

Lawrence Berkeley National Laboratory

LBL Publications

Title

COMMENT ON ""ELECTRONIC STRUCTURE OF UF6"" BY M. BORING, J.H. WOOD, and J.W. MOSKOWITZ J. CHEM. PHYS. 61, 3800 (1974).

Permalink

<https://escholarship.org/uc/item/8tr8m41f>

Author

Edelstein, N.

Publication Date

1975-05-01

0 0 0 4 3 0 7 0 7 7

Submitted to Journal of Chemical Physics

RECEIVED
LIBRARY
BERKELEY LABORATORY

LBL-4016
Preprint c.1

JUL 18 1975

LIBRARY AND
DOCUMENTS SECTION

COMMENT ON "ELECTRONIC STRUCTURE OF UF₆"
BY M. BORING, J. H. WOOD, AND J. W. MOSKOWITZ
J. CHEM. PHYS. 61, 3800 (1974)

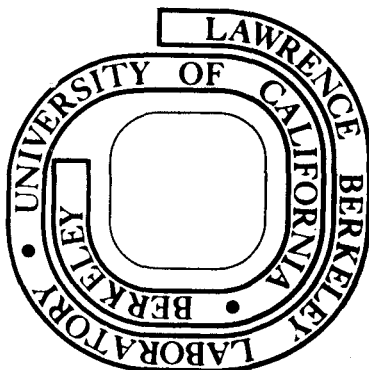
N. Edelstein and D. Karraker

May 1975

Prepared for the U. S. Energy Research and
Development Administration under Contract W-7405-ENG-48

For Reference

Not to be taken from this room



LBL-4016
c.1

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Comment on "Electronic Structure of UF_6^- "

by M. Boring, J. H. Wood, and J. W. Moskowitz
J. Chem. Phys. 61, 3800 (1974)

by

N. Edelstein

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

and

D. Karraker

E. I. duPont de Nemours & Co., Inc.
Savannah River Laboratory
Aiken, South Carolina 29801

In a recent paper Boring, Wood, and Moskowitz report the results of a non-relativistic SCF- $X\alpha$ - scattered wave calculation on the UF_6^- ion. They compare their calculated orbital energy levels with experimental data published on this ion by Reisfeld and Crosby.² We wish to point out the assignments of Reisfeld and Crosby have been questioned and it is now generally agreed some aspects of their analysis were incorrect.³⁻⁷ Furthermore, a straightforward analysis of the optical and magnetic data for this ion based on the crystal field model allows a determination of the 5f orbital energies for a direct comparison with the results of the $X\alpha$ calculation.⁷ The results of such an analysis are shown in Table I. However, if the orbital reduction factors are included in the analysis the 5f orbital energies derived from the data will shift markedly.⁸ At this time there have been no unambiguous determinations of the orbital reduction factors.

The main conclusions (based upon their calculation and its approximations) of Boring, Wood, and Moskowitz are valid. Our objection to their paper is the use of data which has been shown to be incorrect.

References

1. M. Boring, J. H. Wood, and J. W. Moskowitz, *J. Chem. Phys.* 61, 3800 (1974).
2. M. J. Reisfeld and G. A. Crosby, *Inorg. Chem.* 4, 65 (1965).
3. J. L. Ryan, "MTP International Review of Science, Inorganic Chemistry Series One", K. W. Bagnall, Editor (Butterworths, London, 1972), p. 332.
4. C. J. Ballhausen, *Theoret. Chem. Acta (Berl)* 24, 234 (1972).
5. J. Selbin, C. J. Ballhausen, and D. G. Durrett, *Inorg. Chem.* 11, 510 (1972).
6. J. Ryan, *J. Inorg. Nucl. Chem.* 33, 153 (1971).
7. N. Edelstein, D. Brown, and B. Whittaker, *Inorg. Chem.* 13, 563 (1974).
8. N. Edelstein, unpublished results.

Table I. Results of a crystal field analysis on UF_6^- .

$\Gamma_7 - \Gamma_6$	$\Gamma_7 - \Gamma'_8$	$\Gamma_7 - \Gamma'_7$	θ	Δ	ψ
(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})	(cm^{-1})
15900 ^a	13715 ^a	7413 ^a	6882 ^b	4479 ^b	1885 ^b
			13718 ^c	4057 ^c	

^aExperimental assignments from Ref. 6.

^bResults of the crystal field analysis from Ref. 7. Nomenclature as in this reference.

^cResults of the SCF X α calculation from Ref. 1.

LEGAL NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720