ID Card Hexakis[mu-(acetato-O:O')]-µ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate

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 proposed 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	Hexakis[mu-(acetato-O:O')]-µ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate
EC number	259-653-7
CAS number	55466-76-7
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

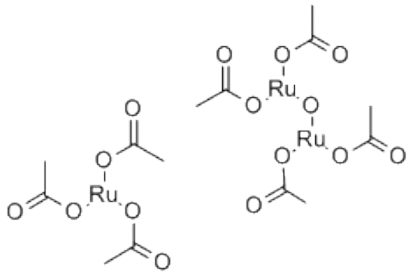
IUPAC name	Ruthenium(3+);heptaacetate
CAS name	
Abbreviations	
Other commercial, brand or international names	
Other identity codes	

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	C12H18O13Ru3.C2H3O2
Structural formula	
Smiles notation	CC(=O)[O-].CC(=O)[O-].CC(=O)[O-].CC(=O)[O-].CC(=O)[O-].CC(=O)[O-]. CC(=O)[O-].[Ru+3].[Ru+3].[Ru+3]
Optical activity	Not applicable
Typical ratio of (stereo) isomers	
Molecular Weight / Molecular Weight range	732,52 g/mol

5. Typical composition of the substance

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%)[§]	Typical concentration (%)[§§]
Main constituent(s)*	Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate	$C_{12}H_{18}O_{13}Ru_3.C_2H_3O_2$	97,5 - 100[$]	> 97,5
Impurities[#]	Water	H_2O	0 – 1,5	< 1,5
	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, Ir, Pd, Pt, Rh, Fe, Ca, Cu, Mg, Na, Si	0 - 1	< 1

* ≥ 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.

[§] Concentration ranges define the substance sameness criteria agreed by all EPMF Members in preparation of the communication with other SIEF members.

[§§] Typical concentration refers to the representative sample used for testing.

[$] Corresponds to 40,4 - 41 % Ru.

The composition given above is typical and should therefore represent the majority of Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate as manufactured and/or imported in the EEA market. Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate containing less than 87 % Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate may still be considered to be the same for the purpose of registration under REACH and may be referred to as impure Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate to distinguish if from the typically pure Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate.

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	Dark green to black crystalline solid
Particle size**	Fine to coarse powder
Does the solid hydrolyse?[#]	Yes / No
Is the solid hygroscopic?[§]	Yes / 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 full definition of a nanomaterial, see http://ec.europa.eu/environment/chemicals/nanotech/index.htm#definition). 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. Cf. also water/moisture content in Table 4.

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

Johnson Matthey is the Lead Registrant for Hexakis[mu-(acetato-O:O')]-µ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate. 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 Raman analysis of a Hexakis[mu-(acetato-O:O')]-µ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate solution.

Instrument: Renishaw inVia

Measurement head: Confocal microscope

Objective: x50 L

Laser: 532 nm

Grating: 1800 lines/mm

Laser power: 100 %

Resolution: 1 cm-1

Sample scans: 1

Scan time: 20 s

Scan range: 50 - 3200 cm-1

The samples are transferred to 2-mm path length Suprasil® quartz cuvettes from Helma, sealed with a PTFE stopper, and run in reflectance mode for ease of analysis. The maximum power of the lasers used is 500 mW.

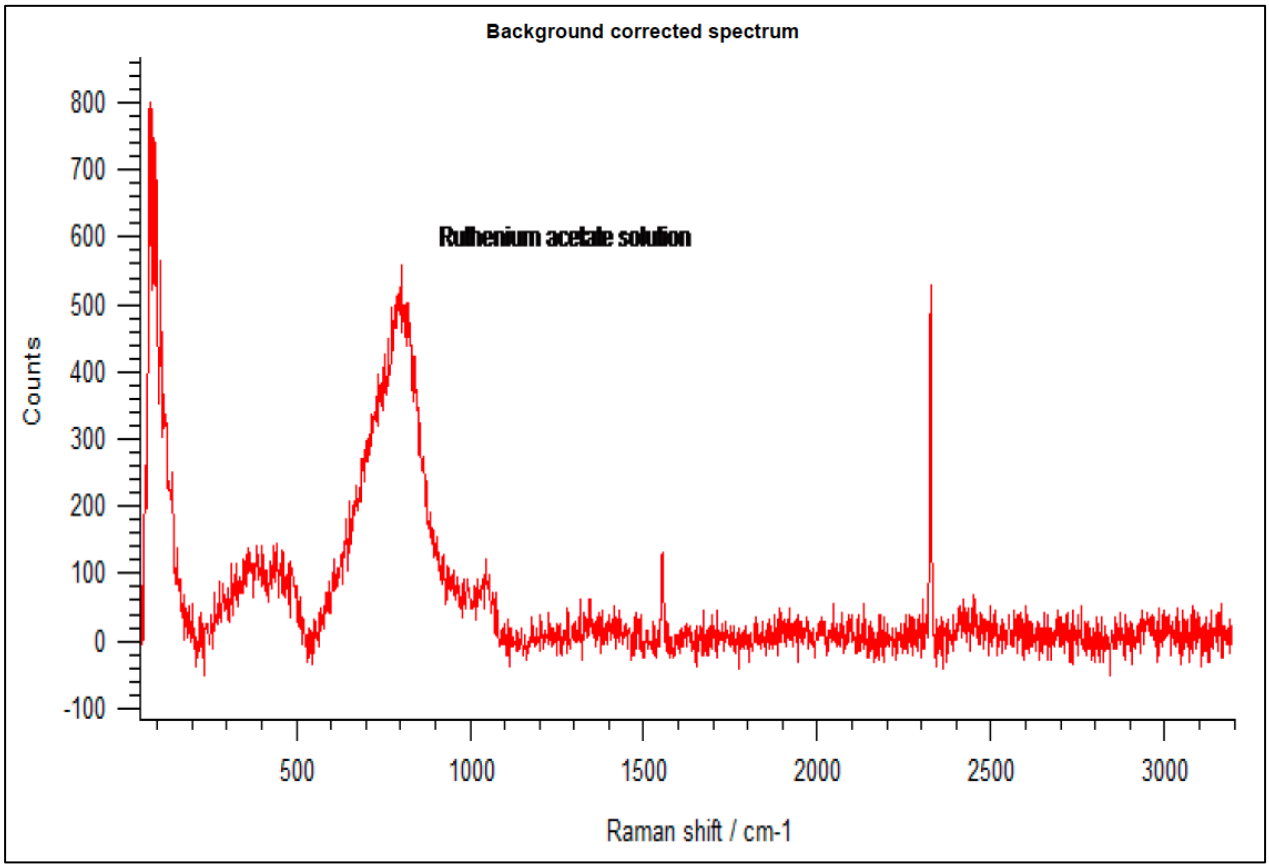


Figure 1. Raman spectrum of Hexakis[mu-(acetato-O:O')]-μ3-oxo-triangulo-triruthenium acetate / Ruthenium acetate