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Niklaus Marti, Bernhard Spingler, Frank Breher, and Roger Schibli*: Comparative Studies of Substitution Reactions of Rhenium(I) Dicarbonyl–Nitrosyl and Tricarbonyl Complexes in Aqueous Media.

Pages 6082−6091. The method of X-ray data collection was incorrectly reported. The last 13 lines of the first paragraph of the Experimental Section have been changed to the following to reflect the actual procedure.

Data collection for the X-ray structure determinations were performed on Stoe IPDS (**3**, **5**, and **6**) or Bruker APEX (**7**, **10**) diffractometer systems, respectively, by using graphite monochromated Mo K_α (0.71073 Å) radiation and a low-temperature device. In order to avoid decomposition, the single crystals were mounted in perfluoro ether oil on top of a glass fiber and then brought into the cold nitrogen stream of a low-temperature device so that the oil solidified. All calculations were performed on PCs by using the SHELXS-97[27] and SHELXL-97[28] software packages. All structures were solved by direct methods and successive interpretation of the difference Fourier maps, followed by full matrix least-squares refinement (against F^2). The collected intensities were corrected for Lorentz and polarization factors, and an absorption correction (numerical: **3**, **5**, and **6**; empirical: **7**, **10** (SADABS, version 2.03)) was applied. All atoms were refined anisotropically, except for three carbon atoms in **7**, which had to be refined using the ISOR restraint. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model. The carboxyl hydrogen atom in **7** could be located in a Fourier difference density map but was restrained to an ideal position during refinement, using the implemented HFIX riding model. Upon convergence, the final Fourier difference map of the X-ray structures showed no significant peaks. For **7** and **10**, some residual electron density was located close to the heavy atom rhenium (∼0.9−1 Å). Relevant data concerning crystallographic data, data collection, and refinement details are compiled in Table 1. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publications CCDC 281452−281456. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K. (Fax: (+44) 1223-336-033. E-mail: deposit@ccdc.cam.ac.uk. Internet: www.ccdc.cam.ac.uk/conts/retrieving.html. ORTEP plots were drawn with the program ORTEP-3 for Windows at a probability of 50%.[29]

In addition to the experimental change, some of the data in Tables 1−4 was updated with the correct data as follows.

Table 1. Crystal Data for Compounds **3**, **5**−**7**, and **10**

	3	**5**	**6**	**7**	**10**
formula	$C_{23}H_{24}N_6O_{13}Re_2$	$C_6H_5N_2O_7Re$	$C_{13}H_{10}N_3O_3Br_2Re$	$C_{13}H_{11}N_2O_7Re$	$C_{14}H_{10}N_2O_3BrRe$
fw	964.88	403.32	602.25	493.44	520.36
temp (K)	183(2)	183(2)	183(2)	200(2)	200(2)
cryst syst	monoclinic	triclinic	triclinic	orthorhombic	monclinic
space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	*Pbca*	$P2_1/c$
a, Å	14.607(1)	6.909(1)	9.823(1)	14.567(1)	12.749(1)
b, Å	8.057(1)	9.882(1)	10.094(1)	13.145(1)	13.302(1)
c, Å	24.721(1)	14.283(1)	12.534(1)	14.865(1)	9.011(1)
α (deg)		89.246(9)	108.679(9)		
β (deg)	107.117(5)	89.420(9)	111.992(9)		107.195(2)
γ (deg)		86.196(9)	95.426(10)		
V (Å^3)	2780.6(2)	973.01(12)	1058.82(15)	2846.4(4)	1459.8(2)
Z	4	4	2	8	4
D_c (g/cm^3)	2.31	2.75	2.13	2.303	2.37
μ (mm^{-1})	8.78	12.51	9.54	8.579	11.07
cryst dimens (mm)	0.33 × 0.28 × 0.11	0.13 × 0.08 × 0.03	0.29 × 0.22 × 0.18	0.20 × 0.08 × 0.06	0.08 × 0.06 × 0.04
F(000)	1832	744	640	1872	968
2θ range (deg)	5.84 ≤ 2θ ≤ 60.84	5.90 ≤ 2θ ≤ 56.56	5.54 ≤ 2θ ≤ 56.56	5.00 ≤ 2θ ≤ 49.42	4.54 ≤ 2θ ≤ 52.74
index range	−20 ≤ h ≤ 20	−8 ≤ h ≤ 9	−13 ≤ h ≤ 13	−17 ≤ h ≤ 17	−15 ≤ h ≤ 15
	−11 ≤ k ≤ 11	−13 ≤ k ≤ 13	13 ≤ k ≤ 13	−15 ≤ k ≤ 15	−16 ≤ k ≤ 16
	−35 ≤ l ≤ 35	−19 ≤ l ≤ 19	−16 ≤ l ≤ 16	17 ≤ l ≤ 13	11 ≤ l ≤ 11
no. of collected reflns	58 828	9756	19 274	14 688	12 965
no. of unique reflns	8302 (R_{int} = 0.0753)	4459 (R_{int} = 0.0404)	4872 (R_{int} = 0.1116)	2431 (R_{int} = 0.0807)	2983 (R_{int} = 0.0458)
no. of params/restraints	399/0	289/0	244/2	209/18	190/0
GOF on F^2	1.089	0.964	1.097	1.168	1.234
R1/wR2[a] (%)	4.05/11.07	6.76/16.27	7.30/17.36	4.95/9.52	4.46/8.66
max/min residual electron density, e/Å^3	3.847/−3.616	2.253/−1.866	2.410/−1.802	2.263/−2.706	1.560/−1.839

[a] $R1 = \sum||F_o| - |F_c||/\sum F_o$; $wR2 = \{[\sum w(F_o - F_c)^2]/\sum wF_o^2]^{1/2}$.

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Table 2. Bond Lengths (Å) and Angles (deg) of Complexes **3** and **7** with Esd's in Parentheses

[Re(L^1)(CO)(NO)] (**3**)		[Re(L^1)(CO)$_3$] (**7**)	
Re(1)−N(1)	1.781(5)	Re(1)−C(12)	1.90(1)
Re(1)−C(1)	1.941(5)	Re(1)−C(11)	1.93(1)
Re(1)−O(3)	2.105(3)	Re(1)−C(13)	1.90(1)
Re(1)−O(5)	2.025(4)	Re(1)−O(1)	2.132(7)
Re(1)−N(3)	2.118(4)	Re(1)−N(1)	2.132(7)
Re(1)−N(2)	2.159(4)	Re(1)−N(2)	2.241(8)
C(1)−O(1)	1.151(6)	C(11)−O(11)	1.12(1)
C(12)−O(12)	1.09(1)	C(13)−O(13)	1.16(1)
N(1)−O(2)	1.193(1)		
N(1)−Re(1)−C(1)	93.3(2)	C(12)−Re(1)−C(11)	88.9(4)
N(1)−Re(1)−O(5)	179(1)	C(12)−Re(1)−O(1)	171.7(3)
N(1)−Re(1)−O(3)	94.1(1)	C(12)−Re(1)−C(13)	87.2(5)
N(1)−Re(1)−N(3)	93.7(1)	C(12)−Re(1)−N(1)	97.6(4)
N(1)−Re(1)−N(2)	99.2(1)	C(12)−Re(1)−N(2)	93.5(4)
C(1)−Re(1)−N(2)	167.5(2)	C(11)−Re(1)−N(2)	170.9(4)
O(1)−C(1)−Re(1)	175.6(5)	O(11)−C(11)−Re(1)	176.3(9)
O(2)−N(1)−Re(1)	177.8(4)	O(12)−C(12)−Re(1)	176(1)
		O(14)−C(13)−Re(1)	179(1)
C(11)−N(3)−Re(1)	127.6(3)	C(5)−N(1)−Re(1)	126.0(6)
C(7)−N(3)−Re(1)	113.1(3)	C(1)−N(1)−Re(1)	115.9(7)

Table 3. Bond Lengths (Å) and Angles (deg) of Complex **5**

Re(1)−N(1)	1.885(9)	Re(1)−N(2)	2.172(7)
Re(1)−C(1)	1.946(9)	C(1)−O(1)	1.11(1)
Re(1)−C(2)	2.01(1)	C(2)−O(2)	1.10(1)
Re(1)−O(4)	2.050(6)	N(1)−O(3)	1.13(1)
Re(1)−O(6)	2.081(6)		
N(1)−Re(1)−C(1)	90.9(4)	N(1)−Re(1)−N(2)	97.8(4)
N(1)−Re(1)−C(2)	90.2(4)	O(1)−C(1)−Re(1)	177.0(8)
C(1)−Re(1)−C(2)	89.7(4)	O(2)−C(2)−Re(1)	178(1)
N(1)−Re(1)−O(4)	176.9(4)	O(3)−N(1)−Re(1)	176(1)
N(1)−Re(1)−O(6)	96.4(4)		

Table 4. Bond Lengths (Å) and Angles (deg) of Complexes **6** and **10** with Esd's in Parentheses

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[ReBr(L^4)(CO)$_2$(NO)]Br (**6**)		[ReBr(L^4)(CO)$_3$] (**10**)	
Re(1)−C(16)	2.018(7)	Re(1)−C(100)	1.98(1)
Re(1)−C(14)	2.030(7)	Re(1)−C(200)	1.949(9)
Re(1)−N(18)	1.784(8)	Re(1)−C(300)	1.880(8)
Re(1)−N(1)	2.198(6)	Re(1)−N(1)	2.192(7)
Re(1)−N(13)	2.179(6)	Re(1)−N(2)	2.198(6)
Re(1)−Br(2)	2.54(1)	Re(1)−Br(1)	2.588(1)
C(16)−O(17)	1.099(9)	C(100)−O(100)	1.05(1)
C(14)−O(15)	1.10(1)	C(200)−O(200)	1.08(1)
N(18)−O(19)	1.17(1)	C(300)−O(300)	1.140(9)
C(14)−Re(1)−N(1)	173.2(3)	C(200)−Re(1)−N(1)	172.9(3)
C(16)−Re(1)−N(13)	173.5(3)	C(100)−Re(1)−N(2)	175.8(3)
N(18)−Re(1)−N(1)	95.6(3)	C(300)−Re(1)−N(1)	96.5(3)
N(18)−Re(1)−N(13)	97.0(3)	C(300)−Re(1)−N(2)	94.1(3)
N(18)−Re(1)−Br(2)	172.6(2)	C(300)−Re(1)−Br(1)	177.9(2)
N(1)−Re(1)−N(13)	83.6(2)	N(1)−Re(1)−N(2)	83.0(2)
C(6)−C(7)−C(8)	114.6(6)	O(5)−C(6)−C(7)	113.3(7)
O(17)−C(16)−Re(1)	179.1(8)	O(100)−C(100)−Re(1)	177.9(8)
O(15)−C(14)−Re(1)	179.3(9)	O(200)−C(200)−Re(1)	177.6(8)
O(19)−N(18)−Re(1)	174.5(6)	O(300)−C(300)−Re(1)	176.3(7)
Re(1)−N(1)−C(6)−C(7)	4(1)	Re(1)−N(1)−C(5)−C(6)	8(1)
Re(1)−N(13)−C(8)−C(7)	0(1)	Re(1)−N(2)−C(7)−C(6)	4(1)

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