Molar Refraction

Extension of the Eisenlohr-Denbigh System of Correlation to Liquid Organoboron Compounds

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Using literature data for 231 organoboron compounds Lorenz-Lorentz and Eisenlohr refraction constants have been computed by least squares for seven species of boron bonds and for the C_{al} C_{ar} bond. The coefficients of variation show that the Eisenlohr system is in definitely better agreement with the observed measurements.

DURING recent years there has been a growing interest in the correlation of refractive index and structure of the liquid organic compounds of boron. The published work has been based exclusively on the classical Lorenz-Lorentz equation. In 1954, Torssell (*59*) derived values ranging from 3.05 to 5.27 for the atomic refractivity R_L of boron in various types of compounds; subsequent values of 2.65, 2.28, and 3.0 were proposed by Abel and others (*2*), by Gerrard, Lappert and Mountfield (*21*), and by Aubrey and Lappert (*4*), respectively.

In 1958, when the convenient and logical Denbigh bond refraction concept (*13, 62*) had attained wide acceptance, McCusker and Ostdick (*45*) published values for the Lorenz-Lorentz refractivities of B—O and B—Cl bonds, as did Hennion (*27*) for that of the B—C bond. In the same year, Christopher and Tully (*10*) calculated values for the refractivities of two boron-containing octets and of B—C_{al} and B—C_{ar} bonds. A more comprehensive study based on the literature data for 172 boron compounds was made in in 1960 by Weidmann and Zimmerman (*65*), who assigned refractivity values to six species of boron-containing octets and to three species of boron bonds.

The present investigation was prompted by the successful utilization of the Eisenlohr molar refraction product (*15*) in conjunction with the Denbigh bond system in correlating refractive index with the structure of liquid organic compounds of phosphorus (*54*) and of tin (*55*). Atomic, group, and bond values from Vogel's tables (*63, 64*) have been used in this work for elements other than boron. The following special values for —CH— and —C— groups and atomic values R_L and R_E for boron were calculated by the least squares method from data on the first 231 boron compounds in Table II, including 16 for which no density measurements are available and which are perforce omitted in calculations based on the Lorenz-Lorentz equation:

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Group or Atom	Atomic Refractivity (Lorenz-Lorentz)	Atomic Refraction Constant (Eisenlohr)
—CH—	3.66	22.80
—C—	2.50	24.57
B	3.44	19.41

More usefulness and interest attach to the corresponding bond values. Thanks largely to Torssell's work (*59*) on tolyl derivatives of boron, sufficient data are available for least squares computation of values for the C_{al}—C_{ar} bond, which is not included in Vogel's table (*64*), as well as for the seven species of boron bonds listed in Table I.

In view of the almost universal adoption at the present time of the Denbigh bond mode of correlation, and in order to save space, the results based on the atomic and group parameters are omitted form Table II, which presents literature data and observed molar values for each compound listed, together with molar values calculated from the bond parameters of Table I in accordance with the Lorenz-Lorentz and with the Eisenlohr systems. For an

Table I. Calculated Parameters

	Bond Refractive (Lorenz-Lorentz)		Bond Refraction Constant (Eisenlohr)	
Bond	No. of Iterations	Value	No. of Iterations	Value
C_{al}—C_{ar}	32	1.424	33	14.26
B—C_{al}	159	2.032	165	13.59
B—C_{ar}	61	3.068	61	16.74
B—Cl	64	6.946	64	56.30
B—F	13	1.681	13	26.98
B—N	59	1.958	65	14.90
B—O	303	1.613	332	17.27
B—S	15	5.378	17	33.77

Table II. Molar Values for Organoboron Compounds

No.	Compound	Lit. 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.
1	$(C_2H_5)_3B$	(57)	98.006	20		0.684	1.3971	34.513	35.124	136.92	137.40
2	$(CH_2=CHCH_2)_3B$	(51)	134.039	20		0.7689	1.4500	46.848	47.634	194.36	195.57
3	$(C_3H_7)_3B$	(32)	140.087	22.5	1.4135	0.7225	1.4147[c]	48.400	49.068	198.18	199.20
4	$(C_4H_9)_3B$	(57)	182.168	20		0.751	1.4285	62.470	63.012	260.23	261.00
5	$[(CH_3)_2CHCH_2]_3B$	(32)	182.168	22.8	1.4188	0.7400	1.4201[c]	62.141	63.012	258.70	261.00
6	$[C_2H_5CH(CH_3)]_3B$	(26)	182.168	25	1.4349	0.7658	1.4371[c]	62.060	63.012	261.79	261.00
7	$[(CH_3)_3C]_2(C_4H_9)B$	(28)	182.168	25	1.4373	0.7608	1.4395[c]	62.768	63.012	262.23	261.00
8	$[(CH_3)_3C][(CH_3)_2CHCH_2](C_5H_{11})B$	(27)	196.195	25	1.4296	0.7506	1.4318[c]	67.467	67.660	280.91	281.60
9	$[(CH_3)_3C]_2(C_5H_{11})B$	(28)	196.195	25	1.4397	0.7668	1.4419[c]	67.393	67.660	282.89	281.60
10	$[(CH_3)_3C](C_5H_{11})_2B$	(27)	210.222	25	1.4333	0.7585	1.4355[c]	72.075	72.308	301.77	302.20
11	$(C_5H_{11})_3B$	(57)	224.249	20		0.760	1.4328	76.655	76.956	321.30	322.80
12	$[(CH_3)_2CHCH_2CH_2]_3B$	(32)	224.249	22.6	1.4321	0.7607	1.4333[c]	76.477	76.956	321.42	322.80
13	$(sym\text{-}C_5H_{11})_3B$	(57)	224.249	20		0.790	1.4455	75.623	76.956	324.15	322.80
14	$(C_6H_{13})_3B$	(57)	266.330	20		0.742	1.4300	92.722	90.900	380.85	384.60
15	$(C_{12}H_{25})_3B$	(57)	518.816	20		0.817	1.4910	183.915	174.564	773.55	755.40
16	$[(CH_3)_2CHCH_2]_2BF$	(29)	144.052	25	1.3816	0.7662	1.3836[c]	43.713	43.689	199.34	200.98
17	$(CLCH=CH)_2BCl$	(3)	169.267	20		1.2759	1.5452	41.957	39.074	261.55	251.34
18	$[(CH_3)_2CHCH_2]_2BCl$	(43)	160.509	25	1.4160	0.8251	1.4182[c]	48.817	48.954	227.63	230.30
19	$(C_6H_5)_2BCl$	(1)	200.489	20		1.116	1.6118	62.433	62.097	323.15	316.52
20	$C_4H_9BF_2$	(36)	105.936	25	1.3268[c]	0.8510	1.3290	25.172	24.367	140.79	140.95
21	$C_5H_{11}BF_2$	(42)	119.963	25	1.3409	0.8550	1.3431[c]	29.480	29.015	161.12	161.55
22	$C_6H_5BF_2$	(44)	125.926	25	1.4441	1.087	1.4463[c]	30.779	30.938	182.13	184.06
23	$p\text{-}CH_3C_6H_4BF_2$	(44)	139.953	25	1.4535	1.055	1.4557[c]	35.890	35.714	203.73	206.06
24	$C_5H_{11}BCl_2$	(41)	152.877	25	1.4204	0.9804	1.4226[c]	39.494	39.543	217.48	220.20
25	$C_6H_5BCl_2$	(1)	158.840	20		1.202	1.5430	41.653	41.467	245.09	242.71
26	$C_6H_{11}BCl_2$	(47)	164.888	20		1.1070	1.4710	41.633	41.979	242.55	242.20
27	$C_6H_{13}BCl_2$	(41)	166.904	25	1.4261	0.9705	1.4283[c]	44.074	44.191	238.39	240.80
28	$p\text{-}CH_3C_6H_4BCl_2$	(44)	172.867	30	1.5452	1.160	1.5497[c]	47.130	46.243	267.89	264.71
29	$(C_4H_9)(C_4H_9O)BF$	(8)	160.052	20		0.888	1.3900	42.725	44.730	222.47	222.12
30	$(C_6H_5)(C_4H_9O)BF$	(8)	180.042	20		0.972	1.4565	50.399	51.302	262.23	265.23
31	$(C_4H_9)(C_4H_9O)BCl$	(8)	176.509	20		0.898	1.4170	49.430	49.995	250.11	251.44
32	$(C_6H_5)(CH_3O)BCl$	(12)	154.418	20		1.086	1.5168	43.003	42.622	234.22	232.75
33	$(C_6H_5)(C_2H_5O)BCl$	(12)	168.445	16	1.5050[c]	1.004	1.5032	49.762	47.270	253.21	253.35
34	$(C_6H_5)(CH_2ClCH_2O)BCl$	(12)	202.894	20		1.158	1.5265	53.823	52.104	309.72	306.28
35	$(C_6H_5)[(CH_3)_2CHO]BCl$	(12)	182.472	20		1.022	1.4928	51.871	51.918	272.39	273.95
36	$(C_6H_5)(C_4H_9O)BCl$	(8)	196.499	20		1.021	1.4996	56.567	56.566	294.67	294.55
37	$(C_6H_5)[(CH_3)_2CHCH_2O]BCl$	(12)	196.499	20		1.009	1.4920	56.500	56.566	293.18	294.55
38	$(C_6H_5)[(CH_3)_3CO]BCl$	(12)	196.499	20		1.021	1.4955	56.173	56.566	293.86	294.55
39	$(C_6H_5)(C_6H_5O)BCl$	(12)	216.489	20		1.151	1.5670	61.443	62.102	339.24	334.51
40	$(C_6H_5)(C_6H_5CH_2O)BCl$	(12)	230.516	16	1.5638[c]	1.136	1.5620	65.782	66.878	360.07	356.51
41	$(C_6H_5)(o\text{-}CH_3C_6H_4O)BCl$	(12)	230.516	16	1.5638[c]	1.156	1.5620	64.644	66.878	360.07	356.51
42	$(C_6H_5)(C_8H_{17}O)BCl$	(12)	252.607	20		0.976	1.4900	74.829	75.158	376.38	376.95
43	$(C_6H_5)[C_6H_{13}CH(CH_3)O]BCl$	(12)	252.607	20		0.963	1.4877	75.536	75.158	355.80	376.95
44	$(C_6H_{11})[(CH_3)_2CHCH_2O]BCl$	(47)	202.547	20		0.951	1.4475	56.961	57.079	293.19	294.04
45	$[(iso\text{-}C_3H_7)_2B]_2O$	(52)	209.996	20		0.7761	1.4222	68.787	68.650	298.66	300.14

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

No.	Compound	Lit. 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.
46	$[(C_4H_9)_2B]_2O$	(*38*)	266.104	25	1.4258	0.7933	1.4280[c]	85.913	87.242	380.00	382.54
47	$[(iso\text{-}C_4H_9)_2B]_2O$	(*52*)	266.104	20		0.7723	1.4230	87.741	87.242	378.67	382.54
48	$[(iso\text{-}C_5H_{11})_2B]_2O$	(*52*)	322.212	20		0.7934	1.4331	105.569	105.834	461.76	464.94
49	$(ClCH{=}CH)_2BOH$	(*5*)	150.818	20		1.2822	1.5832	39.322	35.541	238.77	222.85
50	$(ClCH{=}CH)_2BOC_2H_5$	(*5*)	178.872	20		1.1103	1.4842	46.107	44.877	265.48	261.98
51	$(CH_2{=}CHCH_2)_2BOC_4H_9$	(*51*)	166.082	20		0.8092	1.4303	53.052	53.801	237.55	238.52
52	$(C_4H_9)_2BOC_2H_5$	(*52*)	170.114	20		0.7886	1.4105	53.504	54.757	239.95	240.94
53	$(C_4H_9)_2BOCH_2CH{=}CH_2$	(*24*)	182.125	20		0.8158	1.4279	57.424	58.927	260.06	260.33
54	$(C_4H_9)_2BOC_4H_9$	(*52*)	198.168	20		0.8077	1.4222	62.373	64.053	281.44	282.14
55	$(C_4H_9)_2BOCH_2CH(CH_3)_2$	(*24*)	198.168	20		0.8004	1.4178	62.367	64.053	280.96	282.14
56	$(C_4H_9)_2BOC(CH_3)_3$	(*24*)	198.168	20		0.7998	1.4170	62.309	64.053	280.84	282.14
57	$(C_4H_9)_2BOC_6H_5$	(*52*)	218.158	20		0.8798	1.4760	69.939	69.589	322.00	322.10
58	$(C_4H_9)_2BOCH(CH_3)C_6H_{13}$	(*24*)	254.276	20		0.8099	1.4279	80.758	82.645	363.08	364.54
59	$(C_5H_9)_2BOCH_3$	(*9*)	180.109	20			1.4717			265.07	262.68
60	$(C_5H_{11})_2BOCH_3$	(*9*)	184.141	20			1.4238			262.18	261.54
61	$(CH_3)(C_6H_5)BOC_3H_7$	(*61*)	162.050	25	1.4880	0.8985	1.4902[c]	51.963	52.033	241.49	242.85
62	$(C_2H_5)(C_6H_5)BOC_4H_9$	(*61*)	190.104	25	1.4864	0.8940	1.4886[c]	61.094	61.329	282.99	284.05
63	$(C_6H_5)(o\text{-}CH_3C_6H_4)BOC_3H_7$	(*60*)	238.148	25	1.5440	0.9749	1.5462[c]	77.123	77.324	368.22	369.76
64	$(o\text{-}CH_3C_6H_4)(m\text{-}CH_3C_6H_4)BOC_3H_7$	(*60*)	252.175	25	1.5407	0.9646	1.5429[c]	82.113	82.100	389.08	391.76
65	$(o\text{-}CH_3C_6H_4)(p\text{-}CH_3C_6H_4)BOC_3H_7$	(*60*)	252.175	25	1.5420	0.9648	1.5442[c]	82.260	82.100	389.41	391.76
66	$(o\text{-}CH_3C_6H_4)(p\text{-}ClC_6H_4)BOC_3H_7$	(*60*)	272.597	25	1.5522		1.5544[c]			423.73	422.69
67	$[(C_4H_9)_2BOCH_2\text{-}]_2$	(*38*)	310.158	25	1.4340	0.8266	1.4371[c]	97.715	98.162	445.73	445.80
68	$[(iso\text{-}C_5H_{11})_2BOCH_2\text{-}]_2$	(*38*)	366.266	25	1.4378	0.8267	1.4400[c]	116.257	116.754	527.42	528.20
69	$(C_3H_7)_2BSC_3H_7$	(*48*)	172.153	20		0.8241	1.4546	56.635	57.024	250.41	252.22
70	$(C_3H_7)_2BSC_4H_9$	(*48*)	186.180	20		0.8286	1.4598	61.518	61.672	271.79	278.82
71	$(C_3H_7)_2BSC_6H_5$	(*48*)	206.170	20		0.9252	1.5194	67.679	67.208	313.26	312.78
72	$(C_4H_9)_2BSC_4H_9$	(*48*)	214.234	20		0.8367	1.4548	69.444	70.968	311.67	314.02
73	$(iso\text{-}C_4H_9)_2BSC_4H_9$	(*48*)	214.234	20		0.8213	1.4572	71.068	70.968	312.18	314.02
74	$(iso\text{-}C_5H_{11})_2BSC_4H_9$	(*48*)	242.288	20		0.8219	1.4551	79.997	80.264	352.55	355.22
75	$(C_6H_5)_2BSC_4H_9$	(*48*)	254.214	20		1.001	1.5871	85.361	84.112	403.46	400.24
76	$CH_2{=}CHCH_2B(OCH_2CH{=}CH_2)_2$	(*51*)	166.039	20		0.8931	1.4352	48.532	49.716	238.30	237.85
77	$CH_2{=}CHCH_2B(OC_4H_9)_2$	(*51*)	198.125	20		0.8413	1.4230	59.969	59.968	281.93	281.47
78	$C_4H_9BOCH_2CH_2O$	(*38*)	127.990	25	1.4129	0.9141	1.4151[c]	34.907	35.150	181.12	184.80
79	$C_4H_9B(OC_4H_9)_2$	(*7*)	214.168	20		0.8300	1.4169	64.876	65.094	303.46	303.28
80	$C_4H_9B(OC_8H_{17})_2$	(*7*)	326.384	20		0.8036	1.4312	105.175	102.278	467.12	468.08
81	$C_5H_9B(OCH_3)_2$	(*9*)	142.017	20			1.4300			203.08	200.85
82	$C_5H_{11}B(OCH_3)_2$	(*9*)	144.033	20			1.4025			202.01	200.28
83	$C_6H_5B(OCH_3)_2$	(*59*)	149.996	25	1.4926	1.0024	1.4948[c]	43.458	43.777	224.21	222.79
84	$C_6H_5B(OC_2H_5)_2$	(*7*)	178.050	20		0.9540	1.4785	52.877	53.073	263.25	263.99
85	$C_6H_5B(OCH_2CH_2Cl)_2$	(*12*)	246.948	16	1.5153[c]	1.102	1.5135	67.608	62.741	373.76	369.85
86	$C_6H_5B(OCH_2CCl_3)_2$	(*7*)	384.744	20			1.5333			589.93	581.57
87	$C_6H_5B(OC_3H_7)_2$	(*59*)	206.104	25	1.4738	0.9297	1.4760[c]	62.280	62.369	304.21	305.19
88	$C_6H_5B[OCH(CH_3)_2]_2$	(*12*)	206.104	20		0.9283	1.4632	61.174	62.369	301.57	305.19
89	$C_6H_5B(OC_4H_9)_2$	(*7*)	234.158	20		0.9245	1.4751	71.323	71.665	345.41	346.39
90	$C_6H_5B[OCH_2CH(CH_3)_2]_2$	(*7*)	234.158	20		0.9163	1.4711	71.441	71.665	344.47	346.39

91	$C_6H_5B[OC(CH_3)_3]_2$	(7)	234.158	20		0.9053	1.4635	71.306	71.665	342.69	346.39
92	$C_6H_5B[OCH(CH_3)C_2H_5]_2$	(7)	234.158	20		0.9073	1.4658	71.452	71.665	343.23	346.39
93	$C_6H_5B[OCH_2C(CH_3)_3]_2$	(7)	262.212	20		0.9003	1.4678	80.933	80.961	384.87	387.59
94	$C_6H_5B(OCH_2C_6H_5)_2$	(12)	302.192	16	1.5763[c]	1.110	1.5745	90.130	92.289	475.80	470.30
95	$C_6H_5B(OC_8H_{17})_2$	(12)	346.374	16	1.4718[c]	0.895	1.4700	108.331	108.849	509.17	511.19
96	$C_6H_5B[OCH(CH_3)C_6H_{13}]_2$	(7)	346.374	20		0.8847	1.4666	108.555	108.849	507.99	511.19
97	$C_6H_{11}B[OCH_2CH(CH_3)_2]_2$	(47)	240.206	20		0.8710	1.4383	72.438	72.178	345.49	345.88
98	o-$CH_3C_6H_4B(OCH_3)_2$	(59)	164.023	25	1.4870	0.9798	1.4892[c]	48.147	48.553	244.26	244.79
99	m-$CH_3C_6H_4B(OCH_3)_2$	(59)	164.023	25	1.4926	0.9846	1.4948[c]	48.381	48.553	245.18	244.79
100	p-$CH_3C_6H_4B(OCH_3)_2$	(59)	164.023	25	1.4948	0.9860	1.4970[c]	48.495	48.553	245.54	244.79
101	o-$CH_3C_6H_4B(OC_2H_5)_2$	(59)	192.077	25	1.4737	0.9351	1.4759[c]	57.696	57.849	283.49	285.99
102	m-$CH_3C_6H_4B(OC_2H_5)_2$	(59)	192.077	25	1.4796	0.9388	1.4818[c]	58.080	57.849	284.62	285.99
103	p-$CH_3C_6H_4B(OC_2H_5)_2$		192.077	25	1.4793	0.9389	1.4815[c]	58.043	57.849	284.56	285.99
104	o-$CH_3C_6H_4B(OC_3H_7)_2$	(59)	220.131	25	1.4721	0.9206	1.4743[c]	66.970	67.145	324.54	327.19
105	m-$CH_3C_6H_4B(OC_3H_7)_2$	(59)	220.131	25	1.4757	0.9226	1.4779[c]	67.261	67.145	325.33	327.19
106	p-$CH_3C_6H_4B(OC_3H_7)_2$	(59)	220.131	25	1.4770	0.9225	1.4792[c]	67.425	67.145	325.62	327.19
107	o-$CH_3C_6H_4B(OC_4H_9)_2$	(59)	248.185	25	1.4706	0.9099	1.4728[c]	76.184	76.441	365.53	368.39
108	m-$CH_3C_6H_4B(OC_4H_9)_2$	(59)	248.185	25	1.4744	0.9126	1.4766[c]	76.484	76.441	366.47	368.39
109	p-$CH_3C_6H_4B(OC_4H_9)_2$	(59)	248.185	25	1.4758	0.9127	1.4780[c]	76.669	76.441	366.82	368.39
110	$C_8H_{17}B(OC_8H_{17})_2$	(7)	382.492	20		0.824	1.4288	119.620	120.870	546.50	550.48
111	α-$C_{10}H_7B(OC_4H_9)_2$	(37)	284.218	27		1.5322	1.5353[c]			436.36	437.11
112	$C_3H_7B(SC_4H_9)_2$	(50)	232.273	20		0.9106	1.4956	74.462	74.276	347.39	346.45
113	$C_4H_9B(SC_4H_9)_2$	(50)	246.300	20		0.9045	1.4936	79.219	78.924	367.87	367.05
114	iso-$C_5H_{11}B(SC_4H_9)_2$	(50)	260.327	20		0.8988	1.4871	83.317	83.572	387.13	387.65
115	$C_6H_5B(SC_4H_9)_2$	(50)	266.290	20		0.9865	1.5464	85.526	85.496	411.79	410.16
116	$(ClCH{=}CH)_2BNCH_2CH_2CH_2CH_2CH_2$	(5)	217.953	20		1.077	1.5410	63.592	59.170	335.87	329.10
117	$(CH_2{=}CHCH_2)_2BNHC_4H_9$	(51)	165.098	20		0.8338	1.4697	55.214	56.016	242.64	240.46
118	$(C_3H_7)_2BNHCH_2CH(CH_3)_2$	(52)	169.130	20		0.7724	1.4250	55.990	56.972	241.01	242.88
119	$(C_3H_7)_2BNHC_6H_5$	(52)	189.120	20		0.8859	1.5050	63.318	62.508	284.63	282.84
120	$(C_4H_9)_2BNH_2$	(48)	141.076	20		0.7655	1.4278	47.395	47.486	201.43	203.42
121	$(C_4H_9)_2BNHC_4H_9$	(52)	197.184	20		0.7758	1.4302	65.685	66.268	282.01	284.08
122	$(C_4H_9)_2BNHC_6H_5$	(48)	217.174	20		0.8808	1.5001	72.531	71.804	325.78	324.04
123	$[(C_4H_9)_2BNH-]_2$	(48)	280.136	20		0.8083	1.4495	93.048	93.443	406.06	409.14
124	$(C_4H_9)_2BNHNHC_6H_5$	(48)	232.190	20		0.9150	1.5132	76.296	75.554	351.35	348.11
125	$[(C_4H_9)_2BNHCH_2CH_2CH_2-]_2$	(48)	364.298	20		0.8183	1.4568	121.200	121.185	530.71	532.09
126	$C_3H_7BNHCH_2CH_2NH$	(50)	111.995	20		0.9406	1.4941	34.669	34.933	167.33	168.09
127	iso-$C_5H_{11}BNHCH_2CH_2NH$	(50)	140.049	20		0.9165	1.4872	43.964	44.229	208.28	209.29
128	iso-$C_5H_{11}B(NHC_2H_5)_2$	(49)	170.119	20		0.8040	1.4337	55.069	55.581	243.90	245.37
129	iso-$C_5H_{11}B[N(C_2H_5)_2]_2$	(49)	226.227	20		0.8192	1.4488	74.042	74.553	327.76	324.29
130	iso-$C_5H_{11}B[NHCH_2CH(CH_3)_2]_2$	(49)	226.227	20		0.8028	1.4381	73.989	71.753	325.34	327.77
131	iso-$C_5H_{11}B(NHC_6H_5)_2$	(49)	266.207	20		0.9954	1.5700	87.744	85.245	417.94	407.69
132	$C_6H_5B(NHC_2H_5)_2$	(46)	176.082	20		0.924	1.5120	57.183	57.504	266.24	267.88
133	$C_6H_5B[N(C_2H_5)_2]_2$	(50)	232.190	20		0.9406	1.5183	74.839	76.476	352.53	346.80
134	$(C_2H_5)_2NB(OC_4H_9)_2$	(23)	229.184	20		0.856	1.4233	68.221	68.540	326.20	324.62
135	$(C_4H_9)_2NB(OC_4H_9)_2$	(23)	285.292	21	1.4309		1.4313[c]			408.34	407.02
136	$C_6H_{11}B[N(C_2H_5)_2][OCH_2CH(CH_3)_2]$	(47)	239.222	20		0.8750	1.4500	73.472	74.583	346.87	346.08
137	$[(C_2H_5)_2N]_2BOC_4H_9$	(22)	228.200	20		0.8419	1.4348	70.701	70.945	327.42	324.83

(Continued on page 248)

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

No.	Compound	Lit. Ref.	M	t	n'_D	d'_4	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.
138	$[(C_4H_9)_2N]_2BOC_4H_9$	(22)	340.416	20			1.4470			492.58	489.63
139	$[(C_2H_5)_2N](C_4H_9O)BCl$	(23)	191.525	20			1.4275			273.40	272.78
140	$(CH_3NH)_3B$	(4)	100.973	20		0.8871	1.4465	30.383	30.949	146.06	144.85
141	$(C_2H_5NH)_3B$	(4)	143.054	20		0.833	1.4380	45.082	44.893	205.71	206.65
142	$[(C_2H_5)_2N]_3B$	(22)	227.216	20		0.826	1.4450	73.212	73.351	328.33	325.03
143	$[(CH_3)_2CHNH]_3B$	(4)	185.135	20		0.8000	1.4267	59.380	58.837	264.13	368.45
144	$(C_4H_9NH)_3B$	(4)	227.216	20		0.8347	1.4462	72.619	72.781	328.60	330.25
145	$[C_2H_5(CH_3)CHNH]_3B$	(4)	227.216	20		0.8186	1.4355	72.501	72.781	326.17	330.25
146	$[(CH_3)_3CNH]_3B$	(4)	227.216	20		0.7971	1.4272	73.218	72.781	324.28	330.25
147	$[(C_4H_9)_2N]_3B$	(22)	395.540	20		0.8399	1.4578	128.452	129.127	576.62	572.23
148	$(C_6H_5CH_2NH)_3B$	(4)	329.267	20		1.0479	1.5805	104.645	103.370	520.41	526.12
149	$C_4H_9OBF_2$	(33)	121.936	22	1.3858	1.122	1.3867[c]	25.562	25.407	169.09	162.09
150	$C_2H_5OBCl_2$	(2)	126.796	20		1.125	1.3968	27.130	26.640	177.11	179.54
151	$CH_2ClCH_2OBCl_2$	(14)	161.245	18	1.4438[c]	1.358	1.4429	31.528	31.474	232.66	232.47
152	$C_3H_7OBCl_2$	(20)	140.823	20		1.138	1.4094	30.620	31.288	198.48	200.14
153	$CH_2ClCH_2CH_2OBCl_2$	(2)	175.272	20		1.293	1.4432	35.951	36.122	252.95	253.07
154	$C_4H_9OBCl_2$	(20)	154.850	20		1.079	1.4161	36.022	35.936	219.28	220.74
155	$(CH_3)_2CHCH_2OBCl_2$	(20)	154.850	20		1.046	1.4088	36.584	35.936	218.15	220.74
156	$CH_2ClCH_2CH_2CH_2OBCl_2$	(14)	189.299	20		1.254	1.4522	40.739	40.770	274.90	273.67
157	$C_5H_{11}OBCl_2$	(2)	168.877	20		1.056	1.4170	40.216	40.584	239.30	241.34
158	$(CH_3)_3CCH_2OBCl_2$	(20)	168.877	20		1.032	1.4097	40.518	40.584	238.07	241.34
159	$CH_3ClCH_2CH_2CH_2CH_2OBCl_2$	(2)	203.326	20		1.228	1.4533	44.778	45.418	295.49	294.27
160	$C_8H_{17}OBCl_2$	(20)	210.958	20		1.015	1.4316	53.865	54.528	302.01	303.14
161	$(C_2H_5O)_2BCl$	(2)	136.401	20		0.972	1.3878	33.098	32.443	189.30	190.18
162	$(CH_2ClCH_2O)_2BCl$	(14)	205.099	18	1.4560[c]	1.320	1.4551	42.278	42.111	298.73	296.04
163	$(C_3H_7O)_2BCl$	(34)	164.455	20		0.959	1.4028	41.829	41.739	230.70	231.38
164	$(CH_2ClCH_2CH_2O)_2BCl$	(2)	233.353	20		1.240	1.4564	51.194	51.407	339.86	337.24
165	$(C_4H_9O)_2BCl$	(18)	192.509	20		0.941	1.4141	51.132	51.035	272.23	272.58
166	$[(CH_3)_2CHCH_2O]_2BCl$	(18)	192.509	20		0.938	1.4056	50.368	51.035	270.59	272.58
167	$[C_2H_5CH(CH_3)O]_2BCl$	(34)	192.509	20		0.924	1.4017	50.697	51.035	269.84	272.58
168	$(CH_2ClCH_2CH_2CH_2O)_2BCl$	(2)	261.407	20		1.181	1.4622	60.873	60.703	382.23	378.44
169	$(C_5H_{11}O)_2BCl$	(2)	220.563	20		0.933	1.4202	59.849	60.331	313.24	313.78
170	$[(CH_3)_3CCH_2O]_2BCl$	(34)	220.563	20		0.906	1.4102	60.343	60.331	311.04	313.78
171	$(CH_2ClCH_2CH_2CH_2CH_2O)_2BCl$	(2)	289.461	20		1.127	1.4621	70.623	69.999	423.22	419.64
172	$[(CH_3)_3CCH(CH_3)O]_2BCl$	(34)	248.617	20		0.901	1.4165	69.318	69.627	352.17	354.98
173	$(C_8H_{17}O)_2BCl$	(34)	304.725	20		0.906	1.4380	88.292	88.219	438.19	437.38
174	$[C_6H_{13}CH(CH_3)O]_2BCl$	(34)	304.725	20		0.897	1.4277	87.347	88.219	435.06	437.38
175	$(CH_3O)_3B$	(19)	103.925	20		0.928	1.3610	24.777	24.302	141.44	139.02
176	$(C_2H_5O)_3B$	(11)	146.006	20		0.8635	1.3741	38.624	38.246	200.63	200.82
177	$(CH_2ClCH_2O)_3B$	(31)	249.353	20		1.2780	1.4556	52.998	52.748	362.96	359.61
178	$(CHCl_2CH_2O)_3B$	(2)	352.700	20		1.496	1.4836	67.403	67.250	523.27	518.40
179	$(CH_3OCH_2CH_2O)_3B$	(56)	236.087	28	1.4023[c]	1.0096	1.4059	56.987	57.062	331.91	329.80
180	$(CH_2{=}CHCH_2O)_3B$	(25)	182.039	25	1.4230	0.9280	1.4252[c]	49.952	50.756	259.44	258.99
181	$(C_3H_7O)_3B$	(3)	188.087	20		0.8576	1.3948	52.556	52.190	262.34	262.62
182	$[(CH_3)_2CHO]_3B$	(35)	188.087	20			1.4057			264.39	262.62

183	$(CH_2ClCH_2CH_2O)_3B$	(2)	291.434	20		1.190	1.4571	66.711	66.692	424.65	421.41
184	$(CH_2ClCHClCH_2O)_3B$	(2)	394.781	19	1.4956[c]	1.419	1.4952	81.216	81.194	590.28	580.20
185	$(CHCl_2CH_2O)_3B$	(31)	394.781	20		1.4028	1.4883	81.124	81.194	587.55	580.20
186	$(C_4H_9O)_3B$	(3)	230.168	20		0.8567	1.4080	66.280	66.134	324.08	324.42
187	$[(CH_3)_2CHCH_2CH_2O]_3B$	(35)	230.168	20		0.842	1.4035	66.781	66.134	323.04	324.42
188	$[C_2H_5CH(CH_3)O]_3B$	(35)	230.168	25	1.3946[c]	0.8290	1.3968	66.503	66.134	321.50	324.42
189	$[(CH_3)_3CO]_3B$	(39)	230.168	20		0.8153	1.3879	66.601	66.134	319.45	324.42
190	$(CH_2ClCH_2CH_2CH_2O)_3B$	(14)	333.515	20	1.4618	1.350	1.4622[c]	67.942	80.636	487.67	483.21
191	$(C_5H_{11}O)_3B$	(35)	272.249	20		0.8549	1.4190	80.421	80.078	386.32	386.22
192	$[(CH_3)_2CHCH_2CH_2O]_3B$	(11)	272.249	20		0.8514	1.4156	80.177	80.078	385.40	386.22
193	$[(CH_3)_2C(C_2H_5)O]_3B$	(39)	272.249	20		0.8482	1.4124	79.934	80.078	384.52	386.22
194	$[C_3H_7CH(CH_3)O]_3B$	(56)	272.249	27	1.4044[c]	0.8298	1.4075	80.309	80.078	383.19	386.22
195	$[(CH_3)_2CHCH(CH_3)O]_3B$	(20)	272.249	20		0.844	1.4080	79.577	80.078	383.33	386.22
196	$[(C_2H_5)_2CHO]_3B$	(56)	272.249	28	1.4061[c]	0.8337	1.4097	80.230	80.078	383.79	386.22
197	$[C_2H_5CH(CH_3)CH_2O]_3B$	(56)	272.249	28	1.4134[c]	0.8470	1.4170	80.218	80.078	385.78	386.22
198	$(CH_2ClCH_2CH_2CH_2CH_2O)_3B$	(2)	375.596	20		1.090	1.4626	94.837	94.580	549.35	545.01
199	$(C_6H_{13}O)_3B$	(56)	314.330	28	1.4214[c]	0.8471	1.4250	94.177	94.022	447.92	448.02
200	$[C_4H_9CH(CH_3)O]_3B$	(56)	314.330	25	1.4138[c]	0.7693	1.4160	102.058	80.636	445.09	448.02
201	$[C_3H_7CH(CH_3)CH_2O]_3B$	(56)	314.330	27	1.4230[c]	0.8520	1.4261	93.947	94.022	448.27	448.02
202	$[(CH_3)_2CHCH_2CH(CH_3)O]_3B$	(58)	314.330	24.8	1.4096	0.823	1.4118[c]	94.547	94.022	443.77	448.02
203	$[(C_2H_5)_2CHCH_2O]_3B$	(56)	314.330	28	1.4247[c]	0.8572	1.4283	93.705	94.022	448.96	448.02
204	$[(CH_3)_3CCH(CH_3)O]_3B$	(20)	314.330	20		0.841	1.4151	93.615	94.022	444.81	448.02
205	$(o\text{-}CH_3C_6H_4O)_3B$	(58)	332.219	22	1.5537[c]	1.079	1.5546	98.632	97.070	516.47	510.29
206	$(C_7H_{15}O)_3B$	(3)	356.411	20		0.8398	1.4280	109.188	107.966	508.95	509.82
207	$[C_6H_5CH(CH_3)O]_3B$	(19)	374.300	4	1.5420	1.064	1.5349[c]	110.714	111.014	574.51	572.09
208	$(C_8H_{17}O)_3B$	(3)	398.492	20		0.8548	1.4360	121.890	121.910	572.24	571.62
209	$[C_4H_9CH(C_2H_5)CH_2O]_3B$	(58)	398.492	24	1.4363[c]	0.857	1.4381	121.650	121.910	573.07	571.62
210	$[C_6H_{13}CH(CH_3)O]_3B$	(17)	398.492	4	1.4362[c]	0.8642	1.4289	120.613	121.910	569.41	571.62
211	$(C_{10}H_{21}O)_3B$	(3)	482.654	20		0.8581	1.4440	149.409	149.798	696.95	695.22
212	$(C_{12}H_{25}O)_3B$	(58)	566.816	27	1.4463[c]	0.845	1.4494[c]	178.982	177.676	821.54	818.82
213	$C_4H_9OBOCH_2CH_2O$	(38)	143.990	25	1.4280	0.9976	1.4302[c]	37.134	36.190	205.93	205.94
214	$C_5H_{11}OBOCH_2CH_2O$	(38)	158.017	27	1.4343		1.4374[c]			227.13	226.54
215	$[CH_2(COOC_2H_5)O]_3B$	(16)	320.120	20		1.160	1.4290	71.144	70.910	457.45	455.55
216	$[CH_3CH(COOC_2H_5)O]_3B$	(16)	362.201	20		1.070	1.4215	85.931	84.854	514.87	517.35
217	$[CH_3(COOC_2H_5)CH_2O]_3B$	(16)	362.201	20		1.108	1.4331	84.976	84.854	519.07	517.35
218	$[CH_2(COOC_2H_5)CH(COOC_2H_5)O]_3B$	(16)	578.396	20		1.167	1.4408	130.829	131.462	833.35	833.88
219	$CH_3OBOC_6H_4(o)O$	(21)	149.953	20		1.1890	1.5059	37.463	37.078	225.81	225.30
220	$C_2H_5OBOC_6H_4(o)O$	(21)	163.980	20		1.1316	1.4960	42.331	41.726	245.31	245.90
221	$C_3H_7OBOC_6H_4(o)O$	(21)	178.007	20		1.0937	1.4900	47.056	46.374	265.23	266.50
222	$C_4H_9OBOC_6H_4(o)O$	(21)	192.034	20		1.0707	1.4891	51.773	51.022	285.96	287.10
223	$(CH_3)_2CHCH_2OBOC_6H_4(o)O$	(21)	192.034	20		1.0558	1.4846	52.094	51.022	285.09	287.10

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

No.	Compound	Lit. 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.
224	$C_2H_5CH(CH_3)OBOC_6H_4(o)O$	(*21*)	192.034	20		1.0704	1.4853	51.445	51.022	285.23	287.10
225	$C_5H_{11}OBOC_6H_4(o)O$	(*21*)	206.061	20		1.0578	1.4891	56.232	55.670	306.84	307.70
226	$C_8H_{17}OBOC_6H_4(o)O$	(*21*)	248.142	20		1.0158	1.4856	70.086	69.614	368.64	369.50
227	$C_4H_9SBOC_6H_4(o)O$	(*21*)	208.100	20			1.5334			319.10	318.98
228	$C_8H_{17}SBOC_6H_4(o)O$	(*21*)	264.208	20			1.5198			401.54	401.38
229	$(C_2H_5)_2NBOC_6H_4(o)O$	(*21*)	191.050	20			1.5061			287.74	287.30
230	$(C_4H_9)_2NBOC_6H_4(o)O$	(*21*)	247.158	20			1.4971			370.02	367.70
231	$(CH_3)_3CBOC_6H_4(o)O$	(*21*)	176.034	30	1.4879[c]	1.016	1.4924	49.910	49.982	262.71	265.96
232	$(C_2H_5BO)_3$	(*40*)	167.646	25	1.3958	0.8963	1.3980[c]	44.922	44.791	234.37	241.02
233	$(CH_2=CHCH_2BO)_3$	(*51*)	203.679	20		0.9318	1.4435	58.006	57.301	294.01	299.19
234	$(C_3H_7BO)_3$	(*40*)	209.727	25	1.4080	0.8746	1.4102[c]	59.157	58.735	295.76	302.82
235	$[(CH_3)_2CHBO]_3$	(*40*)	209.727	25	1.4305	0.8558	1.4327[c]	63.371	58.735	300.48	302.82
236	$(C_4H_9BO)_3$	(*40*)	251.808	25	1.4175	0.8718	1.4197[c]	72.712	72.769	357.49	364.62
237	$[(CH_3)_2CHCH_2BO]_3$	(*40*)	251.808	25	1.4127	0.8540	1.4149[c]	73.477	72.769	356.28	364.62
238	$(C_5H_{11}BO)_3$	(*40*)	293.889	25	1.4275	0.8675	1.4297[c]	87.070	86.623	420.17	426.42
239	$(C_6H_{13}BO)_3$	(*40*)	335.970	25	1.4337	0.8654	1.4359[c]	101.041	100.567	482.42	488.22
240	$(CH_3BNH)_3$	(*30*)	122.613	20		0.8681	1.4404	37.254	38.210	176.61	186.80
241	$(C_2H_5BNH)_3$	(*30*)	164.694	20		0.8587	1.4344	49.987	52.154	236.24	248.60
242	$(C_3H_7BNH)_3$	(*30*)	206.775	20		0.8471	1.4484	65.396	66.104	299.49	310.40
243	$[(CH_3)_2CHBNH]_3$	(*30*)	206.775	20		0.8631	1.4434	63.563	66.104	298.46	310.40
244	$[(CH_3)_2CHCH_2CH_2BNH]_3$	(*49*)	290.937	20		0.8485	1.4538	92.819	93.986	422.96	434.00
245	$(C_2H_5BNCH_3)_3$	(*53*)	206.775	22.5	1.4791		1.4802[c]			306.07	305.18
246	$(CH_2=CHCH_2BNCH_3)_3$	(*53*)	242.808	22.5	1.5047		1.5058[c]			365.62	363.35
247	$(C_4H_9BNCH_3)_3$	(*53*)	290.937	22.5	1.4759		1.4770[c]			429.71	428.78
248	$[(C_4H_9)_2B_3Cl](NCH_3)_3$	(*53*)	269.278	22.5	1.4807		1.4818[c]			399.06	398.08
249	$(C_4H_9B_2Cl_2)(NCH_3)_3$	(*53*)	247.619	22.5	1.4876		1.4887[c]			368.63	367.38
250	$(CH_3NHBNCH_3)_3$	(*4*)	209.742	20		1.016	1.5082	61.558	62.493	316.33	312.63
251	$(C_2H_5NHBNC_2H_5)_3$	(*4*)	293.904	20		0.933	1.4826	89.901	90.381	435.74	436.23
252	$[(CH_3)_2CHNHBNCH(CH_3)_2]_3$	(*4*)	378.066	20		0.882	1.4628	118.017	118.269	553.03	559.83
253	$(C_4H_9NHBNC_4H_9)_3$	(*4*)	462.228	20		0.900	1.4730	144.076	146.157	680.86	683.43
254	$[C_2H_5CH(CH_3)NHBNCH(CH_3)C_2H_5]_3$	(*4*)	462.228	20		0.892	1.4695	144.445	146.157	679.24	683.43
255	$[(CH_3)_3CNHBNC(CH_3)_3]_3$	(*4*)	462.228	20		0.883	1.4631	144.206	146.157	676.29	683.43
256	$(C_6H_5CH_2NHBNCH_2C_6H_5)_3$	(*4*)	666.330	20		1.156	1.642	208.188	208.028	1094.11	1055.18
257	$(CH_3OBNCH_3)_3$	(*6*)	212.694	23	1.4610		1.4624[c]			311.04	306.80
258	$(C_2H_5OBNCH_3)_3$	(*6*)	254.775	22.5	1.4540		1.4511[c]			369.70	368.60
259	$(C_3H_7OBNCH_3)_3$	(*6*)	296.856	22	1.4561		1.4570[c]			432.52	430.40
260	$[(CH_3)_2CHOBNCH_3]_3$	(*6*)	296.856	23	1.4460		1.4474[c]			429.67	430.40
261	$(C_4H_9OBNCH_3)_3$	(*6*)	338.937	23	1.4572		1.4586[c]			494.37	492.20

[a] $MR_L = \frac{n^2 - 1}{N^2 + 2}\frac{M}{d}$. [b] $MR_E = Mn_D^{20}$. [c] Corrected by use of coefficient −0.00045°/° C.

impartial comparison of the four systems, the coefficient of variation for each is shown:

	Refractivity (Lorenz-Lorentz)	Refraction Product (Eisenlohr)
Atomic (and group)	0.254	0.086
Bond	0.196	0.049

The superiority of the empirical Eisenlohr system over that of Lorenz-Lorentz is thus indicated to be even greater than that of the bond over the atomic system.

A cursory glance at the data for the 12 tolyl derivatives (Nos. 98 to 109) shows unmistakable dependence of the numerical values for the $C_{al}—C_{ar}$ bond on its ring position. It seems highly probable that future investigation based on a comprehensive study of aromatic compounds will substantiate and amplify this observation.

After the completion of the above work, least squares computations were repeated in which 30 boroxin and borazine derivatives (Nos. 232 to 261) were added to the first 231 compounds of Table II in order to ascertain whether distinctions should be made between cyclic and acyclic B—O and B—N bonds. The results indicated small differences but were so inconclusive that no purpose appears to be served at present in assigning special values to the bonds of ring atoms. Hence data for these cyclic derivatives are listed separately in Table II, and the parameters of Table I were tested further by calculating coefficients of variation for the cyclic compounds alone:

Refractivity (Lorenz-Lorentz)	Refraction Product (Eisenlohr)
0.103	0.073

Omitting Compound 256, for which there is a large discrepancy in the calculated Eisenlohr refraction product, the coefficients are 0.103 and 0.049, respectively.

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