

2/28/2020 DSB

11/17/2020 JJY

Chemistry Report for Case # P-19-0170

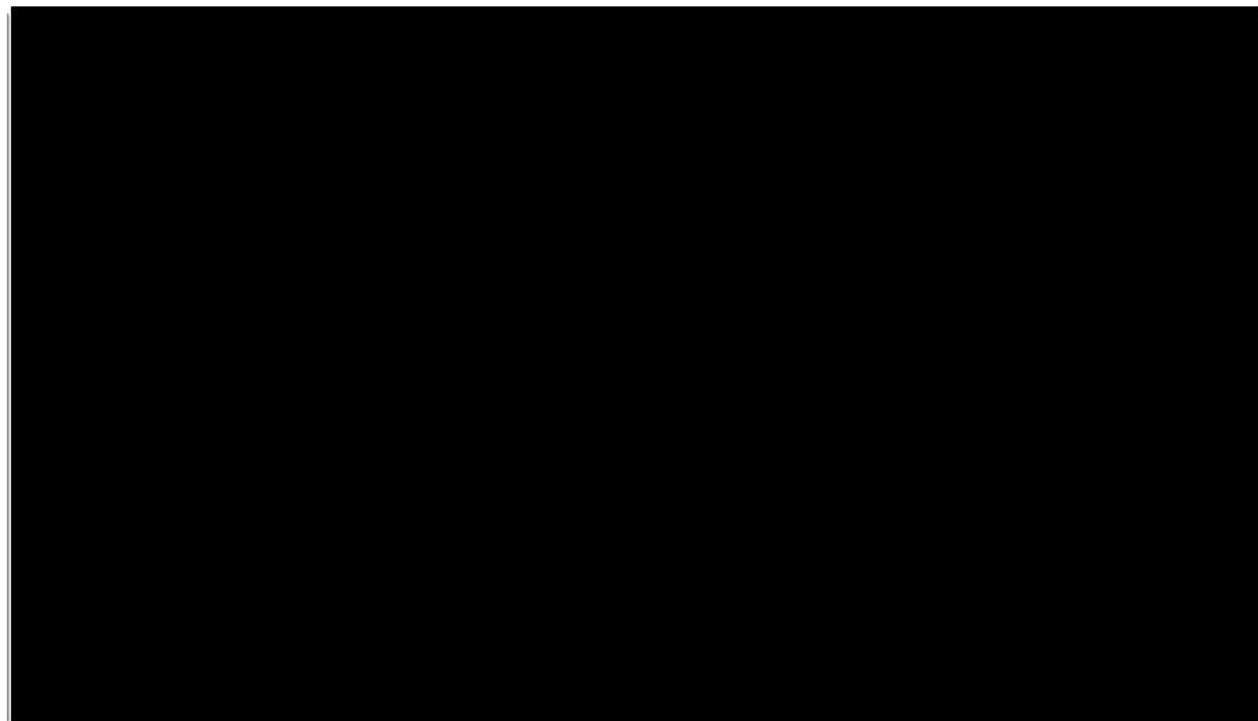
General

Submitter: [REDACTED]	
Contact: [REDACTED]	Contact Telephone No.: [REDACTED]
TS No.: 09MP9S	
Chemist: Schechter, K.	Contractor Support: Y
PV Init (kg/yr): [REDACTED]	PV Max (kg/yr): [REDACTED]
Binding Option: <input type="checkbox"/>	Exposure-Based Review: <input checked="" type="checkbox"/>
Manufacture: <input checked="" type="checkbox"/>	Import: <input type="checkbox"/>

CAS Number: [REDACTED]
Chemical Name [REDACTED]
Trade Name: [REDACTED]
IES Order: [REDACTED]
Generic Name: Heteroatom-substituted alkyl triethoxysilane, reaction products with methylated formaldehyde-melamine polymer

Chemical Structure

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Physical Chemical Properties

Molecular Formula: [REDACTED]	Molecular Weight: [REDACTED]
% < 500: [REDACTED]	% < 1000: [REDACTED]
MP:	MP Estimate:
BP:	BP Pressure:
BP Estimate: >400	
VP (Torr):	VP Estimate (Torr): <0.000001
Water Solubility (g/L):	Water Soluble Estimate (g/L): Reacts
Log P:	Log P Estimate:
Physical State — Neat: Liquid (Sub. Est.)	Physical State — Manuf: Solution: [REDACTED] % PMN material with residual feedstock

Physical State — Processing: Solution: [REDACTED] % PMN material in elastomer formulation

Physical State — End Use: Destroyed

Additional Chemical Info

Composition

by

NAVG MW = with % < 500 and % < 1000 by HPLC and LC/MS.

Submitted Properties: WS = Reacts (Sub.

Est.); pH = 5, Density = 1.2 g/cc.

Estimated Properties: BP = 493 °C

(EPI); VP = 4.3E-8 torr (EPI); WS = Reacts (Ethoxysilyl), 0.00499 g/L

(EPI); logP = 4.06 (EPI). The EPI estimations were performed on the component with on page 1 of this report, having a MW of g/mole, a molecular formula of

and a SMILES of

The PMN

material is expected to hydrolyze with a half-life of hours to give the silanol and ethanol.

Ethoxysilyl FGEW = (Worst case by charge).

Formaldehyde FGEW = (Best case

Amine FGEW = (Best case).

Combined FGEW =

Uses

Consumer Use? No

Use:

Intended Use: Coupling agent in elastomer-based formulations that will be used in molding operations to manufacture different types of rubber articles, including but not limited to rubber tires.

Ethoxysilyl FGEW = (Worst case by charge).

Formaldehyde FGEW = (Best case). Amine FGEW = (Best case).

Combined FGEW = .

Analogues (same use): None.

Patents (same use):

None.

Other Uses:

Analogues

(other use): Analogu

[REDACTED]
Analogues (same use and other use): None.
Patents (other use): None.

Reaction Description

[REDACTED]

Pollution Prevention Analysis(P2 Analysis:)

P2
Claim:
The NCS is developed for silica-filled natural rubber based truck tread formulations as an additive that enables the formulation to match or improve on the wear resistance of traditional carbon black tires while improving the rolling resistance benefits relative to carbon black tires. Both of these qualities, wear resistance and rolling resistance, result in improved gas mileage for vehicles equipped with such tires.

Analogs

Analogues:
[REDACTED]

Comments/Telephone Log

Artifact	Update/Upload Time
[REDACTED]	[REDACTED]