Supplementary Material to the paper

$[TcCl_4(H_2O)_2]$ and $[Cl_3(H_2O)_2TcOTc(H_2O)_2Cl_3]$

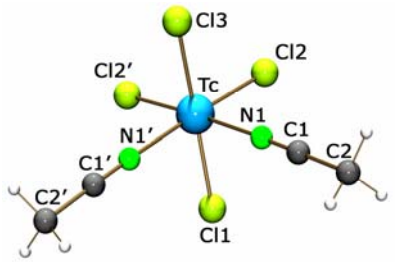
–

Two Molecular Intermediates of the Hydrolysis of Technetium(IV)

*Eda Yegen, Adelheid Hagenbach and Ulrich Abram**

Freie Universität Berlin, Institut für Chemie, Fabeckstr. 34-36, 14195 Berlin, Germany.

Table S1: Bond lengths /Å and angles /° in $[TcCl_4(CH_3CN)_2]$



Tc(1)-N(1)	2.123(5)		N(1)-C(1)	1.121(7)
Tc(1)-Cl(1)	2.323(2)		C(1)-C(2)	1.450(9)
Tc(1)-Cl(2)	2.2787(16)		C(10)-C(11)	1.77(3)
Tc(1)-Cl(3)	2.308(2)		C(11)-N(11)	1.16(3)
N(1)-Tc(1)-N(1)#1	88.1(3)		N(1)-Tc(1)-Cl(2)#1	176.83(13
N(1)-Tc(1)-Cl(2)	88.84(13)		Cl(2)#1-Tc(1)-Cl(2)	94.17(9)
N(1)-Tc(1)-Cl(3)	87.31(14)		Cl(2)-Tc(1)-Cl(3)	93.49(6)
N(1)-Tc(1)-Cl(1)	86.29(14			
Cl(2)-Tc(1)-Cl(1)	92.57(6)		Cl(3)-Tc(1)-Cl(1)	171.09(9)
C(1)-N(1)-Tc(1)	178.0(5		N(1)-C(1)-C(2)	179.5(7)
N(11)-C(11)-C(10)	177(2)			

Symmetry transformations used to generate equivalent atoms: #1 x,-y+3/2,z

Figure S1: Packing diagram of $[TcCl_4(CH_3CN)_2] \cdot CH_3CN$

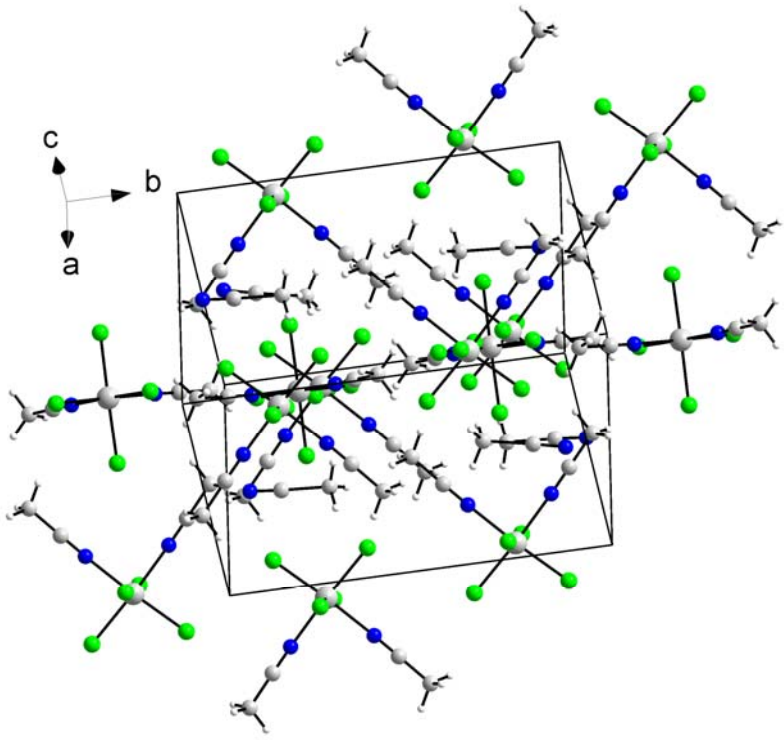
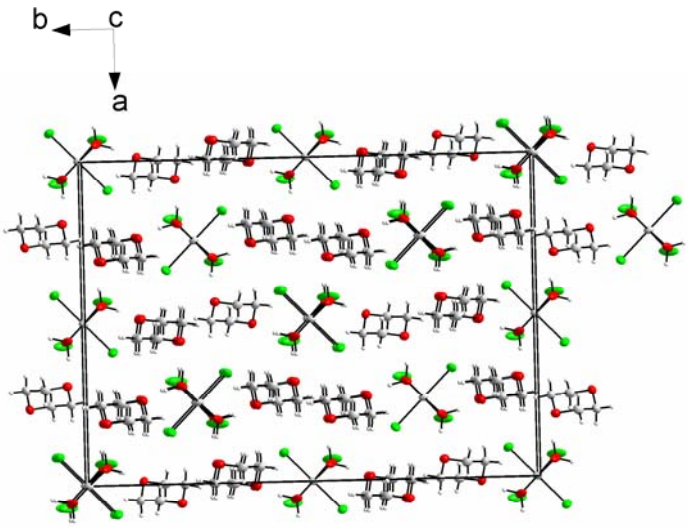


Figure S2: a) Cell plot of $[TcCl_4(H_2O)_2] \cdot 2$dioxane and b) depiction of the direct environment of the complex molecule

a)



b)

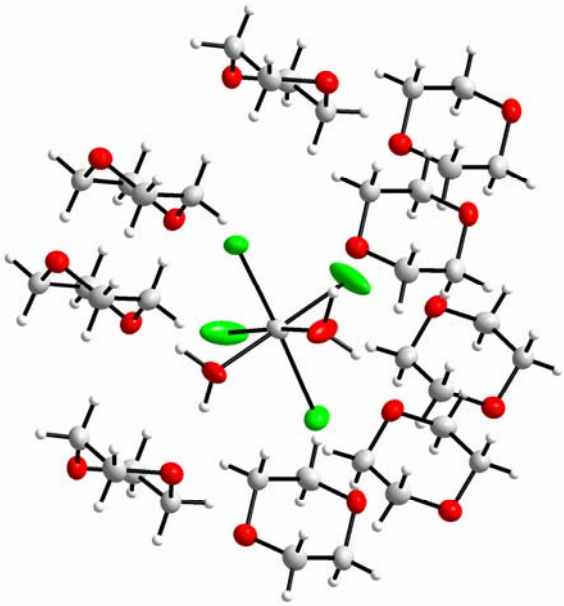
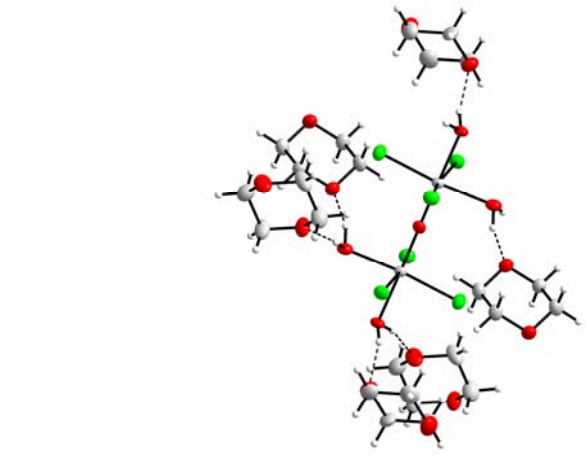


Table S2: Hydrogen bonds in [{$TcCl_3(H_2O)_2$}O] · 6dioxane



D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(20)-H(20A)...O(14)#2	0.96	1.77	2.706(6)	164.2
O(20)-H(20B)...O(21)	0.97	1.81	2.711(5)	153.1
O(30)-H(30A)...O(1)	0.97	1.70	2.632(5)	162.5
O(30)-H(30B)...O(11)	0.96	1.79	2.708(6)	157.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 x,y,z+1

Figure S3: Packing diagram of in [{$TcCl_3(H_2O)_2$}O] · 6dioxane