



# ID Card

## Tetrakis(triphenylphosphine)palladium

Version 5 August 2016

**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).

**DISCLAIMER**

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### 1. Identification of the substance

**Table 1. Identification of the substance**

	Original (in EC inventory)
<b>Name</b>	Tetrakis(triphenylphosphine)palladium
<b>EC number</b>	238-086-9
<b>CAS number</b>	14221-01-3
<b>Description</b>	Not available
<b>Composition type</b>	Mono-constituent substance

### 2. Synonyms and other identifiers of the substance

**Table 2. Synonyms and other identifiers of the substance**

<b>IUPAC name</b>	Palladium;triphenylphosphine
<b>CAS name</b>	Palladium, tetrakis(triphenylphosphine)-, (T-4)-
<b>Abbreviations</b>	Pd(PPh <sub>3</sub> ) <sub>4</sub>
<b>Other commercial, brand or international names</b>	Tetrakis(triphenylphosphine)palladium(0) Palladium-tetrakis(triphenylphosphine) Tetra(triphenylphosphine)palladium
<b>Other identity codes</b>	

### 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

<b>Molecular formula</b>	C72H60P4Pd
<b>Structural formula</b>	
<b>Smiles notation</b>	<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.C1=CC=C(C=C1)P(C2=CC=CC=C2)C3=CC=CC=C3.[Pd]</chem>
<b>Optical activity</b>	Not applicable
<b>Typical ratio of (stereo) isomers</b>	Not applicable
<b>Molecular Weight / Molecular Weight range</b>	1155,56 g/mol

#### 5. Typical composition of the substance

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%)	Typical concentration (%)
<b>Main constituent(s)*</b>	Tetrakis(triphenylphosphine)palladium	C72H60P4Pd	95,5 - 100 <sup>§</sup>	> 97,7
<b>Impurity(ies)#</b>	Triphenylphosphine (CAS# 603-35-0)	C18H15P	0 - 3	< 1,6
	Triphenylphosphine oxide (CAS# 791-28-6)	C18H15OP	0 - 3	< 1,6
	Water	H2O	0 - 2	< 0,5
	Chloride (CAS# 16887-00-6)	Cl	0 - 0,1	< 0,1
	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, Pt, Rh, Ru, Fe, Co, Mn, Na	0 - 0,1	< 0,1

\* ≥ 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 Consortium Members in preparation of the communication



with other SIEF members.

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

§ Corresponds to 8,8-9,2 % Pd.

The composition given above is typical and should therefore represent the majority of Tetrakis(triphenylphosphine)palladium as manufactured and/or imported in the EEA market. Tetrakis(triphenylphosphine)palladium containing less than 95,5% Tetrakis(triphenylphosphine)palladium may still be considered to be the same for the purpose of registration under REACH and may be referred to as impure Tetrakis(triphenylphosphine)palladium to distinguish it from the typically pure Tetrakis(triphenylphosphine)palladium.

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

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

<b>Physical state</b>	Solid
<b>Physical form*</b>	Crystalline
<b>Appearance</b>	Yellow powder
<b>Particle size**</b>	Fine to coarse powder
<b>Does the solid hydrolyse?#</b>	No
<b>Is the solid hygroscopic?§</b>	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
<b>Elemental analysis</b>			
ICP (ICP-MS or ICP-OES)	X		
Atomic absorption spectroscopy (AAS)			
Glow discharge mass spectrometry (GDMS)			
<b>Molecular analysis</b>			
Infrared (IR) spectroscopy	X		
Raman spectroscopy			
<b>Mineralogical analysis</b>			
X-Ray Fluorescence (XRF)		X	
X-Ray Diffraction (XRD)	X		
<b>Morphology and particle sizing</b>			



Electron microscopy (SEM, TEM, REM)* #			
Laser diffraction* #	X		
Particle size by other means (e.g. sieve analysis)#			
Surface area by N-BET* #	X		
<b>Other</b>			

\* 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) volunteers to be the Lead Registrant for Tetrakis(triphenylphosphine)palladium. 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 Tetrakis(triphenylphosphine)palladium 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 Tetrakis(triphenylphosphine)palladium and sets the minimum and maximum set of information that will be gathered and/or produced when preparing the Registration Dossier for Tetrakis(triphenylphosphine)palladium 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
<b>REACH category</b>	Mono-constituent substance
<b>Highest status</b>	Substance
<b>Highest tonnage band</b>	1-10 t/a
<b>Information requirements</b>	Available / Existing + Annex VII Physico-chemical requirements (Annex III exempted substance)
<b>Existing classification*</b>	Aquatic Chronic 4 (H413)
<b>Registration deadline</b>	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<sup>-1</sup>

Resolution: 2 cm<sup>-1</sup>

Scans: 32 scans

Temperature: ambient

Sample preparation: KBr Pellet

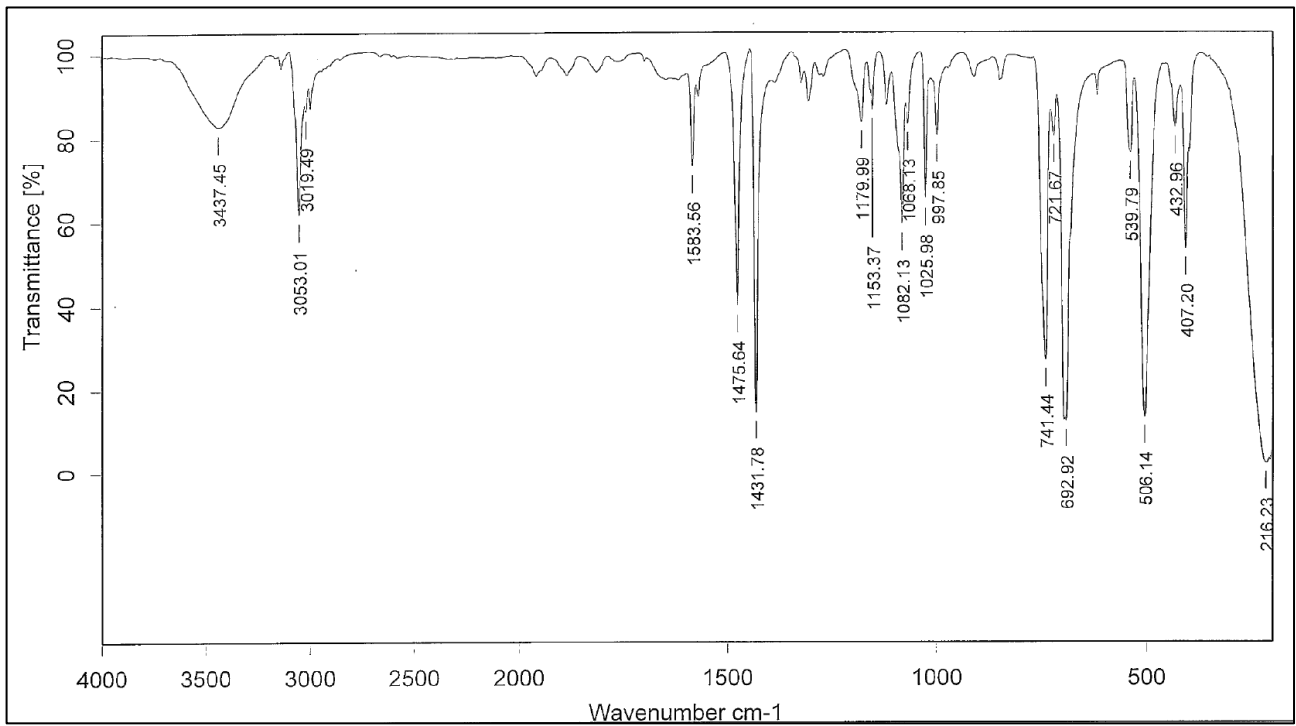


Figure 1. IR spectrum of Tetrakis(triphenylphosphine)palladium