Physical Properties of Hydrocarbons

Part 42—Miscellaneous Cyclic Compounds

From charts you can get these properties for styrene, cyclopentene, cyclohexene and cyclooctadiene:

Vapor Pressure
Heat of Vaporization
Heat Capacity
Density
Viscosity
Surface Tension
Thermal Conductivity

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STYRENE is one of the most important aromatic compounds. In 1968, about 4 billion pounds were produced, almost all of it by dehydrogenation of ethylbenzene. Major producers include Amoco Chemical, Dow Chemical, Foster Grant, Monsanto, Shell, Sinclair-Koppers and Union Carbide. Styrene is used exclusively in the production of polystyrene and styrene copolymers such as styrene-butadiene rubber. Styrene growth will continue to be good.

Cyclopentene, cyclohexene and cycloöctadiene are all specialty compounds. Cycloöctadiene became available in commercial quantities in 1968. It should find application in plastics and flame retardants as the price comes down.

The physical properties of styrene have been well studied by a number of investigators. No physical property data are available on cycloöctadiene. Thus, all its properties were estimated from the molecular structure. These methods will give the same values whether the compound is 1,3-; 1,4-; 1,5-, or 1,6- cycloöctadiene.

Vapor Pressure and Critical Properties. The critical properties of styrene are available from the literature.[1,2] All the critical properties of the other compounds were estimated, except the critical temperature of cyclopentene,[3] by the methods proposed by Lydersen.[4]

No vapor pressure data are reported for cycloöctadiene. The boiling point was estimated from the molecular structure, with a probable error of ±5° C. The vapor pressure of cycloöctadiene over its entire temperature was estimated.[5] Literature data below the boiling point are available on the other compounds.[1,2,6-11] Above the boiling point, estimation methods were used.

Heat of Vaporization. The heats of vaporization of styrene have been measured from 0° C to the boiling point.[2,12,13] Driesbach reports the value at the boiling point for cyclopentene.[9] Giacalone's equation was used to estimate the heat of vaporization at the boiling point for cyclohexene and cycloöctadiene.[4] The values at other temperatures were calculated by Kharbanda's method.[14]

Heat Capacity. Except for experimental data on styrene[15,16] the vapor heat capacities were calculated from their molecular structure.[17]

The liquid heat capacities have been measured from −173 to 226° C for styrene;[2,7,8,12,18] and from −100 to 28° C for cyclopentene and cyclohexene.[19] The heat capacity of cycloöctadiene at 20° C was estimated,[4] and the equation relating density to heat capacity was used to calculate the heat capacities of cyclopentene, cyclohexene and cycloöctadiene at other temperatures. The probable error is about 5 percent.

Density. The liquid densities are reported for styrene from 0 to 145° C;[2,20] for cyclopentene from 0 to 30° C;[8,9,10] and for cyclohexene from 0 to 100° C.[8-11,21] Lydersen's method was used to calculate the densities at other temperatures.[4] For styrene, the error averaged 0.3 percent.

Viscosity. The vapor viscosities were estimated.[22]

Extensive liquid viscosity data are available for styrene,[2,20] The viscosity from 0 to 60° C has been measured for cyclohexene;[21,23] and at room temperature for cyclopentene.[11] Souder's method was used to calculate the viscosity at other temperatures.[4] For cyclohexene, this method gave an average error of 1.1 percent. For cyclopentene, the constant in the equation can be calculated from the experimental data. Thus, the error should be only a few percent over the temperature range. For cycloöctadiene, the constant must be estimated from its molecular structure, with a probable error of 5-10 percent.

Surface Tension. The surface tension of styrene has been measured up to its boiling point.[2] Huckel and Harder have determined the surface tension of cyclopentene from 0 to 35° C and of cyclohexene from 0 to 80° C.[10] Sugden's equation, relating surface tension to density and a molec-

TABLE 42-1—Physical Properties of Miscellaneous Cyclic Compounds

	Boiling Point, °C	Freezing Point, °C	Molecular Weight	Critical Properties Tc °C	Pc psia	dc g/ml
Styrene.....	145.0	− 30.6	104.14	369	552	0.28
Cyclopentene...	44.2	−135.1	68.11	233	695*	0.276*
Cyclohexene....	83.0	−103.5	82.14	287*	630*	0.282*
Cycloöctadiene..	125 *	.....	108.2	337*	555*	0.296*

* Estimated.

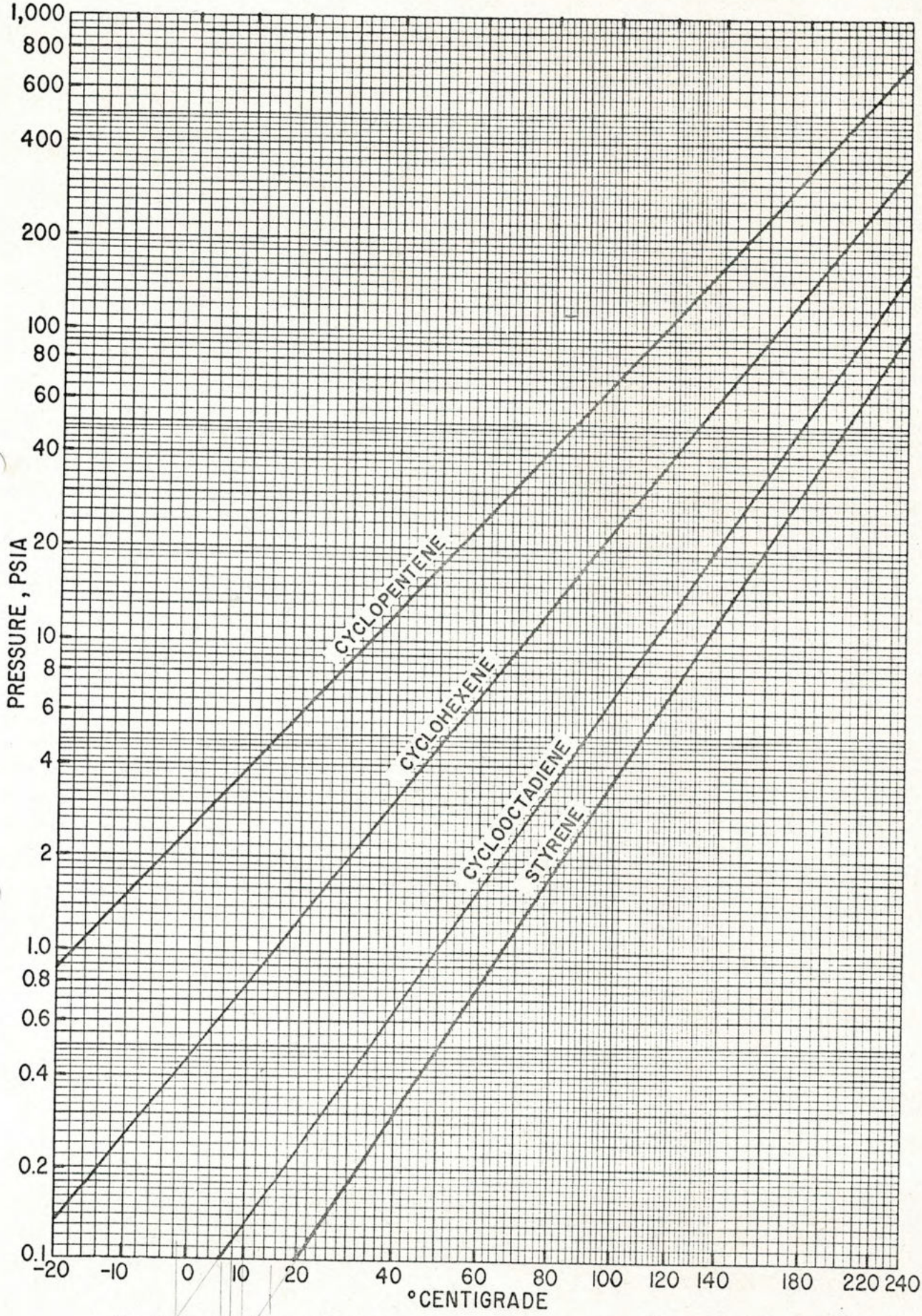

Fig. 42-1—Vapor pressure of miscellaneous cyclic compounds from —20 to 240° C.

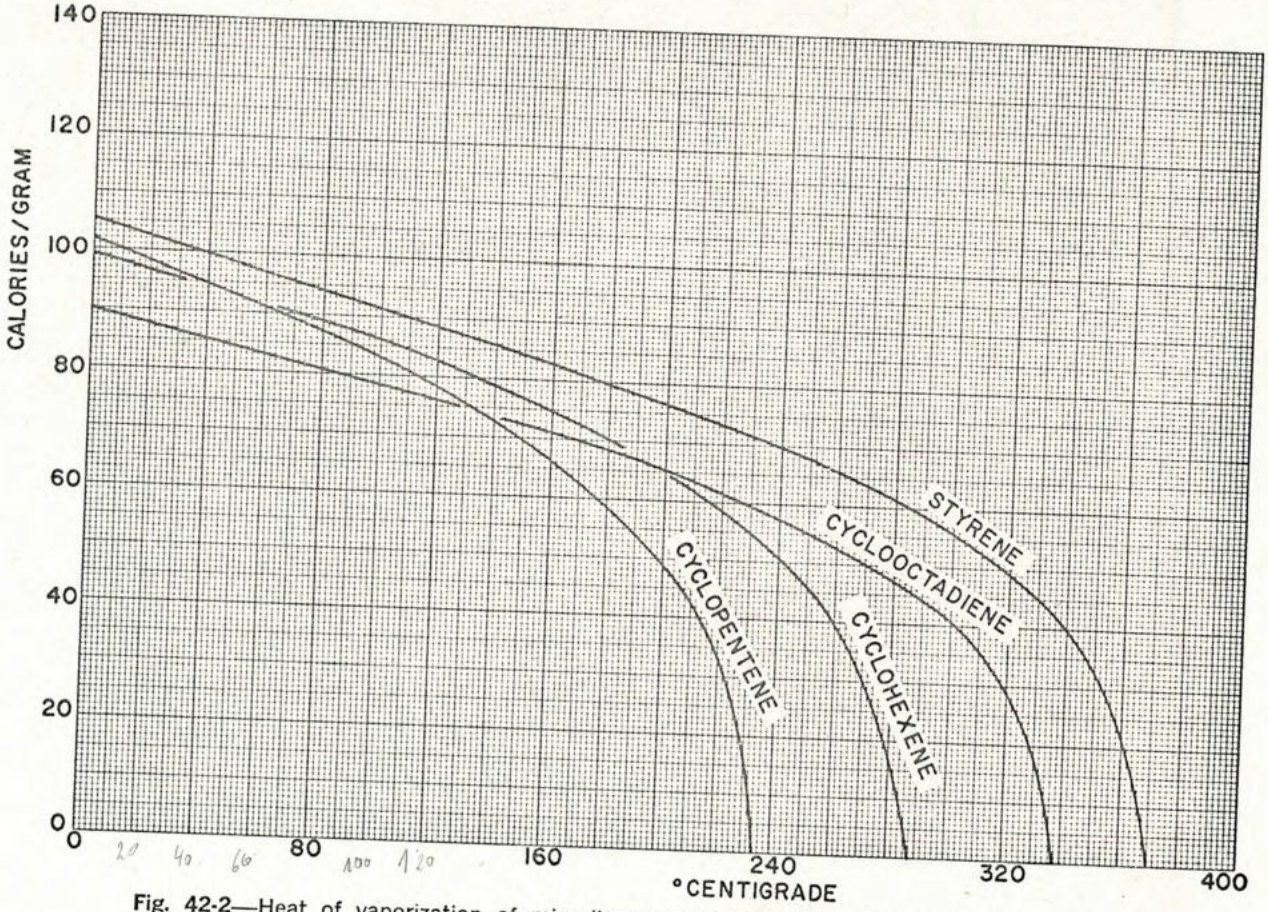

Fig. 42-2—Heat of vaporization of miscellaneous cyclic compounds from 0 to 370° C.

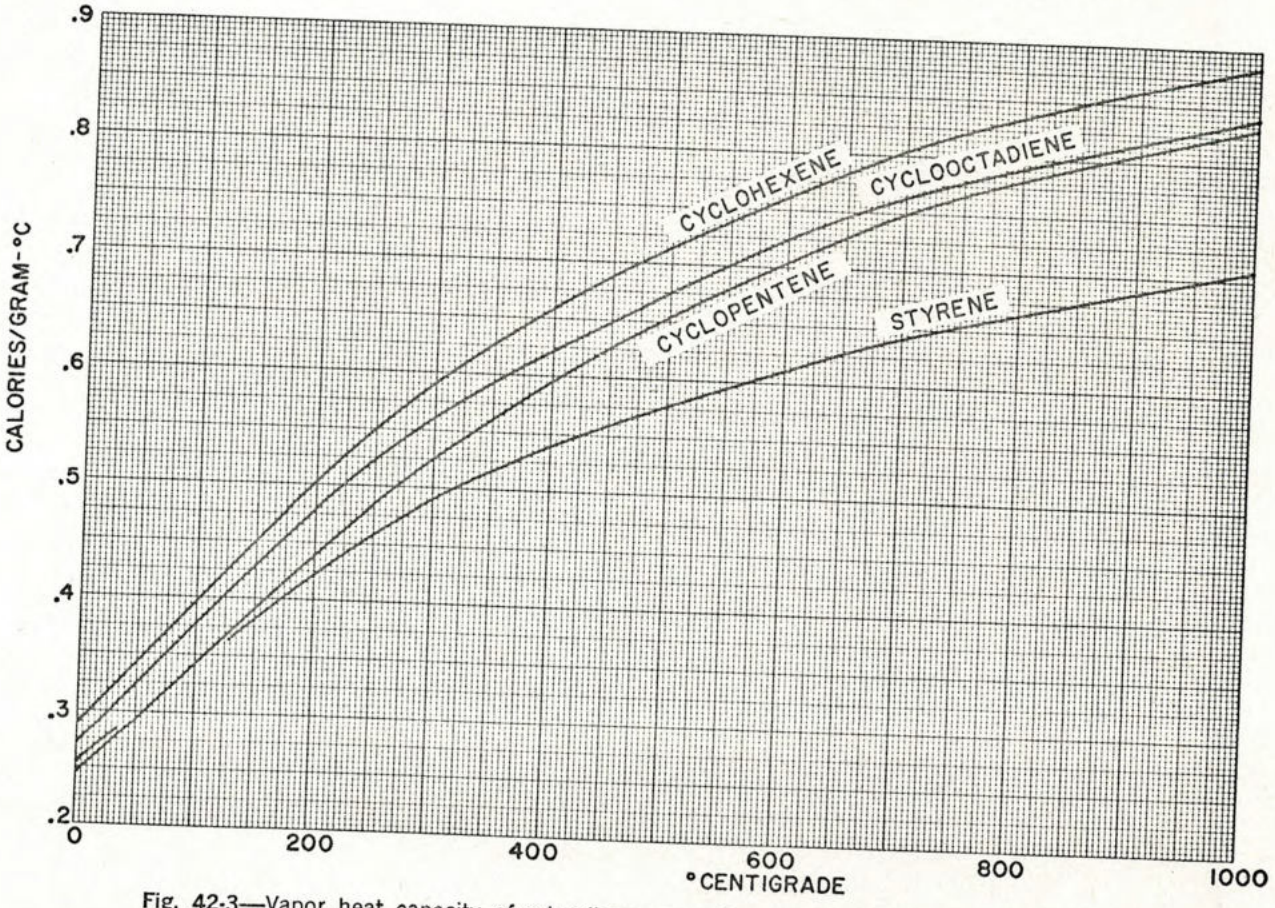

Fig. 42-3—Vapor heat capacity of miscellaneous cyclic compounds from 0 to 1,000° C.

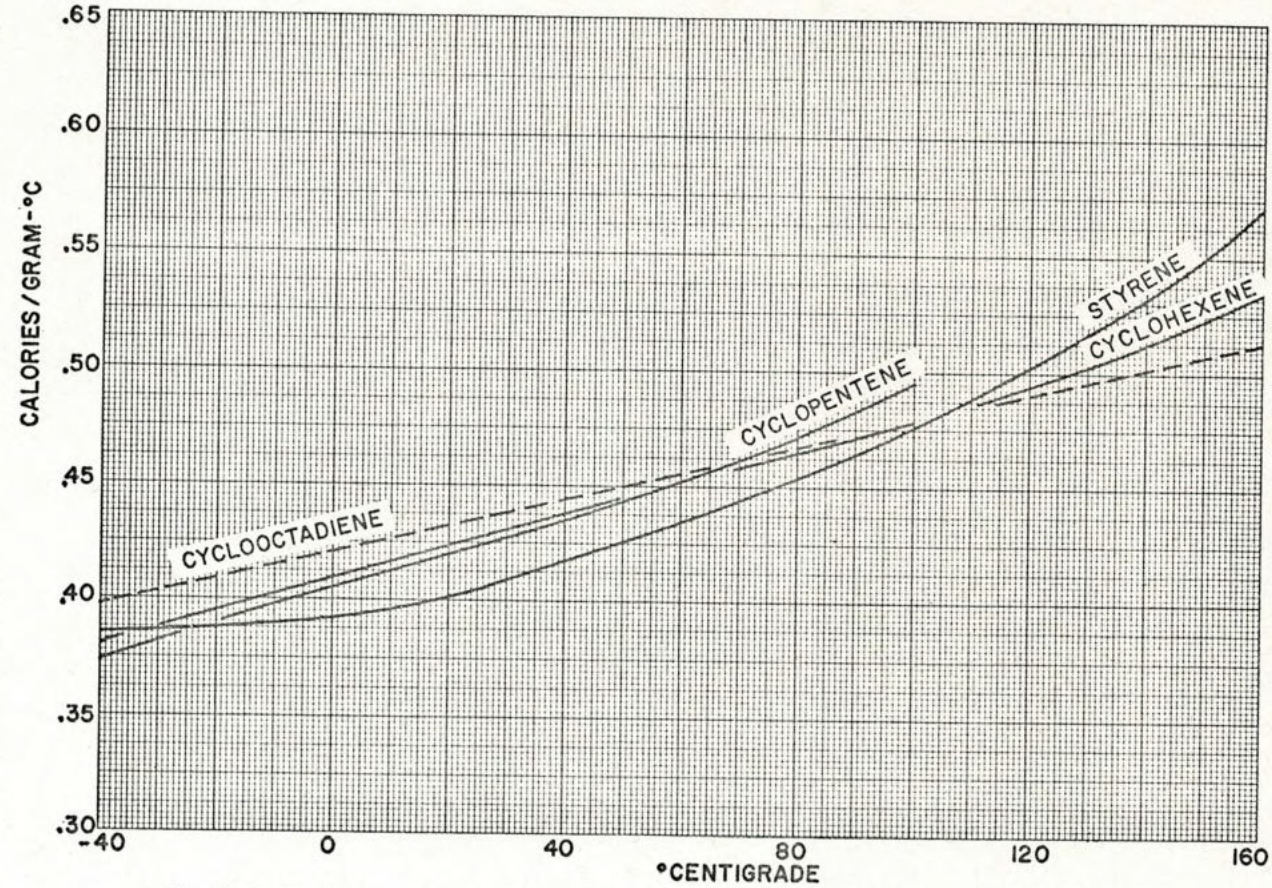

Fig. 42-4—Liquid heat capacity of miscellaneous cyclic compounds from —40 to 160° C.

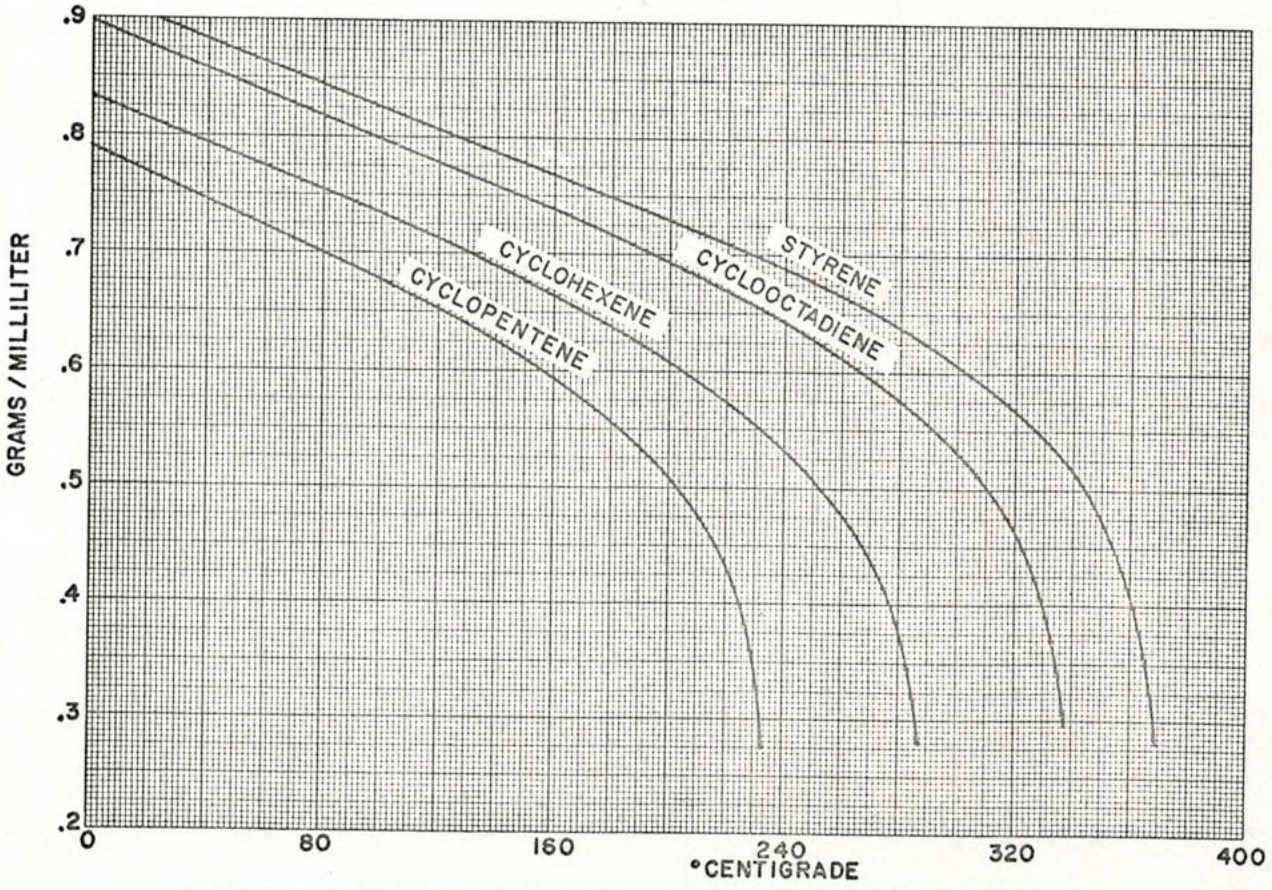

Fig. 42-5—Liquid density of miscellaneous cyclic compounds from 0 to 370° C.

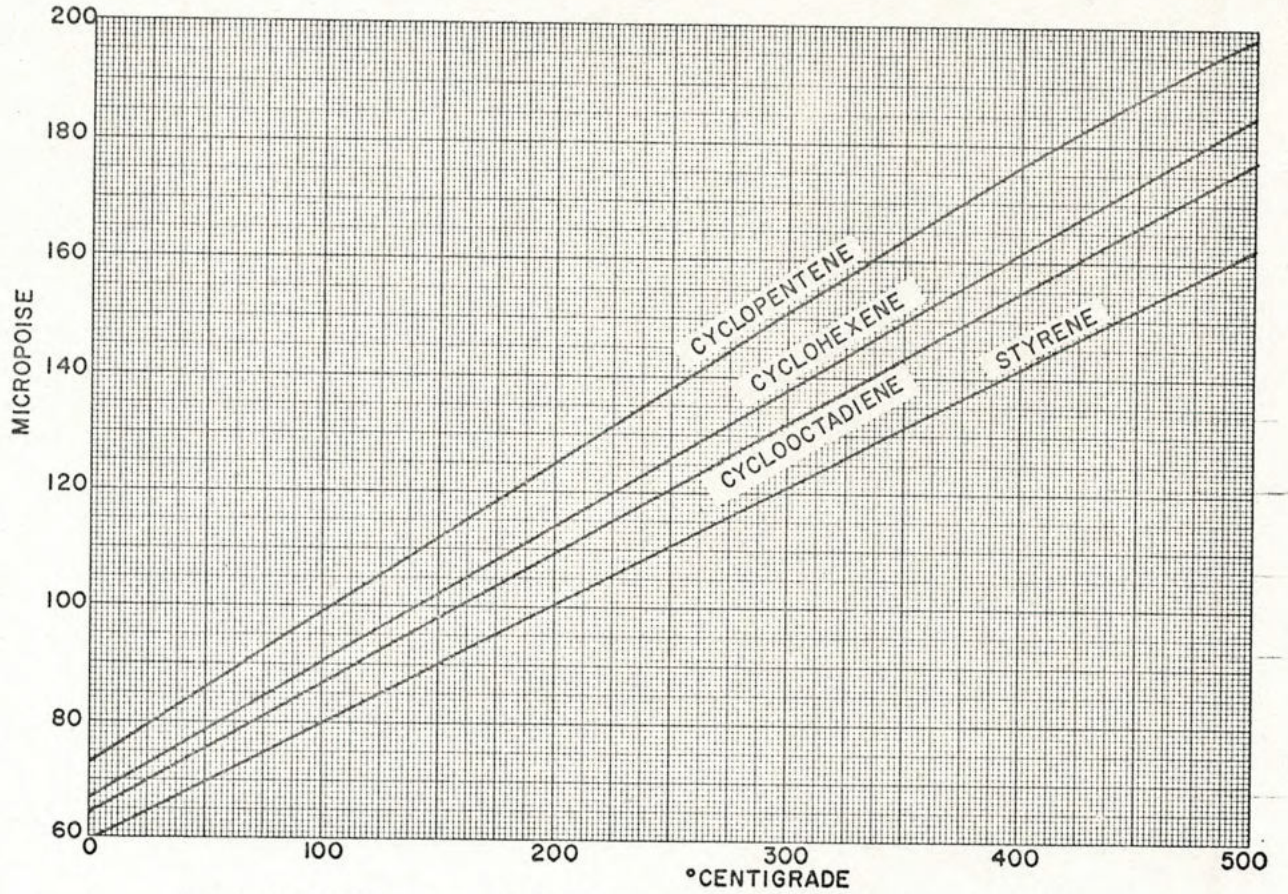

Fig. 42-6—Vapor viscosity of miscellaneous cyclic compounds from 0 to 500° C.

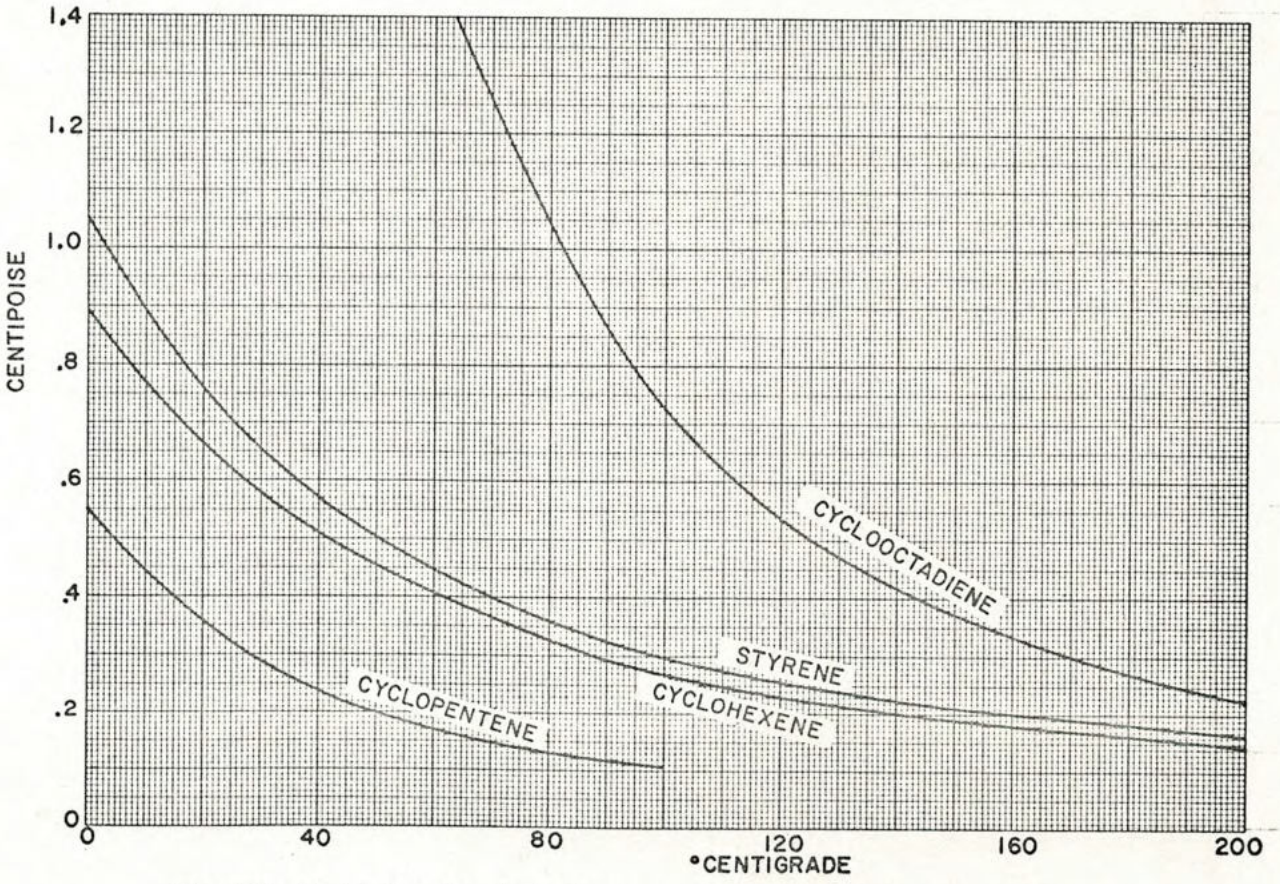

Fig. 42-7—Liquid viscosity of miscellaneous cyclic compounds from 0 to 200° C.

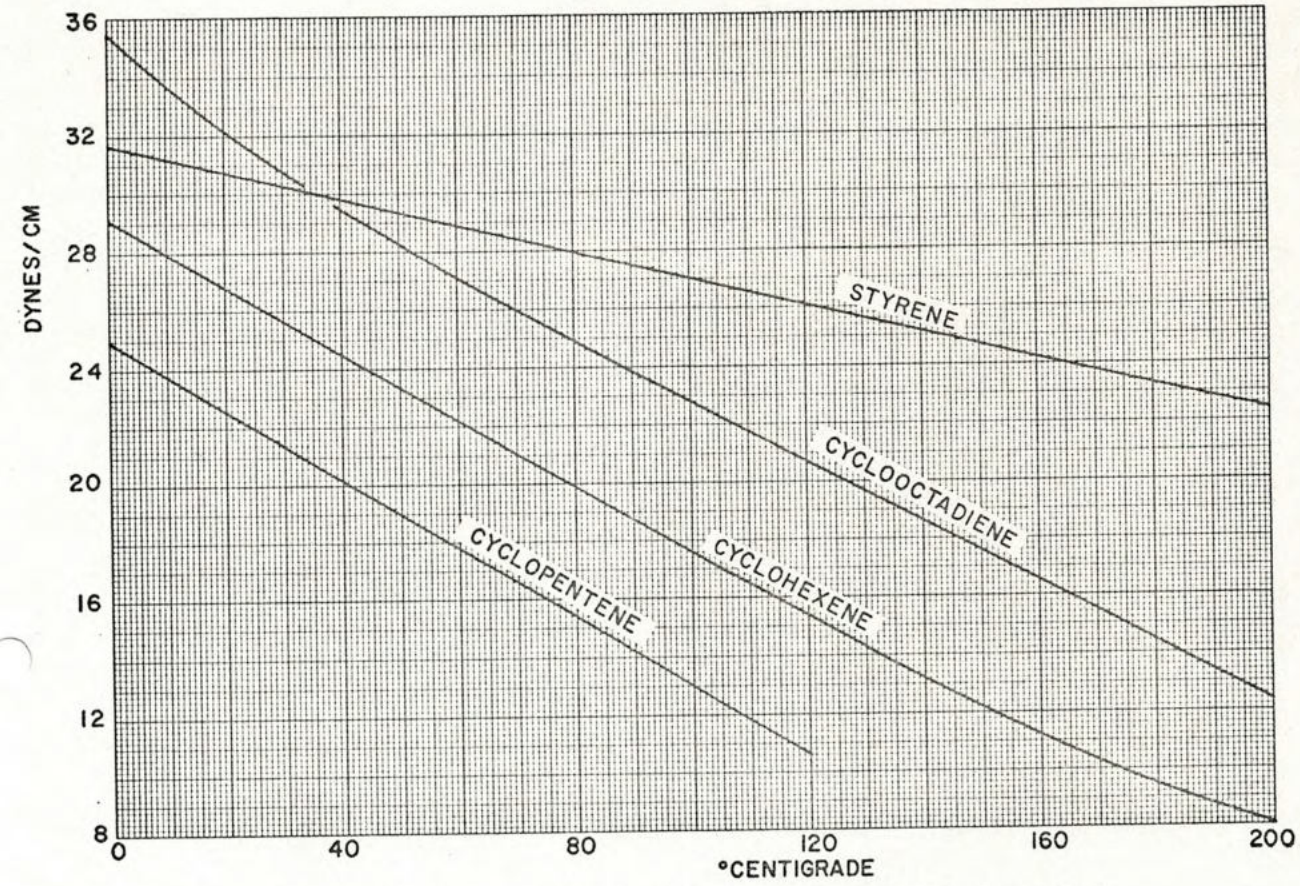

Fig. 42-8—Surface tension of miscellaneous cyclic compounds from 0 to 200° C.

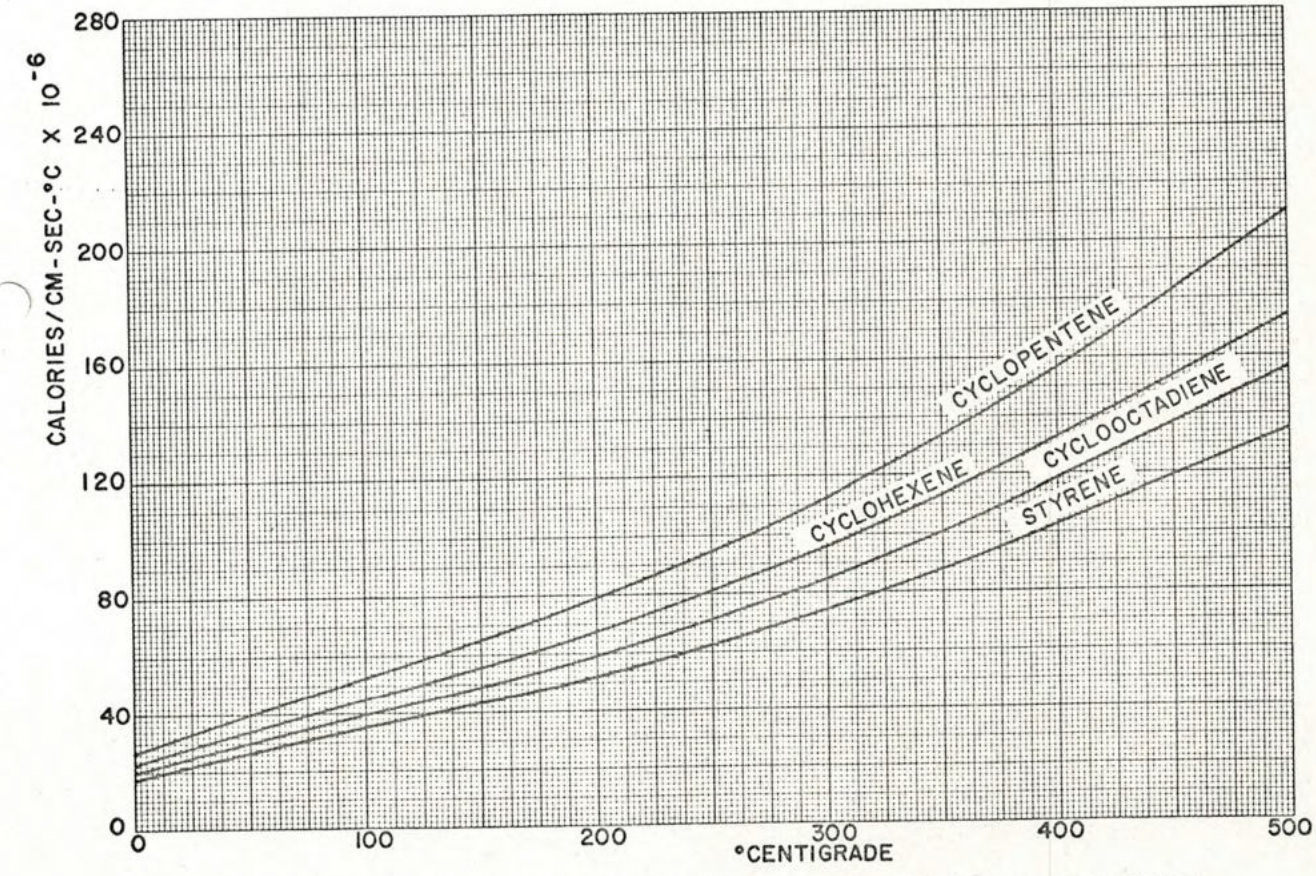

Fig. 42-9—Vapor thermal conductivity of miscellaneous cyclic compounds from 0 to 500° C.

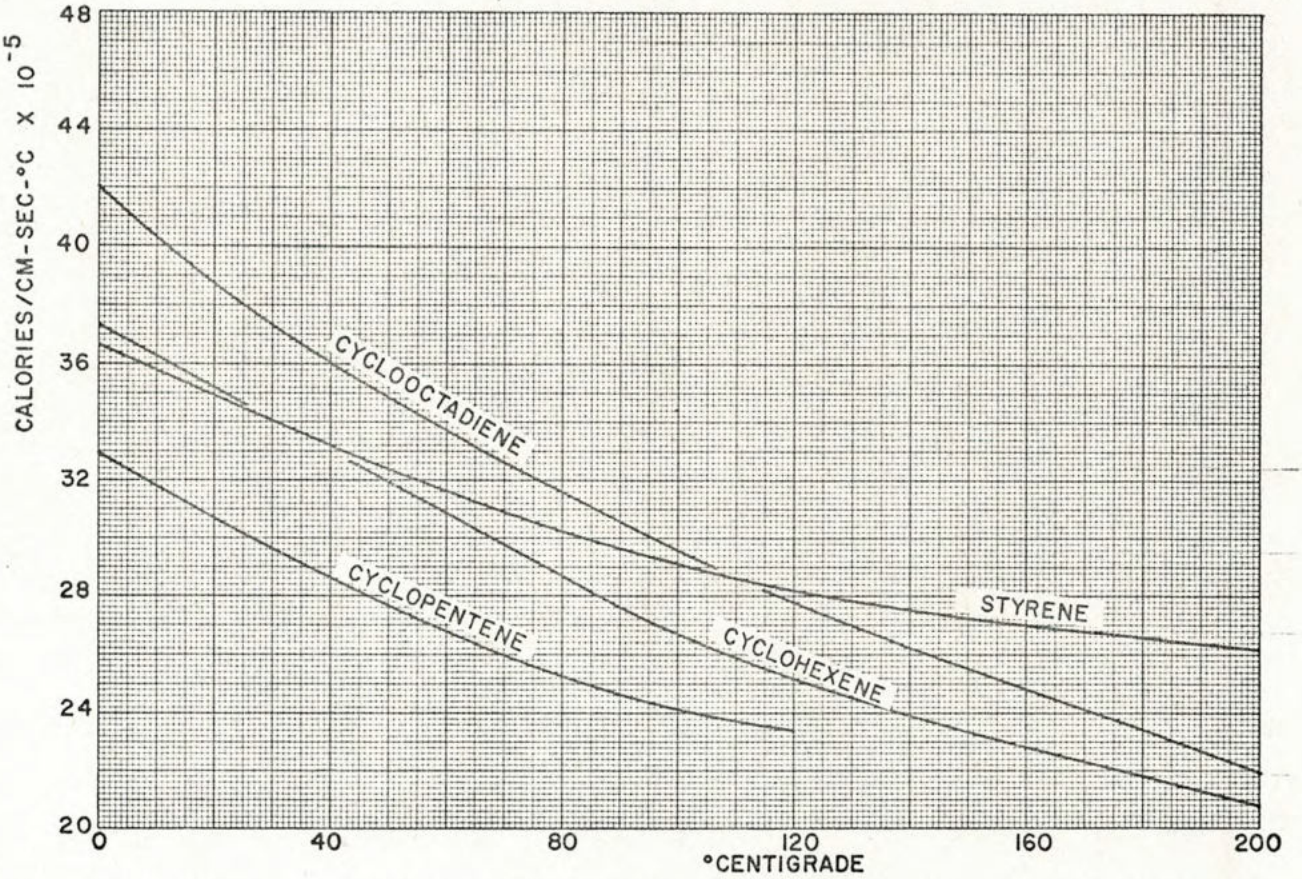

Fig. 42-10—Liquid thermal conductivity of miscellaneous cyclic compounds from 0 to 200° C.

ular constant, was used to calculate the surface tension at other temperatures. For cyclopentene and cyclohexene, the average error was 1.3 percent. The molecular constant had to be estimated for cycloöctadiene, but for cyclopentene and cyclohexene the estimation method was accurate within 1 percent. Thus, the estimated data for cycloöctadiene is probably correct within a few percent.

Thermal Conductivity. The vapor and liquid thermal conductivities were estimated by the method used in previous articles in this series.[24, 25]

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Indexing Terms: Computations-4, Cyclohexene-9, Cyclopentene-9, Cycloctadiene-9, Heat-7, Hydrocarbons-9, Liquid Phase-5, Physical Properties-7, Pressure-6, Properties/Characteristics/-7, Styrene-9, Temperature-6, Vapor Phase-5, Vinyl Compounds-9.

Part 43—Halogenated Aromatics will appear in an early issue.