

**THE UNITED KINGDOM OF GREAT BRITAIN AND NORTHERN IRELAND****THE ROLE OF CAS NUMBERS
IN THE CONTEXT OF THE CHEMICAL WEAPONS CONVENTION****1. Executive Summary**

- 1.1 The Annex on Chemicals to the Chemical Weapons Convention (hereinafter “the Annex on Chemicals”) provides information intended to identify chemicals covered by the Verification Annex to the Chemical Weapons Convention (hereinafter, “the Verification Annex”): this takes the form either of a generic description of a class of chemicals, or of a specific chemical name with a Chemical Abstracts Service (CAS) number. A very large number – even millions- of chemicals may be denoted by the generic description.
- 1.2 There are inherent difficulties associated with attempting to identify uniquely chemicals of significance to the Chemical Weapons Convention (hereinafter, “the Convention) through the use of CAS numbers. The Chemical Abstracts Service sometimes assigns to a chemical a temporary number which is later changed, causing confusion as to the correct CAS number of a particular substance. In addition, CAS numbers can be assigned to mixtures of chemicals, isomers, and isotopically-labelled chemicals. The need for the Convention to cover such forms of chemicals was stated during the negotiations of the Convention.¹ However, by no means has every chemical covered by the Convention’s Schedules of chemicals (hereinafter, “the Schedules”) been assigned a CAS number by the Chemical Abstracts Service.
- 1.3 Reliance on CAS numbers as a primary determinant of whether a chemical is covered by a Schedule would lead to uneven implementation of the Convention by States Parties. We conclude that the primary determinant of whether a chemical should be covered by a Schedule is its chemical structure as indicated by the generic class, if given, or by the specific International Union of Pure and Applied Chemistry (hereinafter, “IUPAC”) or common name. Stereoisomers of scheduled chemicals and isotopically-labelled forms of scheduled chemicals should be viewed as falling within the Schedules for declaration and verification purposes. CAS numbers are not appropriate for use in determining whether a particular chemical falls within the

¹ Ad Hoc Committee on Chemical Weapons, Identification of Chemical Substances, United Kingdom of Great Britain and Northern Ireland, CD/CW/WP.214*/12 December 1988



Schedules, as they cannot be relied upon to uniquely identify a chemical, nor have all relevant chemicals been assigned CAS numbers. However, we recognise that the wording of some of the entries in the Schedules does limit the scope for States Parties to dispense with CAS numbers in determining whether particular forms of a chemical should be subject to declaration and verification.

- 1.4 We recommend that the Executive Council take forward further discussion of this issue, with the aim of developing potential solutions to ensure that CAS numbers are not used to determine whether a chemical is covered by the Schedules. This is essential for consistent implementation of the Convention by all States Parties. One possible way forward would be to make a technical amendment to the Schedules and the Verification Annex, removing all CAS numbers, whilst retaining them for reference purposes within the Declaration Handbook, which could be updated to reflect changes to CAS numbers as required. In establishing a way forward, the Executive Council should take into account the effect that any proposals will have on States Parties' national legislation. Resolution of this issue will enable States Parties to apply verification measures in a consistent manner, leading to increased transparency and confidence in the provisions of the Convention.

2. Preface

- 2.1 Within the Schedules, groups of chemicals are categorised according to chemical class or type. Specific chemicals are identified by their IUPAC name or their common name, and by their CAS registry number. CAS numbers are numerical identifiers assigned to represent chemical substances within the CAS Chemical Registry System, established in 1965. The CAS number bears no relationship to the composition or the molecular structure of the chemical substance itself - numbers are assigned in sequential order upon entry for the first time onto the CAS Registry System.
- 2.2 This paper sets out the technical issues associated with the use of CAS numbers in relation to the Schedules, and concludes that CAS numbers are inappropriate for use as primary identifiers for scheduled chemicals. It also seeks to elucidate the criteria for identifying scheduled chemicals, through reference to specific examples.

3. Shortcomings of CAS numbers for identification purposes

- 3.1 In most cases, CAS numbers have been assigned to chemicals that possess completely defined molecular structures. Different stereoisomers (chemical compounds that have the same molecular formula as each other but a different spatial arrangement of their component atoms) and salts (in general, a stabilised form of a chemical, produced by reacting the chemical with an acid) of a chemical compound have been assigned different CAS numbers, even though they possess essentially the same chemical properties. For example, the (+)-stereo isomer of tabun has the CAS number [93957-08-5], the (-)-stereo isomer has the CAS number [93957-09-6], whilst the racemic mix (a mixture of both isomers) has the CAS number [77-81-6].
- 3.2 However, a CAS number does not always refer to a unique or unambiguously identified substance. Polymers (large molecules consisting of chains of repeating monomer units) differing only in molecular weight, chain length, monomer ratio or

percentage composition may not be differentiated; in these cases all variations bear the same CAS number. Substances for which the structural details cannot be, or have not been, sufficiently defined to establish molecular formulae, may be given a CAS number. In other cases, mixtures have been assigned their own CAS number, without specifying the ratio of compounds contained in the mixture.

- 3.3 CAS numbers can be temporarily assigned and then changed. This can cause confusion as to the correct CAS number of a particular substance.² Changing a CAS number is entirely within the authority of the Chemical Abstracts Service.
- 3.4 Not every identified chemical compound has an assigned CAS number. The Chemical Abstracts Service will assign a number to a compound, and enter its details within their registry, only following a request to do so and payment of a fee from an external body or individual.

4. CAS numbers and the Schedules.

- 4.1 The Annex on Chemicals does not make clear the significance of CAS numbers with respect to the chemicals listed in the Schedules. However, consideration of the organisation of chemicals within the Schedules gives a strong indication on technical grounds that CAS numbers are relatively unimportant in determining whether a specific chemical is covered by the Schedules. A number of individual chemicals are listed in the Schedules according to their IUPAC or common name, along with their CAS numbers. The huge majority of compounds covered by the Schedules, however, are described only by a generic class: examples of that particular class of chemical are then sometimes provided, together with the appropriate CAS number. Therefore, for most of the chemicals within each generic class, and thus the vast majority of chemicals covered by the Schedules, no CAS number is given.
- 4.2 As has already been noted by the Executive Council,³ fewer than 20% of the approximately 1200 (mainly scheduled) chemicals within the OPCW Central Analytical Database have a number assigned to them by CAS. Millions of chemicals are included within the Schedules, and described by a generic class: it is therefore likely that many of those similarly do not have a CAS number. In fact, many of these compounds will never have been synthesised.
- 4.3 It follows, therefore, that the primary determinant of whether a chemical is included in a Schedule should be its chemical structure as indicated by the generic class, or its specific IUPAC or common name, if given - not the CAS number.
- 4.4 It is necessary to clarify the effect of isotopic labelling of a scheduled chemical on its treatment under the Verification Annex. Isotopes are forms of atoms of the same chemical element that contain the same number of protons, but different numbers of neutrons. The chemical properties of isotopically-labelled compounds (those in which one or more atom in a molecule is replaced by an isotope) remain essentially unaltered. If the unlabelled form of a molecule falls within the structural description

² A specific example is that of (+)-saxitoxin, which is assigned the CAS number [35523-89-8], but had previously been successively assigned three different numbers [11017-04-2], [51938-46-6] and [55803-44-6], none of which is now valid.

³ Note by the Acting Director-General, Inclusion of Chemical Abstracts Service Registry Numbers In Lists of New Validated Data (EC-29/DG.6, dated 12 June 2002)

given by the chemical generic class name, then so will the isotopically-labelled form, regardless of the atomic nature of a particular element: the molecule as a whole will still possess a structure described by the generic class name. It should thus be covered within the Schedules for verification and implementation purposes. The same argument applies to those chemicals included within the Schedules that are described by IUPAC or common names.

- 4.5 Stereoisomers are those chemicals that have the same chemical structure as each other, but a different spatial arrangement of their component atoms. In no instance are particular stereoisomers of chemicals that are included within the Schedules specifically excluded from declaration and verification measures. Indeed, under normal conditions many scheduled chemicals exist as mixtures of stereoisomers.⁴ We therefore conclude that stereoisomers of scheduled chemicals, and mixtures thereof, should fall within the scope of the Schedules and should thus be subject to the appropriate verification provisions, regardless of whether a particular stereoisomer has been assigned a CAS number differing from the one in the Annex on Chemicals.

5. Conclusions

- 5.1 We conclude that it is inappropriate to rely upon the CAS number to define a chemical covered by the Schedules. Although relevant as an aid to declaration and verification, the CAS number should not be used as the means to identify a chemical or to determine whether a chemical is included in, or excluded from, a Schedule. Only the molecular structure of a chemical can determine whether it is covered by a Schedule entry.
- 5.2 If a chemical is included within the Schedules, then all isotopically-labelled forms and stereoisomers of the scheduled chemical should also be included, irrespective of whether or not the Chemical Abstracts Service has assigned to them a CAS number which corresponds to that listed in the Schedules. The measures detailed within the Verification Annex should be applied to such chemicals, in the same way as they are for any other scheduled chemical.
- 5.3 We recommend that the Executive Council should now take forward further consideration of these issues, and propose solutions to ensure that CAS numbers not be used to determine a chemical's inclusion within the Schedules. The United Kingdom's preference would be that a technical amendment be made to the Schedules and the Verification Annex, removing all CAS numbers, whilst retaining them for reference purposes within the Declaration Handbook. In establishing a way forward, the Executive Council should take into account the effect that any proposals will have on States Parties' national legislation. Resolution of this concern will enable all States Parties to apply verification measures, according to the provisions of the Verification Annex, in a consistent manner, leading to increased transparency and confidence in the provisions of the Convention.

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The Schedule 1 nerve agents GB, GA and VX all have two enantiomers (forms of a compound that have the same molecular structure except that one form is the mirror image of the other, like a pair of gloves) each, whilst GD has two pairs of enantiomers. For each of these cases, the CAS number provided in Schedule 1 applies only to the racemic mixture (a mixture of the enantiomers). Although individual enantiomers can be synthesised or separated, many racemise quickly under normal conditions. The United Kingdom drew attention to this issue during the negotiation of the Convention.¹