Influence of Polymer Conformations on the Aggregation Behaviour of Alternating Dialkylsilylene-[4,4'-divinyl(cyanostilbene)] Copolymers

Chih-Hsien Chen, *[a] Shern-Long Lee,[a] Tsong-Shin Lim,[b] Chun-hsien Chen,[a] Tien-Yau Luh*[a]

[a] Department of Chemistry, National Taiwan University, Taipei, Taiwan 106

[b] Department of Physics, Tunghai University, Taichung, Taiwan 407

*Corresponding authors: E-mail: tyluh@ntu.edu.tw, chhschen@ntu.edu.tw

Supplementary Information

Table of Contents

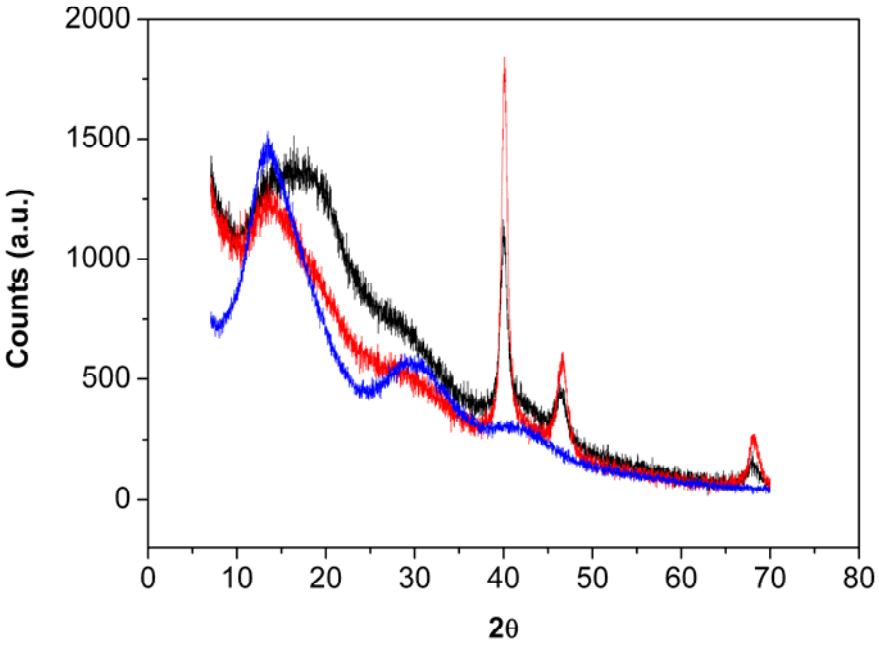

Fig. S1 XRD patterns of **3a** (black), **3b** (red), and blank test (blue).

Crystal size estimation of 3a and 3b.

The crystal sizes (*t*) of **3a** and **3b** were estimated by Scherrer's formula, $t = 0.9\lambda/B\cos\theta$, where λ, B and θ denote the wavelength of X-ray (1.54056 Å), the half width of peaks in radian, and the angle of incident beam, respectively. The results are summarized in Table S1.

Table S1 Crystal size estimation of **3a** and **3b**.

	B (radian)	cosθ	*t*(nm)
3a	0.0149	0.94	9.9
3b	0.0128	0.93	11.5

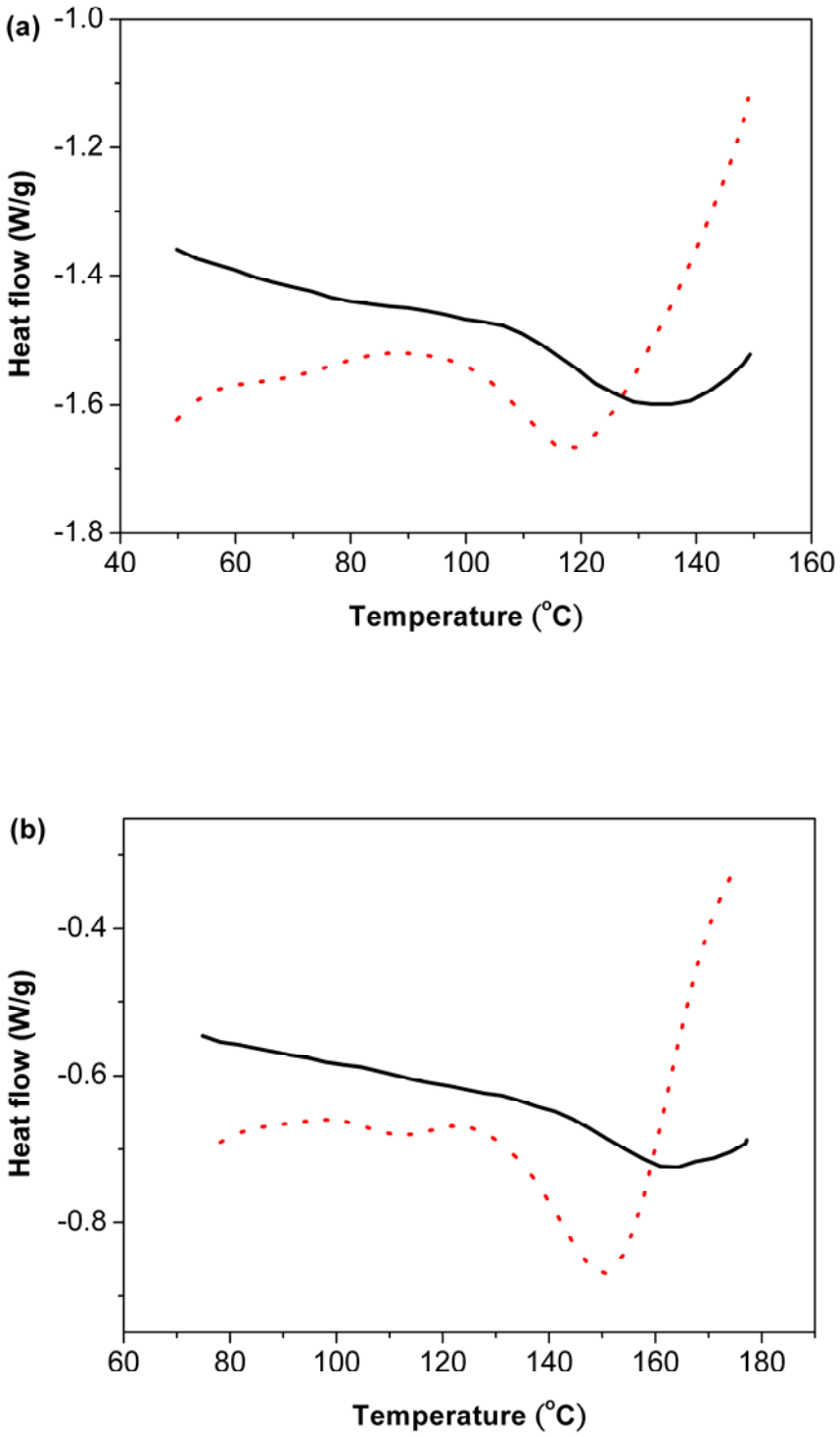

Fig. S2 Normal (black) and first derivative (red) of DSC curves of (a) **3a** and (b) **3b**.

Table S2 Crystal data and structure refinement for **5**.

Identification code	ic14121	
Empirical formula	C25 H31 N Si2	
Formula weight	401.69	
Temperature	295(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.3400(6) Å	α= 90°.
	b = 6.7435(2) Å	β= 102.043(4)°.
	c = 20.8688(7) Å	γ = 90°.
Volume	2524.16(14) $Å^3$	
Z	4	
Density (calculated)	1.057 Mg/m^3	
Absorption coefficient	1.328 mm^{-1}	
F(000)	864	
Crystal size	0.25 x 0.20 x 0.15 mm^3	
Theta range for data collection	4.33 to 68.00°.	
Index ranges	-19<=h<=22, -6<=k<=8, -23<=l<=25	
Reflections collected	9307	
Independent reflections	4565 [R(int) = 0.0266]	
Completeness to theta = 68.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.45060	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4565 / 0 / 253	
Goodness-of-fit on F^2	2.275	
Final R indices [I>2sigma(I)]	R1 = 0.1148, wR2 = 0.3246	
R indices (all data)	R1 = 0.1375, wR2 = 0.3404	
Largest diff. peak and hole	1.253 and -0.625 e.$Å^{-3}$	

Table S3 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	1428(1)	3328(3)	985(1)	78(1)
Si(2)	8544(1)	2472(3)	-3488(1)	78(1)
N(1)	5222(4)	9566(7)	-1109(3)	119(2)
C(1)	5147(3)	7946(8)	-1201(3)	85(2)
C(2)	5079(5)	5870(10)	-1324(5)	179(6)
C(3)	4885(5)	4571(11)	-1261(4)	155(4)
C(4)	4271(3)	5046(14)	-736(3)	104(2)
C(5)	4093(3)	6659(12)	-408(3)	103(2)
C(6)	3575(3)	6528(9)	-7(3)	85(2)
C(7)	3213(2)	4791(8)	67(2)	67(1)
C(8)	3414(3)	3120(10)	-258(3)	91(2)
C(9)	3930(3)	3250(13)	-639(3)	105(2)
C(10)	2639(2)	4741(8)	466(2)	69(1)
C(11)	2208(3)	3236(8)	553(2)	78(1)
C(12)	1258(4)	5935(11)	1208(3)	108(2)
C(13)	590(3)	2389(13)	424(3)	116(3)
C(14)	1634(4)	1780(13)	1733(3)	121(2)
C(15)	5702(3)	5114(11)	-1852(3)	89(2)
C(16)	5947(3)	6639(10)	-2192(3)	87(2)
C(17)	6448(3)	6289(8)	-2582(3)	80(1)
C(18)	6751(2)	4446(8)	-2652(2)	69(1)
C(19)	6495(3)	2908(9)	-2313(3)	84(1)
C(20)	5977(3)	3244(11)	-1934(3)	97(2)
C(21)	7323(2)	4214(8)	-3043(2)	77(1)
C(22)	7765(3)	2703(9)	-3053(2)	81(1)
C(23)	8369(4)	3877(10)	-4259(3)	102(2)
C(24)	9409(3)	3354(15)	-2945(4)	133(3)
C(25)	8645(4)	-244(11)	-3658(3)	117(2)

Table S4 Bond lengths [Å] and angles [°] for **5**.

Si(1)-C(13)	1.840(6)
Si(1)-C(11)	1.845(5)
Si(1)-C(14)	1.850(7)
Si(1)-C(12)	1.862(7)
Si(2)-C(23)	1.837(6)
Si(2)-C(24)	1.845(7)
Si(2)-C(22)	1.852(5)
Si(2)-C(25)	1.882(7)
N(1)-C(1)	1.113(7)
C(1)-C(2)	1.424(8)
C(2)-C(3)	0.965(11)
C(2)-C(15)	1.818(13)
C(3)-C(4)	1.757(12)
C(4)-C(5)	1.361(11)
C(4)-C(9)	1.398(11)
C(5)-C(6)	1.393(7)
C(6)-C(7)	1.371(7)
C(7)-C(8)	1.404(8)
C(7)-C(10)	1.472(5)
C(8)-C(9)	1.358(7)
C(10)-C(11)	1.322(7)
C(15)-C(16)	1.377(9)
C(15)-C(20)	1.382(9)
C(16)-C(17)	1.369(7)
C(17)-C(18)	1.381(7)
C(18)-C(19)	1.392(7)
C(18)-C(21)	1.465(6)
C(19)-C(20)	1.375(7)
C(21)-C(22)	1.306(7)
C(13)-Si(1)-C(11)	107.9(3)
C(13)-Si(1)-C(14)	109.9(4)
C(11)-Si(1)-C(14)	110.5(3)
C(13)-Si(1)-C(12)	108.9(4)
C(11)-Si(1)-C(12)	109.9(3)
C(14)-Si(1)-C(12)	109.7(4)
C(23)-Si(2)-C(24)	110.1(4)

C(23)-Si(2)-C(22)	112.0(3)
C(24)-Si(2)-C(22)	108.9(3)
C(23)-Si(2)-C(25)	110.0(3)
C(24)-Si(2)-C(25)	108.9(4)
C(22)-Si(2)-C(25)	106.9(3)
N(1)-C(1)-C(2)	177.8(8)
C(3)-C(2)-C(1)	152.8(16)
C(3)-C(2)-C(15)	97.1(11)
C(1)-C(2)-C(15)	110.1(8)
C(2)-C(3)-C(4)	102.8(11)
C(5)-C(4)-C(9)	117.2(5)
C(5)-C(4)-C(3)	135.4(7)
C(9)-C(4)-C(3)	107.3(6)
C(4)-C(5)-C(6)	121.1(6)
C(7)-C(6)-C(5)	121.9(6)
C(6)-C(7)-C(8)	116.7(4)
C(6)-C(7)-C(10)	120.2(5)
C(8)-C(7)-C(10)	123.0(5)
C(9)-C(8)-C(7)	121.0(6)
C(8)-C(9)-C(4)	121.9(7)
C(11)-C(10)-C(7)	127.9(5)
C(10)-C(11)-Si(1)	126.1(4)
C(16)-C(15)-C(20)	116.7(4)
C(16)-C(15)-C(2)	114.7(5)
C(20)-C(15)-C(2)	128.6(5)
C(17)-C(16)-C(15)	120.6(6)
C(16)-C(17)-C(18)	123.5(5)
C(17)-C(18)-C(19)	115.5(4)
C(17)-C(18)-C(21)	120.4(4)
C(19)-C(18)-C(21)	124.1(5)
C(20)-C(19)-C(18)	121.1(5)
C(19)-C(20)-C(15)	122.4(5)
C(22)-C(21)-C(18)	127.7(5)
C(21)-C(22)-Si(2)	128.2(4)

Symmetry transformations used to generate equivalent atoms:

Table S5 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	69(1)	104(1)	66(1)	-6(1)	28(1)	-16(1)
Si(2)	66(1)	107(1)	68(1)	-8(1)	26(1)	12(1)
N(1)	192(5)	46(2)	150(5)	-2(3)	104(4)	-6(3)
C(1)	102(4)	54(3)	109(4)	10(3)	43(3)	5(2)
C(2)	197(9)	38(3)	224(10)	17(4)	-131(8)	-11(4)
C(3)	193(8)	46(3)	173(8)	-10(4)	-83(7)	4(4)
C(4)	57(3)	181(7)	76(3)	24(4)	22(2)	16(3)
C(5)	72(3)	130(6)	111(4)	44(4)	28(3)	-9(3)
C(6)	70(3)	93(4)	100(3)	8(3)	35(3)	1(2)
C(7)	55(2)	84(3)	66(2)	0(2)	22(2)	-1(2)
C(8)	71(3)	113(4)	98(4)	-21(3)	39(3)	-7(3)
C(9)	78(3)	149(6)	99(4)	-26(4)	42(3)	11(4)
C(10)	67(2)	77(3)	70(2)	-8(2)	28(2)	-7(2)
C(11)	79(3)	86(3)	76(3)	-8(2)	32(2)	-16(2)
C(12)	118(5)	114(5)	103(4)	-17(4)	47(4)	2(4)
C(13)	83(4)	163(7)	108(5)	-30(5)	33(3)	-34(4)
C(14)	117(5)	140(7)	111(5)	24(5)	33(4)	-29(4)
C(15)	59(3)	132(5)	76(3)	-4(3)	16(2)	24(3)
C(16)	78(3)	102(4)	85(3)	-2(3)	25(3)	22(3)
C(17)	68(3)	82(3)	96(3)	4(3)	30(2)	10(2)
C(18)	57(2)	80(3)	75(2)	1(2)	23(2)	-4(2)
C(19)	78(3)	76(3)	111(4)	2(3)	47(3)	1(2)
C(20)	74(3)	120(5)	106(4)	24(4)	44(3)	-14(3)
C(21)	69(3)	84(3)	84(3)	6(3)	32(2)	4(2)
C(22)	78(3)	91(4)	82(3)	5(3)	34(2)	7(3)
C(23)	108(4)	102(4)	103(4)	14(4)	36(3)	7(3)
C(24)	76(4)	208(10)	118(5)	-40(6)	27(3)	-8(4)
C(25)	142(5)	110(5)	104(4)	-1(4)	39(4)	34(4)

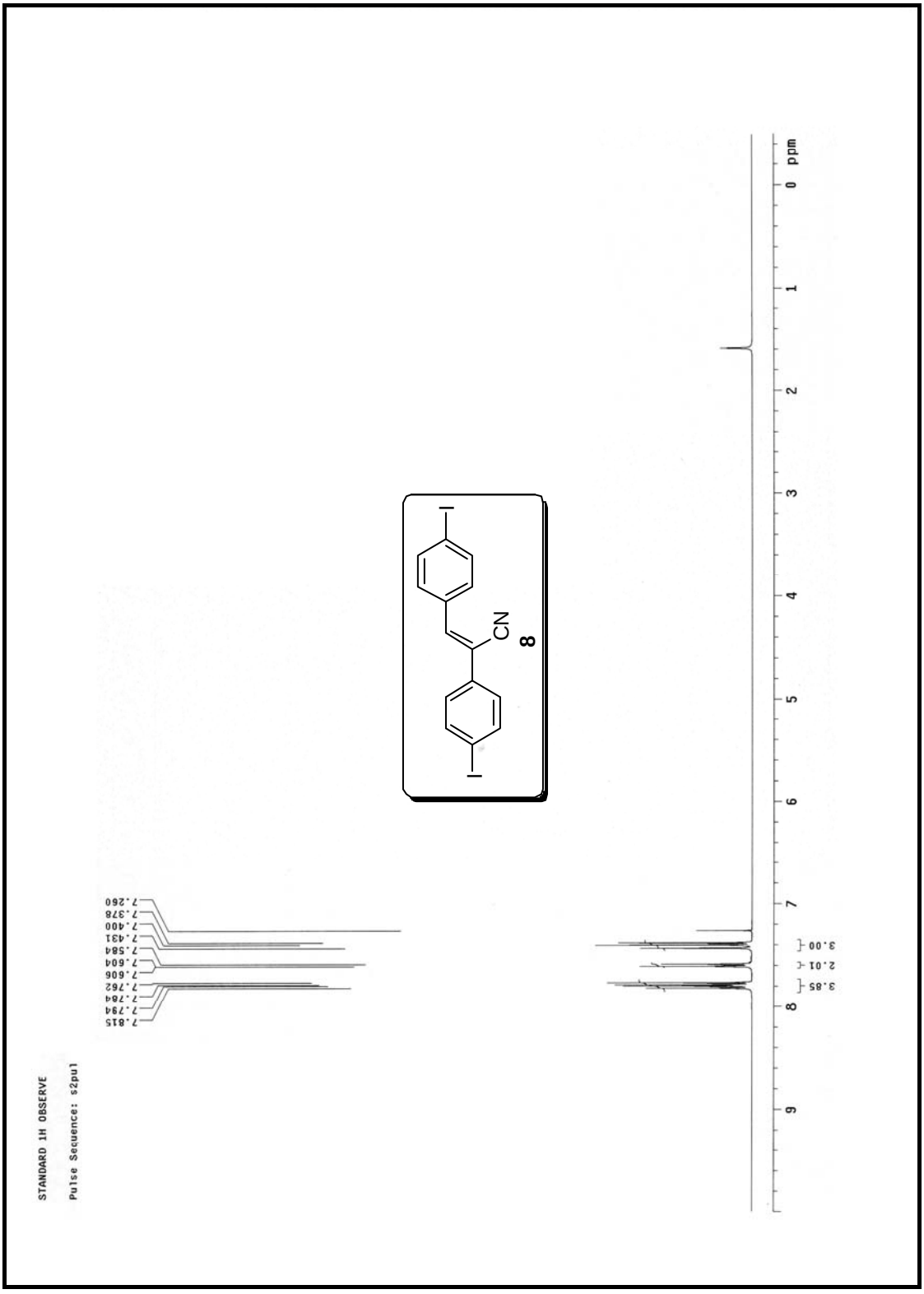

Fig. S3 ^{1}H NMR spectrum of **8**

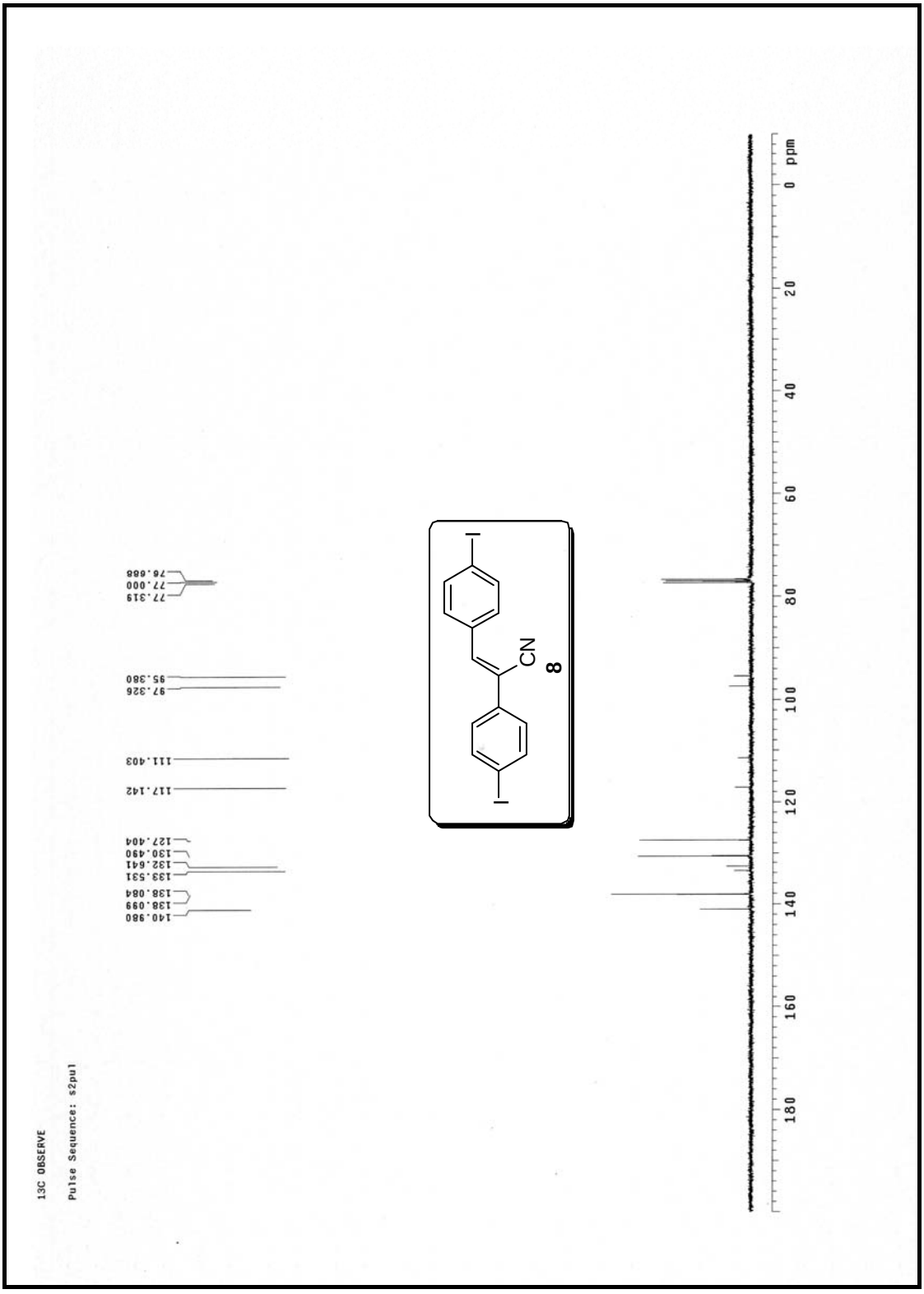

Fig. S4 ^{13}C NMR spectrum of **8**

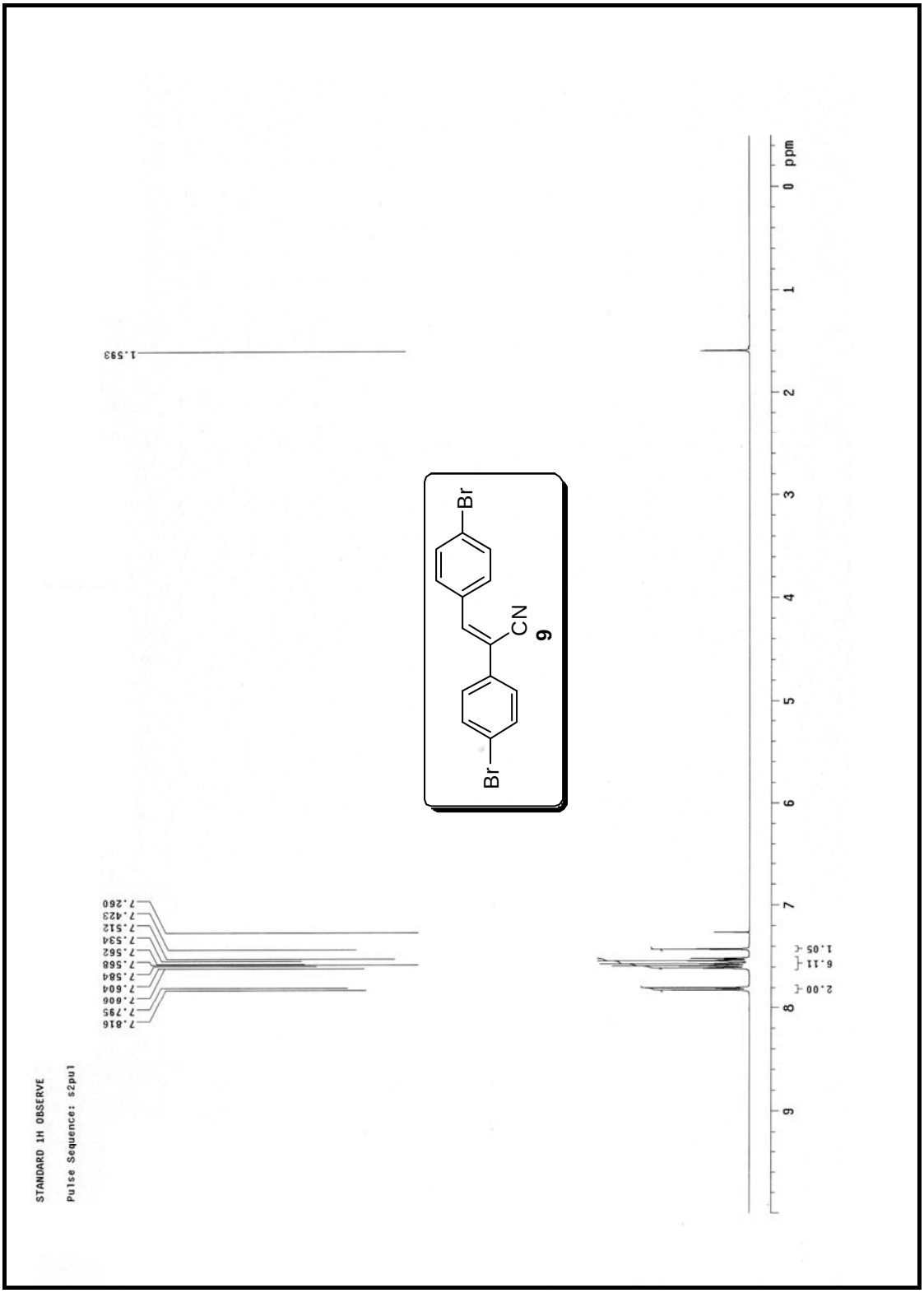

Fig. S5 ^{1}H NMR spectrum of **9**

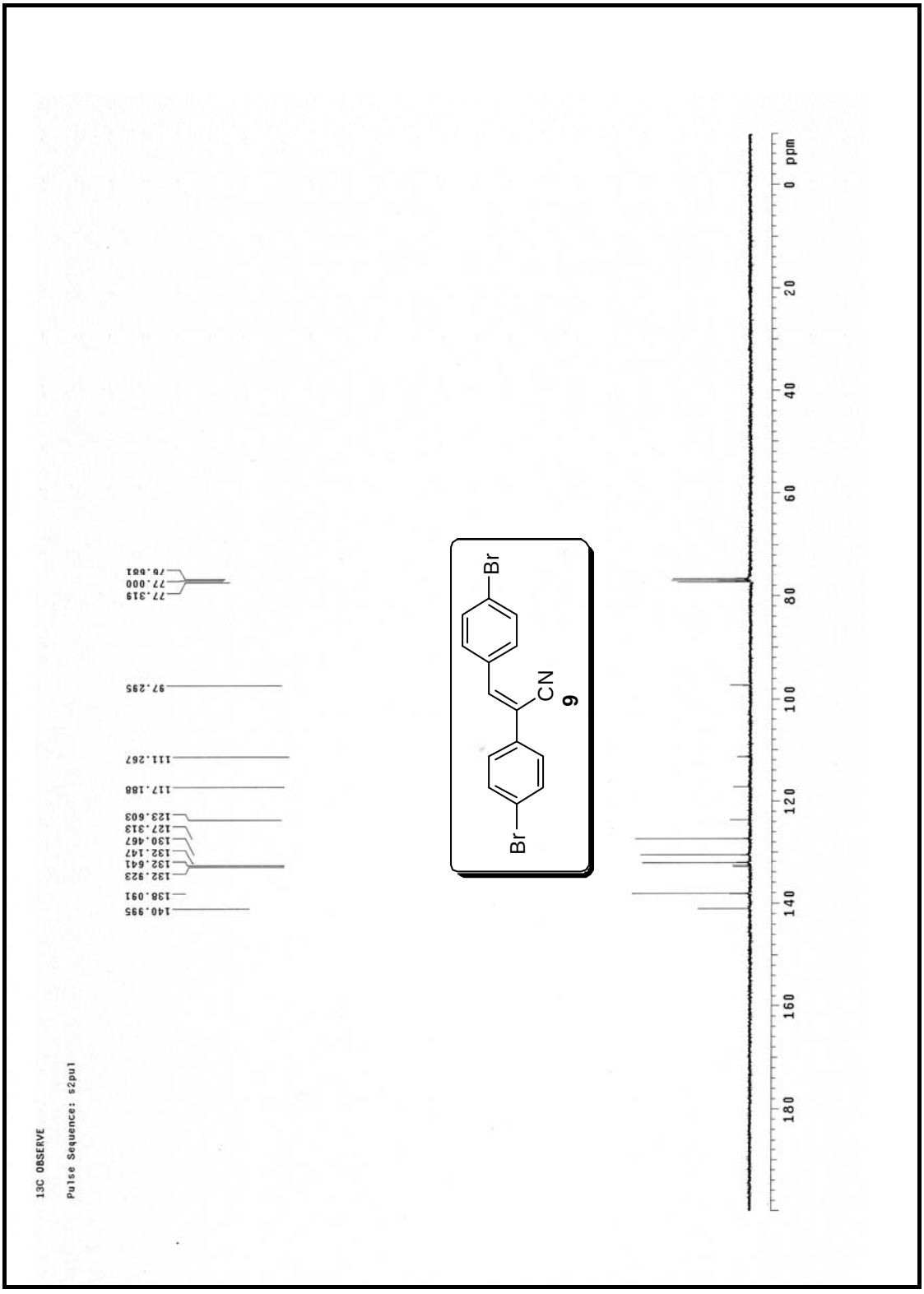

Fig. S6 ^{13}C NMR spectrum of **9**

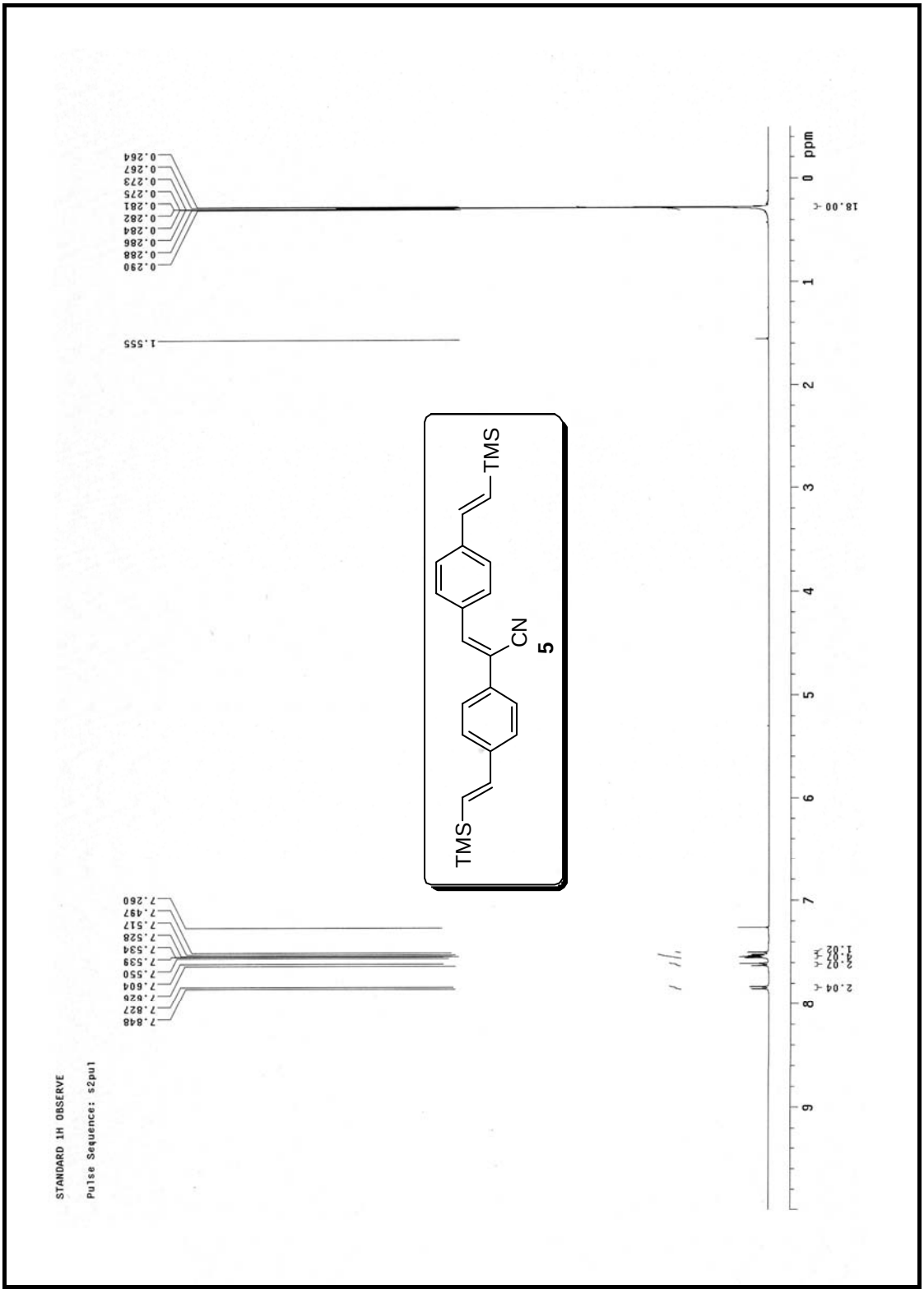

Fig. S7 ^{1}H NMR spectrum of **5**

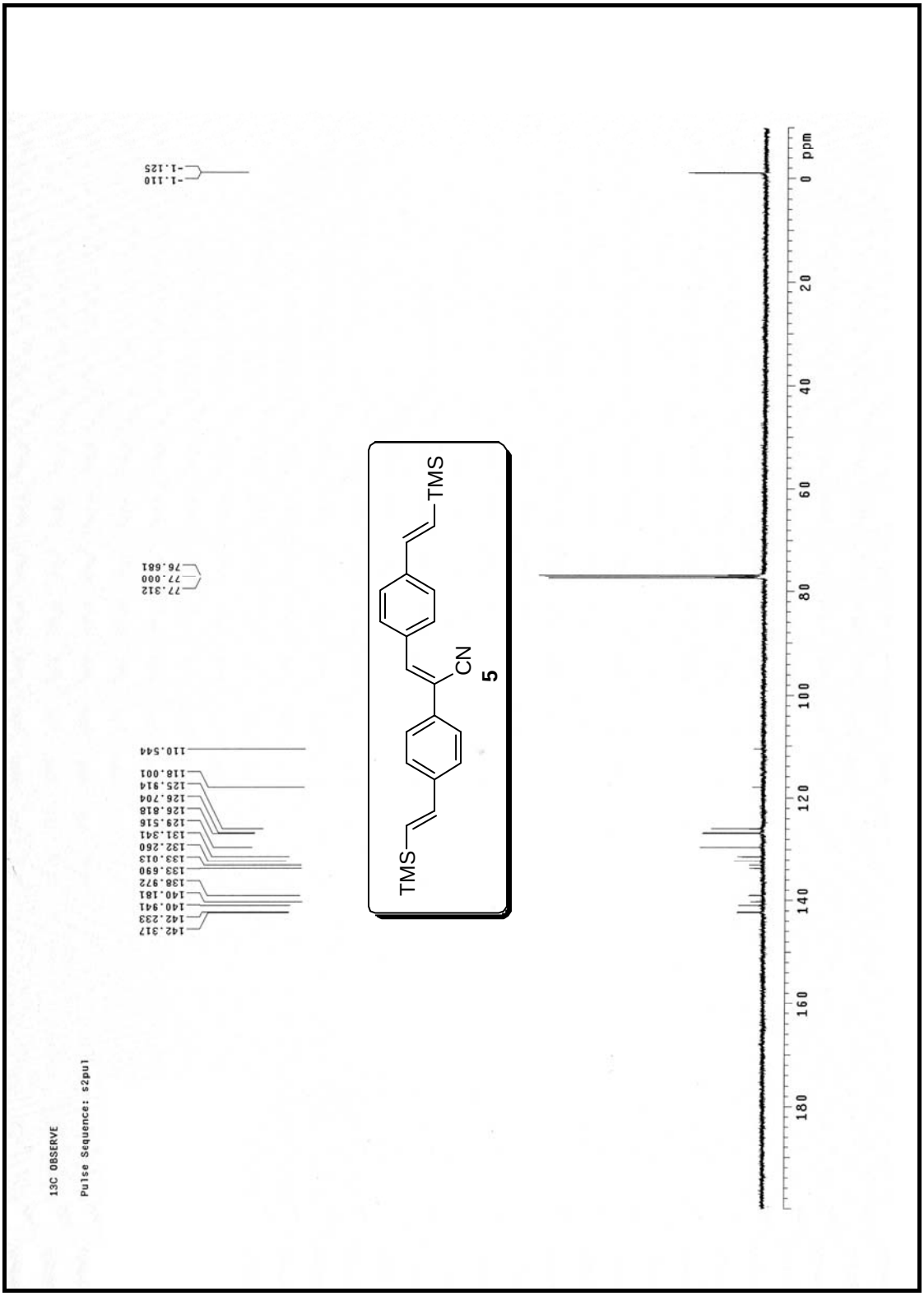

Fig. S8 ^{13}C NMR spectrum of **5**

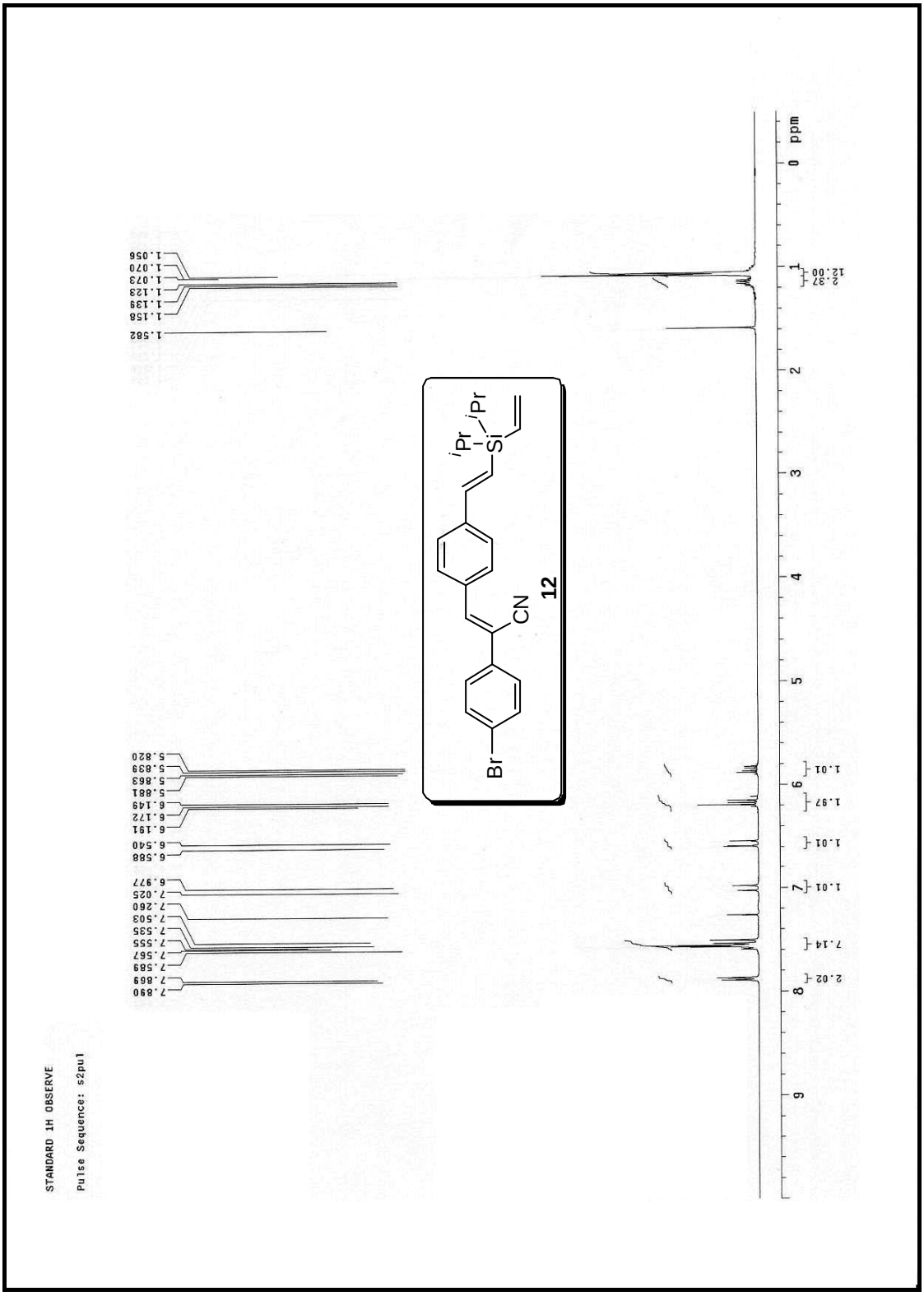

Fig. S9 ^{1}H NMR spectrum of **12**

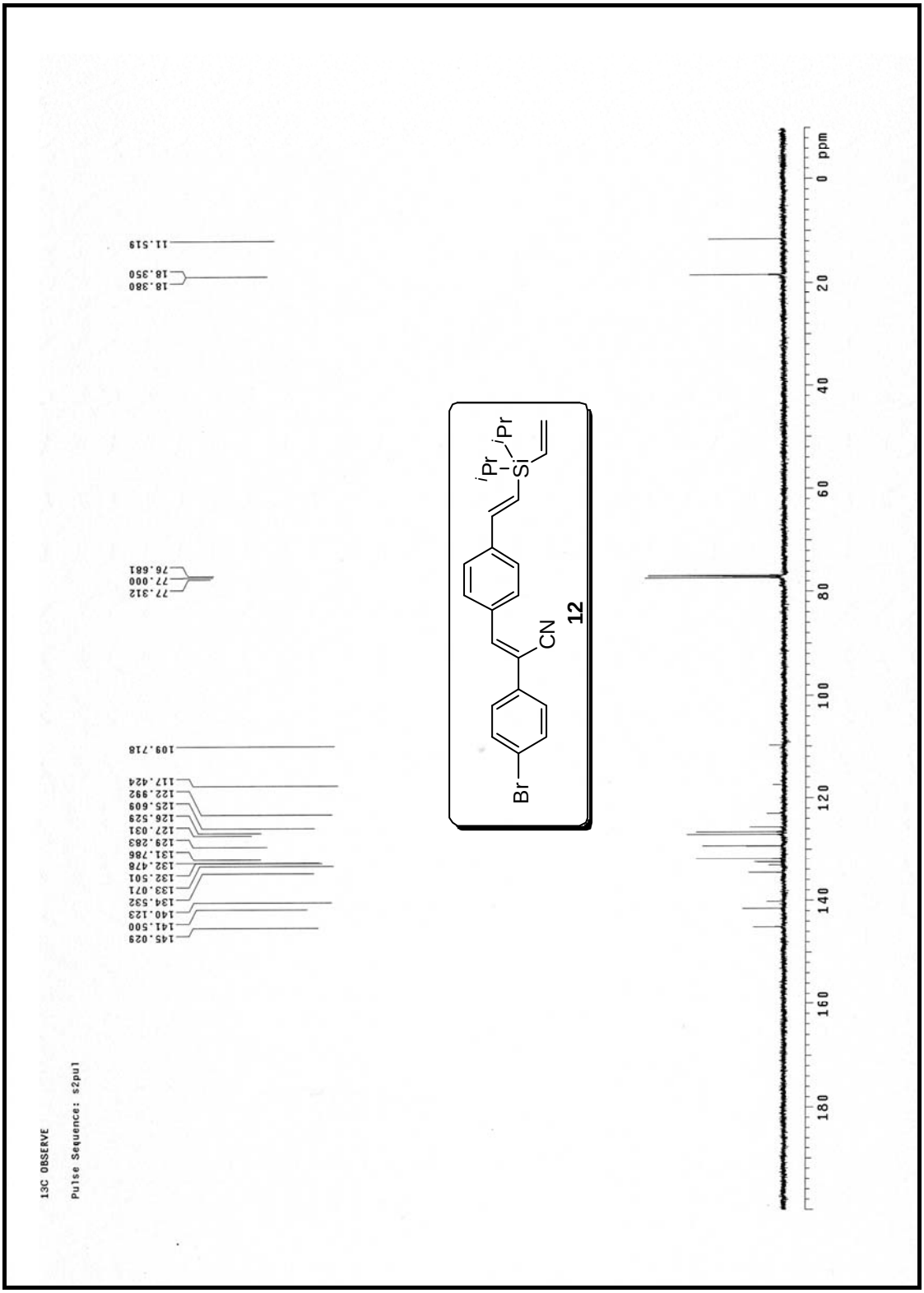

Fig. S10 ^{13}C NMR spectrum of **12**

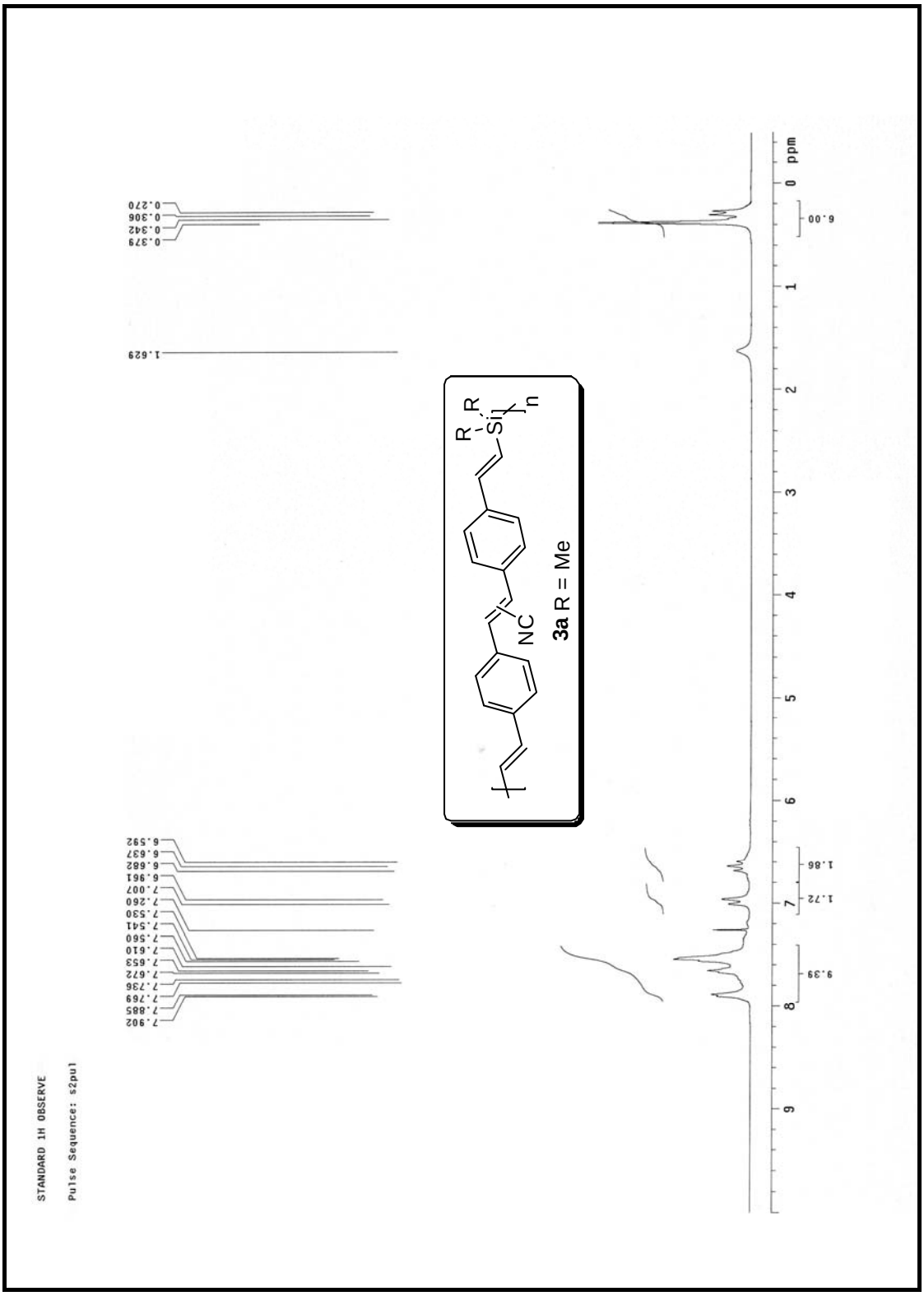

Fig. S11 ^{1}H NMR spectrum of **3a**

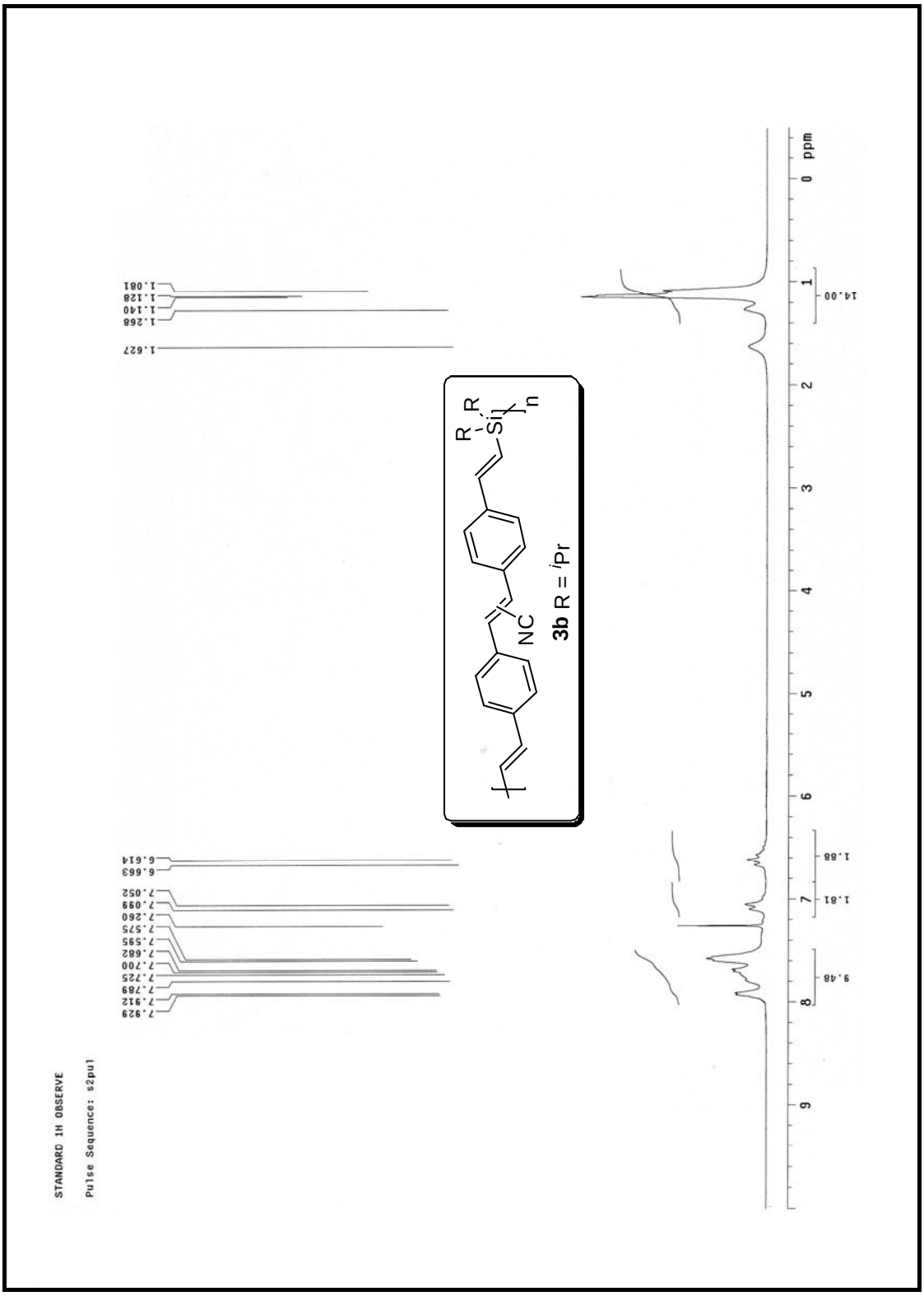

Fig. S12 ^{1}H NMR spectrum of **3b**

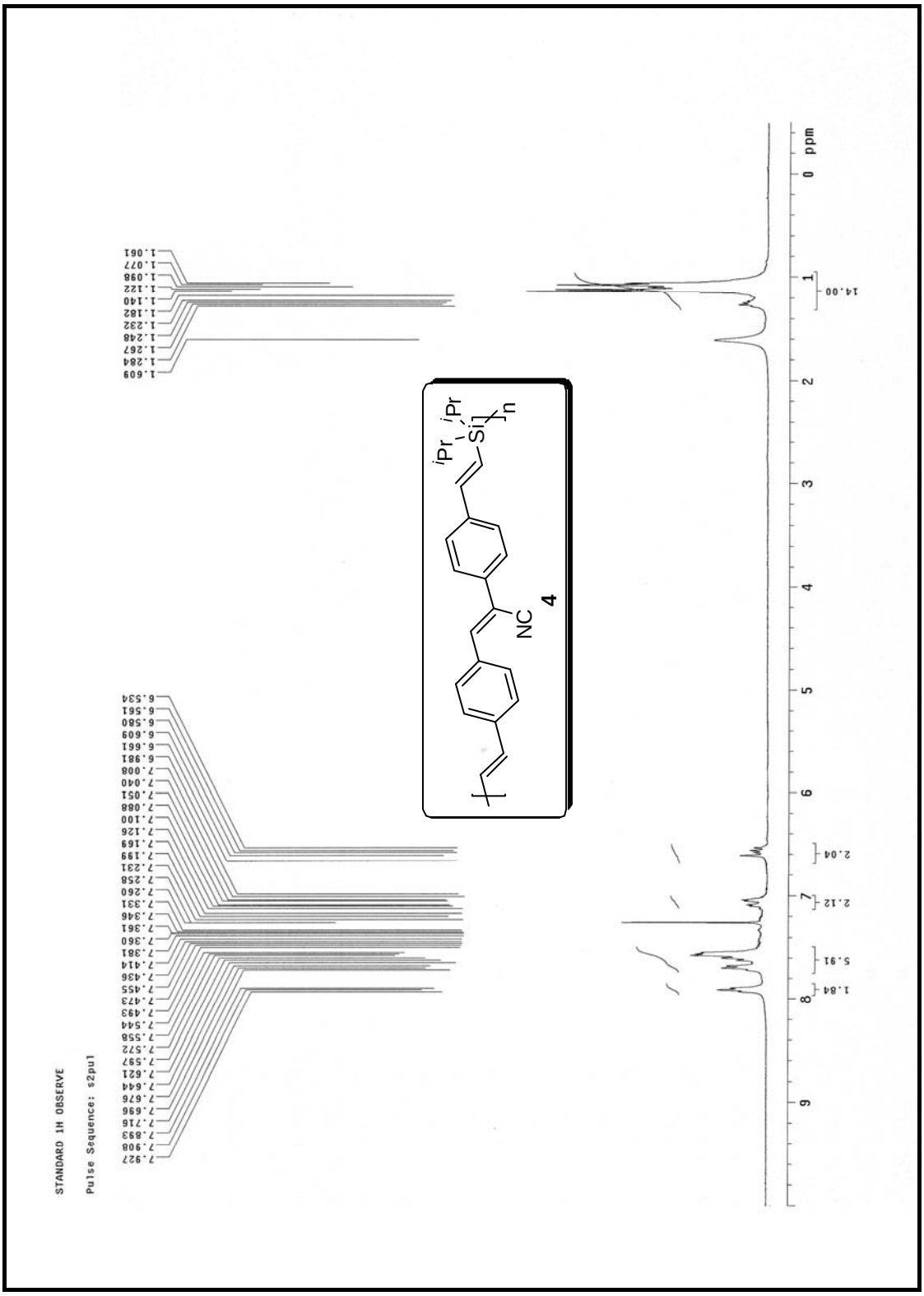

Fig. S13 ^{1}H NMR spectrum of **4**