Registry No.—**5d,** 60967-91-1; **5e** (R_4 = β), 60967-92-2; **6g,** 60967-93-3; **6h** (R_4 = β), 60967-94-4; **7d,** 60967-95-5; **7f,** 60967-96-6; **7g,** 60967-97-7; **7h** (R_4 = α), 60967-98-8; **7h** (R_4 = β), 60967-99-9; **8b,** 60968-00-5; **8c,** 60968-01-6; **8d,** 60968-02-7; **8f,** 60968-03-8; **8g,** 60968-04-9; **8h** (R_4 = α), 60968-05-0; **8h** (R_4 = β), 60968-06-1; **9a,** 38393-90-7; **9b,** 60968-07-2; **9c,** 60968-08-3; **9d,** 60968-09-4; **9f,** 60968-10-7; **9g,** 60968-11-8; **9h** (R_4 = β), 60968-12-9; **10d,** 60968-13-0; **10e** (R_4 = β), 60968-14-1; **11a,** 60968-15-2; **11b,** 60968-16-3; **11c,** 60968-17-4; **11d,** 60968-18-5; **11e** (R_4 = β), 60968-19-6; silver benzoate, 532-31-0; 1,2-dihydroanthracene, 58746-82-0; *N*-bromosuccinimide, 128-08-5; silver acetate, 563-63-3; 3,4-dihydrophenanthrene, 38399-10-9; 1,2-dihydrophenanthrene, 56179-83-0; ethyl acetate, 141-78-6; 10,11-dihydrobenzo[*a*]anthracene, 34501-50-3.

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Aporphines. 19.[1a] Mass Spectrometry of Nitrobenzylisoquinolines. Influence of Positional Isomerism on Fragmentation and Evidence for an Ionically Induced Intramolecular Migration Process[1b]

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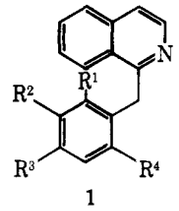
The mass spectra of a series of nitro-substituted benzylisoquinolines were examined under both electron impact and chemical ionization conditions. A number of fragmentation processes have been observed which can be utilized for structural assignments to positional isomers. Isotopic labeling was used to confirm the mechanism of specific fragmentations. The procedures for synthesis of the title compounds are included.

The importance of 1-(2-nitrobenzyl)isoquinolines as key intermediates in the synthesis of aporphine alkaloids and other biologically active molecules has been well documented in the recent literature.[2] The Reissert[3] alkylation method via 2-benzoyl-1,2-dihydroisoquinaldonitriles is used to advantage for the synthesis of many benzylisoquinolines and 1-(2-nitrobenzyl)isoquinolines.[4] Thus, aporphine alkaloids can be conveniently prepared by the reduction of the isoquinolinium salts of 1-(*o*-nitrobenzyl)isoquinolines and Pschorr cyclization.[5,6]

As part of a program aimed at the preparation and biological testing of a variety of new aporphine derivatives, we have synthesized a series of benzylisoquinolines, **1a–h.** This report on the mass spectrometric properties—both under electron impact and chemical ionization conditions—has been prompted, in part, by the relative paucity of mass spectral



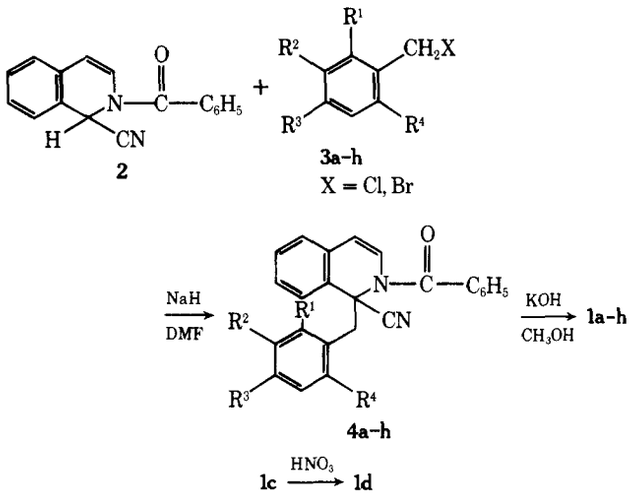
1

	R^1	R^2	R^3	R^4
a	NO_2	H	H	H
b	H	H	NO_2	H
c	H	H	OCH_3	H
d	H	NO_2	OCH_3	H
e	H	NO_2	OCD_3	H
f	NO_2	OCH_3	H	H
g	NO_2	H	OCH_3	H
h	NO_2	H	H	OCH_3

data on compounds of the benzylisoquinoline class. This is in sharp contrast to the partially saturated benzyl- and bisbenzyl-1,2,3,4-tetrahydroisoquinolines, for which a comparative abundance of mass spectrometric information has come to our attention.[7] Furthermore, it was hoped that some analogies might be drawn between the anticipated cleavage of the 1,1′ bond during mass spectral fragmentation and a stereochemically influenced exocyclic carbon–carbon cleavage observed during the reduction of the corresponding isoquinolinium salts.[8] The mass spectrometric investigations of the benzylisoquinolines have brought to light a number of considerations which can be applied to the structural determination of positional isomers of nitrobenzylisoquinolines.

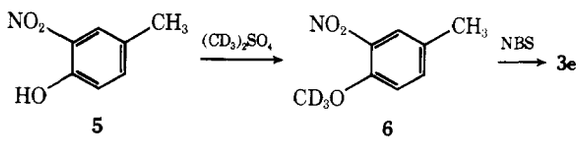
Compounds **1a–h** were prepared via alkylation of 2-benzoyl-1,2-dihydroisoquinaldonitrile (**2**) with the appropriate benzyl halide **3**.[9] The resulting Reissert adducts **4**, which were isolated and characterized in some cases, yielded on hydrolysis the corresponding 1-substituted isoquinoline. In addition, the benzylisoquinoline derivative **1d** was also obtained in 70% yield by nitration of **1c** with concentrated nitric acid (Scheme I). Introduction of the deuteriomethoxy group in **1e** was ac-

Scheme I



complished by the methylation of **5** with dimethyl-d_6 sulfate. The nitroanisole **6** was brominated to the aryl halide **3e** which furnished **1e** according to the procedure described in Scheme II.

Scheme II

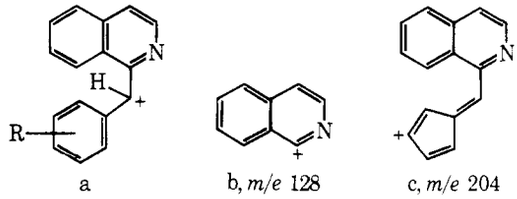


Results and Discussion

Electron Impact Ionization. On examining the electron-impact spectra of the benzylisoquinolines **1a–h** in Figures 1–3 the common features in the fragmentation of these compounds should be considered.

(a) The spectra of compounds containing a 2-nitro substituent exhibit relatively weak molecular ion and $[M - 1]^+$ peaks. This may be attributed, in part, to steric interaction between the NO_2 group and the adjacent methylene group, and is further reflected in the formation of abundant $[M - NO_2]\cdot^+$ ions in the spectra of **1a, 1f, 1g,** and **1h.** The strain introduced from the presence of an ortho substituent on the benzyl ring is also exemplified by the favorable elimination of the 6-methoxy group in compound **1h** to yield the ion at *m/e* 263 $[M - OCH_3]^+$.

(b) Loss of a hydrogen radical from the molecular ion is common to the mass spectra of compounds **1a–h** and presumably involves one of the benzylic hydrogens to produce the resonance stabilized ion a.



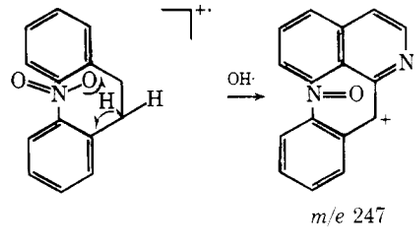
a b, *m/e* 128 c, *m/e* 204

(c) Cleavage of the benzylic–isoquinoline bond, a prominent process in the mass spectra of benzyltetrahydroisoquinolines,[10–12] occurs only to a minor extent in the spectra of the benzylisoquinolines **1a–h.** However, even though of low relative intensity, the presence of a peak at *m/e* 128, corresponding to the isoquinolinyl cation b, is structurally significant as it indicates the presence of that functionality in the molecule. The ions complementary to *m/e* 128 are of moderate abundance in the mass spectra of some of the compounds as noted from the peaks at *m/e* 121 and 166 in the spectra of **1c** and **1g,** respectively. The contrasting behavior of the 1,2,3,4-tetrahydroisoquinolines as opposed to the benzylisoquinoline system has also been noted in a recent publication dealing with the mass spectral behavior of tetrahydroeschscholamidine salts.[13] Similarly, the peak arising from cleavage of the benzylic bond in the spectrum of papaverine *N*-oxide is also of relatively minor intensity.[14]

(d) An ion of *m/e* 204 whose formation involves loss of the benzene ring substituents plus a ring carbon is common to the mass spectra of **1a–h** and a plausible structure for it is depicted by c.

In addition to the variation in the $M\cdot^+$ ion intensity a major qualitative difference in the fragmentation of the two monosubstituted nitro derivatives **1a** and **1b** involves the occurrence of an $[M - OH]^+$ ion (*m/e* 247) in the spectrum of **1a** as compared to the absence of one in the spectrum of the 4-nitro derivative, **1b.** We suggest that the proximity of an oxygen atom of the 2-nitro group and the benzylic hydrogens in **1a** facilitates expulsion of an OH· radical as shown in Scheme III.

Scheme III



m/e 247

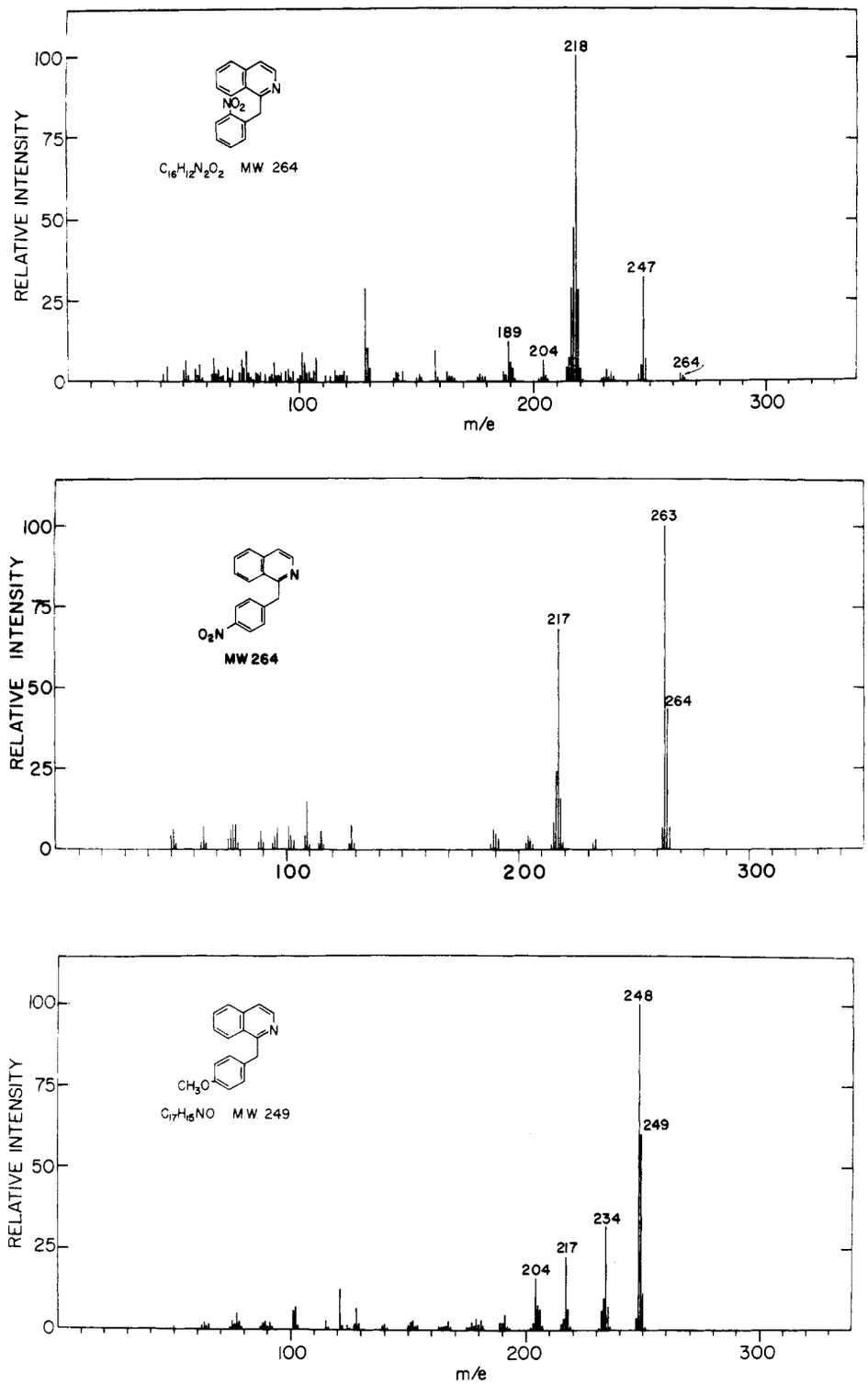


Figure 1. Mass spectra of 1-(2-nitrobenzyl)isoquinoline (**1a**, top spectrum), 1-(4-nitrobenzyl)isoquinoline (**1b**, center), and 1-(4-methoxynitrobenzyl)isoquinoline (**1c**, bottom spectrum).

In the fragmentation of the 4-methoxy derivative **1c** no unique features are apparent. The principal peaks—in addition to ion c (*m/e* 204)—are formed by losses of H· (*m/e* 248), CH_3· (*m/e* 234), and CH_3O· and H· (*m/e* 217) (Figure 1).

The spectrum of 1-(4-methoxy-3-nitrobenzyl)isoquinoline (**1d**) contains fragment ions which are common to the spectra of most of the other isomers, and consequently was examined in greater detail by preparation of the deuterated analogue, 1-(4-methoxy-d_3-3-nitrobenzyl)isoquinoline (**1e**). The mass spectra of **1d** and **1e** are partially summarized in Table I.

Analogous to the monosubstituted benzylisoquinolines **1a–c** the principal fragmentations involve the benzylic hydrogen and the nitro and methoxy substituents. On the basis of metastable transitions and isotopic labeling data (Table I), the sequence and mode of formation of the principal fragment ions in the spectrum of **1d** are shown in Scheme IV. The evidence from metastables supports the formation of $[M - OH]^+$ (*m/e* 277) via a two-step process (*m/e* 294 → 293 → 277). In general, the same mechanisms seem applicable to the formation of ions of the same mass in the spectra of the isomers

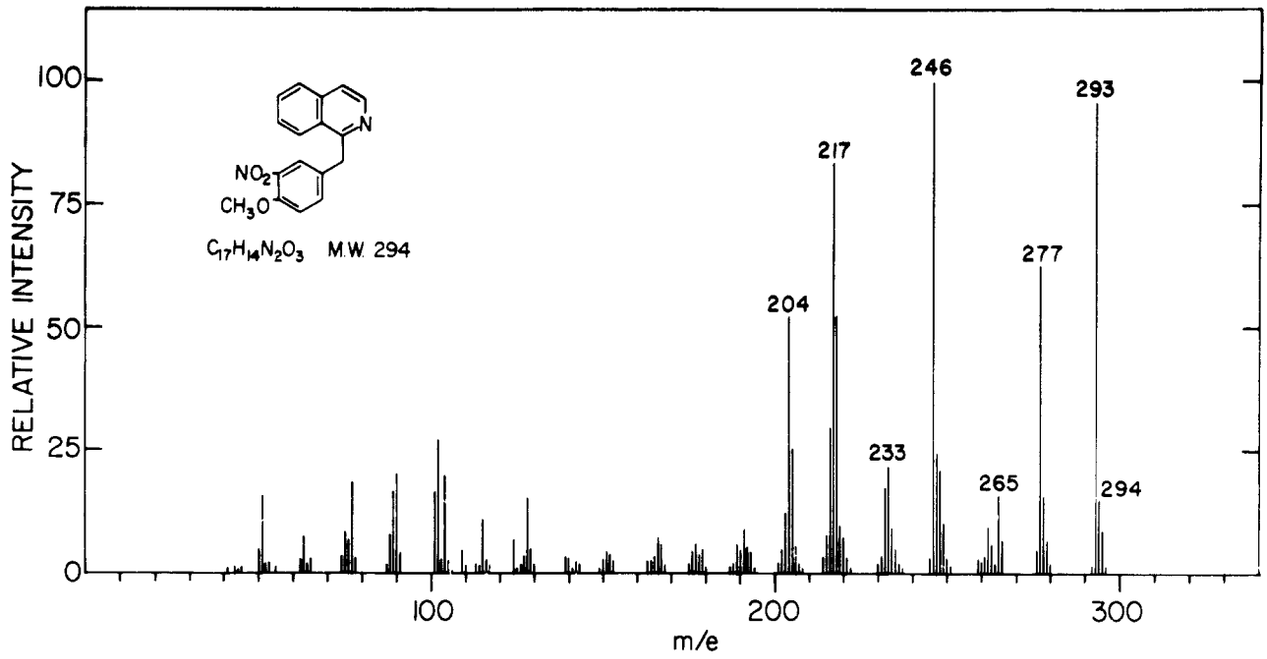


Figure 2. Mass spectrum of 1-(4-methoxy-3-nitrobenzyl)isoquinoline (**1d**).

Scheme IV

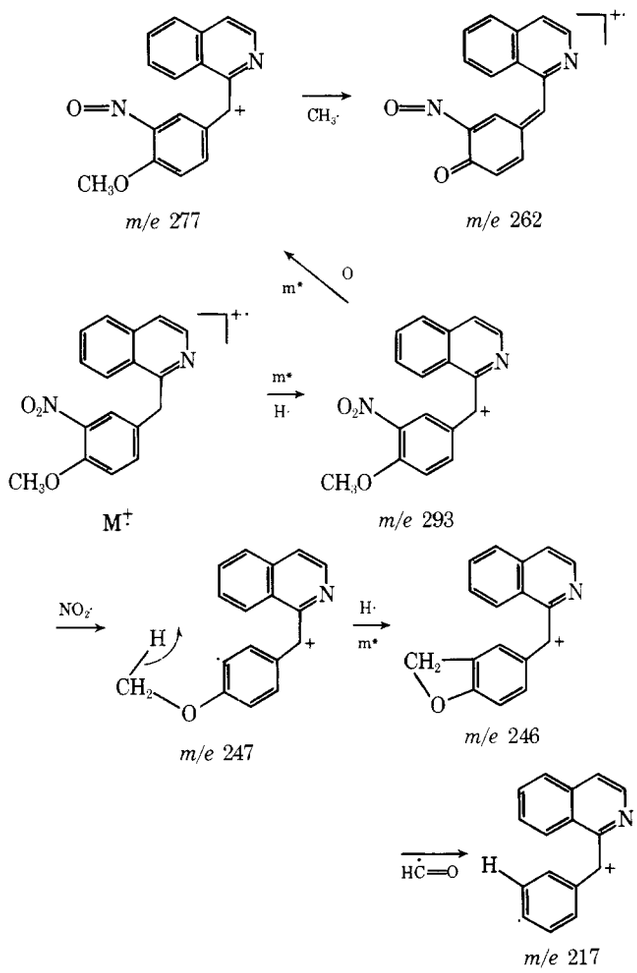


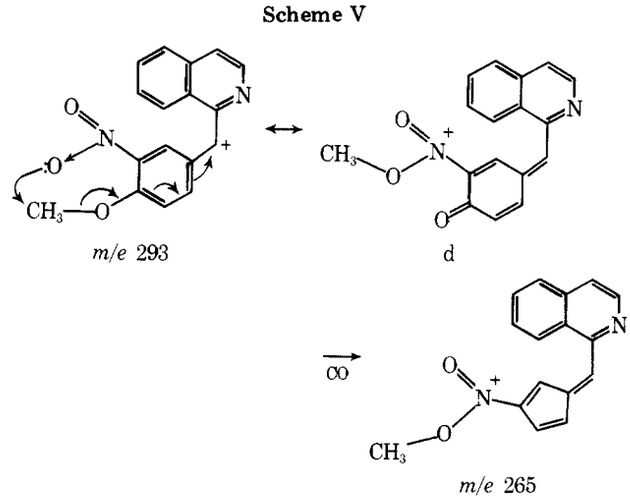
Table I. Mass Shifts of Principal Ions in the Spectra of 1d and 1e

1d	1e	ΔM
294	297	3
293	296	3
277	280	3
265	268	3
262	262	0
246	248	2
233	233	0
217	218	1
204	204	0

1f, 1g, and **1h.**

Of particular mechanistic interest is the occurrence of an ion at *m/e* 265 in the spectrum of **1d.** This ion contains the 4-methoxy group as indicated by the 3-amu shift in the spectrum of the deuterated methoxy derivative, **1e** (see Table I), and is formed by elimination of CO from $[M - H]^+$ (Scheme V). Intramolecular migration of the *O*-methyl group is a requirement for this process and can be induced by interaction with the vicinal nitro group as shown in Scheme V. The postulated alkyl group migration is consistent with previously proposed mechanisms involving intramolecular group transfers in systems containing heteroatoms and/or aromatic ring systems.[15,16] The resulting quinone-type intermediate

Scheme V



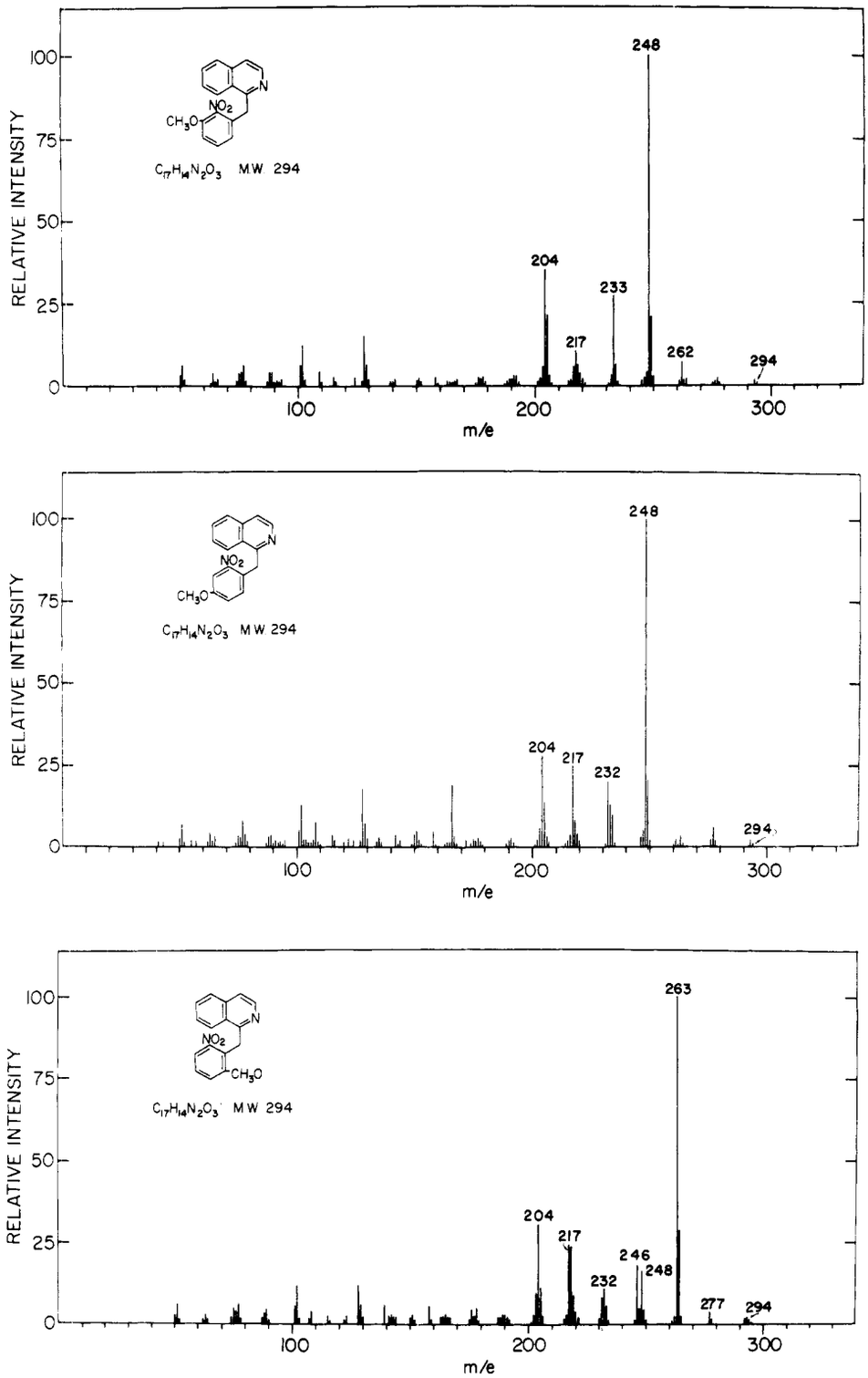
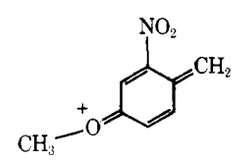


Figure 3. Mass spectra of 1-(3-methoxy-2-nitrobenzyl)isoquinoline (**1f**, top spectrum), 1-(4-methoxy-2-nitrobenzyl)isoquinoline (**1g**, center), and 1-(6-methoxy-2-nitrobenzyl)isoquinoline (**1h**, bottom spectrum).

d is favorably disposed to the elimination of CO, a characteristic process in the spectra of such compounds.[17]

As stated earlier, in the spectra of derivatives containing an ortho nitro group (**1f, 1g**) or a 2-nitro and 6-methoxy group as in **1h**, the $M\cdot^+$ ion and the $[M - 1]^+$ ion intensities are relatively low. In comparing the spectra of **1f** and **1g**, major differences are noted in the peaks at *m/e* 166, 232, and 233. The relatively higher abundance of the *m/e* 166 ion in the spectrum of **1g** in contrast to that of **1f** may be rationalized by the ability of the *p*-methoxy isomer **1g** to contribute the additional

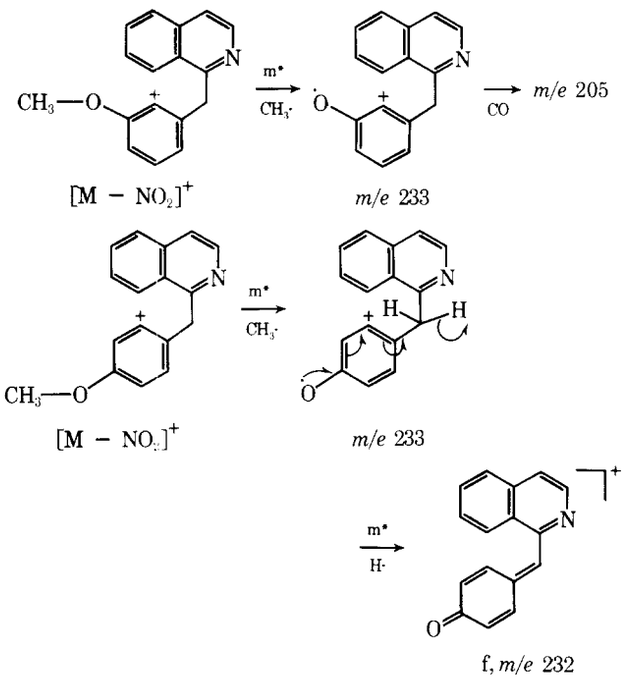


e, *m/e* 166

quinone-type resonance structure e to the stabilization of this fragment ion, following cleavage of the benzyl–isoquinoline linkage. A similar rationale may be applied to explain the

further breakdown of *m/e* 233 to *m/e* 232 in the spectrum of **1g** as opposed to that of **1f** in which only an abundant *m/e* 233 ion is observed. Following loss of the *O*-methyl group further loss of an α-benzyl hydrogen in **1g** is more favorable than **1f** because of the resulting benzoquinone-type ion f. In contrast, the spectrum of **1f** exhibits the competing fragmentation of *m/e* 233 to *m/e* 205 by loss of CO (Scheme VI).

Scheme VI



Chemical Ionization Studies. As noted above, the presence of a substituent in the ortho position of the benzyl ring results in molecular ion peaks of negligible intensity in the EI mass spectra of such compounds. In fact, the facile loss of a hydrogen from $M^{\cdot+}$ introduces an additional complication which hinders identification of the molecular ion peak with the highest degree of confidence. We thus examined the CI[18] mass spectra of these compounds, an approach also used by Fales et al.[19] in their mass spectral studies of related alkaloids containing the aporphine system.

The chemical ionization mass spectra of the benzylisoquinolines **1a–d** and **1f–h** obtained in methane reagent gas are summarized in Table II. As expected, the intensity of the molecular adduct ion peaks is greatly enhanced and, in most cases, these ions dominate the spectra of the respective compounds. It is significant that elimination of HNO_2 and/or CH_3OH from $[M + H]^+$ are the principal fragmentation processes encountered in these mass spectra, and these occur only in cases where the nitro and methoxy groups are present in the ortho position of the benzyl ring (**1a, 1f, 1g,** and **1h**). We suggest that release of the steric strain may be the driving force of this fragmentation process, consistent with the electron impact induced fragmentation.

In summary, the data presented suggest that fragmentation in the mass spectra of benzylisoquinolines is strongly dependent on positional substitution of functional groups. The presence of an ortho substituent on the benzene seems to introduce considerable steric strain and results in molecular ion peaks of very low relative intensity. Conversely, interaction between adjacent nitro and methoxy groups also results in the production of characteristic fragment ions due to intramolecular rearrangement. Thus, these processes can be used for structural characterization of substituted nitrobenzylisoquinolines by mass spectrometry.

Table II. Methane Chemical Ionization Mass Spectra of Benzylisoquinoline Derivatives

	1a	1b	1c	1d	1f	1g	1h
$[M + H]^+$[a]	80[b]	100	100	100	59	100	100
$M^{\cdot+}$	4	2	5	9		2	
$[MH - H_2O]^+$	33	3		10	5	5	3
$[MH - CH_3OH]^+$							29
$[MH - HNO_2]^+$	100	4			100	34	17

[a] Indicates type of ion. [b] Numbers refer to percent relative abundance of indicated ions.

Experimental Section

Melting points were determined on a Thomas-Hoover (Unimelt) apparatus and are uncorrected. All microanalyses were performed by Midwest Microlab, Ltd., Indianapolis, Ind. The analytical values for deuterated compounds were obtained by the Pregl method. NMR spectra were recorded on a Varian T-60 spectrometer with Me_4Si as the internal standard. Mass spectra were obtained with a Nuclide 12-90-G mass spectrometer. The ionizing voltage was 70 eV, accelerating voltage 4.5 kV, and the ion source temperature 225 °C.

2-Benzoyl-1,2-dihydroisoquinaldonitrile (2). This compound was prepared by a modified procedure[8] of Weinstock and Boekelheide,[20] mp 125–126 °C (67%) (lit.[20] mp 125–126 °C).

1-(2-Nitrobenzyl)isoquinoline (1a). The preparation of this compound has been described.[5a]

2-Benzoyl-1-(4-nitrobenzyl)-1,2-dihydroisoquinaldonitrile (4b). The Reissert compound **2** (2.99 g, 11.4 mmol) was alkylated in 40 ml of DMF with 4-nitrobenzyl chloride (2.06 g, 12 mmol) in the presence of NaH (0.6 g, 12.5 mmol, 50% mineral oil suspension) according to the procedure of Uff et al.,[9] and yielded 0.12 g (6%) of **1b** and 0.9 g (20%) of **4b** as off-white needles, mp 200–202 °C. (The compound was previously obtained as an oil, which was hydrolyzed directly to **1b.**)[21] Recrystallization from ethanol gave an analytical sample: mp 203–204 °C; NMR ($CDCl_3$) δ 3.70 (q, J = 30 Hz, 2), 5.60 (d, J = 8 Hz, 1), 6.40 (d, J = 8 Hz, 1) 6.95–7.80 (m, 11), 7.95 (d, J = 8 Hz, 2).

Anal. Calcd for $C_{24}H_{17}N_3O_3$: C, 72.90; H, 4.33; N, 10.63. Found: C, 73.08; H, 4.33; N, 10.67.

1-(4-Nitrobenzyl)isoquinoline (1b). A mixture of 2.0 g (5 mmol) of **4b** in 50 ml of dry CH_3OH and 1.5 g (27 mmol) of finely powdered KOH was stirred at 45 °C for 6 min. After the addition of 100 ml of crushed ice the suspension was extracted with benzene (3 × 50 ml). The organic phase was washed with brine (2 × 30 ml) and 10% HCl (4 × 30 ml). The acid layers were combined and made basic with solid KOH under stirring and cooling in ice. The off-white precipitate was collected, washed neutral with water, and dried to give 1.02 g (76%) of **1b,** mp 96–99 °C. Recrystallization from ether gave mp 99–100 °C (lit.[21] 108–109 °C).

1-(4-Methoxybenzyl)isoquinoline (1c). Following the described procedure 17.3 (66 mmol) of **2** was reacted with equimolar amounts of 4-methoxybenzyl chloride (**3c**) and NaH in 250 ml of dry DMF. Hydrolysis of the oily intermediate **4c** with KOH in CH_3OH was carried out as described for **1h** to give a 69% yield of **1c,** mp 68–69 °C. The product was recrystallized from benzene–petroleum ether, mp 69–70 °C (lit.[21] 68.5–69.5 °C).

α-Bromo-4-methoxy-3-nitrotoluene (3d). In a manner analogous to the preparation of **3e,** 4-methoxy-3-nitrotoluene (10.0 g, 60 mmol), prepared from 4-methyl-2-nitrophenol with dimethyl sulfate, was brominated to yield 9.7 g (65%) of **3d,** mp 102–104 °C. An analytical sample was prepared from benzene–ligroin, mp 103–105 °C.

Anal. Calcd for $C_8H_8BrNO_3$: C, 39.04; H, 3.28; N, 5.69. Found: C, 39.31; H, 3.31; N, 6.01.

1-(4-Methoxy-3-nitrobenzyl)isoquinoline (1d). A. By Reissert Alkylation and Hydrolysis. The procedure employed was identical with that used in the preparation of **1h.** Thus, from 5.2 g (20 mmol) of **2** and equimolar amounts of **3d** and NaH in 80 ml of dry DMF the intermediate **4d** was obtained as an oil. Hydrolysis in 200 ml of dry CH_3OH with 7.5 g of KOH gave 2.64 g (50%) of **1d,** as faint yellow crystals, mp 117–118 °C.

B. By Nitration of 1-(4-Methoxybenzyl)isoquinoline (1c). To 24 ml of nitric acid (70%) was added in small portions, with stirring and cooling in ice, 3.0 g (12 mmol) of **1c.** The yellow solution was stirred at 0 °C for 6 h and at room temperature for 18 h. The mixture was poured onto 100 ml of crushed ice and neutralized with concentrated NH_4OH and the beige precipitate was washed neutral with

water. Trituration with $CHCl_3$ and drying gave 3.5 g (81%) of **1d** as the nitrate salt, mp 137 °C dec. A small sample was recrystallized twice from ethanol to give white needles, mp 142 °C dec.

Anal. Calcd for $C_{17}H_{14}N_2O_3 \cdot HNO_3$: C, 57.14; H, 4.23; N, 11.76. Found: C, 57.26; H, 4.43; N, 11.81.

The free base was liberated from the nitrate in 91% yield by suspending the salt in 20% NaOH at 40 °C. After stirring for 1 h the mixture was extracted with $CHCl_3$. The organic phase was washed neutral with water and dried over Na_2SO_4. Removal of the solvent left faint yellow crystals, mp 116–118 °C. An analytical sample was obtained from ethanol: mp 118–119 °C; NMR ($CDCl_3$) δ 3.73 (s, 3), 4.50 (s, 2), 6.83 (d, J = 8 Hz, 1), 7.20–8.20 (m, 7), 5.40 (d, J = 5 Hz, 1).

Anal. Calcd for $C_{17}H_{14}N_2O_3$: C, 69.37; H, 4.80; N, 9.52. Found: C, 69.39; H, 4.87; N. 9.57.

The NMR and IR spectra of the isoquinoline derivative **1d**, obtained by both methods, were identical. An admixture of the compounds had mp 118–119 °C.

4-Methoxy-d_3-3-nitrotoluene (6). Methylation of **5** (5.26 g, 34 mmol) with dimethyl-d_6 sulfate (10.0 g, 76 mmol, Merck) was carried out at 70–80 °C and pH 8 as described for **3d** to yield 4.83 g (86%) of crude **6**. Distillation [bp 102–104 °C (0.3 mm)] gave an analytical sample: NMR ($CDCl_3$) δ 2.33 (s, 3), 6.95 (d, J = 9 Hz, 1), 7.23 (d, J = 0 Hz, 1), 7.56 (d, J = 2 Hz, 1); mass spectrum (70 eV) m/e 170 ($M^{\cdot+}$, 55%).

Anal. Calcd for $C_8H_6D_3NO_3$: C, 56.46; H, D, 7.10; N, 8.23. Found: C, 56.23; H, D, 7.39; N, 7.95.

α-Bromo-4-methoxy-d_3-3-nitrotoluene (3e). A mixture of 1.85 g (10.9 mmol) of freshly distilled **6**, 1.94 g (10.9 mmol) of recrystallized N-bromosuccinimide, and 50 mg of benzoyl peroxide in 17 ml of dry CCl_4 was refluxed for 3 h under illumination. Without cooling the mixture was filtered, and the mother liquor was concentrated in vacuo to give 1.66 g (61%) of **3e** as a slightly yellow crystalline solid: mp 103–105 °C; NMR ($CDCl_3$) δ 4.46 (s, 2), 7.06 (d, J = 8 Hz, 1), 7.60 (dd, J = 10, 6 Hz, 1), 7.83 (d, J = 2 Hz, 1).

Anal. Calcd for $C_8H_5D_3BrNO_3$: C, 38.57; H, D, 4.45; N, 5.62. Found: C, 38.75; H, D, 4.67; N, 5.77.

1-(4-Methoxy-d_3-3-nitrobenzyl)isoquinoline (1e). Alkylation of **2** (1.35 g, 5.4 nmol) with equimolar amounts of **3e** (1.41 g) and NaH (0.26 g, 50% mineral oil suspension) in 30 ml of dry DMF was carried out as described for the synthesis of **1h**. Hydrolysis in 70 ml of dry methanol with 2.5 g of finely powdered potassium hydroxide yielded 0.63 g (39%) of **1e** as an almost white crystalline solid, mp 118–119 °C. Recrystallization from ethanol gave an analytical sample: mp 119 °C; NMR ($CDCl_3$) δ 4.53 (s, 2), 6.86 (d, J = 8 Hz, 1), 7.20–8.20 (m, 7), 8.43 (d, J = 5 Hz, 1).

Anal. Calcd for $C_{17}H_{11}D_3N_2O_3$: C, 68.67; H, D, 5.76; N, 9.42. Found: C, 68.55; H, D, 5.93; N, 9.57.

1-(3-Methoxy-2-nitrobenzyl)isoquinoline (1f). This compound was prepared as described in the literature.[5g]

1-(4-Methoxy-2-nitrobenzyl)isoquinoline (1g). The synthesis of this compound was carried out as described.[6]

α-Bromo-2-methoxy-6-nitrotoluene (3h). In a similar manner as in the preparation of **1e** the bromination of 2-methyl-3-nitroanisole (20 g, 60 mmol, Aldrich) gave 14.7 g (99%) of **3h**, mp 68–72 °C. Recrystallization from benzene–petroleum ether yielded 12.8 g (87%) of **3h**, mp 75–76 °C.

Anal. Calcd for $C_8H_8BrNO_3$: C, 39.04; H, 3.28; N, 5.69. Found: C, 39.14; H, 3.30; N, 5.58.

1-(2-Methoxy-6-nitrobenzyl)isoquinoline (1h). To a solution of 10.4 g (40 mmol) of **2** and 8.8 g (40 mmol) of **3h** in 160 ml of dry dimethylformamide was added under vigorous stirring and cooling (−20 °C) 1.92 g (40 mmol) of sodium hydride (50% mineral oil suspension) in a nitrogen atmosphere. Stirring was continued for 2 h at −20 °C and 18 h at room temperature. The brown mixture was diluted with 500 ml of chloroform, filtered, washed with water (3 × 100 ml), and dried over Na_2SO_4. Evaporation of the solvent under reduced pressure left an oil which was immediately dissolved in 400 ml of dry methanol. Powdered potassium hydroxide (15 g) was added to the solution and after reflux for 5 min under vigorous stirring the mixture was poured onto 1000 ml of crushed ice. The resulting suspension was extracted with ethyl acetate (3 × 150 ml), the combined organic layers were washed neutral and dried, and the solvent was removed in vacuo to give after cooling in ice 5.0 g (42%) of **1h** as off-white crystals, mp 130–132 °C. Recrystallization from acetonitrile gave an analytical sample: mp 133–134 °C; NMR ($CDCl_3$) δ 3.73 (s, 3), 5.08 (s, 2), 7.0–7.9 (m, 6), 8.18–8.50 (m, 3).

Anal. Calcd for $C_{17}H_{14}N_2O_3$: C, 69.37; H, 4.80; N, 9.52. Found: C, 69.46; H, 4.77; N, 9.63.

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