

REPORT DOCUMENTATION PAGEForm 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) 28 March 2003		2. REPORT TYPE Abstract		3. DATES COVERED (From - To)	
4. TITLE AND SUBTITLE Structural Effects on the Physical Properties of Ionic Liquids				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Greg Drake, Tom Hawkins, John Wilkes				5d. PROJECT NUMBER 2303	
				5e. TASK NUMBER M2C8	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/PRSP 10 E. Saturn Blvd. Edwards AFB, CA 93524-7680				8. PERFORMING ORGANIZATION REPORT NUMBER AFRL-PR-ED-AB-2003-077	
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-2003-077	
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited.					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
20030807 070					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT A	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Sheila Benner
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (include area code) (661) 275-5963

FILE

MEMORANDUM FOR PRS (In-House Publication)

FROM: PROI (STINFO)

31 Mar 2003

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2003-077**
Greg Drake and Tom Hawkins (AFRL/PRSP); John Wilkes (USAF Academy), "Structural Effects on
the Physical Properties of Ionic Liquids"

Drake
5355

AFOSR Molecular Dynamics and Theoretical Chemistry Contractors Meeting (Statement A)
(San Diego, CA, 18-20 May 2003) (Deadline: 14 Apr 2003)

Hawkins

Structural Effects on the Physical Properties of Ionic Liquids

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Recently work using ionic liquids has risen exponentially in both academic research efforts as well as by industrial large-scale organic synthesis. Much of these efforts have centered around the use of di-alkyl substituted imidazolium salts with an array of anions, many of which are commercially available. The pioneering work carried out by the USAF in the last several decades has shed some light upon some of the physical property effect relationships of increasing the alkyl side chain length of these imidazolium cations with viscosities, melting points, hygroscopicity/hydrophobicity, and densities. However, most researchers in the field today are forging efforts in using ionic liquids in various aspects of synthesis and separations, as part of the environmentally driven "green chemistry" efforts. In our efforts we are coming to terms with what really drives the physical properties of ionic liquids and how we are beginning to understand the cation anion interactions. Discussions will focus on factors including size and shape of both the cation and anion, hydrogen bonding, charge delocalization on either/both cation and/or anion, in our quest to design, synthesize and characterize new ionic liquids of interest.

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