ID Card
Diammonium hexachloroiridate

Version 4 July 2023

Notes:

- *This ID card is used to support the substance sameness discussions and to describe the substance to the best of the members' knowledge.*
- *It also aims at grouping communications relevant to the request of available data or information, the approval of the Lead Registrant and the registration strategy.*
- *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	Diammonium hexachloroiridate
EC number	241-007-0
CAS number	16940-92-4
Description	Not available
Composition type	Mono-constituent substance

2. Synonyms and other identifiers of the substance

Table 2. Synonyms and other identifiers of the substance

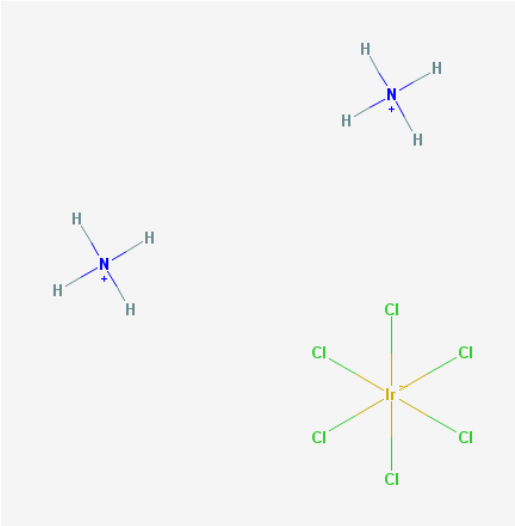
IUPAC name	Diammonium hexachloroiridate(2-)
CAS name	
Abbreviations	
Other commercial, brand or international names	Ammonium hexachloroiridate(IV) Iridium(IV)-ammonium chloride Ammonium chloroiridate Diazanium iridium hexachloride Diammonium iridium hexachloride
Other identity codes	

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	Cl6H8IrN2
Structural formula	
Smiles notation	[NH4+].[NH4+].Cl[Ir-2](Cl)(Cl)(Cl)(Cl)Cl
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	441,01 g/mol

5. Typical composition of the substance

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%)	Typical concentration (%)
Main constituent(s)*	Diammonium hexachloroiridate	Cl6H8IrN2	95- 100	± 98
Impurities#	Several minor (especially metallic) impurities which do not affect the classification of the substance because of their non-hazardous nature or because they do not exceed the classification cut-off limits in the substance	e.g. Ag, Au, Ca, Cu, Fe, Na, Ni, Os, Pd, Pt, Rh, Ru, NH4Cl, …	0 - 3	± 2

* ≥ 80 % (w/w) for mono-constituent substances; ≥ 10 % (w/w) and < 80 % (w/w) for multi-constituent substances.

An impurity is an unintended constituent present in a substance, as produced. It may originate from the starting materials or be the result of secondary or incomplete reactions during the production process. While impurities are present in the final substance, they were not intentionally added.

The composition given above is typical and should therefore represent the majority of Diammonium hexachloroiridate 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 crystalline powder (CRC Handbook)
Particle size**	Fine powder
Does the solid hydrolyse?#	Slowly
Is the solid hygroscopic?§	No

* 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

Mineralogical analysis			
X-Ray Fluorescence (XRF)			
X X-Ray Diffraction (XRD)		X	
Morphology and particle sizing			
Electron microscopy (SEM, TEM, REM)* #			
Laser diffraction* #	X		
Particle size by other means (e.g. sieve analysis)#			
Surface area by N-BET* #	X		
Other			

* 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 (Germany) is the Lead Registrant for Diammonium hexachloroiridate. 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

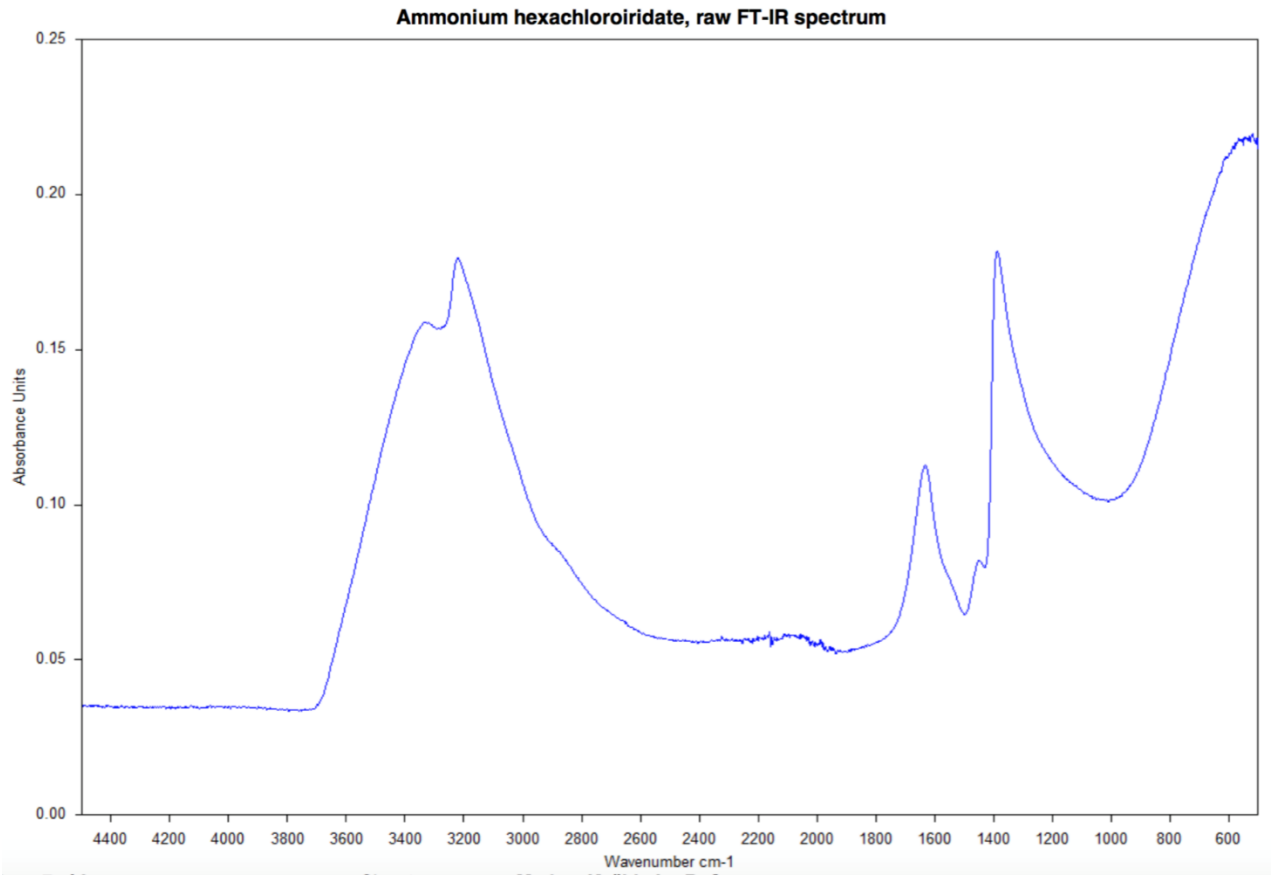
10. Analytical reference information

Below the results of IR analysis of a reference sample used for testing.

FT-IR parameters (solids):

- Instrument: Bruker Tensor 37
- Measurement head: Diamond ATR
- Resolution: 2 cm^{-1}
- Sample scans: 16
- Background scans: 16
- Atmospheric compensation: Off
- Result spectrum: Absorbance
- Source: MIR
- Beam splitter: KBr
- Aperture: 5 mm
- Detector: DLaTGS
- Detector temperature: Ambient
- Scanner velocity: 10 kHz

All samples were analysed under ambient conditions as received.


Ammonium hexachloroiridate, raw FT-IR spectrum
Absorbance Units
0.25
0.20
0.15
0.10
0.05
0.00
4400 4200 4000 3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600
Wavenumber cm-1