



ID Card

Tetrakis(triphenylphosphine)palladium

Version 18 July 2023

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)
Name	Tetrakis(triphenylphosphine)palladium
EC number	238-086-9
CAS number	14221-01-3
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

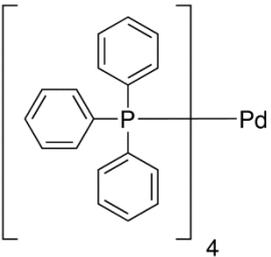
IUPAC name	Palladium;triphenylphosphine
CAS name	Palladium, tetrakis(triphenylphosphine)-, (T-4)-
Abbreviations	Pd(PPh ₃) ₄
Other commercial, brand or international names	Tetrakis(triphenylphosphine)palladium(0) Palladium-tetrakis(triphenylphosphine) Tetra(triphenylphosphine)palladium
Other identity 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	C72H60P4Pd
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.C1=CC=C(C=C1)P(C2=CC=CC=C2)C3=CC=CC=C3.[Pd]</chem>
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	1155,56 g/mol

5. Typical composition of the substance

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%)	Typical concentration (%)
Main constituent(s)*	Tetrakis(triphenylphosphine)palladium	C72H60P4Pd	95,5 - 100 ^s	> 97,7
Impurity(ies)#	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

Physical state	Solid
Physical form*	Crystalline
Appearance	Yellow 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) 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. 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 - 300 cm⁻¹

Resolution: 2 cm⁻¹

Scans: 32 scans

Temperature: ambient

Sample preparation: KBr Pellet

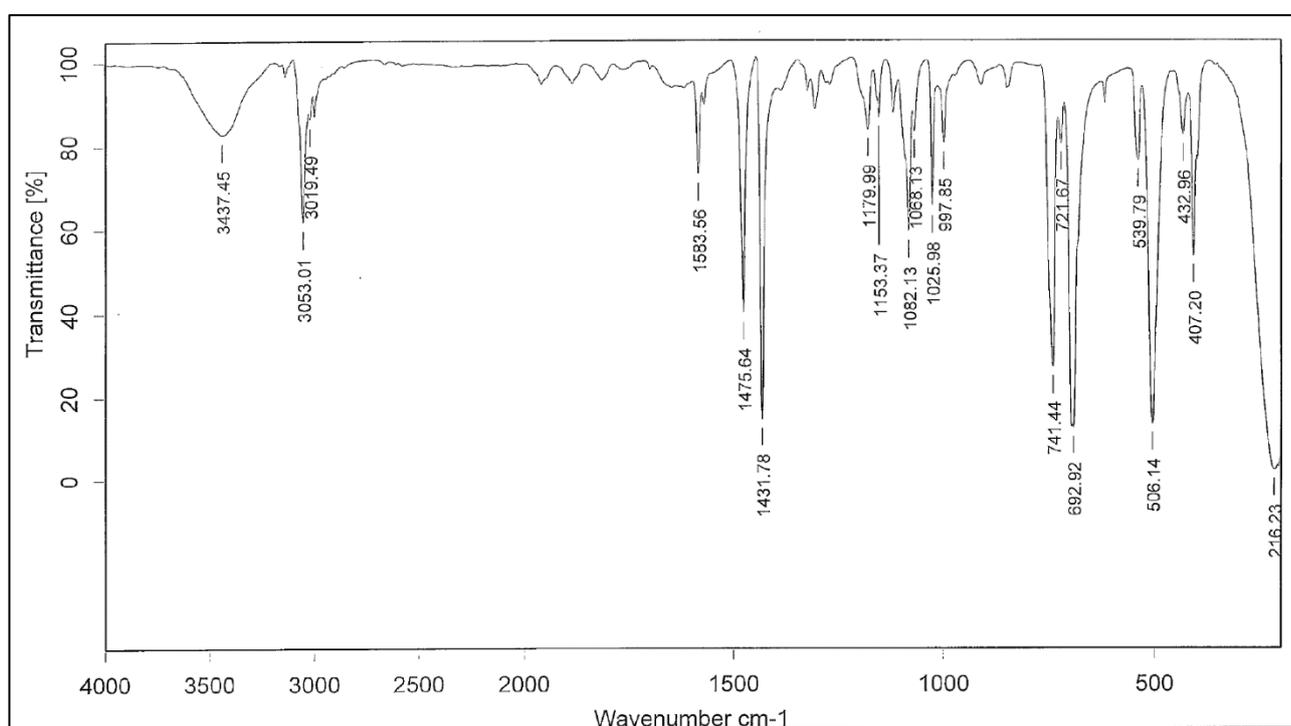


Figure 1. IR spectrum of Tetrakis(triphenylphosphine)palladium