

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. **PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.**

| | | |
|---|---|-------------------------------------|
| 1. REPORT DATE (DD-MM-YYYY) 10 May 2003 | 2. REPORT TYPE Technical Abstract | 3. DATES COVERED (From - To) |
|---|---|-------------------------------------|

| | |
|---|--|
| 4. TITLE AND SUBTITLE Conceptual Problems in Main Group Chemistry | 5a. CONTRACT NUMBER F04611-99-C-0025 |
| | 5b. GRANT NUMBER |
| | 5c. PROGRAM ELEMENT NUMBER |

| | |
|---|-----------------------------------|
| 6. AUTHOR(S) K. Christe, et al. | 5d. PROJECT NUMBER DARP |
| | 5e. TASK NUMBER A205 |
| | 5f. WORK UNIT NUMBER |

| | |
|---|---|
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) ERC, Inc. 10 E. Saturn Blvd. Edwards AFB, CA 93524 | 8. PERFORMING ORGANIZATION REPORT NUMBER |
|---|---|

| | |
|---|--|
| 9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048 | 10. SPONSOR/MONITOR'S ACRONYM(S) |
| | 11. SPONSOR/MONITOR'S NUMBER(S) AFRL-PR-ED-AB-2003-125 |

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

20030616 040

15. SUBJECT TERMS

| | | | | | |
|--|------------------------------------|-------------------------------------|-----------------------------------|----------------------------|--|
| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18. NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON Sheila Benner |
| a. REPORT Unclassified | b. ABSTRACT Unclassified | c. THIS PAGE Unclassified | A | | 19b. TELEPHONE NUMBER (include area code) (661) 275-5693 |

FILE

MEMORANDUM FOR PRS (In-House Contractor Publication)

07 May 2003

FROM: PROI (STINFO)

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2003-125**

K. Christe (AFRL/ERC) et al., "Conceptual Problems in Main Group Chemistry" (abstract only)

5194

226th Nat'l ACS Meeting

(New York, NY, 7-11 September 2003) (Deadline: None provided)

(Statement A)

Corley
5/21/03

Conceptual Problems in Main Group Chemistry

Karl Christe^{1,2}, David A. Dixon,³ and Jerry A. Boatz¹. (1) Air Force Research Laboratory, Edwards AFB, CA 93524, (2) Loker Research Institute, University of Southern California, Los Angeles, (3) William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, P.O. Box 999, Richland, Washington 99352.

Fax: 661-275 5471, karl.christe@edwards.af.mil

During our past work numerous issues concerning bonding situations in main group compounds were encountered that will be highlighted in this talk. Problems to be addressed include:

- (i) The steric activity of free valence electron pairs.
- (ii) The role of semi-ionic, multi-center bonding in complex fluorides, oxofluorides, and compounds containing sterically active free valence electron pairs.
- (iii) How the replacement of fluorine ligands in pentagonal bipyramidal heptafluorides by either doubly bonded oxygen ligands or free valence electron pairs influences the overall bonding.
- (iv) The difficulty of describing in the N_5^+ cation the bonding and charge distribution derived from the experimental data, with resonance structures that satisfy the octet rule.