ID Card
Hexachloroiridic acid

Version 4 July 2023

Notes:

- *This ID card is used to support the substance sameness discussions in SIEFs and to describe the substance to the best of the SIEF members' knowledge.*
- *It also aims at grouping communications relevant to the request of available data or information, the approval of the proposed Lead Registrant and the registration strategy with the SIEF.*
- *It is the responsibility of each individual registrant to identify their substance and to report company-specific identity in their Registration Dossier (section 1 of IUCLID).*

1. Identification of the substance

Table 1. Identification of the substance

	Original (in EC inventory)
Name	Hexachloroiridic acid
EC number	241-012-8
CAS number	16941-92-7
Description	*Dihydrogenhexachloroiridic acid is produced by leading a dissolved salt of hexachloroiridate over an acid cation exchanger. The resulting eluate can be evaporated in order to achieve either a required concentration or to the solid Dihydrogenhexachloroiridic acid hydrate (H2IrCl6.xH2O).* *The resulting H2IrCl6.xH2O contains a variable quantity of H3IrCl6.xH2O. In addition species of H2[IrCl6] and H3[IrCl6] may be formed, in which chlorine is replaced by water like e.g. [IrCl5H2O]3-, [IrCl4(H2O)2]-. The presence of the latter species seems probable due to an analysed molar ratio of Iridium to Chlorine of ca. 1:5, which is lower than the theoretically expected ratio of 1:6.* *Because of the intermediate character of Hexachloroiridic acid and as the H3IrCl6.xH2O hydrate and the chlorine replaced species do not disturb further processing, no additional purification step is carried out.* *Due to the variable content of crystal water of both components H2IrCl6, H3IrCl6, and their chlorine-replaced species, the Hexachloridic acid is regarded as UVCB.*
Composition type	UVCB

2. Synonyms and other identifiers of the substance

Table 2. Synonyms and other identifiers of the substance

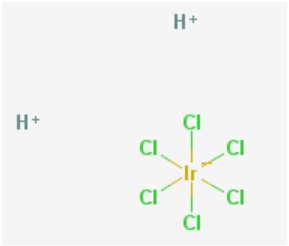
IUPAC name	hexachloroiridium(2-);hydron
CAS name	
Abbreviations	
Other commercial, brand or international names	Chloroiridic(IV) acid Hexachloroiridate Dihydrogen hexachloroiridate(IV) hydrate Hexachloroiridium(IV) acid hydrate Hydrogen iridium hexachloride Iridium(4+) chloride hydrochloride (1:4:2)
Other identity codes	

3. Substances (with core identifiers) also falling under this substance (with justification)

None

4. Information related to molecular and structural formula of the substance

Table 3. Information related to molecular and structural formula of the substance

Molecular formula	Cl6H2Ir.xH2O
Structural formula	
Smiles notation	[H+].[H+].Cl[Ir-2](Cl)(Cl)(Cl)(Cl)Cl
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	406,95 g/mol (anhydrous basis)

5. Usual composition of the substance

Hexachloroiridic acid is preferentially placed on the market in hydrated form as well as hydrochloric acid solution. The Registration Dossier covers the hydrated form only.

The composition given below represents the usual composition available to the Members of the Consortium by the date given above on the document. This usual content represents the majority of the Hexachloroiridic acid that is placed on the EEA market.

In a UVCB substance, the number of constituents is relatively large and/or; the composition is, to a significant part, unknown and/or; the variability of composition is relatively large or poorly predictable. Hence, concentration ranges outside the ones given below do not exclude sameness and are usually referred to as unusual or exceptional situations. Each potential registrant is responsible for performing its own analysis.

Hexachloroiridic acid hydrate

Table 4. Usual constituents

Name	Other names	EC number	Abbreviation / formula	Concentration range (%)	Typical concentration (%)
Dihydrogen hexachloroiridate(IV) hydrate, regarded as anhydrous form [1])		241-012-8	H_2IrCl_6	65 - 85	70,9
Trihydrogen hexachloroiridate(III) hydrate, regarded as anhydrous form [1])		233-044-6	H_3IrCl_6	7 – 20	15,3
Total crystal water [2])			xH20	8 - 25	13,2
Free acid				0 – 1,0	0,2
Several minor, especially metallic constituents	e.g. Ag, Ca, Fe, Na, Ni, Os, Pd, Pt, Rh, Ru, …			0 – 0,5	0,2
Total					**100**

[1]) Dihydrogen hexachloroiridate (H_2IrCl_6) und Trihydrogen hexachloroiridate (H_3IrCl_6) exist in hydrated forms. Both constituents are assumed to have a variable content of crystal water.

Since no analytical method is available for determination of crystal water content by default, the proper amount of crystal water cannot be assigned to the individual constituents and therefore is indicated separately as 'total crystal water'. For this reason, the concentration range and typical concentration of H_2IrCl_6 and H_3IrCl_6 as given in the table above refer formally to the anhydrous form.

Molecular weights (MW) used for calculation purposes:

- MW $(H_2IrCl_6)_{anhyd}$: 406,95 g/mol
- MW $(H_3IrCl_6)_{anhyd}$: 407,96 g/mol
- MW (Ir): 192,22 g/mol

The typical concentration of "anhydrous" H_2IrCl_6 **(%C[H_2IrCl_6]$_{anhyd}$)** and H_3IrCl_6 **(%C[H_3IrCl_6]$_{anhyd}$)** are calculated on basis of the results of the following measurements:

- Total iridium concentration:
  %C(Ir)$_{total}$ = 40,65 %
- Concentration of Ir(IV) **[%C(Ir(IV))]** and Ir(III) **[%C(Ir(III))]**:
  Concentration ratio C%[Ir(IV)] : C%[Ir(III)] = 4,65 : 1
  RV [Ir(IV)] = 4,65
  RV [Ir(III)] = 1

$$\%C[H_2IrCl_6]_{anhyd} = \frac{\%C(Ir)_{total} \times RV\ [Ir(IV)]}{\{RV\ [Ir(IV)] + RV[Ir(III)]\} \times MW[Ir]} \times MW[H_2IrCl_6]_{anhyd}$$

$$\%C[H_3IrCl_6]_{anhyd} = \frac{\%C(Ir)_{total} \times RV\ [Ir(III)]}{\{RV\ [Ir(IV)] + RV[Ir(III)]\} \times MW[Ir]} \times MW[H_3IrCl_6]_{anhyd}$$

[2]) The content of crystal water **%C[xH$_2$O]** is calculated as follows:

$$\%C[xH_2O] = 100 - \{\%C[H_2IrCl_6]_{anhyd} + \%C[H_3IrCl_6]_{anhyd} + \%C[free\ acid] + \%C[minor\ constituents]\}$$

- Concentration of free acid:
  %C(free acid) = 0,2 %
- Concentration of minor constituents:
  %C(minor constituents) = 0,2 %

The composition given above is typical and should therefore represent the majority of Hexachloroiridic acid hydrate as manufactured and/or imported in the EEA market.

6. Information on appearance, physical state and properties of the substance

Table 5. Appearance / physical state / properties of the solid substance

Physical state	Solid
Physical form*	Crystalline
Appearance	Black solid (Harlan 2011)
Particle size**	Coarse powder
Does the solid hydrolyse?#	No
Is the solid hygroscopic?§	Yes

* Crystalline form: solid material whose constituent atoms, molecules, or ions are arranged in an ordered pattern extending in all three spatial dimensions. Amorphous form: solid material whose constituent atoms, molecules, or ions are randomly arranged.

** Nanoform: particles in the size range 1 - 100 nm (for definition of a nanomaterial, see http://ec.europa.eu/environment/chemicals/nanotech/faq/definition_en.htm). Fine powder: particles in the size range 100 – 2.500 nm. Coarse powder: particles in the size range 2.500 nm – 1 mm. Massive object: particles in the size range > 1 mm.

Hydrolysis: decomposition (cleavage of chemical bonds) by the addition of water.

§ Hygroscopic substance: readily attracts moisture from its surroundings in open air, through either absorption or adsorption.

7. Analytical data

Annex VI of REACH requires the registrant to describe the analytical methods and/or to provide the bibliographical references for the methods used for identification of the substance and, where appropriate, for the identification of impurities and additives. This information should be sufficient to allow the methods to be reproduced.

Table 6. Analytical methods for identification of the substance

Parameter / Method	Recommended for substance identification and sameness check	Applicable	Not applicable or not recommended
Elemental analysis			
ICP (ICP-MS or ICP-OES)	X		
Atomic absorption spectroscopy (AAS)			
Glow discharge mass spectrometry (GDMS)			
Molecular analysis			
Infrared (IR) spectroscopy	X		
Raman spectroscopy			X (Raman inactive)
Mineralogical analysis			
X-Ray Fluorescence (XRF)			

X-Ray Diffraction (XRD)			X (X-ray amorphous)
Morphology and particle sizing			
Electron microscopy (SEM, TEM, REM)* #			
Laser diffraction* #			
Particle size by other means (e.g. sieve analysis)#			
Surface area by N-BET* #			
Other			
Ratio of Ir(III) and Ir(IV) by redox titration	X		
Total chlorine content by titration	X		
Free acid by titration	X		

* Analytical techniques particularly (but not exclusively) relevant for nanomaterials.

The choice of the technique for particle size depends on the size of the material as manufactured/imported/placed on the market/used.

8. Lead Registrant

Heraeus Deutschland GmbH & Co. KG (Germany) volunteers to be the Lead Registrant for Hexachloroiridic acid. The EPMF will provide support to the Lead Registrant as laid down in the EPMF Agreement.

9. Scope of the Registration Dossier

The uses included in this Registration Dossier are listed on the EPMF website

10. Analytical reference information

Below the following spectra of a reference sample used for testing:

- IR spectrum

Hexachloroiridic acid - Analytical Reference Information

Hexachloroiridic acid, IR spectrum