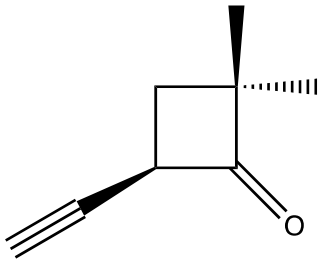
Universitetet i Oslo

Det matematisk-naturvitenskaplige fakultet

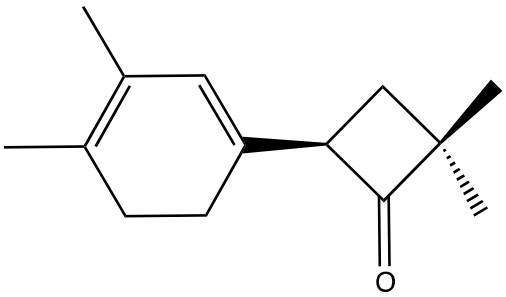
Exam in: **KJM3000 and KJM4000**
Day of exam: **2011-26-08**
Exam hours: **14.30 – 18.30 (4 hours)**
This examination paper consists of 2 page(s).
Appendices: **3 (1, 3 and 2 pages respectively)**
Permitted materials: Ruler, calculator and molecular modelling kit

Make sure that your copy of this examination paper is complete before answering

Question 1 (40%)



I



II

Compound **1** has been synthesized and the following ^{1}H NMR has been recorded: ($CDCl_3$, 300 MHz): δ 1.22 (s, 3H), 1.27 (s, 3H), 1.89 (dd, *J* 7.5 og 9.0 Hz, 1H), 2.13 (dd, *J* 3.5 og 9.0 Hz, 1H), 2.83 (d, *J* 2.5 Hz, 1H), 4.03 (m, 1H).

a) Assign the listed signals in the ^{1}H-NMR spectrum of compound **1** and give a brief explanation of the coupling pattern.

b) Calculate λ_{max} and propose an approximate ε_{max} value for compound **II**.

c) Identify the compound which give rise to the MS spectrum (EI, 70 eV) found in attachment 2. Give a brief explantation.

Question 2 (60%).

a) Identify the compound which gives rise to the spectra found in attachment 3. Assign the signals in the ^{13}C- and ^{1}H-NMR spectra to the molecular structure and give a brief explanation. Draw equations to account for the fragmentation reactions which produce the following ions in the mass spectrum (EI, 70 eV): 141, 97, 69, 39, 29.

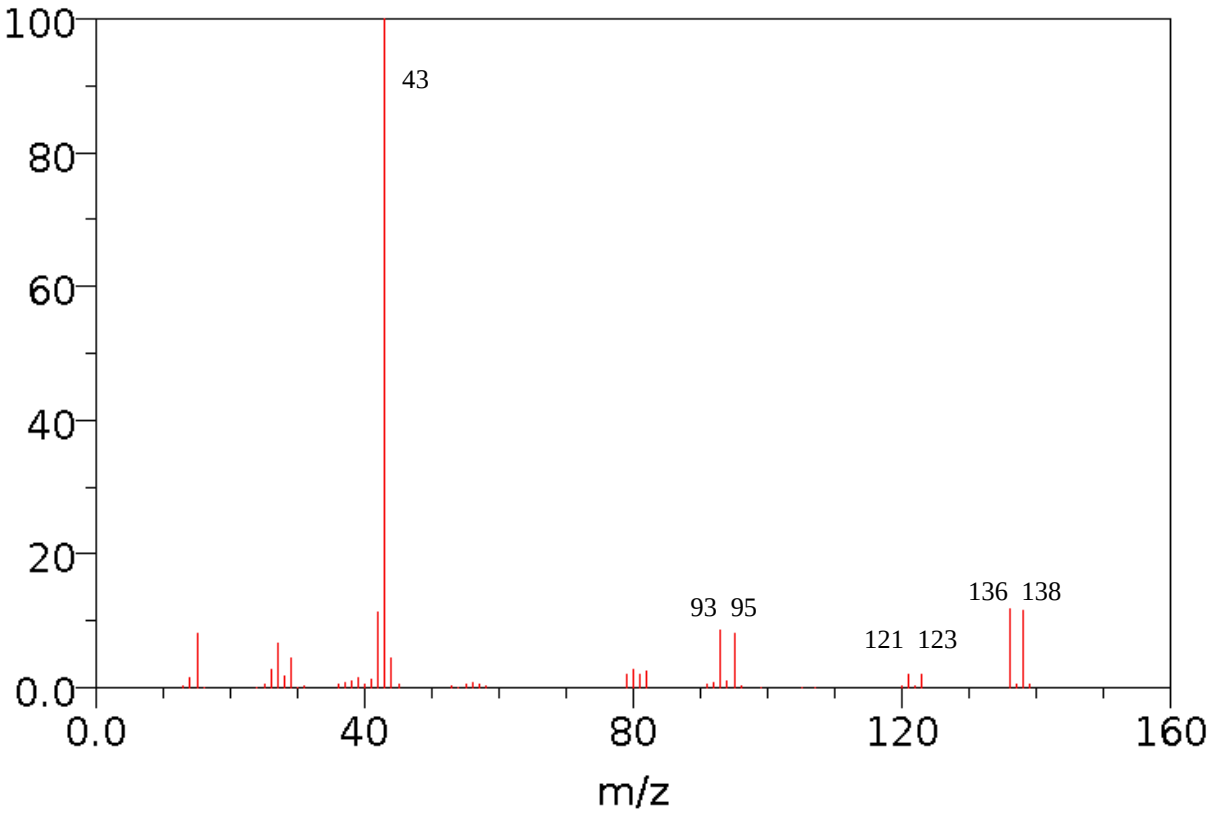
Table 4.3 Atomic weights and approximate natural abundance of some isotopes

Isotope	*Atomic weight* ($^{12}C = 12.000\,000$)	*Natural abundance* (%)
^{1}H	1.007 825	99.985
^{2}H	2.014 102	0.015
^{12}C	12.000 000	98.9
^{13}C	13.003 354	1.1
^{14}N	14.003 074	99.64
^{15}N	15.000 108	0.36
^{16}O	15.994 915	99.8
^{17}O	16.999 133	0.04
^{18}O	17.999 160	0.2
^{19}F	18.998 405	100
^{28}Si	27.976 927	92.2
^{29}Si	28.976 491	4.7
^{30}Si	29.973 761	3.1
^{31}P	30.973 763	100
^{32}S	31.972 074	95.0
^{33}S	32.971 461	0.76
^{34}S	33.967 865	4.2
^{35}Cl	34.968 855	75.8
^{37}Cl	36.965 896	24.2
^{79}Br	78.918 348	50.5
^{81}Br	80.916 344	49.5
^{127}I	126.904 352	100

Table 1.3 Rules for diene and triene absorption

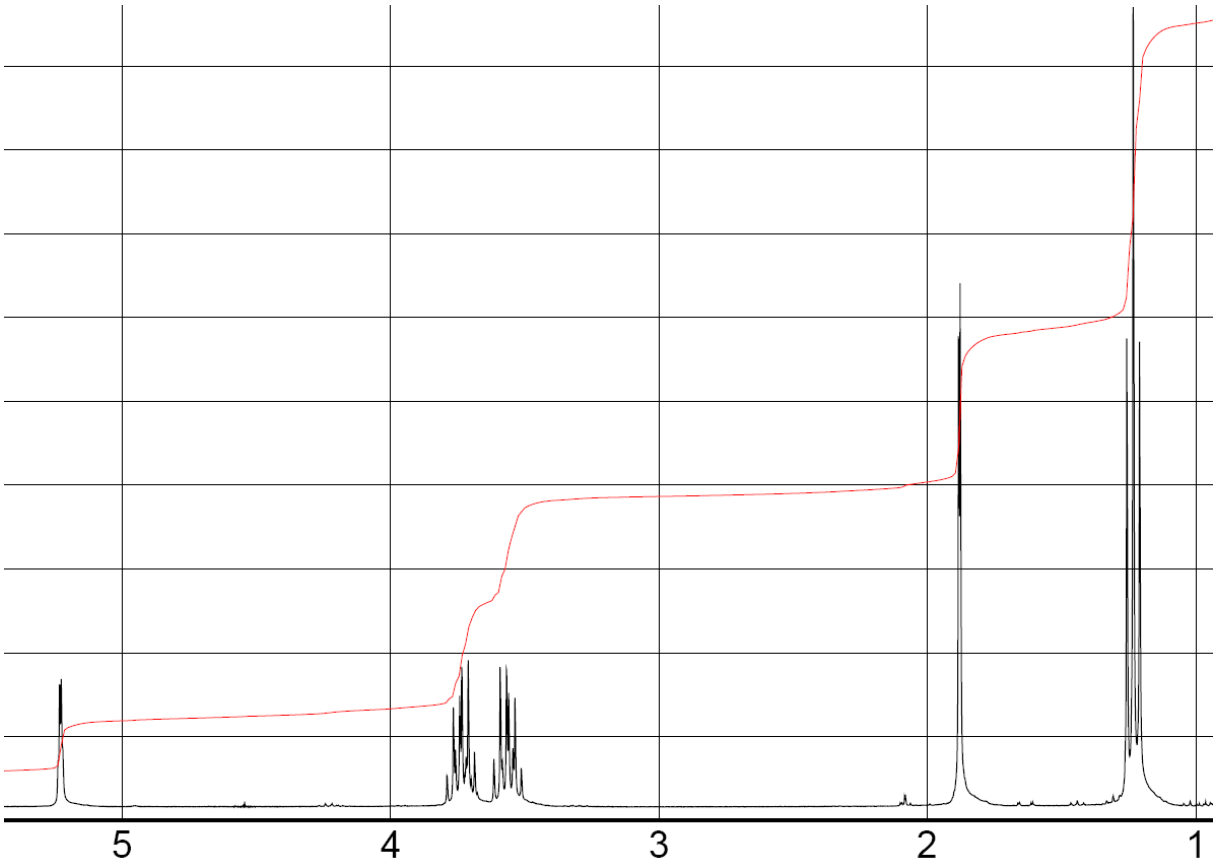
Value assigned to parent heteroannular or open chain diene	214 nm
Value assigned to parent homoannular diene	253 nm
Increment for	
(a) each alkyl substituent or ring residue	5 nm
(b) the exocyclic nature of any double bond	5 nm
(c) a double-bond extension	30 nm
(d) auxochrome —OAcyl	0 nm
—OAlkyl	6 nm
—SAlkyl	30 nm
—Cl, —Br	5 nm
—$NAlkyl_2$	60 nm
λ_{calc} Total	

MS (EI, 70 eV):

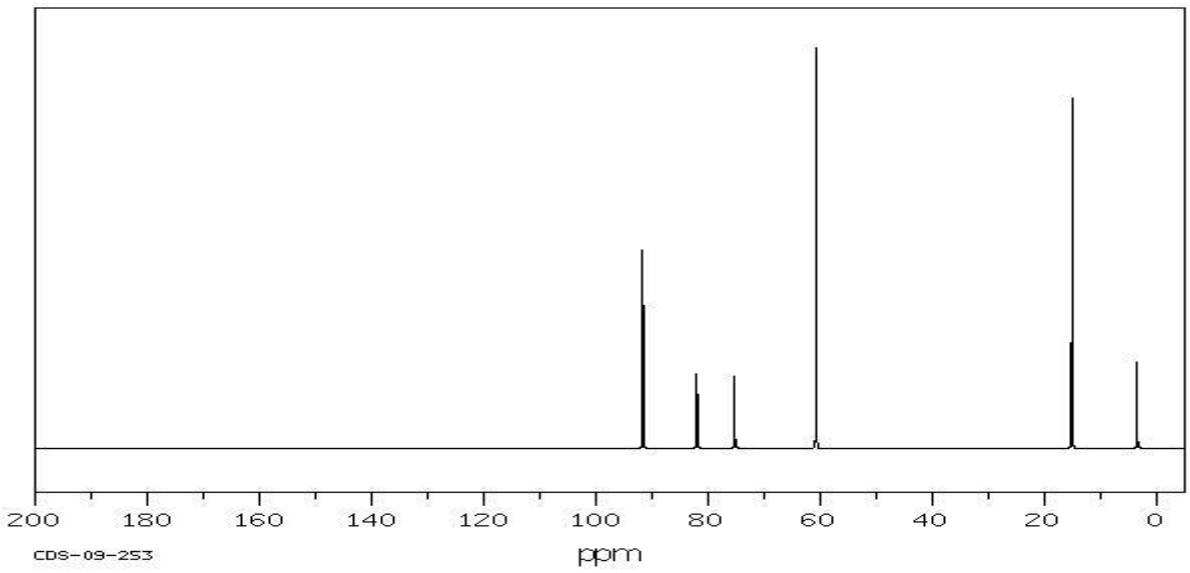


Vedlegg 3 / Attachment 3

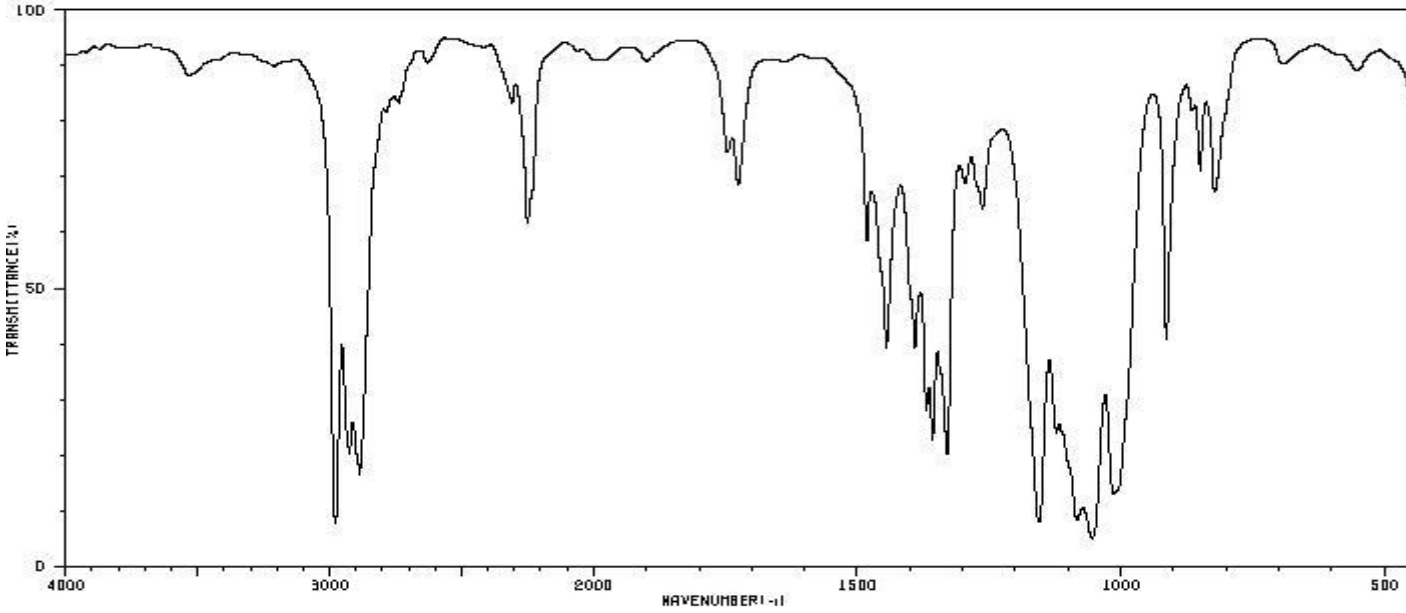
^{1}H-NMR: 300z, in $CDCl_3$
δ: 5.22 (1H, q, *J* = 1.0 Hz), 3.71 (2H, dq, *J* = 9.2 and 6.8 Hz), 3.58 (2H, dq, *J* = 9.2 and 6.8 Hz), 1.88 (3H, d, *J* = 1.0 Hz), 1.23 (6H, t, *J* = 6.8 Hz)



^{13}C-NMR: Broadband decoupled, 22.5 MHz, 0.05 ml in 0.5 ml $CDCl_3$
δ: 91.6, 82.0, 75.2, 60.7, 15.1, 3.5.



IR: Liquid film. Numbers in table indicate frequency and transmittance.



3630	84	1746	72	1330	19	1013	12
2978	7	1726	66	1295	66	914	38
2924	19	1462	57	1263	82	865	79
2886	16	1444	37	1166	7	849	68
2738	79	1391	37	1122	23	823	64
2308	79	1369	26	1083	8	553	86
2260	68	1367	21	1064	4		

MS (CI): 143 (100)

Grunnstoff analyse/Elemental analysis: C:67.51%, H:9.84%.

MS: EI, 70 eV