MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)  26 September 2000


15th Winter Fluorine Conference (St. Petersburg, FL, 14 Jan 2001) (Past Deadline: 14 Sep 2000) (Statement A)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.

Comments: ________________________________________________________________

Signature ___________________________________________ Date ________________

2. This request has been reviewed by the Public Affairs Office for: a.) appropriateness for public release and/or b) possible higher headquarters review

Comments: ________________________________________________________________

Signature ___________________________________________ Date ________________

3. This request has been reviewed by the STINFO for: a.) changes if approved as amended, b.) appropriateness of distribution statement, c.) military/national critical technology, d.) economic sensitivity, e.) parallel review completed if required, and f.) format and completion of meeting clearance form if required

Comments: ________________________________________________________________

Signature ___________________________________________ Date ________________

4. This request has been reviewed by PRS for: a.) technical accuracy, b.) appropriateness for audience, c.) appropriateness of distribution statement, d.) technical sensitivity and economic sensitivity, e.) military/national critical technology, and f.) data rights and patentability

Comments: ________________________________________________________________

______________________________ Date
PHILIP A. KESSEL
Technical Advisor

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This original is for PA files
METHOD FOR SOLVING SOME DISORDERED CRYSTAL STRUCTURES AND ITS APPLICATION TO THE STRUCTURES OF NF2O+ AND SO2F-. Karl O. Christie, Ashwani Vij, Rudiger Mews, Xiongzh Zhang, Jerry Boatz., Air Force Research Laboratory, Edwards AFB, CA 93524 and University of Southern California, Los Angeles, CA 90089, University of Bremen, Bremen, Germany.

Oxygen and fluorine ligands are similar in size and frequently exhibit positional disorder in the crystal structures of oxofluorides, resulting in a partial or complete averaging of the observed bond lengths and angles. The failure to recognize the presence of disorder has resulted in the publication of numerous incorrect structures, while the recognition of disorder problems has generally prompted researchers to abandon these data sets. In this paper, a method is outlined which allows in favorable cases the extraction of the correct individual bond lengths and angles from disordered data. The method is demonstrated for the SO2F- and NOF2+ ions, and the correctness of the derived bond lengths is supported by ab initio calculations for the free ions.

ABSTRACT. Please be BRIEF—150 words maximum if possible. Title of paper should be ALL CAPS; author(s) listed by first name, middle initial, last name; indicate address with zip code.

A. DIVISION OF FLUO Division Member ☒ Yes ☐ No
B. ACS MEMBER ☒ Yes ☐ No
C. TITLE OF PAPER Method for solving some disordered crystal structures and its application to the structures of NF2O+ and SO2F–

Please indicate preference: ☒ Oral ☐ Poster ☐ withdraw if oral/poster format cannot be met
D. AUTHORS

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G. For contributed papers, do authors meet criteria outline in ACS Bylaw VI, Section 6(3)? See instructions.

☐ Yes ☐ No

NOTE: ALL PRESENTING AUTHORS MUST REGISTER FOR THE MEETING—EITHER FULL MEETING REGISTRATION OR ONE-DAY REGISTRATION FOR THE DAY OF PRESENTATION.

H. Specify Equipment Required for Presentation Other than 2" x 2" (35 MM) slide or overhead (transparency) projector. There may be a charge to the individual or division for equipment. Please check with Program Chair.

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