

An Act to Protect Children, Families and Firefighters from Harmful Flame Retardants

Questions from the Department of Environmental Protection (DEP) for the SAB and Definitions requested by the Science Advisory Board (SAB) at its March 2023 meeting

Initial questions from DEP for the SAB:

(Note order of questions is different from March presentation.)

Q1: When flame retardant (FR) chemicals identified in the law are associated with **more than one CAS number**, should all CAS numbers be included in the regulations?

Q2: Should **positional isomers and diastereomers** of the FRs identified in the law (when used as flame retardants themselves) be included in the regulations?

The Board should first consider Q1 and Q2 through the lens of chemical, structural and functional similarity and sameness of the chemicals and the intent of the law, to protect children, families and firefighters from harmful flame retardants. A second way to think about Q1 and Q2 is, do the additional CAS numbers, positional isomers and diastereomers meet the analogue definition?

Q3a: Does each proposed chemical **analogue** (identified by TURI/DEP) meet the analogue definition?

Q3b: Is each proposed **analogue** sufficiently similar to at least one chemical identified in the law such that the proposed analogue would be reasonably anticipated to have similar concerns re: toxic hazard, persistence, bioaccumulation?

Definitions requested at the March SAB meeting

CAS Numbers

CAS is a self-supporting division of the American Chemical Society.

A CAS Registry Number is a unique and unambiguous identifier for a specific substance.

Each CAS Registry Number® (CAS RN®) identifier:

- Is a unique numeric identifier
- Designates only one substance
- Has no chemical significance
- Is a link to a wealth of information about a specific chemical substance

A CAS Registry Number is assigned to a substance when it enters the CAS REGISTRY database. Numbers are assigned in sequential order to unique, new substances identified by CAS scientists for inclusion in the database.

The chemical registry number file assigns CAS registry numbers to unique chemicals for purposes of identification. Assigning a CAS number to a particular chemical facilitates managing and regulating that chemical by universally identifying it with a specific number. (Ideally) Only one CAS number is assigned to each chemical.

Isomers have their own CAS numbers. As an example cis-trans isomers can have different CAS numbers. Different stereoisomers of a substance may also have different CAS numbers while the same substance with unspecified stereochemistry has its own number. Some mixtures have CAS numbers.

The chemical registry number file assigns CAS registry numbers to unique chemicals for purposes of identification. Assigning a CAS number to a particular chemical facilitates managing and regulating that chemical by universally identifying it with a specific number. (Ideally) Only one CAS number is assigned to each chemical. Isomers have their own CAS numbers. Some mixtures have CAS numbers.

There are two possible reasons for a chemical to have multiple numbers.

- The CAS numbers could refer to **different forms** of a chemical where each is considered unique for its particular properties and characteristics. If specific research has been done on a particular form of a chemical, a separate CAS number may be assigned to that particular form to facilitate the search process in the CAS file. For example, sodium hypochlorite is listed with two CAS numbers, 7681-52-9 and 10022-70-5. The former refers to the sodium salt form of hypochlorous acid, sodium hypochlorite, while the latter refers to the pentahydrate form of sodium hypochlorite. Both forms could be called sodium hypochlorite, thus sodium hypochlorite has, in effect, two CAS numbers.
- A chemical may also be listed with multiple CAS numbers when multiple numbers have been **inadvertently assigned** to the same chemical. This multiple assignment can occur when forms of a chemical are originally believed to be unique, but after further review by chemists, are identified as the same chemical. The CAS number first assigned is the more accurate number to use when denoting the chemical. Although all of the CAS numbers will find the chemical, only the more accurate number will prompt the CAS registry file system to display the name, synonyms, and characteristics associated with the chemical. Chromic acid, listed with CAS numbers 1115-74-5 and 7738-94-5, illustrates this situation. After further review by chemists, CAS number 1115-74-5 was deleted as a registry number, but remains on file for future reference. CAS number 7738-94-5 is the more accurate number to identify chromic acid because it was the first registry number assigned.

Related Q&A about the TRI program. Answer provided by EPA.

14. We use a toxic chemical with a CAS number not on the list of Section 313 toxic chemicals. There are similar toxic chemicals on the list, but none with the same CAS number. How can I be sure I do not have to report?

Although CAS numbers are useful, **a covered facility should also use the toxic chemical name to determine if a toxic chemical is listed** on the EPCRA section 313 list. Be aware, however, that mixtures are often assigned CAS numbers. These mixtures may contain individually listed toxic chemicals. The facility should use all available information, including the toxic chemical name as well as process and chemical knowledge, to determine if a component of the mixture is a listed toxic chemical under Section 313. CAS numbers may be of limited use in this case. Also, certain specific compounds (e.g., copper chloride) are not listed individually on the EPCRA section 313 list with a specific CAS number, but are reportable under a compound category.

References: [CAS Registry](#), [EPA TRI Reporting Q&A](#)

Isomers

IUPAC Gold Book definition of isomer: One of several species (or molecular entities) that have the same atomic composition (molecular formula) but different line formulae or different stereochemical formulae and hence different physical and/or chemical properties.

Structural isomers (constitutional isomers) have the same molecular formula with different structures. They may have different bonding and will have different IUPAC names due to the locant (number) or in the substituent (suffix or prefix) (Examples: 2-methylpentane and 3-methylpentane; 1-butene and 2-butene)

- Positional (regioisomers) are a type of structural isomer with the same carbon skeleton, same functional group, differ from each other in the position of the functional group on the carbon chain. (Examples: propyl bromide and isopropyl bromide)

Stereoisomers - isomers that possess identical constitution, but which differ in the arrangement of their atoms in space.

- Diastereoisomers (or diastereomers) are stereoisomers not related as mirror images.

References: IUPAC, Masterorganicchemistry.com, Merriam-webster.com, Sciencedirect.com

Analogues

Analogue definition from the proposed regulations, was discussed among DEP, ORS and TURI:

Chemical Analogue. A compound having a structure similar to that of another compound, but differing from it in respect to a certain aspect. It can differ in one or more atoms, functional groups, or substructures, which are replaced with other atoms, groups, substructures, or in their arrangement.