

Mass spectra of liquid crystals. VI. Alkylbicyclohexyl ethers, dioxanylbenzotrile derivatives and other classes of compounds

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Table 1. Relative abundances of characteristic ions in the EI mass spectra of alkylbicyclohexyl ethers (class I)^a

No.	R ¹	R ²	RMM	m/z													95 +A ^d	93	
				C ^c	C -Et	C -Pr	C -Bu	C -Pe	163 +A ^d	82 +R ¹	81 +R ¹	80 +R ¹	79 +R ¹	66 +R ¹	121	97			96
1	Pr	OMe	238	65	19	e	5	10	31	8	28	39	24	30	15	19	13	27	14
2	Pe	OMe	266	43	17	e	5	e	37	2	14	24	7	19	16	34	23	35	15
3	Pr	OEt	252	63	34	e	5	10	31	6	21	29	21	9	15	13	10	22	12
4	Pe	OEt	280	41	31	2	5	e	40	2	11	21	6	15	16	24	17	28	13
5	Pr	OPr	266	63	41	e	6	10	37	10	20	34	21	29	17	17	10	28	12
6	Pr	OCOPr	294	100	17	e	9	13	51	16	38	57	36	46	26	13	20	37	15
7	Pr	CH ₂ OMe	252	27	27	e	2	5	7	4	7	16	10	19	7	14	22	9	9
8	Pe	CH ₂ OMe	280	16	19	—	—	e	9	—	3	8	3	12	7	32	26	12	11

No.	R ¹	R ²	RMM	m/z													Base Peak ^b		
				83	82	81 +A ^d	80 +A ^d	40 +R ²	27 +R ²	79	69	67	57	55	53	45		43	41
1	Pr	OMe	238	50	51	100	20	70	24	30	60	54	16	72	16	18	34	93	81
2	Pe	OMe	266	47	38	100	20	69	18	29	39	56	16	66	12	14	43	73	81
3	Pr	OEt	252	34	33	70	12	100	15	22	41	42	52	58	11	3	28	60	85
4	Pe	OEt	280	35	30	77	14	100	16	27	33	50	59	67	9	4	46	61	85
5	Pr	OPr	266	39	32	76	13	57	8	24	51	51	100	69	11	10	64	82	57
6	Pr	OCOPr	294	69	84	99	29	—	—	32	86	66	19	73	11	2	99	74	206
7	Pr	CH ₂ OMe	252	33	20	100	26	—	—	19	50	46	9	52	8	52	12	49	95
8	Pe	CH ₂ OMe	280	33	16	100	29	—	—	22	25	54	9	60	10	73	25	56	95

^a Me = methyl, Et = ethyl, Pr = *n*-propyl, Pe = *n*-pentyl.

^b *m/z* of base peak.

^c C = *m/z* (163 + R¹ + A^d).

^d A = 0 (compounds 1–6) or 14 (CH₂, 7 and 8).

^e See *m/z* (163 + A).

^f See *m/z* (166 + R¹).

absence of a peak at *m/z* 58 in the spectrum of 6. In the spectrum of this ester, there is a peak at *m/z* 71 (70%), which corresponds to the ions [COPr]⁺ and not to [H₂C=CHCH=R²]⁺, at *m/z* (40 + R²), as in the spectrum of ether 1.

The mass spectrum of an unsaturated analogue of 4 is given in Fig. 1. Above *m/z* 90, all peaks appear at 2 u less than in the spectrum of ether 4. Below *m/z* 90, both spectra are similar in a qualitative sense. Remarkable are the presence of the molecular ions at *m/z* 278 (10%) and the abundance of the ions at *m/z* 149 (72%) compared with that of *m/z* 151 (21%) in the spectrum of 4. The spectrum of another, all-hydrocarbon derivative of cyclohexylcyclohexene is presented in Fig. 2. The molecular ion is present, and losses of propyl and pentyl radicals from M⁺ are easily discernible (*m/z* 233 and 205, respectively).

The EI spectra of three 1,3-dioxanylbenzonnitriles, 9–11 (class II), are condensed in Table 2. The occurrence of two equally high peaks from the molecu-

lar ions and ions of 1 u less sets apart the spectra of this class of compounds. Another distinct feature in the spectra of these compounds is the presence of peak pairs at *m/z* 130/132 and 102/104. The former pair corresponds to the ions [O≡CC₆H₄CN]⁺ and [HO=CHC₆H₄CN]⁺. The latter pair possibly originates by loss of CO from the former. Small peaks at *m/z* 148 probably represent ions [HO=C(OH)C₆H₄CN]⁺. The base peaks are invariably found at *m/z* 55. Odd-electron alkene ions of *m/z* (R¹ - 1) are abundant. Alkyldioxanyl ions [R¹C₄H₆O₂]⁺ give peaks at *m/z* (86 + R¹). Fragmentation of the dioxanyl ring gives rise to series of ions, of which the most abundant ones yield peaks at *m/z* (40 + R¹), (27 + R¹) and (24 + R¹). These peaks probably correspond to the ions [O=C=CR¹]⁺, [H₂C=CHR¹]⁺ and [C≡CR¹]⁺, respectively.

The mass spectra of two cyclohexenylphenyl derivatives, 12 and 13 (class III), are given in Table 3. The molecular ions are present. The spectra are dominated

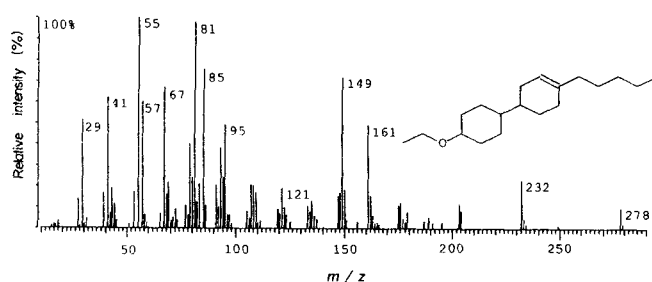


Figure 1. 70 eV EI mass spectrum of 1-ethoxy-4-(4-pentylcyclohex-3-en-1-yl)cyclohexane.

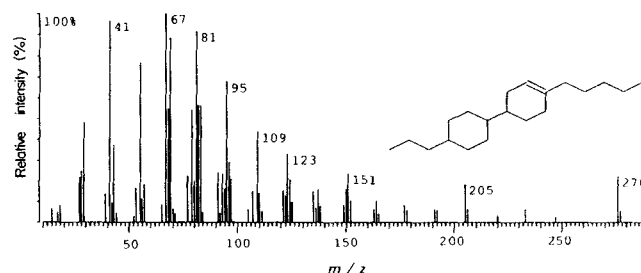


Figure 2. 70 eV EI mass spectrum of 1-pentyl-4-(4-propylcyclohexyl)cyclohexene.

