ID Card – Dihydrogen tetrachloropalladate(2-) (in solution)

Version 18 July 2023

Notes:

- *This ID card is used to support the substance sameness discussions s 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).*

1. Identification of the substance

Table 1. Identification of the substance

	Original (in EC inventory)
Name	Dihydrogen tetrachloropalladate(2-)
EC number	241-047-9
CAS number	16970-55-1
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

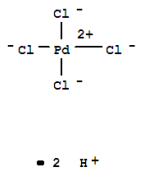
IUPAC name	Palladium(4+) tetrachloride
CAS name	Palladate(2-), tetrachloro-, hydrogen (1:2), (SP-4-1)-
Abbreviations	
Other commercial or international names	Palladium(2+) hydrogen chloride(1:2:4) Dihydrogen palladium tetrachloride Hydrogen chloropalladate Hydrogen tetrachloropalladate(II) Hydrogen tetrachloropalladium (II) Palladate(2-), tetrachloro-, dihydrogen Tetrachloropalladic acid
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	H2Cl4Pd
Structural formula	
Smiles notation	[H+].[H+].Cl[Pd-2](Cl)(Cl)Cl
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	250,25 g/mol

5. Typical composition of the substance

Table 4. Typical composition solution

	Name	Symbol / Formula	Min & Max concentrations (%)§	Typical concentration (%)§§
Main constituent(s)*	Dihydrogen tetrachloropalladate(2-)	H2Cl4Pd	24 - 59$	47
Impurity(ies)#	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 - 0,1	< 0,1
Additives	Water	H2O	28 - 51	35
	Hydrogen chloride	HCl	13 - 25	18

* ≥ 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 10 - 25 % Pd.

Justification for deviation of the rule that for mono-constituent substances the main constituent is expected to be present as a minimum at 80%:

Dihydrogen tetrachloropalladate(2-) (H2[PdCl4], EC 241-047-9, CAS 16970-55-1) is produced by dissolving PdCl2 in diluted solution of hydrochloric acid.

H2[PdCl4] as such cannot be isolated and does not exist in pure form.

H2PdCl4 is only brought on the market in solution (usually with 10 – 25 % Pd content). The most concentrated solution contains 59 % of H2[PdCl4]. When trying to further concentrate the solution, e.g. by evaporation on a water bath, H2O and HCl starts to evolve. In addition, the H2[PdCl4] hydrolyses to Palladium chloride hydroxide moieties and Palladium dihydroxide.

That means, that an amount of 41 % of solvent, in this case a solution of hydrochloric acid (HCl + H2O), is necessary to preserve the stability of H2[PdCl4]. As this minimum quantity of solvent rather acts as stabilizing agent, it is regarded as an additive and not as a solvent only.

Though its typical concentration is below 80 % (w/w), H2PdCl4 is regarded as mono-constituent substance.

Referring to the example 7.1 (pg 63) of the “Guidance for identification and naming of substances under REACH and CLP”, H2[PdCl4] is registered as solution with the lowest concentration of hydrochloric acid solution which guarantees stability of H2[PdCl4]. Hydrochloric acid solution (HCl + H2O) with an upper concentration limit of 41 % is reported as an “Additive” with stabilizing function.

Calculation of the ‘typical concentration’ values of the legal entity composition based on the analytical information as provided in section 1.4:

H2[PdCl4] is usually put on the market in form of diluted hydrochloric acid solutions.

Therefore, it can be assumed that diluted hydrochloric acid solutions are generally used to generate the analytical information required for section 1.4.

Furthermore, it is being expected that the quantitative analytical information is based on the following parameters:

- Pd content

- content of Free acid or Hydrogen chloride (HCl)

- content of impurities

In order to fulfil ECHA requirements on substance identification, the parameter for diluted solutions as given above must be converted into a legal entity specific composition with the highest known content of H2[PdCl4] = 59 % (w/w).

In addition, only the amount of diluted hydrochloric acid (HCl + water) that act both as solvent and as stabilizer may be reported.

To do so, the following information is needed:

Parameters	**Measured concentration, related to the diluted solution (values from section 1.4)**
Pd content	$Pd_{measured}$ [% (w/w)]
MW_{Pd} = 106.42 g/mol	
$MW_{H2PdCl4}$ = 250.25 g/mol	
H2[PdCl4] content	H2[PdCl4] = $Pd_{measured}$ [% (w/w)] x 250.25 / 106.42
Content of Free acid or Hydrogen chloride (HCl)	$HCl_{measured}$ [% (w/w)]
Content of Impurities	$Impurities_{measured}$ [% (w/w)]

According to the following scheme, the measured values can be converted into the typical concentrations of the legal entity composition which is based on the highest known content of H2[PdCl4] = 59 % (w/w):

	Typical concentration(s)
Constituents	
H2PdCl4	59 [% (w/w)]
Impurities	
Several minor impurities / Generic entry to describe…	$Impurities_{converted}$ [% (w/w)] = $Impurities_{measured}$ [% (w/w)] Remark: as the content of impurities is expected to be £ 0.1 % (w/w), no further conversion required
Additives	
HCl	$HCl_{converted}$ [% (w/w)] = 59 [% (w/w)] x $HCl_{measured}$ [% (w/w)] / H2[PdCl4] [% (w/w)]
Water	$Water_{converted}$ [% (w/w)] = 100 – 59 [% (w/w)] - HCl [% (w/w)] – $Impurities_{measured}$ [% (w/w)]

The typical concentration values converted this way are to be specified in the legal entity composition, supplemented by the "justification for deviation of the rule that for mono-constituent substances the main constituent is expected to be present as a minimum at 80 %" in the 'Justification for deviations' field.

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

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

Physical state	Solution
Solvent	Diluted hydrochloric acid (H2O + HCl)
Concentration range of substance in solution	24 - 59 %[$]
pH (range) of the solution	<1
Excess acid	HCl 0-10%

***** For liquid substances (solvent cannot be separated from substance without changing the identity of the substance) and not for mixtures, suspensions, and other non-substance forms in which the substance is manufactured and/or imported under REACH.

[$] Corresponds to 10-25 % 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 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			
Raman spectroscopy	X		
Mineralogical analysis			
X-Ray Fluorescence (XRF)			X
X-Ray Diffraction (XRD)			X
Morphology and particle sizing			
Electron microscopy (SEM, TEM, REM)* #			X
Laser diffraction* #			X
Particle size by other means (e.g. sieve analysis)#			X
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/use

8. Lead Registrant

Heraeus Precious Metals GmbH & Co. KG (Germany) is the Lead Registrant for Dihydrogen tetrachloropalladate(2-). 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 Raman analysis of a reference sample used for testing.

Spectrometer: Bruker RFS 100/S

Laser: NdYAG 1064 nm

Spectral range: 3500 – 50 cm-1

Resolution: 2 cm-1

Scans: 300 scans

Temperature: ambient

Sample preparation: liquid phase (water), glass vail, closed

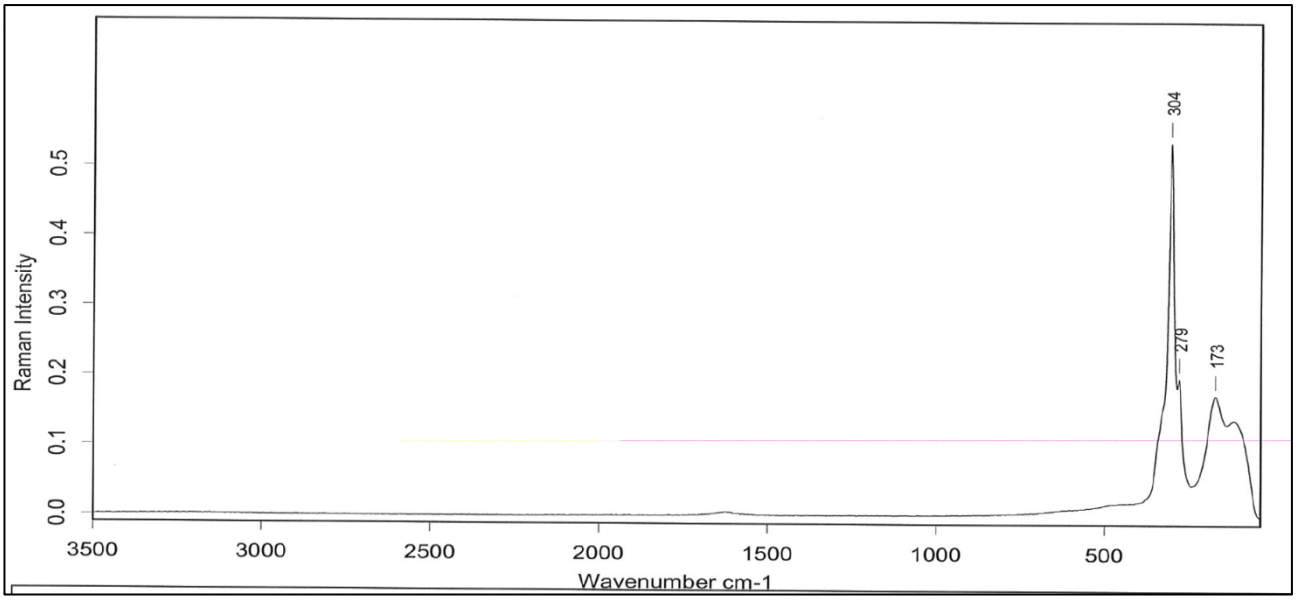


Figure 1. Raman spectrum of Dihydrogen tetrachloropalladate(2-)