SHORT COMMUNICATIONS

THE INFRA-RED SPECTRA OF SOME MIXED BORATE ESTERS*

By R. L. WERNER† and K. G. O'BRIEN‡

In a recent paper|| the infra-red spectra of a series of borate esters have been reported and a strong band at 1340 ± 10 cm^{-1} has been assigned to the B—O stretching frequency.

In connection with work on Boroxole compounds, which will be presented separately, it has been found possible to prepare a series of mixed borate esters of the general formula $(R_1O)(R_2O)_2B$ and the infra-red spectra of these compounds have been examined. In Table 1 the frequencies of the absorption peaks (in wave numbers) of these compounds are given and in Figure 1 the

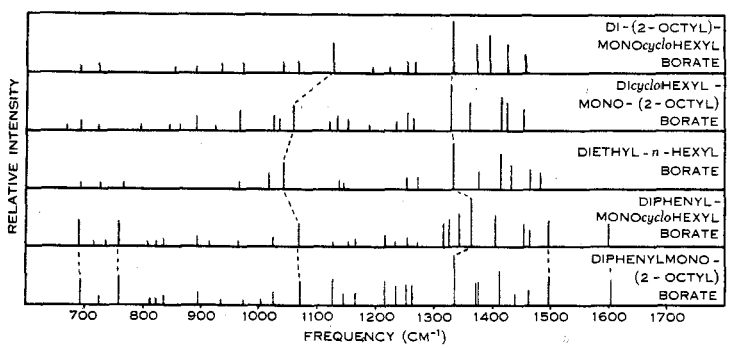

Fig. 1.—The relation of corresponding bands in the infra-red spectra of some asymmetrical borate esters.

relationship of bands is shown. Comparison of these spectra with those obtained earlier shows a similar strong band due to the B—O link, within the range previously reported, except in the case of diphenylmono*cyclo*hexyl borate which is somewhat higher at 1363 cm^{-1}. A tendency of the aryl esters to give rise to a somewhat high value is apparent also in the earlier data|| although the diphenyl mono-(2-octyl)borate now reported is anomalous in this respect.

* Manuscript received August 15, 1955.

† Department of Physical Chemistry, N.S.W. University of Technology, Broadway, Sydney.

‡ Department of Chemistry, Broken Hill Technical College, Broken Hill.

|| Werner, R. L., and O'Brien, K. G. (1955).—*Aust. J. Chem.* **8**: 355.

It is a reasonable inference from the results obtained in the two series of compounds studied, that the B—O band would give rise to a similar band in esters

TABLE 1

THE INFRA-RED SPECTRA OF SOME BORATE ESTERS

Samples were run as capillary film

Di-(2-octyl)-mono-*cyclo*hexyl Borate	Di*cyclo*hexyl-mono-(2-octyl) Borate	Diethyl *n*-Hexyl Borate	Diphenyl-mono-*cyclo*hexyl Borate	Diphenyl-mono-(2-octyl) Borate	Assignment
			1600 (s)	1601 (s)	Phenyl
			1496 (s)	1498 (s)	Phenyl
		1482 (m)	1466 (w)	1460 (m)	
1458 (m)	1452 (m)	1466 (m)	1451 (m)	1440 (m)	C—H bending
1426 (m)	1428 (ms)	1431 (ms)			
1397 (s)	1416 (s)	1414 (s)	1405 (s)	1411 (s)	
1376 (m)	1361 (ms)	1379 (w)		1376, 1371 (ms)	
1332 (vs)	1330 (vs)	1333 (vs)	1363 (vs)	1336 (vs)	B—O stretching
1268 (w)	1266 (w)		1343 (s)	1262, 1252 (m)	
1254 (w)	1255 (m)		1327, 1318 (ms)	1235 (m)	
1225 (w)	1236 (w)	1271 (w)	1272, 1256 (w)	1216 (ms)	
		1252 (w)	1236 (w)		
1194 (w)	1190 (w)		1216 (m)		
	1152 (mw)	1146 (w)	1165, 1152 (w)	1165, 1145 (w)	
	1133 (m)	1138 (w)	1129 (w)	1127 (m)	
	1120 (mw)				
1129 (ms)	1060 (ms)	1040 (ms)	1069 (ms)	1070 (ms)	C—O stretching
1068 (mw)					
1040 (w)	1035 (w)		1035 (w)		
	1025 (mw)	1019 (w)	1023 (mw)	1023 (m)	
				1003 (w)	
971 (w)	968 (m)	967 (w)	965 (w)	973 (w)	
933 (w)	925 (w)		925, 915 (w)	931 (w)	
890 (w)	891 (m)		895 (mw)	896 (mw)	
851 (w)	852, 845 (w)		836, 821, 810 (w)	835, 821, 811 (w)	
	797, 785 (w)		759 (s)	759 (s)	Phenyl
723 (w)	724 (w)	769, 728 (w)	736, 718 (w)	723 (m)	
690 (w)	692 (w) 670 (w)	691 (w)	691 (s)	691 (s)	Phenyl

of the type $R_1R_2R_3O_3B$ and in other compounds in which the BO_3 group is presumed to exist, such as the trialkoxyboroxoles.