ID Card Tris(nitrato-O)nitrosylruthenium

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).

DISCLAIMER

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1. Identification of the substance

Table 1. Identification of the substance

	Original (in EC inventory)
Name	Tris(nitrato-O)nitrosylruthenium
EC number	252-068-8
CAS number	34513-98-9
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	Azanylidyneoxidanium ruthenium(2+) trinitrate
CAS name	Ruthenium, tris(nitrato-□O)nitrosyl-
Abbreviations	Ru(NO)(NO3)3
Other commercial, brand or international names	Ruthenium nitrosyl nitrate Ruthenium(III) nitrosyl nitrate Nitrilooxonium ruthenium(2+) nitrate (1:1:3)
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	N4O10Ru
Structural formula	O, N+:O O O O O O O O O O O O O O O O O O O
Smiles notation	[Ru+2].O=[N+]([O-])[O-].[O-][N+]([O-])=O.[O-][N+]([O-])=O.[O+]#N
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	317,09 g/mol

5. Typical composition of the substance

Table 4. Typical composition of Tris(nitrato-O)nitrosylruthenium

	Name	Symbol / Formula	Min & Max concentrations (%)§	Typical concentration (%)§§
Main constituent(s)*	Tris(nitrato-O)nitrosylruthenium	N ₄ O ₁₀ Ru	85 - 99.9\$	90
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, Ir, Pd, Pt, Rh, Fe, Ca, Cu, Mg, Na, Si	0 – 0.1	< 0.1
	Sodium nitrate	NaNO3	≥0 - 15	10

^{* ≥ 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 27.1 – 31.9 % Ru.



The composition given above is typical and should therefore represent the majority of Tris(nitrato-O)nitrosylruthenium as manufactured and/or imported in the EEA market. Tris(nitrato-O)nitrosylruthenium containing less than 85% Tris(nitrato-O)nitrosylruthenium may still be considered to be the same for the purpose of registration under REACH and may be referred to as impure Tris(nitrato-O)nitrosylruthenium to distinguish it from the typically pure Tris(nitrato-O)nitrosylruthenium.

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	Red / Brown solid
Particle size**	Fine to coarse powder
Does the solid hydrolyse?#	Yes
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.

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			

^{**} 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 **Error! Reference source not found.**.

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

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

8. Lead Registrant

Umicore AG & Co. KG (Germany) is the Lead Registrant for Tris(nitrato-O)nitrosylruthenium. 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.

Spectrometer: Infrared spectrometer Tensor 27; BRUKER Optics

Spectral range: 4000 - 550 cm-1

Resolution: 2 cm-1 Scans: 32 scans

Temperature: ambient

Sample preparation: attenuated total reflection

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

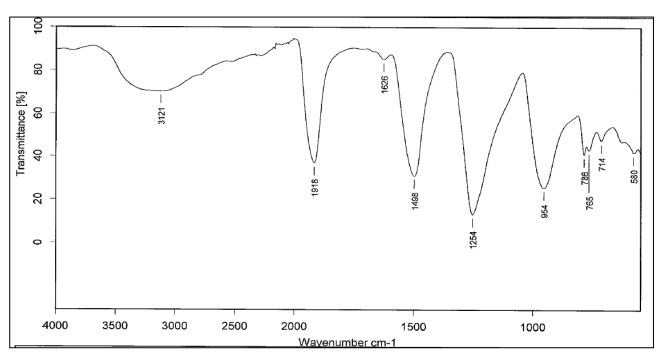


Figure 1. IR spectrum of Tris(nitrato-O)nitrosylruthenium