[1] ERIC PONDER, *Hemolysis and Related Phenomena*, Grune and Stratton, New York, 1948, Ch. 4.
[2] A. TEITEL-BERNARD, *Sang*, 8 (1934) 298.
[3] J. B. BATEMAN, S. S. HSU, J. P. KNUDSON AND K. L. YUDOWITCH, *Arch. Biochem. Biophys.*, 45 (1953) 411.
[4] D. G. DERVICHIAN, *Ann. Chim. Rome*, 40 (1950) 300.
[5] A. F. CULLIS, H. MUIRHEAD, M. F. PERUTZ, M. G. ROSSMAN AND A. C. T. NORTH, *Proc. Roy. Soc. London, Ser. A*, 265 (1962) 161.
[6] J. E. BENNETT, J. F. GIBSON AND D. J. E. INGRAM, *Proc. Roy. Soc. London, Ser. A*, 240 (1957) 67.
[7] J. F. NYE, *Physical Properties of Crystals*, Oxford University Press, New York, 1957, p. 60.
[8] J. J. HERMANS, *Flow Properties of Disperse Systems, Interscience*, New York, 1953, p. 137.
[9] S. J. GILL, C. P. MALONE AND M. DOWNING, *Rev. Sci. Instr.*, 31 (1960) 1299.
[10] E. PONDER, *J. Gen. Physiol.*, 29 (1945) 89.
[11] D. H. WIFFIN, *Free Radicals in Biological Systems*, Academic Press, New York, 1961, p. 227.

Received April 21st, 1962

Preliminary Notes

PN 1197

Ring currents in 3:4-benzpyrene, 1:2-benzanthracene, and 1:2;5:6-dibenzanthracene

The work of the PULLMANS and others aimed at relating the electronic configuration of aromatic hydrocarbons to their carcinogenic potency (a theory well summarized by COULSON[1]) has been at least moderately successful. As some of the theory rests on molecular-orbital calculations it is of interest to re-examine the range of validity of molecular-orbital theory as applied to polycyclic hydrocarbons by making theoretical predictions based on the theory which can be checked directly experimentally. In this note, we shall make use of a modification due to MCWEENY[2] of LONDON's[3] theory of diamagnetic anisotropy in aromatic molecules, which is based directly on molecular-orbital theory. We shall obtain theoretical predictions of the π-electron ring currents in several carcinogenic polycyclic hydrocarbons. As these ring currents are responsible not only for diamagnetic anisotropy but also for nuclear-magnetic-resonance chemical shifts the predictions are subject to rather rigorous experimental test. Similar calculations by BERTHIER *et al.*[4], based on LONDON's unmodified theory, predict the total induced moment, but not the individual ring currents.

MCWEENY has shown that the secondary magnetic field, H', at any point, arising from the diamagnetic effect of ring currents in an aromatic hydrocarbon in the presence of an external magnetic field, H, normal to the plane of the molecule, is given by

$$H' = 2\beta\left(\frac{2\pi e}{hc}\right)^2 \frac{S^2 H}{a^3}(\sigma_1 + \sigma_2),$$

where S is the area of a benzene ring, a is the length of a C–C bond, β is the standard resonance integral, and σ_1 and σ_2 are sums involving bond orders and mutual bond polarizabilities obtained from normal (unperturbed) molecular-orbital theory. The

expression can be simplified for practical calculations by a suitable unitary transformation, and it can be shown that the results can be put in the form

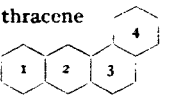
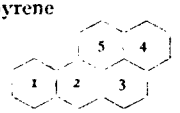
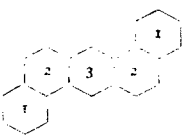
$$H' = -2\beta\left(\frac{2\pi e}{hc}\right)^2 \frac{S^2H}{a^2} \Sigma_l J_l K(\vec{r}_l),$$

where the sum goes over all rings and the $K(\vec{r}_l)$ are defined functions. The J_l are then identified as the ring currents.

We have subjected three polycyclic hydrocarbons to this analysis: the extremely potent carcinogen 3:4-benzpyrene, the mildly carcinogenic 1:2; 5:6-dibenzanthracene; and 1:2-benzanthracene, only very weakly active itself, but numbering among its monomethyl and dimethyl derivatives many carcinogens of widely varying potency. The results are given in Table I (compare with the value 1/9 for benzene).

TABLE I

RING CURRENTS

Molecule	*Ring No.*	*Ring current*
1:2-Benzanthracene 	1	0.1243
	2	0.1412
	3	0.0990
	4	0.1247
3:4-Benzpyrene 	1	0.1338
	2	0.1422
	3	0.0933
	4	0.1435
	5	0.1196
1:2; 5:6-Dibenzanthracene 	1	0.1264
	2	0.1048
	3	0.1432

I should like to acknowledge the assistance of Mr. K. J. FRITZ, who helped with the computer work. This investigation was supported by the National Institute of Health, grant No. C-6401 BBC.

University of South Carolina, Columbia, S.C. (U.S.A.) J. D. MEMORY

[1] C. A. COULSON, *Advan. Cancer Res.*, 1 (1953) 56.
[2] R. MCWEENY, *Mol. Phys.*, 1 (1958) 175.
[3] F. LONDON, *J. Phys. Radium*, 8 (1937) 397.
[4] G. BERTHIER, M. MAYOT, A. PULLMAN AND B. PULLMAN, *J. Phys. Radium*, 13 (1952) 15.

Received September 5th, 1962