

AD

AD-E403 057

Contractor Report ARAET-CR-05005

AQUEOUS SOLUBILITY OF CL-20

P. Karakaya
M. Sidhoum
C. Christodoulatos
Stevens Institute of Technology
Center for Environmental Technology
Castle Point on the Hudson
Hoboken, NJ 07030

Wendy Balas
Steven Nicolich
Project Engineers
ARDEC

August 2005



**ARMAMENT RESEARCH, DEVELOPMENT AND
ENGINEERING CENTER**

Armaments Engineering & Technology Center

Picatinny, New Jersey

Approved for public release; distribution is unlimited.

20050816 093

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinion of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Destroy this report when no longer needed by any method that will prevent disclosure of its contents or reconstruction of the document. Do not return to the originator.

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-01-0188	
The 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 the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the 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) August 2005		2. REPORT TYPE		3. DATES COVERED (From – To)	
4. TITLE AND SUBTITLE AQUEOUS SOLUBILITY OF CL-20				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHORS P. Karakaya, M. Sidhoum, and C. Christofoulatos, Stevens Institute of Technology Wendy Balas and Steven Nicolich, Project Engineers, ARDEC				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Center for Environmental Technology USA ARDEC, AETC Stevens Institute of Technology Energetics, Warheads & Environmental Castle Point on the Hudson Technology (AMSRD-AAR-AEE-W) Hoboken, NJ 07030 Picatinny, NJ 07806-5000				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) USA ARDEC, EM Technical Research Center (AMSRD-AAR-EMK) Picatinny, NJ 07806-5000				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) Contractor Report ARAET-CR-05005	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT The Energetics and Warheads Division of the U.S. Army Armament Research, Development and Engineering Center has been involved in the development of CL-20. An aqueous solubility study was performed to better understand the fate and transport of CL-20 through environmental systems.					
15. SUBJECT TERMS Aqueous solubility CL-20					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			W. Balas/S. Nicolich
U	U	U	SAR	9	19b. TELEPHONE NUMBER (Include area code) (973) 724-4919

CONTENTS

	Page
Introduction	1
Aqueous Solubility Setup	1
Results and Discussion	1
Bibliography	3
Distribution List	6

INTRODUCTION

CL-20, also known as HNIW (2,3,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane), is a high energy, high density material. Concerns regarding the environmental fate and transport of CL-20 are arising due to its potential introduction into soil and water matrices. Work is currently being conducted to study the fate and transport of CL-20 in soil and water matrices. Determination of solubility characteristics of CL-20 in water is a preliminary task necessary to begin other fate and transport studies. The aqueous solubility of CL-20 was measured over a broad temperature range and the data were fitted to a generalized solubility model.

AQUEOUS SOLUBILITY SETUP

The solubility experiments investigated the effects of temperature on the concentration of CL-20 in the aqueous phase. All tests used un-ground CL-20 manufactured by ATK Thiokol Propulsion, Brigham City, Utah. The aqueous solubility of CL-20 was measured at temperatures ranging from 4 to 69°C. Solutions were prepared by adding excess amounts of the solid compound (0.15 g) in flasks containing deionized water (300 mL). Experiments were conducted in a water bath and the temperature was controlled within $\pm 0.5^\circ\text{C}$. A three-blade propeller rotated by an overhead lab stirrer (Stirpak model 4554-10, Cole Parmer) was used to stir the mixture at 150 rpm. Once thermodynamic equilibrium was established at a given temperature, three samples (2 mL each) were withdrawn with a syringe, filtered through 0.2 μ polypropylene filters (Whatman Puradisc 25-PP) and immediately diluted with acetonitrile (1:1 by volume) to avoid precipitation. To overcome CL-20 adsorption losses during filtration, it was necessary to discard the first 0.5 mL of the filtered samples. To avoid re-crystallization of CL-20, all the hardware used for sampling and filtration was equilibrated at the test temperature.

RESULTS AND DISCUSSION

Aqueous solubility data for CL-20 at 12 temperatures are presented in table 1 and plotted in figure 1. The solubility equation used to fit the curve is generally used for compounds that do not ionize or dissociate in solution and where the solid phase is pure. The equation is

$$\ln(x) = A + \frac{B}{T} + C \ln(T) \quad (1)$$

where

$$A = -\ln(\gamma) + \frac{\Delta H_m}{RT_m} - \frac{\Delta C_p}{R} \{\ln(T_m) - 1\} \quad (2)$$

$$B = \frac{\Delta C_p}{R} T_m - \frac{\Delta H_m}{R} \quad (3)$$

$$C = \frac{\Delta C_p}{R} \quad (4)$$

and where x is the solubility expressed in mole fraction at the prevailing absolute temperature $T(^{\circ}\text{K})$. The correlation constants A, B, and C obtained by non-linear analysis of the solubility data versus temperature data ($R^2=0.9991$) are -511.12, 19,063.26, and 75.76, respectively.

The results show that CL-20 solubility increases with temperature. There is about a 17.5-fold increase in solubility as temperature rises from 4 to 69°C. At ambient temperature, the solubility of CL-20 was found to be 4.33 mg/L. The aqueous solubility of CL-20 is significantly lower than that of RDX.

Table 1
Aqueous solubility of CL-20 as a function of temperature

Temperature ($^{\circ}\text{C}$)	Solubility of CL-20	
	(mg/L)	Mole fraction
4	2.27 (± 0.09)	$9.33 \cdot 10^{-8}$
19.5	3.11 (± 0.06)	$1.41 \cdot 10^{-7}$
25	4.33 (± 0.04)	$178 \cdot 10^{-7}$
30	5.46 (± 0.02)	$2.26 \cdot 10^{-7}$
35	6.69 (± 0.01)	$2.86 \cdot 10^{-7}$
39	8.10 (± 0.06)	$3.33 \cdot 10^{-7}$
45	11.30 (± 0.25)	$4.64 \cdot 10^{-7}$
50	14.16 (± 0.47)	$5.82 \cdot 10^{-7}$
55	17.37 (± 0.17)	$7.14 \cdot 10^{-7}$
60	23.98 (± 0.41)	$9.85 \cdot 10^{-7}$
65	32.36 (± 1.03)	$1.33 \cdot 10^{-6}$
69	39.68 (± 0.25)	$1.63 \cdot 10^{-6}$

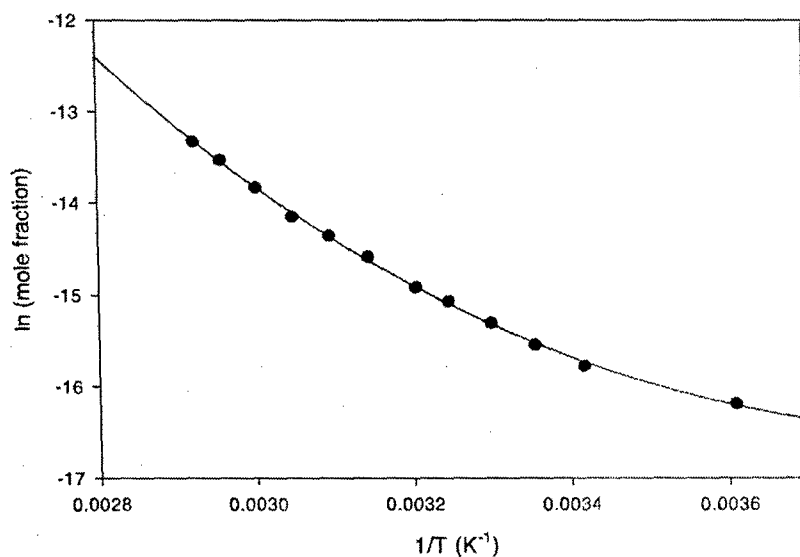


Figure 1
Solubility of CL-20 expressed in mole fraction as a function of temperature
(• experimental data and --- equation 1 fitted to the data)

BIBLIOGRAPHY

1. EPA Water Solubility: Column Elution Method; Shake Flask Method, Product Properties Test Guidelines, OPPTS 830.7840, 1996.
2. Qasim, M.; Flemming, B; and Hansen, L., "An Approximation Methods Study and Comparison of the Chemical and Physical Properties of CL-20 and RDX for Prediction of Reactivities," Proceedings of Curr. Trends Comp. Chem., 184-187, 2000.

DISTRIBUTION LIST

USA ARDEC

ATTN: AMSRD-AAR-EMK (2)
AMSRD-AAR-GC
AMSRD-AAR-AEE, C. Anderson
AMSRD-AAR-AEE-W, W. Balas (5)
S. Nicolich

Picatinny, NJ 07806-5000

Defense Technical Information Center (DTIC)

ATTN: Accessions Division
8725 John J. Kingman Road, Ste 0944
Fort Belvoir, VA 22060-6218

Commander

Soldier and Biological/Chemical Command
ATTN: AMSSB-CII, Library
Aberdeen Proving Ground, MD 21010-5423

Director

U.S. Army Research Laboratory
ATTN: AMSRL-CI-LP, Technical Library
Bldg. 4600
Aberdeen Proving Ground, MD 21005-5066

Chief

Benet Weapons Laboratory, AETC
U.S. Army Research, Development and Engineering Command
Armament Research, Development and Engineering Center
ATTN: AMSRD-AAR-AEW
Watervliet, NY 12189-5000

Director

U.S. Army TRADOC Analysis Center-WSMR
ATTN: ATRC-WSS-R
White Sands Missile Range, NM 88002

Chemical Propulsion Information Agency

ATTN: Accessions
10630 Little Patuxent Parkway, Suite 202
Columbia, MD 21044-3204

GIDEP Operations Center

P.O. Box 8000
Corona, CA 91718-8000

Commander
Naval Surface Warfare Center
Indian Head Division (2)
101 Strauss Avenue
Indian Head, MD 20640

Commander
Air Force Research Laboratory
Munitions Directorate
ATTN: Energetic Materials Branch (2)
Eglin AFB, FL 32542