Provisional Recommendations

IUPAC Seeks Your Comments

Provisional recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols made widely available to allow interested parties to comment before the recommendations are finally revised and published in *Pure and Applied Chemistry*.

There are currently two documents available for review:

Quantities, Terminology, and Symbols in Photothermal and Related Spectroscopies
Comments by 31 July 2002
Chem. Int. 2002, Vol 24, No 2, p. 19

Thermochemistry of Chemical Reactions: Terminology, Symbols, and Experimental Methods for the Determination of Bond Energies
Comments by 30 September 2002
Chem. Int. 2002, Vol 24, No 3, p. 16

If you would like to comment, please visit the IUPAC Web site, where the full texts are available for downloadings as draft pdf files.

www.iupac.org/reports/provisional

Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Critical Evaluation of Proven Chemical Weapon Destruction Technologies (IUPAC Technical Report)

by Graham S. Pearson and Richard S. Magee
Pure and Applied Chemistry, Vol. 74, No. 2, pp. 187-316 (2002)

The Chemical Weapons Convention (CWC), which entered into force on 29 April 1997, prohibits the development, production, transfer, acquisition, stockpiling, and retention of chemical weapons and their use and requires all State Parties to undertake "to destroy chemical weapons it owns or possesses, or that are located in any place under its jurisdiction or control, in accordance with the provisions of this Convention." The CWC opened for signature in January 1993 and, as of May 2002, had 145 State Parties—states which have ratified or acceded to the Convention.

The Requirement for Destruction

Article IV of the Convention requires that:

> "Each State Party shall destroy all chemical weapons. . . Such destruction shall begin not later than two years after this Convention enters into force for it and shall finish **not later than 10 years after entry into force of this Convention.**" [Emphasis added]

Consequently, the deadline for destruction of chemical weapons is 29 April 2007. However, the CWC's Verification Annex includes a provision allowing a State Party to apply to the Executive Council for an extension of the deadline if it believes that it will be unable to ensure destruction of all chemical weapons within the 10-year timeframe. The Convention states that "any extension shall be the minimum necessary but in no case shall the deadline for a State Party to complete its destruction of all chemical weapons be extended beyond 15 years after entry into force of this Convention."

Five years left to destroy chemical weapons

The destruction requirements are further elaborated in Part IV(A) of the Verification Annex which *inter alia* require that the "chemicals are converted in an **essentially irreversible** way to a form unsuitable for production of chemical weapons, and which in an **irreversible** manner renders munitions and other devices unusable as such." [Emphasis added]

This report, published in *Pure and Applied Chemistry*, Vol. 74, No. 2, February 2002, pp. 187-316 is intended to provide policymakers and decisionmakers concerned with the destruction of chemical weapons with information about technologies proven to destroy chemical weapons. The IUPAC Working Party that prepared this report recognized that each country faced with destruction of chemical weapons will need to consider the quantity and nature of their weapons, the CWC requirements, and its own national laws and regulations in deciding where and how to destroy them safely with minimal impact on public health and the environment. Consequently, the report is designed to provide appropriate and relevant information on the proven and available destruction technologies in order to help countries arrive at informed national decisions appropriate for their circumstances.

As already noted, the CWC requires that all declared chemical weapons be destroyed within 10 years after its entry into force, with a possible extension, should that be necessary, for up to five years, which would be until 29 April 2012. The CWC also sets out requirements for the destruction of old and abandoned chemical weapons, which will continue to be found for decades in countries where chemical weapons have been produced, tested, stored, and used. There are, thus, two principal categories of chemical weapons:

1. **Stockpiled chemical weapons**, which have to be destroyed by 29 April 2007 with a possible extension to 29 April 2012; and
2. **Old and abandoned chemical weapons**, in unknown types and quantities, which will be found from time to time and will need to be destroyed also by 29 April 2007 unless the Executive Council decides to modify the provisions on the time limit.

The report starts by addressing in its first chapter the mandate for destruction. The second chapter provides a historical perspective on the type of chemicals that have been used in chemical weapons during the past century and then the third chapter addresses the nature of the problem. The report notes that many chemical weapons have been destroyed or disposed of by methods that are no longer accepted. Indeed, the CWC specifically prohibits "dumping in any body of water, land burial, and open pit burning." During the past 40 years, over 20 000 agent-tonnes of chemical weapons have been destroyed; more than 70% by incineration and the remainder by neutralization. As of October 2001, the United States had destroyed over 20 percent of its stockpiled chemical weapons—around 6 700 agent-tonnes—using incineration. [Note: the unit used in the IUPAC Technical Report for the quantities of chemical weapons destroyed is agent-tonnes and **not** the weight of munitions.]

According to the Organization for the Prohibition of Chemical Weapons (OPCW), as of 30 June 2001, 69 862 agent-tonnes of chemical weapons have been declared and 5 734 agent-tonnes of chemical weapons have been destroyed under OPCW supervision since the CWC entered into force. The principal contributors to the global stockpile are the United States and the Russian Federation. The United States has declared its stockpile to be some 31 495 agent-tons (short tons), which corresponds to 28 570 agent-tonnes. The Russian Federation has declared its stockpile to be about 40 000 agent-tonnes. As India and one other country, known from non-OPCW information to be South Korea, have also declared chemical weapons, the combined stockpiles for these two countries can be deduced to be about 1 500 agent-tonnes.

In addition to stockpiled chemical weapons, there are also quantities of old and abandoned chemical weapons in several countries around the world. The following State Parties to the CWC have made declarations of old and abandoned chemical weapons:

- Belgium
- Canada
- China
- France
- Germany
- Italy
- Japan
- Panama
- Slovenia
- United Kingdom
- United States

The old and abandoned weapons in Europe are primarily from World War I and in China from World War II.

The quantity of chemical weapons that have been destroyed during the past 40 years in a number of countries has been in excess of 20 000 tonnes. The majority, over 16 000 tonnes, has been destroyed by incineration, while 4 000 tonnes have been destroyed by neutralization. Yet, there remain some 64 000 agent-tonnes of declared weapons to be destroyed by 29 April 2007.

Destruction Technologies

It is important to recognize that the destruction technology is only one part of the overall process of safely disposing of chemical weapons. The technology destroys the chemical agents and decontaminates their containers, while creating residual effluent streams of gas, liquid, or solid. The treatment of these effluent streams so they can be discharged to the environment with minimal impact on public health and the environment is as important as the destruction technology itself.

Because these chemical agents were produced to cause harm, steps were never taken to ensure that they were particularly pure. The original considerations were simply that the agent should be effective and should have sufficient stability to be stored for a number of years. Destruction and disposal are consequently made more complex because the agents are likely to contain impurities and materials such as solvents that were present when originally produced, as well as degradation products generated during storage. Many stockpiled chemical weapons are over 40-years old and the nature of their contents is variable and uncertain. Therefore, destruction technologies and effluent treatments must be robust to handle a wide range of impurities and agent compositions.

The fourth chapter of the IUPAC Technical Report addresses the transportation of chemical weapons and bulk agent from storage depots or other locations where chemical weapons have been found to sites at which they are destroyed. In the following chapter, the various options for the removal of the agents from weapons are considered. The next two chapters examine the high-temperature and low-temperature technologies that have been used—or are being considered for use—to destroy chemical agents. The report identifies the following processes as having been sufficiently and successfully demonstrated with actual chemical warfare agents to be considered for use within the timeframe of the CWC requirement.

High-Temperature Destruction of Chemical Agents

- Incineration
- Plasma Pyrolysis
- Molten Metal Technology
- Hydrogenolysis
- Destruction of Arsenical Agents

Low-Temperature Destruction of Chemical Agents

- Hydrolysis of Mustard Agent
- Hydrolysis of Mustard and Nerve Agents using Aqueous Sodium Hydroxide
- Reaction of Mustard and Nerve Agents using Amines and Other Reagents
- Electrochemical Oxidation
- Solvated Electron Technology

It should be noted that there is wide variation in the technical maturity of these technologies. The additional development required for some of these technologies makes it highly problematic that they will be sufficiently advanced to use within the CWC treaty timelines. These technologies may, however, have application for the destruction of old and abandoned chemical weapons. Again, it may be possible for the CWC treaty timeline for these weapons to be modified should the State Party concerned make such a request.

A separate chapter of the report addresses the treatment of gas, liquid, and solid effluent. A subsequent chapter considers how to deal with abandoned chemical weapons, which will be found intermittently in unknown types and quantities in many countries for decades to come. References are provided throughout the report to assist those seeking additional detail.

National Decisions and National Circumstances

A final chapter considers the technologies and constraints that have to be considered by a country faced with making informed decisions about destruction of chemical weapons. The IUPAC Working Party recognized that chemical agents are highly toxic chemicals that primarily became available for use in chemical

weapons programs from ongoing work in chemistry. There is thus a sense in which chemical agents are merely members of a vast array of chemicals of varying toxicity. Consequently, there is a logic in considering the destruction of chemical agents as being no different from the destruction of other highly toxic chemicals. **Chemical agents, therefore, need not be regarded as being a special class of materials whose destruction demands unique precautions—they are merely members of the vast family of chemicals and their destruction, as that of any chemical, requires appropriate precautions to safeguard worker safety, public health, and the environment.**

The working party is acutely aware that much of the information presented in the report is based on U.S. experience. Indeed, one member of the IUPAC Working Party (Richard S. Magee) was chairman of the U.S. National Research Committee’s 1996 Panel on “Review and Evaluation of Alternative Chemical Disposal Technologies.” However, this is hardly surprising as the United States and the Russian Federation had by far the largest stockpiles of chemical weapons and agents anywhere in the world. The United States has made much progress in destroying its stockpile of chemical weapons and agents and has also done more work than any other country to examine alternative technologies for the destruction of chemical weapons and agents. The report, therefore, drew heavily from the U.S. experience. **However, the decisions to be made by countries faced with the destruction of chemical weapons and agents need to be made in light of the particular national conditions and standards—and thus may well result in a decision to use different approaches from those adopted by the United States.** Other countries will need to consider the size and nature of their chemical weapons in deciding both where and how to destroy them in accordance with CWC requirements and how to do this safely with minimal impact on public health and the environment. The aim of the IUPAC Technical Report is to provide information on the available destruction technologies in order to help countries arrive at appropriate, informed decisions.

Graham S. Pearson was chairman of the IUPAC Working Party which prepared this Technical Report and is a professor of international security in the Department of Peace Studies at the University of Bradford, Bradford, West Yorkshire, United Kingdom. Prior to 1995, he was director-general and chief executive of the Chemical and Biological Defence Establishment at Porton Down, United Kingdom.

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www.iupac.org/publications/pac/2002/7402/7402x0187.html

Definitions of Basic Terms Relating to Polymer Liquid Crystals (IUPAC Recommendations 2001)

by M. Barón and R. F. T. Stepto

Pure and Applied Chemistry, Vol. 74, No. 3, pp. 493-509 (2002)

This document provides definitions of the basic terms that are used in the field of liquid-crystalline polymers. It is the result of extensive discussions and evaluations by the former Commission of Macromolecular Nomenclature. It was produced with the cooperation and advice of representatives of the International Liquid Crystal Society.

The recommendations concern terminology relating to the structure of liquid-crystalline polymers. In view of the rapid growth of the field, the terms defined have been restricted to those presently in common usage. They have been selected from the recently published comprehensive document "Definitions of Basic Terms Relating to Low-Molar-Mass and Polymer Liquid Crystals" [(*Pure and Applied Chemistry*, 73(5) 845-895 (2001)].

The recommendations are intended to form a readily usable guide for the reader interested in the structural description of polymer liquid crystals. The more comprehensive document (vide supra) should be used for terminology associated with mesophases and the optical textures and physical characteristics of liquid-crystalline materials. The numbering of terms in the document is consistent within itself and cross-references are made to the numbering of terms in the more comprehensive document.

The document contains the following sections: introduction, general definitions, and liquid-crystalline polymers. It also contains a reference list and an alphabetical index of terms that serves as a subject index. The general definitions section gives the definitions of 27 principal terms and some subsidiary terms concerned mainly with the types of mesophase and types of mesogen; one example is reproduced below. The section dealing specifically with liquid-crystalline polymers defines 12 terms and gives 21 structural examples.

2.7 [2.10] mesogenic group, mesogenic unit, mesogenic moiety

A part of a molecule or macromolecule endowed with sufficient anisotropy in both attractive and repulsive forces to contribute strongly to mesophase or, in particular, LC mesophase formation in low-molar-mass and polymeric substances.

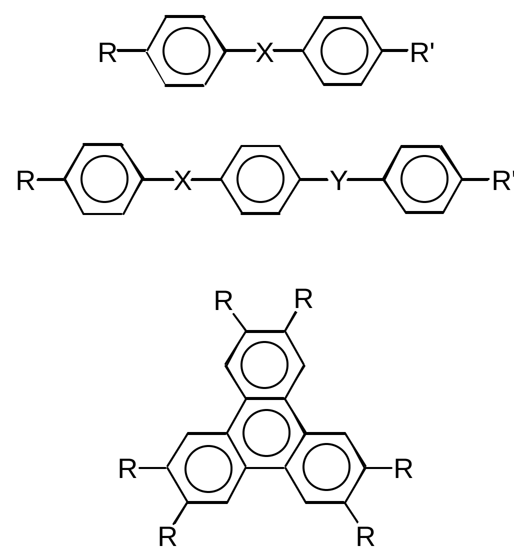
Notes:

1."Mesogenic "is an adjective that in the present document applies to molecular moieties that are structurally compatible with the formation of LC phases by the molecular system in which they exist.

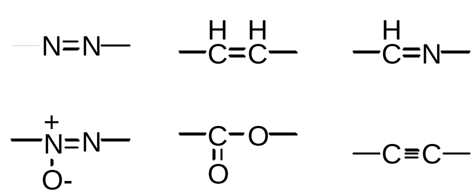
2.Mesogenic groups occur in both low-molar-mass and polymeric compounds.

3.A majority of mesogenic groups consists of rigid rod- or disc-like molecular moieties.

Examples



where X and Y are covalent bonds or linking units such as:



www.iupac.org/publications/pac/2002/7403/7403x0493.html