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MEMORANDUM FOR PR (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

18 Apr 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-075**
Vij, V., Boatz, J.A., Tham, F., Vij, A., and Christe, K.O., "On the Lewis Acidity of LiF" (Abstract)

16th International Symposium of Fluorine Chemistry
(Durham, UK, 23 Jul 00) (Submission Deadline: 18 Apr 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.

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PHILIP A. KESSEL Date
Technical Advisor
Propulsion Science and Advanced Concepts Division

ON THE LEWIS ACIDITY OF LiF

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Based on the recently developed pF^- Lewis acidity scale,¹ free gaseous LiF is a surprisingly strong Lewis acid, comparable to SiF_4 . It was therefore of interest to study whether a strong Lewis base, such as CsF, could transfer a fluoride ion to LiF with formation of a LiF_2^- anion. Theoretical calculations were carried out for LiF_2^- and show that free gaseous LiF_2^- is a linear, vibrationally stable species. Furthermore, the phase-diagram of the LiF/CsF system shows a eutectic at a 1:1 mole ratio that gives a distinct X-ray powder diffraction pattern.² We have prepared this eutectic by fusion of a 1:1 mixture of LiF and CsF in a platinum crucible. Single crystals were obtained by slow cooling of the melt in a dry nitrogen stream. The resulting product was characterized by vibrational spectroscopy, and its crystal structure was determined. It is shown that $CsLiF_2$ does not contain isolated LiF_2^- anions, but exhibits an interesting three-dimensional network of alternating tetra-coordinated LiF_4 and octa-coordinated CsF_8 units.

1. K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy and J. A. Boatz, *J. Fluorine Chem.*, 2000, **101**, 151.
2. D. L. Deadmore and J. S. Machin, *J. Phys. Chem.*, 1960, **64**, 824.