ID Card – 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane and its platinum(0) complexes

(*alternative names: 'Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes' and '**Karstedt Concentrate**'*)

Version 22 August 2019

Notes:

- *This ID card is used to support the substance sameness discussions in the SIEF and to describe the substance/group 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).*

1. Identification of the substance

Table 1. Identification of the substance

	New (in EC inventory)	Original (in EC inventory)
Name	1,3-diethenyl-1,1,3,3-tetramethyldisiloxane and its platinum(0) complexes	Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes
EC number	701-315-2	270-844-4
CAS number		68478-92-2
Description	The reaction of chloroplatinic acid with 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane ($M^{vi}M^{vi}$, hereafter also referred to as 'Dimer') gives a mixture of platinum complexes containing $M^{vi}D_xM^{vi}$ ligands (x = 0-11), whereby D_x = Dimethylsiloxane $(CH_3)_2SiO$. During the reaction the alcohol (Propan-2-ol) and the Sodium bicarbonate serves as reducing agents. The mechanism of reaction is not known in detail. According to Lewis and co-workers (1995) the formation of the Pt(0) olefin complexes happens in two stages, with Pt(II) complexes as an intermediate stage. Some complexes are polynuclear with bridging ligands and no metal-metal bonds, such as $Pt_2(M^{vi}M^{vi})_3$. The conversion of Pt(IV) complexes to Pt(0)	None

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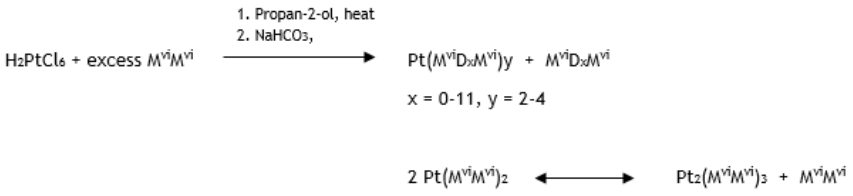
	species results in the net conversion of a silicon-vinyl group to a silicon-oxygen group:  The resulting "Karstedt Concentrate" is composed of Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane, Chloride, Water and Propan-2-ol. Since the exact proportion of each constituent is unknown, "Karstedt concentrate" is registered as UVCB.	
Composition type	UVCB	

2. Synonyms and other identifiers of the substance

Table 2. Synonyms and other identifiers of the substance

IUPAC name	1,3-diethenyl-1,1,3,3-tetramethyldisiloxane and its platinum(0) complexes
CAS name	Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes
Abbreviations	
Other commercial, brand or international names	Karstedt Concentrate Karstedt Catalyst Platinum(0)-1,3-divinyl-1,1,3,3-tetramethyldisiloxane Platinumvinylsiloxane Platinum(0)-1,3-divinyl-1,1,3,3-tetramethyldisiloxane complex Platinum-divinyltetramethyldisiloxane Platinum-divinyltetramethyldisiloxane complex
Other identity codes	

3. Substances (with core identifiers) also falling under this substance (with justification)

None.

4. Usual composition of the substance

The composition given below represents the usual composition available to the Members of the Consortium and SIEF members, by the date given above on the document. This usual content represents the majority of the Karstedt Concentrate that is placed on the EEA market.

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In a UVCB substance, the number of constituents is relatively large and/or; the composition is, to a significant part, unknown and/or; the variability of composition is relatively large or poorly predictable. Hence, concentration ranges outside the ones given below do not exclude sameness and are usually referred to as unusual or exceptional situations. Each potential registrant is responsible for performing its own analysis.

Table 3. Usual composition

	Name	Other names	EC number	Abbreviation / formula	Concentration range (%)	Typical concentration (%)
1	Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes		270-844-4	See below	22 - 85	ca. 70,0
2	1,3-diethenyl-1,1,3,3-tetramethyldisiloxane*	ethenyl[(ethenyldimethylsilyl)oxy]dimethylsilane (IUPAC name); 1,1,3,3-tetramethyl-1,3-divinylsiloxane; 1,3-divinyltetramethyldisiloxane; Divinyltetramethyldisiloxane	220-099-6	$M^{VI}M^{VI}$ $C_8H_{18}OSi_2$	15 - 65	ca. 23,0
3	Chloride			Cl^-	0 – 0,5	ca. 0,0
4	Water		231-791-2	H_2O	0 – 7	ca. 2,0
5	Propan-2-ol **	2-Propanol (IUPAC name); Isopropanol; Isopropyl alcohol; 2-Propyl alcohol	200-661-7	C_3H_8O	0 – 9	ca. 5,0
	Total					**100**

* Excess of 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane is necessary to provide the catalytic functionality of the dissolved complex.
**Other solvents such as methylethylketone may also be used

The resulting ("Karstedt Concentrate") is composed of Platinum, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes, 1,3-diethenyl-1,1,3,3-tetramethyldisiloxane, Chloride, Water and Propan-2-ol.

The **Platinum**, **1,3-diethenyl-1,1,3,3-tetramethylsiloxane complexes** (row 1 in Table 3) consist of:

- **Constituent A:**
  Name: Platinum, bis[1,3-diethenyl-1,1,3,3-tetramethyldisiloxane] complex
  Abbreviation: Pt $(M^{VI}M^{VI})_2$
  Molecular weight: 567,886 g/mol

- **Constituent B:**
  Name: Diplatinum tris[1,3-diethenyl-1,1,3,3-tetramethyldisiloxane] complex
  Abbreviation: $Pt_2(M^{VI}M^{VI})_3$
  Molecular weight: 949,368 g/mol

- **Constituent C (Oligomeric forms):**
  Name: Platinum [diethenyl-tetramethylsiloxane] complexes
  Abbreviation: $Pt(M^{VI}D_xM^{VI})_y$; x = 1-11, y = 2-4 and D_x = Dimethylsiloxane $(CH_3)_2SiO$. The extent of binding of the oligomers to Pt is not known.

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Since the exact proportion of each complex is unknown, the total concentration of the complexes is given in above table, based on the platinum content (typically ca. 23% and ranging from 9% to 30%).

The total silicon content of the Karstedt concentrate is around 20% and ranging from 15% to 30%. The proportion of the silicon content bounded in the Platinum, 1,3-diethenyl-1,1,3,3-tetramethylsiloxane complexes (Constituents A, B, and C) is approximately 15%.

Note:

For the company specific quality assessment, the following values are determined routinely:

Pt content:	$C_{Pt\ measured}$ [%]	(*e.g. by Inductively Coupled Plasma – ICP*)
1,3-diethenyl-1,1,3,3-tetramethyldisiloxane ("Dimer") content:		
	$C_{Dimer\ measured}$ [%]	(*e.g. by gas chromatography*)
Chloride content:	$C_{Cl\ measured}$ [%]	(*e.g. by ion exchange chromatography*)
Water content:	$C_{H2O\ measured}$ [%]	(*e.g. by Karl Fisher titration*)
Propan-2-ol content:	$C_{Propan\text{-}2\text{-}ol\ measured}$ [%]	(*e.g. by gas chromatography*)

Suggested analytical techniques for quantification of the various compounds are added between brackets

Currently neither the concentration of individual constituents nor the concentration of the constituents in total can be determined, so that the lower limit as well as the typical concentration are determined on the following considerations:

- The theoretical lower concentration limit $C_{Constituents\ limit\ low}$ of the Platinum,1,3-diethenyl-1,1,3,3-tetramethyldisiloxane complexes is calculated on the assumption that the complex consists of 100 % of the constituent with the smallest ratio MW_{Const} / $MW_{Platinum}$, multiplied by the measured platinum concentration. The smallest ratio $MW_{Constituent}$ / MW_{Pt} is associated with constituent B ($Pt_2(M^{vi}M^{vi})_3$):

  $C_{Constituents\ limit\ low}$ [%] = $C_{Pt\ measured}$ [%] x $MW_{Constituent\ B}$ [g/mol] / [2 x MW_{Pt}]
  $C_{Pt\ measured}$ = X %
  $MW_{Constituent\ B}$ = 949.4 g/mol
  MW_{Pt} = 195.1 g/mol
  $C_{Constituents\ limit\ low}$ [%] = X [%] x 949.4 [g/mol] / [2 x 195.1] = y %

- The theoretical upper concentration limit $C_{Constituents\ limit\ high}$ results from the calculation

  $C_{Constituents\ limit\ high}$ [%] = 100 [%] - $C_{Dimer\ limit\ low}$ [%], with $C_{Chloride}$, C_{Water} and $C_{Propan\text{-}2\text{-}ol}$ = 0
  $C_{Dimer\ limit\ low}$ = X %
  $C_{Constituents\ limit\ high}$ [%] = 100 [%] - X [%] = y %

- The typical concentration is calculated as 100 % minus the sum of the measured concentrations of the individual components:

  $C_{Constituents\ typical}$ [%] = 100 [%] - $C_{Dimer\ measured}$ [%] - $C_{Cl\ measured}$ [%] - $C_{H2O\ measured}$ [%] - $C_{Propan\text{-}2\text{-}ol\ measured}$ [%]
  $C_{Dimer\ measured}$ = X %
  $C_{Cl\ measured}$ = X %
  $C_{H2O\ measured}$ = X %
  $C_{Propan\text{-}2\text{-}ol\ measured}$ = X %
  $C_{Constituents\ typical}$ [%] = 100 [%] - X [%] – X [%] – X [%] – X [%] = y %

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

Table 4. Appearance / physical state / properties of the substance

Physical state	Liquid
Appearance	

6. 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 5. Analytical methods for identification and characterisation 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)			X
Glow discharge mass spectrometry (GDMS)			X
Molecular analysis			
Infrared (IR) spectroscopy			X
Raman spectroscopy	X		
NMR 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

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Other			
Magnetite analyser			X
DSC-TGA		X	
Separation technique: ion exchange chromatography		X	
Karl Fischer		X	
Headspace GC for solvents/additives		X	

* 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.

Elemental analysis:

- Pt content by ICP-OES or gravimetry
- Si content by ICP-OES
- (Chloride content by potentiometric titration with AgNO3 standard solution or ion exchange chromatography (only for Cl analysis, not speciation)).
- (Water content by Karl Fischer)

Molecular analysis:

- Raman spectroscopy (for 'fingerprinting')
- H-NMR spectroscopy (to assist with sameness by 'fingerprinting')
- C13-NMR spectroscopy (to distinguish complex and free siloxane)
- Pt195-NMR spectroscopy
- (Si-NMR spectroscopy)

In addition, Differential Scanning Calorimetry (DSC) coupled with Thermogravimetric Analysis (TGA): this will give information on phase transitions (melting/ boiling) and can also be used to indicate potential exothermic reactions, assess if the boiling point can be determined at all (e.g., if there is decomposition), assess the amount of volatile organic components, etc.

7. Lead Registrant

Heraeus Deutschland GmbH & Co. KG (Germany) volunteers to be the Lead Registrant for Karstedt Concentrate. The EPMF will provide support to the Lead Registrant as laid down in the EPMF Agreement.

8. REACH Strategy

The table below presents the overall Registration Strategy for Karstedt Concentrate 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 Karstedt Concentrate and sets the minimum and maximum set of information that will be gathered and/or produced when preparing the Registration Dossier for Karstedt Concentrate 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.

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Table 6. REACH strategy for the substance (basis for REACH Registration preparation)

Item	Description	Comment
REACH category	UVCB	Karstedt Concentrate has a variable composition due to the fact that the reaction product of platinum complexes varies according to the stoichiometries of the reactants used.
Highest status	Substance	
Intermediate status	NA	
Highest tonnage band	10-100 t/a	
Information requirements	Annex VII - VIII	
Existing classification	Flam. Liquid 2 (H225) Repr 2 (H361d)	
Registration deadline	2018	

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 following spectra of a reference sample used for testing:

- Raman spectrum
- (H-NMR spectrum – confidential. Spectrum available on request)
- (C-NMR spectrum – confidential. Spectrum available on request)
- (Pt-NMR spectrum – confidential. Spectrum available on request)
- Differential Scanning Colorimetry Analysis (DSC Analysis)

Karstedt concentrate - Analytical Reference Information

Raman spectrum of Karstedt concentrate

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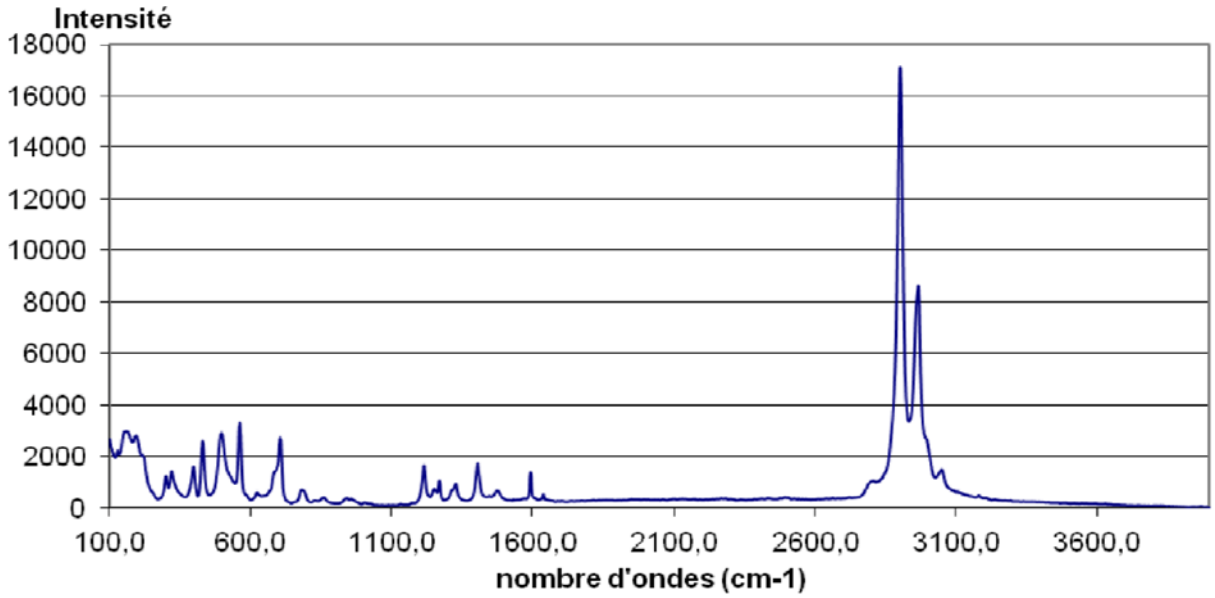

H-NMR of Karstedt concentrate
Confidential. Spectrum available on request

C-NMR of Karstedt concentrate
Confidential. Spectrum available on request

DSC Analysis of Karstedt concentrate:

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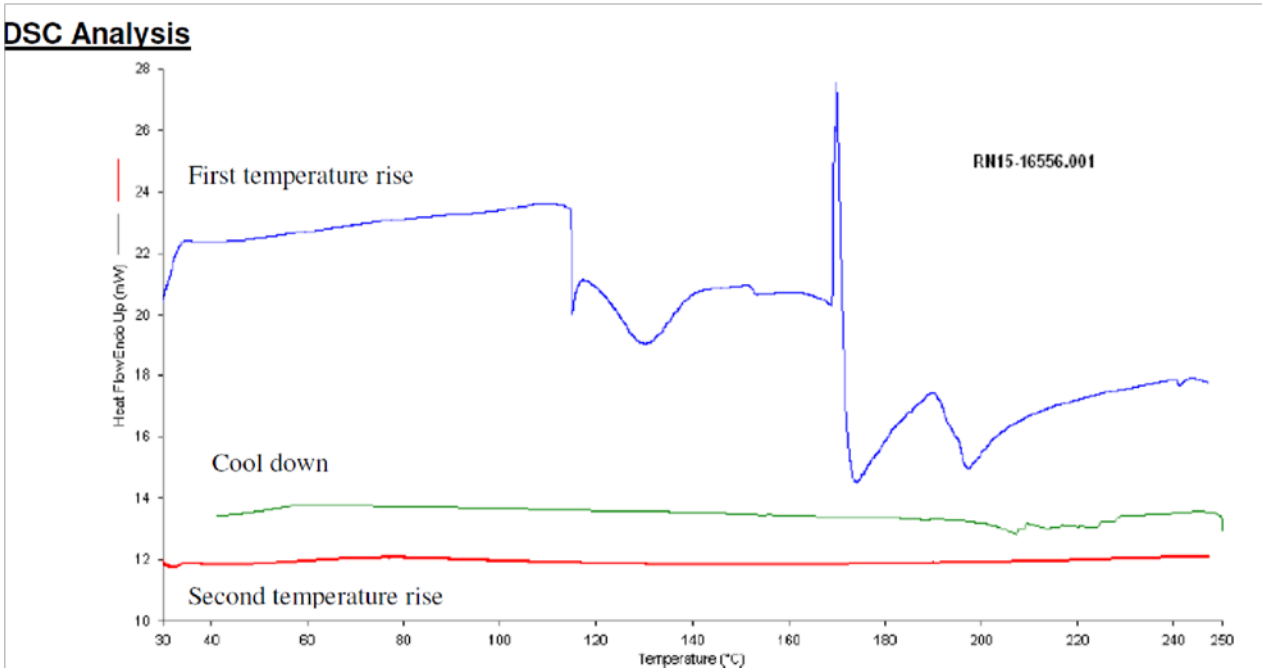
DSC Analysis



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