Table S1. Crystal Data and Structure Refinement for complexes **2a**, **3** and **10**.

Complex	**2a**	**3**	**10**
Empirical formula	$C_{46}\ H_{86}\ N_{10}\ Nb_2\ O$	$C_{25}\ H_{49}\ N_6\ Nb$	$C_{27}\ H_{51}\ N_6\ Nb\ S_2$
Temperature (K)	260	260(2)	260(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Cryst. Syst.	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$
a (Å)	13.28(1)	22.658(5)	11.1088(4)
b (Å)	17.84(2)	9.502(2)	16.4664(6)
c (Å)	22.19(2)	17.340(4)	18.0246(7)
α (deg)	90	90	90
β (deg)	90.39(2)	128.29(1)	91.968(2)
γ (deg)	90	90	90
Volume (Å^3)	5257(9)	2930.4(11)	3295.2(2)
Z	4	4	4
Density (calcd) (g/cm^3)	1.240	1.194	1.243
Abs. coeff (mm^{-1})	0.477	0.432	0.516
F(000)	2088	1128	1312
Crystal size (mm^3)	0.26 x 0.21 x 0.11	0.36 x 0.21 x 0.18	0.23 x 0.19 x 0.15
Index ranges	$-17 \le h \le 16$ $-23 \le k \le 24$ $-30 \le l \le 30$	$-32 \le h \le 32$ $-12 \le k \le 13$ $-24 \le l \le 24$	$-15 \le h \le 15$ $-23 \le k \le 18$ $-24 \le l \le 25$
Reflections collected	43828	26779	27687
Independent reflections	13348 [R(int) = 0.2755]	8896 [R(int) = 0.0985]	10101 [R(int) = 0.0879]
Observed reflections	3932	4572	4106
Data/restraints/params.	13348 / 2 /576	8896 / 0 / 304	10101 / 0 / 339
Goodness-of-fit on F^2	0.849	0.943	0.937
Extinction coef		0.0061(4)	
Final R indices	R1 = 0.0838 wR2 = 0.1742	R1 = 0.0523 wR2 = 0.0940	R1 = 0.0690 wR2 = 0.1580
Largest diff peak hole (eÅ^{-3})	0.700 and -0.630	0.408 and -0.616	0.786 and -0.718