Electronic Supporting information

Group 5 hydride and borohydride complexes supported by cyclopentadienyl-imido ligand sets

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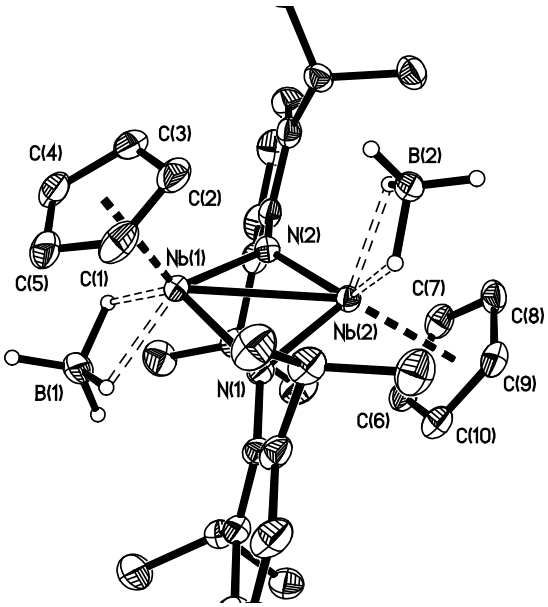

Figure S1. Molecular structure of $[CpNb(\mu\text{-}NAr)(\eta^2\text{-}BH_4)]_2$ (**6**). C-bound hydrogens omitted.

Table S1 Crystal and structure refinement data for $CpTa(NAr)H_2(PMe_3)$ (**5**), $[CpNb(\mu\text{-}NAr)(\eta^2\text{-}BH_4)]_2$ (**6**) and $[CpTa(\mu\text{-}NAr)(\eta^2\text{-}BH_4)]_2$ (**7**).

	5	**6**	**7**	
Empirical formula	$C_{20}H_{31}NNb_{0.18}PTa_{0.82}$	$C_{34}H_{52}B_2N_2Nb_2$	$C_{34}H_{52}B_2N_2Ta_2$	
Formula weight	481.53	696.22	872.32	
colour, habit	Yellow, block		Dark red, block	
Crystal size, mm^3	0.32x0.20x0.06	0.50 x 0.40 x 0.30	0.15 x 0.15 x 0.20	
Crystal system	monoclinic	monoclinic	monoclinic	
Space group	$P\,2_1/n$	$P\,2_1/n$	$P\,2_1/n$	
Unit cell dimensions:				
a, Å	8.8981(2)	10.6798(2)	10.6770(2)	
b, Å	14.3944(3)	20.3557(5)	20.3428(2)	
c, Å	16.7428(5)	15.7752(3)	15.7568(2)	
α, °	90.00	90.00	90	
β, °	97.847(2)	96.568(1)	96.4877(5)	
γ, °	90.00	90.00	90	
Volume, $Å^3$	2124.38(9)	3406.9(1)	3400.46(8)	
Z	4	4	4	
Density (calculated), g/cm^3	1.506	1.357	1.704	
Absorption coefficient, mm^{-1}	4.420	0.697	6.455	
F(000)	961	1448	1694□509	
Diffractometer	'Xcalibur, Sapphire3, Gemini ultra'	Bruker SMART	NONIUS KappaCCD	
Temperature, K	123(2)	100(2)	150(2)	
Radiation, (λ, Å)	(0.71073) Mo K_α	(0.71073) Mo K_α	(0.71073) Mo K_α	
2θ range for data collection, °	2.71 to 30.00	1.64 to 27.00	5.0 to 27.5	
Index ranges	$-12 \le h \le 12$, $-20 \le k \le 19$, $-23 \le l \le 23$	$-13 \le h \le 13$, $-22 \le k \le 26$, $-20 \le l \le 20$	$-13 \le h \le 13$, $0 \le k \le 26$, $0 \le l \le 20$	
Reflections collected	29002	22730	55248	
Independent reflections	4869 [R(int) = 0.0666]	7437 [R(int) = 0.0504]	7965 [R(int) = 0.052]	
Absorption correction	multi-scan	semi-empirical from equivalents	semi-empirical from equivalents	
Max. transmission	0.56437	0.51133	0.27	
Min. transmission	1.00000	0.63503	0.38	
Refinement method	full-matrix least-squares on F^2 (SHELXTL-Plus)	full-matrix least-squares on F^2 (SHELXTL-Plus)	full-matrix least-squares on F (SIR92)	
Data / restraints / parameters	6190/0/98	7437 / 0 / 569	5841/8/385	
Goodness-of-fit on F^2 (**5** and **6**) or F (**7**)	1.072	1.135	1.037	
Final R indices [$I>2\sigma(I)$] (**5** and **6**) or [$I>3\sigma(I)$] (**7**)	R_1 = 0.0513, wR_2 = 0.1236	R_1 = 0.0348, wR_2 = 0.0802	R_1 = 0.0256 , R_w = 0.0294	
R indices (all data)	R_1 = 0.0700, wR_2 = 0.1326	R_1 = 0.0432, wR_2 = 0.0865	R_1 = 0.0407 , R_w = 0.0480	
Largest diff. peak and hole, $e.Å^{-3}$	3.89 and -1.42	0.95 and -0.61	1.40 and -1.54	