



ID Card

Tris(triphenylphosphine) rhodium (I) chloride

Version 14 January 2021

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).

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1. Identification of the substance

Table 1. Identification of the substance

	Original (in EC inventory)
Name	Tris(triphenylphosphine) rhodium (I) chloride
EC number	238-744-5
CAS number	14694-95-2
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	rhodium;triphenylphosphane;chloride
CAS name	Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)-
Abbreviations	RhCl(PPh ₃) ₃ Rh(PPh ₃) ₃ Cl
Other commercial, brand or international names	Chlorotris(triphenylphosphine)rhodium(I) Rhodium(I) tris(triphenylphosphine) chloride Rhodium, chlorotris(triphenylphosphine) Tris(triphenylphosphine)chlororhodium Wilkinson's catalyst Wilkinson's complex
Other identity codes	PubChem ID: 84599



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	C ₅₄ H ₄₅ ClP ₃ Rh
Structural formula	
Smiles notation	<chem>C1=CC=C(C=C1)P(C2=CC=CC=C2)C3=CC=CC=C3.C1=CC=C(C=C1)P(C2=CC=CC=C2)C3=CC=CC=C3.C1=CC=C(C=C1)P(C2=CC=CC=C2)C3=CC=CC=C3.[Cl].[Rh]</chem>
Optical activity	Not applicable
Typical ratio (stereo) isomers of	Not applicable
Molecular Weight / Molecular Weight range	925,21 g/mol

5. Typical composition of the substance

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%) [§]	Typical concentration (%) ^{§§}
Main constituent(s)*	Tris(triphenylphosphine) rhodium (I) chloride	C ₅₄ H ₄₅ ClP ₃ Rh	90 - 98 [§]	95
Impurities##	Bis(triphenylphosphine)rhodium chloride dimer (CAS# 14653-50-0)	C ₇₂ H ₆₀ Cl ₂ P ₄ Rh ₂	2 - 10	3,5
	Triphenylphosphine (CAS# 603-35-0)	C ₁₈ H ₁₅ P	0 - 3	0,75
	Triphenylphosphine oxide (CAS# 791-28-6)	C ₁₈ H ₁₅ OP	0 - 3	0,75



	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, Cu, Ir, Pd, Pt, Ru, Ca, Fe, Mg	0 – 0,1	< 0,1
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* $\geq 80\%$ (w/w) for mono-constituent substances; $\geq 10\%$ (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 10-10,9 % Rh.

The composition given above is typical and should therefore represent the majority of Tris(triphenylphosphine) rhodium (I) chloride as manufactured and/or imported in the EEA market. Tris(triphenylphosphine) rhodium (I) chloride containing less than 90 % Tris(triphenylphosphine) rhodium (I) chloride may still be considered to be the same for the purpose of registration under REACH and may be referred to as impure Tris(triphenylphosphine) rhodium (I) chloride to distinguish it from the typically pure Tris(triphenylphosphine) rhodium (I) chloride.

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	Red/brown powder
Particle size**	Fine to coarse powder
Does the solid hydrolyse?#	No
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 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			
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

Umicore AG & Co. KG (Germany) is the Lead Registrant for Tris(triphenylphosphine) rhodium (I) chloride. The EPMF will provide support to the Lead Registrant as laid down in the EPMF Agreement.

9. REACH Strategy

The table below presents the overall Registration Strategy for Tris(triphenylphosphine) rhodium (I) chloride based on the information available to the EPMF by the date given above on the document.

The Registration Dossier will be prepared for the highest substance status (information requirements associated to a substance or Article 10 Registration being higher than an intermediate handled under strictly controlled conditions or Article 17 or 18 one) and associated tonnage band.

The recap below therefore reflects the scope of work of the EPMF for Tris(triphenylphosphine) rhodium (I) chloride and sets the minimum and maximum set of information that will be gathered and/or produced when preparing the Registration Dossier for Tris(triphenylphosphine) rhodium (I) chloride as described in this ID Card.

If higher information requirements are necessary, these can be included in the Registration dossier (if EPMF is made aware of these additional requirements in-time) as an update to the already submitted dossier.

Table 7. REACH strategy for the substance (basis for REACH Registration preparation)

Item	Description
REACH category	Mono-constituent substance
Highest status	Substance
Highest tonnage band	1-10 t/a
Information requirements	Available / Existing + Annex VII
Existing classification*	Aquatic Chronic 2 (H411)
Registration deadline	2018

* For the pure form

10. Scope of the Registration Dossier

The uses included in this Registration Dossier are listed on the [EPMF website](#).

11. 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 - 300 cm⁻¹
 Resolution: 2 cm⁻¹
 Scans: 32 scans
 Temperature: ambient
 Sample preparation: KBr Pellet

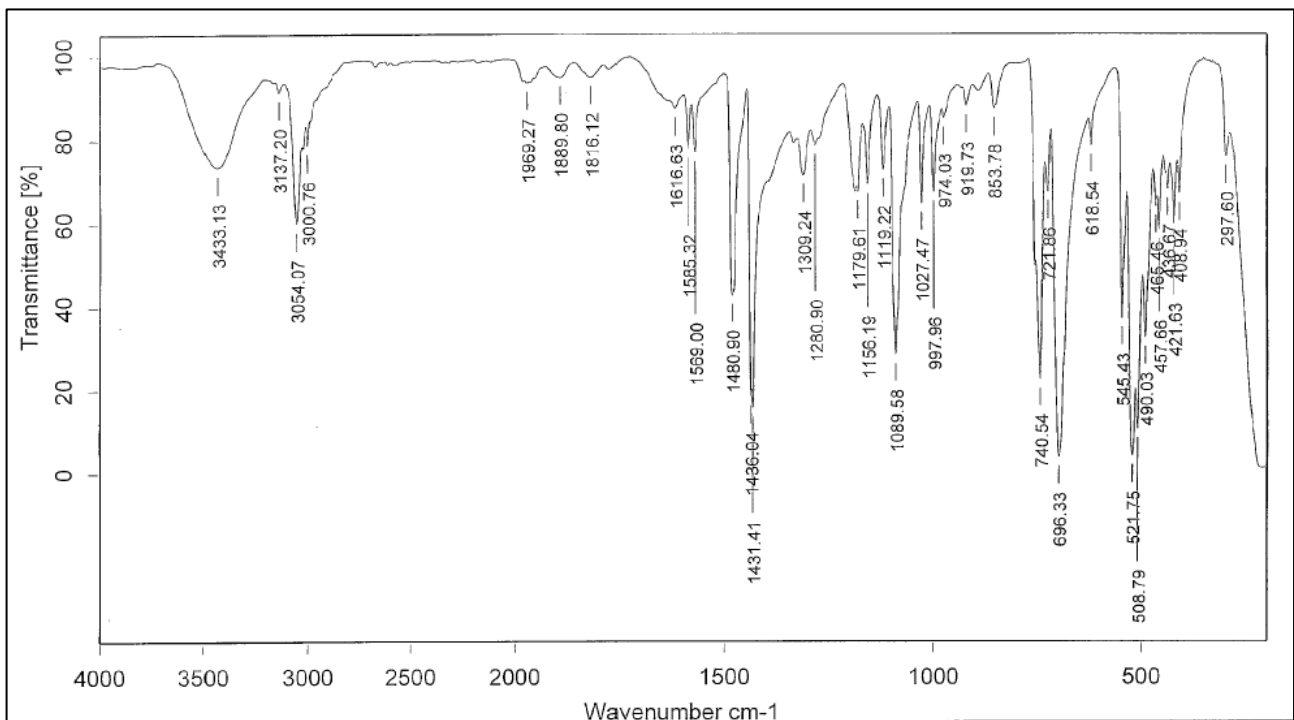


Figure 1. IR spectrum of Tris(triphenylphosphine) rhodium (I) chloride