

## Supporting Information

### Enediyne Isomers of Tetraethynylethene ( $C_{10}H_4$ )

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**General.** THF, previously distilled from CaH<sub>2</sub>, was freshly distilled from Na/benzophenone. Benzene and CH<sub>2</sub>Cl<sub>2</sub> were freshly distilled from CaH<sub>2</sub>. Air sensitive reactions were run under an atmosphere of N<sub>2</sub> and glassware was oven-dried overnight or flame-dried. Flash chromatography was conducted on silica gel. <sup>1</sup>H NMR spectra (300 MHz) and <sup>13</sup>C NMR spectra (75.4 MHz) were obtained in CDCl<sub>3</sub> and referenced to internal SiMe<sub>4</sub>.

**1,5-Bis(trimethylsilyl)-1,4-pentadiyn-3-ol (5).** Using the procedure of Rubin,<sup>1</sup> 21.2 mmol *n*-BuLi in hexane was added to a solution of trimethylsilylacetylene (21.2 mmol) in 60 mL THF at 0 °C. The colorless mixture was stirred for 15 min. at 0 °C. Methyl formate (10.6 mmol) was then added dropwise, and the bright yellow mixture was heated to near reflux using a heat gun. Once cooled to room temperature, the red mixture was poured into a separatory funnel containing 50 mL ethyl acetate and 50 mL sat. aqueous NH<sub>4</sub>Cl solution. The contents were mixed. The layers were separated and the organic layer was washed with 50 mL water and then 50 mL brine. The organic phase was dried with MgSO<sub>4</sub>, filtered and concentrated to reveal a deep red oil. This oil was purified via flash chromatography (CHCl<sub>3</sub>, silica) yielding 2.15 g (9.58 mmol, 90% yield) of **5** as a yellow oil. <sup>1</sup>H NMR δ 5.13 (d, *J* = 6.9 Hz, 1 H), 2.58 (d, *J* = 6.9 Hz, 1 H) 0.22 (s, 18 H). <sup>13</sup>C NMR δ 102.0, 89.7, 53.1, -0.2. EIMS (70 eV) *m/z*: M<sup>+</sup> 224 (17), 209 (19), 193 (30), 181 (62), 169 (75), 155 (25), 141 (75), 134 (94), 110 (49), 97 (82), 73 (100).

**1,5-Bis(trimethylsilyl)-1,4-pentadiyn-3-one (6).** Using the oxidation procedure of Rubin,<sup>1</sup> 5.0 mmol BaMnO<sub>4</sub> was added to a solution of 1,5-bis(trimethylsilyl)-1,4-pentadiyn-3-ol (**5**) (2.96 mmol) in 10 mL CH<sub>2</sub>Cl<sub>2</sub>. Thin layer chromatography indicated that this reaction was complete after two hours. The mixture was filtered through a short plug of silica gel. The filtrate was dried with MgSO<sub>4</sub>, filtered and concentrated to yield **6** (0.586 g, 2.63 mmol, 89%

yield) as colorless needles. When necessary, flash chromatography ( $\text{CHCl}_3$ , silica) can be used for further purification.  $^1\text{H}$  NMR  $\delta$  0.26 (s, 18 H).  $^{13}\text{C}$  NMR  $\delta$  160.5, 102.8, 99.5, -0.9. EIMS (70 eV)  $m/z$ :  $\text{M}^+$  222 (11), 207 (93), 179 (100), 155 (64), 97 (51), 73 (76).

**3-(Dibromomethylidene)-1,5-bis(trimethylsilyl)penta-1,4-diyne (7).**<sup>2</sup> Addition of triphenylphosphine (8.0 mmol) to a solution of carbon tetrabromide (4.0 mmol) in 100 mL dry  $\text{CH}_2\text{Cl}_2$  caused the solution to turn bright orange. A solution of 1,5-bis(trimethylsilyl)-1,4-pentadiyn-3-one (**6**) (2.63 mmol) in  $\text{CH}_2\text{Cl}_2$  (5 mL) was added to this mixture dropwise, resulting in a further color change to dark orange-red. After stirring for 1 h at room temperature, the reaction was complete, as monitored by TLC. The mixture was concentrated under reduced pressure to approximately 5-10 mL. After the addition of hexane (~10 mL), the reaction mixture was filtered through a short plug of silica. The filtrate was dried with  $\text{MgSO}_4$ , filtered and concentrated to reveal a yellow oil. This oil was further purified by flash chromatography (hexane, silica) yielding **7** (0.702 g) as a colorless oil (1.86 mmol, 71 % yield).  $^1\text{H}$  NMR  $\delta$  0.23 (s, 18 H).  $^{13}\text{C}$  NMR  $\delta$  114.5, 110.6, 102.8, 100.3, -0.26. EIMS  $m/z$ :  $\text{M}^+$  380/378/376 (5/9/5), 365/363/361 (6/13/6), 174 (8), 145 (100), 139/137 (24/24), 73 (29).

**1,6-Bis(trimethylsilyl)-3,4-bis[(trimethylsilyl)ethynyl]hex-3-ene-1,5-diyne (8).**<sup>2</sup> To a flask containing 3-(dibromomethylidene)-1,5-bis(trimethylsilyl)penta-1,4-diyne (**7**) (0.217 g, 0.574 mmol) was added 10 mL benzene, 0.232 mL *n*-BuNH<sub>2</sub> (2.28 mmol), 10.39 mg CuI (0.05 mmol), 31.5 mg Pd(PPh<sub>3</sub>)<sub>4</sub> (0.027 mmol) and 0.19 mL trimethylsilylacetylene (1.34 mmol). This mixture was stirred at room temperature for 12 h. The mixture was diluted with hexane, washed with 0.1 M HCl, water, and sat. aq. NaHCO<sub>3</sub> solution. The organic phase was dried with  $\text{MgSO}_4$ , filtered and concentrated under reduced pressure to reveal a black, oily solid, which was further purified via flash chromatography (3:1 hexane: $\text{CH}_2\text{Cl}_2$ ). The product **8** was isolated as

tan plates (131 mg, 0.317 mmol, 55% yield).  $^1\text{H}$  NMR  $\delta$  0.23 (s, 36 H).  $^{13}\text{C}$  NMR  $\delta$  119.0, 105.5, 101.2, 0.0. EIMS  $m/z$ : M<sup>+</sup> 412 (22), 309 (7), 73 (100). UV/vis  $\lambda_{\max}$  ( $\varepsilon$ , M<sup>-1</sup>cm<sup>-1</sup>) (MeOH) = 349.7 (24,746), 335.1 (17,438), 326.0 (13,596), 314.2 (8575), 285.5 (6026), 270.3 (6257), 261.8 (4790), 224.3 (10,377), 214.6 (7880) nm. IR (relative intensity) 2962 (41), 2900 (20), 2165 (17), 2146 (17), 1409 (11), 1251 (98), 1204 (73), 1037 (65), 849 (100) cm<sup>-1</sup>.

**3-(Bromomethylidene)-1,5-bis(trimethylsilyl)penta-1,4-diyne (9).**<sup>3</sup> A solution of dibromoolefin (**7**) (1.86 mmol) in THF (15 mL) was cooled to -78 °C. A 2.3 M *n*-BuLi solution in hexane (1.86 mmol) was added dropwise to this solution (turning first dark pink, then dark purple). This mixture was stirred at -78 °C for 1 h. Solid NH<sub>4</sub>Cl (1.0 g) was added at -78 °C and sat. NH<sub>4</sub>Cl solution was slowly added with warming to room temperature. Ether (30 mL) was added and the layers separated. The organic phase was dried with MgSO<sub>4</sub>, filtered, and concentrated to reveal **9** as a yellow oil. This oil was purified via flash chromatography (hexane, silica). Compound **9** was isolated as a pale yellow oil (0.327 g, 1.10 mmol) in 59% yield.  $^1\text{H}$  NMR  $\delta$  7.00 (s, 1 H), 0.25 (s, 9 H), 0.21 (s, 9H).  $^{13}\text{C}$  NMR  $\delta$  125.0, 112.6, 102.5, 100.0, 99.3, 95.9, -0.10, -0.13. EIMS (70 eV)  $m/z$ : M<sup>+</sup> 298/300 (42/44), 283/285 (47/49), 97 (38), 73 (31).

## Notes and References

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- (3) Eisler, S.; Chahal, N.; McDonald, R.; Tykwinski, R. R. *Chem. Eur. J.* **2003**, 9, 2542-2550.

**Table S1.** Results of B3LYP/6-31G\* calculations: energy (Hartrees), relative energy vs. enyne **3** (kcal/mol), dipole moment (in Debye), and Cartesian coordinates.

<b>3,4-Diethynyl-hex-3-ene-1,5-diyne (1)</b>			
E = -383.161917348 Hartrees			
Relative Energy = 22.4 kcal/mol			
Dipole Moment = 0.0 D			
C	0.000000	2.219124	2.110229
C	0.000000	1.214437	1.435871
H	0.000000	3.113996	2.690366
C	0.000000	0.000000	0.691609
C	0.000000	-1.214437	1.435871
C	0.000000	-2.219124	2.110229
H	0.000000	-3.113996	2.690366
C	0.000000	0.000000	-0.691609
C	0.000000	-1.214437	-1.435871
C	0.000000	-2.219124	-2.110229
H	0.000000	-3.113996	-2.690366
C	0.000000	1.214437	-1.435871
C	0.000000	2.219124	-2.110229
H	0.000000	3.113996	-2.690366

<b>3-Ethynyl-oct-3-ene-1,5,7-triyne (2)</b>			
E = -383.179829356 Hartrees			
Relative Energy = 11.2 kcal/mol			
Dipole Moment = 0.16 D			
C	-3.299417	2.399979	0.000000
C	-2.374839	1.619371	0.000000
H	-4.113055	3.089526	0.000000
C	-1.300701	0.678275	0.000000
C	-1.644606	-0.706725	0.000000
C	-1.967703	-1.872315	0.000000
H	-2.238889	-2.903808	0.000000
C	0.000000	1.113010	0.000000
H	0.175521	2.186777	0.000000
C	1.123882	0.274153	0.000000
C	2.133734	-0.414680	0.000000
C	3.252830	-1.190136	0.000000
C	4.251435	-1.881711	0.000000
H	5.128727	-2.487816	0.000000

**Table S1.** (continued)

<b><i>trans-Dec-5-ene-1,3,7,9-tetrayne (3)</i></b>			
E = -383.197629685 Hartrees			
Relative Energy = 0.0 kcal/mol			
Dipole Moment = 0.0 D			
C	-0.156162	5.620038	0.000000
C	-0.008986	4.414546	0.000000
H	-0.284477	6.678570	0.000000
C	0.156162	3.062318	0.000000
C	0.298756	1.848765	0.000000
C	0.504504	0.456724	0.000000
H	1.535707	0.106154	0.000000
C	-0.504504	-0.456724	0.000000
H	-1.535707	-0.106154	0.000000
C	-0.298756	-1.848765	0.000000
C	-0.156162	-3.032318	0.000000
C	0.008986	-4.414546	0.000000
C	0.156162	-5.620038	0.000000
H	0.284477	-6.678570	0.000000

<b><i>cis-Dec-5-ene-1,3,7,9-tetrayne (4)</i></b>			
E = -383.196334083 Hartrees			
Relative Energy = 0.8 kcal/mol			
Dipole Moment = 0.10 D			
C	0.000000	3.804149	-2.045287
C	0.000000	3.067944	-1.079514
H	0.000000	4.450259	-2.893470
C	0.000000	2.242837	0.004449
C	0.000000	1.496013	0.971113
C	0.000000	0.680804	2.117990
H	0.000000	1.189444	3.080965
C	0.000000	-0.680804	2.117990
H	0.000000	-1.189444	3.080965
C	0.000000	-1.496013	0.971113
C	0.000000	-2.242837	0.004449
C	0.000000	-3.067944	-1.079514
C	0.000000	-3.804149	-2.045287
H	0.000000	-4.450259	-2.893470

**Table S2.** Results of MP2 calculations: energy (Hartrees), relative energy vs. enyne **3** (kcal/mol), dipole moment (Debye) and Cartesian coordinates.

<b>3,4-Diethynyl-hex-3-ene-1,5-diyne (1)</b>			
E = -380.707698118 Hartrees			
Relative Energy = 14.0 kcal/mol			
Dipole Moment = 0.0 D			
C	0.000000	2.259496	2.073959
C	0.000000	1.221387	1.425455
H	0.000000	3.164153	2.640313
C	0.000000	0.000000	0.690445
C	0.000000	-1.221387	1.425455
C	0.000000	-2.259496	2.073959
H	0.000000	-3.164153	2.640313
C	0.000000	0.000000	-0.690445
C	0.000000	-1.221387	-1.425455
C	0.000000	-2.259496	-2.073959
H	0.000000	-3.164153	-2.640313
C	0.000000	1.221387	-1.425455
C	0.000000	2.259496	-2.073959
H	0.000000	3.164153	-2.640313

<b>3-Ethynyl-oct-3-ene-1,5,7-triyne (2)</b>			
E = -380.719059229 Hartrees			
Relative Energy = 6.8 kcal/mol			
Dipole Moment = 0.09 D			
C	3.211006	-2.562326	0.000000
C	2.200559	-1.872365	0.000000
H	4.082996	-3.177655	0.000000
C	1.023574	-1.062075	0.000000
C	-0.241771	-1.724686	0.000000
C	-1.323835	-2.295946	0.000000
H	-2.266367	-2.796781	0.000000
C	1.122619	0.304829	0.000000
H	2.116755	0.750329	0.000000
C	0.000000	1.155944	0.000000
C	-0.964345	1.927295	0.000000
C	-2.038272	2.772477	0.000000
C	-3.004767	3.529033	0.000000
H	-3.841989	4.191032	0.000000

**Table S2.** (continued)

<b><i>trans-Dec-5-ene-1,3,7,9-tetrayne (3)</i></b>			
E = -380.729968586 Hartrees			
Relative Energy = 0.0 kcal/mol			
Dipole Moment = 0.0 D			
C	-0.165006	5.642321	0.000000
C	-0.004980	4.425759	0.000000
H	-0.291766	6.702123	0.000000
C	0.165006	3.068627	0.000000
C	0.318590	1.844256	0.000000
C	0.515607	0.444272	0.000000
H	1.538776	0.069692	0.000000
C	-0.515607	-0.444272	0.000000
H	-1.538776	-0.069692	0.000000
C	-0.318590	-1.844256	0.000000
C	-0.165006	-3.068627	0.000000
C	0.004980	-4.425759	0.000000
C	0.165006	-5.642321	0.000000
H	0.291766	-6.702123	0.000000

<b><i>cis-Dec-5-ene-1,3,7,9-tetrayne (4)</i></b>			
E = -380.728364548 Hartrees			
Relative Energy = 1.0 kcal/mol			
Dipole Moment = 0.18 D			
C	0.000000	3.646754	-2.126972
C	0.000000	2.948252	-1.118044
H	0.000000	4.243224	-3.012032
C	0.000000	2.175948	0.010406
C	0.000000	1.460630	1.016068
C	0.000000	0.680874	2.195361
H	0.000000	1.203021	3.151111
C	0.000000	-0.680874	2.195361
H	0.000000	-1.203021	3.151111
C	0.000000	-1.460630	1.016068
C	0.000000	-2.175948	0.010406
C	0.000000	-2.948252	-1.118044
C	0.000000	-3.646754	-2.126972
H	0.000000	-4.243224	-3.012032

**Table S3.** Computed vibrational frequencies (B3LYP/6-31G\*).

3,4-Diethynyl-hex-3-ene-1,5-diyne (1)		3-Ethynyl-oct-3-ene-1,5,7-triyne (2)	
frequency (cm <sup>-1</sup> )	intensity (km/mol)	frequency (cm <sup>-1</sup> )	intensity (km/mol)
3494.2587	0.0000	3494.3540	29.2625
3494.1176	119.3012	3493.4264	208.5236
3493.3014	177.8918	3493.2959	55.4862
3493.0903	0.0000	3181.7639	7.2261
2237.6689	3.1972	2308.9029	1.2736
2215.0515	26.9280	2224.1940	3.6170
2210.4365	0.0000	2216.1285	8.7553
2208.9666	0.0000	2168.9445	4.7288
1544.7773	0.0000	1593.5779	2.1022
1307.3458	0.0000	1368.5518	8.3308
1175.6358	46.2219	1246.1736	3.6684
995.4174	23.4379	1192.6047	24.5803
752.5746	0.0000	875.6250	19.9750
633.1083	39.9512	814.8421	13.8356
631.6827	0.0000	788.9690	2.1664
631.3570	0.0000	726.9660	0.5613
630.5867	106.9679	681.5752	3.1508
629.2753	34.5128	675.9321	0.3871
619.0083	0.0000	638.2477	42.2588
594.1227	1.3585	631.0840	34.5787
586.9823	0.0000	590.3846	2.4880
583.5934	148.2395	588.5716	10.1107
576.1358	0.0000	581.9545	46.2958
568.4864	0.0000	580.8584	62.7778
517.6437	0.0000	578.5341	60.7716
517.0633	0.0000	496.0925	0.0793
466.2974	0.0000	460.9838	1.9722
419.9798	6.7745	427.1202	3.3257
391.7788	0.0000	385.8763	0.0006
275.7213	0.0000	273.0084	1.0364
256.8944	0.0000	266.6766	6.7402
151.9281	5.2097	190.0834	0.0008
145.7719	3.4613	173.0861	1.0305
122.3087	0.0000	130.2700	1.7886
112.5485	0.1677	66.6482	0.7138
75.4927	0.0000	56.5537	0.3169

**Table S3.** (continued)

<b><i>trans</i>-Dec-5-ene-1,3,7,9-tetrayne (<b>3</b>)</b>	<b><i>cis</i>-Dec-5-ene-1,3,7,9-tetrayne (<b>4</b>)</b>
frequency (cm <sup>-1</sup> )	intensity (km/mol)
3494.9300	0.0000
3494.5122	313.1642
3173.4365	17.0689
3166.2222	0.0000
2326.4744	0.0491
2295.8131	0.0000
2173.6167	8.9317
2167.8240	0.0000
1636.2742	0.0000
1329.8440	3.3268
1324.2245	0.0000
1252.8973	1.2495
1205.8200	0.0000
963.5838	38.4831
864.9420	0.0000
856.3632	0.0000
734.2790	10.3262
717.6531	3.9288
704.2626	0.0000
671.7046	0.5904
667.8461	0.0000
586.1346	101.5152
585.3824	0.0000
578.5644	95.9845
576.9169	0.0000
500.8577	1.8333
487.0433	3.8426
416.0659	0.0000
382.4834	0.0000
257.1422	0.0000
232.2055	6.0260
229.4849	4.2446
151.6821	0.0000
110.3650	0.0000
44.8204	0.4450
43.4791	0.4024
	3494.7264
	3494.2657
	3177.6522
	3162.2902
	2326.1874
	2299.0884
	2173.6158
	2169.4401
	1621.8445
	1453.5034
	1277.1816
	1227.0496
	1144.7564
	945.2625
	860.2243
	777.9594
	716.8071
	697.6365
	679.4351
	663.5131
	660.3894
	608.3283
	580.6758
	579.6527
	579.4988
	578.7112
	551.1763
	417.0151
	380.1641
	291.6904
	290.6612
	195.9472
	162.3739
	109.2286
	99.6082
	34.5358
	109.9968
	127.0994
	15.8565
	3.9673
	0.6536
	3.9010
	6.1137
	3.6939
	8.8242
	8.1686
	0.0720
	1.7575
	0.6466
	0.0000
	14.6857
	30.4042
	0.0000
	0.0291
	1.2332
	0.0451
	1.7213
	7.3908
	35.0501
	101.1420
	0.0000
	56.1355
	0.0000
	0.5458
	0.2264
	0.0000
	0.3930
	2.5875
	8.0093
	2.5090
	0.0000
	0.0617

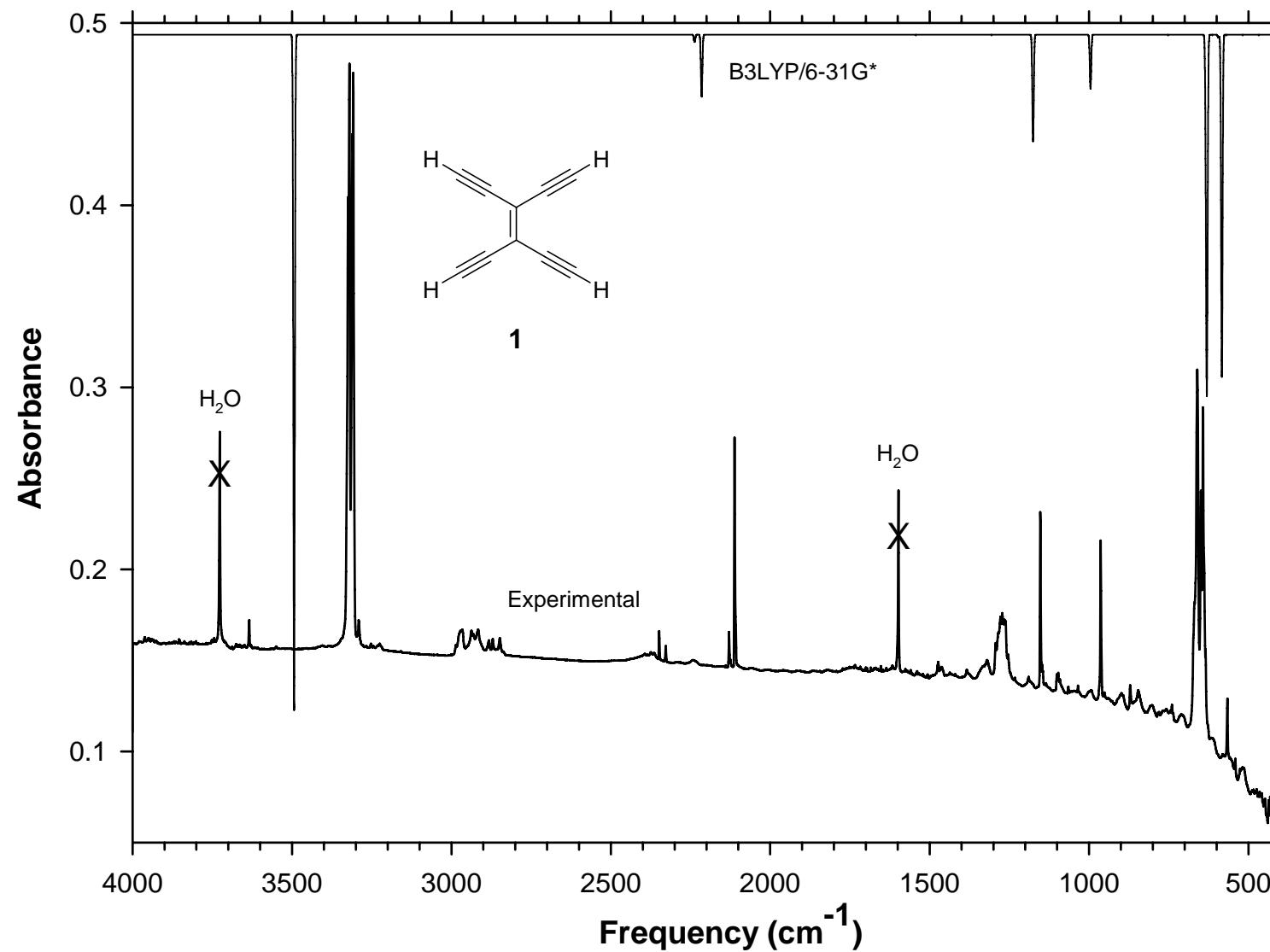
**Table S4.** Observed infrared frequencies for **1-4**.

<b>3,4-Diethynyl-hex-3-ene-1,5-diyne (1)</b> frequency (cm <sup>-1</sup> )	intensity (relative)	<b>3-Ethynyl-oct-3-ene-1,5,7-triyne (2)</b> frequency (cm <sup>-1</sup> )	intensity (relative)
3324.9	75	3312.3	100
3320.1	100	2206.4	1
3311.5	88	2122.3	3
3308.3	66	1325.0	4
2129.0	6	1196.8	7
2111.8	38	1162.0	14
1153.2	28	852.5	4
963.6	25	769.8	4
660.6	56	758.9	3
649.0	38	670.2	23
642.9	50	647.8	21

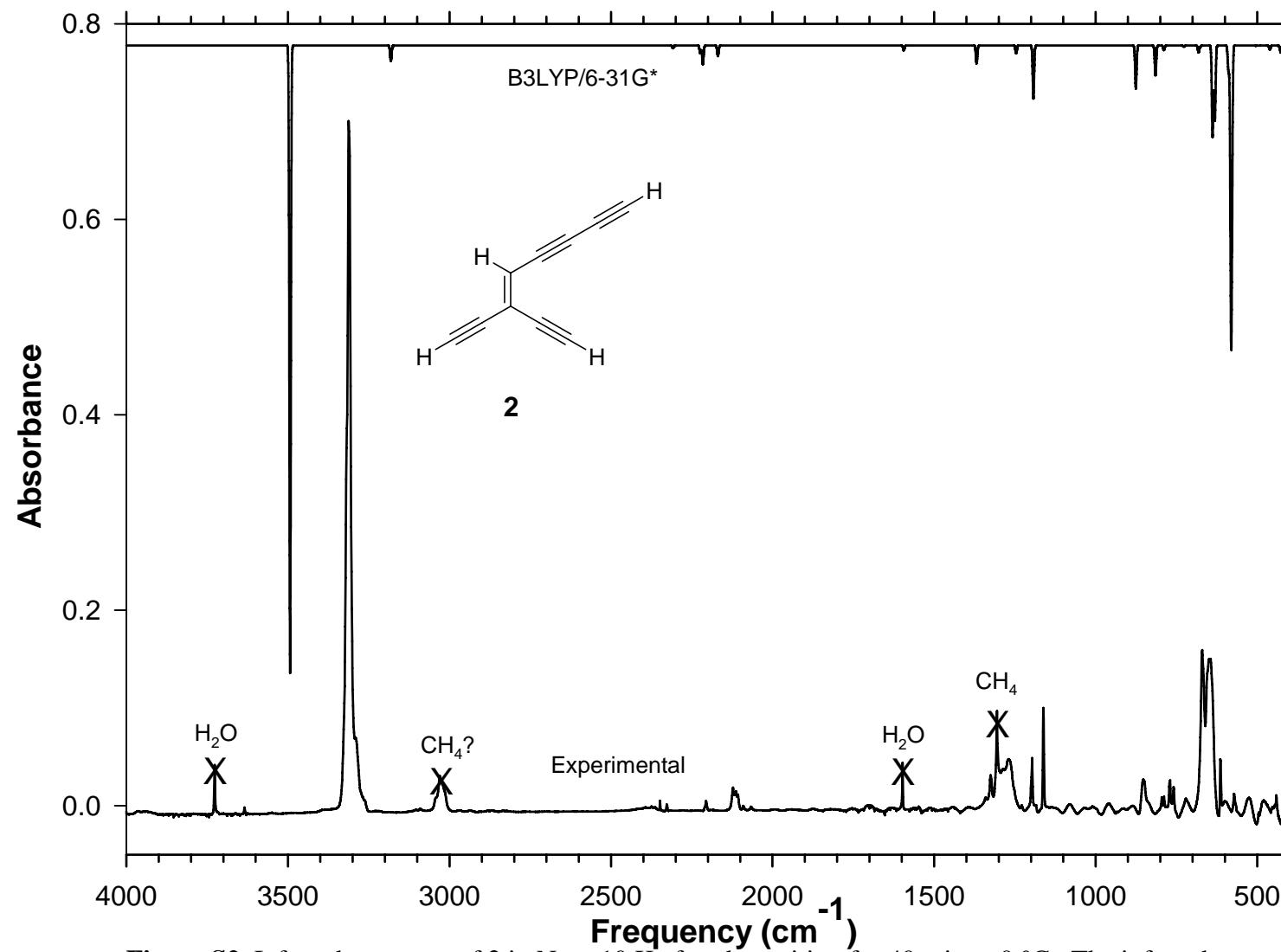
<b>trans-Dec-5-ene-1,3,7,9-tetrayne (3)</b> frequency (cm <sup>-1</sup> )	intensity (relative)	<b>cis-Dec-5-ene-1,3,7,9-tetrayne (4)</b> frequency (cm <sup>-1</sup> )	intensity (relative)
3320.8	66	3316.5	100
3315.7	100	3305.0	97
3309.5	66	2193.0	3
3302.6	84	2188.0	3
2068.3	3	2066.9	3
1254.7	32	1685.1	7
1206.3	13	1571.0	3
1203.4	13	1401.4	7
948.7	3	1258.1	17
938.3	18	1179.5	10
934.3	18	834.2	7
643.3	45	750.0	23
637.3	50	634.4	73
632.3	66		

**Table S5.** Observed absorption maxima for the electronic spectra of **1-4**.

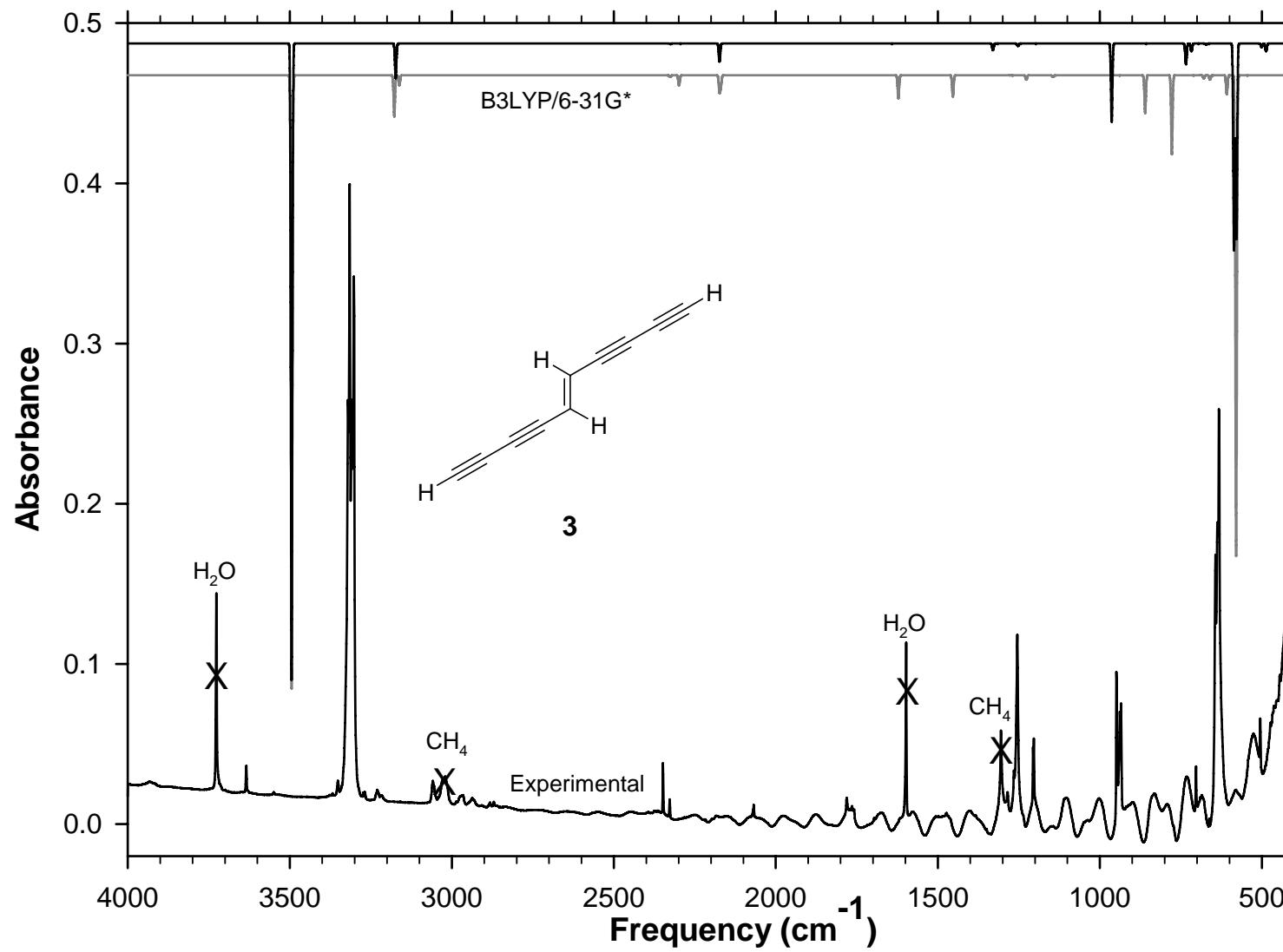
<b>1</b> $\lambda_{\text{max}}$ (nm)	<b>2</b> $\lambda_{\text{max}}$ (nm)	<b>3</b> $\lambda_{\text{max}}$ (nm)	<b>4</b> $\lambda_{\text{max}}$ (nm)
330.5	315.0	322.2	322.9
317.0	303.1	315.5	316.0
309.0	296.0	302.2	305.6
305.0	285.2	295.9	302.4
298.0	278.9	284.2	296.4
293.8	269.4	278.5	284.4
290.9	263.8	267.7	279.0
287.0	232.0	263.2	268.2
282.8	224.7	234.3	263.5
280.4	220.9	223.5	235.5
277.0	210.0	212.6	223.5
273.9		212.4	213.5
271.0		203.4	204.5



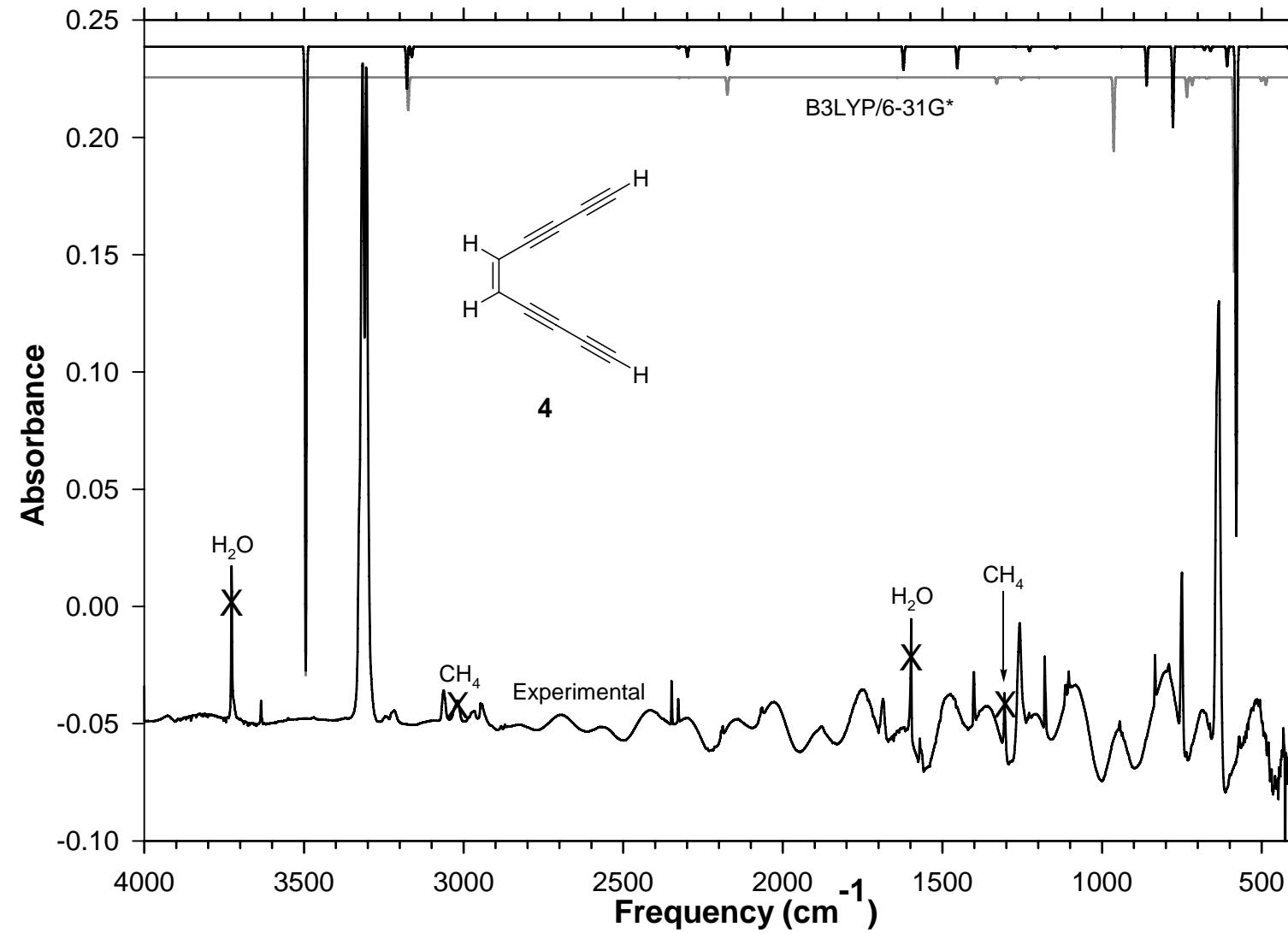
**Figure S1.** Infrared spectrum of **1** in N<sub>2</sub> at 10 K after deposition for 40 min at 0 °C. The experimental infrared frequencies of tetraethynylethene (**1**) correlate well with those predicted by density functional theory (B3LYP/6-31G\* (unscaled)).



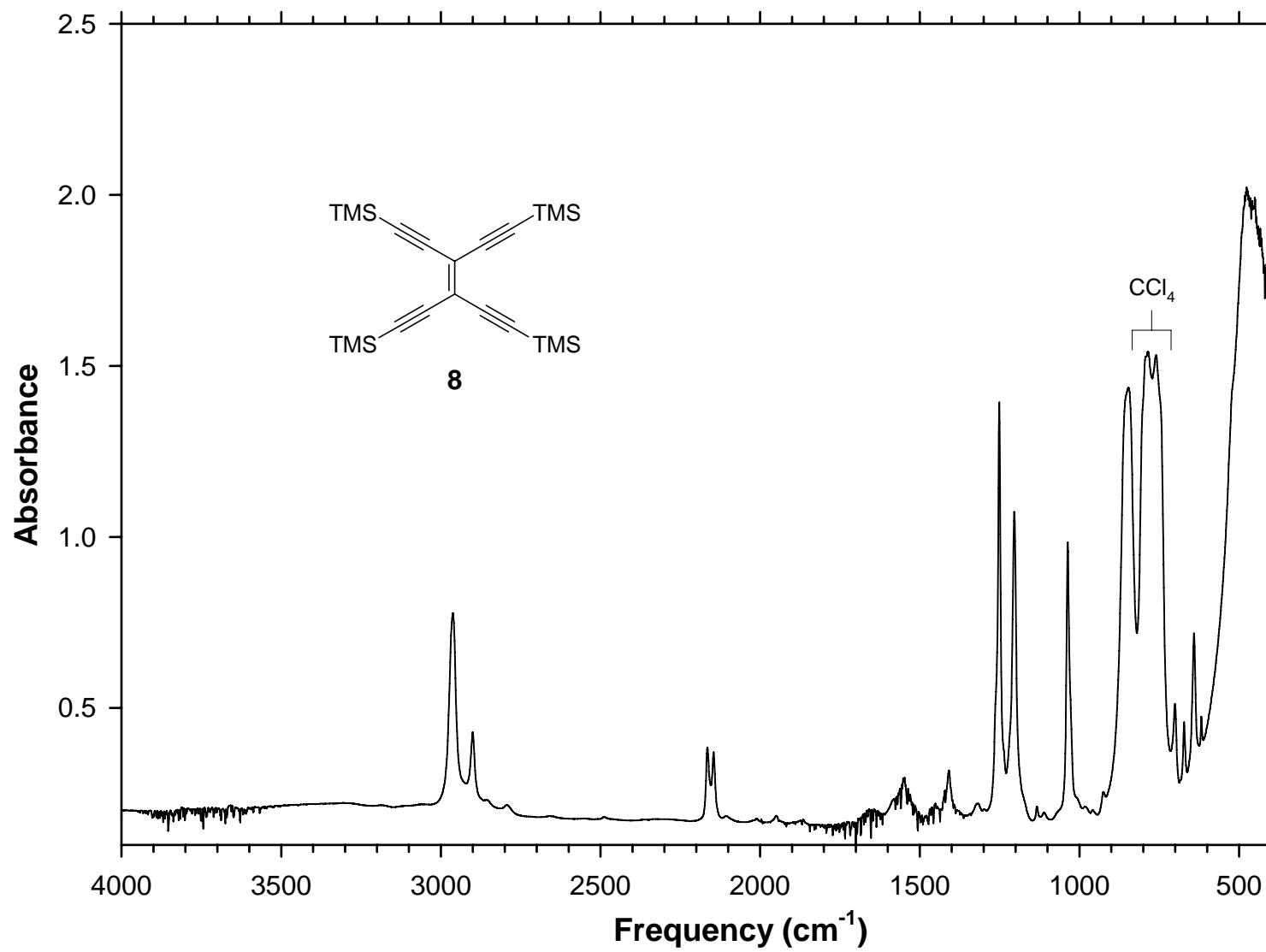
**Figure S2.** Infrared spectrum of **2** in  $\text{N}_2$  at 10 K after deposition for 40 min at 0 °C. The infrared frequencies observed for **2** are in reasonable agreement with those computed using density functional theory (B3LYP/6-31G\* (unscaled)). The methane contaminant from prior experiments may be overlapping with a vinyl C-H stretch.



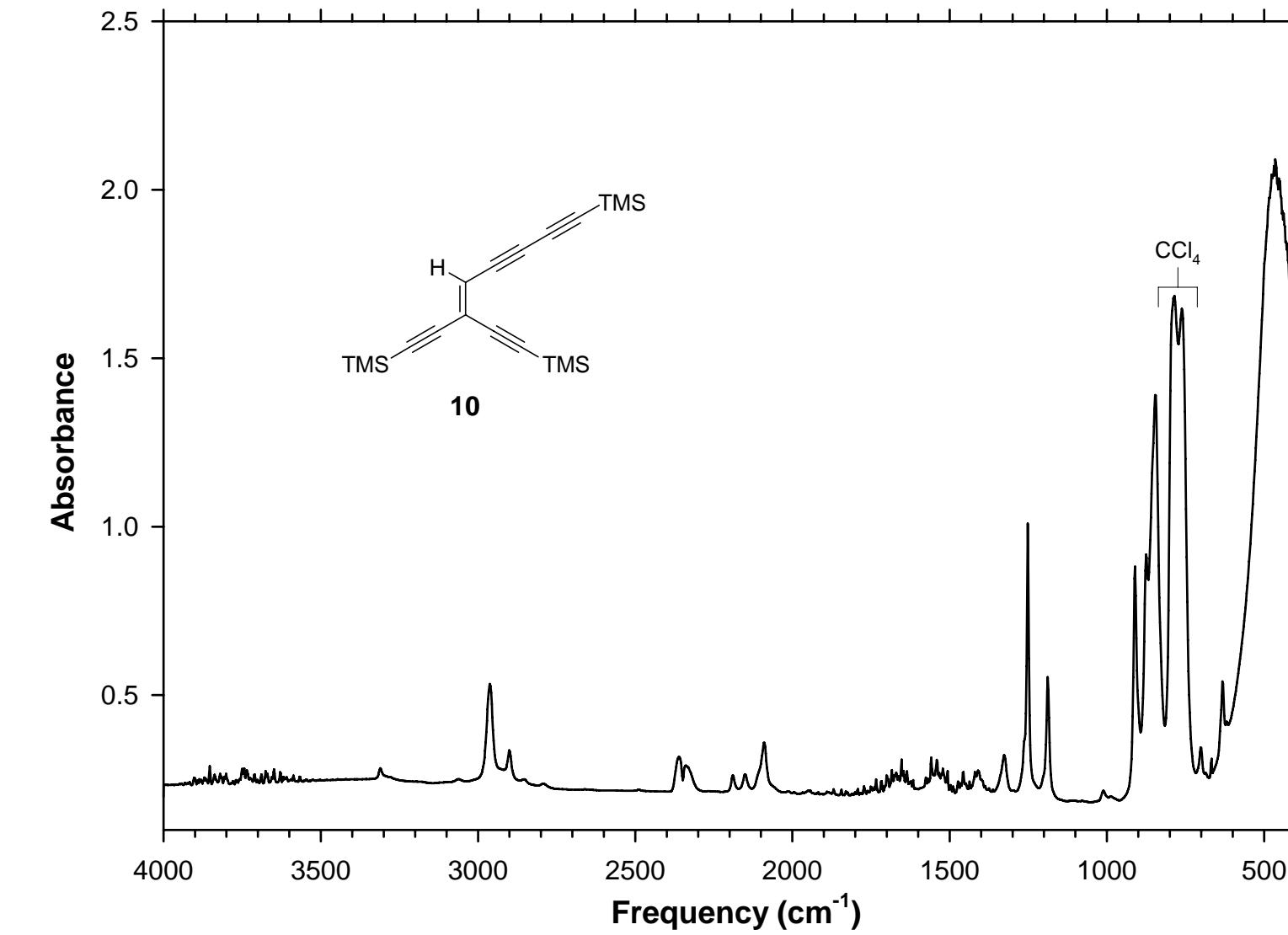
**Figure S3.** An infrared spectrum of **3** in N<sub>2</sub> at 10 K after deposition for 60 min at 0 °C. The spectrum of **3** correlates well with the computed frequencies (B3LYP/6-31G\*) for **3** (black) and not as well with those computed for **4** (gray). The absorptions in the 1200 cm<sup>-1</sup> region likely represent combination bands, and therefore, are not predicted by our calculations. The methane contaminant is a remnant from a previous study.



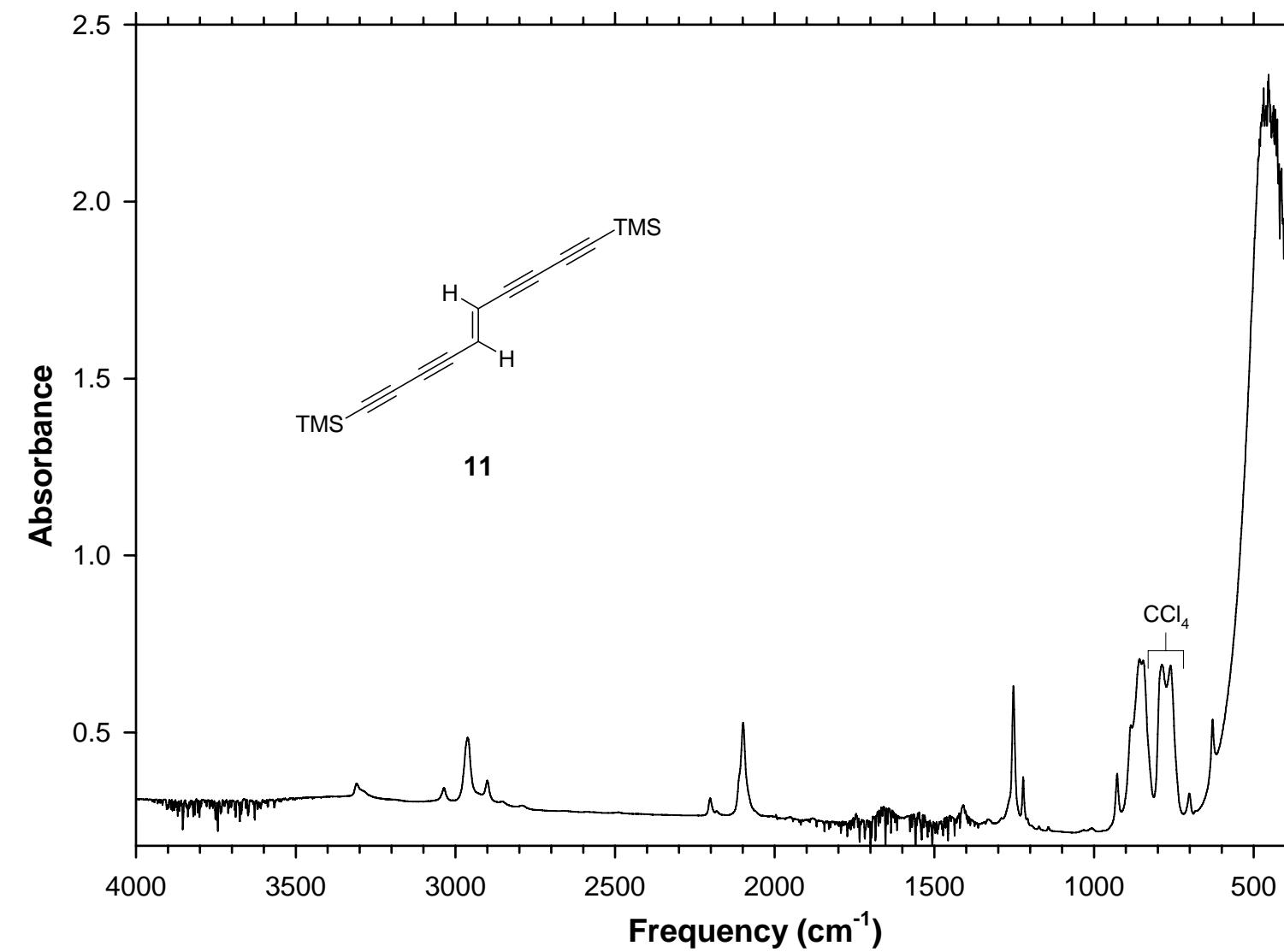
**Figure S4.** Infrared spectrum of **4** in  $\text{N}_2$  at 10 K after deposition for 45 min at 0 °C. The observed vibrational frequencies for **4** correlate well with the computed frequencies (B3LYP/6-31G\*) for **4** (black) and not as well with those computed for **3** (gray). The absorptions in the  $1200 \text{ cm}^{-1}$  region likely represent combination bands, and therefore, are not predicted by our calculations. The methane contaminant is a remnant from a previous study and can be disregarded.



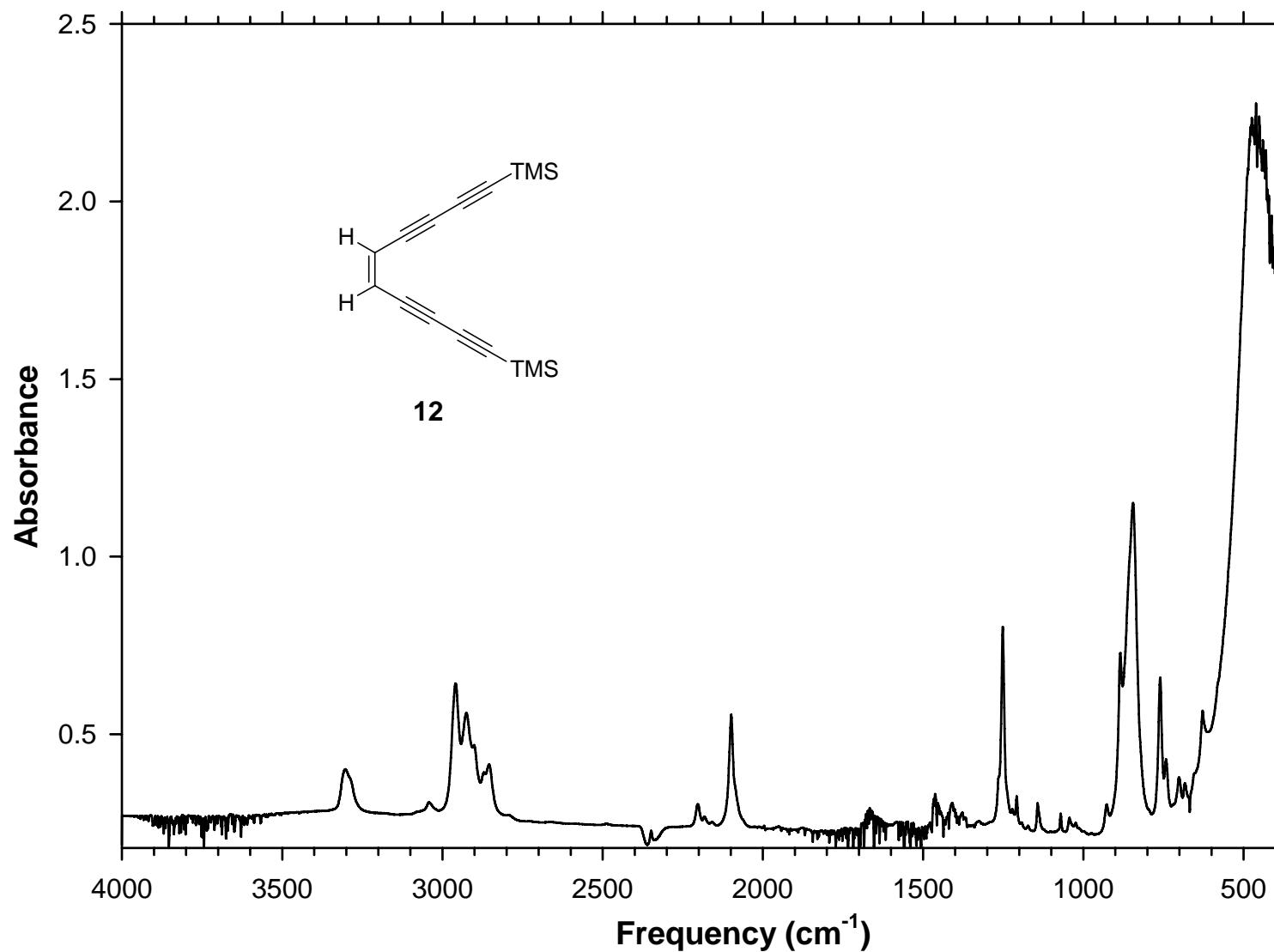
**Figure S5.** Infrared spectrum of **8** in CCl<sub>4</sub> at room temperature.



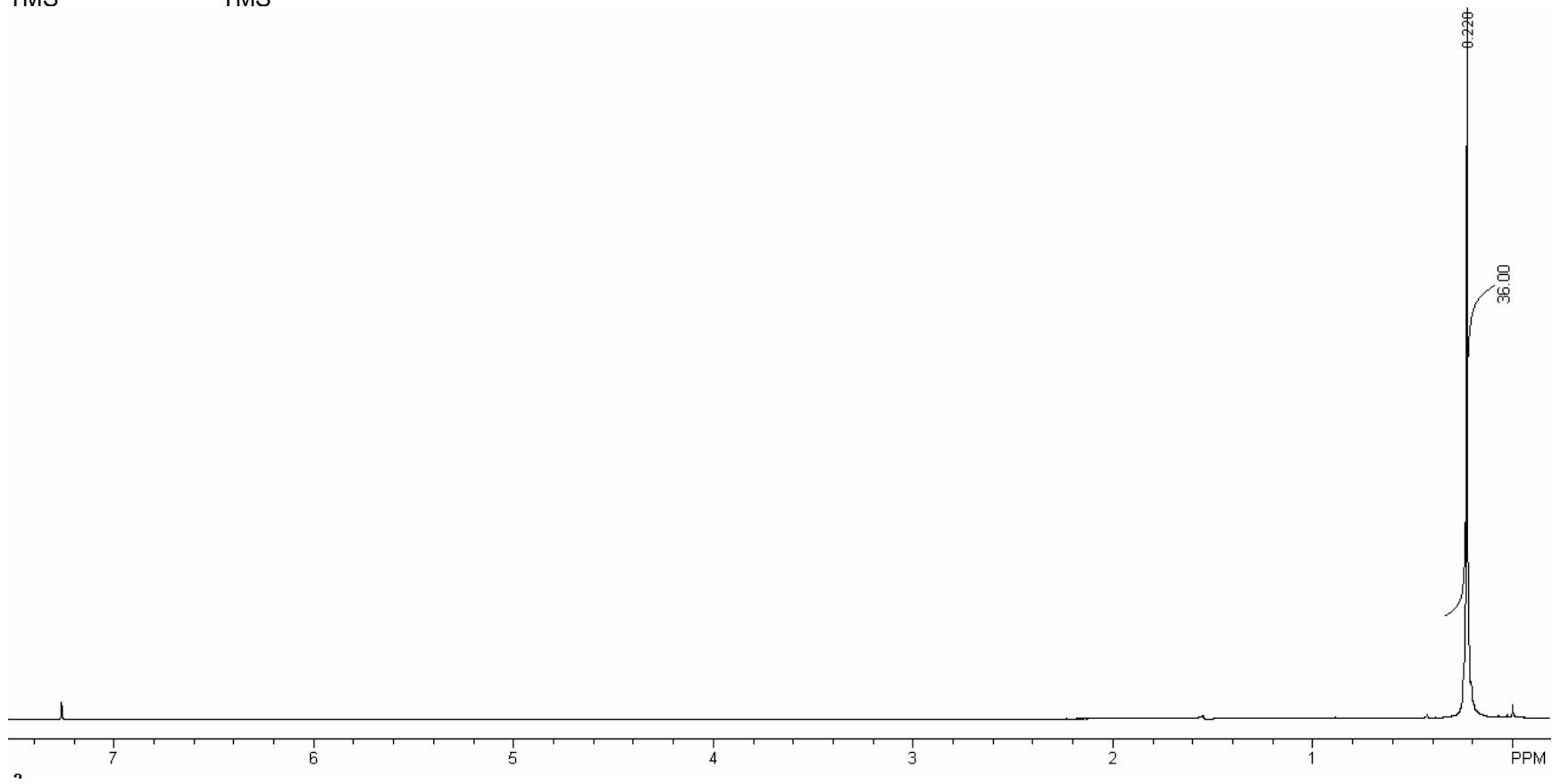
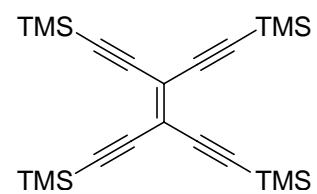
**Figure S6.** Infrared spectrum of **10** in  $\text{CCl}_4$  at room temperature.

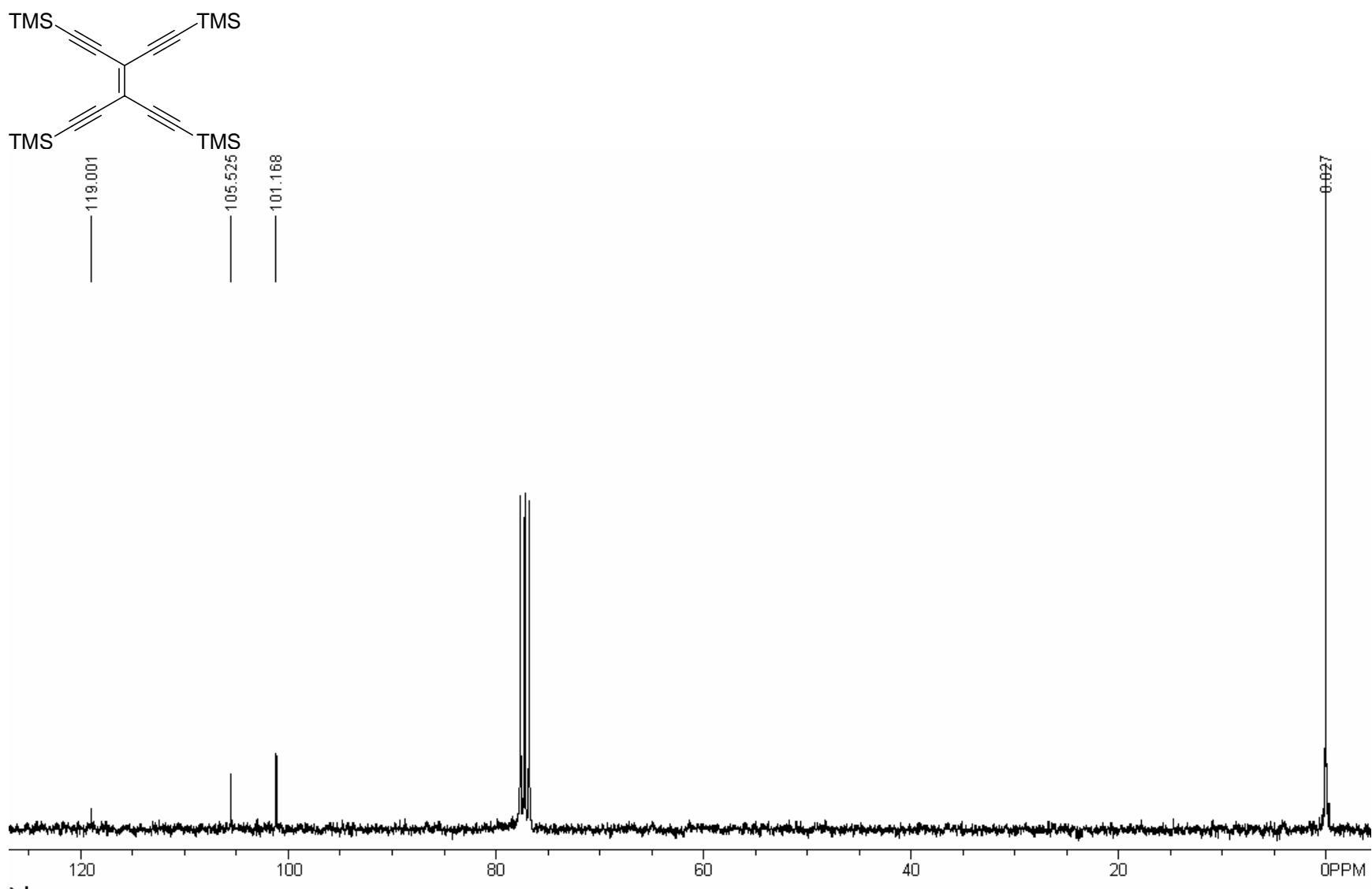


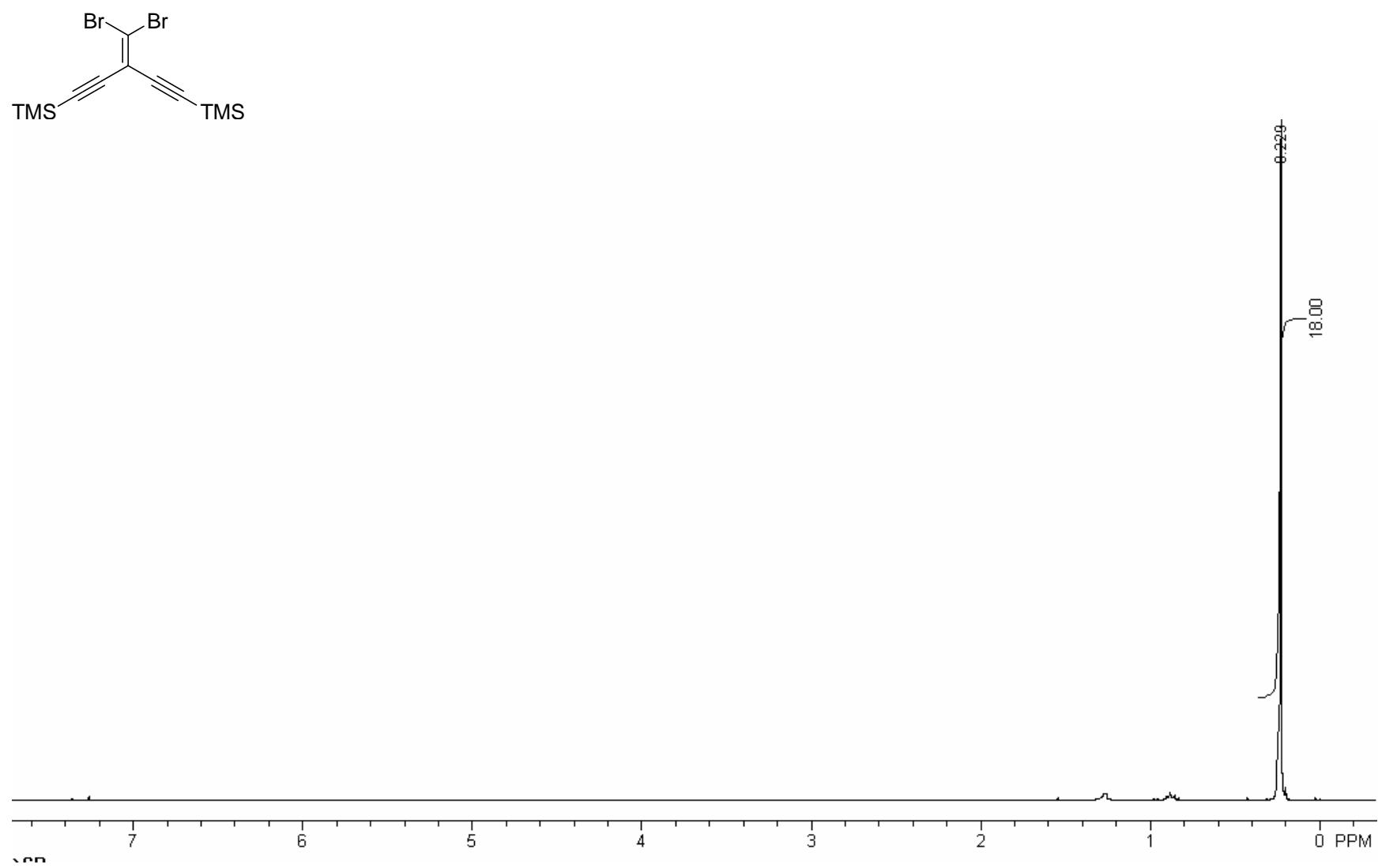
**Figure S7.** Infrared spectrum of **11** in  $\text{CCl}_4$  at room temperature.

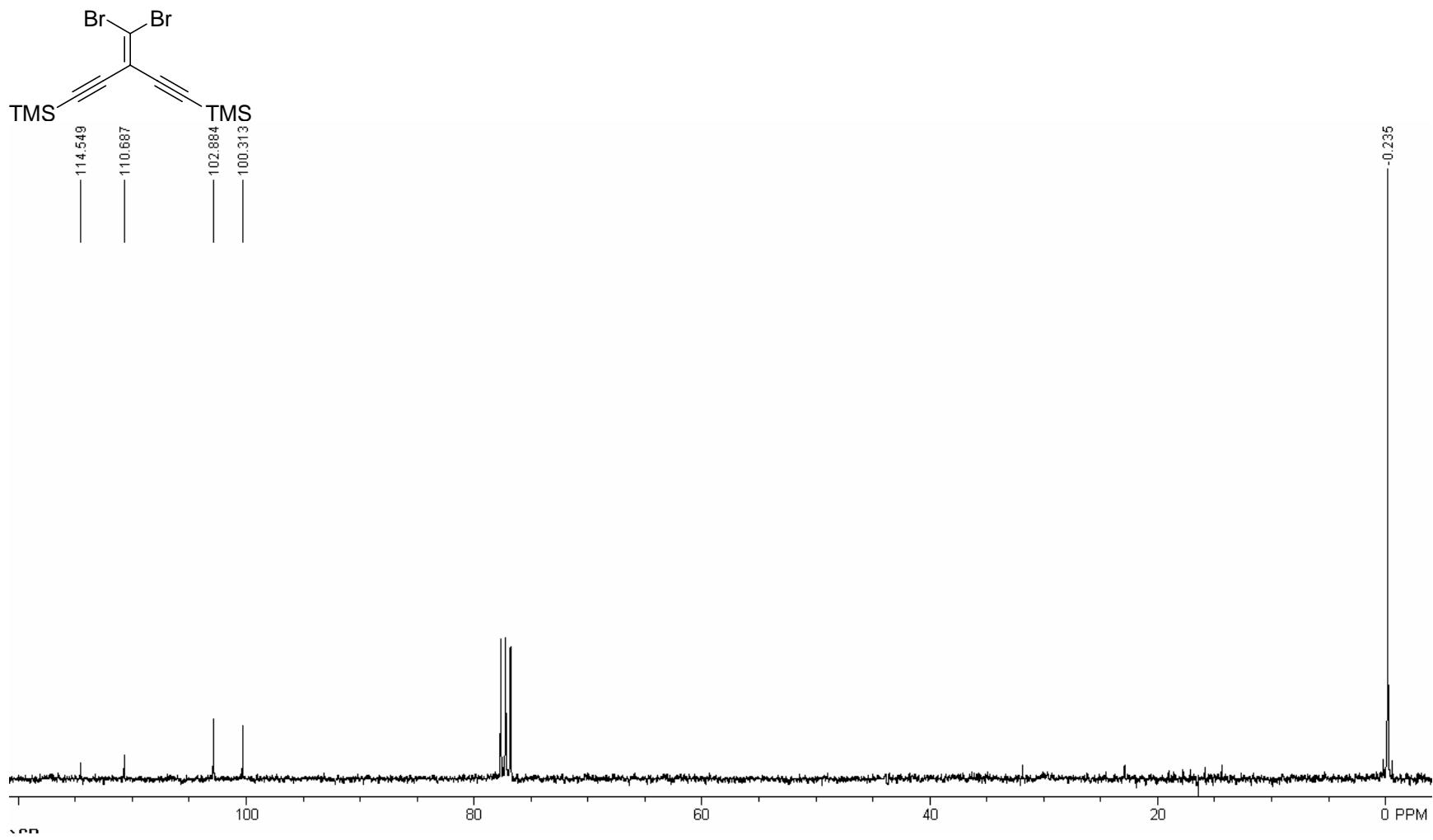


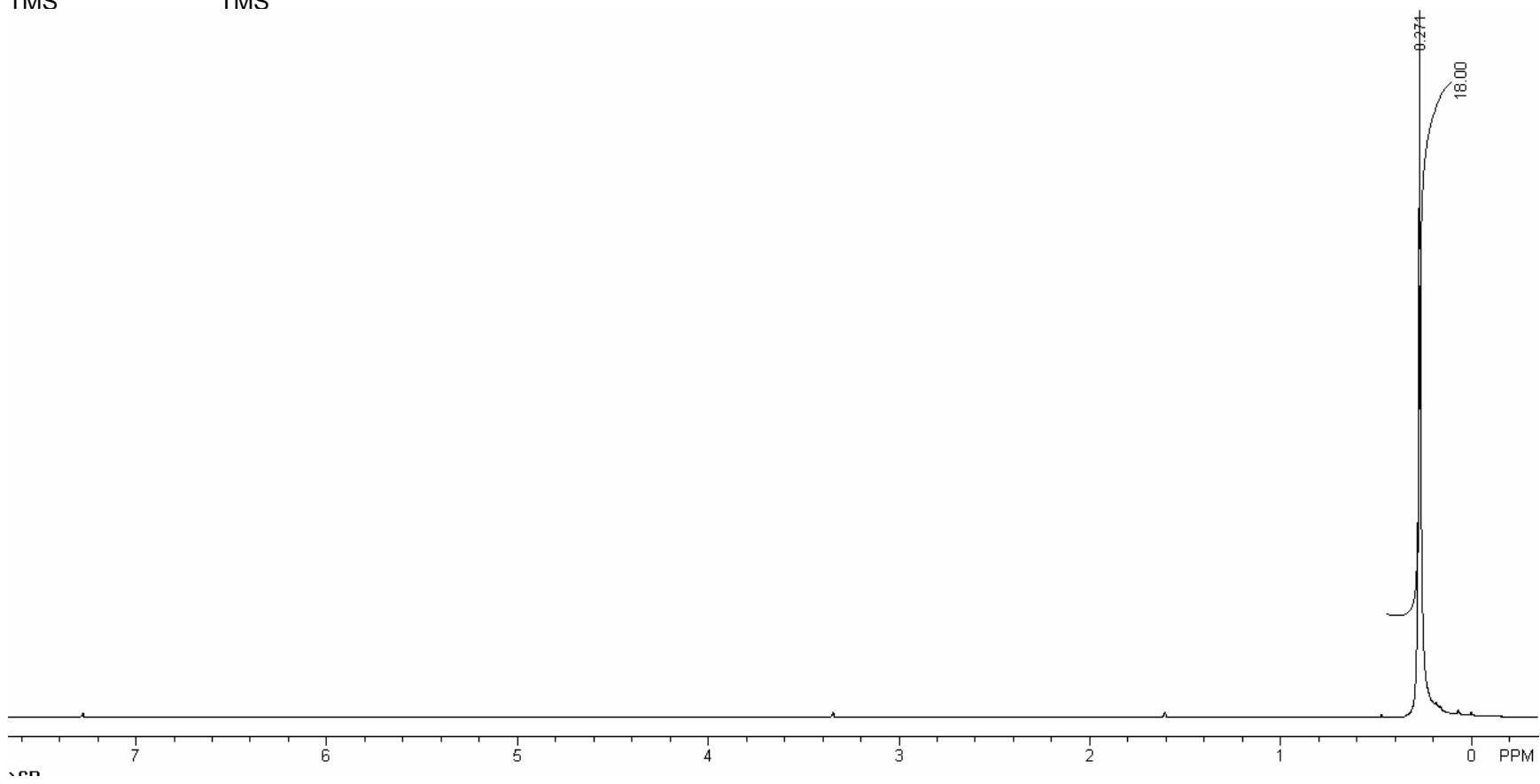
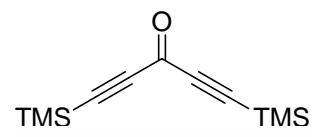
**Figure S8.** Infrared spectrum of **12** (neat) at room temperature.

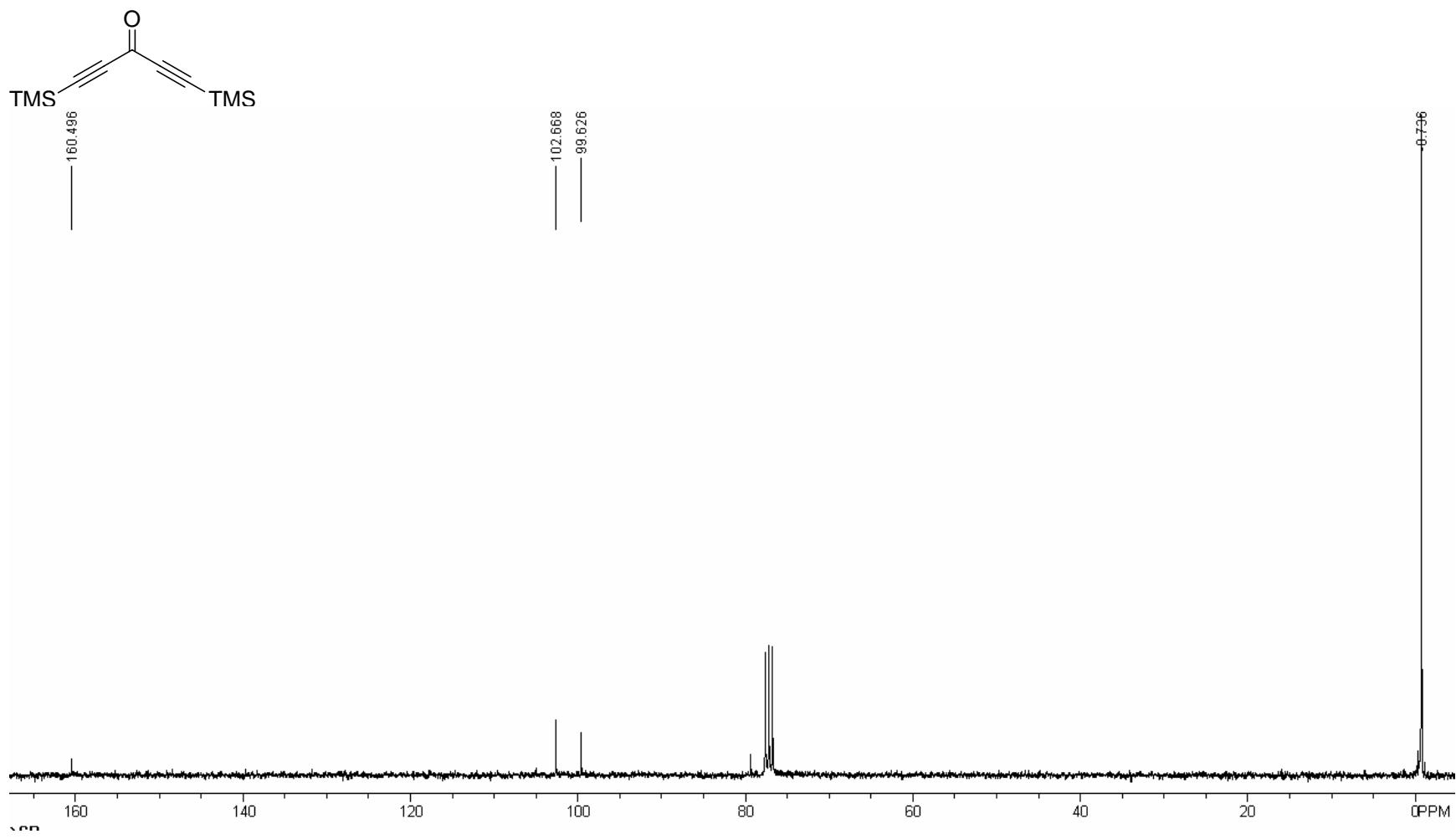


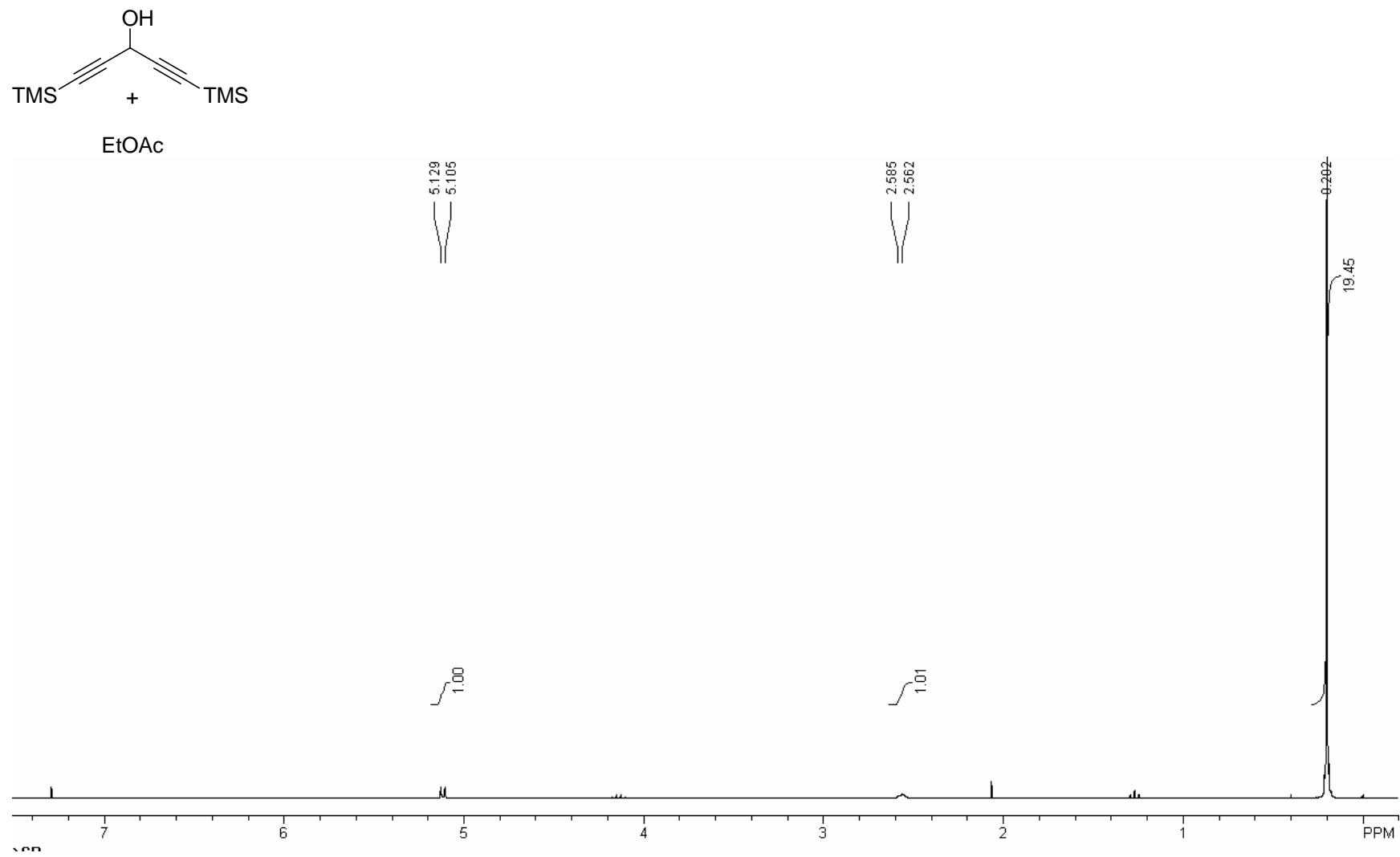


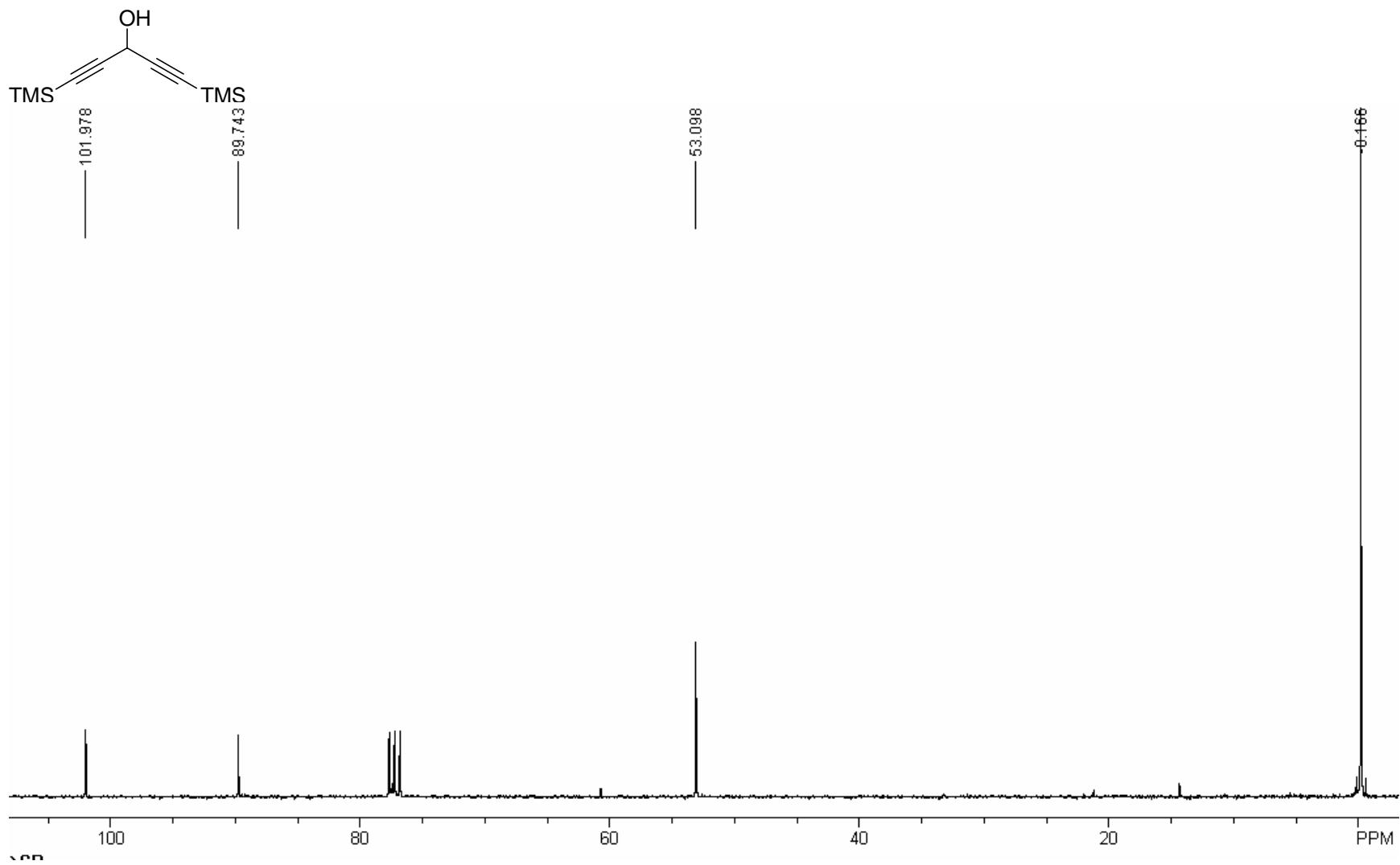


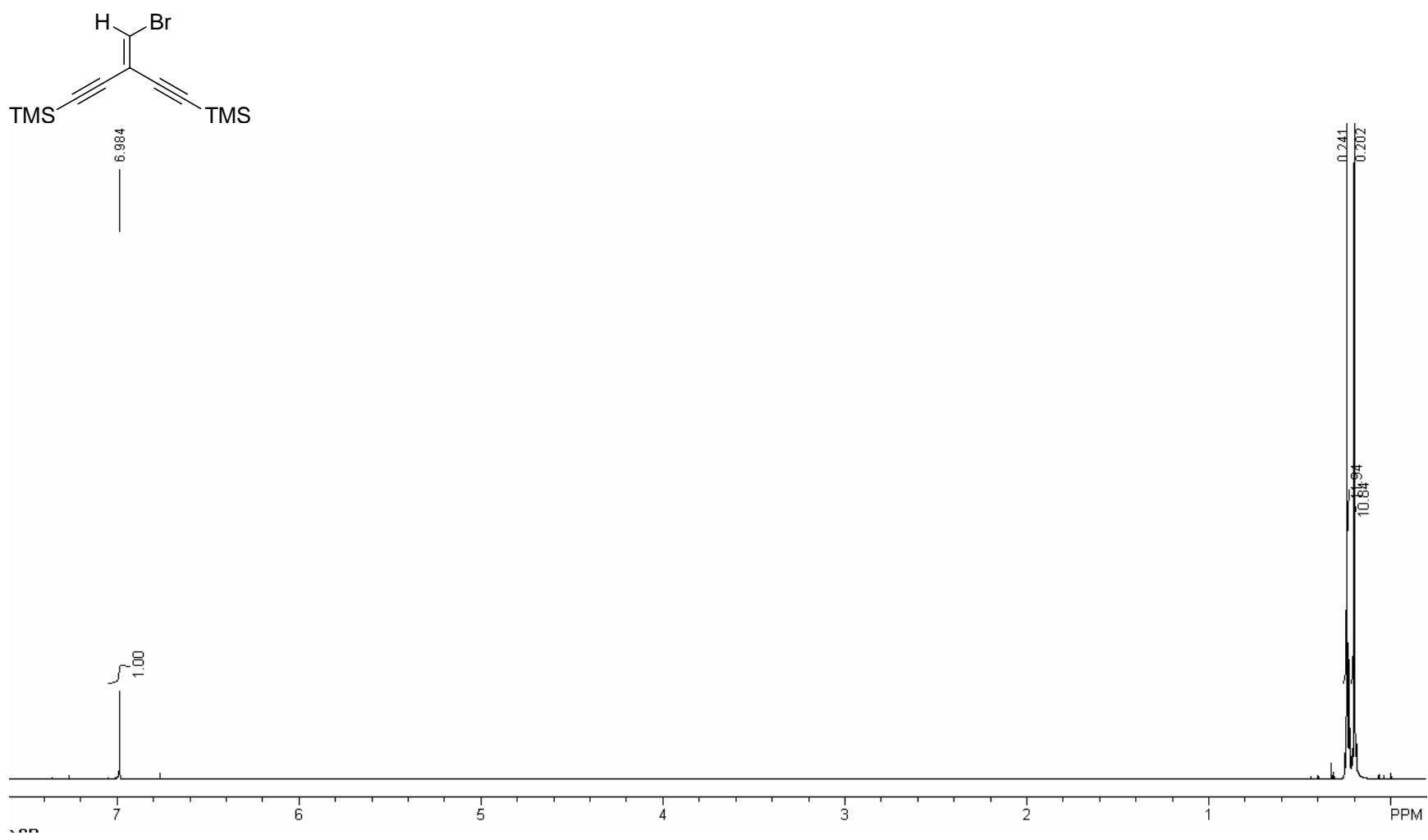


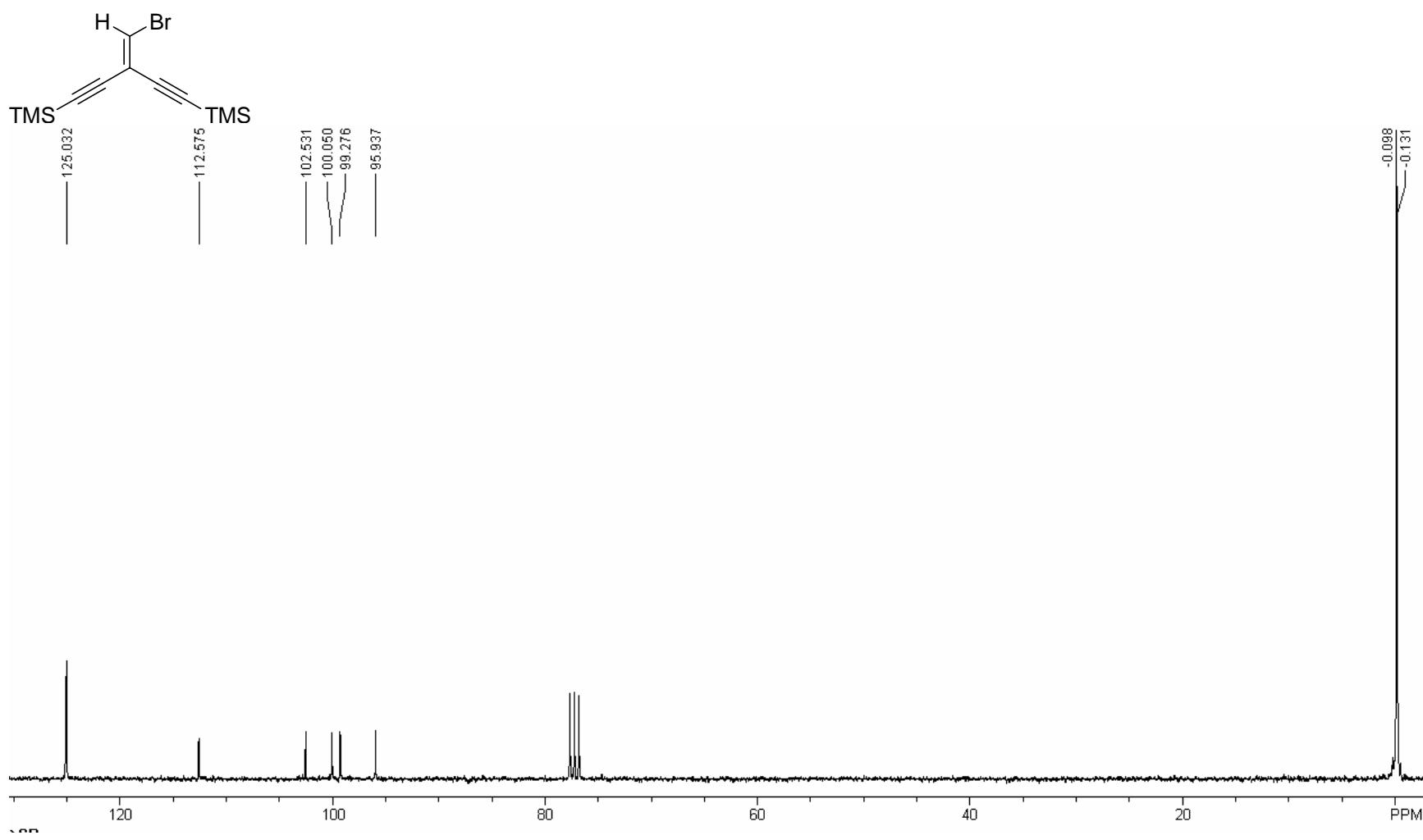


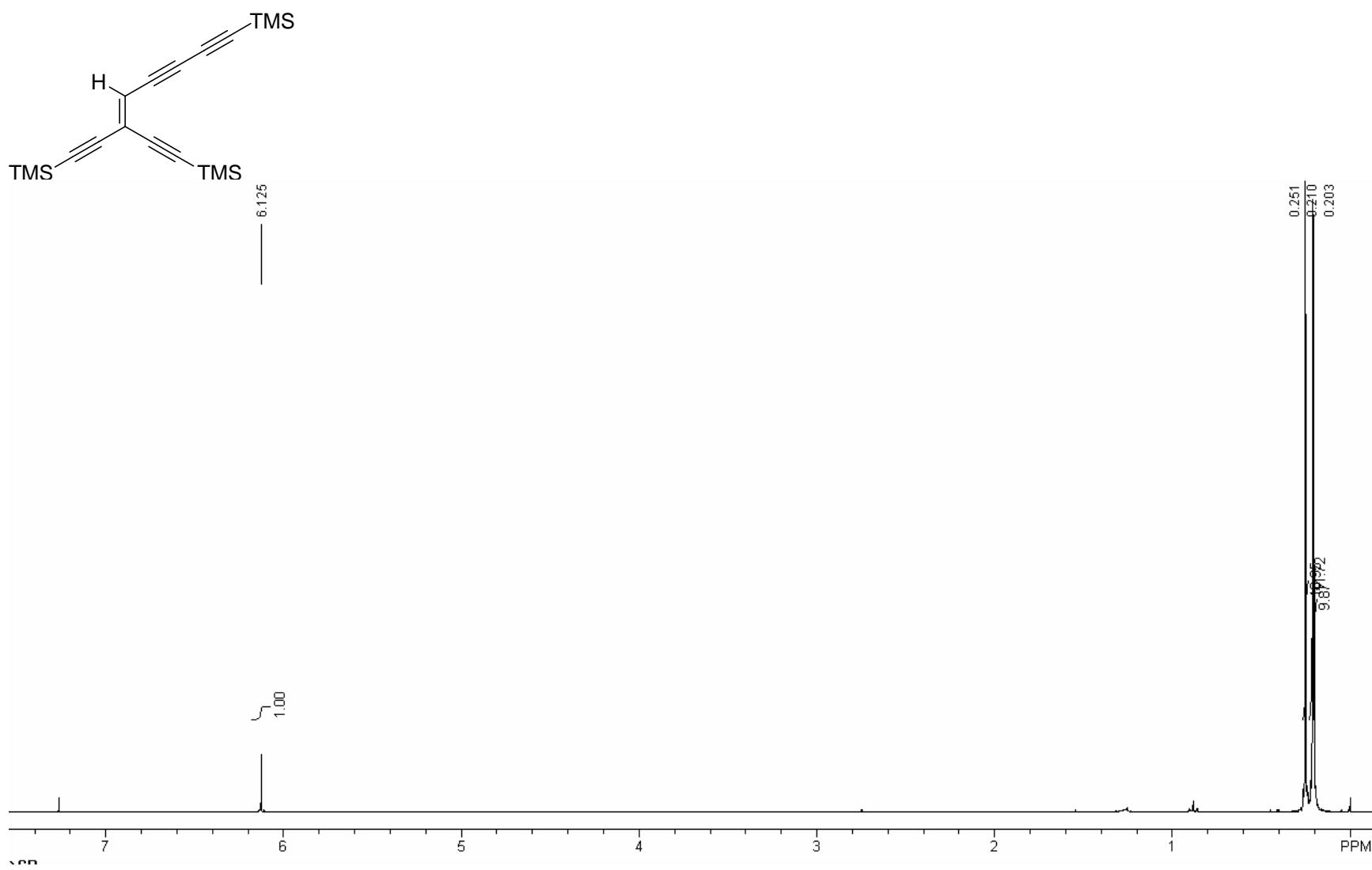


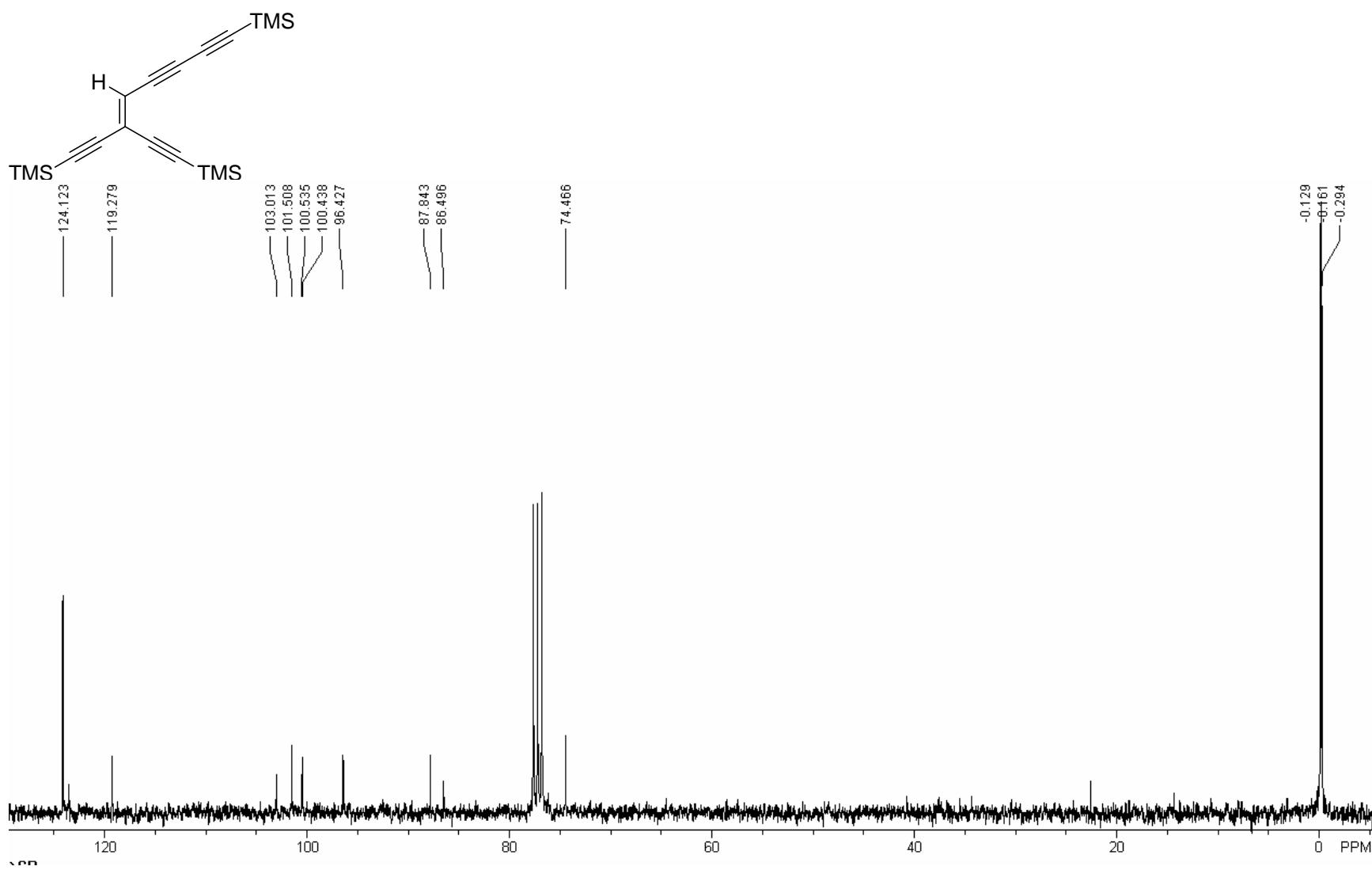


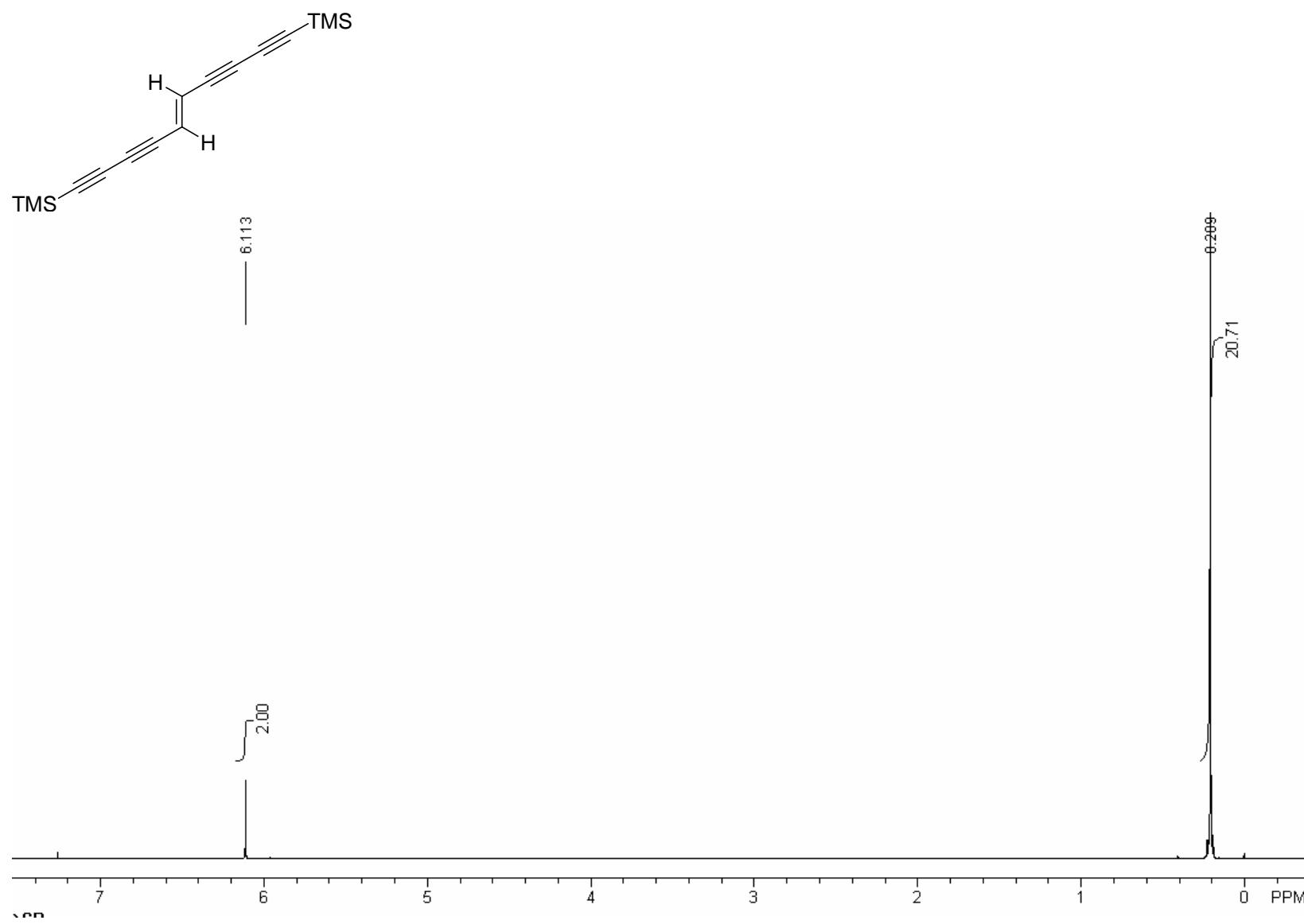


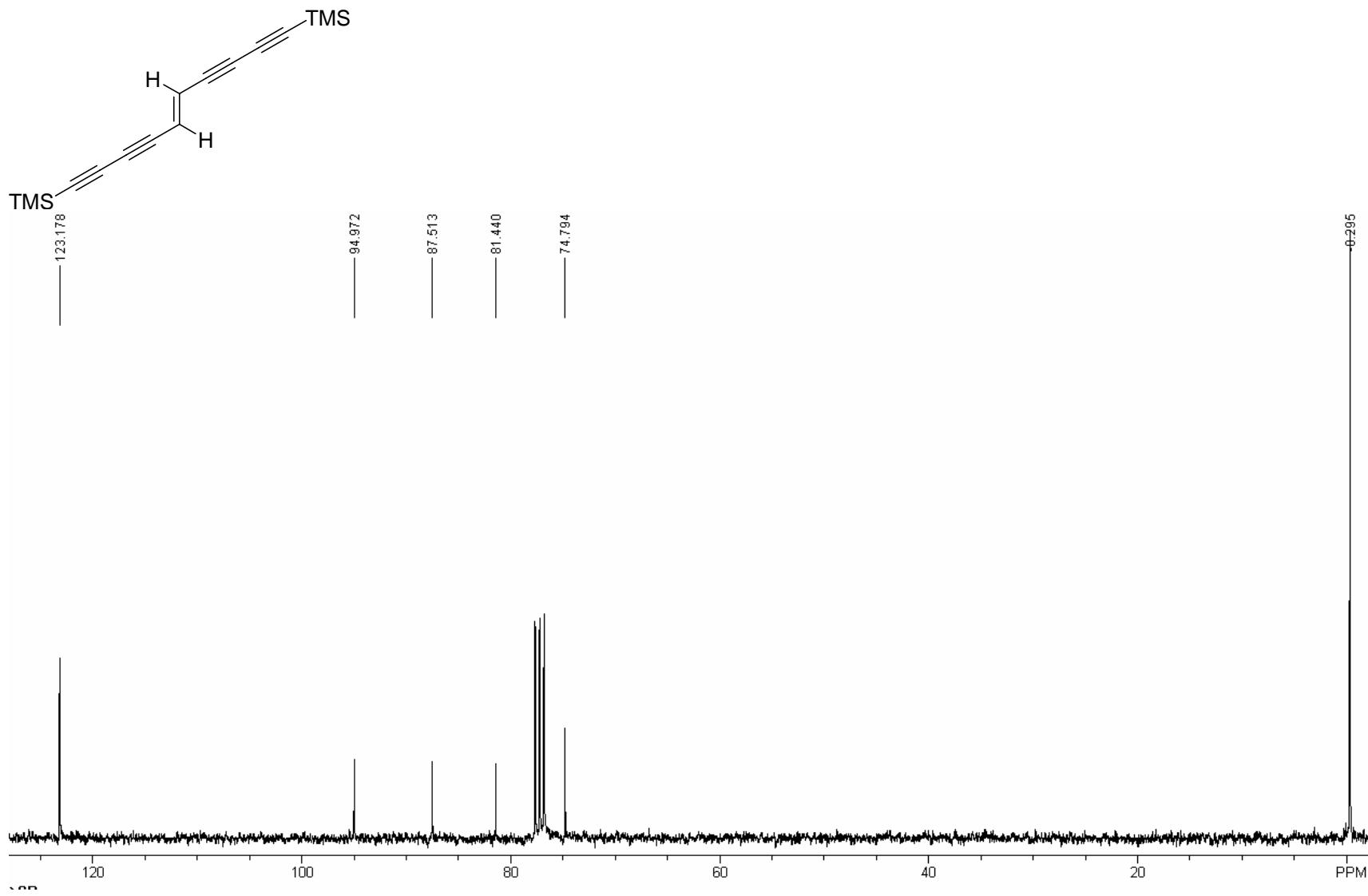


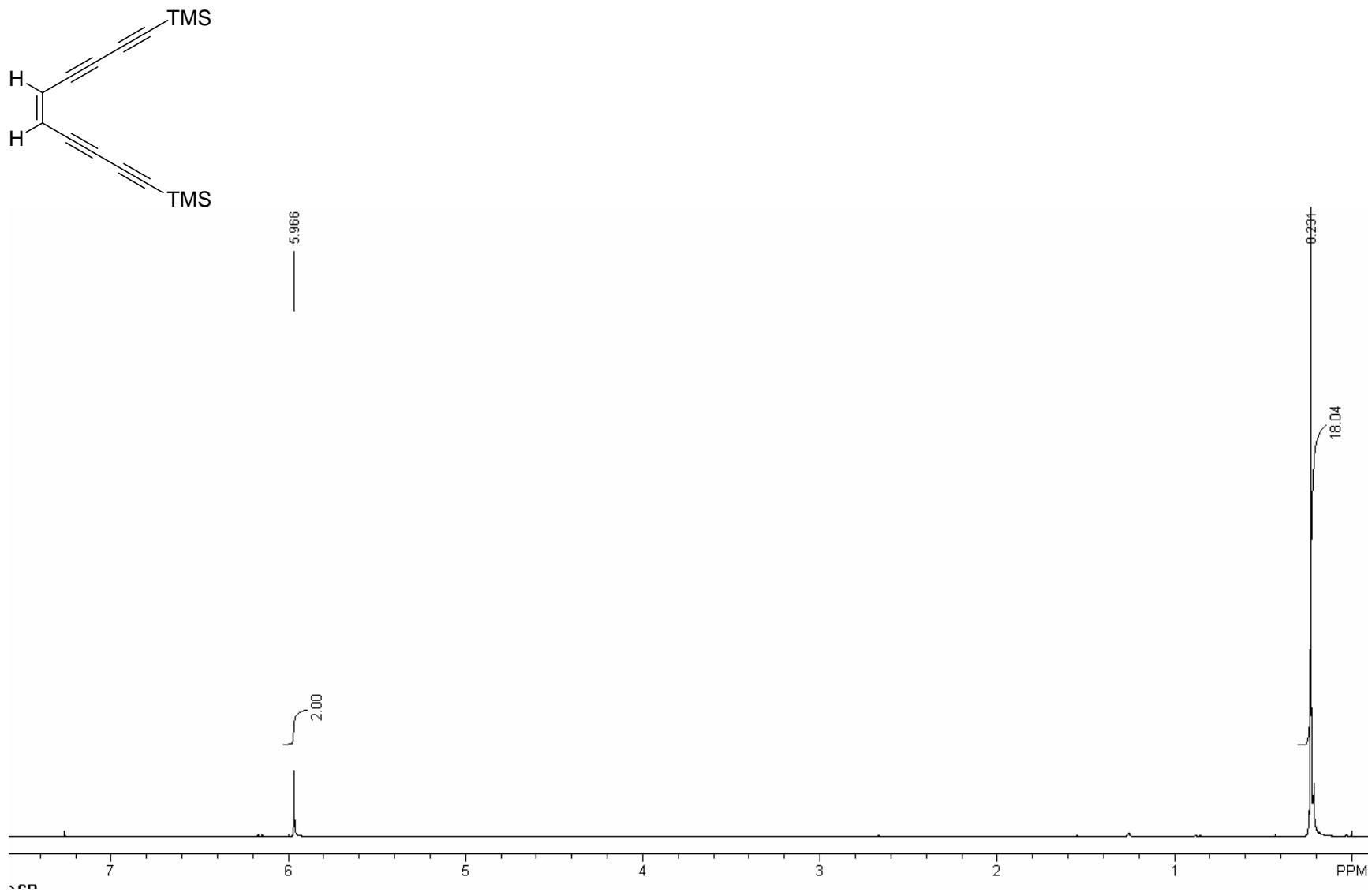


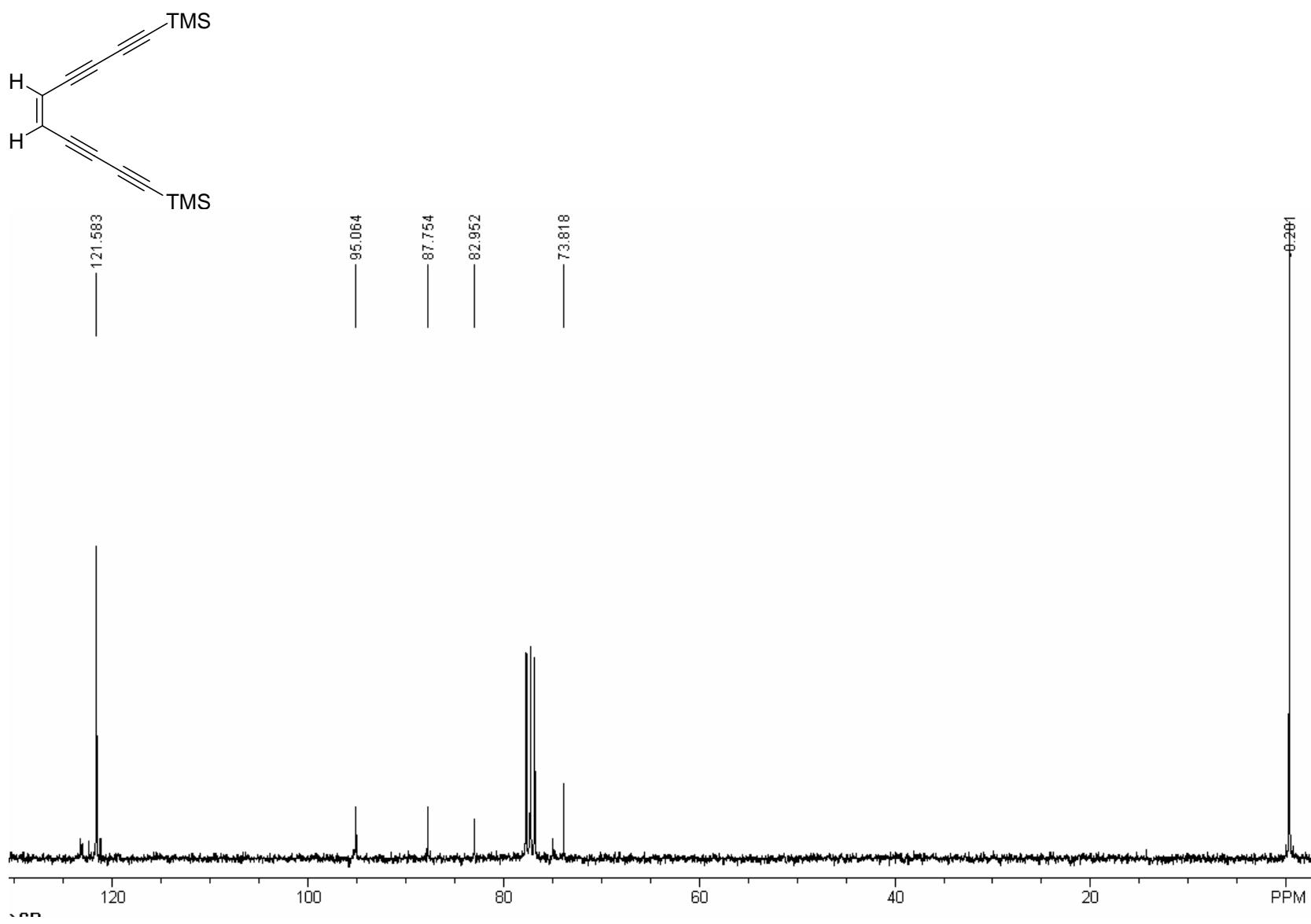


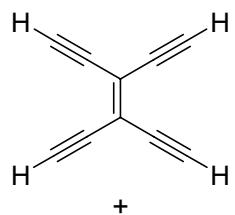




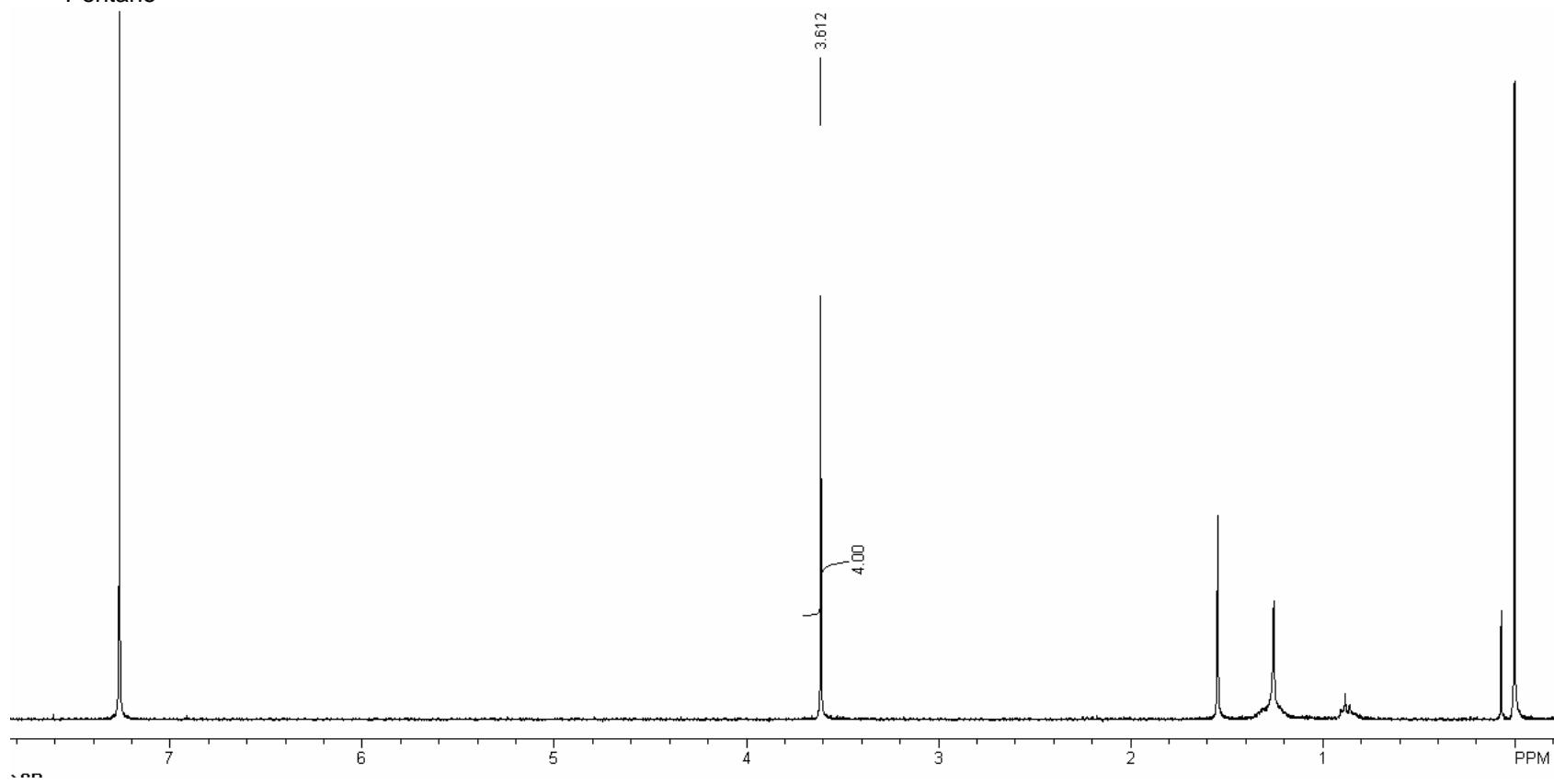


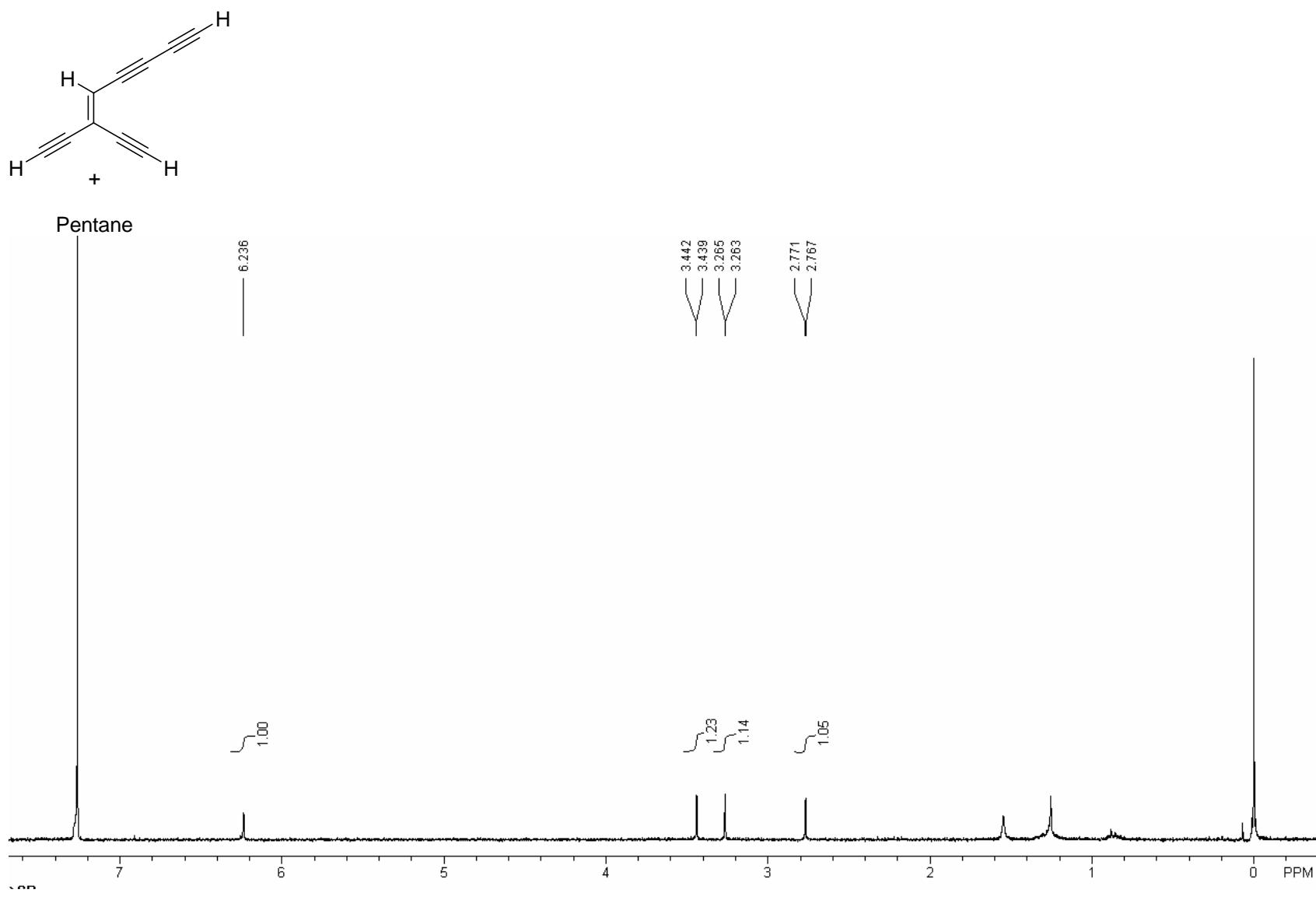


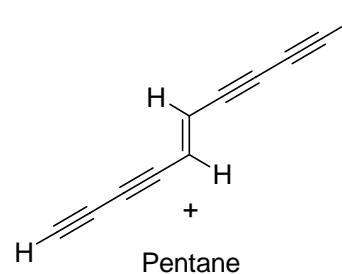




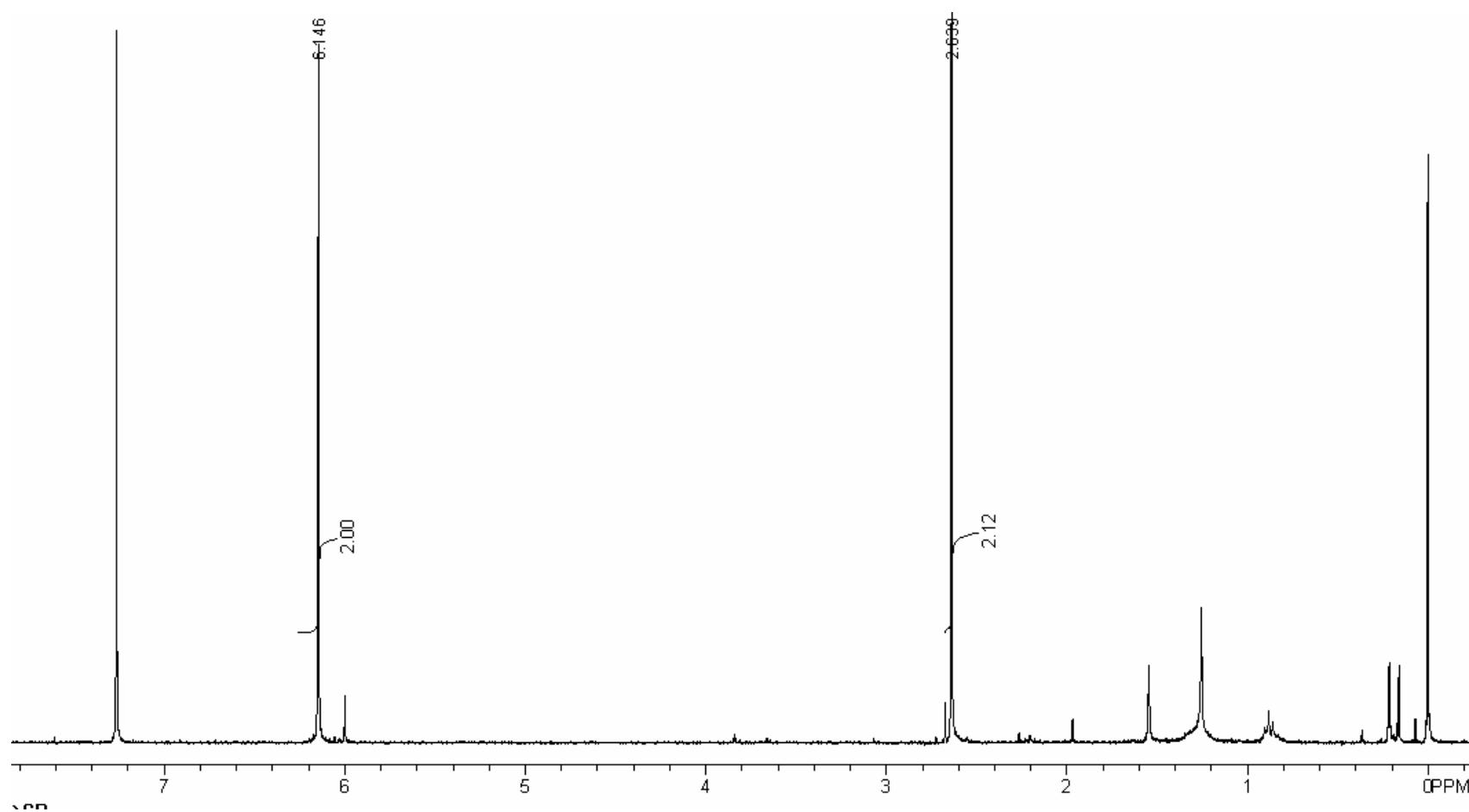
Pentane

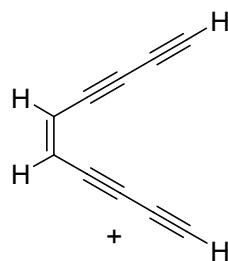






Resonances at  $\delta = 2.67$  and  $6.00$  ppm arise from the *cis* isomer as a minor contaminant (see p. S40). The TMS-substituted precursor depicted on p. S33, which did not contain the *cis* impurity, was the source of the sample used to obtain IR and UV/vis spectra under matrix isolation conditions. The IR spectrum of the *trans* isomer (p. S15) establishes that the *cis* isomer is not present as a contaminant in the matrix samples. The sample depicted in this spectrum was obtained by deprotection of a different batch of TMS-substituted precursor, which presumably contained a small amount of the *cis* isomer by virtue of incomplete chromatographic separation of the isomers.





Pentane

