The Molar Refraction of Liquid Organosilicon Compounds

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Computation of least squares values for 11 species of silicon bonds from literature data on 255 compounds demonstrates that the Eisenlohr molal refraction MR_E provides better correlation of refractive index with molecular structure than is afforded by the classical Lorenz-Lorentz expression.

MODERN ATTEMPTS to correlate refractive index with molecular structure of liquid organosilicon compounds began with a 1946 article of Sauer (*39*), who used the literature data of 49 silicon compounds to devise a system which involved both group and bond refractions. Later in the same year, Warrick (*62*), in extending the Denbigh (*7*) concept of bond refraction to 72 silicon compounds, calculated values for 10 species of silicon bonds, using Denbigh's values for bonds of elements other than silicon. Results differing only slightly from Warrick's were obtained from 139 silicon compounds by Vogel, Cresswell, and Leicester (*58*), who used values from Vogel's table (*57*) for elements other than silicon. In all of this prior work, the classical Lorenz-Lorentz equation

$$MR_L = \frac{(n^2 - 1)}{(n^2 + 2)} \cdot \frac{M}{d}$$

was the basis for the calculations, inasmuch as it is the only relation resting on accepted theoretical considerations.

As the concluding investigation of a series begun in 1957 on the molar refraction of liquid organometallic compounds, the present work aimed at providing further support for the strong inference already drawn from the results of calculations on compounds of phosphorus (*40*), of tin (*41*), and of boron (*42*)—namely, that the empirical Eisenlohr "molecular refraction coefficient" (*11*) $MR_E = Mn_D^{20}$ is more in accord with the facts of nature than is the Lorenz-Lorentz equation. Literature data for 255 representative silicon compounds served for the calculations, in which the values R_L = 1.424 and R_E = 14.26 were used for the C_{al}—C_{ar} bond (*42*), supplementing those from Vogel's table (*57*) for elements other than silicon. Both Lorenz-Lorentz and Eisenlohr values for 11 species of silicon bonds were computed by the method of least squares. Table I shows that the new Lorenz-Lorentz values are in fairly close agreement with those of Warrick and of Vogel.

The literature data and observed molar refractions of each compound are listed in Table II, together with the molar refractions calculated from the newly derived parameters of Table I. For comparison of the precision of the two systems under consideration, the coefficient of variation, C_v, was calculated for each—Lorenz-Lorentz = 0.0450, Eisenlohr = 0.0271.

Of the two systems investigated, that of Eisenlohr, aside from its other advantages, is clearly the more precise in its application to silicon compounds, as it has already been shown to be for the other principal classes of liquid organometallics; by a fairly reasonable inference, it seems likely that the same relative superiority obtains for all organic liquids. However, the evidence so far rests on calculations in which a substantial and sometimes preponderant part of the molar values is contributed by various carbon bonds, and of these the only ones derived by the method of least squares are C—C and C—H, obtained by Vickery and Denbigh (*56*) from eight *n*-alkanes and by Vogel from 12 *n*-alkanes and a considerable number of alkyl halides including both straight-chain and branched compounds. Although the 35 values, mostly of carbon bonded with other elements, given in Vogel's table (*57*) have been eminently useful, it is believed that reliance on molar refraction in research will eventually require that all bond values be computed by the least squares method from thoroughly reliable data, and that finer distinctions than those now in use be drawn between bond species. In particular, the numerous subspecies of C_{al}—C_{al} bonds should be clearly differential rather than lumped together as most of them have been in the past. Hence, the present work merely completes the preliminary portion of a comprehensive study of organic compounds in general, the next phase of which is already in progress on the molar refraction of liquid alkanes.

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Table I. Calculated Parameters

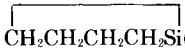
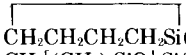
	Lorenz-Lorentz Refractions				Eisenlohr Refractions	
			Present Work			
Bond	Warrick (*62*)	Vogel (*58*)	Number of iterations	Values	Number of iterations	Values
Si—C_{al}	2.50	2.52	656	2.47	689	18.57
Si—C_{ar}	2.56	2.93	30	2.93	31	23.68
Si—H	3.20	3.17	96	3.17	96	10.39
Si—F	1.50	1.7	28	1.95	33	32.26
Si—Cl	7.20	7.11	81	7.33	85	62.21
Si—Br	10.20	10.08	39	10.31	39	135.19
Si—I			9	15.92	10	213.77
Si—N	2.00	2.16	74	2.10	83	20.59
Si—O	1.75	1.80	157	1.83	158	21.93
Si—S	6.25	6.14	70	5.94	70	40.96
Si—Si	5.65	5.89	26	5.85	27	30.02

Table II. Molar Values for Organosilicon Compounds

No.	Compound	Ref.	M	t	n'_D	d_4^t	n_D^{20}	Lorenz-Lorentz Molar Refractivity[a] Obsd.	Lorenz-Lorentz Molar Refractivity[a] Calcd.	Eisenlohr Molar Refraction Product[b] Obsd.	Eisenlohr Molar Refraction Product[b] Calcd.
1	$(CH_3)_4Si$	(*50*)	88.230	20		0.6426	1.3582	30.166	29.987	119.83	120.72
2	$(CH_3)_3SiC_2H_5$	(*64*)	102.257	20		0.6849	1.3820	34.746	34.645	141.32	141.32
3	$(CH_3)_3SiCH_2CH=CH_2$	(*47*)	114.268	20			1.4074	39.140	38.815	160.82	160.71
4	$(CH_3)_3SiC_3H_7$	(*64*)	116.284	20		0.7020	1.3929	39.525	39.294	161.97	161.92
5	$(CH_3)_3SiC_4H_9$	(*64*)	130.311	20		0.7181	1.4030	44.283	43.941	182.83	182.52
6	$(C_2H_5)_3SiCH_3$	(*64*)	130.311	20		0.7437	1.4160	43.971	43.941	184.52	182.52
7	$(CH_3)_2Si(C_3H_7)_2$	(*50*)	144.338	20		0.7399	1.4146	48.809	48.589	204.18	203.12
8	$(CH_3)_3SiC_5H_{11}$	(*64*)	144.338	20		0.7313	1.4096	48.859	48.589	203.46	203.12
9	$(C_2H_5)_4Si$	(*64*)	144.338	20		0.7662	1.4268	48.347	48.589	205.94	203.12
10	$(CH_3)_3SiC_6H_{13}$	(*64*)	158.365	20		0.7422	1.4154	53.477	53.237	224.15	223.72
11	$(C_2H_5)_3SiC_3H_7$	(*64*)	158.365	20		0.7724	1.4308	53.050	53.237	226.59	223.72
12	$(CH_3)_3SiC_7H_{15}$	(*64*)	172.392	20		0.7506	1.4201	58.134	57.885	244.81	244.32
13	$(C_2H_5)_3SiC_4H_9$	(*64*)	172.392	20		0.7786	1.4348	57.753	57.885	247.35	244.32
14	$(CH_3)_3SiCH_2CHClCH_2Cl$	(*47*)	185.182	20		1.030	1.4581	49.067	48.961	270.01	267.78
15	$(CH_3)_3SiC_8H_{17}$	(*64*)	186.419	20		0.7581	1.4242	62.773	62.533	265.50	264.92
16	$(C_2H_5)_3SiC_5H_{11}$	(*64*)	186.419	20		0.7835	1.4377	62.422	62.533	268.01	264.92
17	$(CH_3)_3SiCH_2CH_2CH_2Br$	(*47*)	195.192	20		1.113	1.4580	47.853	47.007	284.59	282.56
18	$(C_3H_7)_4Si$	(*27*)	200.446	20		0.7870	1.4378	66.833	67.181	288.20	285.52
19	$(C_2H_5)_3SiC_6H_{13}$	(*64*)	200.446	20		0.7880	1.4400	67.040	67.181	288.64	285.52
20	$(CH_3)_3SiC_{10}H_{21}$	(*64*)	214.473	20		0.7705	1.4310	72.052	71.829	306.91	306.12
21	$(C_2H_5)_3SiC_7H_{15}$	(*64*)	214.473	20		0.7907	1.4422	71.797	71.829	309.31	306.12
22	$(C_2H_5)_3SiC_8H_{17}$	(*64*)	228.500	20		0.7971	1.4438	76.117	76.477	329.91	326.72
23	$(CH_3)_3SiCH_2CH_2CH_2I$	(*47*)	242.186	20			1.496			362.31	360.51
24	$(CH_3)_3SiC_{12}H_{25}$	(*64*)	242.527	20		0.7800	1.4358	81.265	81.125	348.22	347.32
25	$(C_4H_9)_3SiC_3H_7$	(*32*)	242.527	20		0.7949	1.4462	81.393	81.125	350.74	347.32
26	$(C_2H_5)_3SiC_{10}H_{21}$	(*64*)	256.554	20		0.8036	1.4472	85.334	85.773	371.28	367.92
27	$(CH_3)_3SiC_{14}H_{29}$	(*64*)	270.581	20		0.7911	1.4410	90.321	90.421	389.91	385.52
28	$CH_3CH[Si(CH_3)_3]_2$	(*34*)	174.444	20		0.7821	1.4340	58.086	57.939	250.02	246.56
29	$CH_2CH_2CH_2CH_2Si(CH_3)_2$	(*18*)	114.268	20		0.7931	1.4330[c]	37.445	37.237	163.75	167.04
30	$CH_2CH_2CH_2CH_2Si(C_2H_5)_2$	(*18*)	142.322	20		0.8256	1.4471	46.068	46.533	205.95	208.24
31	$(CH_3)_3SiOH$	(*38*)	90.203	20		0.8112	1.3880	26.239	25.983	125.20	125.62
32	$(CH_3)SiOCH_3$	(*47*)	104.230	20			1.3634			142.11	141.54
33	$(CH_3)_3SiOC_2H_5$	(*38*)	118.257	20		0.7573	1.3743	35.687	35.459	162.52	162.14
34	$(CH_3)_3SiOC_3H_7$	(*21*)	132.284	20		0.7682	1.3838	40.243	40.107	183.05	182.74
35	$(C_2H_5)_3SiOH$	(*16*)	132.284	20		0.8647	1.4329	39.752	39.927	189.55	187.42
36	$(CH_3)_3SiOC_4H_9$	(*38*)	146.311	20		0.7774	1.3925	44.867	44.755	203.74	203.34
37	$(CH_3)_3SiOC_5H_{11}$	(*21*)	160.338	20		0.7849	1.4000	49.522	49.403	224.47	223.94
38	$CH_3CHCl(C_2H_5)_2SiOH$	(*45*)	166.733	20		1.0238	1.4607	44.663	44.761	243.55	240.35
39	$(C_3H_7)_3SiOC_2H_5$	(*18*)	202.419	20		0.8169	1.4242	63.255	63.347	288.28	285.74
40	$(CH_3)_3SiOC_{10}H_{21}$	(*21*)	230.473	20		0.8068	1.4228	72.713	72.673	327.92	326.94
41	$(C_4H_9)_3SiOC_2H_5$	(*18*)	244.500	20		0.8322	1.4350	76.665	77.291	350.86	347.54
42	$[(CH_3)_3Si]_2O$	(*38*)	162.390	20		0.7619	1.3774	49.069	48.647	223.68	224.94
43	$[(C_2H_5)_3Si]_2O$	(*49*)	246.552	25	1.4323	0.8402	1.4345[c]	76.158	76.535	353.68	348.54

(*Continued on page 148*)

Table II. Molar Values for Organosilicon Compounds *(Continued)*

No.	Compound	Ref.	M	t	n^t_D	d^t_4	n^{20}_D	Lorenz-Lorentz Molar Refractivity[a] Obsd.	Lorenz-Lorentz Molar Refractivity[a] Calcd.	Eisenlohr Molar Refraction Product[b] Obsd.	Eisenlohr Molar Refraction Product[b] Calcd.
44	$[(C_3H_7)_3Si]_2O$	(27)	330.714	20		0.8381	1.4412	104.243	104.423	476.62	472.14
45	$(CH_3)_2Si(OC_2H_5)_2$	(18)	148.284	20		0.8410	1.3815	40.985	40.922	204.85	203.55
46	$(C_2H_5)_2Si(OC_2H_5)_2$	(18)	176.338	20		0.8622	1.4022	49.822	50.218	247.26	244.75
47	$(C_3H_7)_2Si(OC_2H_5)_2$	(18)	204.392	20		0.8558	1.4100	59.173	59.514	288.19	285.95
48	$(C_4H_9)_2Si(OC_2H_5)_2$	(18)	232.446	20		0.8510	1.4182	68.863	68.810	329.65	327.15
49		(18)	146.268	20		0.9623	1.4269	39.018	38.866	208.71	208.67
50		(18)	174.322	20		0.9468	1.4300	47.562	48.162	249.28	249.87
51	$CH_3[(CH_3)_2SiO]_2Si(CH_3)_3$	(31)	236.550	20		0.8200	1.3848	67.572	67.297	327.57	329.15
52	$CH_3[(CH_3)_2SiO]_3Si(CH_3)_3$	(31)	310.710	20		0.8536	1.3895	86.188	85.946	431.73	433.36
53	$CH_3[(CH_3)_2SiO]_4Si(CH_3)_3$	(31)	384.870	20		0.8755	1.3925	104.799	104.596	535.93	537.58
54	$CH_3[(CH_3)_2SiO]_5Si(CH_3)_3$	(31)	459.030	20		0.8910	1.3948	123.456	123.246	640.25	641.79
55	$[(CH_3)_2SiO]_4$ (Cyclic)	(31)	290.640	20		0.9558	1.3968	73.195	74.599	405.97	416.86
56	$[(CH_3)_2SiO]_5$ (Cyclic)	(31)	370.800	20		0.9593	1.3982	93.332	93.248	518.45	521.07
57	$[(CH_3)_2SiO]_6$ (Cyclic)	(31)	444.960	20		0.9672	1.4015	111.897	111.898	623.61	625.29
58	$[(CH_3)_2SiO]_7$ (Cyclic)	(31)	519.120	20		0.9730	1.4040	130.481	130.548	728.84	729.50
59	$(C_4H_9O)_3SiNHC_6H_5$	(17)	339.560	20		0.9598	1.4664	98.056	96.706	497.93	494.12
60	$(CH_3)_2Si[N(CH_3)_2]_2$	(3)	146.316	22	1.4169	0.809	1.4178[d]	45.473	45.581	207.45	206.02
61	$(CH_3)_2Si(NHC_2H_5)_2$	(23)	146.316	20		0.8067	1.4151	45.429	45.201	207.05	209.50
62	$[(CH_3)_3C]_2Si(NH_2)_2$	(46)	174.370	20			1.4534			253.43	254.18
63	$(CH_3)_2Si(NHCH_2C_6H_5)_2$	(23)	270.458	20		1.0090	1.5409	84.217	84.417	416.75	415.82
64	$(CH_3)_2Si(NHC_7H_{15})_2$	(23)	286.586	20		0.8297	1.4425	91.482	91.681	413.40	415.50
65	$[(CH_3)_3C](C_{16}H_{33})Si(NH_2)_2$	(46)	342.694	20			1.4604			500.47	501.38
66	$C_3H_7Si(NHCH_3)_3$	(51)	161.332	20		0.8884	1.4427	48.115	48.155	232.75	233.28
67	$CH_3Si[N(CH_3)_2]_3$	(3)	175.359	22	1.4324	0.850	1.4333[d]	53.553	53.373	251.34	248.66
68	$C_3H_7Si(NHC_2H_5)_3$	(51)	203.413	20		0.8545	1.4380	62.590	62.099	292.51	295.08
69	$C_3H_7Si(NHC_3H_7)_3$	(51)	245.494	20		0.8545	1.4436	76.256	76.043	354.39	356.88
70	$C_2H_5Si[N(C_2H_5)_2]_2$	(53)	273.548	20		0.8773	1.4595	85.320	85.909	399.24	392.86
71	$C_3H_7Si[N(C_2H_5)_2]_3$	(53)	287.575	20		0.8752	1.4599	89.978	90.557	419.83	413.46
72	$C_3H_7Si(NHC_4H_9)_3$	(51)	287.575	20		0.8527	1.4474	90.179	89.987	416.24	418.68
73	$C_3H_7Si(NHCH_2C_6H_5)_3$	(52)	389.626	20		1.0503	1.5665	121.097	120.923	610.35	604.56
74	$[(CH_3)_3Si]_2NH$	(38)	161.406	20		0.7742	1.4080	51.432	50.947	227.26	229.52
75	$[(CH_3)_2SiNH]_3$ (Cyclic)	(6)	219.528	20		0.9196	1.4448	63.511	62.848	317.17	326.39
76	$[(C_2H_5)_2SiNH]_3$ (Cyclic)	(6)	303.690	20		0.9287	1.4670	90.735	90.736	445.57	449.99
77	$[(C_2H_5)_2SiNH]_4$ (Cyclic)	(6)	404.920	20		0.9521	1.4769	120.148	120.982	598.03	599.98
78	$(CH_3)_3SiCl$	(37)	108.652	20		0.8581	1.3884	29.906	29.825	150.85	152.75
79	$CH_3(C_2H_5)(CH_2=CH)CH_2SiCl$	(26)	148.717	20		0.9109	1.4380	42.858	43.291	213.85	213.34
80	$(C_2H_5)_3SiCl$	(8)	150.733	20		0.8967	1.4314	43.547	43.769	215.76	214.55
81	$CH_3(C_2H_5)(CH_2ClCH_2CH_2)SiCl$	(26)	185.182	20		1.0408	1.4548	48.255	48.603	269.40	267.48
82	$CH_3[(CH_3)_3CNH]_2SiCl$	(53)	222.846	20		0.9259	1.4419	63.669	63.621	321.32	323.93
83	$CH_3[(C_2H_5)_2N]_2SiCl$	(53)	222.846	20		0.9343	1.4453	63.518	64.001	322.08	320.45
84	$C_2H_5[(CH_3)_3CNH]_2SiCl$	(53)	236.873	20		0.9280	1.4465	68.133	68.269	342.64	344.53
85	$C_2H_5[(C_2H_5)_2N]_2SiCl$	(53)	236.873	20		0.9395	1.4517	67.978	68.649	343.87	341.05
86	$C_3H_7[(CH_3)_3CNH]_2SiCl$	(51)	250.900	20		0.9153	1.4468	73.212	72.917	363.00	365.13
87	$C_3H_7[(C_2H_5)_2N]SiCl$	(51)	250.900	20		0.9323	1.4530	72.740	73.297	364.56	361.65
88	$C_3H_7[CH_3(C_6H_5)N]_2SiCl$	(51)	318.934	20			1.5675			499.93	482.77

89	$CH_2CH_2CH_2CH_2SiCl_2$	(*18*)	155.112	20		1.1505	1.4651	37.278	36.892	227.25	231.10
90	$CH_3(CH_2{=}CHCH_2)SiCl_2$	(*26*)	155.112	20		1.0686	1.4406	38.301	38.480	223.45	224.77
91	$CH_3[CH_2{=}C(CH_3)CH_2]SiCl_2$	(*26*)	169.139	20		1.0521	1.4470	42.954	43.118	244.74	245.37
92	$C_2H_5(CH_2{=}CHCH_2)SiCl_2$	(*26*)	169.139	20		1.0529	1.4483	43.029	43.118	244.96	245.37
93	$CH_3(CH_2ClCH_2CH_2)SiCl_2$	(*26*)	191.577	20		1.2040	1.4585	43.458	43.782	279.42	278.91
94	$C_2H_5(CH_2ClCH_2)SiCl_2$	(*33*)	191.577	20		1.2174	1.4678	43.729	43.782	281.20	278.91
95	$C_2H_5(CH_3CHCl)SiCl_2$	(33)	191.577	20		1.2017	1.4578	43.484	43.782	279.28	278.91
96	$C_2H_5(CH_2ClCH_2CH_2)SiCl_2$	(*26*)	205.604	20		1.1810	1.4663	48.244	48.430	301.48	299.51
97	$[(CH_3)_3C]_2SiCl_2$	(*55*)	213.236	20		1.009	1.4561	57.459	57.540	310.49	308.38
98	$C_3H_7[(i\text{-}C_3H_7)_2N]SiCl_2$	(*51*)	242.279	20		1.0192	1.4557	64.582	65.332	352.69	351.05
99	$C_3H_7[(C_6H_{11})_2N]SiCl_2$	(*54*)	322.409	20			1.499			483.29	477.45
100	$CH_2{=}CHSiCl_3$	(*34*)	161.507	20		1.2426	1.4295	33.542	33.649	230.87	236.20
101	$CH_2{=}CHCH_2SiCl_3$	(*26*)	175.534	20		1.2224	1.4445	38.181	38.297	253.36	256.80
102	$CH_2{=}C(CH_3)SiCl_3$	(*34*)	175.534	20		1.2398	1.4412	37.403	38.297	252.98	256.80
103	$CH_2{=}C(CH_3)CH_2SiCl_3$	(*26*)	189.561	20		1.2036	1.4535	42.610	42.945	275.53	277.40
104	$CH_2ClCH_2CH_2SiCl_3$	(*26*)	211.999	20		1.3590	1.4668	43.269	43.609	310.96	310.94
105	$CH_3CH(SiCl_3)_2$	(*34*)	296.976	20		1.5059	1.4820	56.222	56.902	440.12	438.75
106	$(CH_3)_2C(SiCl_3)_2$	(*34*)	311.003	20		1.3733	1.4927	65.781	61.550	464.23	459.35
107	$(CH_3)_3SiSC_2H_5$	(*1*)	134.323	20		0.832	1.4512	43.487	42.722	194.93	196.55
108	$CH_3SiSC_3H_7$	(*1*)	148.350	20		0.844	1.4524	47.453	47.370	215.46	217.15
109	$(CH_3)_3SiSC_4(CH_3)_2$	(*1*)	148.350	20		0.824	1.4497	48.355	47.370	215.06	217.15
110	$(CH_3)_3SiSC_4H_9$	(*1*)	162.377	20		0.854	1.4550	51.588	52.018	236.26	237.75
111	$(CH_3)_3SiSC(CH_3)_3$	(*1*)	162.377	20		0.834	1.4570	53.025	52.018	236.58	237.75
112	$(CH_3S)_4Si$	(*4*)	216.494	35	1.5989	1.1888	1.6057[d]	62.209	62.305	347.62	341.65
113	$(C_2H_5S)_4Si$	(*4*)	272.602	25	1.5638	1.0860	1.5661[d]	81.619	80.897	426.92	424.05
114	$(C_3H_7S)_4Si$	(*4*)	328.710	25	1.5431	1.0328	1.5454[d]	100.335	99.489	507.99	506.45
115	$[(CH_3)_2CHS]_4Si$	(*4*)	328.710	35	1.5350	1.0099	1.5418[d]	101.334	99.489	506.80	506.45
116	$(C_2H_5)_3SiH$	(*50*)	116.284	20		0.7318	1.4119	39.530	39.609	164.18	162.74
117	$C_6H_5CH_2(CH_3)_2SiH$	(*16*)	150.301	20		0.9486	1.5040	46.917	49.921	226.05	224.70
118	$(C_3H_7)_3SiH$	(*63*)	158.365	20		0.7601	1.4284	53.647	53.553	226.21	224.54
119	$(C_4H_9)_3SiH$	(*63*)	200.446	20		0.7793	1.4380	67.521	67.497	288.24	286.34
120	$CH_3(C_6H_5CH_2)_2SiH$	(*16*)	226.399	20		0.9936	1.5650	74.219	74.177	354.31	348.46
121	$(C_5H_{11})_3SiH$	(*63*)	242.527	20		0.7894	1.4436	81.546	81.441	350.11	348.14
122	$(C_2H_5)_2(C_2H_5O)SiH$	(*18*)	132.284	20		0.7897	1.4000	40.609	40.422	185.20	183.55
123	$C_2H_5(C_2H_5O)_2SiH$	(*18*)	148.284	20		0.8465	1.3869	41.231	41.237	205.66	204.37
124	$(CH_2{=}CH_2CH_2O)_3SiH$	(*17*)	200.317	25	1.4270	0.9836	1.4284[d]	52.289	54.561	286.13	283.36
125	$[C_2H_5C(CH_3)O]_3SiH$	(*17*)	248.446	20		0.8661	1.4054	70.369	69.939	349.17	348.79
126	$(C_5H_{11}O)_3SiH$	(*17*)	290.527	27	1.4195	0.8710	1.4210[d]	84.328	83.883	412.84	410.59
127	$(C_6H_5O)_3SiH$	(*17*)	308.416	26	1.5621	1.1158	1.5636[d]	89.652	86.547	482.24	468.67
128	$(C_6H_{13}O)_3SiH$	(*17*)	332.608	25	1.4270	0.8701	1.4284[d]	98.146	97.827	475.10	472.39
129	$(C_7H_{15}O)_3SiH$	(*17*)	374.689	26	1.4315	0.8713	1.4330[d]	111.427	111.771	536.93	534.19
130	$[(C_2H_5O)_2SiH]_2O$	(*17*)	254.444	25	1.3850	0.9442	1.3864[d]	63.152	61.830	352.76	351.03
131	$(CH_3S)_3SiH$	(*66*)	170.401	25	1.5671	1.1423	1.5693[d]	48.738	49.895	267.41	266.63
132	$(C_2H_5S)_3SiH$	(*66*)	212.482	25	1.5440	1.0484	1.5462[d]	63.980	63.839	328.54	328.43
133	$(C_3H_7S)_3SiH$	(*66*)	254.563	25	1.5278	0.9991	1.5300[d]	78.432	77.783	389.48	390.23
134	$[(CH_3)_2CHS]_3SiH$	(*66*)	254.563	25	1.5221	0.9864	1.5243[d]	78.722	77.783	388.03	390.23
135	$(C_4H_9S)_3SiH$	(*66*)	296.644	25	1.5160	0.9819	1.5182[d]	91.251	91.727	450.36	452.03

(*Continued on page 150*)

Table II. Molar Values for Organosilicon Compounds *(Continued)*

No.	Compound	Ref.	M	t	n'_D	d'_4	n^{20}_D	Lorenz-Lorentz Molar Refractivity[a] Obsd.	Lorenz-Lorentz Molar Refractivity[a] Calcd.	Eisenlohr Molar Refraction Product[b] Obsd.	Eisenlohr Molar Refraction Product[b] Calcd.
136	$[(CH_3)_2CHCH_2S]_3SiH$	(66)	296.644	25	1.5160	0.9694	1.5182[d]	92.427	91.727	450.36	452.03
137	$Cl(CH_3)(C_6H_5CH_2)SiH$	(16)	170.723	27	1.5129[d]	1.0020	1.5160	51.202	49.748	258.82	256.73
138	$Cl[(CH_3)_3CNH]_2SiH$	(53)	208.819	20		0.9261	1.4379	59.179	59.288	300.26	303.14
139	$Cl[(C_2H_5)_2N]_2SiH$	(53)	208.819	20		0.9354	1.4433	59.218	59.668	301.39	300.66
140	$Cl(C_4H_9S)_2SiH$	(66)	242.919	25	1.5030	1.0358	1.5052[d]	69.328	69.534	365.64	367.03
141	$Cl[(CH_3)_3CS]_2SiH$	(66)	242.919	25	1.5040	1.0222	1.5062[d]	70.368	69.534	365.88	367.03
142	$Cl_2(CH_2=CH)SiH$	(34)	127.058	20		1.1222	1.4160	28.413	29.489	179.91	184.39
143	$Cl_2[CH_2=C(CH_3)]SiH$	(34)	141.085	20		1.0787	1.4310	33.855	34.137	201.89	204.99
144	$Cl_2(CH_3CHCl)SiH$	(33)	163.523	20		1.2614	1.4484	34.731	34.801	236.85	238.53
145	$(C_2H_5)_2SiH_2$	(12)	88.230	20		0.6832	1.3918	30.738	30.628	122.80	122.35
146	$(CH_2=CHCH_2)_2SiH_2$	(35)	112.252	20		0.7533	1.4420	39.428	38.968	161.87	161.13
147	$(C_3H_7)_2SiH_2$	(12)	116.284	20		0.7194	1.4112	40.151	39.924	164.10	163.55
148	$(C_4H_9)_2SiH_2$	(63)	144.338	20		0.7458	1.4241	49.395	49.220	205.55	204.75
149	$(C_5H_{11})_2SiH_2$	(63)	172.392	20		0.7636	1.4324	58.604	58.516	246.93	245.95
150	$CH_2=CHCH_2SiH_3$	(35)	72.187	20		0.6764	1.4050	26.157	25.817	101.42	101.35
151	$C_3H_7SiH_3$	(12)	74.203	20		0.6434	1.3759	26.457	26.295	102.10	102.56
152	CH_2ClSiH_3	(35)	80.598	20		0.9286	1.4157	21.767	21.833	114.10	114.29
153	$C_4H_9SiH_3$	(50)	88.230	20		0.6786	1.3922	30.975	30.943	122.83	123.16
154	$(CH_3)_2CHCH_2SiH_3$	(50)	88.230	20		0.6753	1.3905	31.006	30.943	122.68	123.16
155	$CH_3CHClSiH_3$	(33)	94.625	20		0.8846	1.4147	26.770	26.481	133.87	134.89
156	$C_5H_{11}SiH_3$	(63)	102.257	20		0.7019	1.4042	35.645	35.591	143.59	143.76
157	$CH_3CHClCH_2SiH_3$	(35)	108.652	20		0.8983	1.4305	31.277	31.129	155.43	155.49
158	$C_6H_{11}SiH_3$	(30)	114.268	25	1.4464	0.7958	1.4486[d]	38.320	38.027	165.53	165.76
159	$C_6H_{13}SiH_3$	(63)	116.284	20		0.7189	1.4131	40.343	40.239	164.32	164.36
160	$CH_3CH[SiH(CH_3)_2]_2$	(34)	146.390	20		0.7597	1.4252	49.292	49.273	208.63	206.99
161	$(CH_3)_3SiCH_2SiH(CH_3)_2$	(54)	146.390	20		0.7454	1.4158	49.263	48.958	207.26	206.18
162	$(CH_3)_2C[SiH(CH_3)_2]_2$	(34)	160.417	20		0.7779	1.4360	53.919	53.921	230.36	227.59
163	$(CH_3)_3SiCH(CH_3)SiH(CH_3)_2$	(34)	160.417	20		0.7756	1.4288	53.299	53.606	229.20	226.78
164	$(CH_3)_3SiC(CH_3)_2SiH(CH_3)_2$	(34)	174.444	20		0.7939	1.4378	57.658	58.254	250.82	247.38
165	$Cl_3SiCH(CH_3)SiHCl_2$	(34)	262.527	20		1.4310	1.4740	51.558	52.742	386.96	386.93
166	$(CH_3)_3SiBr$	(24)	153.111	25	1.4211	1.1727	1.4233[d]	33.116	32.805	217.92	225.73
167	$CH_3(C_2H_5)_2SiBr$	(25)	181.165	25	1.4464	1.1515	1.4486[d]	41.987	42.101	262.44	266.93
168	$(C_2H_5)_3SiBr$	(61)	195.192	20		1.1454	1.4573	46.438	46.749	284.45	287.53
169	$H(CH_3S)_2SiBr$	(67)	203.216	25	1.5660	1.5041	1.5682[d]	44.072	44.626	318.68	316.41
170	$H(C_2H_5S)_2SiBr$	(67)	231.270	25	1.5408	1.3717	1.5430[d]	52.964	53.922	356.85	357.61
171	$(CH_3S)_3SiBr$	(67)	249.309	25	1.5978	1.4988	1.6000[d]	56.736	57.035	398.89	391.43
172	$H[(CH_3)_2CHS]_2SiBr$	(67)	259.324	25	1.5195	1.2720	1.5217[d]	61.929	63.218	394.61	398.81
173	$H[(CH_3)_2CHCH_2S]_2SiBr$	(67)	287.378	25	1.5159	1.2481	1.5181[d]	69.535	72.514	436.27	440.01
174	$(C_2H_5S)_3SiBr$	(67)	291.390	25	1.5628	1.3508	1.5650[d]	70.039	70.979	456.03	453.23
175	$(C_3H_7S)_3SiBr$	(67)	333.471	25	1.5418	1.2444	1.5440[d]	84.312	84.923	514.88	515.03
176	$[(CH_3)_2CHS]_3SiBr$	(67)	333.471	25	1.5410	1.2244	1.5432[d]	85.584	84.923	514.61	515.03
177	$C_3H_7[CH_3(C_6H_5)N]_2SiBr$	(53)	369.393	20		1.2126	1.5770	99.312	96.645	573.07	555.74
178	$[(CH_3)_2CHCH_2S]_3SiBr$	(67)	375.552	25	1.5282	1.1823	1.5304[d]	97.842	98.867	574.74	576.83
179	$(CH_3)_2SiBr_2$	(24)	217.992	25	1.4696	1.6952	1.4718[d]	35.852	35.612	320.84	330.74
180	$(C_2H_5)_2SiBr_2$	(24)	246.046	25	1.4850	1.5767	1.4872[d]	44.725	44.908	365.92	371.94

181	$(C_2H_5S)_2SiBr_2$	(67)	310.178	25	1.5658	1.6541	1.5680[d]	61.151	61.062	486.36	482.41
182	$[(CH_3)_2CHCH_2S]_2SiBr_2$	(67)	366,286	25	1.497	1.3566	1.4992[d]	79.009	79.654	549.14	564.81
183	CH_3SiBr_3	(24)	282.873	25	1.5152	2,2130	1.5174[d]	38.558	38.419	429.23	435.75
184	$C_2H_5SiBr_3$	(24)	296.900	25	1.5155	2.0671	1.5177[d]	43.347	43.067	450.60	456.35
185	$C_2H_5(CH_3)_2SiF$	(10)	106.222	25	1.3570		1.3592[d]			144.38	143.40
186	$(C_2H_5)_3SiF$	(59)	134.276	20		0.8360	1.3900	38.074	38.394	186.64	184.60
187	$CH_2ClCH_2(C_2H_5)_2SiF$	(45)	168.925	20		1.0100	1.4277	43.004	43.228	241.17	237.53
188	$CH_3CHCl(C_2H_5)_2SiF$	(45)	168.925	20		0.9955	1.4208	43.013	43.228	240.01	237.53
189	$(C_3H_7)_3SiF$	(59)	176.357	20		0.8384	1.4117	52.307	52.338	248.96	246.40
190	$(C_4H_9)_3SiF$	(59)	218.438	20		0.8404	1.4238	66.297	66.282	311.01	308.20
191	$CH_2=CH(C_2H_5)SiF_2$	(36)	122.198	20		0.9578	1.3356	26.429	29.017	163.21	165.87
192	$(C_2H_5)_2SiF_2$	(36)	124.214	20		0.9357	1.3398	27.811	28.199	166.42	166.08
193	$[(CH_3)_2CH]_2SiF_2$	(10)	152.168	22	1.3663		1.3672[d]			208.04	207.28
194	$CH_3ClCH_2(C_2H_5)SiF_2$	(36)	158.663	20		1.1467	1.3900	32.799	33.033	220.54	219.01
195	$CH_3CHCl(C_2H_5)SiF_2$	(36)	158.663	20		1.1155	1.3790	32.869	33.033	218.80	219.01
196	$(C_4H_9)_2SiF_2$	(48)	180.322	25	1.4049	0:881	1.4071[d]	50.155	46.791	253.73	248.48
197	$CH_2ClCH_2SiF_3$	(36)	148.601	20		1.3661	1.3418	22.910	22.838	199.39	200.49
198	$CH_3CHClSiF_3$	(36)	148.601	20		1.2606	1.3180	23.251	22.838	195.86	200.49
199	$C_6H_{11}SiF_3$	(48)	168.244	25	1.3689	1.1012	1.3702[d]	34.390	34.384	230.53	231.36
200	$CH_2[Si(CH_3)_2F]_2$	(5)	168.347	20			1.3780			231.98	230.12
201	$H_3SiC_6H_5$	(12)	108.220	20		0.8681	1.5125	37.438	36.940	163.68	168.23
202	$H_3SiC_6H_4OCH_3$	(30)	138.247	25	1.5251	0.9797	1.5273[d]	43.252	43.212	211.14	210.89
203	$(CH_3)_3SiC_6H_5$	(22)	150.301	20		0.8748	1.4918	49.829	49.938	224.22	227.59
204	$H_3SiC_{10}H_7(a—)$	(30)	158.280	25	1.6030	1.0054	1.6052[d]	54.075	55.104	254.07	258.95
205	$C_6H_4CH_3(p—)$	(15)	164.328	20		0.8666	1.4910	54.919	54.714	245.01	249.59
206	$HO(C_2H_5)_2SiC_6H_5$	(44)	180.328	20		0.9905	1.5170	55.079	55.220	273.56	273.68
207	$(CH_3)_3SiC_6H_4Cl(p—)$	(15)	184.750	20		1.0002	1.5090	55.153	54.772	278.79	280.52
208	$BrH_2SiC_6H_5$	(24)	187.128	25	1.5555	1.3632	1.5577[d]	44.092	44.080	291.49	293.02
209	$(C_2H_5)_3SiC_6H_5$	(13)	192.382	20		0.8816	1.5024	64.443	63.882	289.03	289.39
210	$(CH_3)_3SiC_6H_4N(CH_3)_2(p—)$	(15)	193.371	20		0.9249	1.5338	64.969	63.028	296.59	290.47
211	$[(CH_3)_3C](NH_2)_2SiC_6H_5$	(46)	194.360	20			1.5198			295.39	299.24
212	$Cl(C_2H_5)_2SiC_6H_5$	(44)	198.777	20		1.0252	1.5130	58.277	59.061	300.75	300.82
213	$Br(CH_3)_2SiC_6H_5$	(25)	215.182	25	1.5294	1.2666	1.5316[d]	52.429	52.746	329.57	332.60
214	$CH_3CHCl(C_2H_5)_2SiC_6H_5$	(45)	226.831	20		1.0109	1.5229	68.534	68.716	345.44	342.32
215	$Br_2HSiC_6H_5$	(24)	266.036	25	1.5778	1.7293	1.5800[d]	51.039	51.220	420.34	417.72
216	$(C_4H_9)_3SiC_6H_5$	(15)	276.544	20		0.8719	1.4891	91.557	91.770	411.80	412.99
217	$Br_3SiC_6H_5$	(22)	344.944	25	1.5970	2.0228	1.5992[d]	58.102	58.360	551.63	542.61
218	$Br_3SiC_6H_4OCH_3(p$ -)	(24)	374.971	25	1.5958	1.9089	1.5980[d]	66.819	64.632	599.20	585.27
219	$[(C_2H_5)_2C_6H_5Si]_2O$	(44)	342.640	20		0.9828	1.5214	106.228	107.121	521.29	521.07
220	$H_2Si(C_6H_5)_2$	(63)	184.318	20		1.0027	1.5802	61.193	61.214	291.26	294.88
221	$(CH_3)_2Si(C_6H_5)_2$	(22)	212.372	20		0.9880	1.5639	69.903	69.879	332.13	334.45
222	$(C_2H_5O)_2Si(C_6H_5)_2$	(18)	272.426	20		1.0334	1.5235	80.595	80.803	415.04	417.29
223	$Br_2Si(C_6H_5)_2$	(24)	342.134	25	1.6179	1.5869	1.6201[d]	75.527	75.494	554.29	544.47
224	$[(CH_3)_3Si—]_2$	(60)	146.390	20		0.7268	1.4229	51.279	50.846	208.30	211.11
225	$(CH_3)_3Si—Si(CH_3)_2F$	(20)	150.355	20		0.8083	1.4031	45.403	45.299	210.96	213.18
226	$[(CH_3)_2FSi—]_2$	(20)	154.320	20		0.9120	1.3837	39.535	39.752	213.53	215.26

(Continued on page 152)

Table II. Molar Values for Organosilicon Compounds (*Continued*)

No.	Compound	Ref.	M	t	n_D^t	d_4^t	n_D^{20}	Lorenz-Lorentz Molar Refractivity[a] Obsd.	Lorenz-Lorentz Molar Refractivity[a] Calcd.	Eisenlohr Molar Refraction Product[b] Obsd.	Eisenlohr Molar Refraction Product[b] Calcd.
227	$(CH_3)_3Si$–$Si(CH_3)_2Cl$	(*43*)	166.812	20			1.4430			240.71	243.14
228	$(CH_3)_2ClSi$—$Si(CH_3)_2F$	(*20*)	170.777	20		0.9623	1.4201	44.920	45.126	242.52	245.20
229	$(CH_3)_3Si$—$Si(OC_2H_5)(CH_3)_2$	(*20*)	176.417	20		0.7993	1.4229	56.192	56.318	251.02	252.52
230	$CH_2Cl(CH_3)_2Si$—$Si(CH_3)_3$	(*19*)	180.839	20		0.8837	1.4576	55.796	55.680	263.59	264.04
231	$[(CH_3)_2ClSi-]_2$	(*20*)	187.234	20		1.0103	1.4545	50.234	50.501	272.33	275.17
232	$CH_2Cl(CH_3)_2Si$—$Si(C_2H_5)(CH_3)_2$	(*19*)	194.866	20		0.8933	1.4662	59.993	60.439	284.93	285.71
233	$CH_2Cl(CH_3)_2Si$—$SiCl(CH_3)_2$	(*19*)	201.161	20		1.0206	1.4735	55.343	55.507	296.41	296.07
234	$[(CH_3)_2(C_2H_5O)Si-]_2$	(*20*)	206.444	20		0.8507	1.4240	61.924	61.770	293.98	293.94
235	$(CH_3)_3Si$–$Si(CH_3)_2C_6H_5$	(*14*)	208.461	20		0.8738	1.5056	70.831	70.787	313.86	317.91
236	$[(C_2H_5)_3Si-]_2$	(*60*)	230.552	20		0.8351	1.4790	78.288	78.734	340.99	334.71
237	$(CH_3)_2(C_2H_5O)Si$–$Si(OC_2H_5)_2CH_3$	(*20*)	236.471	20		0.8873	1.4220	67.724	67.233	336.26	335.36
238	$[(CH_3O)_3Si-]_2$	(*28*)	242.390	20		1.095	1.4070	54.491	55.731	341.04	336.00
239	$[CH_3(C_2H_5O)_2Si-]_2$	(*20*)	266.498	20		0.9282	1.4200	72.657	72.695	378.43	376.77
240	$(CH_3)_3Si$—$Si(CH_3)(C_6H_5)_2$	(*14*)	270.532	20		0.9678	1.5606	90.467	90.728	422.19	424.84
241	$[(C_3H_7)_3Si-]_2$	(*60*)	314.714	20		0.8291	1.4721	106.311	106.622	463.29	458.31
242	$[(C_2H_5O)_3Si-]_2$	(*29*)	326.552	20		0.9728	1.4102	83.205	83.619	460.50	459.60
243	$[(C_4H_9)_3Si-]_2$	(*60*)	398.876	20		0.8306	1.4694	133.837	134.510	586.11	581.91
244	$[(i\text{-}C_5H)_3Si-]_2$	(*60*)	483.038	20		0.8260	1.4667	162.174	162.398	708.47	705.51
245	$[(C_6H_{13})_3Si-]_2$	(*60*)	567.200	20		0.8366	1.4691	188.848	190.286	833.27	829.11
246	$(CH_3)_3SiSi(CH_3)_2Si(CH_3)_3$	(*65*)	204.550	20		0.7763	1.4612	72.330	71.695	298.89	301.49
247	$[(CH_3)_3SiSi(CH_3)_2-]_2$	(*65*)	262.710	20		0.8066	1.4877	93.789	92.543	390.83	391.88
248	$(CH_3)_3SiI$	(*1*)	200.105	20			1.4742			294.99	307.91
249	Cl_2CH_3SiI	(2)	240.949	20		1.903	1.5044	37.517	38.032	362.48	368.38
250	$(C_2H_5)_3SiI$	(*61*)	242.186	20		1.351	1.4949	52.268	52.357	362.04	366.11
251	$(C_3H_7)_3SiI$	(*61*)	284.267	20		1.229	1.4880	66.640	66.301	422.99	427.91
252	$[(CH_3)_2CHCH_2CH_2]_3SiI$	(*61*)	368.429	20		1.117	1.4842	94.399	94.189	546.82	551.51
253	$(C_6H_{13})_3SiI$	(*61*)	410.510	20		1.086	1.4810	107.573	108.133	607.96	613.31
254	$ClCH_3SiI_2$	(2)	332.402	20		2.451	1.600	46.396	46.657	531.84	519.94
255	$(C_2H_5)_2SiI_2$	(9)	340.034	20		1.9711	1.5714	56.713	56.126	534.33	529.11

[a] $MR_L = \frac{(n^2-1)}{(n^2+2)} \cdot \frac{M}{d}$ [b] $MR_E = Mn_D^{20}$

[c] The refractive index of Compound 29 is given as 1.5330 on Page 17 and in C.A. (*18*); this is obviously a typographical error, since Page 13 gives 1.4330, and 37.41 for MR_L. [d] Corrected by use of coefficient-0.00045/° C.

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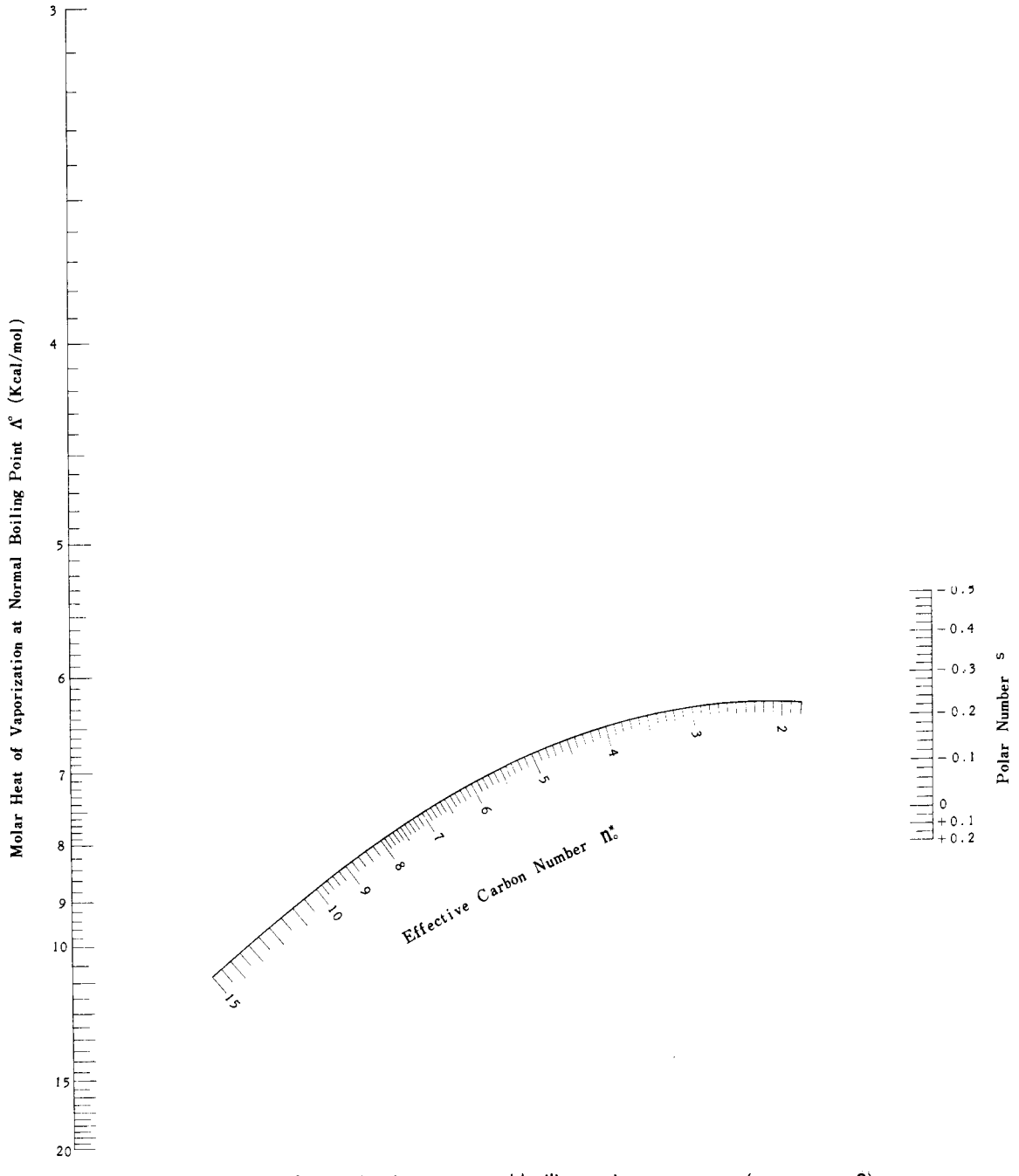

Figure 6. Heat of vaporization at normal boiling point nomogram (nomogram 3)

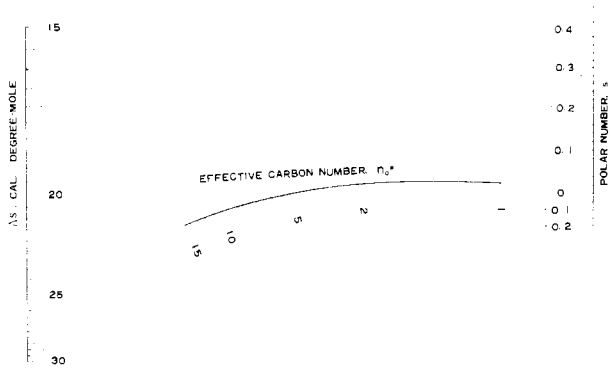

Figure 7. Entropy of vaporization at normal boilint point nomogram (nomogram 4)

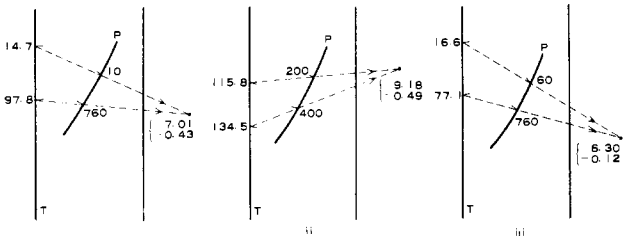

Figure 8. Determination of point representing each compound on nomogram

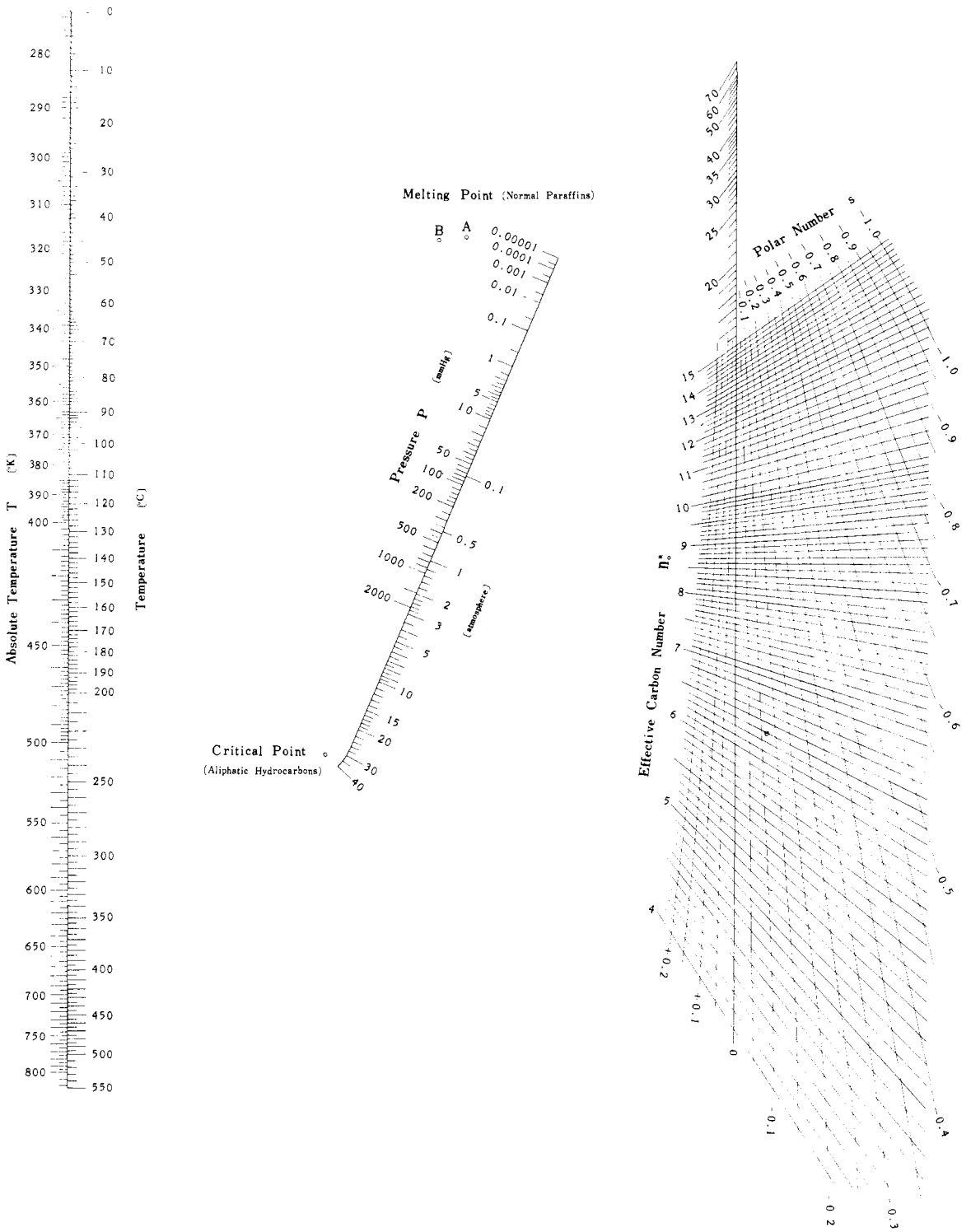

Figure 5. Generalized vapor pressure nomogram II (nomogram 2)

CORRECTION:

In the article, "Generalized Vapor Pressure Nomogram for Organic Liquids," [J. CHEM. ENG. DATA 8, 355 (1963)], the figures and captions were not in proper order. The figures with their correct captions are published from pages 154–157.

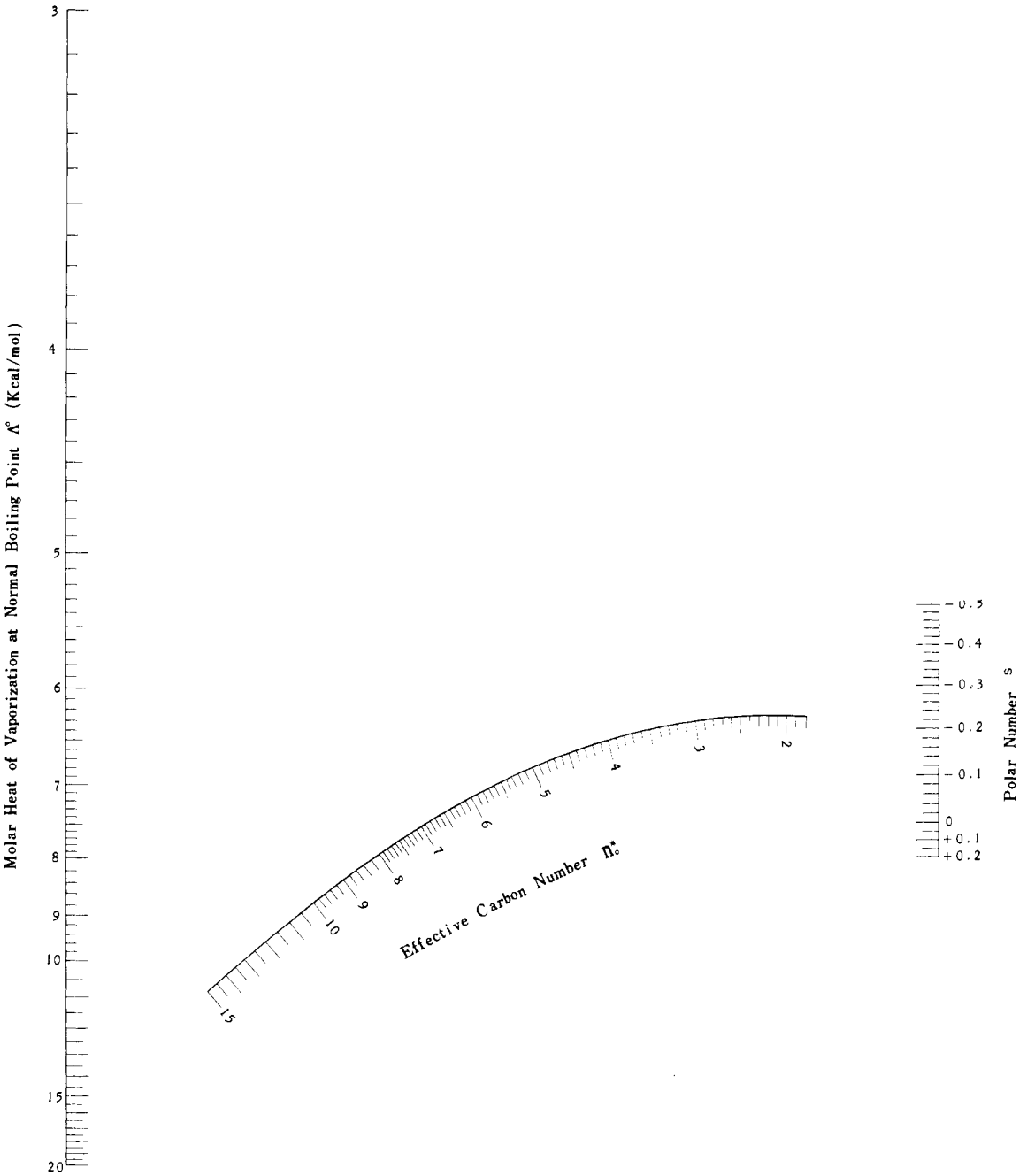

Figure 6. Heat of vaporization at normal boiling point nomogram (nomogram 3)

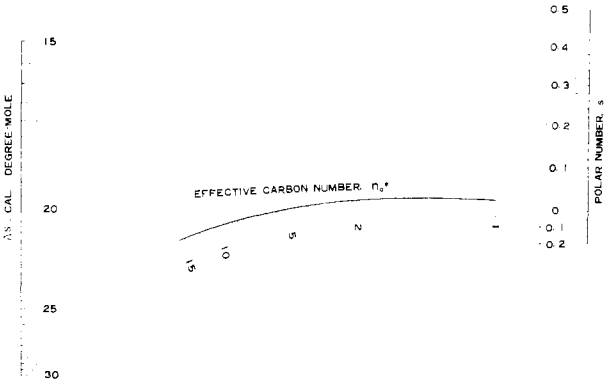

Figure 7. Entropy of vaporization at normal boilint point nomogram (nomogram 4)

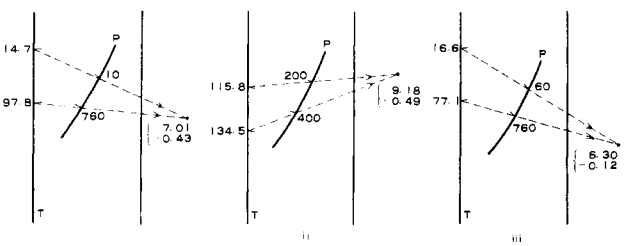

Figure 8. Determination of point representing each compound on nomogram

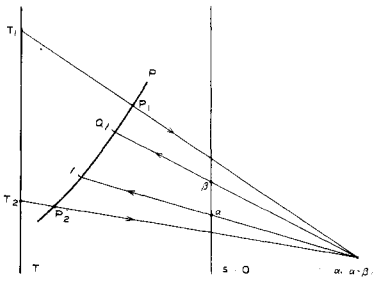

Figure 9. Determination of n_o^* and s on nomogram

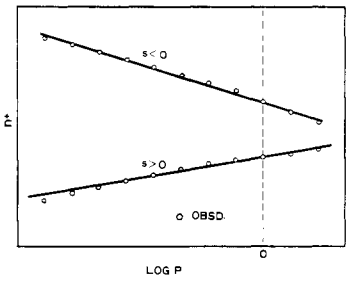

Figure 10. Detailed analysis of n^* vs. log P data

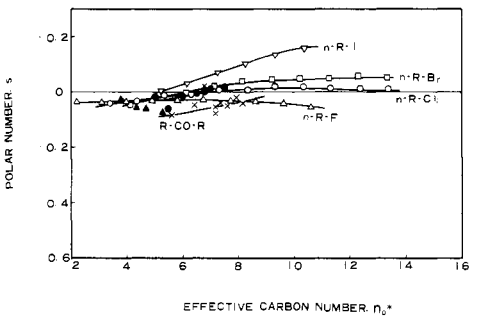

Figure 11. s vs. n_o^* relationship in mono-substituted alkane homologs (1) R- and R'- are alkyl groups and n-R-, normal alkyl group: closed marks are RX

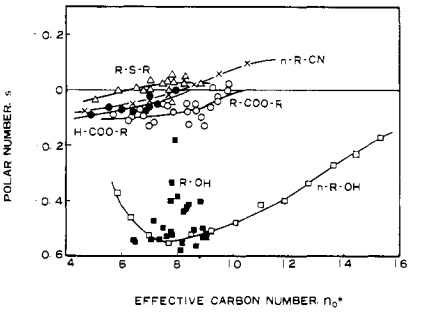

Figure 12. s vs. n_o^* relationship in mono-substituted alkane homologs (2)

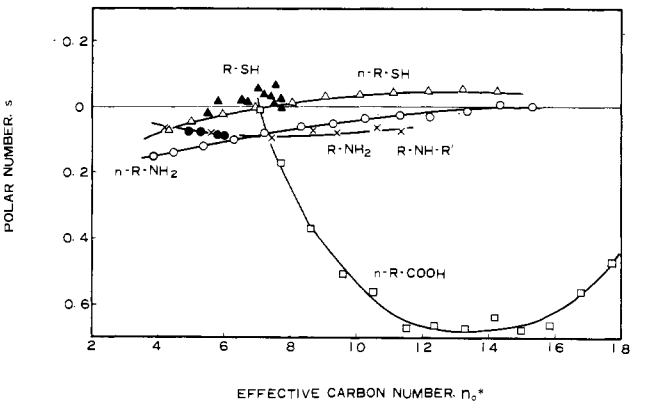

Figure 13. s vs. n_o^* relationship in mono-substituted alkane homologs (3)

CORRECTION:

In the article "Vapor-Liquid Equilibria" [J. CHEM. ENG. DATA 8, 549 (1963)] the name of one of the coauthors is misspelled. A.K. Keshpande should read as A.K. Deshpande. The same error is made in the index, p. 63; on the front cover the name appears as A.K. Koshpande.

CORRECTION:

In the article entitled, "A Generalized Equation for Diffusion in Liquids," by Ramalingam Sitaraman, S.H. Ibrahim, and N.R. Kuloor [J. CHEM. ENG. DATA 8, 198 (1963)], there are two errors. In Equation 1 the term $(XM_s)^{1/2}$ should read $(XM_s)^{1/2}$. In equation 2 the term $L_s^{0.3}$ should read $L^{0.3}$