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Enthalpy of Fusion of Nematogens†

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(*Received January 6, 1977*)

The enthalpy of fusion of nematic compounds is an important parameter related to the use of such materials in displays. Since no single material is adequate in nematic range for use in displays, a substantial amount of work is required in preparation and evaluation of mixtures. One valuable method of estimating the nematic range of liquid crystal mixtures is based on the Schroeder–Vanlaar equation,[1–5]

$$\ln x = \frac{\Delta H}{R}\left(\frac{1}{T} - \frac{1}{Tm}\right) \tag{1}$$

which relates the melting temperature of a solution (Tm) to the mole fraction, x, of solute of melting temperature T and enthalpy of fusion ΔH, and the gas constant, R.

In order to make use of this method, it is clear that enthalpies of fusion must be known. Since these values are scarce in the literature, we synthesized a large number of compounds and determined their melting enthalpies. These data, as well as some previously obtained in this laboratory, are presented in this paper.

The compounds were synthesized using available or easily adaptable procedures and were purified by recrystallization and/or molecular distillation to constant melting behavior. Satisfactory elemental analysis were obtained. Enthalpies of fusion were determined using a duPont Model 900 Thermal Analyzer equipped with a calibrated (Ga, In, Sn) differential scanning calorimeter cell. Integration of endothermic maxima was accomplished with a Keuffel and Esser 0.01 in^2 compensating polar planimeter.

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† Presented at the Sixth International Conference on Liquid Crystals, Kent, Ohio, August 1976, Abstract No. H-4.

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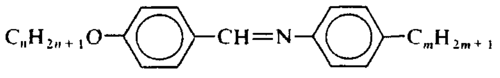
The data are presented in the following tables. The wide variations[7] observed within homologous series indicate that there is very little correlation with molecular structure. Odd–even effects are in general not observed. This is to be expected, since crystal structure and lattice energy of organic compounds are only slightly influenced by molecular structure.[8] It is also clear that there is no simple relationship between melting point and enthalpy of melting, as has been suggested.[3]

TABLE I

Enthalpy of fusion of Schiff bases of structure

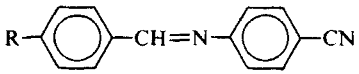


Kcal/mole

	m					
n	2	3	4	5	6	7
1	3.4	3.6	3.2	3.2	6.9	9.1
2	4.7	3.5	5.8	6.0	7.6	6.7
3		3.8	5.5	2.5	7.4	7.7
4	1.9	3.2	0.8	1.8	0.8	0.4
5	3.6	2.3	0.8	0.5	5.0	0.6
6	3.7	3.5	3.2	3.8	0.7	0.4
7	3.7	2.5	8.1	5.4	3.6	8.2
8	6.1	5.5	5.0	8.4	12.9	16.1

TABLE II

Enthalpy of fusion of Schiff bases of structure



Kcal/mole

	R		
n	C_nH_{2n+1}	$C_nH_{2n+1}O$	$C_nH_{2n+1}CO$[a]
1		5.6	7.6
2	4.9	5.3	10.6
3		7.1	7.3
4		6.2	13.2
5	4.8	6.8	8.0
6		6.0	7.6
7	4.7	11.7	6.7
8		8.2	

[a] Data of J. A. Castellano and M. T. McCaffrey, private communication.

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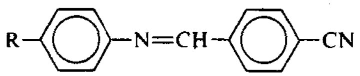
TABLE III

Enthalpy of fusion of Schiff bases of structure

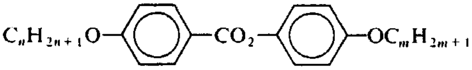


Kcal/mole

	R	
n	C_nH_{2n+1}	$C_nH_{2n+1}O$
1		5.6
2	5.7	5.4
3	5.1	6.2
4	8.9	9.4
5	8.1	9.0
6	4.7	7.1
7	16.9	

TABLE IV

Enthalpy of fusion of esters of structure

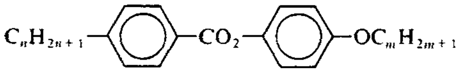


Kcal/mole

	m			
n	2	4	5	6
2	7.3	8.8	12.4	9.3
4	9.3	7.1	4.3	6.6
5	7.2	6.1	5.9	9.1
6	10.2	7.9	6.0	4.1
8	7.9	8.6	8.9	7.7

TABLE V

Enthalpy of fusion of esters of structure



Kcal/mole

	m			
n	2	4	5	6
4	7.8	7.7	7.1	4.7
5	7.3	6.8	4.5	6.1
6	6.4	8.0	5.8	5.7

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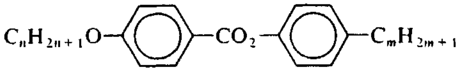
TABLE VI

Enthalpy of fusion of esters of structure

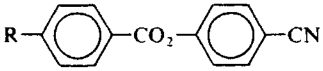


Kcal/mole

	m		
n	4	5	6
4	8.3	7.7	7.5
5	7.4	8.2	8.2
6	6.4	3.8	6.0

TABLE VII

Enthalpy of fusion of esters of structure



Kcal/mole

	R	
n	C_nH_{2n+1}	$C_nH_{2n+1}O$
4	6.7	8.2
5	6.0	7.7
6	8.6	8.3
7	8.7	8.2

Enthalpies of fusion for individual compounds were reproducible to within a few percent in duplicate runs. Due to the errors inherent in cell calibration, however, we are only confident of the accuracy of the data to ±10%. Using our computer program, which solves Eq. (1) by the Newton–Raphson Method,[6] errors of 10% in enthalpies were found to translate to changes of about 2°C in predicted eutectic temperature and of 2–5% in predicted eutectic compositions.

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