Supporting Information

Two Scandium coordination polymers: rapid synthesis and catalytic property

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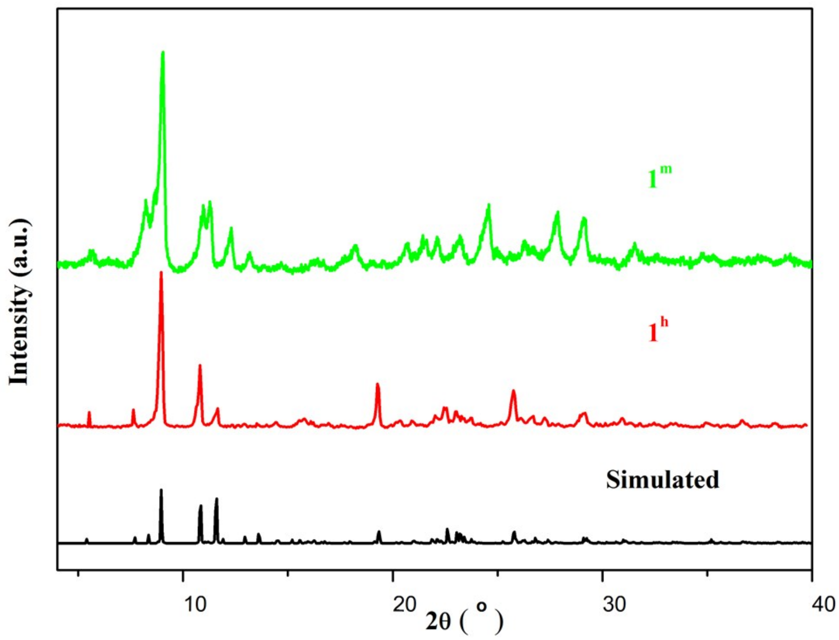


Fig. S1 PXRD patterns for $\mathbf{1^h}$ and $\mathbf{1^m}$.

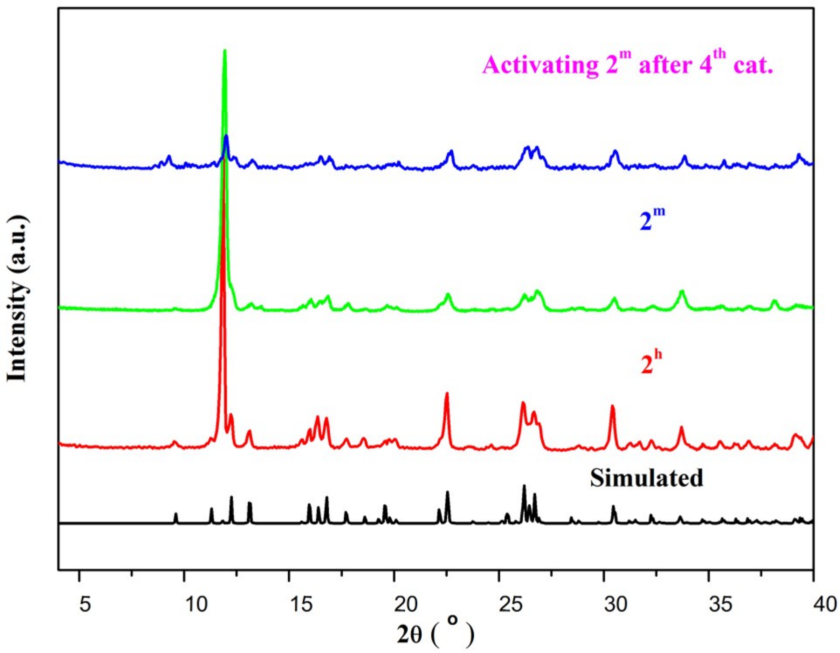


Fig. S2 PXRD patterns for $\mathbf{2^h}$ and $\mathbf{2^m}$.

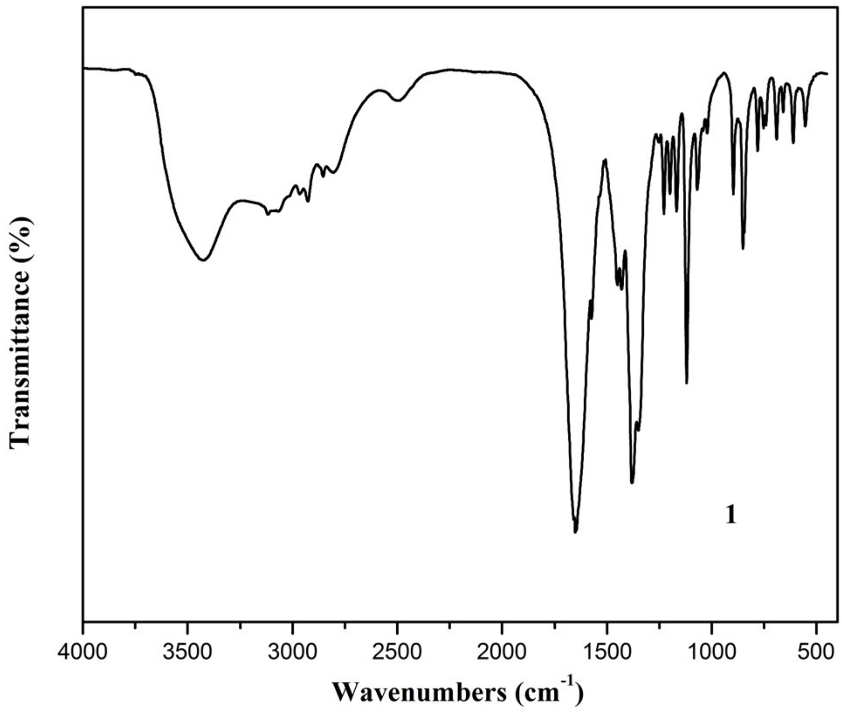


Fig. S3 The IR spectrum of **1**.

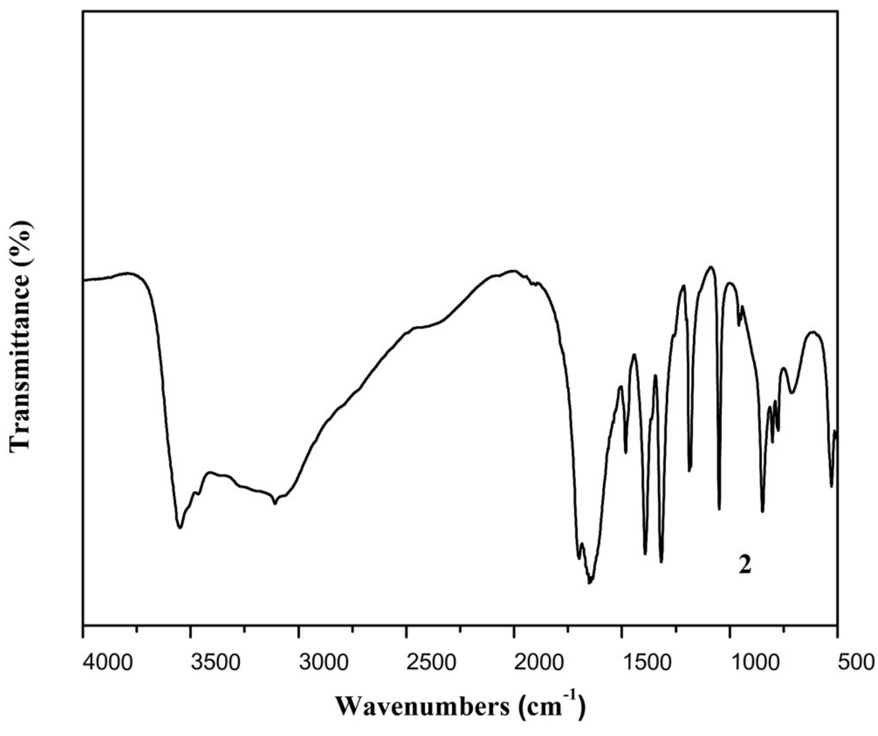


Fig. S4 The IR spectrum of **2**.

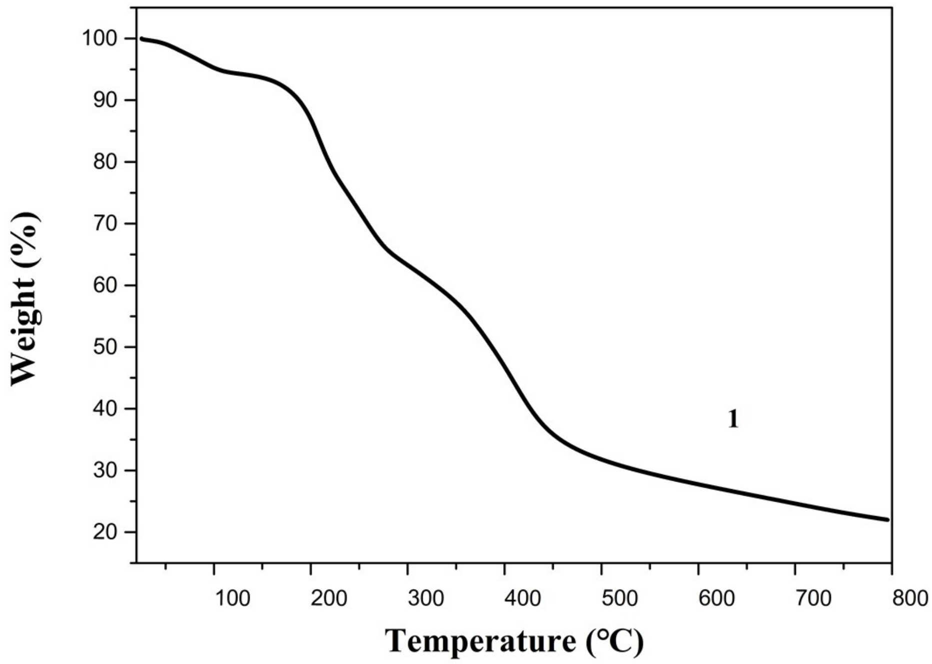


Fig. S5 The TGA curve for **1**.

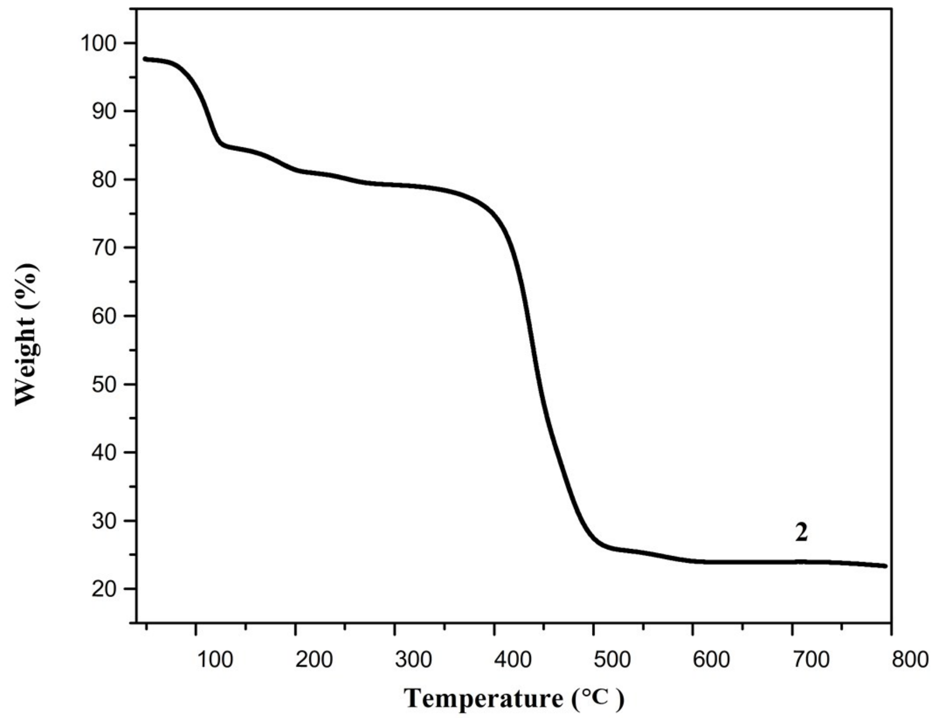


Fig. S6 The TGA curve for **2**.

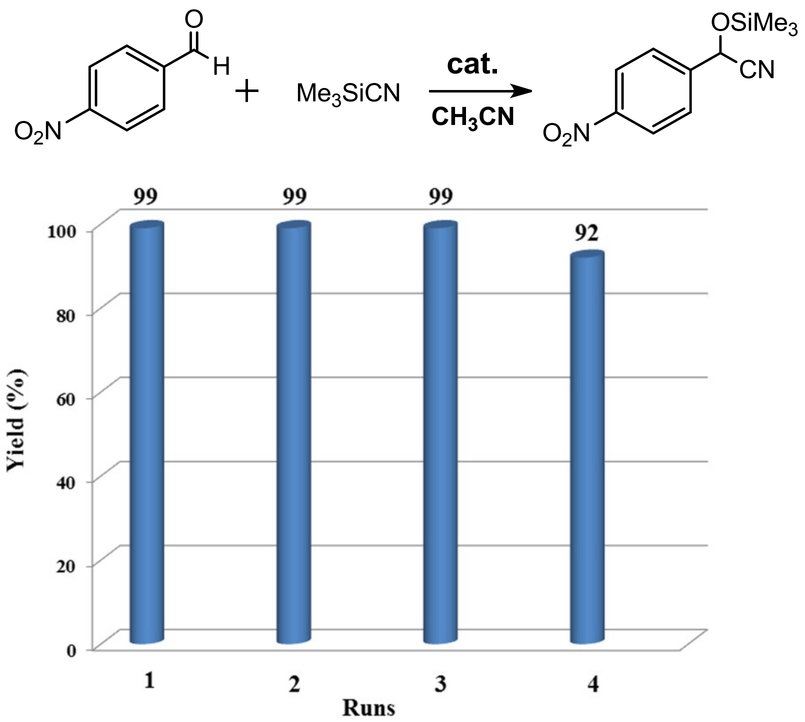


Fig. S7 The study on the recycling of **2**^{m} for the heterogeneous cyanosilylation.

Table S1 The crystal data and structure refinement for **1** and **2**.

Complex	**1**	**2**
Formula	$C_{15}H_{10}N_5O_9Sc$	$C_7H_8N_2O_9Sc$
Fw (g·mol^{-1})	449.24	309.1
Temperature (K)	293(2)	293(2)
Wave length (Å)	0.71073	0.71073
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a (Å)	12.1982(9)	8.0179(5)
b (Å)	12.6561(10)	8.1281(6)
c (Å)	17.4615(13)	10.1235(8)
α (°)	79.068(5)	67.896(4)
β (°)	69.577(4)	77.329(5)
γ (°)	65.464(4)	87.356(4)
Volume (Å^3)	2295.0(3)	595.89(7)
Z	4	2
D_{calc} (g·cm^{-3})	1.300	1.617
F (000)	912	292
θ range (°)	1.771 to 25.075	2.225 to 25.018
Index range (°)	-14<=h<=14	-9<=h<=9
	-15<=k<=13	-8<=k<=9
	-19<=l<=20	-10<=l<=12
Refl. Collected/ unique	13126 / 8125	3361/2087
R_{int}	0.0537	0.0332
Completeness	97.9 %	96.6 %
Goodness-of-fit on F^2	0.784	1.085
R_1, wR_2 [$I > 2\sigma(I)$]	0.0506, 0.1099	0.0317, 0.0932
R_1, wR_2 (all data)	0.1154, 0.1229	0.0352, 0.0957
Largest diff. peak and hole (eÅ^{-3})	0.456, -0.269	0.777, -0.275
CCDC Number	1054439	1054440

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$

Table S2. The selected bond length [Å] and angle [°] data for **1** and **2**.

		1	
N(1)-Sc(1)	2.422(3)	O(1)-Sc(2)	2.085(3)
N(3)-Sc(1)	2.497(4)	O(7)-Sc(2)#3	2.133(3)
N(5)-Sc(2)	2.464(3)	O(9)-Sc(2)	2.113(3)
N(7)-Sc(2)#3	2.438(3)	O(11)-Sc(2)	2.142(3)
O(2)-Sc(1)	2.124(3)	O(15)-Sc(2)	2.035(3)
O(6)-Sc(1)	2.117(3)	Sc(1)-O(18)#4	2.064(3)
O(12)-Sc(1)	2.163(3)	O(13)-Sc(1)	2.033(3)
O(13)#2-Sc(1)-O(18)#4	177.16(13)	O(15)#1-Sc(2)-O(1)	179.56(13)
O(13)#2-Sc(1)-O(6)	90.39(13)	O(15)#1-Sc(2)-O(9)	92.22(12)
O(18)#4-Sc(1)-O(6)	92.01(12)	O(1)-Sc(2)-O(9)	87.44(12)
O(13)#2-Sc(1)-O(2)	85.60(12)	O(15)#1-Sc(2)-O(7)#3	91.89(12)
O(18)#4-Sc(1)-O(2)	93.52(12)	O(1)-Sc(2)-O(7)#3	88.55(12)
O(6)-Sc(1)-O(2)	140.28(11)	O(9)-Sc(2)-O(7)#3	141.93(11)
O(13)#2-Sc(1)-O(12)	93.39(12)	O(15)#1-Sc(2)-O(11)	91.89(12)
O(18)#4-Sc(1)-O(12)	83.78(11)	O(1)-Sc(2)-O(11)	88.21(12)
O(6)-Sc(1)-O(12)	140.70(12)	O(9)-Sc(2)-O(11)	141.40(12)
O(2)-Sc(1)-O(12)	79.02(11)	O(7)#3-Sc(2)-O(11)	76.20(11)
O(13)#2-Sc(1)-N(1)	94.23(12)	O(15)#1-Sc(2)-N(7)#3	87.56(12)
O(18)#4-Sc(1)-N(1)	87.96(12)	O(1)-Sc(2)-N(7)#3	92.61(12)
O(6)-Sc(1)-N(1)	72.01(11)	O(9)-Sc(2)-N(7)#3	73.26(11)
O(2)-Sc(1)-N(1)	68.92(11)	O(7)#3-Sc(2)-N(7)#3	69.13(11)
O(12)-Sc(1)-N(1)	146.30(12)	O(11)-Sc(2)-N(7)#3	145.28(12)
O(13)#2-Sc(1)-N(3)	86.20(12)	O(15)#1-Sc(2)-N(5)	88.70(12)
O(18)#4-Sc(1)-N(3)	93.33(12)	O(1)-Sc(2)-N(5)	90.92(11)
O(6)-Sc(1)-N(3)	67.23(12)	O(9)-Sc(2)-N(5)	68.90(11)
O(2)-Sc(1)-N(3)	151.24(12)	O(7)#3-Sc(2)-N(5)	149.04(12)
O(12)-Sc(1)-N(3)	74.01(12)	O(11)-Sc(2)-N(5)	72.85(12)
N(1)-Sc(1)-N(3)	139.24(12)	N(7)#3-Sc(2)-N(5)	141.78(12)

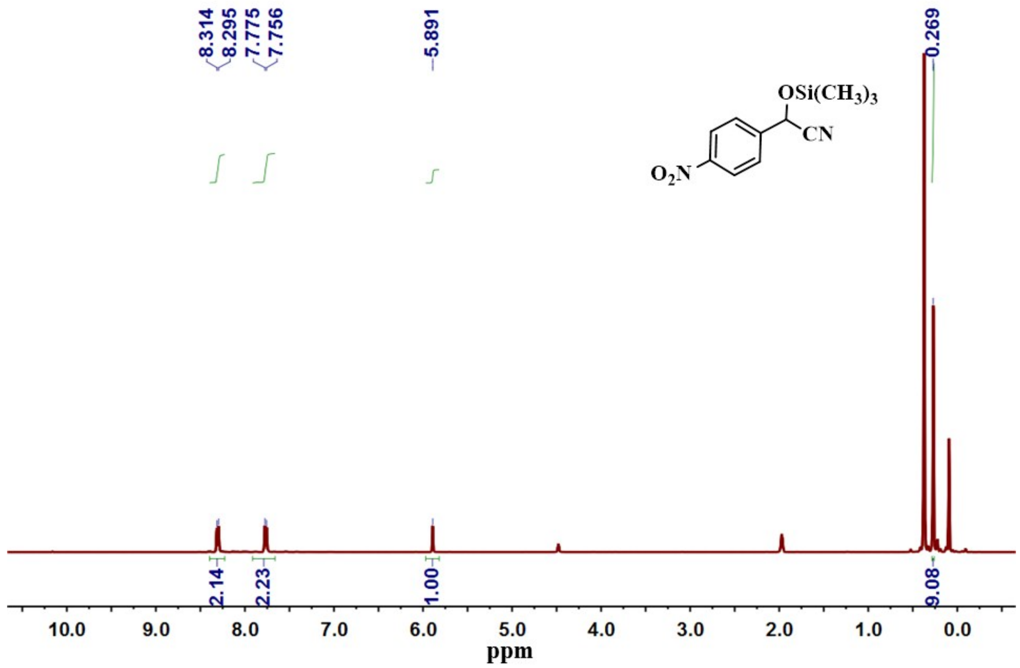
Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1; #2 -x+1,-y+1,-z; #3 -x,-y+2,-z+1; #4 -x+2,-y,-z

	2		
Sc(1)-O(1)	2.1529(17)	Sc(1)-O(5)	2.1402(16)
Sc(1)-O(2)	2.2164(18)	Sc(1)-O(6)	2.2767(16)
Sc(1)-O(3)	2.1601(18)	Sc(1)-N(1)	2.4463(19)
Sc(1)-O(4)	2.2068(18)	Sc(1)-N(2)	2.480(2)
O(1)-Sc(1)-O(2)	88.11(7)	O(5)-Sc(1)-O(6)	133.95(6)
O(1)-Sc(1)-O(3)	86.81(7)	O(1)-Sc(1)-N(1)	68.87(6)
O(1)-Sc(1)-O(4)	95.37(7)	O(2)-Sc(1)-N(1)	75.85(6)
O(1)-Sc(1)-O(6)	74.04(6)	O(3)-Sc(1)-N(1)	141.74(7)
O(2)-Sc(1)-O(6)	143.92(6)	O(4)-Sc(1)-N(1)	70.53(6)
O(3)-Sc(1)-O(2)	74.21(7)	O(5)-Sc(1)-N(1)	76.81(6)
O(3)-Sc(1)-O(4)	143.48(7)	O(6)-Sc(1)-N(1)	123.23(6)
O(3)-Sc(1)-O(6)	73.72(6)	O(1)-Sc(1)-N(2)	145.16(7)
O(4)-Sc(1)-O(2)	142.19(7)	O(2)-Sc(1)-N(2)	117.00(7)
O(4)-Sc(1)-O(6)	71.94(6)	O(3)-Sc(1)-N(2)	78.26(7)
O(5)-Sc(1)-O(1)	144.99(6)	O(4)-Sc(1)-N(2)	79.51(7)
O(5)-Sc(1)-O(2)	76.79(6)	O(5)-Sc(1)-N(2)	68.40(6)
O(5)-Sc(1)-O(3)	118.04(7)	O(6)-Sc(1)-N(2)	71.61(6)
O(5)-Sc(1)-O(4)	79.15(6)		

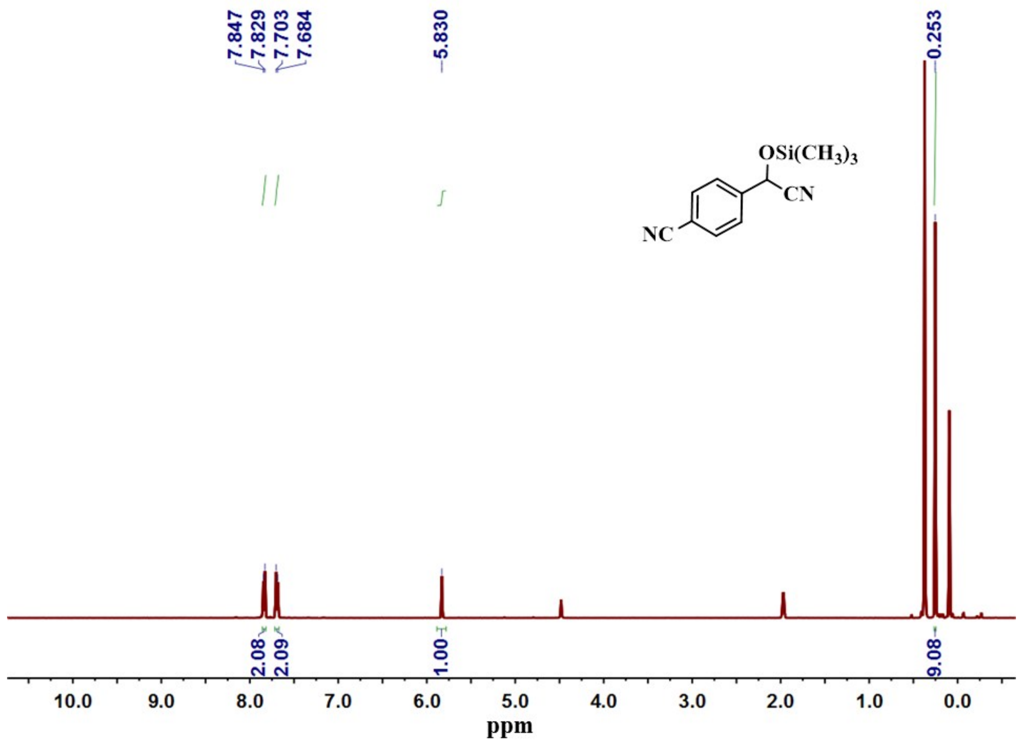
Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z; #2 -x+1,-y,-z+1; #3 -x+2,-y,-z+1

Fig. S8 The ^{1}H NMR data for the cyanosilylation reaction products.

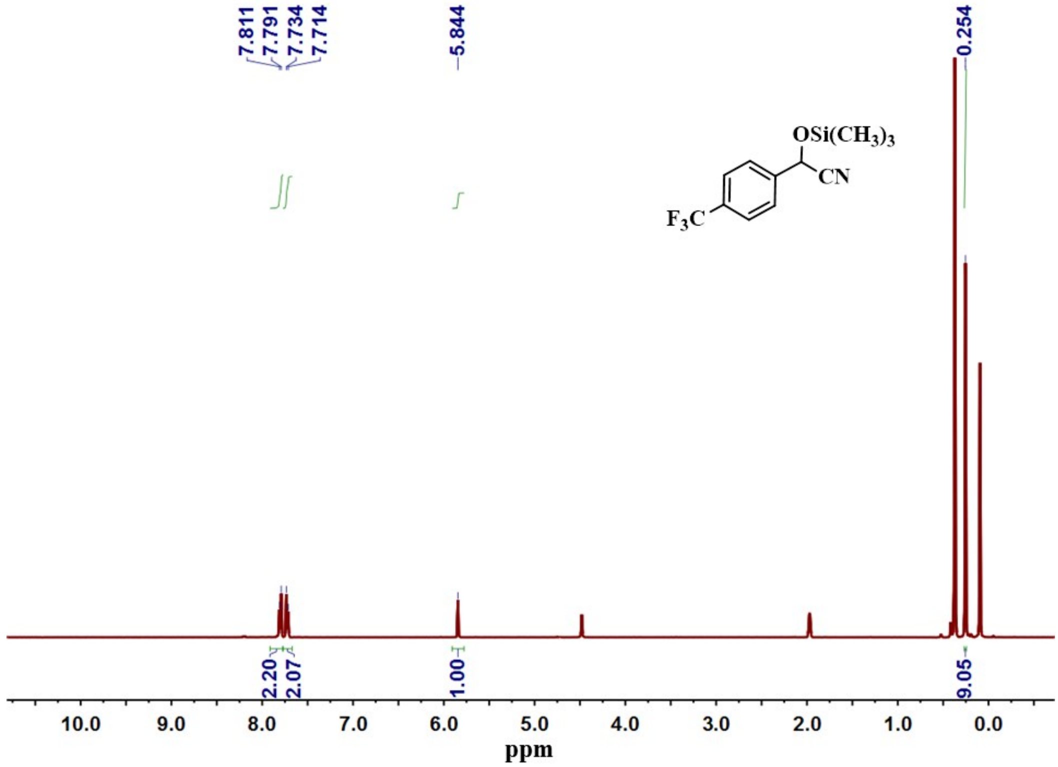
^{1}H NMR (400 MHz, CD_3CN) δ = 8.30 (d, J = 7.6 Hz, 2H), 7.77 (d, J = 7.6 Hz, 2H), 5.89 (s, 1H), 0.27 (s, 9H).



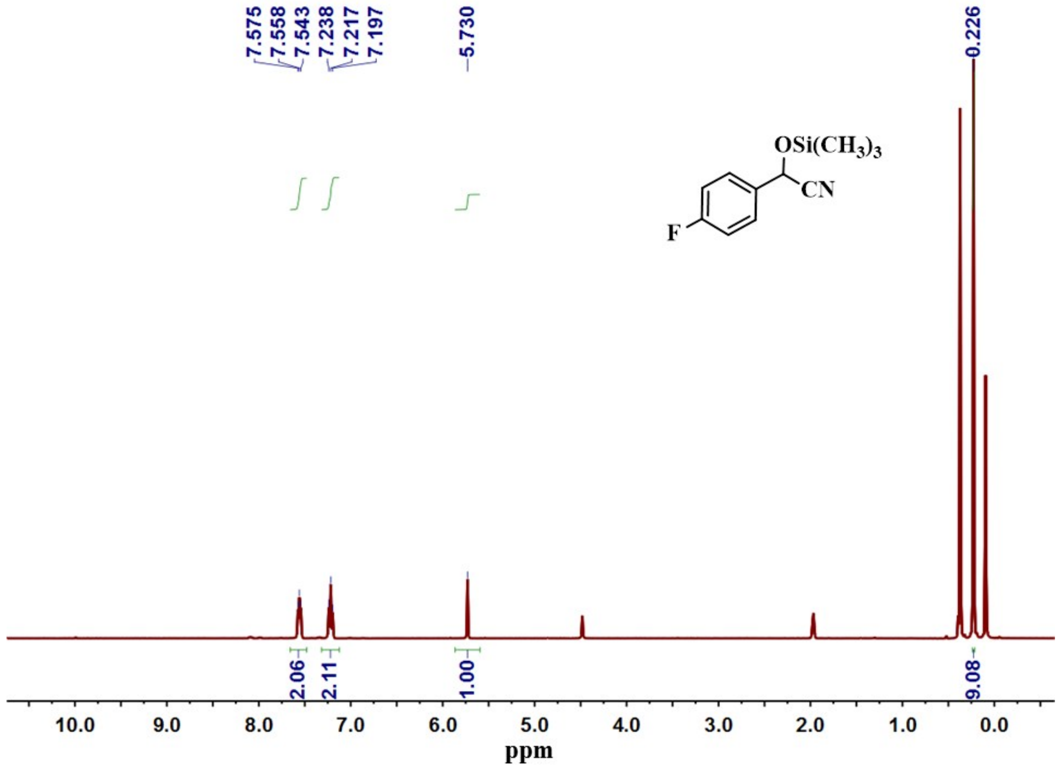
^{1}H NMR (400 MHz, CD_3CN) δ = 7.84 (d, J = 7.2 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 5.83 (s, 1H), 0.25 (s, 9H).



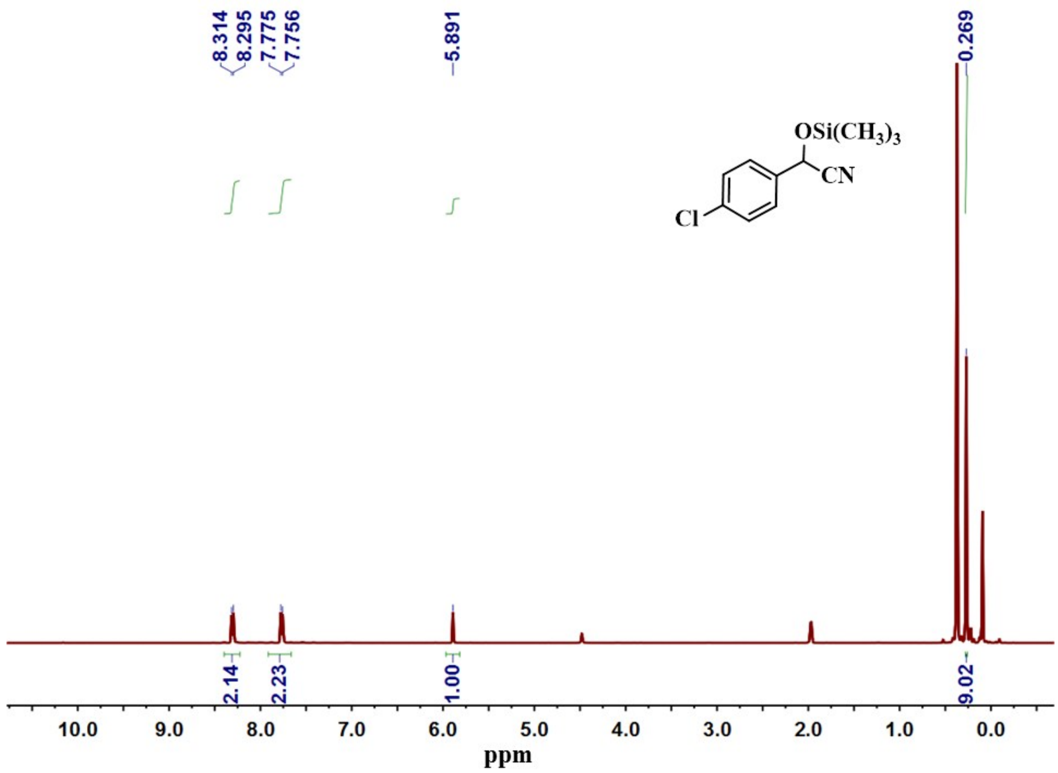
^1H NMR (400 MHz, CD_3CN) δ = 7.80 (d, J = 8.0 Hz, 2H), 7.72 (d, J = 8.0 Hz, 2H), 5.84 (s, 1H), 0.25 (s, 9H).



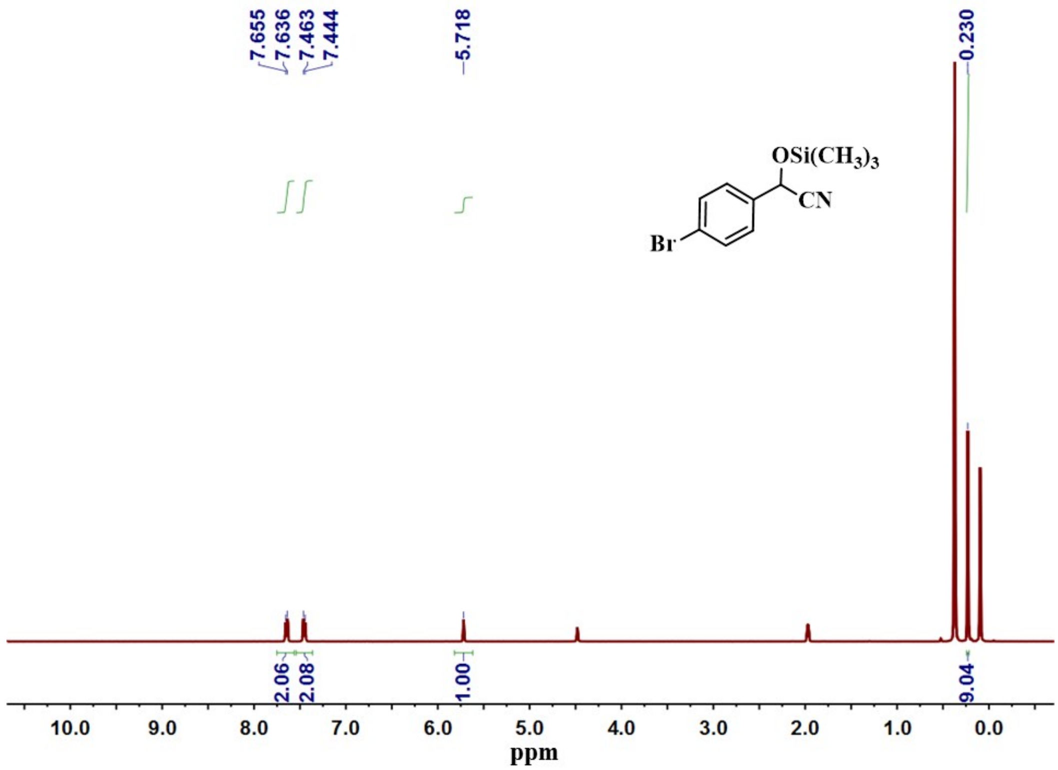
^1H NMR (400 MHz, CD_3CN) δ = 7.56 (m, 2H), 7.22 (t, J = 8.2 Hz, 2H), 5.73 (s, 1H), 0.23 (s, 9H).



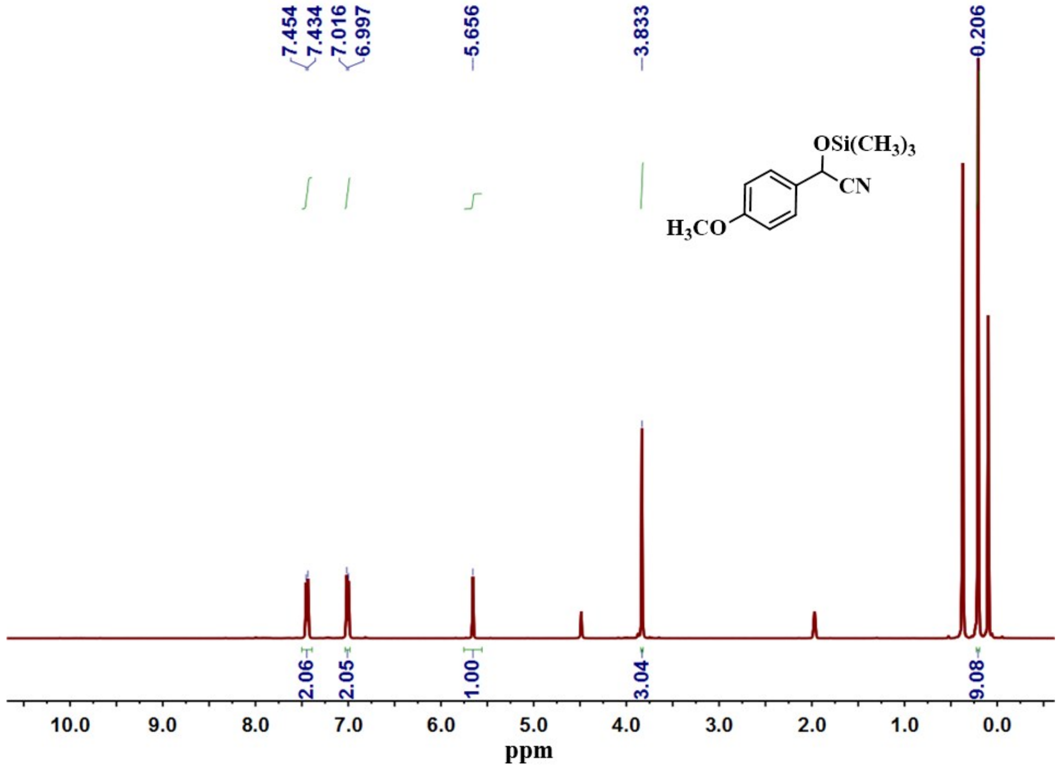
^1H NMR (400 MHz, CD_3CN) δ = 8.30 (d, J = 7.6 Hz, 2H), 7.77 (d, J = 7.6 Hz, 2H), 5.89 (s, 1H), 0.27 (s, 9H).



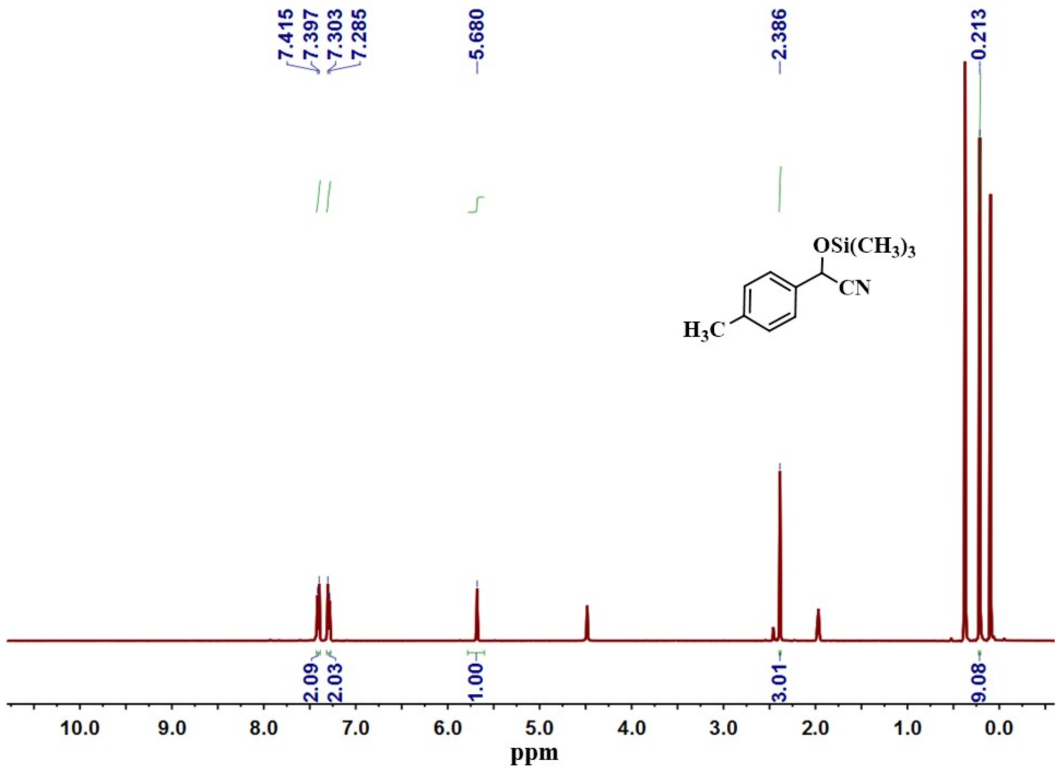
^1H NMR (400 MHz, CD_3CN) δ = 7.65 (d, J = 7.6 Hz, 2H), 7.45 (d, J = 7.6 Hz, 2H), 5.72 (s, 1H), 0.23 (s, 9H).



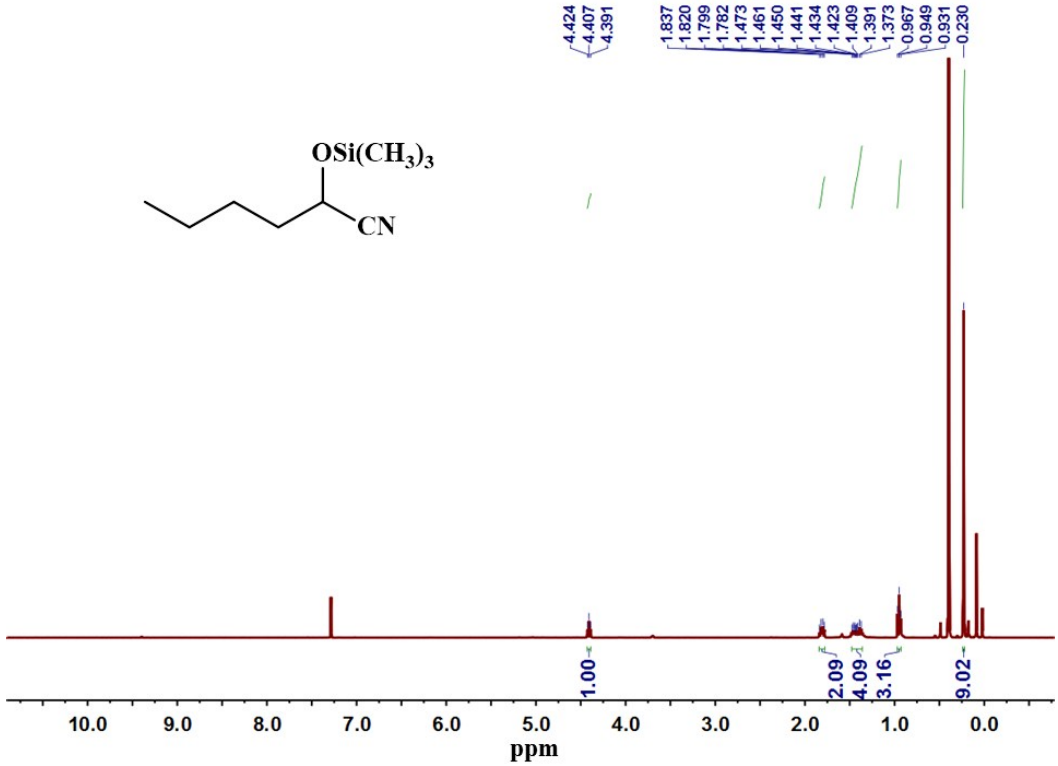
^{1}H NMR (400 MHz, CD_3CN) δ = 7.44 (d, J = 8.0 Hz, 2H), 7.01 (d, J = 7.6 Hz, 2H), 5.66 (s, 1H), 3.83 (s, 3H), 0.21 (s, 9H).



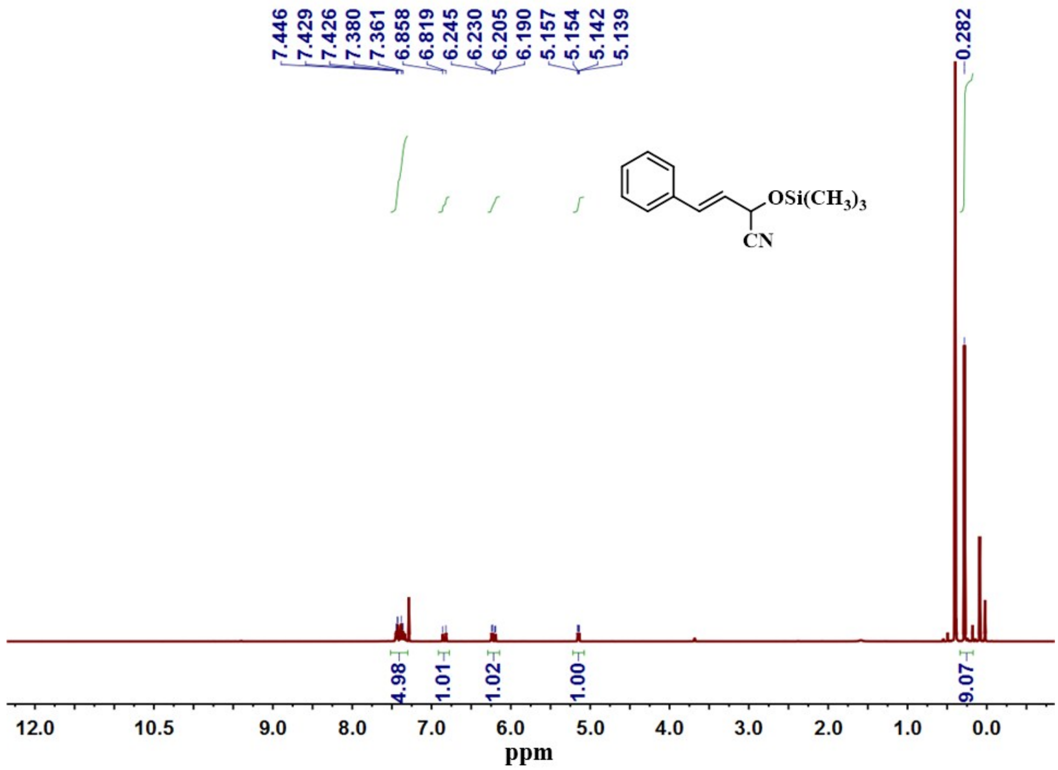
^{1}H NMR (400 MHz, CD_3CN) δ = 7.41 (d, J = 7.2 Hz, 2H), 7.29 (d, J = 7.2 Hz, 2H), 5.68 (s, 1H), 2.39 (s, 3H), 0.21 (s, 9H).



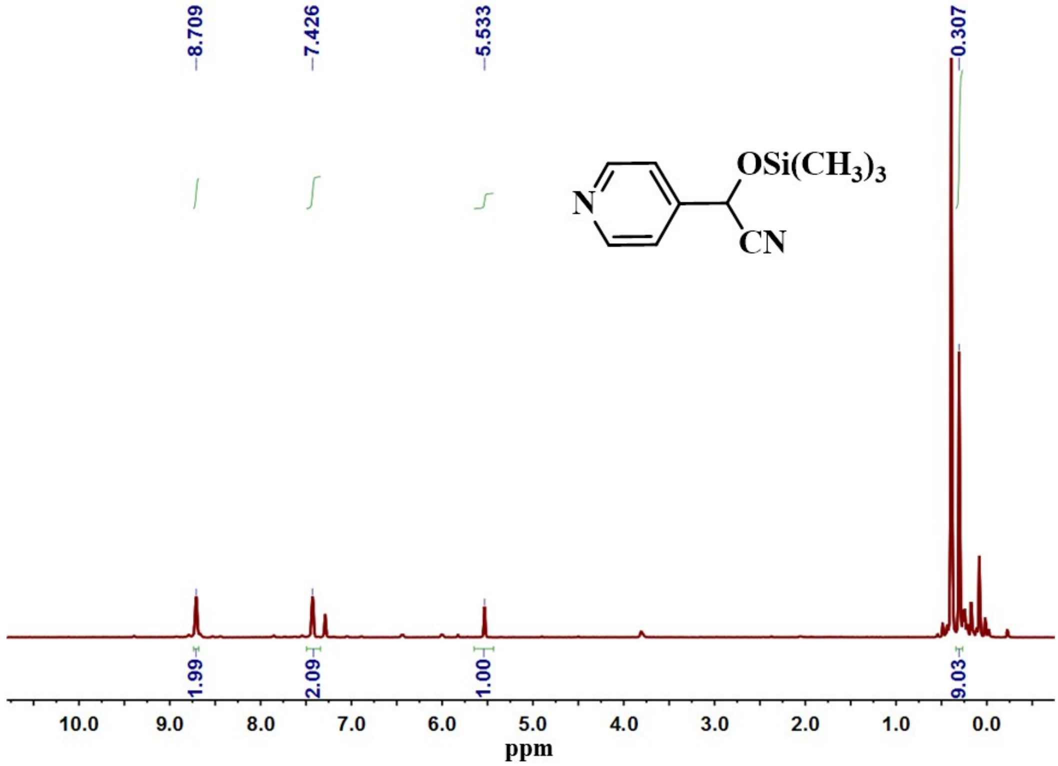
^1H NMR (400 MHz, $CDCl_3$) δ = 4.41 (t, J = 6.6 Hz, 1H), 1.81 (dd, J = 15.2, 6.8 Hz, 2H), 1.43 (m, 4H), 0.95 (t, J = 7.2 Hz, 3H), 0.23 (s, 9H).



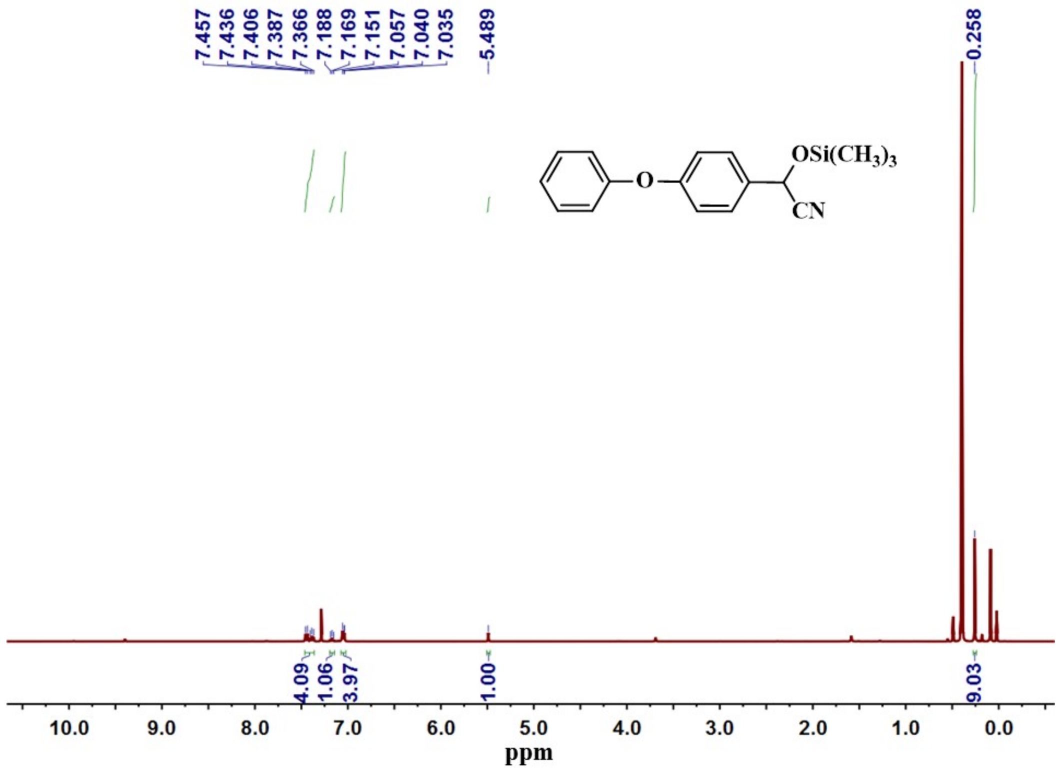
^1H NMR (400 MHz, $CDCl_3$) δ = 7.41 (m, 5H), 6.84 (d, J = 15.6 Hz, 1H), 6.22 (dd, J = 16.0, 6.0 Hz 1H), 5.15 (dd, J = 6.0, 1.2 Hz 1H), 0.28 (s, 9H).



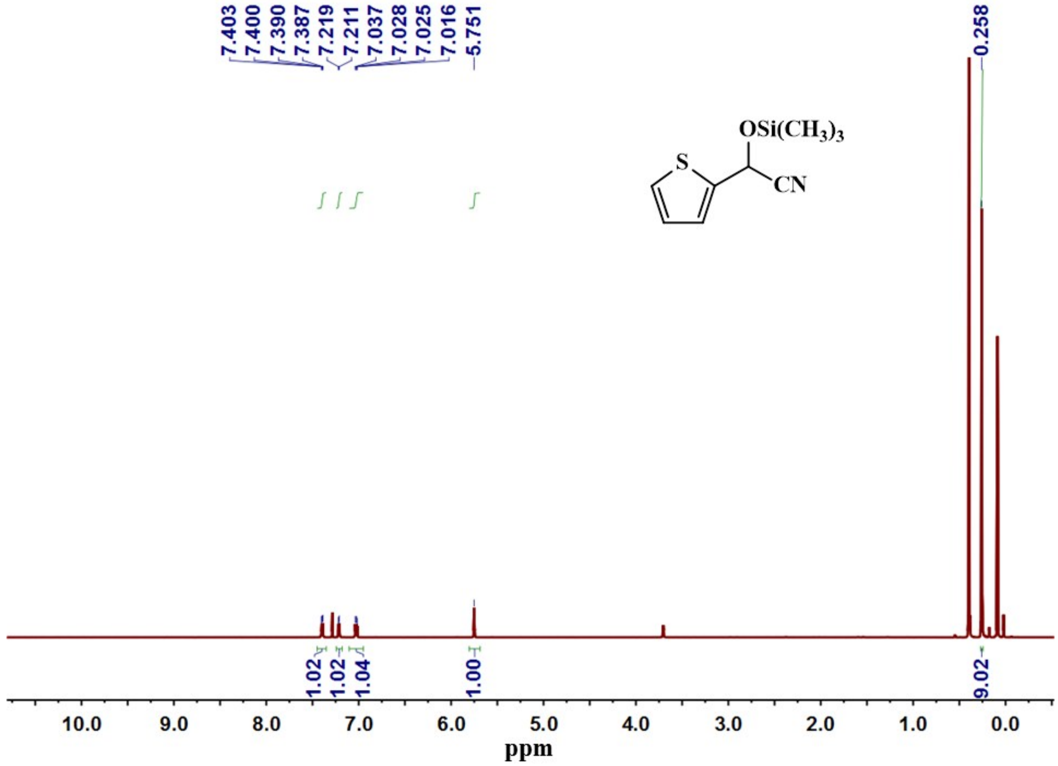
^1H NMR (400 MHz, $CDCl_3$) δ = 8.71 (s, 2H), 7.43 (s, 2H), 5.53 (s, 1H), 0.31 (s, 9H).



^1H NMR (400 MHz, $CDCl_3$) δ = 7.41 (m, 4H), 7.17 (t, J = 7.4 Hz, 1H), 7.04 (m, 4H), 5.49 (s, 1H), 0.26 (s, 9H).



^1H NMR (400 MHz, $CDCl_3$) δ = 7.39 (dd, J = 5.2, 1.2 Hz, 1H), 7.21 (d, J = 3.2 Hz, 1H), 7.03 (dd, J = 4.8, 3.6 Hz, 1H), 5.75 (s, 1H), 0.26 (s, 9H).



^1H NMR (400 MHz, $CDCl_3$) δ = 8.20 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 7.2 Hz, 1H), 7.64 (m, 1H), 7.59 (m, 1H), 7.51 (m, 1H), 6.08 (s, 1H), 0.23 (s, 9H).