

June 24, 2013

Ms. Lara Phelps Director, Forum on Environmental Measurements United States Environmental Protection Agency Office of the Science Advisor 109 TW Alexander Drive (E234-05) Research Triangle Park, NC 27709

**RE: Compound Identification Inconsistency** 

Dear Ms. Phelps:

Recently, the Environmental Laboratory Advisory Board (ELAB), a standing Federal Advisory Committee to the U.S. Environmental Protection Agency (EPA or the Agency), was made aware of the inconsistent naming and identification of a specific organic compound of concern among EPA programs and program offices that has resulted in the inconsistent reporting of a frequently targeted organic compound. This inconsistency is causing considerable frustration among laboratories and data users and requires prompt corrective action by the Agency.

ELAB has prepared recommendations to address this issue, which are detailed in the attached document. ELAB is requesting that the Forum on Environmental Measurements initiate prompt action to resolve this situation based on ELAB's recommendations.

ELAB appreciates the opportunity to bring this matter to the Agency's attention and provide input for resolution. If any additional assistance is needed, ELAB is available to aid in establishing a solution.

Sincerely,

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Patsy Root Chair, Environmental Laboratory Advisory Board



## COMPOUND NAMING AND IDENTIFICATION INCONSISTENCY 2, 2'-oxybis (1-chloropropane) vs. bis (2-chloroisopropyl) ether

## Background.

The nomenclature and identity of a frequently monitored semivolatile organic compound has been tagged with conflicting compound names and Chemical Abstracts Registry Numbers (CAS) depending on the EPA program office responsible for preparing the regulated compound list. The compound, 2, 2'-oxybis (1-chloropropane) with CAS number 108-60-1, has been an EPA semivolatile compound of interest since at least the beginning of the EPA Contract Laboratory Program (CLP). The inconsistent names and CAS number assignments have caused confusion among laboratories and data users and in many cases have resulted in the inaccurate reporting of the compound in regulatory monitoring situations.

EPA has attempted to resolve the issue. Unfortunately, each program office that was involved addressed the solution independently. Accordingly, the solutions implemented by the CLP, Office of Water, and Office of Resource Conservation and Recovery (ORCR) all differ. Data users are understandably confused and insist that laboratories report the analytical results for an incorrectly listed compound.

## Nomenclature and Identity Inconsistencies.

The identity issues seem to have originated when compound CAS 108-60-1 was incorrectly assigned the name bis (2-chloroisopropyl) ether. This name is more appropriately assigned to CAS 39638-32-9 based on its chemical structure as depicted in the following structural diagrams.



CAS 108-60-1



CAS 39638-32-9

The most logical choice for the name and CAS number of the intended target compound is 2, 2'oxybis (1-chloropropane), which is the only one of the two compounds in question that has ever been in industrial production. Bis (2-chloroisopropyl) ether has never been produced and is therefore unlikely to be a compound of monitoring concern. Furthermore, it is not possible to procure standard reference materials for the compound with CAS 39638-32-9. Accordingly, the compound of regulatory concern for all EPA program offices should be 2, 2'-oxybis (1chloropropane), CAS 108-60-1. <u>The CLP Solution</u>. Exhibit C of OLM 4.x in the CLP Statement of Work lists 2, 2'-oxybis (1-chloropropane) with CAS 108-60-1. This is the correct name and the correct CAS. There is a footnote stating that the compound was formerly called bis (2-chloroisopropyl) ether.

<u>The 40 CFR 136 Solution</u>. Table 1C lists 2, 2'-oxybis (2-chloropropane), and the CAS is not listed. This is the incorrect compound, and the error likely the result of an erroneous literal translation from bis (2-chloroisopropyl) ether.

<u>The ORCR Solution</u>. Method 8270D lists bis (2-chloroisopropyl) ether with CAS 39638-32-9. This is a change of CAS number from previous versions, which had 108-60-1. The name, which was originally incorrect, was not changed; the CAS number, which was correct, was changed.

Method 8270E lists bis (2-chloro-1-methylethyl) ether with CAS 108-60-1; a footnote indicates that the name was changed in ISIS from bis (2-chloroisopropyl) ether in 2007. Although the name is correct, it is nonstandard terminology. 2, 2'-oxybis (1chloropropane) is superior and unambiguous. It also lists the correct CAS number.

## **Recommended Remedy.**

Prompt, coordinated action among all involved EPA program offices is required to resolve the confusion. ELAB strongly recommends that the CLP solution be implemented in all program offices employing the name 2, 2'-oxybis (1-chloropropane) and CAS 108-60-1 as the intended target compound. In particular, incorrect compound nomenclature at 40 CFR 136 and within SW-846 Method 8270 is responsible for much of the inaccurate data reporting. However, the incorrect nomenclature is not limited to those documents and exists in other CFR references. ELAB also recommends that all references to bis (2-chloroisopropyl) ether with CAS 39638-32-9 in regulatory compound lists be stricken from record as it is likely that this compound was never a pollutant of concern.