References

1. Amos, A. T., and L. C. Snyder: J. chem. Physics **41**, 1773 (1964).
2. Snyder, L. C., and A. T. Amos: J. chem. Physics **42**, 3670 (1965).
3. Harriman, J. E.: J. chem. Physics **40**, 2827 (1964). — Sando, K. M., and J. E. Harriman: J. chem. Physics **47**, 130 (1967); **48**, 5138 (1968).
4. See, for example, Hinchliffe, A.: Theoret. chim. Acta (Berl.) **5**, 451 (1966). — Atherton, N. M., and A. Hinchliffe: Molecular Physics **12**, 349 (1967).
5. Hinchliffe, A.: Theoret. chim. Acta (Berl.) **8**, 300 (1967).
6. Pariser, R., and R. G. Parr: J. chem. Physics **21**, 466, 767 (1953). — Pople, J. A.: Trans. Farad. Soc. **49**, 1375 (1953).
7. Mataga, N., and K. Nishimoto: Z. physik. Chem. **13**, 140 (1957).
8. Parr, R. G.: J. chem. Physics **20**, 1499 (1952).
9. Fessenden, R. W., and R. H. Schuler: J. chem. Physics **39**, 2147 (1963).
10. Koutecký, J.: J. chem. Physics **46**, 2443 (1967).

Dr. D. R. Burnham
Department of Chemistry
University of York
Heslington, York, England

Theoret. chim. Acta (Berl.) 13,432 (1969)

Erratum

Calculation of Hyperfine Field and Quadrupole Splitting in Ferriprotoporphyrin IX Chloride (Hemin)

M. F. RETTIG, P. S. HAN, and T. P. DAS

Theoret. chim. Acta (Berl.) **12**, 178—182 (1968)

Received March 17, 1969

The sign of q in Eq. (7) is incorrect, necessitating the following changes: 1. the summation in Eq. (7) should be preceded by a minus sign; 2. the first two lines after Eq. (8) should have $q = -.6626 a_0^{-3}$ and $\Delta E = -.73$ mm/sec; 3. in the table on p. 181, the column headings should be preceded by minus signs; 4. in the first line after this table, replace the word "positive" by "negative", and in the third line replace "negative" by "positive".

In view of these corrections, our remarks concerning good agreement of experimental and theoretical field gradient no longer apply. The conclusions concerning hyperfine field at iron are unchanged, however. Further discussion of the experimental and theoretical field gradients will be given in a forthcoming paper on N^{14} hyperfine and quadrupole interactions in hemin, to be submitted to this journal.

We are grateful to Dr. T. Moss of the IBM-Watson Laboratory, New York, for bringing the error to our attention.