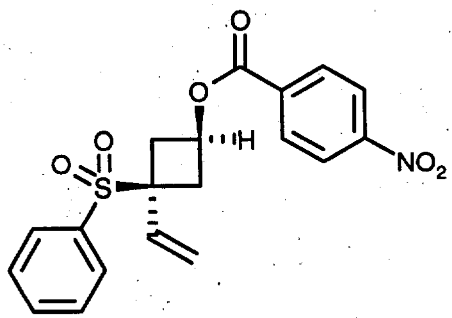

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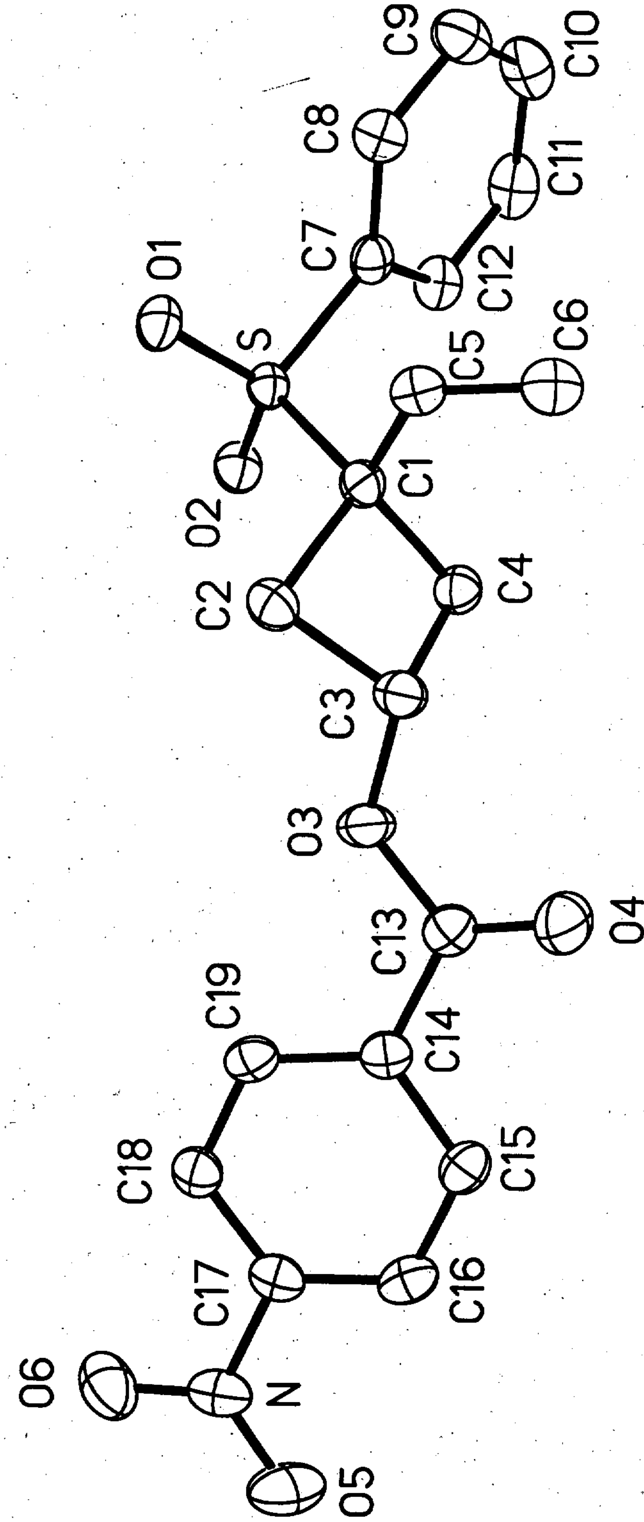

O1
S
O2
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
O3
C13
O4
C14
C15
C16
C17
C18
C19
N
O5
O6

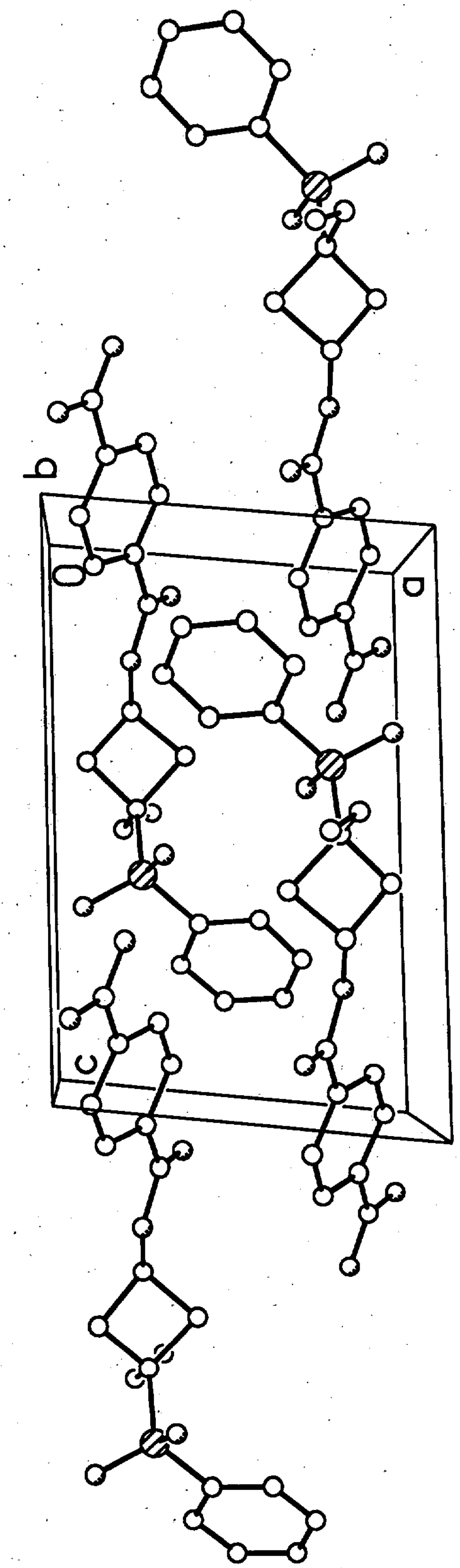

b
0
a
c

Table 1. Crystal data for Functionalized cyclobutane.

Identification code	mn651
Empirical formula	$C_{19}H_{17}NO_6S$
Formula weight	387.40
Crystal size	0.28 x 0.14 x 0.075 mm
Crystal habit	plate
Crystal color	colorless
Crystal system	$P\bar{1}$
Space group	triclinic
Unit cell dimensions	a = 7.846(2) Å α = 86.94(2)°
	b = 9.444(2) Å β = 83.56(2)°
	c = 12.110(2) Å γ = 84.05(2)°
Volume	886.1(3) $Å^3$
Z	2
Density (calculated)	1.452 $Mg{\bullet}m^{-3}$
Absorption coefficient	1.961 mm^{-1}
F(000)	404
Absorption correction[1]	XABS2
Max. and min. transmission	0.88 and 0.76

1) XABS2: an empirical absorption correction program. Parkin, S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* **1995**, 28, 53-56.

Table 2. Data collection for Functionalized cyclobutane.

Diffractometer	Syntex P2~1~
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
θ range for data collection	3.68 to 57.07°
Scan type	$2\theta-\omega$
Index ranges	$-8 \le h \le 8$, $-10 \le k \le 10$, $0 \le \ell \le 13$
Reflections collected	2399
Independent reflections	2399
Standard reflections	2
Percent decay of standards	< 1%

Table 3. Solution and refinement of Functionalized cyclobutane.

System for solution	SHELXTL v. 5 (Sheldrick, 1994)
Structure solution	direct
System for refinement	SHELXTL v. 5 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	2399 / 0 / 245
Goodness-of-fit on F^2	1.051
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0796P)^2 + 0.4869P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0538, wR2 = 0.1305
R indices calcd from obsd data	R1 = 0.0463, wR2 = 0.1222
Observed data (>2sigma(I))	2092
Largest diff. peak and hole	0.423 and -0.474 $e\text{Å}^{-3}$

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) Goodness-of-Fit = $[\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	y	z	U(eq)
S	2475(1)	3522(1)	6066(1)	21(1)
O(1)	820(3)	3503(2)	6718(2)	28(1)
O(2)	3054(3)	4879(2)	5689(2)	27(1)
O(3)	2265(3)	3927(2)	2274(2)	36(1)
O(4)	3448(3)	2437(2)	954(2)	48(1)
O(5)	1913(4)	8175(3)	-2773(2)	50(1)
O(6)	465(3)	9344(3)	-1434(2)	47(1)
N	1341(3)	8280(3)	-1802(2)	32(1)
C(1)	2364(4)	2485(3)	4874(2)	22(1)
C(2)	994(4)	3239(3)	4142(2)	30(1)
C(3)	2264(4)	2815(3)	3136(2)	29(1)
C(4)	3754(4)	2659(3)	3868(2)	24(1)
C(5)	1988(4)	999(3)	5251(2)	23(1)
C(6)	2837(4)	-177(3)	4866(2)	30(1)
C(7)	4043(4)	2591(3)	6849(2)	22(1)
C(8)	3534(4)	1534(3)	7618(2)	28(1)
C(9)	4774(4)	804(3)	8235(3)	34(1)
C(10)	6455(4)	1141(4)	8071(3)	36(1)
C(11)	6929(4)	2205(3)	7314(3)	34(1)
C(12)	5723(4)	2952(3)	6681(2)	26(1)
C(13)	2785(4)	3587(3)	1223(2)	27(1)
C(14)	2408(4)	4823(3)	440(2)	23(1)
C(15)	3135(4)	4766(3)	-662(2)	28(1)
C(16)	2781(4)	5902(3)	-1407(2)	29(1)
C(17)	1702(4)	7061(3)	-1022(2)	24(1)
C(18)	948(4)	7137(3)	57(2)	26(1)
C(19)	1303(4)	6000(3)	791(2)	26(1)

Table 5. Bond lengths [Å] for Functionalized cyclobutane.

S-O(2)	1.438(2)	S-O(1)	1.444(2)
S-C(7)	1.770(3)	S-C(1)	1.801(3)
O(3)-C(13)	1.338(4)	O(3)-C(3)	1.440(3)
O(4)-C(13)	1.199(4)	O(5)-N	1.216(3)
O(6)-N	1.231(4)	N-C(17)	1.475(4)
C(1)-C(5)	1.501(4)	C(1)-C(4)	1.556(4)
C(1)-C(2)	1.561(4)	C(2)-C(3)	1.528(4)
C(3)-C(4)	1.536(4)	C(5)-C(6)	1.314(4)
C(7)-C(12)	1.386(4)	C(7)-C(8)	1.387(4)
C(8)-C(9)	1.395(4)	C(9)-C(10)	1.379(5)
C(10)-C(11)	1.376(5)	C(11)-C(12)	1.396(4)
C(13)-C(14)	1.490(4)	C(14)-C(19)	1.392(4)
C(14)-C(15)	1.392(4)	C(15)-C(16)	1.391(4)
C(16)-C(17)	1.380(4)	C(17)-C(18)	1.375(4)
C(18)-C(19)	1.383(4)		

Table 6. Bond angles [°] for Functionalized cyclobutane.

O(2)-S-O(1)	118.33(12)	O(2)-S-C(7)	108.50(13)
O(1)-S-C(7)	107.83(13)	O(2)-S-C(1)	108.91(12)
O(1)-S-C(1)	105.91(13)	C(7)-S-C(1)	106.80(13)
C(13)-O(3)-C(3)	119.0(2)	O(5)-N-O(6)	123.7(3)
O(5)-N-C(17)	118.2(3)	O(6)-N-C(17)	118.1(3)
C(5)-C(1)-C(4)	117.5(2)	C(5)-C(1)-C(2)	112.4(2)
C(4)-C(1)-C(2)	88.3(2)	C(5)-C(1)-S	109.7(2)
C(4)-C(1)-S	117.1(2)	C(2)-C(1)-S	109.8(2)
C(3)-C(2)-C(1)	86.7(2)	O(3)-C(3)-C(2)	111.2(2)
O(3)-C(3)-C(4)	117.8(3)	C(2)-C(3)-C(4)	90.2(2)
C(3)-C(4)-C(1)	86.6(2)	C(6)-C(5)-C(1)	125.5(3)
C(12)-C(7)-C(8)	122.4(3)	C(12)-C(7)-S	119.0(2)
C(8)-C(7)-S	118.5(2)	C(7)-C(8)-C(9)	118.3(3)
C(10)-C(9)-C(8)	120.0(3)	C(11)-C(10)-C(9)	120.8(3)
C(10)-C(11)-C(12)	120.6(3)	C(7)-C(12)-C(11)	117.8(3)
O(4)-C(13)-O(3)	124.2(3)	O(4)-C(13)-C(14)	125.1(3)
O(3)-C(13)-C(14)	110.8(2)	C(19)-C(14)-C(15)	120.2(3)
C(19)-C(14)-C(13)	120.7(3)	C(15)-C(14)-C(13)	119.0(3)
C(16)-C(15)-C(14)	119.8(3)	C(17)-C(16)-C(15)	118.3(3)
C(18)-C(17)-C(16)	123.2(3)	C(18)-C(17)-N	118.2(3)
C(16)-C(17)-N	118.6(3)	C(17)-C(18)-C(19)	118.2(3)
C(18)-C(19)-C(14)	120.4(3)		

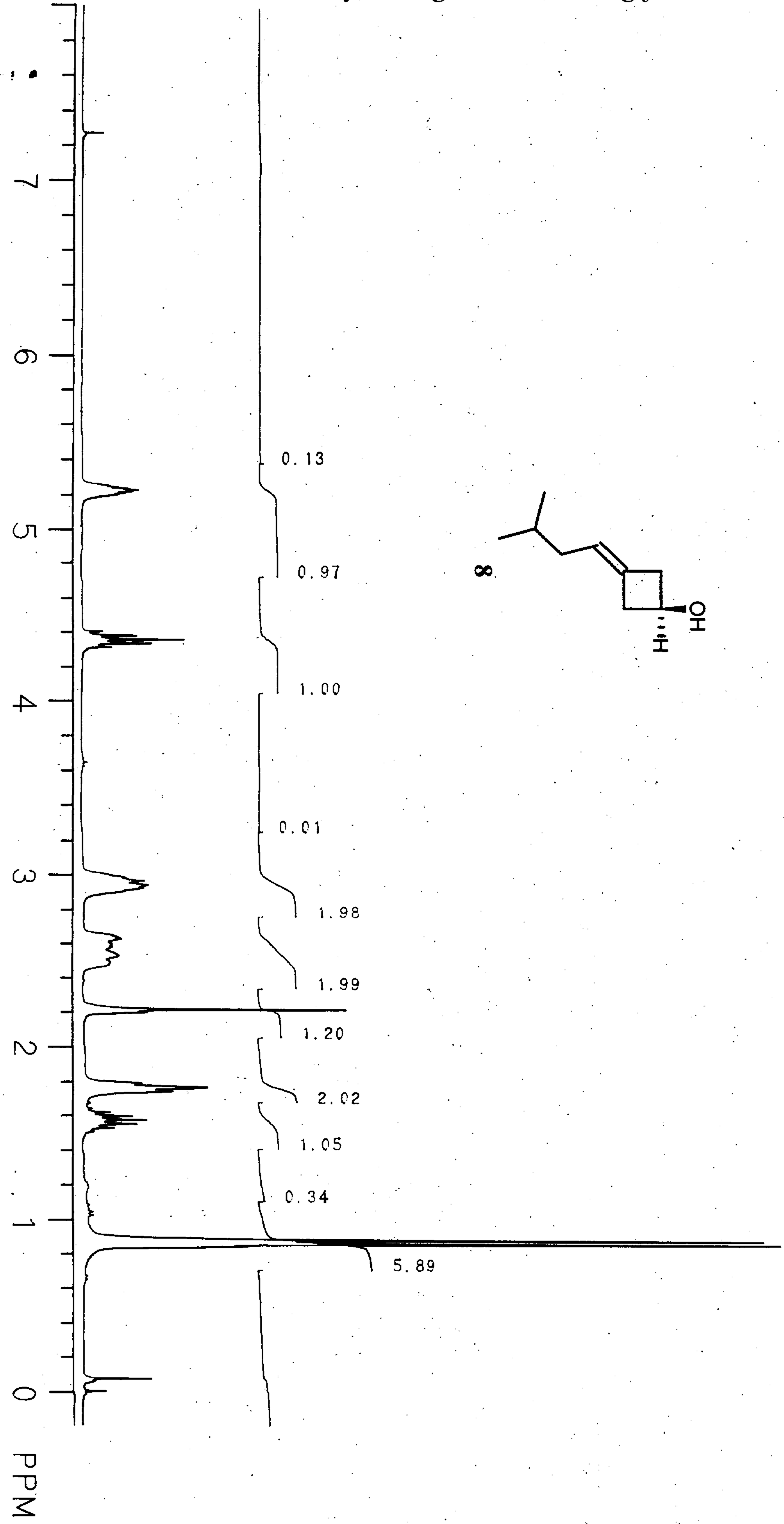
Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for Functionalized cyclobutane.

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
S	19(1)	21(1)	23(1)	-2(1)	-1(1)	-1(1)
O(1)	21(1)	33(1)	28(1)	-3(1)	1(1)	2(1)
O(2)	27(1)	21(1)	31(1)	0(1)	0(1)	-4(1)
O(3)	58(2)	28(1)	20(1)	-0(1)	-6(1)	4(1)
O(4)	70(2)	30(1)	37(1)	0(1)	6(1)	9(1)
O(5)	71(2)	50(2)	30(1)	10(1)	-7(1)	-15(1)
O(6)	40(2)	42(2)	55(2)	14(1)	2(1)	4(1)
N	29(2)	39(2)	30(2)	8(1)	-8(1)	-14(1)
C(1)	18(2)	26(2)	22(2)	-1(1)	-3(1)	0(1)
C(2)	27(2)	33(2)	28(2)	-1(1)	-8(1)	3(1)
C(3)	36(2)	26(2)	23(2)	1(1)	-6(1)	1(1)
C(4)	25(2)	23(2)	25(2)	0(1)	0(1)	-3(1)
C(5)	22(2)	27(2)	22(2)	-1(1)	-4(1)	-7(1)
C(6)	31(2)	28(2)	31(2)	0(1)	-5(1)	-8(1)
C(7)	23(2)	21(2)	22(2)	-6(1)	-3(1)	-1(1)
C(8)	28(2)	28(2)	29(2)	-2(1)	-5(1)	-5(1)
C(9)	42(2)	31(2)	32(2)	2(1)	-11(2)	-2(2)
C(10)	36(2)	36(2)	40(2)	-10(2)	-20(2)	4(2)
C(11)	24(2)	38(2)	42(2)	-14(2)	-7(1)	-5(2)
C(12)	26(2)	23(2)	32(2)	-6(1)	-3(1)	-6(1)
C(13)	27(2)	30(2)	27(2)	-3(1)	-4(1)	-5(1)
C(14)	23(2)	25(2)	24(2)	-4(1)	-7(1)	-7(1)
C(15)	29(2)	28(2)	26(2)	-6(1)	-2(1)	-5(1)
C(16)	29(2)	37(2)	23(2)	-1(1)	-1(1)	-14(2)
C(17)	21(2)	27(2)	28(2)	2(1)	-9(1)	-10(1)
C(18)	23(2)	29(2)	28(2)	-3(1)	-6(1)	-4(1)
C(19)	24(2)	32(2)	22(2)	-2(1)	-4(1)	-8(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Functionalized cyclobutane.

	x	y	z	U(eq)
H(2A)	-94(4)	2782(3)	4198(2)	35
H(2B)	770(4)	4280(3)	4230(2)	35
H(3)	2052(4)	1881(3)	2852(2)	34
H(4A)	4365(4)	3524(3)	3873(2)	29
H(4B)	4574(4)	1800(3)	3733(2)	29
H(5)	1058(4)	900(3)	5815(2)	28
H(6A)	3776(4)	-126(3)	4302(2)	35
H(6B)	2513(4)	-1078(3)	5152(2)	35
H(8)	2372(4)	1313(3)	7723(2)	34
H(9)	4460(4)	75(3)	8767(3)	41
H(10)	7295(4)	631(4)	8487(3)	43
H(11)	8089(4)	2433(3)	7221(3)	41
H(12)	6043(4)	3684(3)	6153(2)	32
H(15)	3871(4)	3953(3)	-904(2)	33
H(16)	3269(4)	5882(3)	-2161(2)	35
H(18)	203(4)	7949(3)	292(2)	32
H(19)	789(4)	6023(3)	1539(2)	31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5.89
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4
3
2
1
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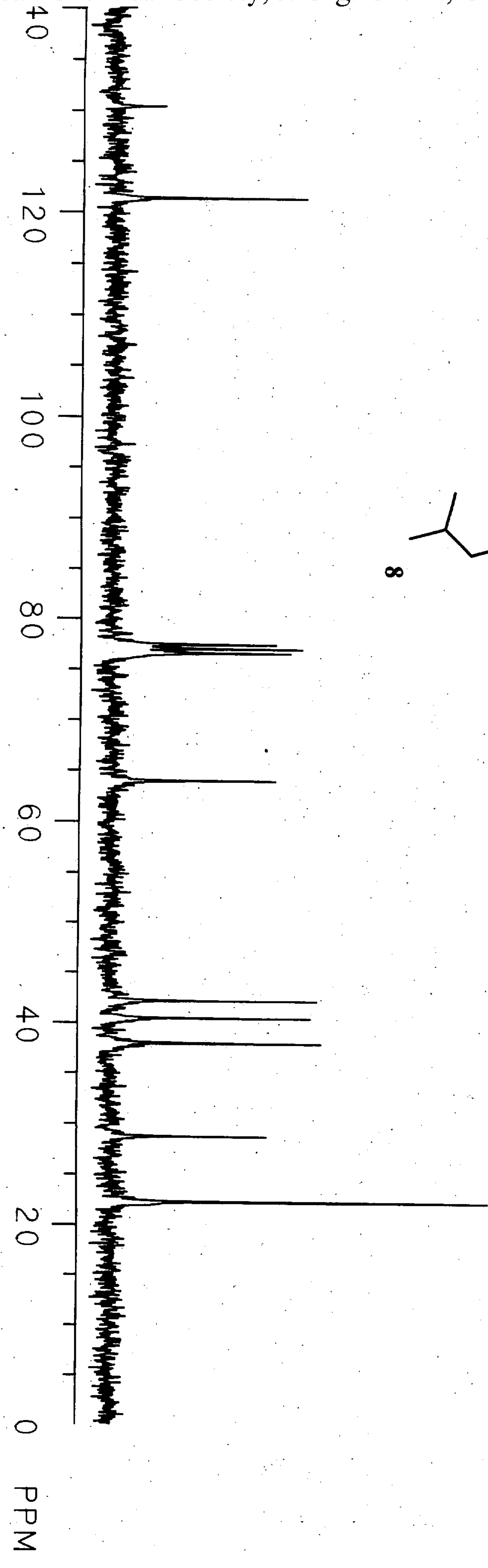
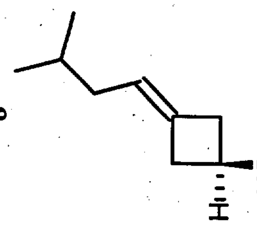
PPM
OH
H
8

14





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