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MEMORANDUM FOR PRS (In-House/Contractor Publication)

FROM: PROI (STINFO)

12 June 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2002-140**
Karl Christe (ERC) et al., "Nitrogen Fluoride Chemistry" (abstract)
↳ 55194 (unofficial notification)
ACS Meeting
(20 August 2002, Boston, MA)

(Statement A)

Dr. Corley
55881

Nitrogen Fluoride Chemistry

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The isomerization of trans-N_2F_2 to cis-N_2F_2 going through $N_2F^+AsF_6^-$ is unpredictable, erratic, requires 2 steps, and consumes an equimolar amount of AsF_5. It was found that catalytic amounts of SbF_5 at 30C can achieve this isomerization, but still result in substantial N_2F_2 losses due to $N_2F^+SbF_6^-$ formation. When the reaction is carried out at 60C, surprisingly $NF_4^+SbF_6^-.nSbF_5$ is formed. The crystal structures of $N_2F^+SbF_6^-$ (disordered), $N_2F^+SbF_6^-$ (disordered), $N_2F^+Sb_2F_{11}^-$ (ordered), and $NF_4^+Sb_2F_{11}^-$ were determined and are discussed. AlF_3 was also studied as a catalyst for the N_2F_2 isomerization and was found to be an ideal catalyst resulting in very high conversions of trans-N_2F_2 and high yields of cis-N_2F_2. The AlF_3 can be used repeatedly without loss of activity or N_2F^+ salt formation. Cis-N_2F_2 forms with SnF_4 at low temperatures a 2:1 salt, $(N_2F^+)2SnF_6^{2-}$, that slowly loses N_2F_2 at room temperature to give $N_2F^+SnF_5^-$. The crystal structure of $H_3NF^+CF_3SO_3^-$ was also determined and exhibits a relatively long N-F bond.

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