

SUPPORTING INFORMATION

for

**C4'-Spiroalkylated Nucleosides Having Sulfur Incorporated at the Apex
Position**

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Copies of high-field ^1H NMR spectra of all compounds, together with tables
giving the crystallographic details and structure refinement for **8** and **13**.

(38 pages)

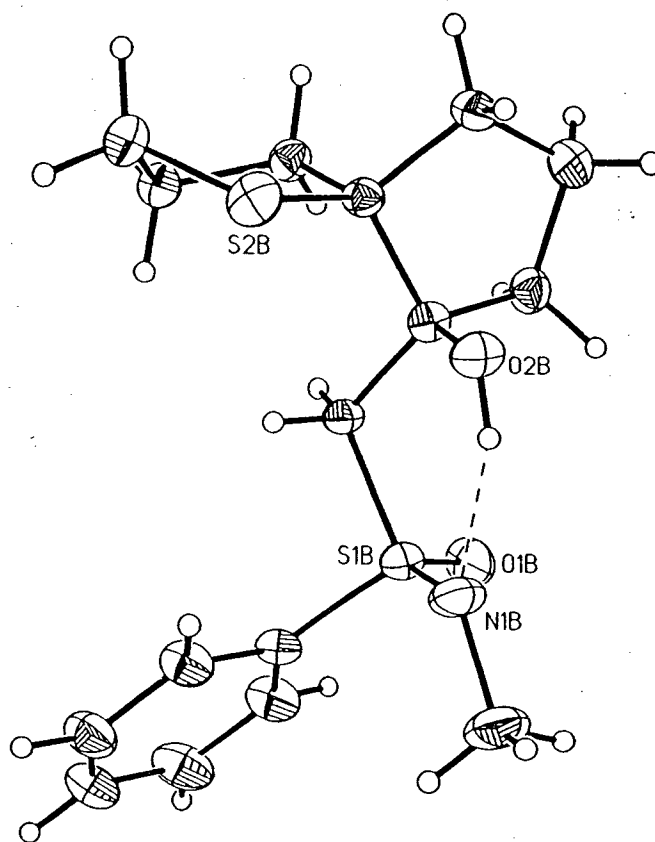


Figure 1. Computer-generated perspective drawing of the final X-ray model of **8**.

Table 1. Crystal Data and Structure Refinement for **8**.

Compound	8
Color / Shape	colorless / fragment
Empirical formula	C ₁₆ H ₂₃ NO ₂ S ₂
Formula weight	325.47
Temperature	173(2) K
Crystal system	Orthorhombic
Space group	P2 ₁ ² ₁ ² ₁
Unit cell dimensions	a = 10.4524(1) Å α = 90°
(6695 reflections	b = 17.8099(2) Å β = 90°
in full θ range)	c = 18.1935(1) Å γ = 90°
Volume	3386.83(5) Å ³
Z	8
Density (calculated)	1.277 Mg/m ³
Absorption coefficient	0.318 mm ⁻¹
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1392
Crystal size	0.38 x 0.52 x 0.90 mm
θ range for data collection	1.60 to 27.87°
Index ranges	-13 ≤ h ≤ 10, -21 ≤ k ≤ 23, -23 ≤ l ≤ 22
Reflections collected	21518
Independent / observed refls.	7857(R _{int} = 0.0223) / 7134([I>2σ(I)])
Absorption correction	SADABS
Range of relat. transm. factors	0.97 and 0.83
Refinement method	Full-matrix least-squares on F ²
Computing	SHELXTL, Ver. 5 ²
Data / restraints / parameters	7853 / 0 / 384
Goodness-of-fit on F ²	1.044
SHELX-93 weight parameters	0.0319, 0.6163
Final R indices [I>2σ(I)]	R1 = 0.0288, wR2 = 0.0648
R indices (all data)	R1 = 0.0359, wR2 = 0.0692
Absolute structure parameter	0.01(4)
Extinction coefficient	0.0010(2)
Largest diff. peak and hole	0.243 and -0.191 eÅ ⁻³

Table 2. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **8**.

Atom	x/a	y/b	z/c	U(eq)
S(1A)	5291(1)	10846(1)	3874(1)	22(1)
S(2A)	2805(1)	8948(1)	2395(1)	31(1)
O(1A)	6007(1)	10626(1)	4527(1)	31(1)
O(2A)	5341(1)	9723(1)	2488(1)	26(1)
N(1A)	5992(1)	11053(1)	3164(1)	25(1)
C(1A)	4233(2)	10115(1)	3590(1)	22(1)
C(2A)	4939(2)	9465(1)	3199(1)	21(1)
C(3A)	6083(2)	9125(1)	3611(1)	28(1)
C(4A)	6298(2)	8351(1)	3241(1)	36(1)
C(5A)	5098(2)	8207(1)	2767(1)	29(1)
C(6A)	4093(2)	8766(1)	3055(1)	22(1)
C(7A)	3413(2)	8454(1)	3747(1)	24(1)
C(8A)	2295(2)	7983(1)	3485(1)	33(1)
C(9A)	1572(2)	8465(1)	2931(1)	40(1)
C(10A)	7001(2)	11631(1)	3217(1)	35(1)
C(11A)	4241(2)	11577(1)	4181(1)	25(1)
C(12A)	4066(2)	11681(1)	4935(1)	33(1)
C(13A)	3267(2)	12255(1)	5173(1)	39(1)
C(14A)	2655(2)	12713(1)	4668(1)	41(1)
C(15A)	2829(2)	12599(1)	3919(1)	38(1)
C(16A)	3628(2)	12025(1)	3670(1)	29(1)
S(1B)	2904(1)	8874(1)	6442(1)	25(1)
S(2B)	805(1)	10075(1)	4358(1)	31(1)
O(1B)	2378(1)	8633(1)	7142(1)	39(1)
O(2B)	1130(1)	8625(1)	5040(1)	29(1)
N(1B)	3246(2)	8306(1)	5838(1)	36(1)
C(1B)	1844(1)	9505(1)	5990(1)	21(1)
C(2B)	711(1)	9146(1)	5586(1)	20(1)
C(3B)	-288(2)	8766(1)	6083(1)	28(1)
C(4B)	-1532(2)	8758(1)	5626(1)	38(1)
C(5B)	-1280(2)	9269(1)	4956(1)	30(1)

Table 2 (continued)

C(6B)	-91(2)	9740(1)	5162(1)	22(1)
C(7B)	-442(2)	10457(1)	5607(1)	24(1)
C(8B)	471(2)	11093(1)	5398(1)	30(1)
C(9B)	584(2)	11065(1)	4570(1)	35(1)
C(10B)	4293(2)	7776(1)	6002(1)	51(1)
C(11B)	4269(2)	9442(1)	6656(1)	24(1)
C(12B)	4966(2)	9765(1)	6086(1)	30(1)
C(13B)	6041(2)	10186(1)	6247(1)	35(1)
C(14B)	6436(2)	10271(1)	6970(1)	36(1)
C(15B)	5745(2)	9944(1)	7531(1)	40(1)
C(16B)	4650(2)	9532(1)	7380(1)	33(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond Lengths (Å) and Angles (°) for **8**.

S(1A)-O(1A)	1.4581(12)	S(1A)-N(1A)	1.5297(13)
S(1A)-C(1A)	1.786(2)	S(1A)-C(11A)	1.791(2)
S(2A)-C(9A)	1.831(2)	S(2A)-C(6A)	1.833(2)
O(2A)-C(2A)	1.436(2)	N(1A)-C(10A)	1.477(2)
C(1A)-C(2A)	1.546(2)	C(2A)-C(3A)	1.535(2)
C(2A)-C(6A)	1.549(2)	C(3A)-C(4A)	1.550(3)
C(4A)-C(5A)	1.544(3)	C(5A)-C(6A)	1.538(2)
C(6A)-C(7A)	1.548(2)	C(7A)-C(8A)	1.516(2)
C(8A)-C(9A)	1.525(3)	C(11A)-C(16A)	1.383(2)
C(11A)-C(12A)	1.398(2)	C(12A)-C(13A)	1.389(3)
C(13A)-C(14A)	1.385(3)	C(14A)-C(15A)	1.389(3)
C(15A)-C(16A)	1.396(3)	S(1B)-O(1B)	1.4522(14)
S(1B)-N(1B)	1.537(2)	S(1B)-C(1B)	1.779(2)
S(1B)-C(11B)	1.791(2)	S(2B)-C(9B)	1.819(2)
S(2B)-C(6B)	1.836(2)	O(2B)-C(2B)	1.429(2)
N(1B)-C(10B)	1.475(2)	C(1B)-C(2B)	1.533(2)
C(2B)-C(3B)	1.537(2)	C(2B)-C(6B)	1.555(2)
C(3B)-C(4B)	1.543(3)	C(4B)-C(5B)	1.543(3)
C(5B)-C(6B)	1.545(2)	C(6B)-C(7B)	1.555(2)
C(7B)-C(8B)	1.529(2)	C(8B)-C(9B)	1.513(2)
C(11B)-C(16B)	1.386(2)	C(11B)-C(12B)	1.392(2)
C(12B)-C(13B)	1.382(2)	C(13B)-C(14B)	1.387(3)
C(14B)-C(15B)	1.379(3)	C(15B)-C(16B)	1.386(3)
O(1A)-S(1A)-N(1A)	120.43(8)	O(1A)-S(1A)-C(1A)	110.98(7)
N(1A)-S(1A)-C(1A)	103.19(7)	O(1A)-S(1A)-C(11A)	104.82(7)
N(1A)-S(1A)-C(11A)	112.42(8)	C(1A)-S(1A)-C(11A)	103.94(8)
C(9A)-S(2A)-C(6A)	94.88(8)	C(10A)-N(1A)-S(1A)	117.08(12)
C(2A)-C(1A)-S(1A)	112.54(11)	O(2A)-C(2A)-C(3A)	109.80(13)
O(2A)-C(2A)-C(1A)	108.30(12)	C(3A)-C(2A)-C(1A)	116.30(13)
O(2A)-C(2A)-C(6A)	105.80(12)	C(3A)-C(2A)-C(6A)	102.11(12)
C(1A)-C(2A)-C(6A)	113.96(13)	C(2A)-C(3A)-C(4A)	104.61(14)
C(5A)-C(4A)-C(3A)	105.74(14)	C(6A)-C(5A)-C(4A)	104.90(13)
C(5A)-C(6A)-C(7A)	111.05(13)	C(5A)-C(6A)-C(2A)	100.79(13)
C(7A)-C(6A)-C(2A)	114.42(12)	C(5A)-C(6A)-S(2A)	113.09(11)
C(7A)-C(6A)-S(2A)	104.98(11)	C(2A)-C(6A)-S(2A)	112.79(11)

Table 3 (continued)

C(8A)-C(7A)-C(6A)	107.33(13)	C(7A)-C(8A)-C(9A)	106.10(14)
C(8A)-C(9A)-S(2A)	105.53(13)	C(16A)-C(11A)-C(12A)	121.5(2)
C(16A)-C(11A)-S(1A)	119.61(13)	C(12A)-C(11A)-S(1A)	118.90(14)
C(13A)-C(12A)-C(11A)	118.9(2)	C(14A)-C(13A)-C(12A)	120.3(2)
C(13A)-C(14A)-C(15A)	120.2(2)	C(14A)-C(15A)-C(16A)	120.3(2)
C(11A)-C(16A)-C(15A)	118.8(2)	O(1B)-S(1B)-N(1B)	121.34(9)
O(1B)-S(1B)-C(1B)	110.86(8)	N(1B)-S(1B)-C(1B)	103.30(8)
O(1B)-S(1B)-C(11B)	106.13(8)	N(1B)-S(1B)-C(11B)	110.02(8)
C(1B)-S(1B)-C(11B)	103.93(8)	C(9B)-S(2B)-C(6B)	94.68(8)
C(10B)-N(1B)-S(1B)	116.66(14)	C(2B)-C(1B)-S(1B)	116.09(11)
O(2B)-C(2B)-C(1B)	111.53(12)	O(2B)-C(2B)-C(3B)	109.33(13)
C(1B)-C(2B)-C(3B)	115.29(13)	O(2B)-C(2B)-C(6B)	105.16(12)
C(1B)-C(2B)-C(6B)	111.76(12)	C(3B)-C(2B)-C(6B)	103.00(12)
C(2B)-C(3B)-C(4B)	105.09(13)	C(5B)-C(4B)-C(3B)	105.98(14)
C(4B)-C(5B)-C(6B)	105.47(14)	C(5B)-C(6B)-C(2B)	100.62(12)
C(5B)-C(6B)-C(7B)	112.44(13)	C(2B)-C(6B)-C(7B)	115.30(13)
C(5B)-C(6B)-S(2B)	113.19(11)	C(2B)-C(6B)-S(2B)	109.98(10)
C(7B)-C(6B)-S(2B)	105.55(10)	C(8B)-C(7B)-C(6B)	109.40(13)
C(9B)-C(8B)-C(7B)	105.72(14)	C(8B)-C(9B)-S(2B)	104.67(12)
C(16B)-C(11B)-C(12B)	120.7(2)	C(16B)-C(11B)-S(1B)	120.09(14)
C(12B)-C(11B)-S(1B)	119.20(12)	C(13B)-C(12B)-C(11B)	119.4(2)
C(12B)-C(13B)-C(14B)	120.2(2)	C(15B)-C(14B)-C(13B)	119.9(2)
C(14B)-C(15B)-C(16B)	120.7(2)	C(11B)-C(16B)-C(15B)	119.1(2)

Table 4. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **8**.

Atom	U11	U22	U33	U23	U13	U12
S(1A)	26(1)	21(1)	19(1)	-2(1)	0(1)	-2(1)
S(2A)	34(1)	30(1)	29(1)	1(1)	-6(1)	-5(1)
O(1A)	37(1)	33(1)	23(1)	-1(1)	-6(1)	1(1)
O(2A)	35(1)	24(1)	19(1)	-1(1)	8(1)	-6(1)
N(1A)	27(1)	26(1)	22(1)	-2(1)	4(1)	-5(1)
C(1A)	24(1)	20(1)	23(1)	-2(1)	4(1)	-4(1)
C(2A)	24(1)	21(1)	17(1)	-1(1)	5(1)	-1(1)
C(3A)	23(1)	29(1)	32(1)	3(1)	1(1)	1(1)
C(4A)	30(1)	27(1)	50(1)	1(1)	4(1)	7(1)
C(5A)	35(1)	21(1)	32(1)	-3(1)	8(1)	2(1)
C(6A)	25(1)	21(1)	20(1)	-1(1)	2(1)	0(1)
C(7A)	30(1)	21(1)	22(1)	1(1)	6(1)	-5(1)
C(8A)	39(1)	29(1)	32(1)	-5(1)	10(1)	-11(1)
C(9A)	29(1)	43(1)	47(1)	-5(1)	1(1)	-10(1)
C(10A)	35(1)	33(1)	38(1)	2(1)	-1(1)	-13(1)
C(11A)	27(1)	20(1)	26(1)	-5(1)	4(1)	-4(1)
C(12A)	38(1)	32(1)	28(1)	-7(1)	4(1)	-4(1)
C(13A)	45(1)	36(1)	37(1)	-13(1)	12(1)	-7(1)
C(14A)	36(1)	26(1)	61(1)	-12(1)	16(1)	-4(1)
C(15A)	35(1)	23(1)	55(1)	5(1)	4(1)	-2(1)
C(16A)	32(1)	23(1)	31(1)	-1(1)	3(1)	-5(1)
S(1B)	22(1)	26(1)	27(1)	4(1)	-4(1)	2(1)
S(2B)	37(1)	36(1)	20(1)	4(1)	3(1)	2(1)
O(1B)	33(1)	49(1)	36(1)	19(1)	-2(1)	-6(1)
O(2B)	32(1)	28(1)	27(1)	-11(1)	-4(1)	8(1)
N(1B)	31(1)	30(1)	46(1)	-10(1)	-11(1)	11(1)
C(1B)	20(1)	22(1)	22(1)	0(1)	-4(1)	3(1)
C(2B)	22(1)	21(1)	18(1)	-2(1)	0(1)	2(1)
C(3B)	29(1)	26(1)	30(1)	5(1)	4(1)	-3(1)
C(4B)	24(1)	34(1)	56(1)	9(1)	-1(1)	-5(1)
C(5B)	24(1)	30(1)	37(1)	-2(1)	-9(1)	1(1)
C(6B)	21(1)	24(1)	21(1)	1(1)	0(1)	1(1)
C(7B)	24(1)	23(1)	25(1)	0(1)	2(1)	3(1)

Table 4 (continued)

C(8B)	28(1)	24(1)	37(1)	1(1)	-3(1)	0(1)
C(9B)	36(1)	30(1)	37(1)	11(1)	-1(1)	-3(1)
C(10B)	36(1)	38(1)	80(2)	-12(1)	-15(1)	18(1)
C(11B)	19(1)	30(1)	23(1)	0(1)	-3(1)	4(1)
C(12B)	27(1)	42(1)	22(1)	2(1)	-1(1)	0(1)
C(13B)	23(1)	47(1)	33(1)	7(1)	2(1)	-2(1)
C(14B)	23(1)	46(1)	39(1)	-3(1)	-5(1)	-4(1)
C(15B)	31(1)	63(1)	26(1)	-5(1)	-8(1)	-2(1)
C(16B)	28(1)	50(1)	22(1)	2(1)	0(1)	2(1)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}] .$$

Table 5. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **8**.

Atom	x	y	z	U(eq)
H(1AO)	5650(1)	10181(1)	2554(1)	34(5)
H(1C)	3780(2)	9914(1)	4025(1)	27
H(1D)	3583(2)	10326(1)	3252(1)	27
H(3A)	5886(2)	9065(1)	4140(1)	34
H(3B)	6850(2)	9447(1)	3559(1)	34
H(4A)	7076(2)	8360(1)	2930(1)	43
H(4B)	6396(2)	7953(1)	3617(1)	43
H(5A)	5282(2)	8300(1)	2241(1)	35
H(5B)	4796(2)	7684(1)	2825(1)	35
H(7A)	4012(2)	8143(1)	4038(1)	29
H(7B)	3105(2)	8872(1)	4059(1)	29
H(8A)	1733(2)	7848(1)	3903(1)	40
H(8B)	2603(2)	7515(1)	3250(1)	40
H(9A)	1017(2)	8833(1)	3186(1)	48
H(9B)	1033(2)	8149(1)	2608(1)	48
H(10A)	7452(8)	11668(5)	2746(3)	53
H(10B)	7608(7)	11493(4)	3604(5)	53
H(10C)	6612(2)	12117(2)	3335(7)	53
H(12A)	4486(2)	11365(1)	5280(1)	39
H(13A)	3140(2)	12333(1)	5684(1)	47
H(14A)	2114(2)	13106(1)	4835(1)	49
H(15A)	2403(2)	12914(1)	3576(1)	45
H(16A)	3748(2)	11944(1)	3158(1)	35
H(1BO)	1824(1)	8383(1)	5194(1)	60(7)
H(1BC)	1503(1)	9860(1)	6360(1)	25
H(1BD)	2344(1)	9801(1)	5630(1)	25
H(3BA)	-408(2)	9055(1)	6543(1)	34
H(3BB)	-21(2)	8249(1)	6209(1)	34
H(4BA)	-1736(2)	8241(1)	5464(1)	46
H(4BB)	-2257(2)	8952(1)	5920(1)	46
H(5BA)	-2024(2)	9599(1)	4862(1)	36
H(5BB)	-1112(2)	8965(1)	4511(1)	36

Table 5 (continued)

H(7BA)	-1334(2)	10606(1)	5498(1)	29
H(7BB)	-375(2)	10352(1)	6140(1)	29
H(8BA)	123(2)	11584(1)	5558(1)	36
H(8BB)	1317(2)	11019(1)	5631(1)	36
H(9BA)	1325(2)	11364(1)	4399(1)	41
H(9BB)	-201(2)	11260(1)	4334(1)	41
H(10D)	4487(10)	7479(6)	5563(3)	77
H(10E)	4032(6)	7441(6)	6402(6)	77
H(10F)	5056(5)	8058(1)	6151(8)	77
H(12B)	4706(2)	9696(1)	5590(1)	36
H(13B)	6510(2)	10418(1)	5862(1)	42
H(14B)	7182(2)	10555(1)	7079(1)	43
H(15B)	6021(2)	10001(1)	8025(1)	48
H(16B)	4167(2)	9315(1)	7768(1)	40

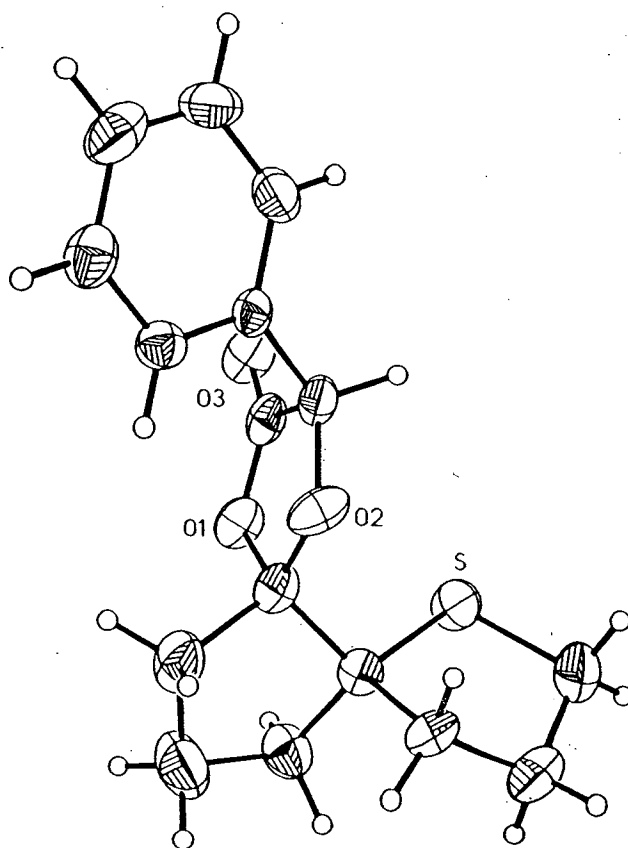


Figure 2. Computer-generated perspective drawing of the final X-ray model of **13**.

Table 6. Crystal Data and Structure Refinement for **13**.

Compound	13
Color / Shape	colorless / fragment
Empirical formula	$C_{16}H_{18}O_3S$
Formula weight	290.36
Temperature	173(2) K
Crystal system	Orthorhombic
Space group	$P2_1^2 2_1^2 1$
Unit cell dimensions	$a = 6.3920(1) \text{ \AA} \quad \alpha = 90^\circ$
(4786 reflections	$b = 8.7808(2) \text{ \AA} \quad \beta = 90^\circ$
in full θ range)	$c = 26.063 \text{ \AA} \quad \gamma = 90^\circ$
Volume	$1462.85(4) \text{ \AA}^3$
Z	4
Density (calculated)	1.318 Mg/m^3
Absorption coefficient	0.226 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoK α (graphite monochrom.) / 0.71073 \AA
F(000)	616
Crystal size	$0.24 \times 0.38 \times 0.54 \text{ mm}$
θ range for data collection	1.56 to 27.85°
Index ranges	$-8 \leq h \leq 7, -11 \leq k \leq 11, -26 \leq l \leq 34$
Reflections collected	9155
Independent / observed refls.	3383 ($R_{\text{int}} = 0.0304$) / 2843 ($[I > 2\sigma(I)]$)
Absorption correction	SADABS
Range of relat. transm. factors	0.97 and 0.87
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5 ²
Data / restraints / parameters	3379 / 0 / 182
Goodness-of-fit on F^2	1.231
SHELX-93 weight parameters	0.0158, 0.8444
Final R indices $[I > 2\sigma(I)]$	$R1 = 0.0518, wR2 = 0.0910$
R indices (all data)	$R1 = 0.0699, wR2 = 0.1017$
Absolute structure parameter	0.12(11)
Extinction coefficient	0.0053(9)
Largest diff. peak and hole	0.226 and -0.218 e\AA^{-3}

Table 7. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **13**.

Atom	x/a	y/b	z/c	U(eq)
S	-1027(1)	-3973(1)	-1599(1)	44(1)
O(1)	530(3)	-7153(2)	-1713(1)	37(1)
O(2)	2508(3)	-6228(2)	-1047(1)	40(1)
O(3)	-1830(3)	-8547(2)	-1285(1)	45(1)
C(1)	-296(6)	-2084(4)	-1372(1)	58(1)
C(2)	1845(5)	-1767(3)	-1598(1)	46(1)
C(3)	3059(4)	-3255(3)	-1546(1)	34(1)
C(4)	1637(4)	-4512(3)	-1781(1)	29(1)
C(5)	1958(5)	-4687(3)	-2360(1)	42(1)
C(6)	3928(6)	-5726(4)	-2409(1)	61(1)
C(7)	4160(5)	-6544(3)	-1891(1)	48(1)
C(8)	2228(4)	-6112(3)	-1586(1)	31(1)
C(9)	-336(4)	-7707(3)	-1283(1)	33(1)
C(10)	917(4)	-7156(3)	-825(1)	34(1)
C(11)	1813(4)	-8464(3)	-522(1)	30(1)
C(12)	630(5)	-9144(3)	-136(1)	43(1)
C(13)	1408(6)	-10384(3)	133(1)	51(1)
C(14)	3367(6)	-10966(4)	20(1)	53(1)
C(15)	4556(5)	-10290(3)	-358(1)	42(1)
C(16)	3804(4)	-9038(3)	-626(1)	33(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 8. Bond Lengths (Å) and Angles (°) for **13**.

S-C(1)	1.823(3)	S-C(4)	1.829(3)
O(1)-C(9)	1.341(3)	O(1)-C(8)	1.457(3)
O(2)-C(8)	1.420(3)	O(2)-C(10)	1.425(3)
O(3)-C(9)	1.206(3)	C(1)-C(2)	1.516(5)
C(2)-C(3)	1.526(4)	C(3)-C(4)	1.554(3)
C(4)-C(5)	1.531(4)	C(4)-C(8)	1.541(4)
C(5)-C(6)	1.560(4)	C(6)-C(7)	1.537(5)
C(7)-C(8)	1.516(4)	C(9)-C(10)	1.517(4)
C(10)-C(11)	1.508(4)	C(11)-C(12)	1.393(4)
C(11)-C(16)	1.396(4)	C(12)-C(13)	1.387(4)
C(13)-C(14)	1.384(5)	C(14)-C(15)	1.378(4)
C(15)-C(16)	1.389(4)		
C(1)-S-C(4)	94.63(14)	C(9)-O(1)-C(8)	110.2(2)
C(8)-O(2)-C(10)	110.6(2)	C(2)-C(1)-S	105.8(2)
C(1)-C(2)-C(3)	105.5(2)	C(2)-C(3)-C(4)	106.0(2)
C(5)-C(4)-C(8)	101.5(2)	C(5)-C(4)-C(3)	112.3(2)
C(8)-C(4)-C(3)	112.0(2)	C(5)-C(4)-S	113.9(2)
C(8)-C(4)-S	112.3(2)	C(3)-C(4)-S	105.0(2)
C(4)-C(5)-C(6)	104.4(2)	C(7)-C(6)-C(5)	106.2(2)
C(8)-C(7)-C(6)	105.4(2)	O(2)-C(8)-O(1)	105.9(2)
O(2)-C(8)-C(7)	113.4(2)	O(1)-C(8)-C(7)	109.3(2)
O(2)-C(8)-C(4)	114.9(2)	O(1)-C(8)-C(4)	108.4(2)
C(7)-C(8)-C(4)	104.8(2)	O(3)-C(9)-O(1)	123.0(3)
O(3)-C(9)-C(10)	128.0(3)	O(1)-C(9)-C(10)	108.9(2)
O(2)-C(10)-C(11)	112.2(2)	O(2)-C(10)-C(9)	103.9(2)
C(11)-C(10)-C(9)	111.8(2)	C(12)-C(11)-C(16)	118.8(3)
C(12)-C(11)-C(10)	120.0(3)	C(16)-C(11)-C(10)	121.2(2)
C(13)-C(12)-C(11)	120.4(3)	C(14)-C(13)-C(12)	120.4(3)
C(15)-C(14)-C(13)	119.5(3)	C(14)-C(15)-C(16)	120.6(3)
C(15)-C(16)-C(11)	120.2(3)		

Table 9. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **13**.

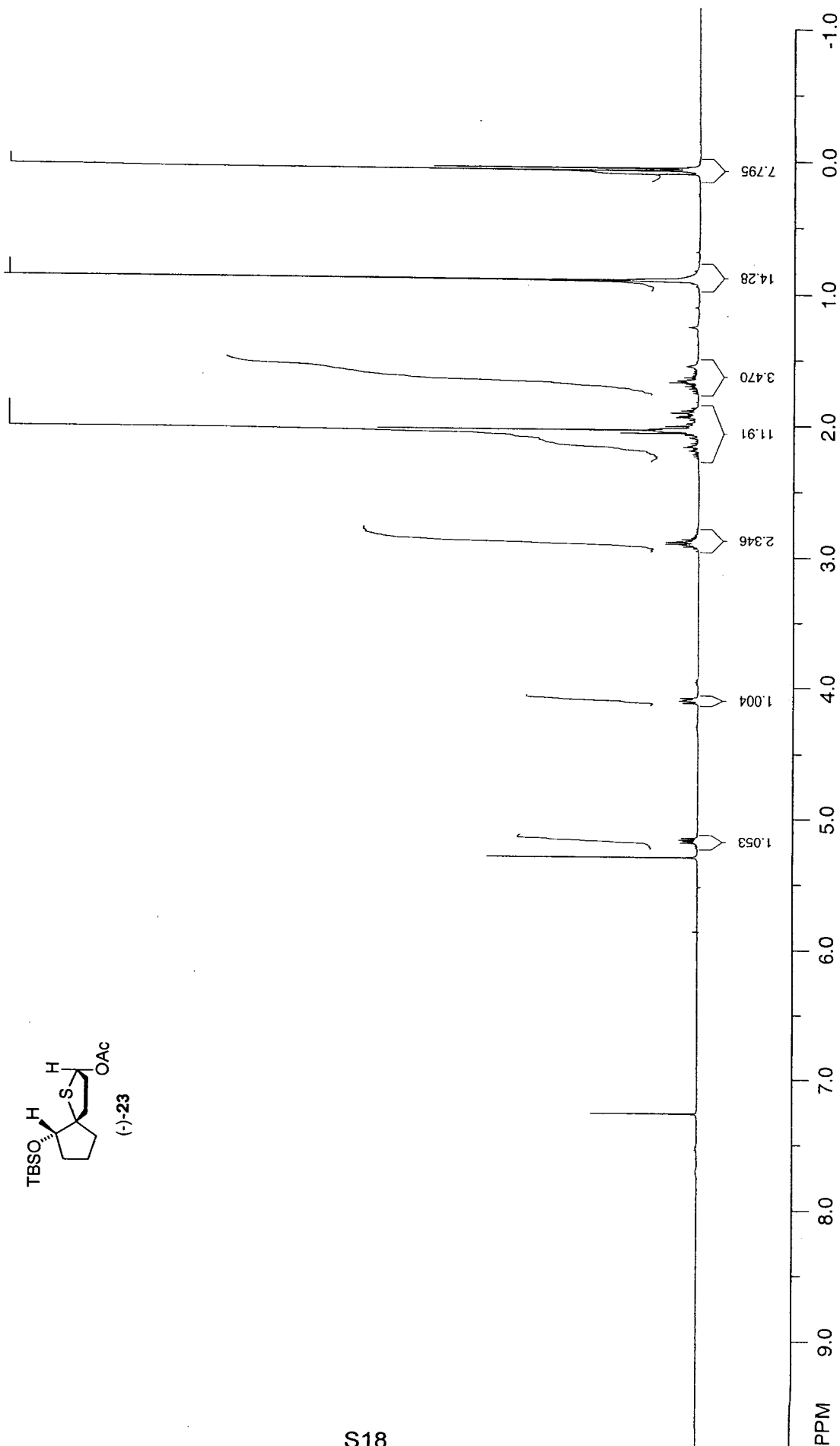
Atom	U11	U22	U33	U23	U13	U12
S	26(1)	42(1)	62(1)	5(1)	6(1)	6(1)
O(1)	34(1)	32(1)	44(1)	-5(1)	-9(1)	-8(1)
O(2)	44(1)	32(1)	43(1)	9(1)	-18(1)	-13(1)
O(3)	23(1)	38(1)	75(2)	1(1)	-3(1)	-3(1)
C(1)	77(3)	39(2)	57(2)	-3(2)	15(2)	14(2)
C(2)	58(2)	31(1)	49(2)	3(1)	-11(2)	-2(1)
C(3)	34(1)	29(1)	39(2)	9(1)	-8(1)	-5(1)
C(4)	19(1)	32(1)	35(1)	-1(1)	-4(1)	0(1)
C(5)	43(2)	50(2)	33(2)	0(1)	-2(1)	7(2)
C(6)	58(2)	69(2)	58(2)	-5(2)	16(2)	18(2)
C(7)	32(2)	40(2)	72(2)	-1(2)	4(2)	8(1)
C(8)	27(1)	28(1)	39(1)	-4(1)	-8(1)	-3(1)
C(9)	24(1)	25(1)	51(2)	-2(1)	-4(1)	6(1)
C(10)	32(1)	24(1)	44(2)	-5(1)	3(1)	2(1)
C(11)	35(1)	23(1)	32(1)	-7(1)	3(1)	-3(1)
C(12)	46(2)	41(2)	43(2)	-10(1)	14(1)	-6(2)
C(13)	77(3)	43(2)	34(2)	4(1)	13(2)	-15(2)
C(14)	81(3)	33(2)	43(2)	4(1)	-17(2)	0(2)
C(15)	43(2)	38(2)	43(2)	-2(1)	-9(1)	8(1)
C(16)	34(1)	32(1)	32(1)	1(1)	1(1)	-4(1)

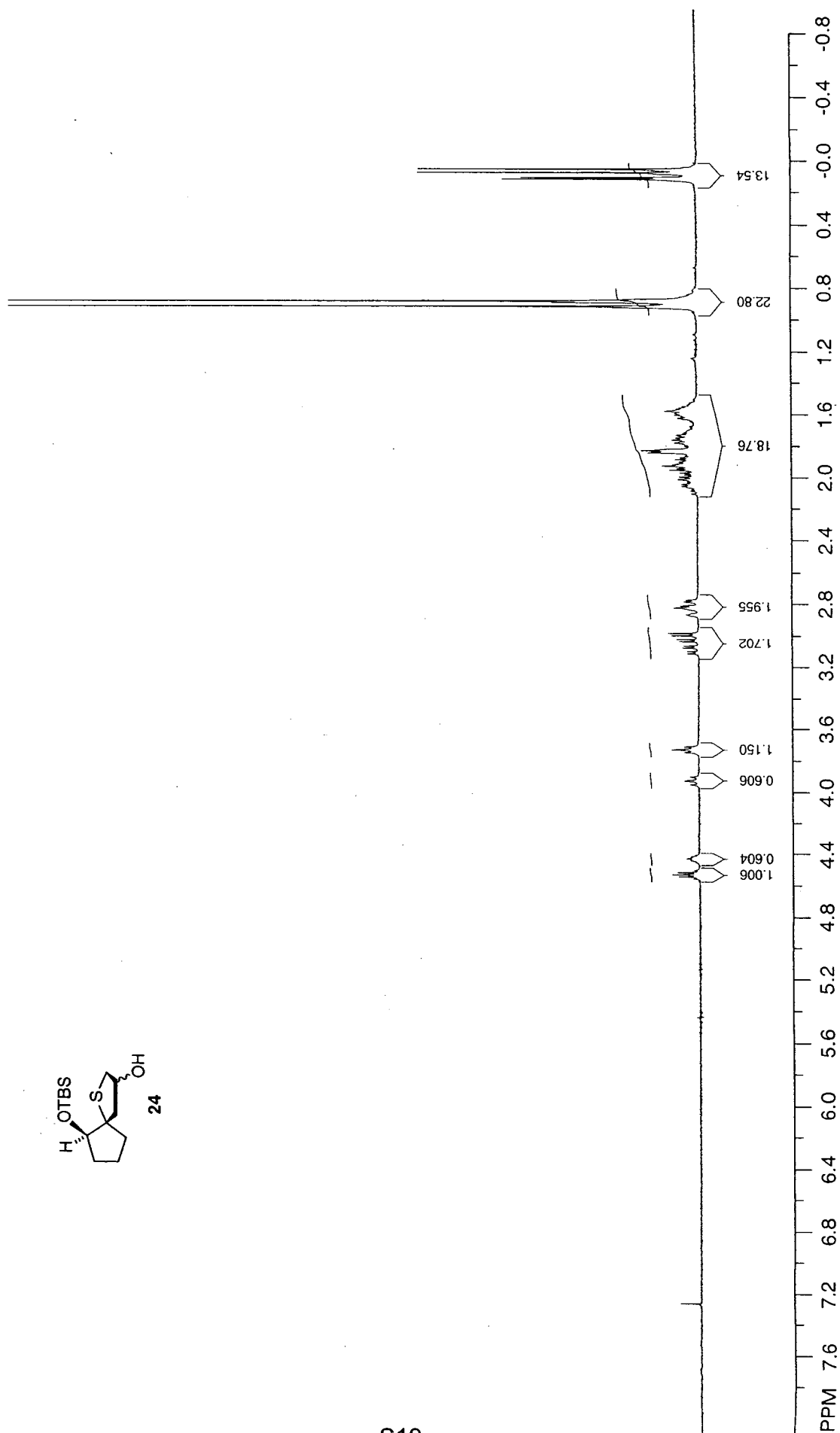
The anisotropic displacement factor exponent takes the form:

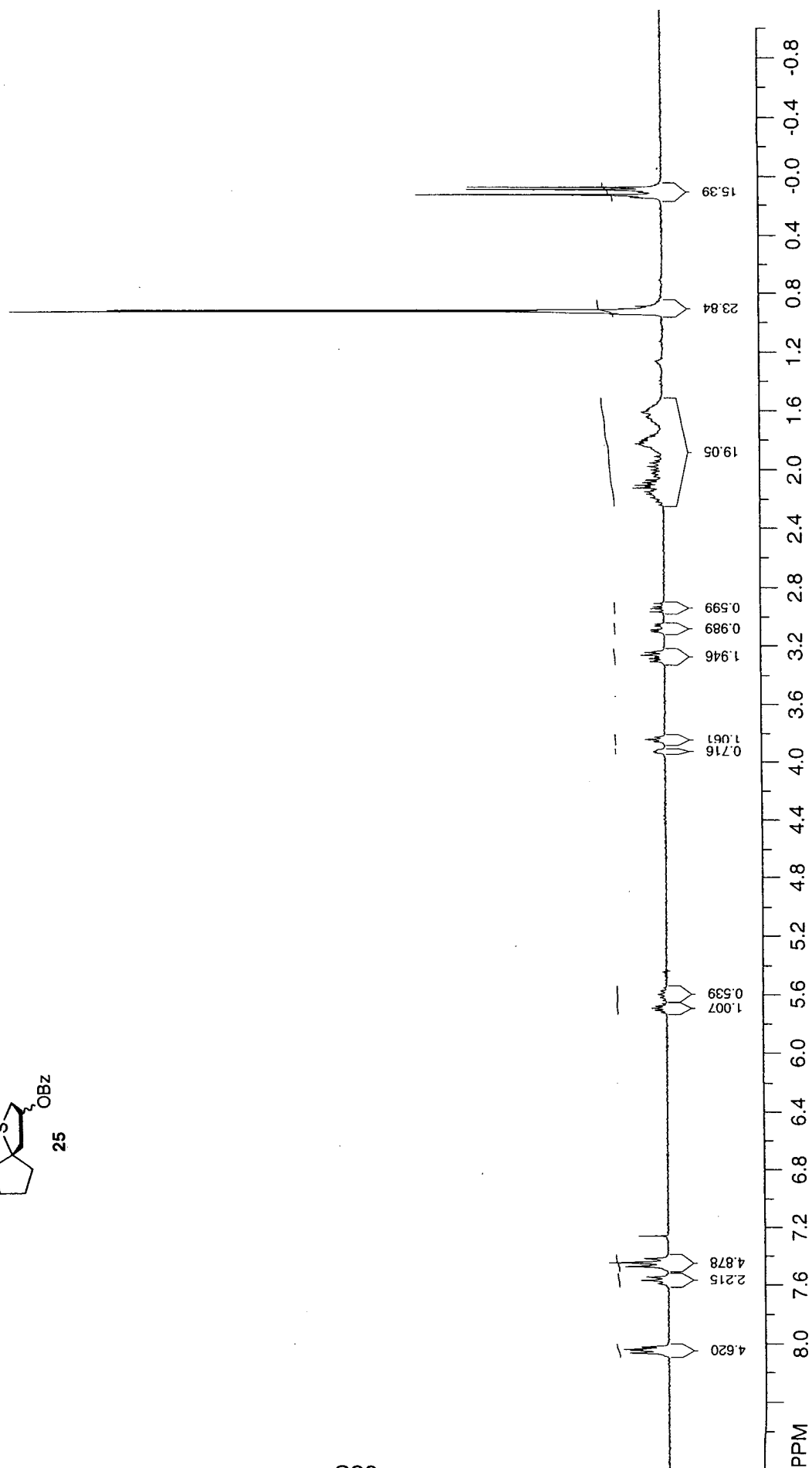
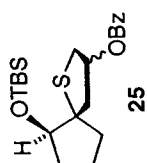
$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}].$$

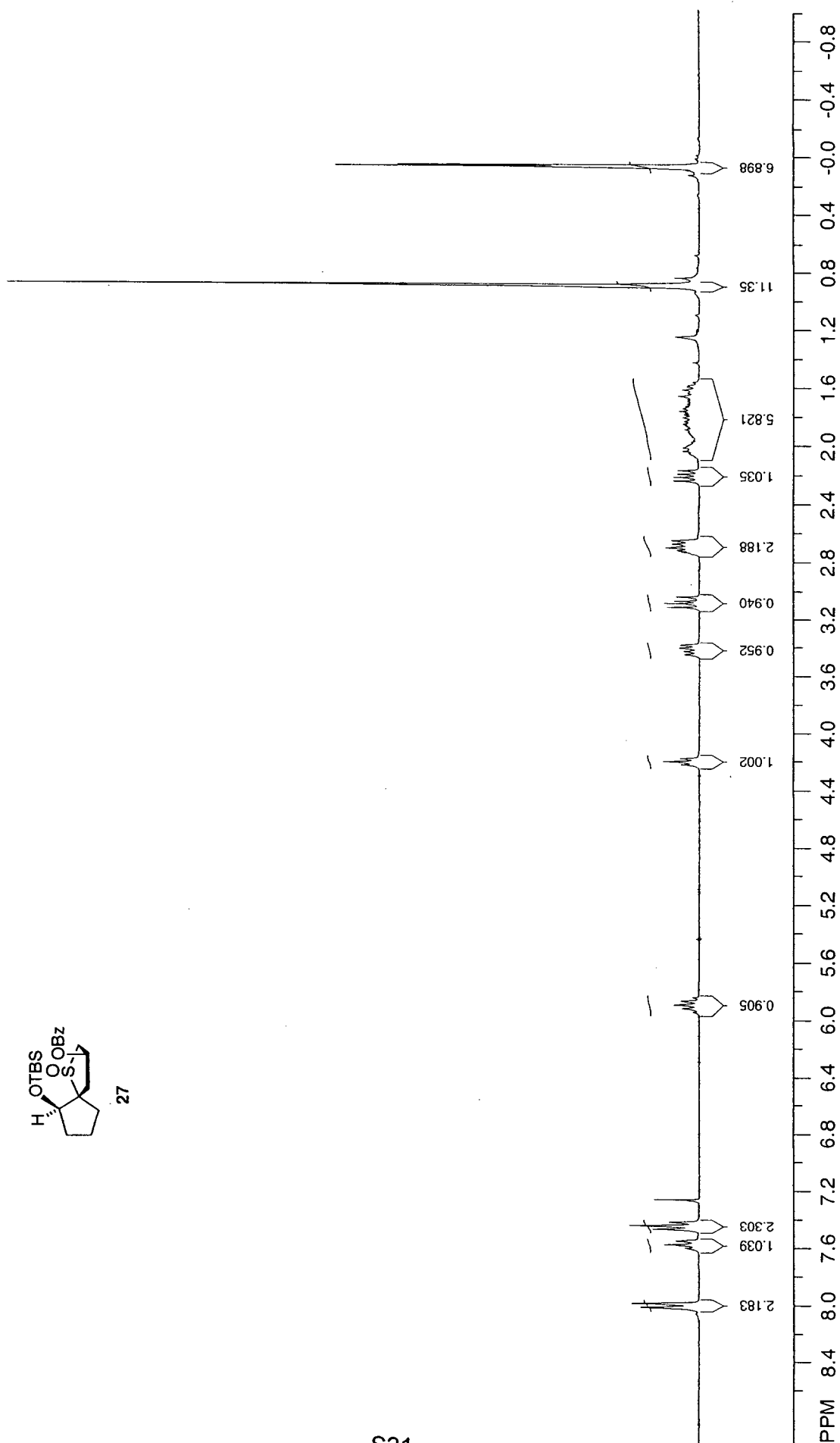
Table 10. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 13.

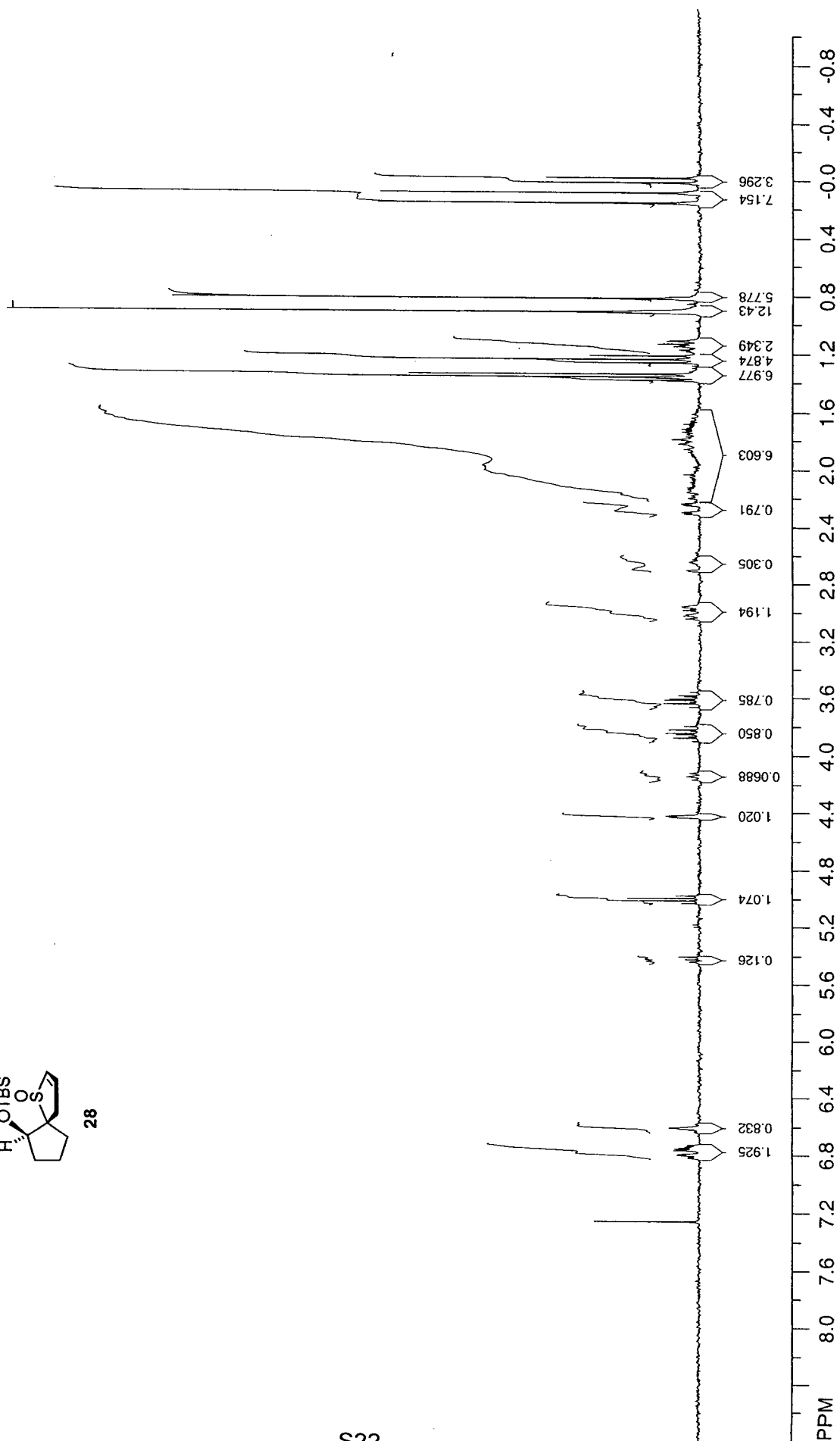
Atom	x	y	z	U(eq)
H(1A)	-1321(6)	-1314(4)	-1489(1)	69
H(1B)	-237(6)	-2064(4)	-992(1)	69
H(2A)	2553(5)	-938(3)	-1408(1)	55
H(2B)	1723(5)	-1468(3)	-1963(1)	55
H(3A)	3355(4)	-3476(3)	-1181(1)	41
H(3B)	4402(4)	-3195(3)	-1734(1)	41
H(5A)	2204(5)	-3685(3)	-2523(1)	50
H(5B)	725(5)	-5170(3)	-2522(1)	50
H(6A)	3737(6)	-6475(4)	-2689(1)	74
H(6B)	5186(6)	-5107(4)	-2484(1)	74
H(7A)	4231(5)	-7660(3)	-1940(1)	57
H(7B)	5444(5)	-6203(3)	-1712(1)	57
H(10A)	7(4)	-6520(3)	-598(1)	40
H(12A)	-718(5)	-8755(3)	-56(1)	52
H(13A)	591(6)	-10838(3)	396(1)	62
H(14A)	3887(6)	-11825(4)	201(1)	63
H(15A)	5903(5)	-10685(3)	-436(1)	50
H(16A)	4648(4)	-8570(3)	-881(1)	39

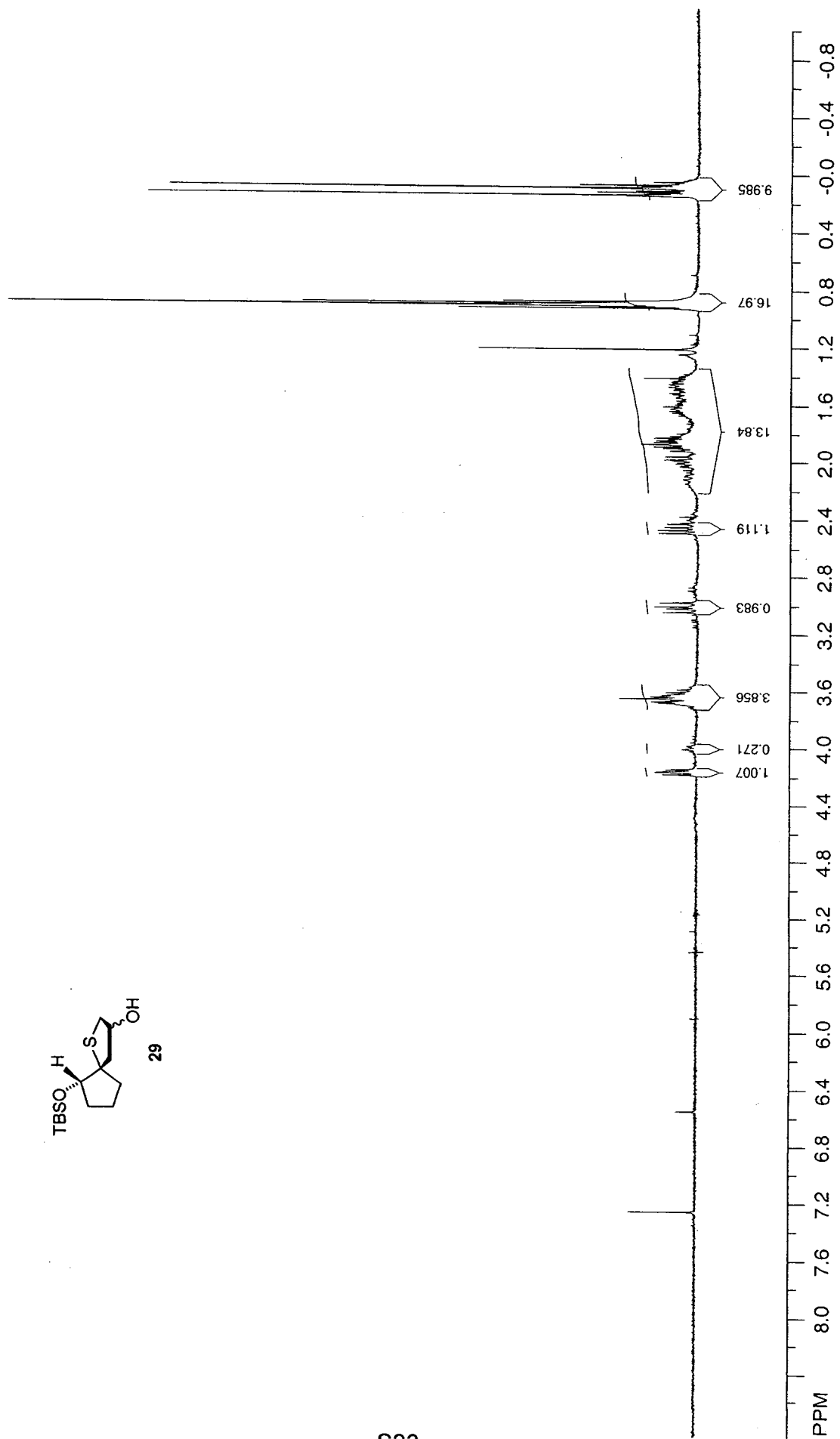


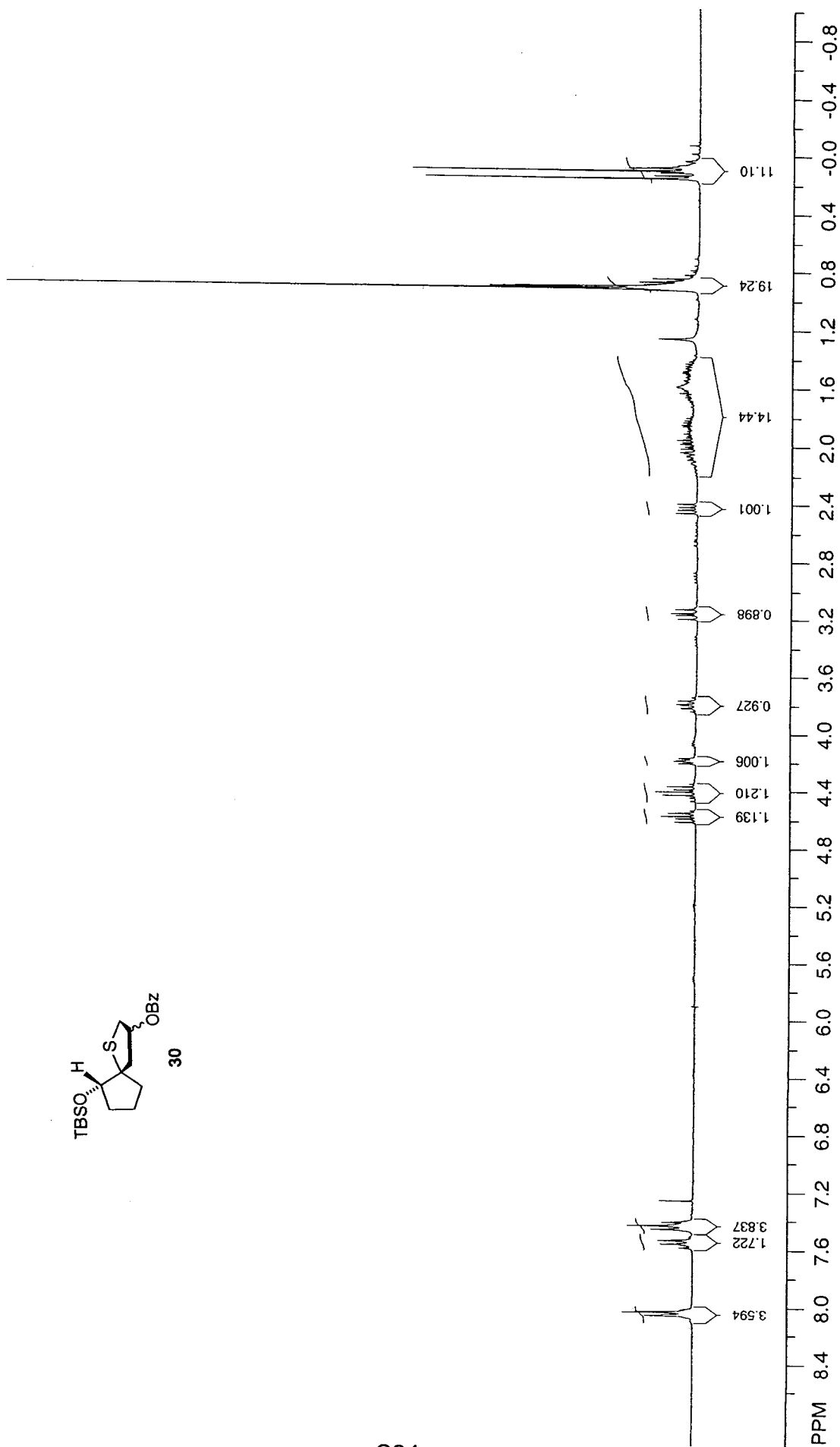


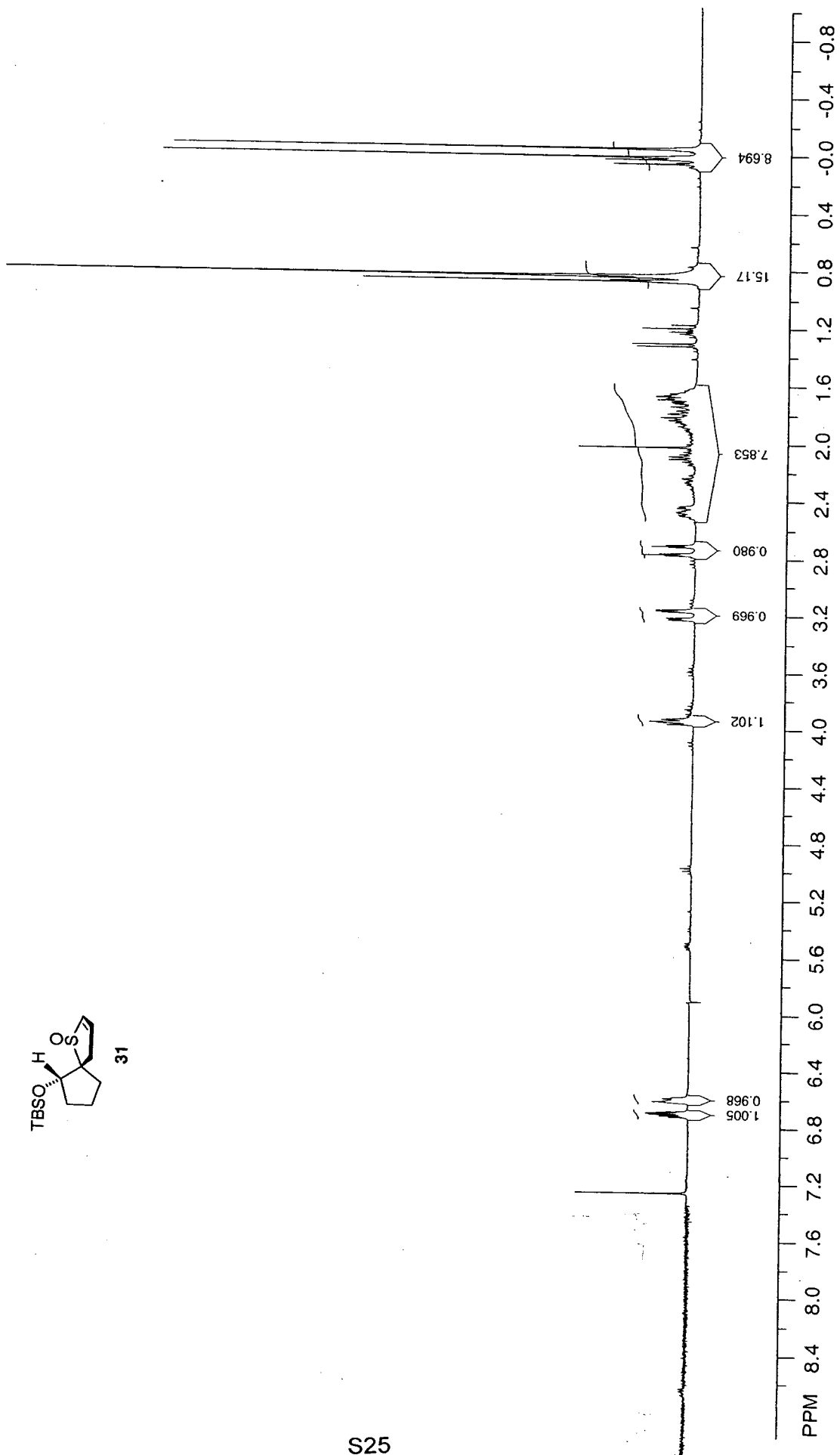


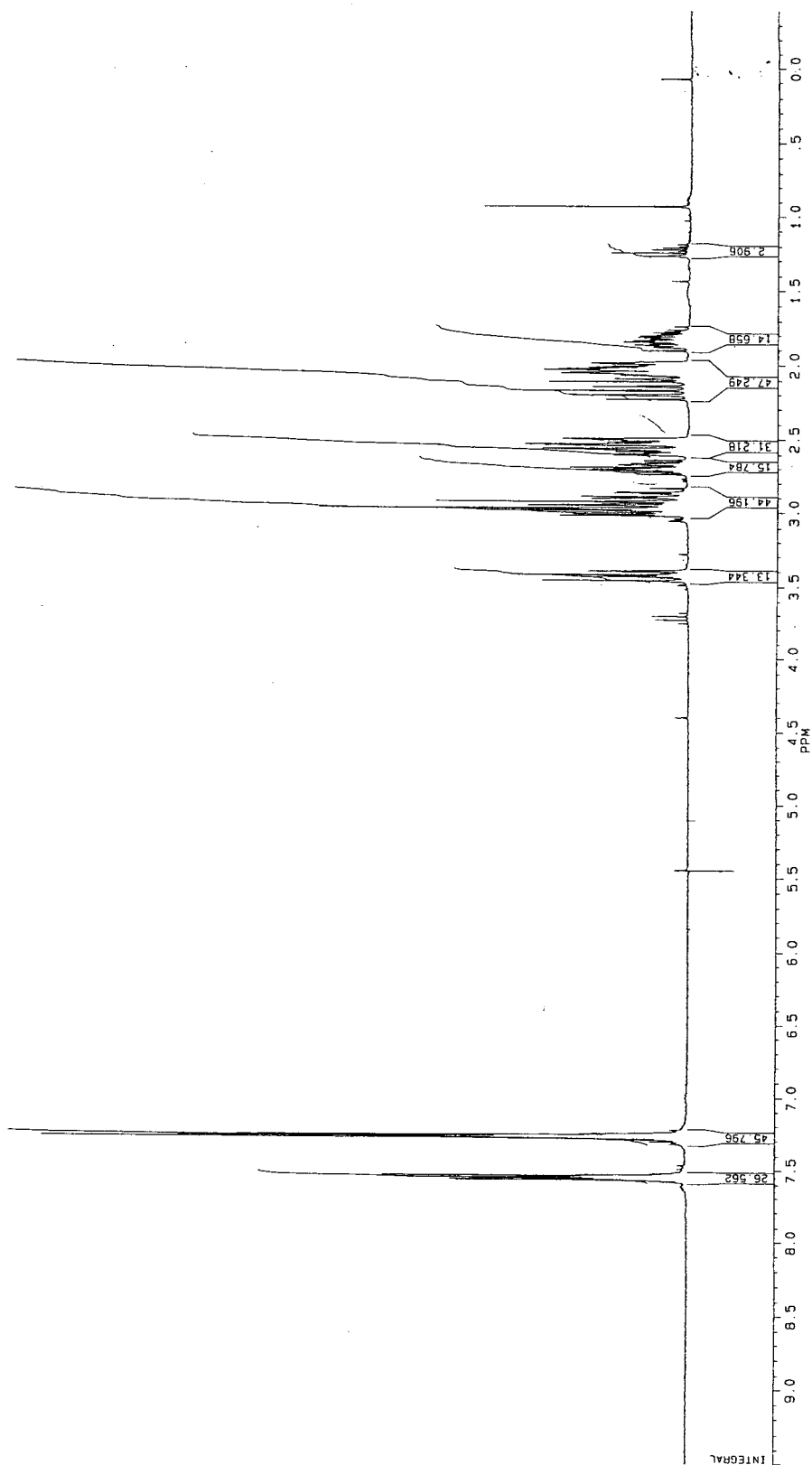
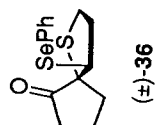


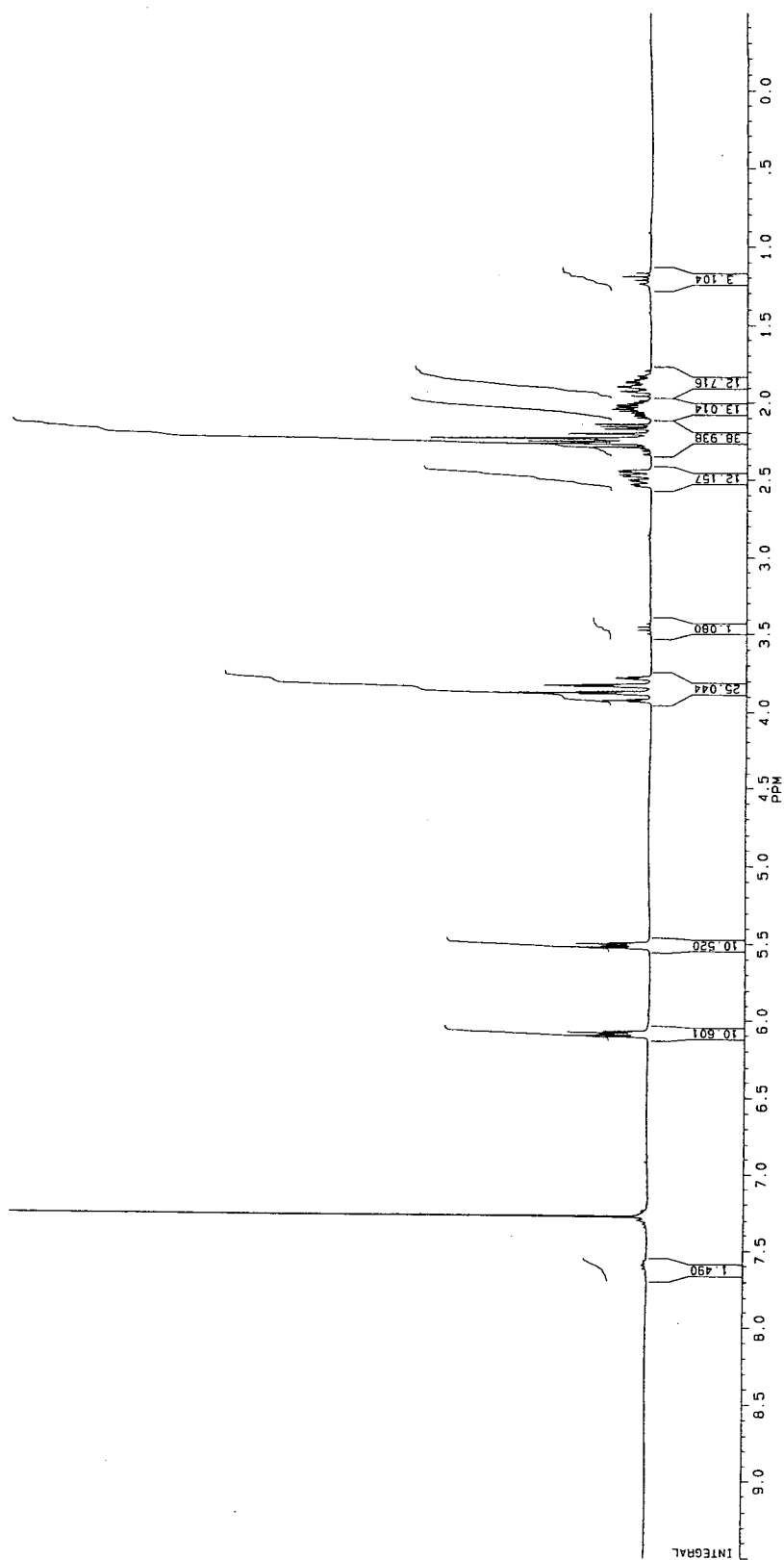
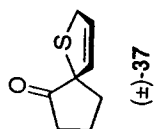


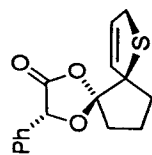












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