# Molecular Polarisability. The Electronic Anisotropy of the $C_{Ar}$ -CF<sub>3</sub> Group

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Molar Kerr constants and apparent dipole moments at 25° are recorded for the molecules  $p-XC_{B}H_{4}$ ·CF<sub>a</sub> (X = H, F, CI, CF<sub>3</sub>), C<sub>6</sub>F<sub>5</sub>·CF<sub>3</sub>, and m-C<sub>6</sub>H<sub>4</sub>·(CX<sub>3</sub>)<sub>2</sub> (X = H, F) in carbon tetrachloride and the data have been analysed to provide the anisotropic electron polarisability for the  $C_{Ar}$ -CF<sub>3</sub> group. The results are compared with those for  $C_{Ar}$ -CX<sub>3</sub> (X = H, CH<sub>3</sub>, CI) for evidence of hyperconjugation.

PREVIOUSLY <sup>1,2</sup> we have investigated the mesomeric and hyperconjugative effects of  $C_{Ar}$ -CX<sub>3</sub> systems (X = H, Me, Cl). In this context the  $C_{Ar}$ -CF<sub>3</sub> group is of interest since there is much discussion in the literature<sup>3</sup> on the existence and magnitude of any interaction between this group and the benzene ring. We here report

 <sup>1</sup> M. J. Aroney, K. E. Calderbank, R. J. W. Le Fèvre, and R. K. Pierens, J. Chem. Soc. (B), 1969, 159.
 <sup>2</sup> M. J. Aroney, K. E. Calderbank, R. J. W. Le Fèvre, and R. K. Pierens, J. Chem. Soc. (B), 1970, 1120.
 <sup>3</sup> J. D. Roberts, R. L. Webb, and E. A. McElhill, J. Amer. Chem. Soc., 1950, 72, 408; W. A. Sheppard, Trans. New York Acad. Sci., 1967, 29, 700; R. T. C. Brownlee, R. E. J. Hutchinson, A. R. Katritzky, T. T. Tidwell, and R. D. Topsom, J. Amer. Chem. Soc., 1968, 90, 1757; G. R. Howe, J. Chem. Soc. (B), 1971, 984. 984.

the anisotropic electron polarisability of the aromatic trifluoromethyl substituent.

## EXPERIMENTAL

Materials, Apparatus, etc.-The solutes were dried and redistilled immediately before use; the b.p.s being in accord with literature values. Apparatus, techniques, and symbols used are given in refs. 4-6. Sulphur-free carbon

<sup>4</sup> R. J. W. Le Fèvre, 'Dipole Moments,' Methuen, London,

<sup>•</sup> R. J. W. Le Fèvre, <sup>•</sup> Dipole Moments, <sup>•</sup> Methuen, London, 3rd edn., 1953. <sup>5</sup> C. G. Le Fèvre and R. J. W. Le Fèvre, (a) Rev. Pure Appl. Chem. (Australia), 1955, **5**, 261; (b) Ch. XXXVI in 'Physical Methods of Organic Chemistry,' ed. A. Weissberger, Interscience, New York, 3rd edn., vol. I, p. 2459. <sup>6</sup> R. J. W. Le Fèvre and G. L. D. Ritchie, J. Chem. Soc., 1062, 4032.

1963, 4933.

tetrachloride was fractionated and dried with calcium chloride, the following solvent constants apply at 25°:  $\varepsilon_1 = 2.2270$ ;  $d_1 = 1.58454$ ;  $(n_1)_D = 1.4575$ ;  $10^7(B_1)_D =$ 0.083;  $10^{14}(_{\rm S}K_1) = 0.894$ . N.m.r. spectra were recorded at 40 °C on a Varian A60 spectrometer, tetramethylsilanc being used as internal reference.

*Previous Measurements.*—Apart from *m*-xylene<sup>7</sup> and *p*-dichlorobenzene<sup>8</sup> the molar Kerr constants for these compounds have not previously been recorded as solutes in carbon tetrachloride, nor does McClellan<sup>9</sup> list their dipole moments in this solvent.

#### DISCUSSION

The determination of molecular polarisabilities  $b_1$ ,  $b_2$ , and  $b_3$  in the general case requires three equations (e.g. 22, 23, and 30 on pp. 44-47 of ref. 10) and from these molecular polarisabilities, bond or group polarisabilities  $b_{\rm L}$ ,  $b_{\rm T}$  and  $b_{\rm v}$  can be obtained.

Unfortunately light-scattering depolarisation data are available for relatively few simple molecules.<sup>11</sup> In certain cases this limitation may be overcome by choosing molecules of suitable symmetry. For bonds or groups, axial symmetry can sometimes be assumed in order to obtain the bond polarisability parameters.<sup>2</sup> The suitability of this assumption is then verified by the calculation of molar Kerr constants ( $_{\rm m}K_{\rm cale}$ ) for a similar molecule containing that bond or group and comparison with the observed value.

In previous work we have investigated hyperconjugative effects in  $C_{\Lambda r}$ -CX<sub>3</sub> systems by making use of the principle that where there is no electronic interaction between the substituents and the phenyl group in substituted benzenes, then the observed molecular polarisabilities  $b_i$  should agree with those obtained by additivity of the isolated component bond and group semi-axes. We now suggest an alternative procedure for the estimation of the anisotropic group polarisabilities where the group is in an aromatic environment. In this approach the three equations used for their derivation are those involving (i) the total group polarisabilities  $(b_{\rm L} + b_{\rm T} +$  $b_{\rm v}$ ) obtained from the electronic polarisation  $_{\rm E}P$  for the group, (ii) the observed molar Kerr constant  $_{\infty}(_{\rm m}K_2)$  of the monosubstituted benzene, and (iii) the  $_{\infty}(_{m}K_{2})$  value of the meta-disubstituted compound. The meta-compound is here chosen because it is polar and therefore has a  $\theta_2$  term (equation 26 of ref. 10) and further any mesomeric or spatial interaction is minimal.

Calculation of  $b_L$ ,  $b_T$ , and  $b_v$  for  $C_{Ar}$ -Cl and  $C_{Ar}$ -CH<sub>3</sub>.— The  $C_{Ar}$ -Cl and the  $C_{Ar}$ -CH<sub>3</sub> groups have been chosen to illustrate the above procedure because the group polarisability ellipsoid semi-axes have been previously estimated and shown to be reasonable parameters.<sup>12</sup> In the calculation of  $b_i(C_{Ar}$ -Cl) the following data are

<sup>7</sup> C. G. Le Fèvre and R. J. W. Le Fèvre, J. Chem. Soc., 1954, 1577.
<sup>8</sup> M. L. Kemp and R. J. W. Le Fèvre, J. Chem. Soc., 1965,

#### TABLE 1

Incremental dielectric constants, densities, refractive indices, and Kerr constant for solutions in carbon tetrachloride at 25 °C

		n	n-Xylene							
$10^{5}w_{2}$	1647	3291	<b>4050</b>	5320	6656	9310				
$10^{11}\Delta B$	163	304	371	485	607	835				
$10^4$ Δε		82	102	135	170	231				
$-10^{5}\Delta d$	2196	4314	5258	6841	8474	11,608				
$10^4\Delta n$	13	27	30	40	49	69				
whence	- 107AR -	- 0.951	0.72	2. 540	$ \Sigma_m  = 0$	959.				
whene	$\Lambda d = 1.9$	2500 10	$\frac{1}{2} - 0.137$	$\mathcal{D}_2^-, \ \Delta \Delta \mathcal{E}_1^-$	$\Delta w_2 = 0.075$	202;				
	$\Delta u \sim 1.0$	$55w_2 + 0$	$5.52w_2^{-},$	$\Delta\Delta n/\Delta w_2$	= 0.015					
		Trifluor	omethylb	enzene						
1 0570	1085	1706	9164	9498	9179	9200				
101178	1961	2025	2104	2400	20220	3008				
104 \ a	975	1970	2074	2927	0009 0520	4402				
10542	807	1379	1945	1974	2002	2919				
$-10^{\circ}\Delta u$	007	309	1240	1400	1017	2058				
$-10^{-}\Delta n$	4	12	14	15	22	25				
whenc	$\approx 10^7 \Delta B$	= 11.45u	$v_2 + 20.8$	$w_{2}^{2}$ ; $\Sigma\Delta\epsilon$	$\Sigma w_2 = 8$	·09;				
	$\Sigma \Delta d / \Sigma w_{\rm c}$	$_{2} = -0.5$	570; ΣΔn	$\Sigma w_2 = -$	-0.067					
		<u> </u>								
		Octai	luorotolu	ene						
$10^{5}w_{2}$	577	768	1005	1197	1943					
$10^{11}\Delta B$	78	100	133	158	256					
$10^4\Delta\epsilon$	19	30	36	39	51					
$-10^{5}\Delta d$	14	18	19	<b>22</b>	38					
$-10^4\Delta n$	7	8	13	15	24					
111	honce $\Sigma 1$	$07 \Lambda R / \Sigma_{ab}$	- 1.29.	$\sum A_{-} \sum a_{+}$	0.20					
	$\sum d \sum m$		2 = 1.02	1200/20	$_{2}^{2} = 0.32$					
	22u/2w	$_{2} = -0.0$	$20; \Delta n$	$/\Delta w_2 = -$	-0.122					
	<b>カ-</b> F	Shorotrif	uoromet	vlbenzen	ie.					
1.05	702	1169	1619	9094	0460					
$10^{1} \omega_{2}$	106	1102	1015	2034	2400					
1044	190	140	409	010 024	010					
10-AE	102	148		204	310					
$-10^{\circ}\Delta a$	-330	4/3	009	800	1026					
$-10^{\circ}\Delta n$	1	11	15	18	22					
1 44	nence 21	$0'\Delta B/\Sigma w$	$_{2} = 2.50$	$\Sigma \Delta \epsilon / \Sigma w$	a = 1.29:					
W1	$\sum \Delta d / \sum w$	$\Delta B/\Sigma w_{s} = -0.4$	$_{2}=2.50;$ 16; $\Sigma\Delta n$	$\Sigma \Delta \varepsilon / \Sigma w$ $\Sigma w_{2} = -$	$_{2} = 1.29;$ -0.090					
W1	$\sum \Delta d / \sum w_{i}$	$\frac{1}{2} = -0.4$	2 = 2.50; 16; $\Sigma \Delta n$	$\frac{\Sigma\Delta\varepsilon/\Sigma w}{\Sigma w_2} = -$	2 = 1.29; -0.090					
Ŵ	$\frac{1}{\Sigma\Delta d/\Sigma w}$	$2^{2} = -0.4$	$2_2 = 2.50;$ 16; $\Sigma \Delta n$ uorometl	$\Sigma \Delta \epsilon / \Sigma w$ $/\Sigma w_2 = -$ nylbenzen	$_{2} = 1.29;$ -0.090					
10 <sup>5</sup> w <sub>2</sub>	$\frac{\sum \Delta d}{\sum \Delta d} \frac{\sum D}{\sum w_{i}}$	$\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351	2 = 2.50; $16; \Sigma \Delta n;$ 10; uorometh; 3198;	$\frac{\Sigma\Delta\varepsilon/\Sigma w}{\Sigma w_2} = -$ hylbenzen $\frac{4252}{\Sigma}$	$_{2} = 1.29;$ -0.090 ne 5374	6362				
$10^{5}w_{2}$ $10^{11}\Delta B$	hence $\Sigma I f$ $\Sigma \Delta d / \Sigma w_{f}$ p - C 1299 503	$2^{\Delta B/\Sigma w_3}_2 = -0.4$ Chlorotrifl 2351 913	$2_2 = 2.50;$ $16; \Sigma \Delta n;$ 100  uorometh; 3198; 1245;	$\Sigma \Delta \varepsilon / \Sigma w_2 = -$ nylbenzen $4252$ 1653	2 = 1.29; - 0.090 te 5374 2100	6362 2464				
$10^{5}w_{2}$ $10^{11}\Delta B$ $10^{4}\Delta \varepsilon$	hence $\Sigma d / \Sigma w_{1}$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165	$2^{\Delta B/\Sigma w_3}_2 = -0.4$ Chlorotrifi 2351 913 296	${}_{2}=2{\cdot}50;$ 16; $\Sigma\Delta n$ uorometl 3198 1245 399	$\frac{\Sigma\Delta\varepsilon/\Sigmaw}{/\Sigmaw_2} = -$ hylbenzen $\frac{4252}{1653}$ 536	2 = 1.29; - 0.090 ne 5374 2100 675	6362 2464 797				
$10^{5}w_{2}$ $10^{11}\Delta B$ $10^{4}\Delta \varepsilon$ $-10^{5}\Delta d$	hence $\Sigma 11 \\ \Sigma \Delta d / \Sigma w_{2} \\ p - C \\ 1299 \\ 503 \\ 165 \\ 466 \\ 466 \\ c = 11 \\ c =$	$2^{\circ}\Delta B/\Sigma w_{2}$ $2^{\circ} = -0.4$ Chlorotrifi 2351 913 296 812	$z_2 = 2 \cdot 50;$ $z_16; \Sigma \Delta n,$ $z_10; \Sigma \Delta n,$ $z_108,$ $z_1245,$ $z_1245,$ $z_1073,$ $z_1073,$	$\Sigma\Delta\epsilon/\Sigmaw_2 = -$ $2w_2 = -$ $4252$ $1653$ $536$ $1426$	2 = 1.29; -0.090 the 5374 2100 675 1783	6362 2464 797 2111				
$10^{5}w_{2}$ $10^{11}\Delta B$ $10^{4}\Delta \varepsilon$ $-10^{5}\Delta d$ $-10^{4}\Delta w$	hence $\Sigma 1^{+}$ $\Sigma \Delta d / \Sigma w_{\pm}$ p - C 1299 503 165 466 5	$2^{0}\Delta B/\Sigma w_{4}^{2} = -0.4$ Chlorotrifi 2351 913 296 812 8	${}_{2}=2{\cdot}50;\ {}_{2}=2{\cdot}50;\ {}_{2}=2{\cdot}5$	$\Sigma\Delta\varepsilon/\Sigmaw_2 = -$ hylbenzen $4252$ 1653 $536$ 1426 $12$	2 = 1.29; -0.090 the 5374 2100 675 1783 16	6362 2464 797 2111 17				
$     \begin{array}{r} 10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       - 10^{5}\Delta d \\       - 10^{4}\Delta n   \end{array} $	hence $\Sigma \Pi$ $\Sigma \Delta d / \Sigma w_{,}$ p-C 1299 503 165 466 5	$2^{\circ}\Delta B/\Sigma w_{2}$ $2^{\circ} = -0.4$ Chlorotriff 2351 913 296 812 8 8	$2_2 = 2 \cdot 50;$ $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9	$\sum \Delta \varepsilon / \Sigma w_2 = -$ hylbenzen $4252$ 1653 536 1426 12 $\sum \Delta \varepsilon / \Sigma w_2$	2 = 1.29; -0.090 e 5374 2100 675 1783 16	6362 2464 797 2111 17				
$     \begin{array}{r} 10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       - 10^{5}\Delta d \\       - 10^{4}\Delta n \\       \qquad \qquad$	hence $\Sigma I^{+}$ $\Sigma \Delta d / \Sigma w_{2}$ p - C 1299 503 165 466 5 hence $\Sigma I^{+}$	$0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{2}$	$2_{2} = 2 \cdot 50;$ $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 2 = 3.89; 2 = 3.89;	$\sum \Delta \varepsilon / \Sigma w$ $/ \Sigma w_2 = -$ nylbenzen $4252$ 1653 536 1426 12 $\Sigma \Delta \varepsilon / \Sigma w$	$_{2} = 1.29;$ -0.090 the 5374 2100 675 1783 16 $_{2} = 1.26;$	6362 2464 797 2111 17				
$     \begin{array}{r} 10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       - 10^{5}\Delta d \\       - 10^{4}\Delta n \\       wl     \end{array} $	hence $\Sigma II' \\ \Sigma \Delta d / \Sigma w_{2} \\ p - C \\ 1299 \\ 503 \\ 165 \\ 466 \\ 5 \\ hence \Sigma I \\ \Sigma \Delta d / \Sigma w_{2} \\ \end{cases}$	$0^{7}\Delta B/\Sigma w_{2}$ 2 = -0.4 Chlorotrift 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{2}$ 2 = -0.3	${}_{2} = 2.50;$ ${}_{16}; \Sigma \Delta n;$ ${}_{10}$ uorometl ${}_{3198}$ ${}_{1245}$ ${}_{399}$ ${}_{1073}$ ${}_{9}$ ${}_{2} = 3.89;$ ${}_{336}; \Sigma \Delta n;$	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w_2 = - \\ & \text{hylbenzen} \\ & 4252 \\ & 1653 \\ & 536 \\ & 1426 \\ & 12 \\ & \Sigma \Delta \varepsilon / \Sigma w_2 = - \end{split}$	$_{2} = 1.29;$ -0.090 te 5374 2100 675 1783 16 $_{2} = 1.26;$ -0.029	6362 2464 797 2111 17				
$     \begin{array}{r} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ w \end{array} $	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ p - C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$	$0^{7}\Delta B/\Sigma w_{2}$ 2 = -0.4 Chlorotrift 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{2}$ 2 = -0.3 2 Biotecie	$z_2 = 2.50;$ $z_16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 $z_2 = 3.89;$ $36; \Sigma \Delta n$	$\sum \Delta \varepsilon / \Sigma w_2 = -$ hylbenzen $4252$ 1653 536 1426 12 $\sum \Delta \varepsilon / \Sigma w_2 = -$	$_{2} = 1.29;$ -0.090 te 5374 2100 675 1783 16 $_{2} = 1.26;$ -0.029	6362 2464 797 2111 17				
$     \begin{array}{c}       10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       -10^{5}\Delta d \\       -10^{4}\Delta n \\       wl     \end{array} $	hence $\Sigma 11'' \Sigma \Delta d / \Sigma w_{2}$ p - C 1299 503 165 466 5 hence $\Sigma 11'' \Sigma \Delta d / \Sigma w_{2}$ 1,3	$0^{7}\Delta B/\Sigma w_{*}$ $_{2}^{2} = -0.4$ Chlorotrifl 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{*}$ $_{2}^{2} = -0.3$ 3-Bistriflu	$z_{2} = 2.50;$ $z_{16}; \Sigma\Delta n$ $z_{16}; \Sigma\Delta n$ $z_{198}$ $z_{1245}$ $z_{399}$ $z_{1073}$ $y_{2} = 3.89;$ $z_{36}; \Sigma\Delta n$ $z_{10}$	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{nylbenzen} \\ & 4252 \\ & 1653 \\ & 536 \\ & 1426 \\ & 12 \\ & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{ylbenzene} \end{split}$	$2_{2} = 1.29;$ -0.090 ae 5374 2100 675 1783 16 $2_{2} = 1.26;$ -0.029 -0.029	6362 2464 797 2111 17				
$     \begin{array}{c}       10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       -10^{5}\Delta d \\       -10^{4}\Delta n \\       w]     \end{array} $	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ p - 0 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ 1,: 1560	$0^{7}\Delta B/\Sigma w_{1}$ $_{2}^{2} = -0.4$ Chlorotrifl 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{1}$ $_{2}^{2} = -0.3$ 3-Bistriflu 2396	2 = 2.50; $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 2 = 3.89; $36; \Sigma \Delta n$ norometh 3504	$\Sigma \Delta \varepsilon / \Sigma w$ $/ \Sigma w_2 = -$ nylbenzen $4252$ $1653$ $536$ $1426$ $12$ $\Sigma \Delta \varepsilon / \Sigma w$ $/ \Sigma w_2 = -$ $ylbenzene$ $3707$	2 = 1.29; -0.090 10 675 1783 16 2 = 1.26; -0.029 5728	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ - 10^5 \Delta d \\ - 10^4 \Delta n \\ \end{array} \\ \\ \end{array} \\ \\ \begin{array}{c} w1 \\ 10^5 w_2 \\ 10^{11} \Delta B \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,5 1560 1096	$0^{\prime}\Delta B/\Sigma w_{,2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{,2}$ $_{2} = -0.3$ 3-Bistriffu 2396 1672	2 = 2.50; $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 2 = 3.89; $336; \Sigma \Delta n$ norometh 3504 2442	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{nylbenzen} \\ & 4252 \\ & 1653 \\ & 536 \\ & 1426 \\ & 12 \\ & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{ylbenzene} \\ & 3707 \\ & 2586 \end{split}$	$\begin{array}{c} {}_{2}=1.29;\\ -0.090\\ {}_{2}\\ {}_{2}\\ {}_{3}\\ {}_{3}\\ {}_{3}\\ {}_{1}\\ {}_{3}\\ {}_{1}\\ {}_{3}\\ {}_{2}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{3}\\ {}_{1}\\ {}_{2}\\ {}_{2}\\ {}_{1}\\ {}_{2}\\ {}_{2}\\ {}_{1}\\ {}_{2}\\ {}_{2}\\ {}_{1}\\ {}_{2}\\ {$	6362 2464 797 2111 17				
$\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$	hence $211$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,1 1560 1096 804	$0^{\prime}\Delta B/\Sigma w, \ _{2}=-0.4$ Chlorotrifi 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w, \ _{2}=-0.3$ 3-Bistrifit 2396 1672 1242	$2_{2} = 2.50;$ $16; \Sigma \Delta n$ uorometh 3198 1245 399 1073 9 2 = 3.89; $336; \Sigma \Delta n$ norometh 3504 2442 1821	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w_2 = - \\ & (\Sigma \omega_2 = - \\ & (\Sigma \omega_2 = - \\ 1) \\ & (\Sigma \omega_2 = - \\ 1653 \\ & (\Sigma \omega_2 = - \\ 12 \\ & (\Sigma \omega_2 = - \\ 12 \\ & (\Sigma \omega_2 = - \\ 2) \\ & (\Sigma \omega_2 = - \\ 12 \\ & (\Sigma \omega_2 = - \\ 2) \\ & ($	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{abs} \\ 5728 \\ 4006 \\ 2976 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ w \end{array}$	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ 1,560 1096 804 505	$0^{\prime}\Delta B/\Sigma w, \ _{2}=-0.4$ Chlorotrifl 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w, \ _{2}=-0.3$ 3-Bistriflu 2396 1672 1242 757	2 = 2.50; $16; \Sigma \Delta n$ uorometh 3198 1245 399 1073 9 2 = 3.89; $336; \Sigma \Delta n$ norometh 3504 2442 1821 1097	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ 1ylbenzen \\ 4252 \\ 1653 \\ 536 \\ 1426 \\ 12 \\ \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ ylbenzen \\ 3707 \\ 2586 \\ 1925 \\ 1150 \end{array}$	$2_{2} = 1.29;$ -0.090 ae 5374 2100 675 1783 16 $2_{2} = 1.26;$ -0.029 5728 4006 2976 1760	6362 2464 797 2111 17				
$ \begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ - 10^5 \Delta d \\ - 10^4 \Delta n \end{array} \\ \\ \end{array} \\ \\ \begin{array}{c} w \\ 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ - 10^5 \Delta d \\ - 10^4 \Delta n \end{array} $	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w_{2}$ 1,5 1560 1096 804 505 18	$0^{\prime}\Delta B/\Sigma w_{,2} = -0.4$ $2^{\prime} = -0.4$ Chlorotrifi 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{,2}$ $2^{\prime} = -0.3$ 3-Bistriflu 2396 1672 1242 757 29	$\begin{array}{r} 2 = 2 \cdot 50; \\ 16;  \Sigma \Delta n \\ \text{uorometl} \\ 3198 \\ 1245 \\ 399 \\ 1073 \\ 9 \\ 2 = 3 \cdot 89; \\ 36;  \Sigma \Delta n \\ 10rometh \\ 3504 \\ 2442 \\ 1821 \\ 1097 \\ 42 \end{array}$	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ \mathrm{aylbenzen} \\ 4252 \\ 1653 \\ 536 \\ 1426 \\ 12 \\ \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ \mathrm{ylbenzene} \\ 3707 \\ 2586 \\ 1925 \\ 1150 \\ 46 \end{array}$	2 = 1.29; -0.090 100 1783 16 2 = 1.26; -0.029 5728 4006 2976 1760 68	6362 2464 797 2111 17				
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$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ \end{array} \\ \\ \end{array} \\ \\ \begin{array}{c} wl \\ \\ 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \end{array} \\ \end{array}$	hence $\Sigma I = \frac{1}{\Sigma \Delta d / \Sigma w}$ p - C 1299 503 165 466 5 hence $\Sigma I = \frac{1}{\Sigma \Delta d / \Sigma w}$ 1,: 1560 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$	$0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.4$ Chlorotrifi 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$ 3-Bistriflu 2396 1672 1242 757 29 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$	2 = 2.50; $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 2 = 3.89; $36; \Sigma \Delta n$ 1000 meth 3504 2442 1821 1097 42 2 = 6.99; $12: \Sigma \Delta n$	$\begin{split} &\Sigma\Delta\epsilon/\Sigma w\\ &\Sigma\Delta\epsilon/\Sigma w_2=-\\ &\Sigma w_2=-\\ &\Sigma w_2=-\\ &1000000000000000000000000000000000000$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{te} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{te} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \end{array}$ $\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^{41} \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \end{array}$ wi	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ;	$0^{r}\Delta B/\Sigma w, \ _{2}=-0.4$ Chlorotriff 2351 913 296 812 8 $0^{r}\Delta B/\Sigma w, \ _{2}=-0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{r}\Delta B/\Sigma w, \ _{2}=-0.3$	$2_{2} = 2.50;$ $16; \Sigma \Delta n$ uorometh 3198 1245 399 1073 9 2 = 3.89; $36; \Sigma \Delta n$ norometh 3504 2442 1821 1097 42 2 = 6.99; $112; \Sigma \Delta n$	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ 1 \\ \gamma \\ 2 \\ 1653 \\ 536 \\ 1426 \\ 12 \\ \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ \gamma \\ $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{de} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{dot} \\ 2976 \\ 1760 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $W$	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ; $\Sigma \Delta d / \Sigma w$ ; $\Sigma \Delta d / \Sigma w$ ; $\Sigma \Delta d / \Sigma w$ ; L;	$0^{\prime}\Delta B/\Sigma w_{,2} = -0.4$ $2^{\prime} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{,2}$ $2^{\prime} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w_{,2}$ $2^{\prime} = -0.3$ 4-Bistriffu	$_{2} = 2.50;$ $_{16}; \Sigma \Delta m$ uorometl 3198 1245 399 1073 9 $_{2} = 3.89;$ $36; \Sigma \Delta m$ 10rometh 3504 2442 1821 1097 42 $_{2} = 6.99;$ $512; \Sigma \Delta m$ 10rometh	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{aylbenzen} \\ & 4252 \\ & 1653 \\ & 536 \\ & 1426 \\ & 12 \\ & \Sigma \Delta \varepsilon / \Sigma w_2 = - \\ & \text{ylbenzene} \\ & 3707 \\ & 2586 \\ & 1925 \\ & 1150 \\ & 46 \\ & \Sigma \Delta \varepsilon / \Sigma w_2 = - \\ & \text{ylbenzene} \end{split}$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ 100 \\ 100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ 300 \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ 300 $	6362 2464 797 2111 17				
$     \begin{array}{c}       10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       -10^{5}\Delta d \\       -10^{4}\Delta n \\       w1 \\       10^{5}w_{2} \\       10^{11}\Delta B \\       10^{4}\Delta \varepsilon \\       -10^{5}\Delta d \\       -10^{4}\Delta n \\       w1 \\       10^{5}\Delta d \\       w1 \\       10^{5}w_{2} \\       10^{4}\Delta n \\       w1 \\       10^{5}w_{2} \\       w1 \\       w1 \\       10^{5}w_{2} \\       w1 \\       w$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,3 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w_{2}$ 1,3 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w_{2}$ 1,3 1067 1096	$0^{\prime}\Delta B/\Sigma w_{,2} = -0.4$ 2 = -0.4 Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{,2}$ 2 = -0.3 3-Bistriflu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w_{,2}$ 2 = -0.3 4-Bistriflu 1362	2 = 2.50; $16; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 2 = 3.89; $36; \Sigma \Delta n$ 1000meth 3504 2442 1821 1097 42 2 = 6.99; $112; \Sigma \Delta n$ 1000meth 1916	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw \\ \Sigma\Delta\epsilon/\Sigmaw_{2} = - \\ 1/\Sigmaw_{2} = - \\ 1/\Sigma$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{be} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ \text{be} \\ 3022 \end{array}$	6362 2464 797 2111 17				
$10^{5}w_{2}$ $10^{11}\Delta B$ $10^{4}\Delta \varepsilon$ $-10^{5}\Delta d$ $-10^{4}\Delta n$ $10^{5}w_{2}$ $10^{11}\Delta B$ $10^{4}\Delta \varepsilon$ $-10^{5}\Delta d$ $-10^{4}\Delta n$ wi $10^{5}w_{2}$ $10^{14}\Delta B$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,: 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w_{2}$ 1,: 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w_{2}$ 1,: 1046	$0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.4$ Chlorotrifi 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$ 3-Bistrifit 2396 1672 1242 757 29 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$ 4-Bistrifit 1362 $_{20}^{0}$	$_{2} = 2.50;$ $_{16}; \Sigma \Delta n$ uorometl 3198 1245 399 1073 9 $_{2} = 3.89;$ $36; \Sigma \Delta n$ 1000 meth 3504 2442 1821 1097 42 $_{2} = 6.99;$ 1252 1252 1252 1252 1252 1000 meth 1916 952	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w_2 = - \\ & / \Sigma w_2 = - \\ & 1 \\ & 1 \\ & 1 \\ & 1 \\ & 2 \\ & 1 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{ae} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ \text{ae} \\ 3022 \\ 55 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ \\ \end{array} \\ \\ \begin{array}{c} w \\ w \\ 10^5 w_2 \\ 10^{11} \Delta B \\ -10^4 \Delta s \\ \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,21 $\Sigma \Delta d / \Sigma w_{2}$ 1,21 $\Sigma \Delta d / \Sigma w_{2}$	$0^{\prime}\Delta B/\Sigma w,$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w,$ $_{2} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w,$ $_{2} = -0.3$ 4-Bistriffu 1362 20 30	$\begin{array}{r} 2 = 2 \cdot 50;\\ 16;  \Sigma \Delta n,\\ 10;  \Sigma \Delta n,\\ 1245\\ 399\\ 1073\\ 9\\ 2 = 3 \cdot 89;\\ 36;  \Sigma \Delta n,\\ 1070 \text{ meth}\\ 3504\\ 2442\\ 1821\\ 1097\\ 42\\ 2= 6 \cdot 99;\\ 112;  \Sigma \Delta n,\\ 1070 \text{ meth}\\ 1916\\ 25\\ 43\end{array}$	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigma w \\ \Sigma\Delta\epsilon/\Sigma w_2 = - \\ 1/\Sigma w_2 = -$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ie} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{o} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ \text{o} \\ 3022 \\ 55 \\ 63 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ -10^{4}\Delta \varepsilon \\ -10^{4}\Delta \epsilon \\ -10^{4}\Delta \epsilon \end{array}$	hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma II$ $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ; 1,21 $\Sigma \Delta d / \Sigma w$ ; 1,32 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ; 1,42 1096 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ; 1,63 804 505 18 hence $\Sigma I$ $\Sigma \Delta d / \Sigma w$ ; 1,63 1096 804 505 18 hence $\Sigma I$	$0^{\prime}\Delta B/\Sigma w_{,2} = -0.4$ $2^{\prime} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{,2}$ $2^{\prime} = -0.3$ 3-Bistriflu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w_{,2}$ $2^{\prime} = -0.3$ 4-Bistriflu 1362 20 30 436	$_{2} = 2.50;$ $_{16}; \Sigma \Delta m$ uorometl 3198 1245 399 1073 9 $_{2} = 3.89;$ $36; \Sigma \Delta m$ 1070meth 3504 2442 1821 1097 42 $_{2} = 6.99;$ $512; \Sigma \Delta m$ 1070meth 1916 25 43 616	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{nylbenzen} \\ & 4252 \\ & 1653 \\ & 536 \\ & 1426 \\ & 12 \\ & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & \text{ylbenzene} \\ & 3707 \\ & 2586 \\ & 1925 \\ & 1150 \\ & 46 \\ & \Sigma \Delta \varepsilon / \Sigma w \\ & z = - \\ & \text{ylbenzene} \\ & 2873 \\ & 40 \\ & 60 \\ & 921 \\ \end{split}$	2 = 1.29; -0.090 100; 1783; 16; 2 = 1.26; -0.029; 5728; 4006; 2976; 1780; 68; 2 = 5.19; -0.120; 55; 63; 96; 3022; 55; 63; 96; 65; 65; 63; 96; 65; 65; 1783; 16; 2976; 1760; 68; 25; 63; 96; 65; 63; 96; 65; 63; 96; 65; 178; 120;	6362 2464 797 2111 17				
$\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} w_{1} \\ w_{2} \\ 10^{11}\Delta B \\ -10^{4}\Delta n \\ \end{array}$ $\begin{array}{c} w_{1} \\ w_{2} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ $	hence 211 $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence 211 $\Sigma \Delta d / \Sigma w_{2}$ 1,560 1096 804 505 18 hence 21 $\Sigma \Delta d / \Sigma w_{2}$ 1,6 1046 276 9	$0^{\prime}\Delta B/\Sigma w,$ $_{2}^{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w,$ $_{2}^{2} = -0.3$ 3-Bistriflu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w,$ $_{2}^{2} = -0.3$ 4-Bistriflu 1362 20 30 436 16	$_{2} = 2.50;$ $_{16}; \Sigma \Delta m$ uorometh 3198 1245 399 1073 9 $_{2} = 3.89;$ $36; \Sigma \Delta m$ 1000 meth 3504 2442 1821 1097 42 $_{2} = 6.99;$ $112; \Sigma \Delta m$ 1000 meth 1916 25 43 616 25	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ 1653 \\ 536 \\ 1426 \\ 12 \\ \Sigma\Delta\epsilon/\Sigmaw \\ /\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ 2586 \\ 1925 \\ 1150 \\ 46 \\ \Sigma\Delta\epsilon/\Sigmaw \\ \gamma/\Sigmaw_2 = -\\ 2873 \\ 40 \\ 60 \\ 921 \\ 35 \end{array}$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{be} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ \text{be} \\ 3022 \\ 555 \\ 63 \\ 965 \\ 36 \end{array}$	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ \end{array} \\ \\ \hline \\ 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ \hline \\ w \\ \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,299 1,3 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1046 276 9 	$0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{7}\Delta B/\Sigma w_{i}$ $_{2}^{2} = -0.3$ 4-Bistriffu 1362 20 30 436 16 16	$_{2} = 2.50;$ $_{16}; \Sigma \Delta n;$ $_{10}; \Sigma \Delta n;$ $_{10}; \Sigma \Delta n;$ $_{1245};$ $_{399};$ $_{1245};$ $_{399};$ $_{1073};$ $_{99};$ $_{2} = 3.89;$ $_{136}; \Sigma \Delta n;$ $_{100};$ $_{100};$ $_{12}; \Sigma \Delta n;$ $_{100};$ $_{12}; \Sigma \Delta n;$ $_{100};$ $_{12}; \Sigma \Delta n;$ $_{10};$ $_{12}; \Sigma \Delta n;$ $_{10};$ $_$	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & 1 \\ & 1 \\ & 1 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \end{array}$ $\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \end{array}$ $\begin{array}{c} wl \\ 10^5 w_2 \\ 10^{11} \Delta B \\ -10^4 \Delta n \\ wl \\ \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w_{2}$ 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$	$0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 4-Bistriffu 1362 20 30 436 16 $7\Delta B/\Sigma w_{2}$	$\begin{array}{c} 2 = 2 \cdot 50;\\ 16;  \Sigma \Delta n \\ \text{uorometl} \\ 3198 \\ 1245 \\ 399 \\ 1073 \\ 9 \\ 2 = 3 \cdot 89;\\ 36;  \Sigma \Delta n \\ 1070 \\ 1070 \\ 1070 \\ 1087 \\ 2442 \\ 1821 \\ 1097 \\ 42 \\ 2442 \\ 1821 \\ 1097 \\ 42 \\ 2 = 6 \cdot 99;\\ 112;  \Sigma \Delta n \\ 1070 \\ 1097 \\ 42 \\ 1821 \\ 1097 \\ 42 \\ 1821 \\ 1097 \\ 42 \\ 1821 \\ 1097 \\ 42 \\ 25 \\ 1070 \\ 1$	$\begin{split} & \Sigma \Delta \varepsilon / \Sigma w \\ & / \Sigma w_2 = - \\ & 1 \\ & 1 \\ & 1 \\ & 1 \\ & 2 \\ & 1 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ & 2 \\ & 2 \\ & 1 \\ & 2 \\ $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{abs} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ \text{abs} \\ 2 = 5.19; \\ -0.120 \\ \text{abs} \\ 3022 \\ 55 \\ 63 \\ 965 \\ 36 \\ \text{abs} \\ -0.22 \\ \text{abs} \\ 2 = -0.22 \\ \text{abs} \\ 36 \\ 36 \\ 36 \\ 36 \\ 36 \\ 36 \\ 36 \\ 3$	6362 2464 797 2111 17				
$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ - 10^5 \Delta d \\ - 10^4 \Delta n \\ \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ - 10^5 \Delta d \\ - 10^4 \Delta n \\ \\ \\ 10^5 w_2 \\ 10^{11} \Delta B \\ - 10^4 \Delta s \\ - 10^4 \Delta n \\ \\ - 10^5 \Delta d \\ - 10^4 \Delta n \\ \\ \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma 1$ ; $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,2 1046 276 9 ence $\Sigma 10$ $\Sigma \Delta d / \Sigma w$	$0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{\prime}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 4-Bistriffu 1362 20 30 436 16 $7\Delta B/\Sigma w_{2}$ $_{2} = -0.3$	$\begin{array}{c} 2 = 2 \cdot 50; \\ 2 = 2 \cdot 50; \\ 16;  \Sigma \Delta n, \\ 100; 100; 100; 100; 100; 100; 100; 10$	$\begin{split} & \sum \Delta \varepsilon / \sum w_2 = - \\ & \sum \omega $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ 100 \\ 100 \\ 1783 \\ 160 \\ 2 = 1.26; \\ -0.029 \\ 300 \\ 2976 \\ 1783 \\ 160 \\ 2976 \\ 1783 \\ 160 \\ 2976 \\ 1760 \\ 68 \\ 2976 \\ 1760 \\ 100 $	6362 2464 797 2111 17				
$\begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array} \\ w] \\ \begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ 10^{4}\Delta \varepsilon \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array} \\ w] \\ \begin{array}{c} 10^{5}w_{2} \\ 10^{11}\Delta B \\ -10^{4}\Delta n \\ -10^{5}\Delta d \\ -10^{5}\Delta d \\ -10^{4}\Delta n \\ \end{array} \\ wh \end{array}$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,7 1046 276 9 ence $\Sigma 10$ $\Sigma \Delta d / \Sigma w$ ;	$0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 3-Bistriffu 2396 1672 1242 7257 29 $0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 4-Bistriffu 1362 20 30 436 16 $7\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 4-Disch	$_{2} = 2.50;$ $_{16}; \Sigma \Delta m$ uorometh 3198 1245 399 1073 9 $_{2} = 3.89;$ $36; \Sigma \Delta m$ 1000 meth 3504 2442 1821 1097 42 $_{2} = 6.99;$ $512; \Sigma \Delta m$ 1000 meth 1916 25 43 616 25 $= 0.15; \Sigma \Delta m$	$\begin{array}{l} \Sigma\Delta\epsilon/\Sigmaw\\/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ 1653\\536\\1426\\12\\\Sigma\Delta\epsilon/\Sigmaw\\/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -\\ 2873\\40\\60\\921\\35\\\Sigma\Delta\epsilon/\Sigmaw_2 = -\\ \gamma/\Sigmaw_2 = -$	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ 100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ 3022 \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 2 = 5.19; \\ -0.120 \\ 3022 \\ 55 \\ 63 \\ 965 \\ 36 \\ = -0.22 \\ -0.118 \end{array}$	6362 2464 797 2111 17				
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$\begin{array}{c} 10^5 w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta \varepsilon \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ 10^{5} w_2 \\ 10^{11} \Delta B \\ 10^4 \Delta s \\ -10^5 \Delta d \\ -10^4 \Delta n \\ \\ \\ 10^{5} w_2 \\ 10^{11} \Delta B \\ -10^4 \Delta n \\ \\ \\ \\ \\ 10^5 \omega_2 \\ -10^4 \Delta n \\ \\ \\ \\ \\ \\ \\ \\ 10^5 w_2 \\ \\ \\ \\ 10^5 w_2 \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	hence $\Sigma 11$ $\Sigma \Delta d / \Sigma w$ ; p-C 1299 503 165 466 5 hence $\Sigma 11$ ; $\Sigma \Delta d / \Sigma w$ ; 1,560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,7 1560 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,9 $\Sigma \Delta d / \Sigma w$ 1,1 $\Sigma \Delta d / \Sigma w$ 1,1 $\Sigma \Delta d / \Sigma w$ 1,1 $\Sigma \Delta d / \Sigma w$ 1,2 1,5 1096 804 505 18 hence $\Sigma 1$ $\Sigma \Delta d / \Sigma w$ 1,1 $\Sigma \Delta d / \Sigma w$ 1,1 $\Sigma \Delta d / \Sigma w$ 1,1 1,2 $\Sigma \Delta d / \Sigma w$ 1,1 1,2 $\Sigma \Delta d / \Sigma w$ 1,1 1,2 1,2 1,2 1,2 1,2 1,2 1,2	$0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.4$ Chlorotriff 2351 913 296 812 8 $0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 3-Bistriffu 2396 1672 1242 757 29 $0^{7}\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ 4-Bistriffu 1362 20 30 436 16 $7\Delta B/\Sigma w_{2}$ $_{2} = -0.3$ $\phi$ -Dich 2047	$\begin{array}{c} 2 = 2 \cdot 50; \\ 16;  \Sigma \Delta n, \\ \text{uorometl} \\ 3198 \\ 1245 \\ 399 \\ 1073 \\ 9 \\ 2 = 3 \cdot 89; \\ 36;  \Sigma \Delta n, \\ 1070 \\ 1070 \\ 1070 \\ 1070 \\ 1097 \\ 42 \\ 1821 \\ 1097 \\ 42 \\ 1821 \\ 1097 \\ 42 \\ 2 = 6 \cdot 99; \\ 112;  \Sigma \Delta n, \\ 1070 \\ 1$	$\begin{split} & \sum \Delta \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / \sum \omega \varepsilon / \sum w_2 = - \\ & \sum \omega \varepsilon / $	$\begin{array}{c} 2 = 1.29; \\ -0.090 \\ \text{ae} \\ 5374 \\ 2100 \\ 675 \\ 1783 \\ 16 \\ 2 = 1.26; \\ -0.029 \\ \text{abs} \\ 5728 \\ 4006 \\ 2976 \\ 1760 \\ 68 \\ 965 \\ 36 \\ 965 \\ 36 \\ 2976 \\ 1760 \\ 1760 \\ 68 \\ 965 \\ 36 \\ 2976 \\ 1760 \\ 1760 \\ 100 \\ $	6362 2464 797 2111 17				
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<sup>11</sup> R. J. W. Le Fèvre and B. Purnachandra Rao, *J. Chem. Soc.*, 1958, 1465.

<sup>3463.</sup> <sup>9</sup> A. L. McClellan, 'Tables of Experimental Dipole Moments,' Provide San Departmental 1922.

Freeman, San Francisco, 1963. <sup>10</sup> R. J. W. Le Fèvre, Adv. Phys. Org. Chem., 1965, **3**, 1.

<sup>&</sup>lt;sup>12</sup> K. E. Calderbank, R. J. W. Le Fèvre, and R. K. Pierens, *J. Chem. Soc.* (B), 1969, 968.

used: for chlorobenzene,  $\mu = 1.59 \text{ D},^{13} 10^{12} \text{ }_{\infty}(\text{m}K_2) =$ 137,<sup>14</sup>  $_{\rm E}P = 29.87 \text{ cm}^{3 \text{ 15}}$  whence  $\Sigma b_i = 35.52$ ; \*  $b_{\rm L}(C_6H_5)$  $b_{\rm T}(C_6H_5) = 10.50$ ,  $b_{\rm v}(C_6H_5) = 6.79$ ,<sup>16</sup> and  $b_{\rm L}(CH) = b_{\rm T}(CH) = b_{\rm v}(CH) = 0.65$ ;<sup>17</sup> and for *m*-dichlorobenzene  $\mu = 1.41$  D and  $10^{12} \text{m}(\text{m}K_2) = 64.4$ .<sup>12</sup> Applying the above data we have three simultaneous equations (1)— (3), where  $\theta_1$  and  $\theta_2$  have the usual significance.<sup>10</sup> Of

$$\Sigma b_i(C_{Ar} - Cl) = \Sigma b_i(C_6 H_5 Cl) - \Sigma b_i(C_6 H_5) \qquad (1)$$

 $(_{\mathrm{m}}K_{2})(\mathrm{C}_{6}\mathrm{H}_{5}\mathrm{Cl}) = 2\pi N(\theta_{1} + \theta_{2})/9$ (2)

 $(_{\rm m}K_2)(m-C_6H_4Cl_2) = 2\pi N(\theta_1 + \theta_2)/9$ (3)

the four roots obtained by solving the resulting quartic equation for  $b_{\rm L}(C_{\rm Ar}-Cl)$  only one positive value is obtained. Substituting this value back into the above relationships yields  $b_{\rm T}$  and  $b_{\rm y}$  for the bond. The values thus obtained are  $b_L(C_{Ar}-Cl) = 4.23$ ,  $b_T(C_{Ar}-Cl) = 1.98$ , and  $b_v(C_{Ar}-Cl) = 1.51$ , which are in good agreement p-chlorotoluene using the above group polarisability parameters together with those for the phenyl group listed earlier. In each case the agreement between calculated and observed values is better than those obtained hitherto.1,8,16

Calculation of  $b_L$ ,  $b_T$  and  $b_{\tau}$  for the  $C_{Ar}$ -CF<sub>3</sub> Group.--Using an analogous equation to (1)  $\Sigma b_i(C_{Ar}-CF_3)$  is larger than estimates obtained from similar considerations of p-fluoro-, p-chloro-, m- and p-trifluoromethyltrifluoromethylbenzene. It would appear that there is an added polarisability of this group in trifluoromethylbenzene. This exaltation of polarisability  $(0.3 \times 10^{-24})$ cm<sup>3</sup>) arising from mesomeric interactions can be readily obtained from  $\Sigma b_i(C_{Ar}-CF_3)$  observed minus  $\Sigma b_i(C_{Ar}-CF_3)$ calculated.

Application of the data for trifluoromethylbenzene and 1,3-bistrifluoromethylbenzene from Table 2 yields

#### TABLE 2

Polarisations, refractions, dipole moments, and molar Kerr constants (from observations in carbon tetrachloride at 25°)

				/				
Solute	οC ε	β	γ	δ	$_{\infty}P_2/\mathrm{cm}^3$	$R_{ m D}/{ m cm^3}$	μ/D *	$10^{12} \infty ({}_{\rm m}K_2)$
<i>m</i> -Xylene	0.25	-0.843	0.05	11.5	38.7	36.3		12.4
Trifluoromethylbenzene	8.09	-0.360	-0.05	137.9	161.7	$31 \cdot 1$	2.52	177
Octafluorotoluene	0.32	-0.013	-0.08	15.9	51.8	32.5	0.93	36
<i>p</i> -Fluorotrifluoromethylbenzene	1.29	-0.563	-0.06	30.2	60.5	30.8	1.17	<b>45</b>
<i>p</i> -Chlorotrifluoromethylbenzene	1.26	-0.212	-0.05	46.8	64.1	35.9	1.14	77
1,3-Bistrifluoromethylbenzene	5.19	-0.192	-0.08	$84 \cdot 2$	164.6	35.7	$2 \cdot 49$	159
1,4-Bistrifluoromethylbenzene	-0.52	-0.198	-0.08	1.8	39.8	35.7		<b>4</b> ·8
p-Dichlorobenzene	0.28 †	-0.225 †	-0.08 †	20.0	37·4 †	36·4 †		$27 \cdot 6$
	* Calmate	(	ala at D	1 05 0	A Dans and 6	00		

\* Calculated on the basis of  $_{\rm D}P = 1.05 R_{\rm D}$ . † From ref. 20.

with the bond polarisability anisotropy obtained previously <sup>11</sup> ( $b_L = 4.3$ ,  $b_T = 2.0_5$ ,  $b_v = 1.5$ ) from polarisation and light scattering. A similar procedure applied to toluene and *m*-xylene can be used for the  $C_{Ar}$ -CH<sub>3</sub> group, [the relevant data needed: for toluene  $\mu =$ 0.37 D,  $10^{12}_{\infty}({}_{\rm m}K_2) = 13.7$  and  $\Sigma b_i = 35.55$ ; <sup>16</sup> and for *m*-xylene  $\mu = 0.26$  D,  $710^{12} \text{}_{\infty}(\text{}_{\text{m}}K_2) = 12.4$  (from Table 2)]. The results obtained,  $b_{\rm L}(C_{\rm Ar}-CH_3) = 3.39$ ,  $b_{\rm T}(C_{\rm Ar}-CH_3)$ = 2.04 and  $b_{\tau}(C_{Ar}-CH_3) = 2.33$  are in close agreement with those earlier derived <sup>16</sup> ( $b_{\rm L} = 3.4$ ,  $b_{\rm T} = 2.0$ ,  $b_{\rm T} =$ 2.3).

#### TABLE 3

Calculated molecular polarisabilities and molar Kerr constants for p-xylene, p-dichlorobenzene, and p-chlorotoluene 1010 17 1010 77

	$b_1$	$b_2$	$b_3$	$10^{12} \text{m} K$	$10^{12} \text{m} K$
	(calc.)	(calc.)	(calc.)	(calc.)	(obs.)
ρ-C <sub>6</sub> H₄Me₂	16.63	13.93	10.80	12.3	10.8 4
p-C <sub>6</sub> H₄Cl <sub>2</sub>	18.31	13.81	9.16	31	<b>28</b>
p-ClC <sub>6</sub> H₄Me	17.48	13.89	9.99	237	237 <sup>b</sup>
	ª Fron	n ref. 12.	<sup>b</sup> From ref. 1.		

Table 3 summarises the results of calculations for the molar Kerr constants of p-xylene, p-dichlorobenzene, and

\* The polarisability semi-axes of bonds or groups  $b_{L}$ ,  $b_{T}$ , or  $b_{v}$ or of molecules  $b_1$ ,  $b_2$ , or  $b_3$  are quoted throughout in  $10^{-24}$  cm<sup>3</sup> units.

13 C. G. Le Fèvre and R. J. W. Le Fèvre, J. Chem. Soc., 1953,

4041. <sup>14</sup> R. J. W. Le Fèvre, D. V. Radford, G. L. D. Ritchie, and P. J. Stiles, *J. Chem. Soc.* (*B*), 1968, 148.

 $b_{\rm L}(C_{\rm Ar}-CF_3) = 2.6$ ,  $b_{\rm T}(C_{\rm Ar}-CF_3) = 2.5$ , and  $b_{\rm v}(C_{\rm Ar}-CF_3)$  $= 2 \cdot 2$ . The <sub>m</sub>K values calculated using these values together with the observed quantities are listed in Table 4.

### TABLE 4

Calculated molecular polarisabilities and molar Kerr constants for molecules  $p-XC_6Y_4$ ·CF<sub>3</sub> in carbon tetrachloride solutions

		$b_1$	$b_2$	$b_3$	$10^{12} K$	$10^{12} MK$
X	Y	(calc.)	(calc.)	(calc.)	(calc.)	(obs.)
CF <sub>3</sub>	н	15.0	14.9	$10.5_{5}$	9.7	4.8
Cl	н	16.7	$14.3_{5}$	$9.8_{5}^{\circ}$	84	77
$\mathbf{F}$	н	13·2 <sub>5</sub> ª	13·1 <sup>°</sup> , a	8·6, "	46	45
F	$\mathbf{F}$	13·1 <sup>°</sup>	13·5 <sup>°</sup>	7.8 <sup>3</sup> 5	38	36

<sup>a</sup> Calc. using  $b_l(C_{Ar}-F)$  from ref. 11. <sup>b</sup> Calc. using  $b_L(C_6F_5) = 11\cdot16$ ,  $b_T(C_6F_5) = 11\cdot64$ ,  $b_v(C_6F_5) = 6\cdot29$ , M. J. Aroney, G. Cleaver, and R. J. W. Le Fèvre, unpublished data.

For the  $C_{Ar}$ -CH<sub>3</sub> group our calculations give  $b_T < b_r$ , whereas for  $C_{Ar}$ -CF<sub>3</sub> (where negative hyperconjugation has been postulated) show  $b_{\rm T} > b_{\rm v}$ . This is to be compared with our earlier results<sup>2</sup> for CAr-CMe<sub>3</sub> and  $C_{Ar}$ -CCl<sub>3</sub> where the assumption that  $b_T = b_y$  was satisfactory. If hyperconjugation were to exist to some extent we would expect this to be displayed in the

<sup>15</sup> R. J. W. Le Fèvre and K. D. Steel, Chem. and Ind., 1961,

670. <sup>16</sup> R. J. W. Le Fèvre and L. Radom, J. Chem. Soc. (B), 1967,

1295. <sup>17</sup> R. J. W. Le Fèvre, B. J. Orr, and G. L. D. Ritchie, *J. Chem.* 

relative magnitude of  $b_{\rm T}$  to  $b_{\rm v}$ . Kostelnik *et al.*<sup>18</sup> from an n.m.r. study of trifluoromethylbenzene state that the hyperconjugation of the -CF<sub>3</sub> group with the aromatic ring is, if not equal, at least comparable (or complementary) to that of the -CH<sub>3</sub> group, while Grynkiewicz *et al.*<sup>19</sup> conclude (from a kinetic study) that the -CCl<sub>3</sub> group is a substituent without significant hyperconjugative interaction with the ring. Hence it would appear that the sign of  $b_{\rm v}$  —  $b_{\rm T}$  of the group C<sub>Ar</sub>-CX<sub>3</sub> may be an indicator of the type and degree of hyperconjugation.

Trifluoromethylbenzene in Benzene Solution.—Trifluoromethylbenzene has also been studied in benzene solution  $[10^{12}_{\infty}(_{m}K_{2}) = +206,^{20} 10^{12}_{\infty}(_{m}K_{2}) = +215$ <sup>6</sup>]. Further, the <sup>1</sup>H n.m.r. spectrum for this solute in C<sub>6</sub>D<sub>6</sub> shows all

<sup>18</sup> R. J. Kostelnik, M. P. Williamson, D. I. Wisnosky, and S. M. Castellano, *Canad. J. Chem.*, 1969, **47**, 3313.

the peaks have been shifted up field relative to those in the spectrum with  $CCl_4$  as solvent. This finding is in accord with those of Kostelnik *et al.*<sup>18</sup> for trifluoromethylbenzene, neat liquid (which corresponds to an aromatic environment) and in carbon tetrachloride solution. These results can be attributed to stereospecific solute-solvent interactions <sup>14</sup> involving transient complexes having parallel arrangement of the aromatic rings.

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