



# ID Card

## Tetraamminepalladium(2+) diacetate

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**

All data and information contained in this document shall be treated by the receiving party (i) in full confidence with the adequate respect of any confidential and/or proprietary nature of such information and (ii) only in the framework of the purpose of agreeing on substance sameness, Lead Registrant and overall REACH Strategy for the concerned Substance under REACH (the 'Purpose').

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## 1. Identification of the substance

**Table 1. Identification of the substance**

	Original (in EC inventory)
<b>Name</b>	Tetraamminepalladium(2+) diacetate
<b>EC number</b>	262-819-1
<b>CAS number</b>	61495-96-3
<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**

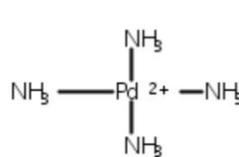
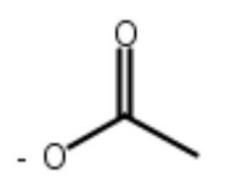
<b>IUPAC name</b>	azane;palladium(2+);diacetate
<b>CAS name</b>	Palladium(2+), tetraammine-, (SP-4-1)-, acetate (1:2)
<b>Abbreviations</b>	
<b>Other commercial, brand or international names</b>	Palladium tetraammine diacetate Tetraamminepalladium(II) acetate
<b>Other identity codes</b>	

### 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>	C4H18N4O4Pd
<b>Structural formula</b>	<p>15974-14-8 H<sub>12</sub> N<sub>4</sub> Pd</p>  <hr/> <p>71-50-1 C<sub>2</sub> H<sub>3</sub> O<sub>2</sub></p> 
<b>Smiles notation</b>	[Pd+2].[O-]C(=O)C.[O-]C(=O)C.N.N.N.N
<b>Optical activity</b>	Not applicable
<b>Typical ratio of (stereo) isomers</b>	Not applicable
<b>Molecular Weight / Molecular Weight range</b>	292,63 g/mol

### 5. Typical composition of the substance

**Table 4. Typical composition solid**

	Name	Symbol / Formula	Min & Max concentrations (%) <sup>§</sup>	Typical concentration (%) <sup>§§</sup>
<b>Main constituent(s)*</b>	Tetraamminepalladium(2+) diacetate	C4H18N4O4Pd	82 - 100 <sup>§</sup>	91
<b>Impurity(ies)<sup>#</sup></b>	Chloride	Cl	0 - 0,5	< 0,1
	Water	H <sub>2</sub> O	0 - 10	< 5
	Ammonium acetate	C <sub>2</sub> H <sub>7</sub> NO <sub>2</sub>	0 - 8	< 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, Cu, Ir, Pb, Pt, Rh, Ru	0 - 0,5	< 0,5
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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 Consortium Members in preparation of the communication with other SIEF members.

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

§ Corresponds to 30-36.4 % Pd.

The composition given above is the composition of the solid substance. In practice, Tetraamminepalladium(2+) diacetate is only brought on the market in solution (usually with 15 – 20 % Pd content). The solvent can however be separated without affecting the chemical stability of the substance. The solid form is thus considered the same substance as the substance in solution; the solutions are considered mixtures under REACH.

## 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>	White / Pale yellow crystals
<b>Particle size**</b>	Fine to coarse powder
<b>Does the solid hydrolyse?#</b>	No
<b>Is the solid hygroscopic?§</b>	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.

**Table 6. Appearance / physical state / properties of the substance in solution**

<b>Physical state</b>	Solution
<b>Solvent</b>	Water
<b>Concentration range of substance in solution</b>	41-55%§
<b>pH (range) of the solution</b>	7 - 9
<b>Excess acid</b>	

§ Corresponds to 15-20 % Pd.

## 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 7. 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 (solid)		
Raman spectroscopy	X (solution)		
<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 Tetraamminepalladium(2+) diacetate. 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 (solid) and Raman (solution) analysis of a reference sample.

### **IR analysis solid form**

Spectrometer: Infrared spectrometer Tensor 27, BRUKER Optics

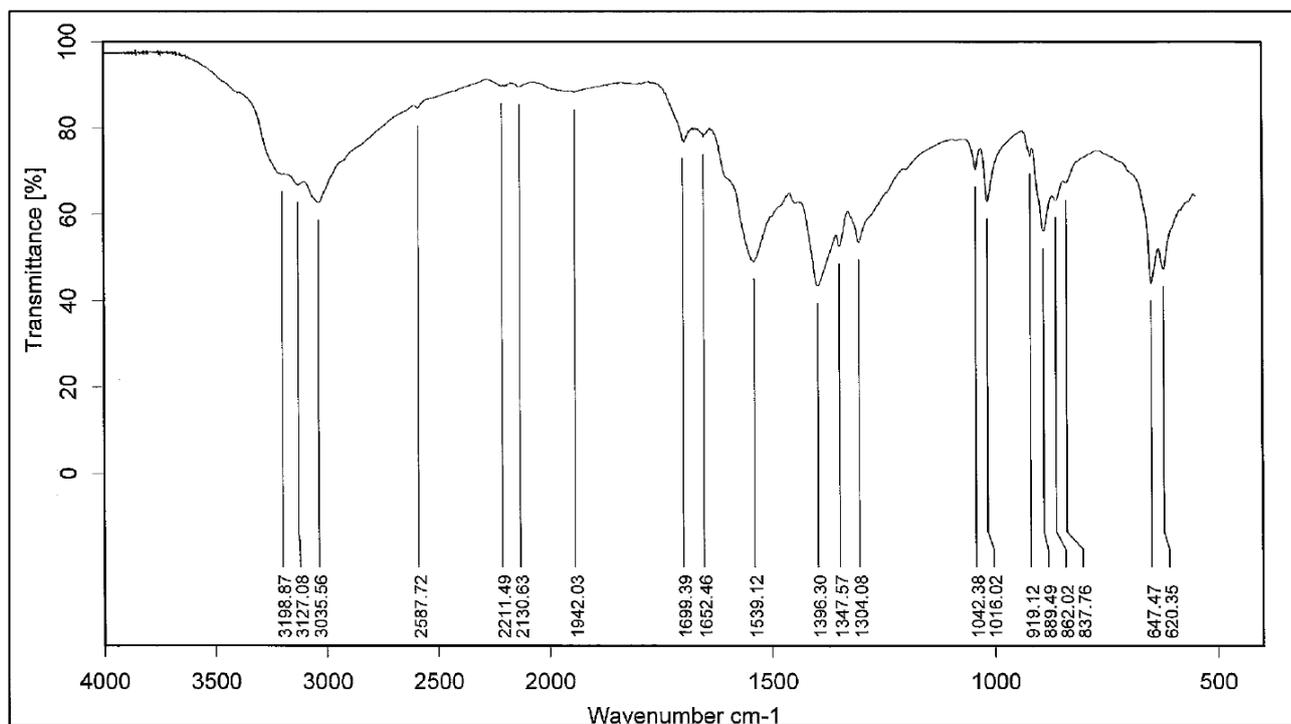
Spectral range: 4000 - 300 cm<sup>-1</sup>

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

Scans: 32 scans

Temperature: ambient

Sample preparation: attenuated total reflection



**Figure 1. IR spectrum of Tetraamminepalladium(2+) diacetate (solid)**

### **Raman analysis solution**

Spectrometer: Bruker RFS 100/S

Spectral range: 3500 – 50 cm<sup>-1</sup>

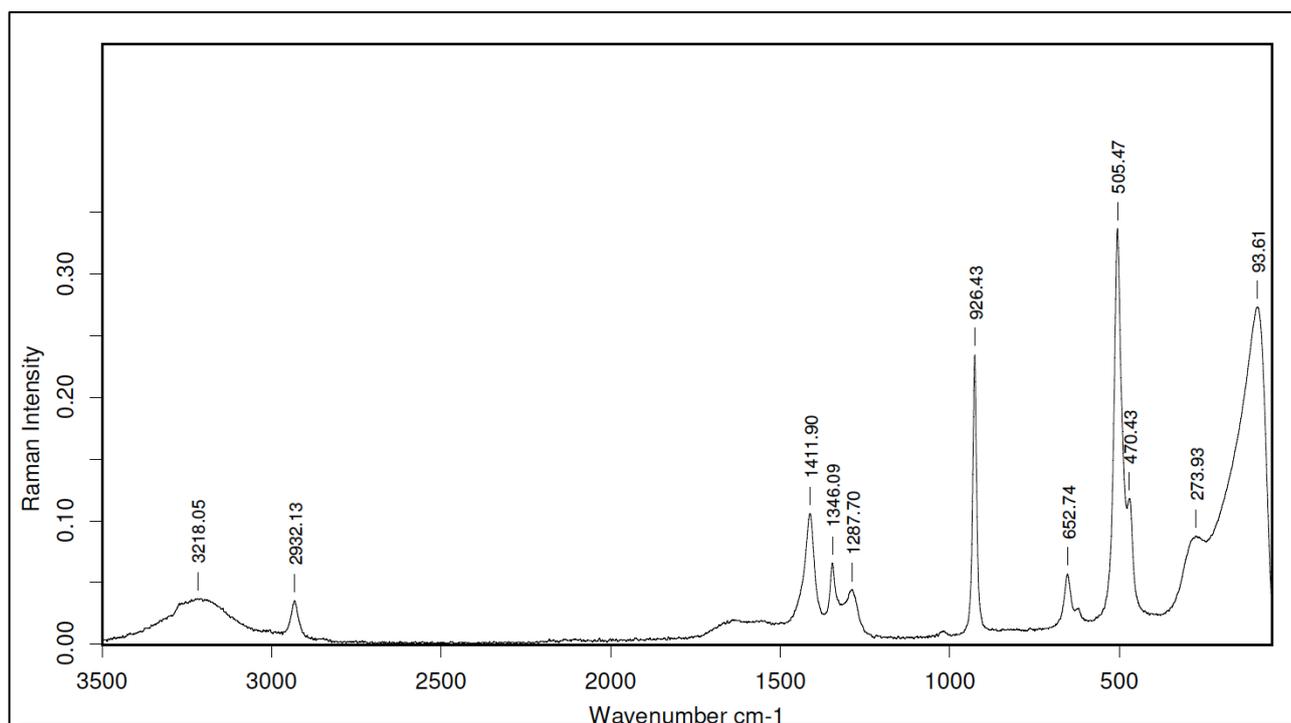
Resolution: 2 cm<sup>-1</sup>

Scans: 100 scans

Laser: 1003 mW

Temperature: ambient

Sample preparation: liquid, glass vial



**Figure 2. Raman spectrum of Tetraamminepalladium(2+) diacetate (solution)**