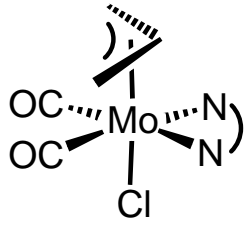
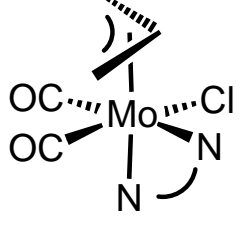
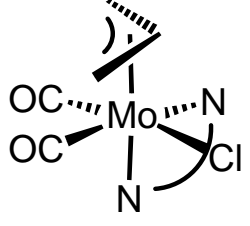


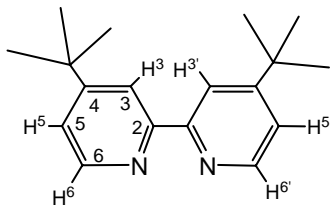
Electronic Supplementary Information

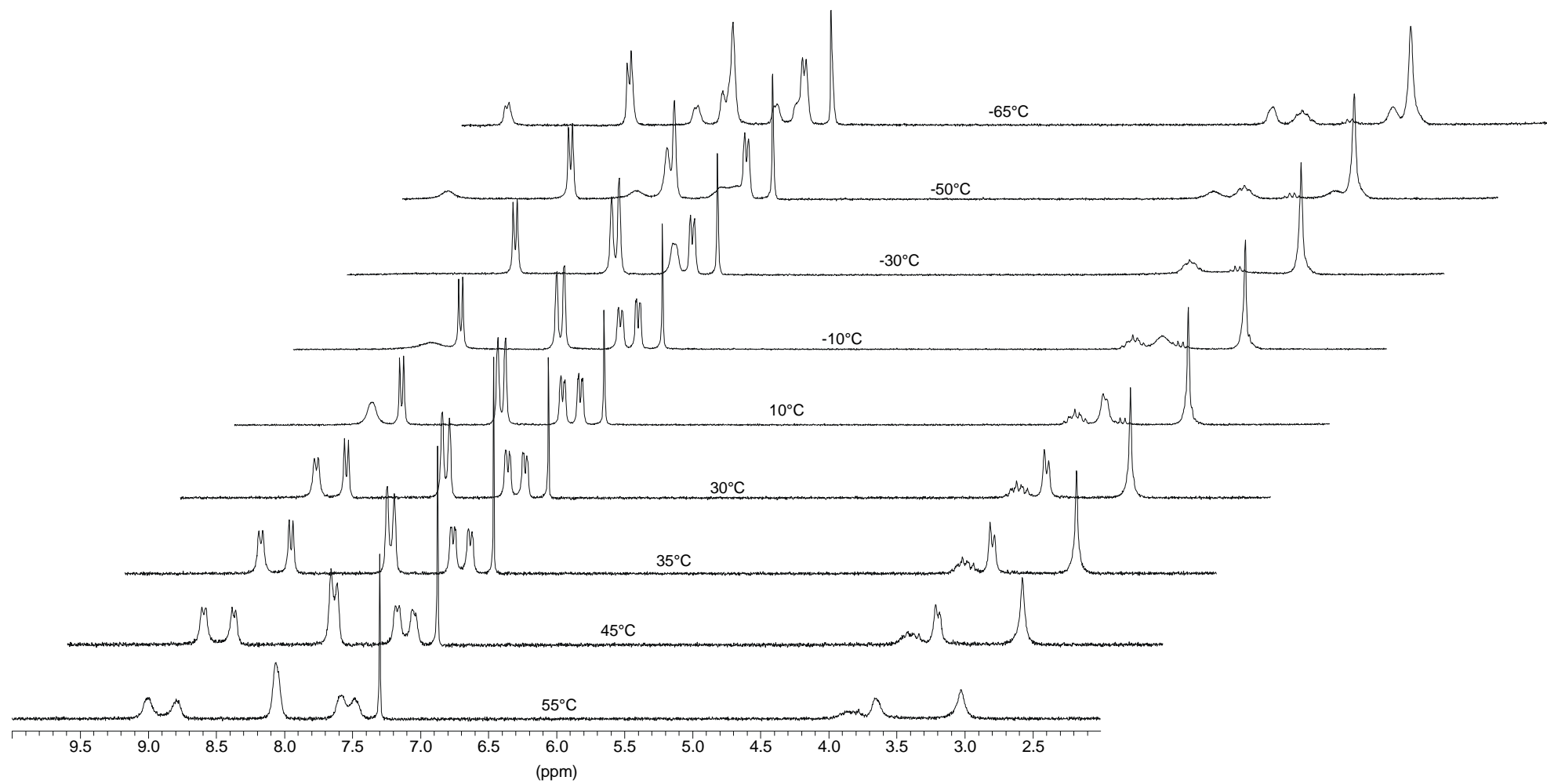
Experimental evidence supporting identification of 1

Appearance	red solid
Yield	75%
Formula	$C_{23}H_{29}ClMoN_2O_2$
Molecular Mass	496.88 g/mol
EA (%)	calc.: C 55.60; H 5.88; N 5.64; Cl 7.14 found: C 55.25; H 5.90; N 5.49; Cl 7.40
MS (FAB _{pos}) m/z [Frag.]	958 (7%) [$M^+ + 3 \text{ NBA}$], 498 (7%) [M^+], 464 (26%) [$M^+ - Cl$], 443 (100%) [$M^+ - t\text{Bu}$]
IR (KBr) [cm^{-1}]	2965 (m), 1938 (vs), 1849 (vs), 1612 (m), 1483 (m), 1409 (m), 1254 (w), 843 (w), 801 (m), 604 (w), 567 (m), 465 (m)
$^{13}\text{C}\{^1\text{H}\}$ -NMR (CDCl_3)(30°C):	226.33 (s, 2 C, CO), 226.16 (s, 2 C, CO), 163.26 (s, 2 C, $C^{2,2'}$), 163.23 (s, 2 C, $C^{2,2'}$), 153.96 (s, 2 C, $C^{4,4'}$), 153.60 (s, 2 C, $C^{4,4'}$), 152.22 (s, 2 C, $C^{6,6'}$), 151.53 (s, 2 C, $C^{6,6'}$), 124.02 (s, 2 C, $C^{5,5'}$), 123.73 (s, 2 C, $C^{5,5'}$), 119.26 (s, 2 C, $C^{3,3'}$), 119.02 (s, 2 C, $C^{3,3'}$), 73.13 (s, 1 C, C_m), 71.18 (s, 1 C, C_m), 68.37 (s, 2 C, C_t), 53.92 (s, 2 C, C_t), 35.79 (s, 2 C, C_{iso-Bu}), 35.77 (s, 2 C, C_{iso-Bu}), 30.77 (br, 12 C, C_{t-Bu}).

Temperature (°C)	30	-60		
 <p>A</p>	H _{t-Bu}	1.44 (s)	1.44 (s)	
	H _a	superposed by H _{t-Bu}	superposed by H _{t-Bu}	
	H _m	3.03 (br)	3.03 (br)	
	H _s	3.03 (br)	3.03 (br)	
	H ^{5,5'}	7.47 (d) ³ J _{H-H} = 5.00 Hz	7.47 (d) ³ J _{H-H} = 5.00 Hz	
	H ^{3,3'}	8.02 (s)	8.02 (s)	
	H ^{6,6'}	8.78 (d) ³ J _{H-H} = 5.80 Hz	8.78 (d) ³ J _{H-H} = 5.80 Hz	
 <p>B</p>	H _{t-Bu}	1.46 (s)	1.46 (br)	
	H _a	superposed by H _{t-Bu}	superposed by H _{t-Bu} 1.68 (br) ³ J _{H-H} = 9.22 Hz	
	H _m	3.83 (m)	3.83 (m)	
	H _s	3.65 (d) ³ J _{H-H} = 6.49 Hz	3.19 (br) 4.08 (br)	
	H ^{5,5'}	7.59 (d) ³ J _{H-H} = 5.00 Hz	7.70 (br) 7.55 (sh)	
	H ^{3,3'}	8.07 (s)	8.08 (br) 8.04 (sh)	
	H ^{6,6'}	9.00 (d) ³ J _{H-H} = 5.40 Hz	8.28 (br) 9.67 (br) ³ J _{H-H} = 3.41 Hz	
	 <p>C</p>			

Experimental evidence supporting identification of **2**

Appearance	red solid
Yield	44%
Formula	$C_{72}H_{114}F_6Mo_2N_4O_{26}S_2$
Molecular Mass	1821.69 g/mol
EA (%)	calc.: C 47.47; H 6.31; N 3.08 found: C 48.01; H 6.48; N 3.04
MS (FAB _{pos}) m/z [Frag.]	942 (6%) [$\{Mo({}^3-C_3H_5)(CO)_2(bipy^*)\}_2H_2O\}^+$], 463 (42%) [$\{Mo({}^3-C_3H_5)(CO)_2(bipy^*)\}^+$], 422 (31%) [$\{Mo(CO)_2(bipy^*)\}^+$], 405 (38%) [$\{Mo({}^3-C_3H_5)(bipy^*)\}^+$], 392 (17%) [$\{Mo(CO)(bipy^*)\}^+$], 362 (7%) [$\{Mo(bipy^*)\}^+$]
IR (KBr) [cm^{-1}]	3423 (m,br), 2955 (w), 2897 (w), 1944 (vs), 1854 (vs), 1615 (s), 1545 (m), 1474 (m), 1410 (m), 1553 (m), 1262 (vs), 1158 (m), 1103 (m), 1026 (s), 953 (m), 843 (m), 801 (m), 752 (m), 637 (vs), 567 (m), 509 (m)
1H -NMR (CDCl ₃)	9.07 (d, ${}^3J_{H-H} = 5.12$ Hz, 4 H, $\underline{H}^{6,6'}$), 8.05 (s, 4 H, $\underline{H}^{3,3'}$), 7.65 (d, ${}^3J_{H-H} = 5.12$ Hz, 4 H, $\underline{H}^{5,5'}$), 4.04 (m, 2 H, \underline{H}_m), 3.69 (br, 52 H, \underline{H}_s + 18-crown-6), 1.57 (d, ${}^3J_{H-H} = 7.85$ Hz, 4 H, \underline{H}_a), 1.46 (s, 36 H, \underline{H}_{t-Bu})
$^{13}C\{^1H\}$ -NMR (CDCl ₃)	225.97 (s, 4 C, CO), 164.79 (s, 4 C, $C^{2,2'}$), 154.14 (s, 4 C, $C^{4,4'}$), 152.16 (s, 4 C, $C^{6,6'}$), 124.30 (s, 4 C, $C^{5,5'}$), 119.18 (s, 4 C, $C^{3,3'}$), 73.89 (s, 2 C, C_m), 71.02 (s, 24 C, 18-crown-6), 61.00 (s, 4 C, C_t), 36.00 (s, 4 C, C_{iso-Bu}), 30.71 (s, 12 C, C_{Me})
	



$^1\text{H-NMR}$ in CDCl_3

Temperature dependent $^1\text{H-NMR}$ spectrum (200.13 MHz) of **1** in CDCl_3

Temperature dependent ^1H -NMR spectrum (200.13 MHz) of **1** in CD_2Cl_2

