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Errata

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Errata

"Orientation and Structure of Pyrazine, Pyrimidine, and Pyridazine in a Lyotropic Liquid Crystal", by Robert C. Long, Jr., Kathryn R. Long and J. H. Goldstein

In our recent paper on the orientation and structure of pyrazine, pyrimidine, and pyridazine in a lyotropic liquid crystal,† an error was discovered which modifies the values of distance ratios and parameters determined for pyrimidine. The appropriate corrections are as follows:

1) Page 303 line 12 should read: The values of J_{13} and J_{24} were 1.42 Hz and 2.50 Hz, respectively, as determined from analysis of the isotropic spectrum of pyrimidine in the mesophase after addition of a small amount of water to transform the mesophase to the isotropic liquid.

2) Table 2 (page 304) should be replaced by revised Table 2.

3) Replace Table 4 (page 309) with the revised Table 4. Discussion Section A, line 8, replace 6.6 Hz by 6.7 Hz; line 10, replace 1.25 ppm by 1.26 ppm.

4) Page 310, last paragraph, should read: In view of the quoted experimental uncertainty in the pyrimidine distance ratios the present values are not significantly different from te values of Khetrapal and co-workers [10] obtained using thermotropic media. The NMR results are slightly different from the microwave values.

5) Page 311, first paragraph, second sentence, should read: Although geometries deduced from microwave and NMR methods are expected to be slightly different [22] we have observed very close agreement between values determined by both methods in the case of furan and thiophene[5].

6) Page 311, in the section on orientation, $P_{293}(\theta, \varphi)$ and $P_{294}(\theta, \phi)$ should be

$$P_{293}(\theta, \phi) = 0.07825 + 0.00406 \cos^2\theta + 0.000456 \sin^2\theta \cos 2\theta$$
$$P_{294}(\theta, \phi) = 0.07947 + 0.00040 \cos^2\theta + 0.00365 \sin^2\theta \cos 2\phi$$

† *Molecular Crystals and Liquid Crystals*, 21, 299 (1973).

TABLE 2

NMR parameters and motional constants for pyrimidine

	293° K	305° K	311° K	315° K
$\delta\ (\omega_3-\omega_1)$	1.64±0.001	1.65±0.001	1.65±0.002	1.66±0.001
$\delta\ (\omega_3-\omega_2)$	1.25±0.001	1.26±0.001	1.26±0.002	1.27±0.001
J_{12}	0.51±0.02	0.40	0.36± .10	0.20
J_{13}	1.42	1.42	1.42	1.42
J_{23}	7.1± .5	7.56	5.50± .31	6.47
J_{24}	2.5	2.5	2.5	2.5
D_{12}	-12.89± .03	-10.22	-8.85±0.06	-7.92
D_{13}	-14.32± .05	-11.75	-10.53±0.09	-9.73
D_{23}	20.68± .49	20.65	23.24±0.30	22.90
D_{24}	13.99± .04	12.78	12.26±0.04	12.03
$C_{3z^2-r^2}$	0.01522 ±0.00006	0.01248	0.01120 ±0.00007	0.01025
$C_{x^2-y^2}$	0.00296 ±0.00005	0.00353	0.00382 ±0.00006	0.00418

TABLE 4

Distance ratios for pyrazine, pyrimidine and pyridazine

	NMR lyotropic	NMR thermotropic	X-ray	Microwave
Pyrazine				
(r_{14}/r_{12})	1.65±0.004	1.66±0.02	1.703	–
Pyrimidine				
(r_{12}/r_{23})	1.642±0.011	1.62±0.01	1.670	1.695
(r_{13}/r_{23})	1.930±0.009	1.90±0.02	1.957	1.979
(r_{24}/r_{23})	1.701±0.005	1.706±0.004	1.720	1.712
Pyridazine				
(r_{12}/r_{23})	0.983±0.015	0.988±0.010	–	1.030
(r_{13}/r_{23})	1.692±0.008	1.693±0.007	–	1.759
(r_{14}/r_{23})	1.897±0.004	1.890±0.004	–	2.033