

Electronic supplementary information

SYNTHESIS AND CHARACTERIZATION OF TRIS(ALKOXY) YTTRIUM AND SCANDIUM COMPLEXES COORDINATED BY SCHIFF-BASE LIGANDS

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Table S1. Crystal data and structure refinement parameters for complex **1**

	1
Empirical formula	C ₆₉ H ₉₀ N ₃ O ₆ Y
Formula Weight	1146.34 g/mol
<i>T</i> , K	120
Crystal System	Monoclinic
Space Group	<i>P</i> 2 ₁ / <i>n</i>
Unit Cell Dimensions	a = 12.538(9)Å b = 18.583(13)Å c = 30.54(2)Å α = 90° β = 99.552(15)° γ = 90°
<i>V</i> , Å ³	7016(9)
<i>Z</i>	4
<i>d</i> _{calc} , Mg/m ³	1.085
μ, mm ⁻¹	0.878
<i>F</i> ₀₀₀	2448
Crystal Size, mm	0.25x0.15x0.03
θ Range for Data Collection, °	1.673-24.997
Index Ranges	-14 ≤ h ≤ 14, -22 ≤ k ≤ 22, -36 ≤ l ≤ 36
Reflns Collected	82567
Independent Reflns	12309
Observed Reflns	5028
Completeness to θ, %	99.8
Parameters	737
<i>GOF</i> on <i>F</i> ²	0.958
Final <i>R</i> Indices (<i>I</i> > 2σ(<i>I</i>))	R ₁ = 0.00828, wR ₂ = 0.1754
<i>R</i> Indices (all data)	R ₁ = 0.2040, wR ₂ = 0.2359
Largest Diff Peak and Hole, e/Å ³	0.576 and -0.589

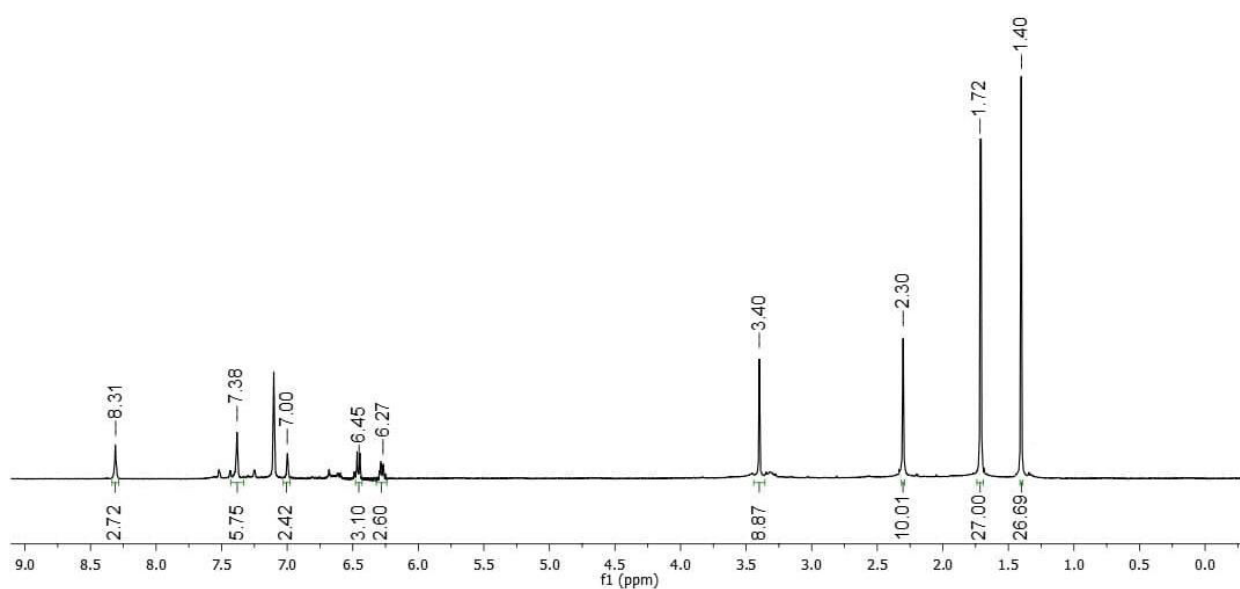


Figure S1. ^1H NMR spectrum (400 MHz, benzene- d_6 , 293 K) of **1**

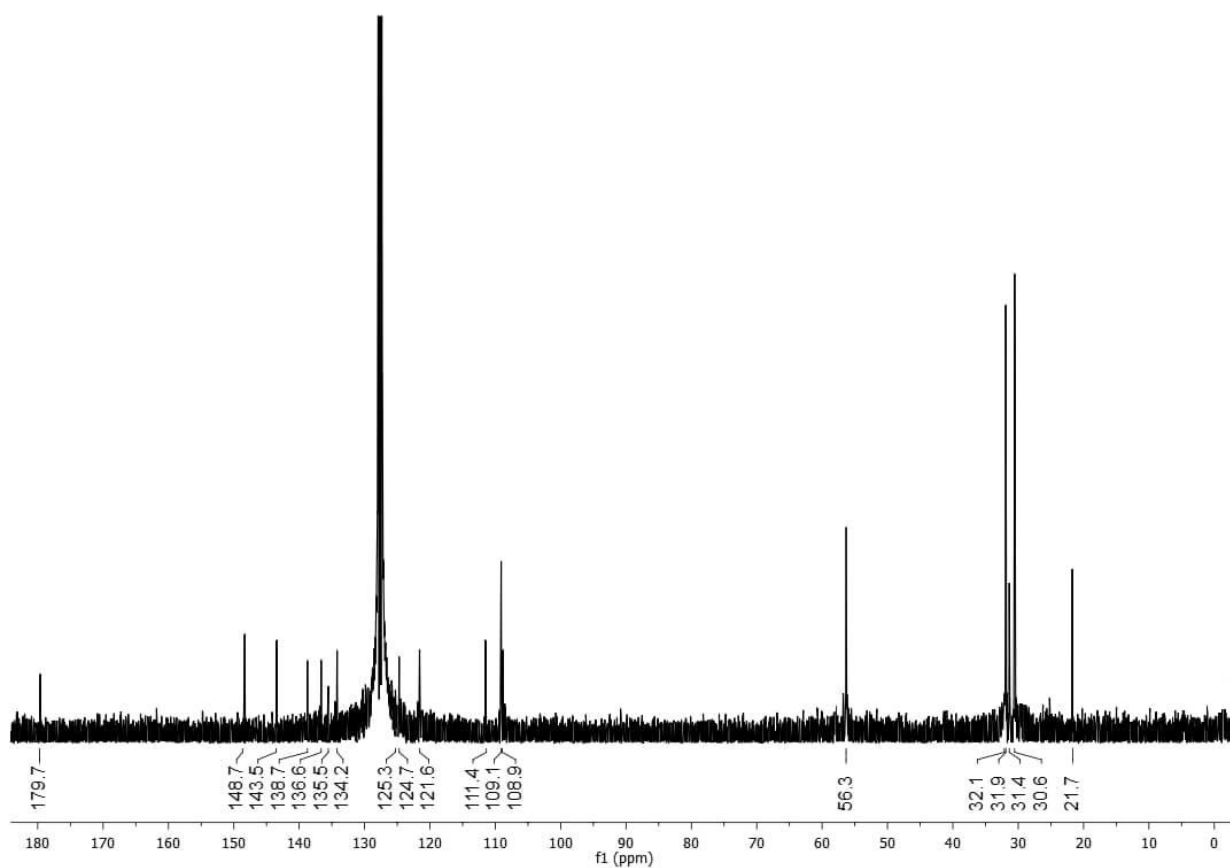


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, benzene- d_6 , 293 K) of **1**

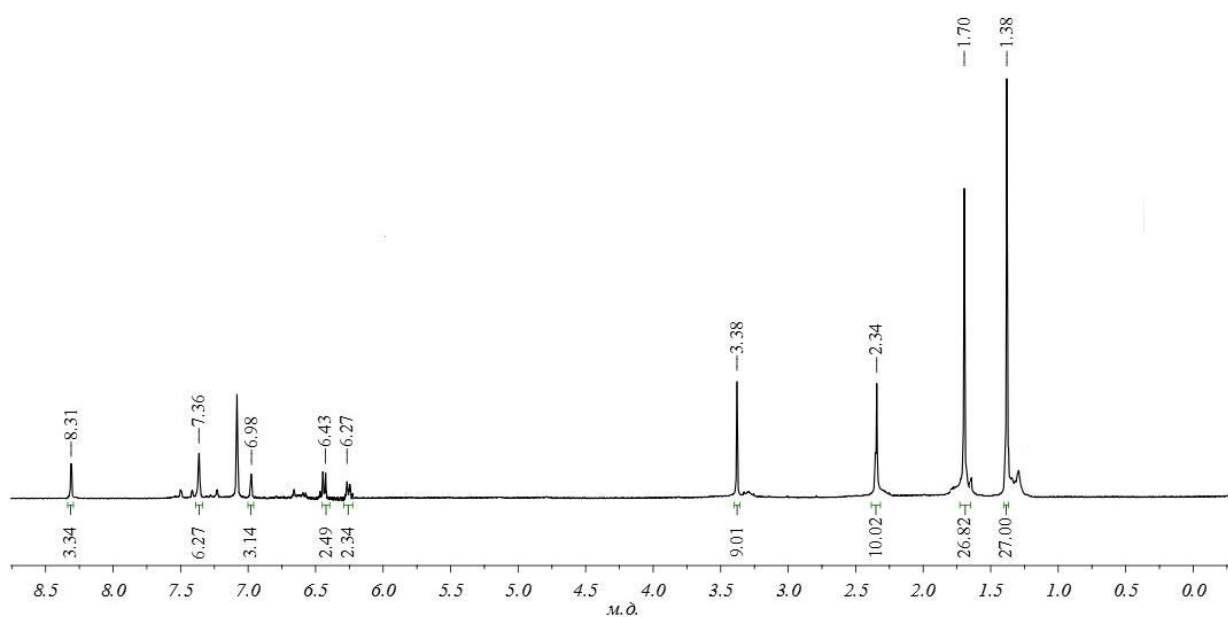


Figure S3. ^1H NMR spectrum (400 MHz, benzene- d_6 , 293 K) of **2**

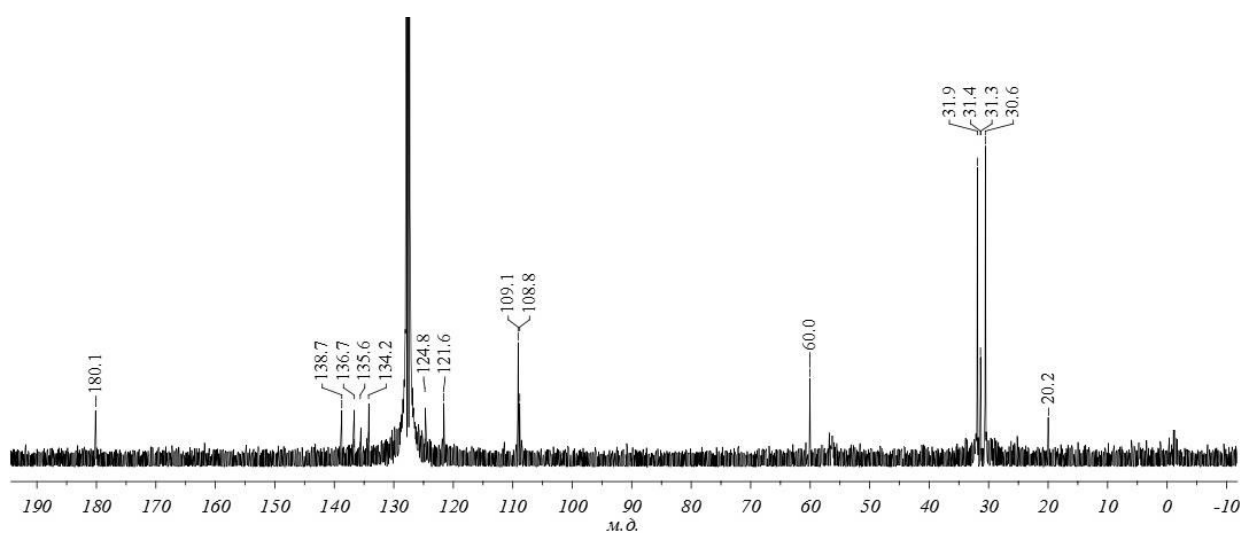


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, benzene- d_6 , 293 K) of **2**