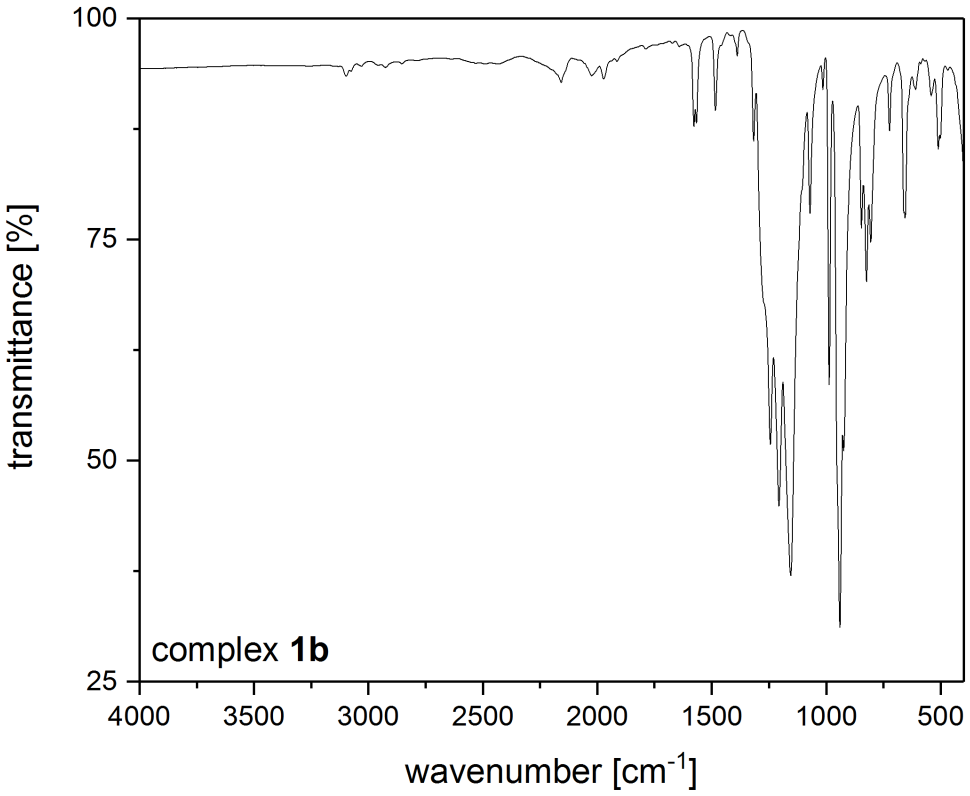

Fig. 1 IR spectrum of complex **1b**. Recorded on a Varian FTIR-670 spectrometer with ATR sampling technique.

[4-(trifluoromethoxy)phenyl]trioxorhenium(VII) ***2b***

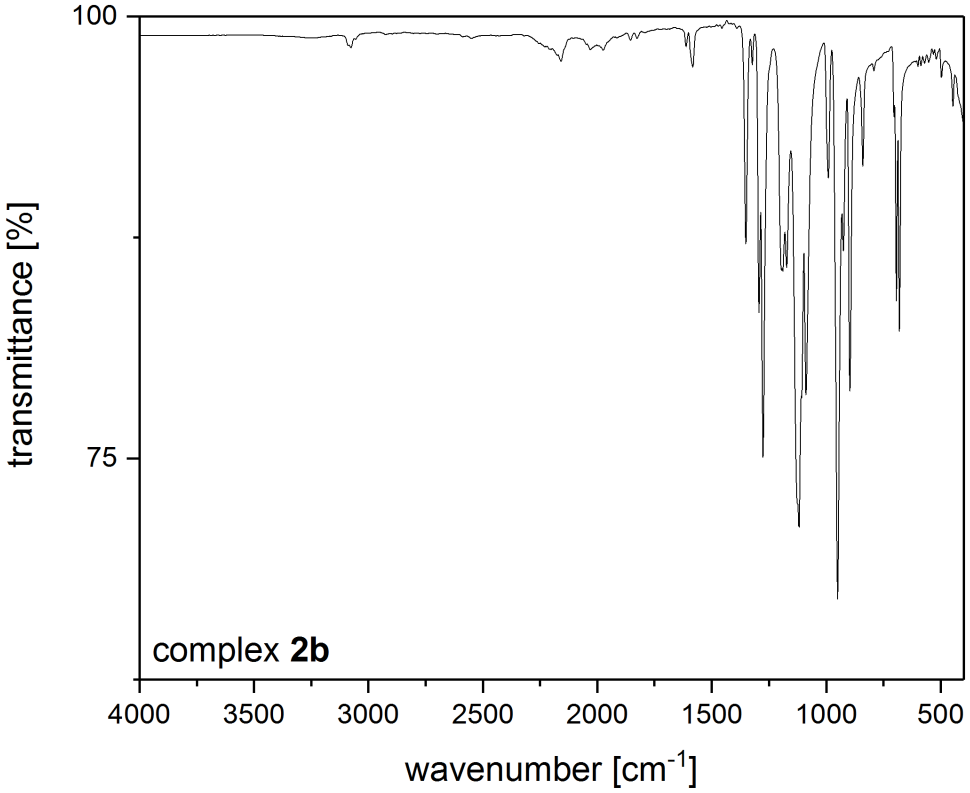

Fig. 2 IR spectrum of complex **2b**. Recorded on a Varian FTIR-670 spectrometer with ATR sampling technique.

[4-(trifluoromethyl)tetraflurophenyl]trioxorhenium(VII)(THF) ***3b · THF***

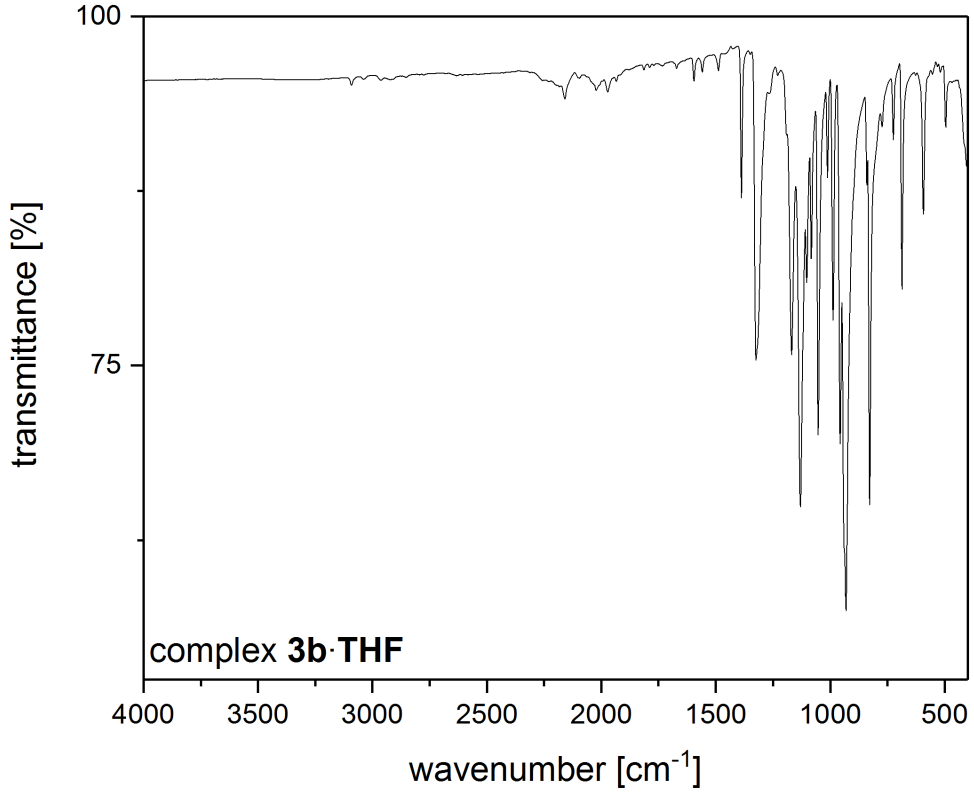

Fig. 3 IR spectrum of complex **3b·THF**. Recorded on a Varian FTIR-670 spectrometer with ATR sampling technique.

(2,2,6,6-tetramethylpiperidin-1-yl)trioxorhenium(VII) ***5***

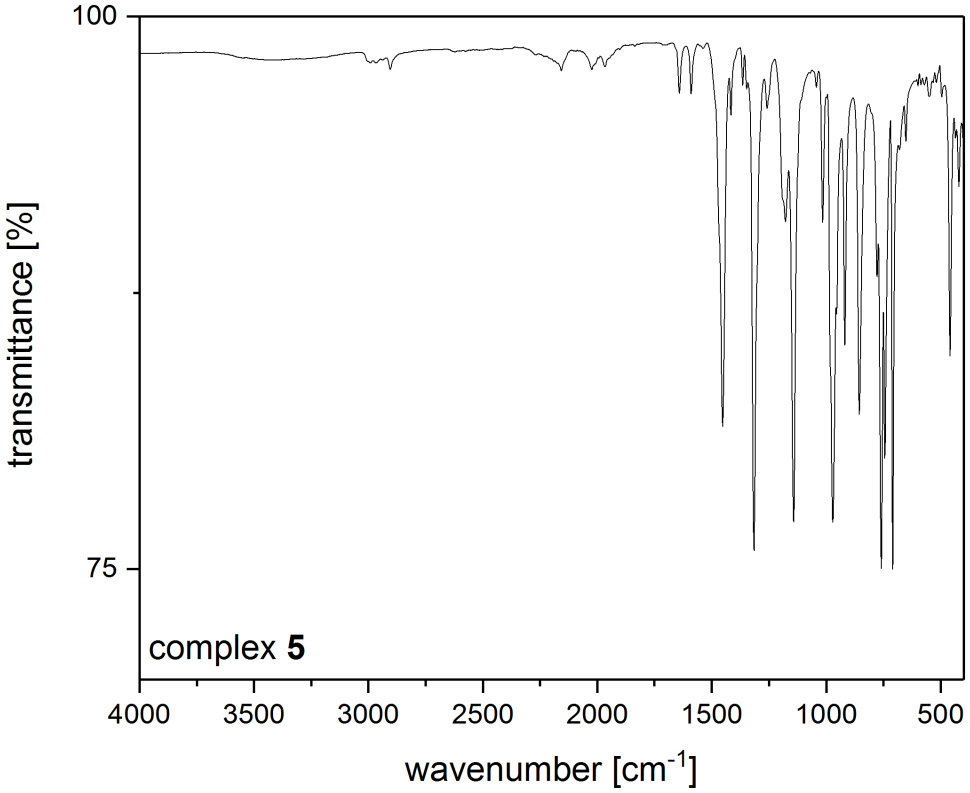

Fig. 4 IR spectrum of complex **5**. Recorded on a Varian FTIR-670 spectrometer with ATR sampling technique.

2. Crystallographic data

Table 1. Crystallographic data and structure refinement parameters.

Substance identification	**Complex (1b·THF)**	**Complex (2b·THF)**	**Complex (5)**
CCDC	1846360	1846358	1846359
Empirical formula	$C_{11}H_{12}F_3O_4Re$	$C_{11}H_{12}F_3O_5Re$	$C_9H_{18}NO_3Re$
Fw [g mol^{-}]	451.47	467.42	374.45
T [K]	123(1)	123(1)	123(1)
Crystal system	triclinic	monoclinic	orthorhombic
Space group	*P* -1	*C* 2/c	*P n m a*
a [Å]	6.6339(6)	16.0247(4)	10.2640(3)
b [Å]	9.8331(9)	6.6973(1)	13.0928(4)
c [Å]	10.7312(10)	24.9223(6)	8.2318(2)
α [deg]	106.871(4)	90	90
β [deg]	94.897(4)	91.1148(11)	90
γ [deg]	94.758(4)	90	90
V [Å^3]	663.17(11)	2674.21(10)	1106.23(5)
Z	2	8	4
Density (calcd) [g cm^{-3}]	2.261	2.322	2.248
μ [mm^{-1}]	9.204	9.139	10.968
F (000)	424	1760	712
Crystal size (mm^3)	0.13 × 0.24 × 0.32	0.20 × 0.23 × 0.28	0.30 × 0.34 ×0.41
ϑ range for data collection [deg]	2.00 to 25.53	1.63 to 25.49	2.92 to 36.46
Reflections collected	16656	26944	85048
Independent reflections	2446 [R(int) = 0.0266]	2496 [R(int) = 0.0320]	2782 [R(int) = 0.0581]
Data/restrains/parameters	2446 / 97 / 229	2496 / 0 / 182	2782 / 0 / 73
GOF on F^2	1.202	1.160	1.106
Final R1	R1 = 0.0203,	R1 = 0.013,	R1 = 0.0138
wR2 [I > 2σ(I)]	wR2 = 0.0491	wR2 = 0.0290	wR2 = 0.0290
Largest diff. peak and hole [eÅ^{-3}]	1.412 and -0.756	0.532 and -0.481	1.515 and -1.726

3. References

[1] APEX suite of crystallographic software. APEX 2 Version 2008.4. Bruker AXS Inc., Madison, Wisconsin, USA (**2008**).

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[3] G.M. Sheldrick, Sadabs (verion 2008/1), Program for Empirical Absorption Correction of Area Detector Data, University of Göttingen (Germany) (**2008**).

[4] G. M. Sheldrick, "SHELXL-97", University of Göttingen, Göttingen, Germany, **1998**.

[5] International Tables for Crystallography, Vol. C, Tables 6.1.1.4 (pp. 500–502), 4.2.6.8 (pp. 219–222), and 4.2.4.2 (pp. 193–199), A. J. C. Wilson (Ed.), Kluwer Academic Publishers, Dordrecht, The Netherlands, **1992**.

[6] A. L. Spek, "PLATON", A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, **2010**.