Supporting Information

New Volatile Tantalum Imido Precursors with Carboxamide Ligands

Jeong Min Hwang,[a] Sung Kwang Lee,[a,b] Sunyoung Shin,[a] Ji-Seoung Jeong,[a,b] Hae Sun Kim,[a,b] Ji Yeon Ryu,[a] Taeyong Eom,[a] Bo Keun Park,[a] Chang Gyoun Kim,[a] and Taek-Mo Chung*[a]

[a] Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea

[b] Department of Chemistry and Department of Energy Science, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon-si, Gyenggi-do 16419, Republic of Korea

Figure S1. H-NMR spectrum of Tantalum Complex **1**. $TaCl_2(N^tBu)(py)(edpa)$ (C_6D_6, 500 MHz, R.T.)

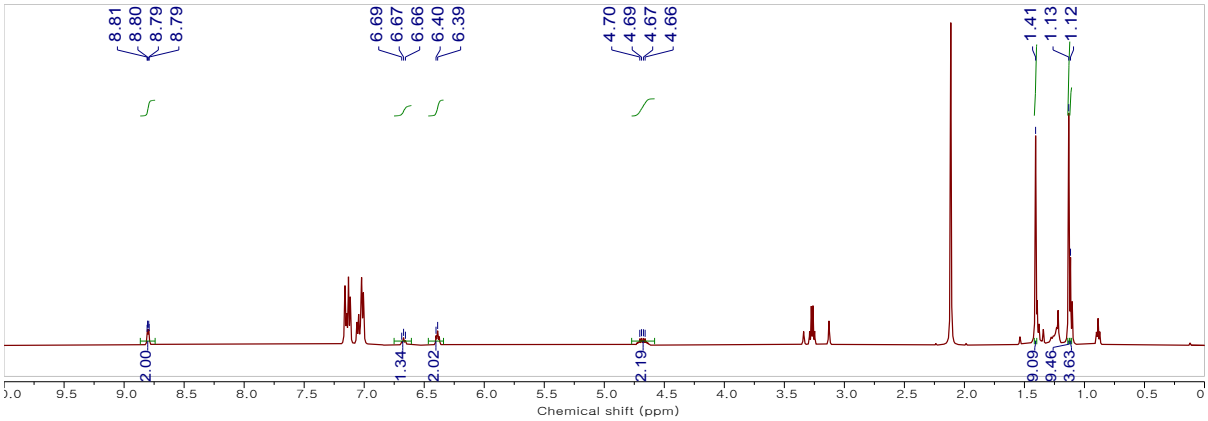

Figure S2. H-NMR spectrum of Tantalum Complex **2**. $TaCl(N^tBu)(edpa)_2$ (C_6D_6, 500 MHz, R.T.)

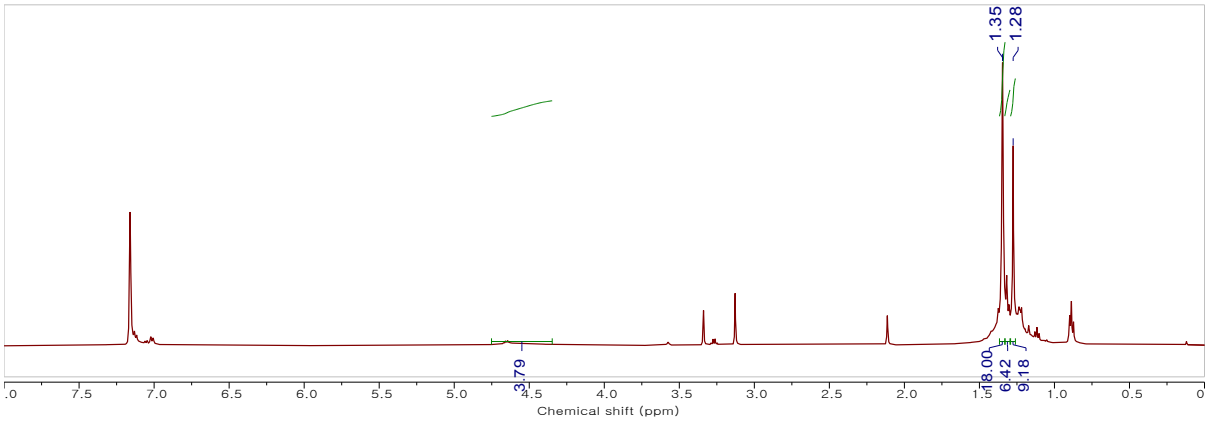

Figure S3. H-NMR spectrum of Tantalum Complex **3**. Ta(N^{t}Bu)(edpa)$_3$ (C_6D_6, 500 MHz, R.T.)

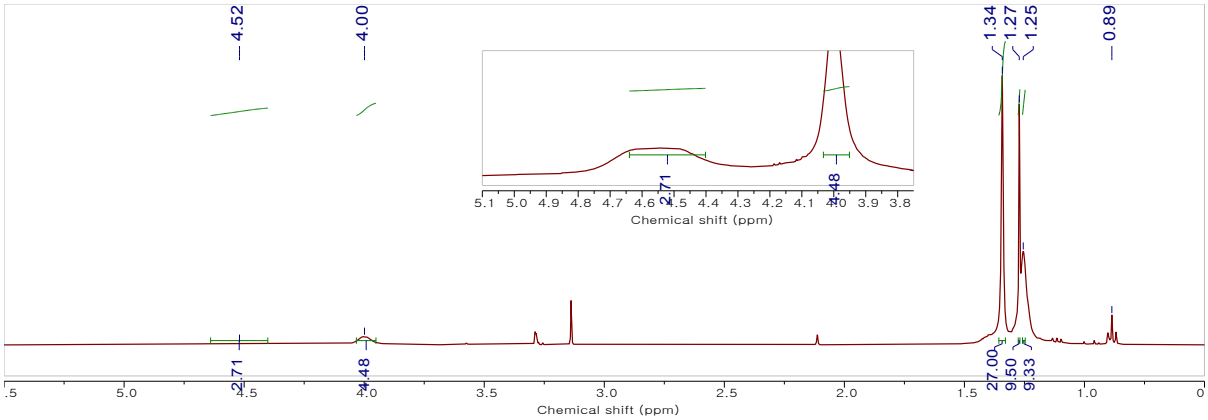

Figure S4. H-NMR spectrum of Tantalum Complex **4**. $TaCl_2$(N^{t}Bu)(py)(mdpa) (C_6D_6, 500 MHz, R.T.)

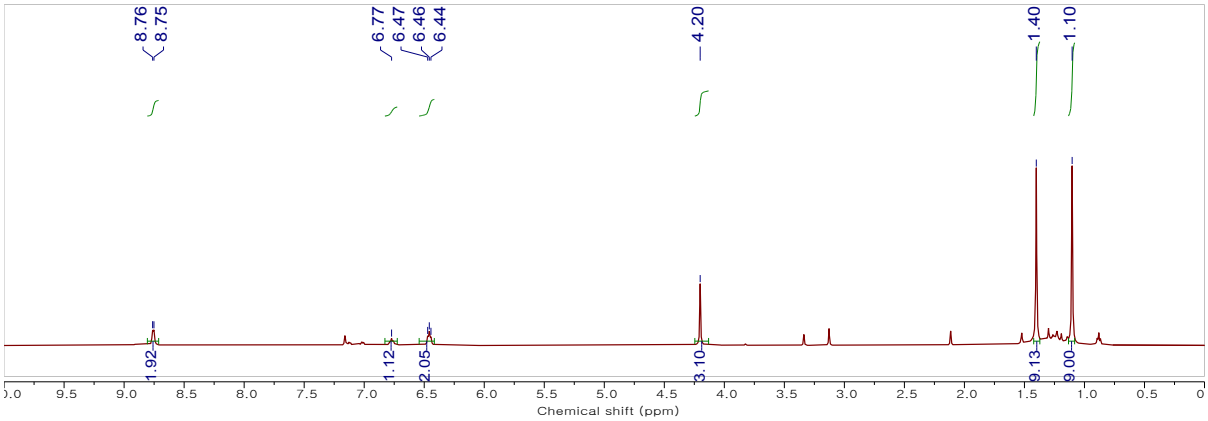

Figure S5. H-NMR spectrum of Tantalum Complex **5**. Ta(N^{t}Bu)(mdpa)$_3$ (C_6D_6, 500 MHz, R.T.)

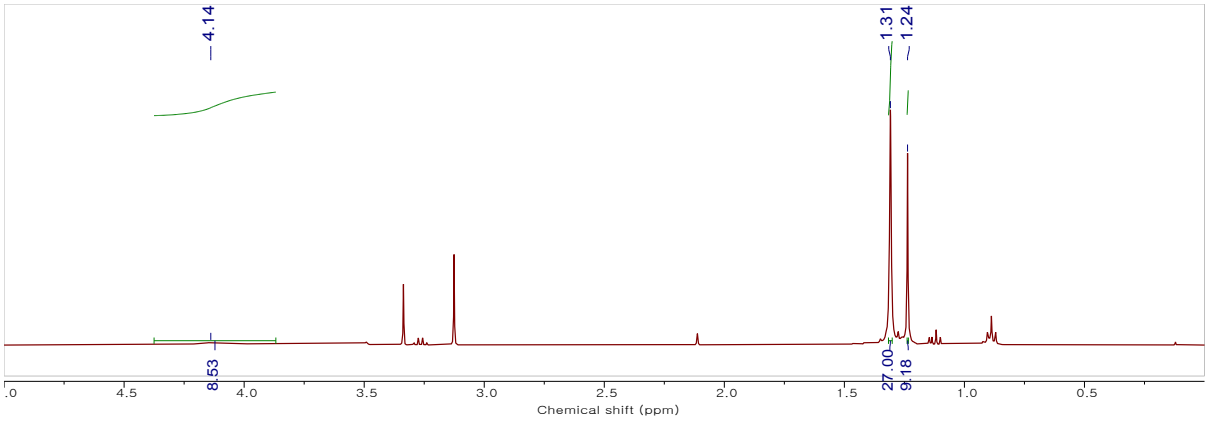

Figure S6. C-NMR spectrum of Tantalum Complex **1**. $TaCl_2(N^tBu)(py)(edpa)$ (C_6D_6, 500 MHz, R.T.)

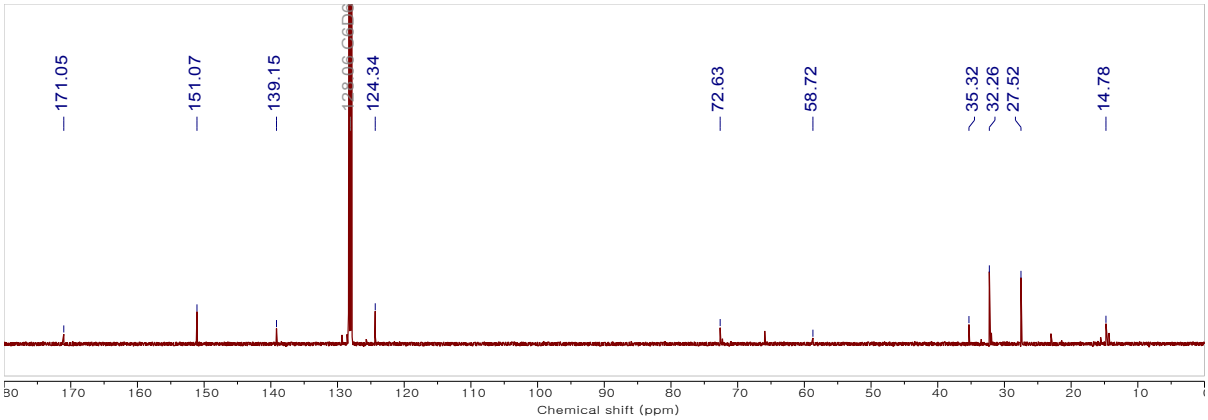

Figure S7. C-NMR spectrum of Tantalum Complex **2**. $TaCl(N^tBu)(edpa)_2$ (C_6D_6, 500 MHz, R.T.)

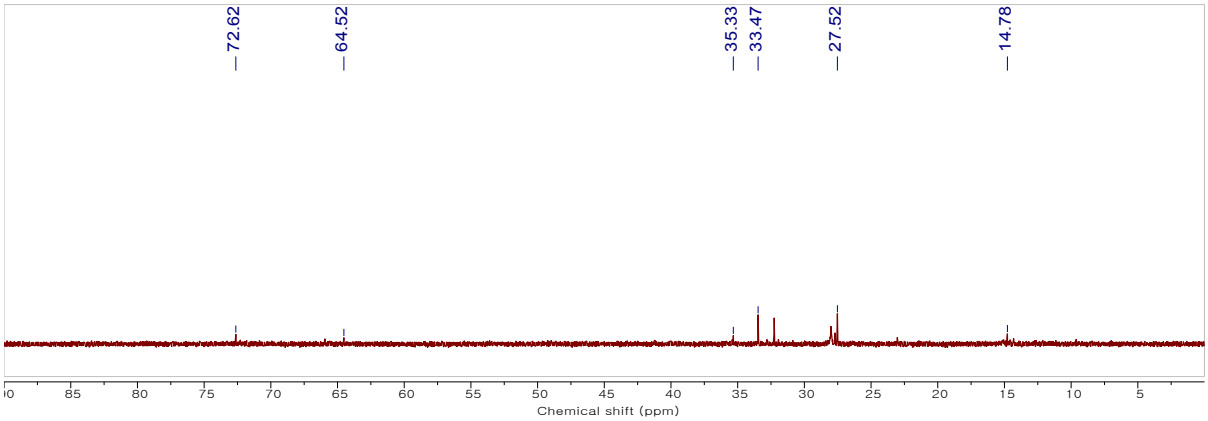

Figure S8. C-NMR spectrum of Tantalum Complex **3**. $Ta(N^tBu)(edpa)_3$ (C_6D_6, 500 MHz, R.T.)

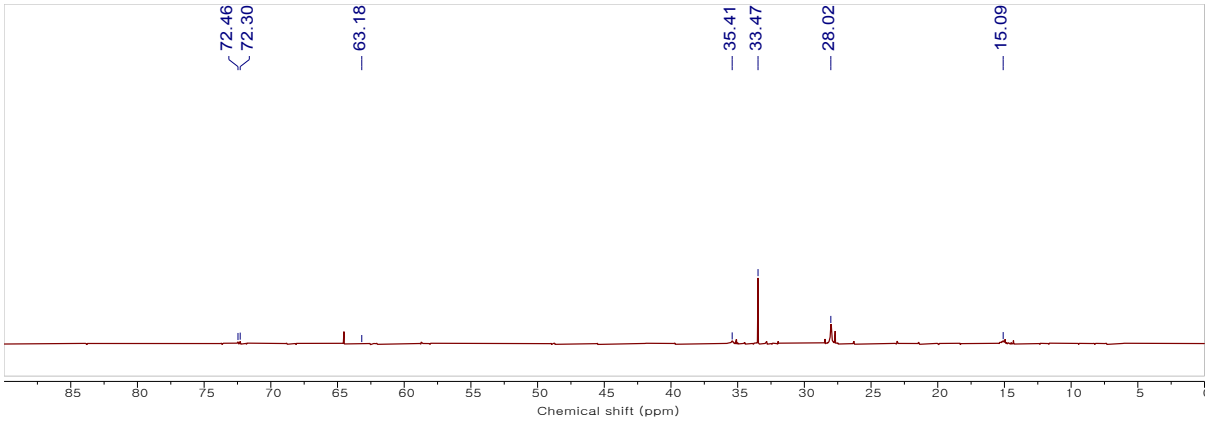

Figure S9. C-NMR spectrum of Tantalum Complex **4**. $TaCl_2(N^tBu)(py)(mdpa)$ (C_6D_6, 500 MHz, R.T.)

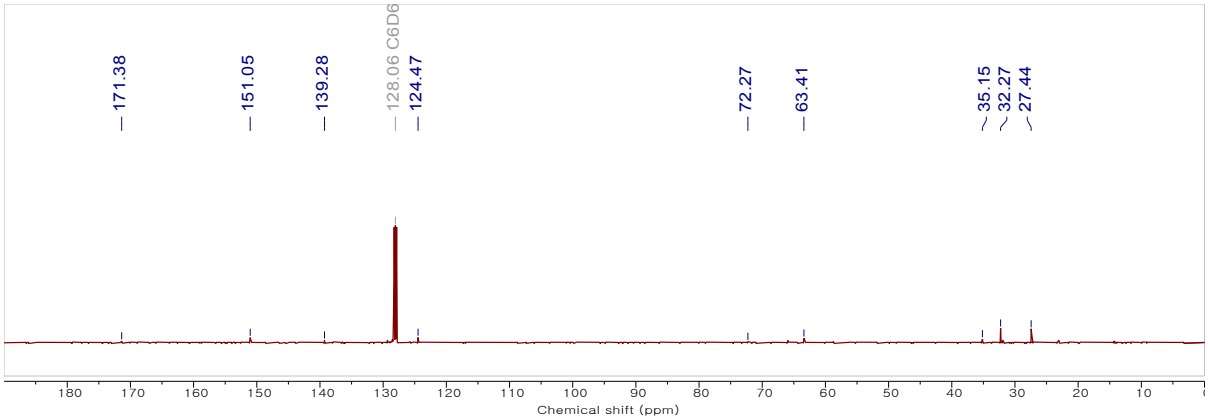

Figure S10. C-NMR spectrum of Tantalum Complex **5**. $Ta(N^tBu)(mdpa)_3$ (C_6D_6, 500 MHz, R.T.)

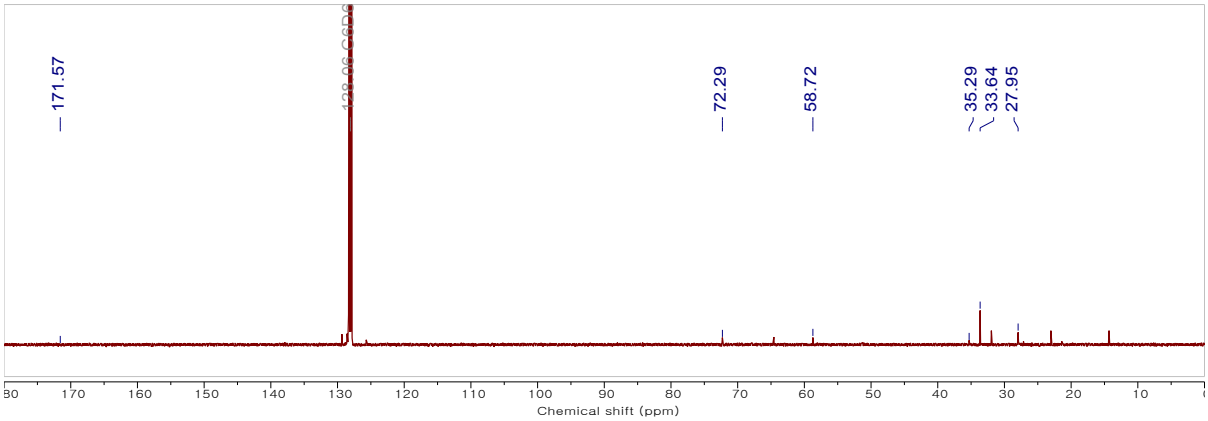

Figure S11. VT-NMR spectrum of complex **5** at room temperature, 5 °C and – 5 °C. (toluene d_8, 400 MHz)

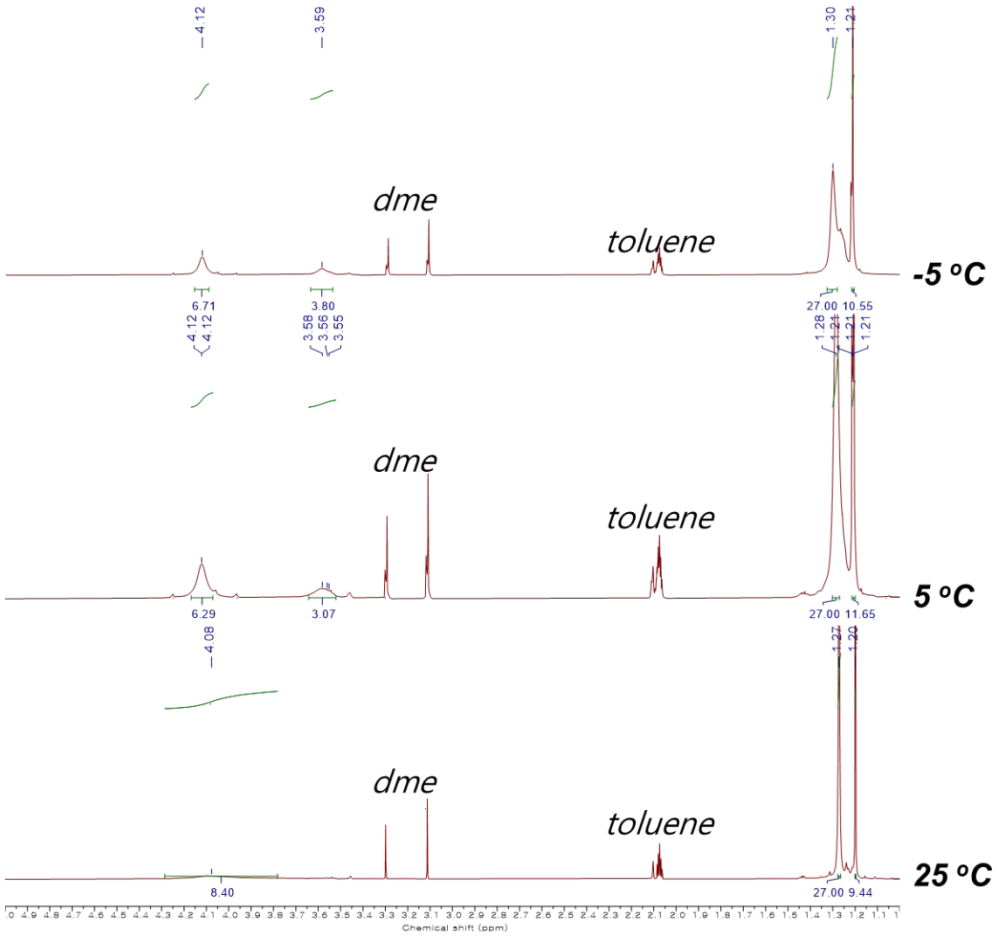

Figure S12. H-NMR spectrum of Tantalum mixture of complex **4, 5** and TaCl(N^{t}Bu)(mdpa)$_2$ (C_6D_6, 500 MHz, R.T.)

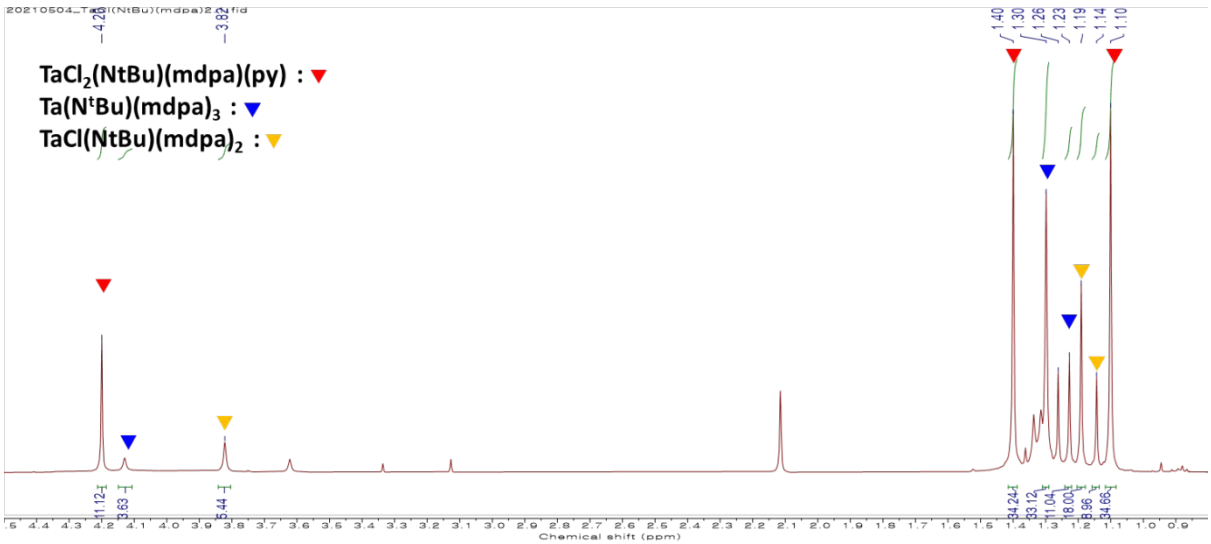

Figure S13. H-NMR spectrum of Tantalum Complex **6**. $[Ta(\mu_2-O)(edpa)_3]_2$ (C_6D_6, 500 MHz, R.T.)

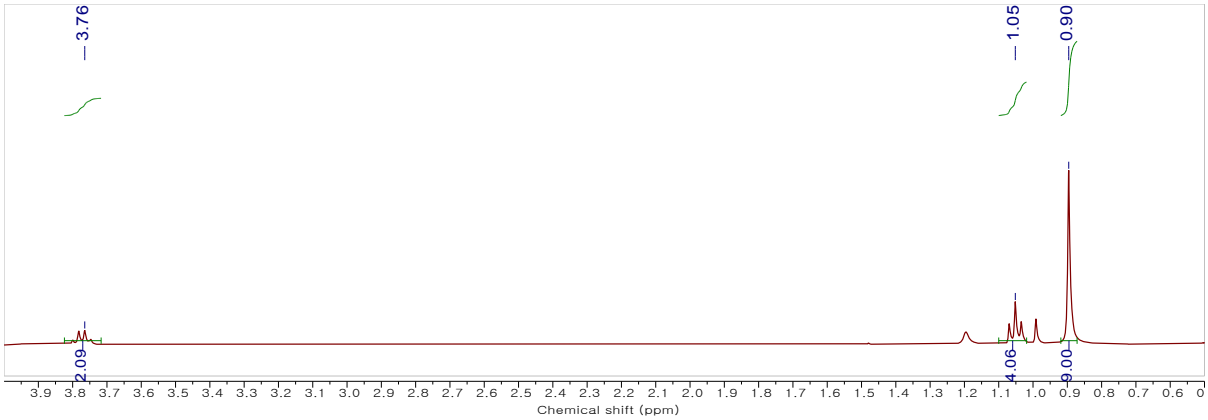

Figure S14. H-NMR spectrum of Tantalum Complex **7**. $[Ta(\mu_2-O)(mdpa)_3]_2$ (C_6D_6, 500 MHz, R.T.)

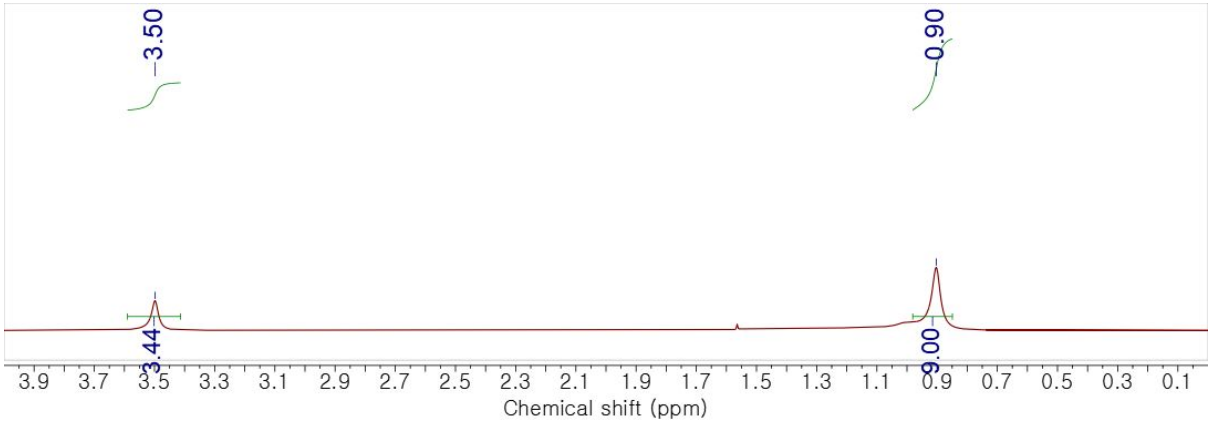

Figure S15. C-NMR spectrum of Tantalum Complex **6**. $[Ta(\mu_2-O)(edpa)_3]_2$ (C_6D_6, 500 MHz, R.T.)

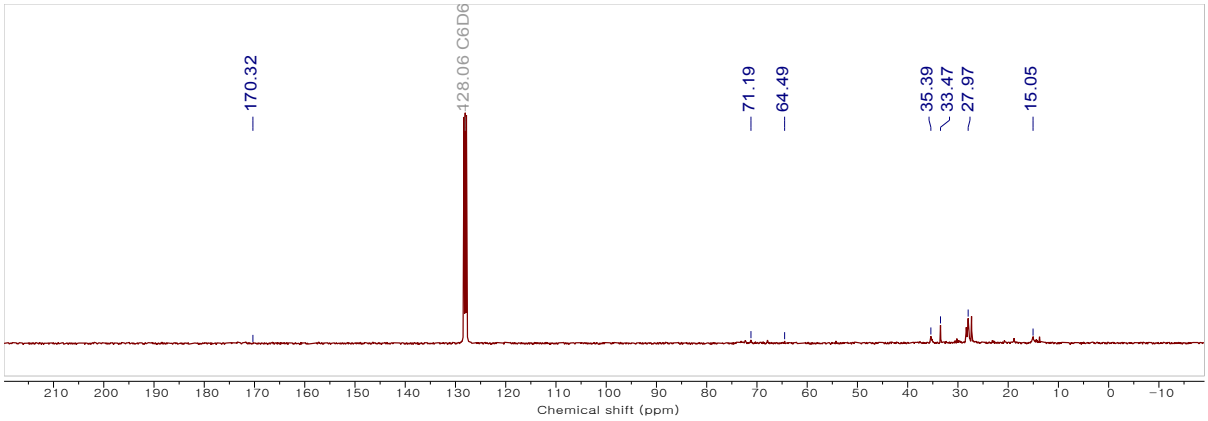

Figure S16. C-NMR spectrum of Tantalum Complex **7**. $[Ta(\mu_2{-}O)(mdpa)_3]_2$ (C_6D_6, 500 MHz, R.T.)

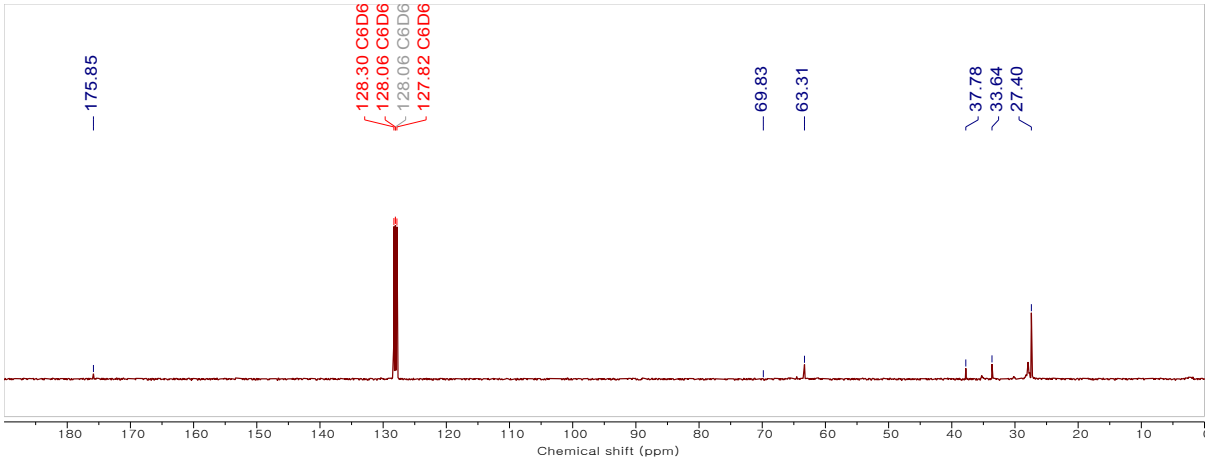

Table S1. X-ray data collection and structure refinement for **6**

	Complex **6**
Empirical formula	$C_{42}H_{84}N_6Ta_2O_{14}$
Formula weight	1259.05
Temperature (K)	100(1)
Crystal system	Monoclinic
Space group	C2/c
a (Å)	24.0890(12)
b (Å)	13.5356(7)
c (Å)	18.7495(9)
α (°)	90
β (°)	95.6888(17)
γ (°)	90
V (Å^3)	105.603(2)
Z	4
ρ (Mg m^{-3})	1.420
μ (mm^{-1})	3.771
F(000)	2544
θ range (°)	1.943 – 26.000
No. of reflections collected	45001
No. of reflections independent	5737
No. of reflections with $I > 2\sigma(I)$	5737

$T_{maximum}$	0.75
$T_{minimum}$	0.63
No. of parameters	302
Goodness-of-fit on F^2	1.093
R^a	0.0228
$wR2^b$	0.0564
Maximum in $\Delta\rho$ (e Å^{-3})	2.114
Minimum in $\Delta\rho$ (e Å^{-3})	-0.593

$^aR = \sum[|F_o| - |F_c|]/\sum|F_o|]$, $^bwR2 = \{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

Table S2. Selected bond lengths (Å) and bond angles (°) for complex 6.

Bond lengths (Å)			
Ta1-O1	2.0345(19)	Ta1-O7	1.9896(18)
Ta1-O2	2.274(2)	Ta1-O7A	1.8931(19)
Ta1-O3	2.031(2)	Ta1-Ta1A	3.0464(2)
Ta1-O4	2.323(2)		
Ta1-O5	1.9981(19)		
Ta1-O6	2.3916(19)		
Bond angles (°)			
O1-Ta1-O2	91.23(4)	O7-Ta1-O7A	92.5(3)
O3-Ta1-O4	103.20(7)	Ta1-O7-Ta1A	103.34(8)
O5-Ta1-O6	172.25(9)		