Factors Influencing the Stabilities of Nematic Liquid Crystals[1]

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Abstract: A number of potentially mesomorphic esters and thio esters have been prepared in which the central *p*-phenylene ring of bis(*p*-methoxyphenyl) terephthalate, or dithioterephthalate, is replaced by 1,4-bicyclo[2.2.2]octadiyl, 1,4-bicyclo[2.2.2]octenediyl, 1,4-cyclohexadiyl, 1,4-cyclohexa-1,3-dienediyl, 1,4-cyclohexa-1,4-dienediyl, ethene-1,2-diyl, 2-butene-1,4-diyl, 2,5-pyridinediyl, 1,3-butadiene-1,4-diyl, 2,4- or 2,5-furandiyl, or 2,4- or 2,5-thiophenediyl. The nematic → liquid transition temperatures indicate that the predominant factors in determining mesophase stability are geometric, polarity having little or no beneficial effect. The possible value of 1,4-bicyclo[2.2.2]octenediyl as a central group, and of the thio ester moiety (-COS-) as a linking group, in liquid crystals, is pointed out.

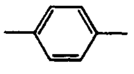
Early studies[3] suggested that compounds tend to form nematic mesophases if their molecules are rod-shaped and possess polar terminal groups. It was suggested that the determining factor was the tendency for such molecules to adhere to one another sideways, this lateral adhesion being assisted by their shape and by dipole-dipole attractions. It was found that lateral projections from a rod-shaped molecule decrease the stability of the nematic phase, presumably by geometrical interference with the necessary parallel orientation. It was also suggested that the *p*-phenylene group (**1**) might favor lateral attractions in molecules containing it, partly by enhanced van der Waals attractions, due to the presence of polarizable π electrons, and partly through enhanced polarity due to conjugation with adjacent groups. The majority of known liquid crystals do indeed contain *p*-phenylene groups but this could be due to other factors. In the first place, a rod-shaped molecule can be obtained most easily by linkage of rigid linear units; *p*-phenylene is both rigid and perfectly linear. And second, a wide variety of 1,4-disubstituted benzenes can be obtained easily and cheaply by standard methods.

Since the publication of Gray's classic monograph[3] there has been a great upsurge of interest in liquid crystals, due to the discovery of important technological applications. Most of this work has, however, been directed toward the synthesis of new compounds of possible practical value or to the study of their physical properties with a view to improving devices based on them. Very little further experimental work has been reported on the relationship between molecular structure and mesophase stability.[4,5]

The work reported here was intended to provide further information concerning the relative importance of four features of molecules that have been thought to contribute to mesophase stability, i.e., rigidity, linearity, polarizability, and enhancement of polarity by conjugation. In the course of this we have also prepared a number of new types of liquid crystal that are of interest in their own right.

Results and Discussion

Our research followed on from a recent study here[5] of the effects of structural changes on a typical liquid crystal, *p*-phenylene di-*p*-anisate (**2a**), the central *p*-phenylene (**1**) group being replaced either by 1,4-bicyclo[2.2.2]octylene (**3**), a group which is as linear and rigid as benzene but saturated, or by *trans*-1,4-cyclohexylene (**4**),[6] a group which is linear and saturated but rather flexible. The results seemed to suggest that rigidity is more important than unsaturation, replacement of **1** by **4** having a much more damaging effect on the stability of the nematic mesophase of **2a** than replacement by **3**.



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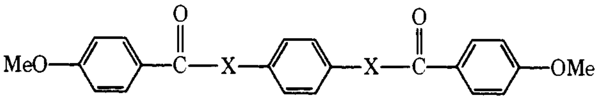
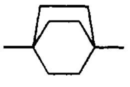


2a, X = O
b, X = S



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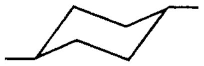

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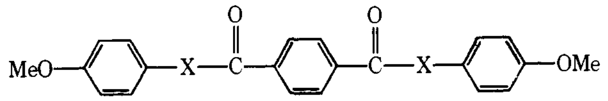
The ester linkage has advantages[7] over others that have been used in constructing liquid crystals in that esters are easily prepared and thermally stable. We therefore decided to study structural variations in a series of diesters analogous to **2a**. However, since we wished to study the effect of changes in the central ring, and since dicarboxylic acids are in general more accessible than corresponding diols, we decided to base our study on an analog of **2a** in which the ester groups are inverted, i.e., bis-*p*-methoxyphenyl terephthalate[7b] (**5a**). The nematic → liquid transition temperature of **5a** had been reported[7b] to be lower than that of **2a** by 22°, a difference attributed to enhanced polarity of the carbonyl and methoxy groups in **2a** as a result of mutual conjugation *via* the terminal benzene rings.

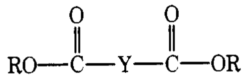
Our first objective was to study in more detail the specific role of the π electrons in the central group of **5a**. We therefore prepared a series of analogs (**6**) of **5a** in which the central phenylene unit was replaced by some other linear nonpolar group. The first two of these (**7a, 8a**) corresponded to the previously prepared[5] analogs of **2a** while the rest (**9a–13a**) differed in the size, rigidity, and unsaturation of the central group. The melting points and transition temperatures are shown in Table I together with those of **5a** for comparison. All except **12a** and **13a** melted to nematic mesophases while **12a** showed a monotropic nematic → liquid transition.

The results for **7a** and **8a** support the earlier conclusion[5] that rigidity is more important than the presence of π electrons in the central group Y of **6**. Thus replacement of the central phenylene in **5a** by **3** lowers the nematic → liquid transition temperature by 16° whereas replacement by **4** lowers it by 40°.

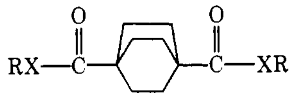
Introduction of a double bond into the bicyclooctylene moiety of **7a** leads to an *increase* in mesophase stability, the nematic → liquid transition temperature of **9a** being only



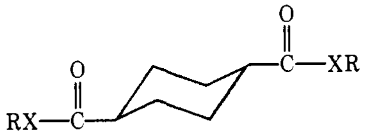
5a, X = O
b, X = S



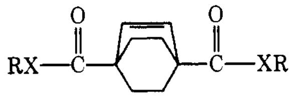
6, R = p-C$_6$H$_4$OMe



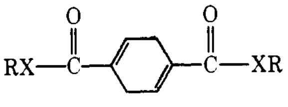
7a, X = O
b, X = S



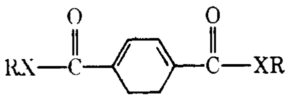
8a, X = O
b, X = S



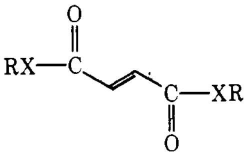
9a, X = O
b, X = S



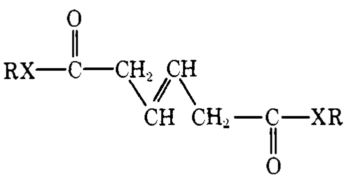
10a, X = O
b, X = S



11a, X = O
b, X = S



12a, X = O
b, X = S



13a, X = O
b, X = S

9° less than that of **5a.** This difference cannot be due to conjugation or polarizability since the polarizability of bicyclo[2.2.2]octene must be very little greater than that of bicyclo[2.2.2]octane. One possible factor might be the enhancement of electrostatic interactions between molecules of **9a** due to polarity of the bicyclooctene moiety in it, sp^3-sp^2 carbon-carbon bonds being polar. However, the corresponding dipole moments are so small that this effect should be minimal. Subsequent work here[8] suggests that the difference between **7a** and **9a** arises from reduced symmetry, the saturated central group (**3**) in **7a** having D_{3h} symmetry whereas the unsaturated central group in **9a** is only D_2.

The results for **10a** and **11a** are interesting. Both 1,3- and 1,4-cyclohexadiene are more rigid than cyclohexane so both **10a** and **11a** might be expected to have higher nematic → liquid transition temperatures than that of **8a.** This is the case, but while the difference between **8a** and **10a** is large (28°), the nematic phase of **10a** being as stable as that of **7a,** the difference between **8** and **11** is only 6°.

The reason for this probably lies in the nonplanarity of the double bonds in 1,3-cyclohexadiene. Examination of models shows that the butadiene moiety in it must be severely twisted and this undoubtedly is responsible for the fact that it is little, if any, more stable than the unconjugated isomer, 1,4-cyclohexadiene.[9] Conjugation between each carbonyl group in **11a** and the adjacent double bond will tend to make them coplanar, so the nonplanarity of the double bonds will be reflected by a corresponding nonplanarity of the carboxyl groups. The molecules of **11a** are therefore kinked, unlike those of **5a** or **7a–10a,** and this presumably interferes with the "packing" of molecules in the nematic liquid crystal.

Table I. Melting Points and Nematic → Liquid Transition Temperatures for Diesters and Bis(thio esters)

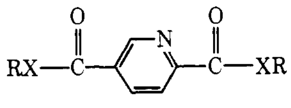
	Diester (a series)		Bis(thio ester) (b series)	
Compd	Mp[a]	Nematic → liquid transition temp[a]	Mp[a]	Nematic → liquid transition temp
2	213	297	178	312
5	209	285	210	311
7	152	269	162	>310
8	142[d]	245[d]	202	241
9	125	276	150	>310
10	205	273	194	273
11	144	251	185	245
12	174	139[b]	176	143[b]
13	133–134	*c*	106–107	*c*
14	175	256	203	270 dec
15			179–180	*c*

[a] In °C. [b] Monotropic transition. [c] No nematic phase observed. [d] See ref 5. Transition temperatures of 143 and 242° are reported.

The fact that **13a** failed to give a detectable nematic phase was not unexpected since the molecules should exist as a number of rotational conformers of comparable stability, only one of which will be linear. It is, however, somewhat surprising that the nematic phase of **12a** should be so unstable, the compound exhibiting only a monotropic transition at a temperature (143°) less by 142° than that for **5a.** This seems to suggest that an important factor in mesophase stability may be the presence of molecules which are not only rigid and rod-shaped but also have more or less uniform cross-sections. The vinylene group in **12a** is much narrower than in phenylene group in **5a.** It is of course well known[3,4] that lateral substituents that project beyond the edges of a rod-shaped molecule lower the stability of the nematic mesophase.

The importance of rigidity is further indicated by comparison of our data for **7a** and **8a** with those of Dewar and Goldberg[5] for the corresponding analogs of **2a** where the central ring is replaced by **3** or **4**. In the case of the bicyclooctylene moiety **3** the two transition temperatures were the same (269°), while in the case of cyclohexylene (**4**) our ester (**8a**) had a much higher transition temperature (245° vs. 195°). In **8a** the groups attached to the cyclohexane ring are much bulkier and will therefore enforce a chair conformation in which both are equatorial whereas the analog of **2a** has more opportunities for conformational isomerism.

It has been generally believed that polarity of the central part of a rod-shaped molecule tends to enhance the stability of the corresponding mesophase by strengthening the lateral intermolecular attractions. Indeed, the greater stability of the mesophase in **2a** than in **5a** had been attributed to the greater polarity of the former. It therefore seemed likely that an increase in polarity of the central segment of **5a** might increase the stability of the mesophase; we accordingly synthesized the pyridine-2,5-dicarboxylic analog **14a.** Much to our surprise the nematic → liquid transition temperature for this was *lower* by no less than 29° than that for **5a** (Table I), being indeed only 11° higher than that of the flexible 1,4-cyclohexylene derivative **8a.** Evidently polarity



14a, X = O
b, X = S

is not in itself necessarily advantageous; on the contrary, one might conclude from this example that it is if anything disadvantageous.[10]

This result was of interest in view of a preliminary report by Elser[11] concerning the effects of replacing oxygen atoms in various alkyl cholesteryl carbonates by sulfur. In all cases, introduction of sulfur led to an increase in the smectic → cholesteric transition temperature although it might be expected to lead also to a decrease in polarity of the ester group.

We therefore decided to prepare the thio ester analogs **5b–14b** of **5a–14a** to see if replacement of oxygen by sulfur would have a similarly favorable effect on the stabilities of their mesophases. These thio esters were in any case of inherent interest since few sulfur-containing mesomorphic compounds have as yet been reported[12] and since the thio ester moiety could represent a useful linking group, being thermally and chemically stable. These compounds were prepared without difficulty from the appropriate dicarboxylic acid chloride and *p*-methoxythiophenol. Their melting points and nematic → liquid transition temperatures are listed in Table I, together with the transition temperatures of the oxygen analogs (**5a–14a**) for comparison.

It will be seen that the nematic phases of the thio esters were in most cases much more stable than those of their oxygen analogs, the differences between pairs of corresponding transition temperatures being mostly greater than 20°. Since the melting points of the thio esters are comparable with those of the corresponding esters, the thio ester linking group may prove generally superior for the preparation of materials with long nematic mesophases.

We also prepared the dithioester analog (**2b**) of **2a**. This again had a higher nematic → liquid transition temperature than the oxygen analog. However, whereas the transition temperature of **2a** is greater by 12° than that of **5a**, those for the sulfur analogs **2b** and **5b** were almost identical. This seems to throw doubt on the explanation of the greater nematic stability of **2a** in terms of polarity;[7] for one might expect a similar difference in polarity between **2b** and **5b**. We now believe that the difference in mesophase stability between **2a** and **5a**, and between the esters (**2a, 5a–14a**) and thio esters (**2b, 5b–14b**), may be due to steric effects rather than to polarity as a result of the nonlinearity of the ester (-COO-) and thio ester (-COS-) groups.

The terminal bonds in these groups are not only not collinear but also not even parallel, for whereas the bond angles of the carbonyl carbon are ca. 120°, those at the divalent oxygen or sulfur are much less. The deviation from parallelism is moreover greater for sulfur (bond angle 95–100°) than for oxygen (bond angle ca. 105°).

As Figure 1a shows, **2a** can adopt an almost ideal linear geometry with an almost uniform cross-section. Indeed, if the bond angles at the carbonyl carbon and divalent oxygen are 120 and 105°, respectively, the terminal MeO-C bonds are *exactly* collinear! The best geometry for **5a** (Figure 1b) on the other hand is distinctly S shaped. The fact that **2a** forms the more stable nematic phase can be explained very well in terms of this difference in geometry without any recourse to polarity.

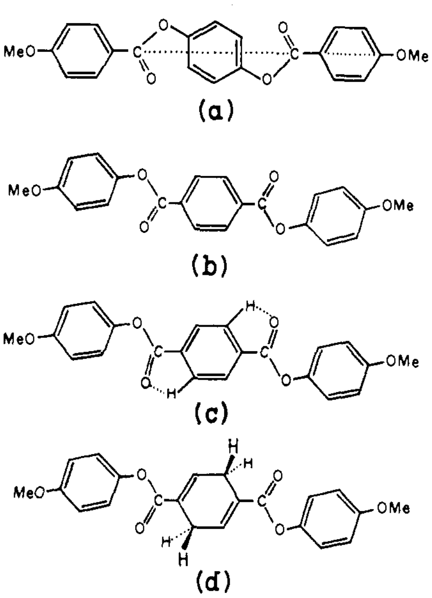


Figure 1. Geometries of (a) **2a** and (b) **5a**, (c) carbonyl-hydrogen interaction in **5a**, and (d) lack of carbonyl-hydrogen interactions in **10a**.

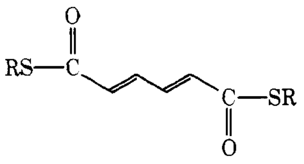
The fact that the thio esters (**5b–14b**) form more stable mesophases than the corresponding esters (**5a–14a**) can also be explained in terms of geometry alone. In the esters there must be quite a severe steric interaction between the carbonyl oxygen and the *ortho* hydrogen atom of the anisyl moiety (Figure 1c); this will tend to force the benzene rings out of coplanarity and so upset the overall linearity of the molecule. Steric effects should be much less important in the thio esters, because although the bond angle of sulfur is somewhat smaller, the CS bond is much longer. The smaller bond angle of sulfur may also improve the overall linearity of the molecule, compensating better for the offset at the terminal bonds in the ester or thio ester groups.

We can also explain in this way why the mesophases from **2b** and **5b** are similar in stability whereas that from **2a** is much more stable than that from **5a**. In the case of **2b** the bond angle at sulfur is too small for perfect linearity while the smaller bond angle probably makes **5b** more linear than **5a**. Consequently, **2b** and **5b** are comparably nonlinear and so have similar transition temperatures.

These arguments also explain why the mesophases from **8a** and **8b**, from **10a** and **10b**, and from **11a** and **11b** differ little in stability. Thus **10a** can adopt a planar configuration (Figure 1d) to which oxygen-hydrogen interactions no longer present an obstacle since each carbonyl oxygen is now opposite a methylene group instead of an *ortho* methine in a benzene ring. Here the advantage of sulfur is correspondingly attenuated. The same situation arises even more strongly in the case of **8a**; here the transition temperatures for the diester and dithio ester are identical. And finally, in the case of **11a**, where one carbonyl group will be forced out of planarity with the adjacent double bond by a methine interaction, this twist is positively advantageous, for it will compensate for the twist due to the nonplanarity of the 1,3-cyclohexadiene ring.

The remaining cases where sulfur fails to show any advantage over oxygen (**12, 13**) can be explained likewise, sulfur again conferring no steric advantage. We also prepared the *trans-trans*-muconic acid dithio ester **15** to see if an extension of the polyene system might lead to the formation of a nematic mesophase; none was observed.

These results seemed to suggest that geometrical factors are of paramount importance in determining the stabilities of mesophases, unsaturation and polarity playing relatively unimportant roles. In view of the importance of this conclusion, we decided to test it by replacing the central benzene ring in **5** by a polar nonlinear heteroaromatic ring. We



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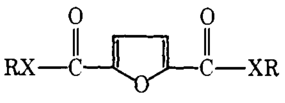
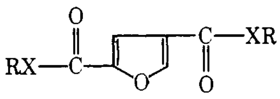
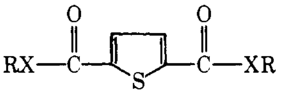


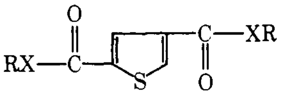
16a, X = O
b, X = S



17a, X = O
b, X = S



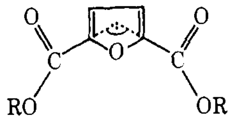
18a, X = O
b, X = S



19a, X = O
b, X = S

therefore prepared the 2,4- and 2,5-furan and thiophene diesters and dithio esters **16–19**.

Of these only **17b** and **18b** melted to nematic mesophases although **17a** showed a monotropic nematic → liquid transition a few degrees below its melting point. The transition temperatures for the other compounds were found by extrapolating the nematic → liquid transition line in the phase diagram for a binary system of the compound in question with one forming a nematic mesophase.[14] Figure 2 shows the corresponding plots for (**18b** + **19a**) and (**18b** + **19b**). Table II shows the melting points and nematic → liquid transition temperatures for the eight compounds. Table II also shows values of the angle θ between the CC bonds linking the central ring to the two adjacent ester groups (see, eg., **20**). These were estimated from Dreiding models or (in



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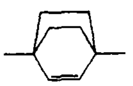
the case of the diesters **16a–19a**) from MINDO/2[15] calculations. The two sets of values for **16a–19a** agreed closely.

The results in Table II show very clearly the deleterious effect of bending an otherwise linear molecule, the nematic → liquid temperatures of **16–19** being lower by 100-250° than those for **5**. Moreover the relative stabilities of the 2,4- and 2,5-diesters and -dithio esters are inverted on passing from furan to thiophene, in agreement with the inverted order of the corresponding angles θ.

Summary

The two results of most potential practical value that arise from this work are the discovery of the first possibly superior alternative to *p*-phenylene groups in liquid crystals, i.e., 1,4-bicyclo[2.2.2]octenylene (**21**), and the demonstration of the utility of a new linking group, i.e., -COS-.



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The results for **5** and **9** seem to suggest that replacement of *p*-phenylene by **21** may leave the nematic → liquid transition temperatures unchanged while greatly lowering the melting point. The possible significance of this for the synthesis of new "room temperature" liquid crystals is self-evident.

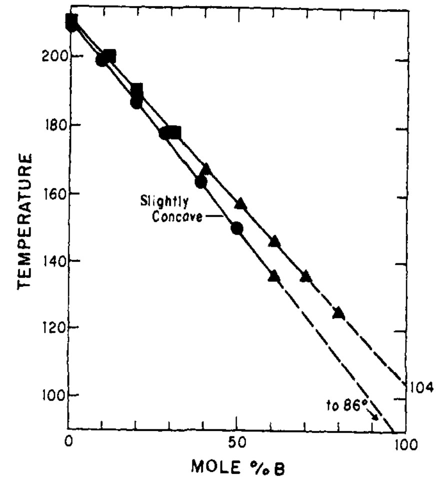

Figure 2. Nematic → liquid transition lines in the binary phase diagrams for (a) **19a** and **18b** (●, ▲) and (b) **19b** and **18b** (■, ▲). In each case the points ●, and ■ denote reversible transitions and the others (▲) monotropic ones.

Table II. Melting Points, Nematic → Liquid Transition Temperatures, and Interbond Angles θ (see 20) for Furan and Thiophene Diesters

	Diester (a series)		Bis(thio ester) (b series)		
Compd	Mp[a]	Nematic → liquid transition temp[a]	Mp[a]	Nematic → liquid transition temp	θ, deg
5	209	285	210	311	180
16	163	62[b]	179	62[b]	137
17	140	140[c]	115	179	160
18	160	153[b]	133	208	148
19	185	86[b]	181	104[b]	140

[a] In °C. [b] By extrapolation of the nematic → liquid transition line in a binary phase diagram. [c] Monotropic transition.

Likewise the results in Table II seem to suggest that thio esters may form more stable mesophases than esters while retaining their advantages of thermal and chemical stability, and without any necessary increase in melting point.

On the theoretical side, our results seem to indicate the paramount importance of geometry in determining the stabilities of nematic mesophases, the essential requirement being a linear rod-shaped molecule of more or less uniform cross-section. Polarity seems to play a minor, and not necessarily favorable, role; hence the superiority of azoxy (-NO=N-) to azo (-N=N-) as a linking group may be due solely to the absence of a "waist" (cf. **12** and **15**) in molecules containing the former and the superiority of the ester and thio ester linkages to vinylene (-CH=CH-) or azo may also be due to this.

Experimental Section

Melting points and transition temperatures (all corrected) were determined with a Thomas-Hoover capillary melting point apparatus and a Leitz Ortholux II Polarising microscope fitted with a hot stage. Elemental analyses were carried out by Galbraith Laboratories, Knoxville, Tenn. All the compounds studied gave satisfactory elemental analyses. Proton NMR spectra were measured with a Varian A60 spectrometer and ir spectra with a Beckman IR8 spectrometer. The NMR and ir spectra of all the compounds studied were consistent with their assigned structures.

The majority of the normal diesters were prepared by adding the diacid chloride slowly to a stirred solution of *p*-methoxyphenol

(10% excess) in dry pyridine and isolated by pouring the solution into ice water.

The fumaric diester (**12a**) was prepared by simultaneous dropwise addition of fumaryl chloride and triethylamine to a solution of *p*-methoxyphenol in dry ether.

The *trans*-β-dihydromuconate diester (**13a**) was prepared by adding the diacid chloride to a solution of *p*-methoxyphenol and pyridine (10% excess of each) in dry ether. This procedure was also used for the furan and thiophene derivatives **16a–19a**.

The thio esters **5b–19b** were prepared in the same way as the corresponding esters, substituting *p*-methoxythiophenol for *p*-methoxyphenol.

Full details of the experimental procedures and references to the literature will be found in a thesis by one of us.[16,17]

References and Notes

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(2) Robert A. Welch Predoctoral Fellow.

(3) See G. W. Gray, "Molecular Structure and the Properties of Liquid Crystals", Academic Press, New York, N.Y., 1962.

(4) Gray et al. have studied the effects of lateral substituents, and of changes in the terminal groups, on the stability of mesophases: see G. W. Gray, *Mol. Cryst. Liq. Cryst.*, **1**, 333 (1966); **7**, 127 (1969); G. W. Gray and K. J. Harrison, *ibid.*, **13**, 37 (1971); *Symp. Faraday Soc.*, **5**, 54 (1971).

(5) Dewar and Goldberg have studied the effect of rigidity on liquid crystallinity: M. J. S. Dewar and R. S. Goldberg, *J. Am. Chem. Soc.*, **92**, 1582 (1970).

(6) 1,4-Cyclohexylene di-*p*-anisate has been prepared by W. E. Baron and G. H. Brown, *Mol. Cryst. Liq. Cryst.*, **6**, 155 (1969).

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(9) R. B. Bates, R. H. Carninghan, and C. E. Staples, *J. Am. Chem. Soc.*, **85**, 3030 (1963).

(10) For a detailed discussion of the reasons for the low nematic mesophase stability in **14a** see ref 8.

(11) W. Elser, *Mol. Cryst. Liq. Cryst.*, **8**, 219 (1969).

(12) Thus of the 1400 compounds listed by Kast[13] as forming mesophases, less than 1% contain sulfur.

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(14) A. Bogojawlensky and N. Winogradow, *Z. Phys. Chem.*, **64**, 229 (1908); R. Walter, *Ber. Dtsch. Chem. Ges.*, **58**, 2803 (1925); J. S. Dave and M. J. S. Dewar, *J. Chem. Soc.*, 4305 (1955).

(15) Personal communication, Dr. N. Bodor.

(16) R. M. Riddle, Ph.D. Dissertation, the University of Texas at Austin, Austin, Texas, 1971.

(17) The transition temperatures in the range >250° reported in this dissertation[16] seems to be uniformly too low, in cases where they were determined by the Thomas-Hoover apparatus. The values listed in the tables were determined by Griffin[8] and checked by DTA. The error was probably due to a defective thermometer in the Thomas-Hoover melting point apparatus; we were unable to check this since the thermometer in question had been accidentally destroyed.

A Thermodynamic Study of the Role of the Central Group on the Stability of Nematic Liquid Crystals[1,2]

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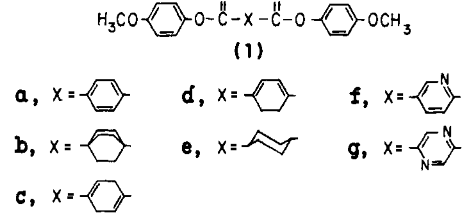
Abstract: Studies of the effect of changes in the central parts of "nematic" molecules indicate that the corresponding changes in nematic → isotropic transition temperatures arise from changes in the entropy of transition, not in the heat of transition as previously supposed. This is true also for the effects of projecting substituents. The results lead to some general conclusions concerning the relationship between structure and mesophase stability.

It has been generally assumed that the stability of nematic liquid crystals depends primarily on the anisotropy of intermolecular forces, the lateral attractions between rod-shaped molecules making them tend to adopt a parallel arrangement. Attempts to correlate structure with mesophase stability have consequently been largely based on considerations of the nature and magnitude of the intermolecular forces favoring such lateral associations. The importance of geometrical factors has of course been recognized but these have been regarded as operating by helping or hindering lateral adhesion of the molecules in question.

Recent work in these laboratories[3] has, however, led to the conclusion that intermolecular forces, due to dipole-dipole attractions, etc., are not the most important factors in determining mesophase stability and that enhanced intermolecular attractions may indeed lead to a decrease in the stability of the nematic phase. The matter is of some practical importance since the strategy followed in searching for new and better liquid crystals must depend on theories concerning the relationship between structure and mesophase stability. The purpose of the work reported here was to study this problem in more detail.

In order to avoid complications from varying end group associations, we decided to study a series of compounds of type **1** where only the central group X is varied. Since our purpose was to determine the relative importance of energetic and other factors in determining mesophase stability, the most promising approach seemed to lie in determining thermodynamic parameters for nematic → liquid phase transitions. We decided to use differential thermal analysis (DTA) since this seems the simplest of the procedures that have been found effective.[4] Few systematic studies had been previously reported on the effect of variations in the central groups of molecules such as **1** on the stability of the corresponding nematic mesophases[3,5-7] and no systematic study of the thermodynamic parameters for their N → I (nematic → isotropic) phase transitions had been reported.



The first series of compounds studied were those in which X is a 1,4-phenylene group (**1a**) or a group structurally related to this (**1b–g**). The observed melting points, N → I transition temperatures, and thermodynamic parameters