SUPPLEMENTARY MATERIALS

Flowback verses First-Flush: New Information on the Geochemistry of Produced Water from Mandatory Reporting

By

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Table S-1. Chemical constituents used in well stimulations in California, May 5, 2015 – June 29, 2016, sorted by frequency of use in well stimulations. There were 618 stimulations conducted at 596 wells. The number of unique constituents is 178. TT= used as a tracer (chemical was used in a treatment where tracers were used), AF=used in acid fracturing, MA=used in matrix acidizing.

Chemical name	CASRN	Stimu-lations
Water	7732-18-5	618
Crystalline silica (quartz)	14808-60-7	617
Guar gum	9000-30-0	617
Ammonium persulfate	7727-54-0	577
2-Butoxypropan-1-ol	15821-83-7	522
1-Butoxy-2-propanol	5131-66-8	522
Prolonium chloride	55636-09-4	522 (AF)
Paraffinic petroleum distillate, hydrotreated light	64742-55-8	522
Isotridecanol, ethoxylated	9043-30-5	522
Magnesium nitrate	10377-60-3	521
Crystalline silica (cristobalite)	14464-46-1	521
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	521
2-Methyl-3(2H)-isothiazolone	2682-20-4	521
Hydrotreated light petroleum distillate	64742-47-8	521
Magnesium chloride	7786-30-3	521
Diatomaceous earth, calcined	91053-39-3	521
Sodium hydroxide	1310-73-2	519
Sodium tetraborate decahydrate	1303-96-4	493
Ethylene glycol	107-21-1	447
Phosphonic acid	13598-36-2	411
Nitrilotris (methylene phosphonic acid)	6419-19-8	410
Hemicellulase enzyme concentrate	9025-56-3	288
Glycerol	56-81-5	287
Sodium chloride	7647-14-5	276
Beta mannanases	37288-54-3	233
Methanol	67-56-1	84
Boric acid	10043-35-3	79
Methyl borate	121-43-7	79
Potassium bicarbonate	298-14-6	79
Potassium carbonate	584-08-7	79
Hemicellulase enzyme	9012-54-8	61
Non-crystalline silica (impurity)	7631-86-9	55
Isopropanol	67-63-0	53
Calcium magnesium sodium phosphate frit	65997-18-4	49
Choline chloride	67-48-1	49
Tetrakis hydroxymethyl phosphonium sulfate	55566-30-8	46
1,2-benzisothiazolin-3-one	2634-33-5	42

Chemical name	CASRN	Stimu-lations
Sodium polyacrylate	9003-04-7	41
Ammonium chloride	12125-02-9	40
Sodium sulfate	7757-82-6	40
Sodium persulfate	7775-27-1	40
Monoethanolamine borate	26038-87-9	39
Polydimethyl diallyl ammonium chloride	26062-79-3	39
Lactose	63-42-3	39
Sodium bisulfite	7631-90-5	39
Acetic acid	64-19-7	34
Triethanolamine	102-71-6	31
Zinc sulfate	7733-02-0	28
Xanthan gum	11138-66-2	22
Propylene glycol	57-55-6	22
Sodium citrate	68-04-2	22
Triethylene glycol	112-27-6	21 (AF)
Castor oil, ethoxylated	61791-12-6	21 (AF)
Alcohols, C12-15 ethoxylated	68131-39-5	21 (AF)
1,2-Ethanediamine, N1-(2-aminoethyl)-N2-(2-((2-aminoethyl)amino)ethyl)-, polymer with 2-methyloxirane and oxirane	68815-65-6	21 (AF)
Poly(oxy-1,2-ethanediyl), .alpha.-2,4,6-tris(1-phenylethyl)phenyl-.omega.-hydroxy-	70559-25-0	21 (AF)
Sorbitan stearate	1338-41-6	20
2-Propenoic acid, 2-ethylhexyl ester, polymer with 2-hydroxyethyl 2-propenoate	36089-45-9	20
Tetrahydro-3,5-dimethyl-1,3,5-thiadiazine-2-thione	533-74-4	20
Dimethyl siloxanes and silicones	63148-62-9	20
Siloxanes and silicones, dimethyl, reaction products with silica	67762-90-7	20
Fatty acids, C18-unsatd., dimers, ethoxylated propoxylated	68308-89-4	20
Siloxanes and Silicones, di-Me, 3-hydroxypropyl Me, ethoxylated propoxylated	68937-55-3	20
Sodium nitrite	7632-00-0	20
Sodium carboxymethylcellulose	9004-32-4	20
Sorbitan monooleate, ethoxylated	9005-65-6	20
Citrus terpenes	94266-47-4	19
Potassium chloride	7447-40-7	15
Polypropylene glycol	25322-69-4	9
Citric acid	77-92-9	9
Glutaraldehyde	111-30-8	8
MBNPA (2-bromo-3-nitrilopropionamide)	1113-55-9	8
D-limonene	5989-27-5	8
2,2 Dibromo-3-nitrilopropionamide	10222-01-2	7
Lauryl hydroxysultaine	13197-76-7	7

Chemical name	CASRN	Stimu-lations
Acetic acid etheynl ester, polymer with ethene	24937-78-8	5
Diatomaceous earth, natural (kieselguhr)	61790-53-2	5
Heavy aromatic naphtha	64742-94-5	5
Olefin/maleic ester	68188-50-1	5
Mineral oil	8042-47-5	5
Naphthalene	91-20-3	5
1,2,4-Trimethylbenzene	95-63-6	5
Acrylonitrile	107-13-1	4
Potassium acetate	127-08-2	4
Potassium hydroxide	1310-58-3	4
Potassium borate	1332-77-0	4
4-Chlorobenzophenone	134-85-0	4 (TT)
Magnesium silicate hydrate (talc)	14807-96-6	4
Vinylidene chloride/methylacrylate copolymer	25038-72-6	4
Polyethylene glycol monohexyl ether	31726-34-8	4
Polytetrafluoroethylene	9002-84-0	4
2-propenoic acid, polymer with 2-propenamide	9003-06-9	4
1,4-Dibromobenzene	106-37-6	3 (TT)
1-bromo-3,5-dichlorobenzene	19752-55-7	3 (TT)
Poly(dimethylaminoethylmethylacrylate) dimethyl sulphate quat.	27103-90-8	3
2,5-Dibromothiophene	3141-27-3	3 (TT)
1-Bromo-4-iodobenzene	589-87-7	3 (TT)
Dicoco dimethyl quaternary ammonium chloride	61789-77-3	3
4-Iodotoluene	624-31-7	3 (TT)
1,3,5-Tribromobenzene	626-39-1	3 (TT)
2,4,6-Tribromotoluene	6320-40-7	3 (TT)
1,2,4,5-Tetrabromobenzene	636-28-2	3 (TT)
1-Chloro-4-iodobenzene	637-87-6	3 (TT)
Orange terpenes	68647-72-3	3 (AF)
Ethoxylated alcohol C11-14	78330-21-9	3
Phenolic resin	9003-35-4	3
1-Iodonaphthalene	90-14-2	3 (TT)
2-Ethylhexan-1-ol	104-76-7	2
Ethoxylated alcohol C6	104780-82-7	2
2-Butoxyethanol	111-76-2	2
Disodium octaborate tetrahydrate	12008-41-2	2
Corundum	1302-74-5	2
Ulexite	1319-33-1	2
Mullite	1327-36-2	2
3,5-Dibromotoluene	1611-92-3	2 (TT)
2,4,5-Tribromotoluene	3278-88-4	2 (TT)
1,2-Diiodobenzene	615-42-9	2 (TT)

Chemical name	CASRN	Stimu-lations
Hydrochloric acid	7647-01-0	2
Hydrofluoric acid	7664-39-3	2
Zirconium dichloride oxide	7699-43-6	2
Ethoxylated alcohol C7-9-iso, C8	78330-19-5	2
Polyethylene, polypropylene ether glycol copolymer	9003-11-6	2
Calcium chloride	10043-52-4	1
Quaternary ammonium compound	100765-57-9	1 (AF)
Cinnamaldehyde	104-55-2	1 (AF)
Propargyl alcohol	107-19-7	1
1-Methoxy-2-propanol	107-98-2	1
Methyl isobutyl ketone	108-10-1	1 (AF)
Diethanolamine	111-42-2	1
2,2"-oxydiethanol (impurity)	111-46-6	1
1-Tetradecene	1120-36-1	1
Oleic acid	112-80-1	1
1-Octadecene	112-88-9	1
Ammonium fluoride	12125-01-8	1
2-Propenoic acid, polymer with sodium phosphinate	129898-01-7	1
Ammonium bifluoride	1341-49-7	1
Potassium oleate	143-18-0	1
2-Iodobiphenyl	2113-51-1	1 (TT)
5-Iodo-m-xylene	22445-41-6	1 (TT)
Polyethylene oxide	25322-68-3	1
Dodecylbenzene sulfonic acid	27176-87-0	1
Etidronic acid	2809-21-4	1
4-Iodo-o-xylene	31599-61-8	1 (TT)
1-Eicosene	3452-07-1	1
Aziridine, polymer with methyloxirane and oxirane	52501-07-2	1 (AF)
Hydroxylamine hydrochloride	5470-11-1	1 (MA)
Polyurethane resin	57029-46-6	1
9-Bromophenanthrene	573-17-1	1 (TT)
Dioctyl sulfosuccinate sodium salt	577-11-7	1
2-Bromonaphthalene	580-13-2	1 (TT)
3-aminopropyl (sileanetriol)	58160-99-9	1
Fatty acids, tall-oil	61790-12-3	1
Amines, hydrogenated tallow alkyl, acetates	61790-59-8	1
Fatty acids, tall-oil, ethoxylated	61791-00-2	1 (AF)
1-Hexadecene	629-73-2	1
Ethanol	64-17-5	1
Formic acid	64-18-6	1
Benzoic acid	65-85-0	1 (AF)
Alcohols, C10-14, ethoxylated	66455-15-0	1
Sulferized polyolefin	68037-13-8	1 (AF)

Chemical name	CASRN	Stimu-lations
Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	68123-18-2	1
Silanetrio; (3-aminopropyl, homopolymer	68400-07-7	1
Ethoxylated alcohol C6-12	68439-45-2	1
Thiourea, polymer with formaldehyde and 1-phenylethanone	68527-49-1	1
Alcohols, C12-16, ethoxylated	68551-12-2	1
Ethoxylated alcohol C8-10	68603-25-8	1 (AF)
Alcohols, C14-C15, ethoxylated	68951-67-7	1
2,4-Dibromomesitylene	6942-99-0	1 (TT)
Tar bases, quinoline derivs., benzyl chloride quaternized	72480-70-7	1 (AF)
Copper dichloride	7447-39-4	1 (MA)
Ethylene oxide	75-21-8	1
Sulfuric acid	7664-93-9	1
Potassium iodide	7681-11-0	1
Triisobutylene (mixed isomers)	7756-94-7	1 (AF)
Tricalcium phosphate	7758-87-4	1
Polyethylene glycol trimethyl nonyl ether	84133-50-6	1
Erythorbic acid	89-65-6	1