Table S1. Crystal Data and Structure Refinement for compounds **1a** and **3dH$_2$**.

Compound	**1a**	**3dH$_2$**
Empirical formula	C_{31} H_{42} Br N_4 Nb	C_{20} H_{36} N_6
Temperature (K)	260(2)	300(2)
Wavelength (Å)	0.71073	0.71073
Cryst. Syst.	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a (Å)	11.992(1)	9.648(1)
b (Å)	18.927(2)	16.467(1)
c (Å)	15.034(2)	8.442(1)
α (deg)	90	90
β (deg)	112.579(1)	98.015(5)
γ (deg)	90	90
Volume (Å^3)	3150.7(7)	1328.0(2)
Z	4	2
Density (calcd) (g/cm^3)	1.357	0.902
Abs. coeff (mm^{-1})	1.675	0.056
F(000)	1328	396
Crystal size (mm^3)	0.35 x 0.17 x 0.14	0.17 x 0.14 x 0.10
Index ranges	$-13 \le h \le 14$ $-22 \le k \le 22$ $-17 \le l \le 12$	$-11 \le h \le 11$ $-19 \le k \le 18$ $-10 \le l \le 10$
Reflections collected	20346	11614
Independent reflections	5509 [*R*(int) = 0.0913]	2354 [*R*(int) = 0.0651]
Observed reflections	3840	1244
Data/restraints/params.	5509 / 0 / 345	2354/ 1 / 126
Goodness-of-fit on F^2	0.873	0.921
Extinction coef		0.054(9)
Final *R* indices	R1 = 0.0348 wR2 = 0.0672	R1 = 0.0678 wR2 = 0.1809
Largest diff peak hole (eÅ^{-3})	0.332 and -0.529	0.176 and -0.213