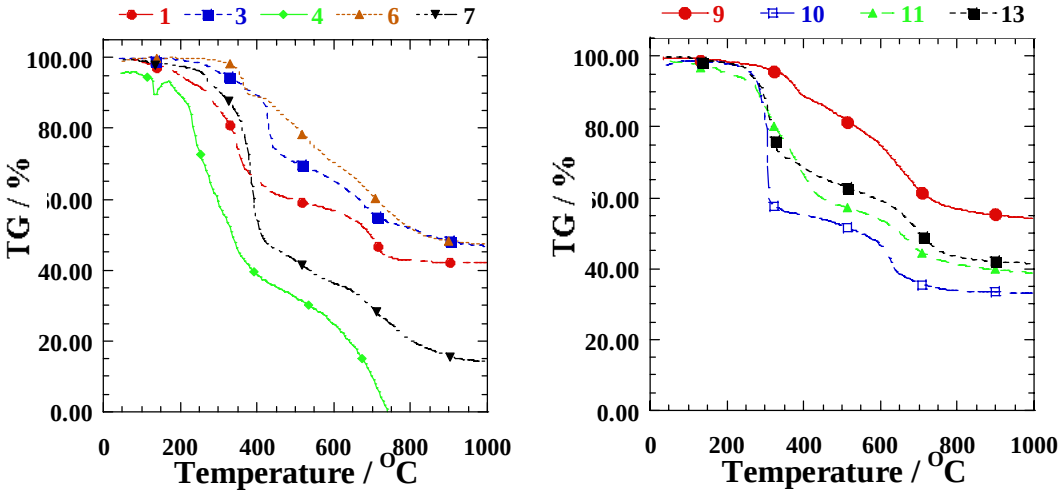

Figure S1 TGA curves of $MoO_2Cl_2L_2$-type complexes

Table S1 ^{1}H NMR spectroscopic data for complexes **1-13** and corresponding free ligands

Complex	$\delta_{py\text{-}H}$				substituted-group	Solvent
	$H^{3,3'}$	$H^{6,6'}$	$H^{4,4'}$	$H^{5,5'}$		
1	-	8.34(d,2H)	7.74(d,2H)	7.32(dd,2H)	1.89(s,6H,CH_3)	DMSO-d_6
$C_{12}H_{12}N_2$	-	8.23(d,2H)	7.52(d,2H)	7.1(dd,2H)	1.83(s,6H,CH_3)	DMSO-d_6
3	8.1(m,2H)	8.64(s,2H)	8.46(m,2H)	-	2.41(d,6H,CH_3)	DMSO-d_6
$C_{12}H_{12}N_2$	7.71(d,2H)	8.49(s,2H)	8.24(d,2H)	-	2.34(s,6H,CH_3)	DMSO-d_6
4	7.59(d,2H)	-	7.28(t,2H)	6.76(d,2H)	1.98(s,6H,CH_3)	DMSO-d_6
$C_{12}H_{12}N_2$	7.31(d,2H)	-	6.97(t,2H)	6.44(d,2H)	1.71(s,6H,CH_3)	DMSO-d_6
6	8.60(s,2H)	8.00(d,2H)	-	9.20(d,2H)	-	CD_3NO_2-d_3
$C_{10}H_6N_2Br_2$	8.50(d,2H)	7.62(dd,2H)	-	8.57(d,2H)	-	CD_3NO_2-d_3
7	8.13(d,2H)	9.44(d,2H)	8.40(d,2H)	-	-	CD_3NO_2-d_3
$C_{10}H_6N_2Br_2$	7.94(dd,2H)	8.62(d,2H)	8.21(d,2H)	-	-	CD_3NO_2-d_3
9	8.71(s,2H)	8.06(d,2H)	7.31(d,2H)	-	6.26(b,4H)	DMSO-d_6
$C_{10}H_{10}N_4$	7.91(s,2H)	7.86d(d,2H)	6.95(dd,2H)		5.33(b,4H)	DMSO-d_6
10	9.14(dd,2H)	10.23(s,2H)	8.94(d,2H)	-	-	CD_3NO_2-d_3
$C_{11}H_6N_2O$	8.78(d,2H)	9.51(d,2H)	8.73(dd,2H)	-	-	CD_3NO_2-d_3
11	9.96(s,2H)	8.88(dd,2H)	8.73(d,2H)	-	4.51(q,4H, CH_2), 1.44(t,6H, CH_3)	CD_3NO_2-d_3
$C_{14}H_{16}N_2O_4$	9.26(s,2H)	8.60(d,2H)	8.48(dd,2H)	-	4.46(q,4H, CH_2), 1.45(t,6H, CH_3)	CD_3NO_2-d_3

	$H^{6'}$	$H^{6''}$	$H^{2''}$	H^5	$H^{3,3'}$	$H^{4,4'}$	$H^{3''}$,$H^{4''}$,$H^{5''}$	$H^{5'}$	
12	8.74(s,1H)	8.62(d,1H)	8.08(s,1H)	8.37(s,1H)	8.25(d,2H)	8.04(s,2H)	7.54(m,3H)	7.48(d,2H)	DMSO-d_6
$C_{12}H_{12}N_2$	7.88(d,1H)	6.72(t,2H)		7.75(d,1H)	7.41(d,2H)	6.66(m,2H)	7.18(m,3H)	7.52(t,1H)	DMSO-d_6

	$H^{6,6'}$	$H^{3,3'}$	$H^{3''}$, $H^{5''}$	$H^{5,5'}$	$H^{4''}$	$H^{4,4'}$	
13	9.04(d,2H)	8.84(d,2H)	8.71(s,2H)	8.65(d,2H)	8.44(t,1H)	8.14(s,2H)	CD_3NO_2-d_3
$C_{15}H_{11}N_3$	8.70(m,4H)		8.50(d,2H)	8.01(m,2H)	8.07(m,1H)	7.46(m,2H)	CD_3NO_2-d_3