BMF 101 | 0722

Quaternary ammonium compounds (Quats)

Quaternary ammonium compounds (quats) are a group of chemicals that share a similar molecular structure, with one of several long chain hydrocarbons and short chain substitutions such as methyl, ether, and benzyl. Although useful in many products, especially those used in the fight against COVID-19, quats have become a cause for concern due to their impact on human and environmental health.

Disinfectants have been increasingly used during the COVID-19 pandemic, as individuals focused on improving their own personal hygiene to prevent the spread of the disease.

Health professionals recommended regular washing of hands with soap, alongside the use of alcohol-based sanitizers to minimize the risk of contracting the virus. Disinfectants were also extensively used to mitigate COVID-19 transmission.

Whilst higher levels of personal hygiene have been widely embraced by the public, there is now concern over the effects that exposure to these disinfectants can have on human health.

Common disinfectants that have been recommended to stop the spread of COVID-19, contain chemicals that can have a damaging impact on human health and our environment. These frequently used disinfectants belong to a chemical group called quats.

Quaternary ammonium compounds (Quats) are almost inert to degradation and are now beginning to accumulate in our environment. The chemicals have been detected in wastewater sludge, surface waters, sediments, and soils[1]. Recent studies have indicated that extensive disinfecting practices can have a strong effect on indoor chemical levels[2].

The increased use of these chemicals may be associated with adverse effects on reproductive and respiratory systems. There is also concern of a risk of antibiotic resistance, which may be affected due to the increased use of disinfectants[3].

Measures should be taken to investigate the use and impact of quats to protect the public from the possible health and safety risks connected to disinfectants.

What are Quats?

Quats, also known as QACs, are salts of quaternary ammonium cations, with one of several long chain hydrocarbons and short chain substitutions such as methyl, ether, and benzyl.

The EPA (The US Environmental Protection Agency) has combined quats into four groups, for testing and registration purposes. Assigning them in this way aids efforts to build a database, that will support the registration of the entire family of quats.[4]

The EPA grouping of currently registered quat compounds:

Group 1: The alkyl or hydroxyalkyl (straight chain) substituted quats

Group 2: The non-halogenated benzyl substituted quats (includes hydroxybenzyl, ethylbenzyl, hydroxyethybenzyl, napthylmethyl, dodecylbenzyl, and alkyl benzyl)

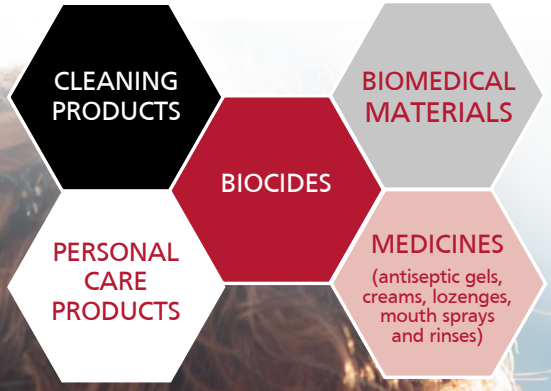
Group 3: The di- and tri- chlorobenzyl substituted

Group 4: Quats with unusual substituents (charged heterocyclic ammonium compounds)

Applications

Quats have a variety of applications, including as surfactants and as active ingredients in disinfectants and sanitizing products. They are commonly found in products used in multiple environments, including transportation, hospitals, nursing homes, wastewater treatment facilities, and general households. They are also a staple ingredient in the pharmaceutical industry as an active pharmaceutical ingredient (API).

QUATS have antimicrobial activity and are applied in:



Quats have been recommended for use to protect against SARS-CoV-2 by the US Centers for Disease Control and Prevention (CDC) and EPA.

In March 2020, the EPA issued List N: Disinfectants for Use Against SARS-CoV-2, which identified approximately 250 surface disinfectants that met that EPA's criteria for efficacy under the Emergency Viral Pathogen Guidance for Antimicrobial Pesticides.

As of August 2020, 482 surface disinfectants met the EPA's criteria for efficacy against SARS-CoV-2. Approximately 81% of these disinfectants contained a single active ingredient, of which 48% contained quats. The remaining disinfectants contained a mixture of two or more active ingredients.[5].

In addition to being used as disinfectants, quats are also applied as:

PHASE TRANSFER CATALYSTS IN CHEMICAL REACTIONS
(due to their surfactant properties)

HAIR CONDITIONERS

FABRIC SOFTENERS

What are the concerns?

It has been reported that the increased use of these chemicals may be associated with adverse effects on reproductive and respiratory systems. There are also concerns relating to risk of antibiotic resistance, which may be affected due to the increased use of disinfectants.

The use and effect of quats should be monitored and further investigated to understand their true impact on human and environmental health.

Quats have been detected in outdoor environments, including wastewater sludge, surface waters, sediments, and soils. Recent studies have indicated that extensive disinfecting practices can also have a strong effect on indoor chemical levels.

The degradation and metabolism of quats is a concern. It is known that alkyl quats are very persistent and do not easily degrade in the environment. Replacements to alkyl quats have been introduced for some applications, such as fabric softeners.

However, little has been reported on the degradation of quats and trialkylamines in the environment.

Oxidation to carboxylic acid in the omega alkyl moiety is one possible degradation route. Benzyl quats may rearrange at elevated temperature following the Sommelet-Hauser rearrangement.[6,7]

Trialkylquats may also rearrange following the Stevens rearrangement.[8] However, there is little information about whether this happens under normal degradation or metabolism conditions.

Potential health effects:

INCREASE IN ASTHMA TRIGGERS

BREATHING PROBLEMS, SUCH AS PULMONARY CELL DAMAGE AND INFLAMMATION

SKIN IRRITATION

DECREASED FERTILITY

Other news

The Covid-19 pandemic has highlighted the importance of personal protective equipment (PPE) in mitigating virus transmission. Research has shown that the virus can survive on PPE, such as surgical masks, and methods are needed to inactivate the live virus on contaminated material.

In a recent study, which embedded quats into surgical masks during the manufacturing, live SARS-CoV-2 was found to be inactivated within minutes.

The benefit of this approach is the inactivation of the virus on the surface of the face mask, ultimately increasing its protective capabilities and mitigating the accidental spread of the virus to the individual wearing the mask, or to other PPE.

The data gathered highlighted the effectiveness of PPE infused with anti-viral compounds. However, there is the concern of potential toxicity to the wearer of the infused surgical mask.

To address this concern, the coating was applied only to the outside of the 3-layers mask. The ensuing polymeric film concentrated the disinfectant materials in the outer layer of the mask, preventing the inhalation of infectious particles. Additionally, this lessened the risk of contact of the quats the skin.

The data suggests that quats placed on PPE can be used to inactive the SARS-CoV-2 virus in an effective and safe manner.[9]

Regulations

Despite their extensive use during the pandemic, many active ingredients in antimicrobial products such as surface disinfectants, are lacking in Occupational Exposure Limits (OELs), which are used to support health professionals in identifying risks associated with exposure to these chemicals.

In a recent case study[10], three potential OELs were acquired based on irritation toxicity data, developmental and reproductive toxicity data (DART), and modification of an existing health-based exposure limits (HBELs). The lowest of value of the three approaches was adopted as the final OEL for the evaluated quat containing product, resulting in a recommended OEL of 0.1 mg/m^3.

In Europe, uses of quats have been limited in food products and consumer hand and body washes.[10]

Published methods

ASTM D5070-90(2014) Standard Test Method for Synthetic Quaternary Ammonium Salts in Fabric Softeners by Potentiometric Titrations

ASTM D5806-95(2017) Standard Test Method for Disinfectant Quaternary Ammonium Salts by Potentiometric Titration

ISO - ISO 2871-1:2010 - Surface active agents — Detergents — Determination of cationic-active matter content — Part 1: High-molecular-mass cationic-active matter

ISO - ISO 2871-2:2010 - Surface active agents — Detergents — Determination of cationic-active matter content — Part 2: Cationic-active matter of low molecular mass (between 200 and 500)

Chiron offer a comprehensive range of reference materials for quats, trialkylamines, and surfactants, including isotopic labelled internal standards.

References:

1. Lennart Kaj, Petra Wallberg, Eva Brorström-Lundén Quaternary ammonium Compounds Analyses in a Nordic cooperation on screening; ISBN 978-92-893-3813-4 (PRINT), Nordic Council of Ministers 2014.
2. Guomao Zheng, Gabriel M. Filippelli, and Amina Salamova, Incresded Indoor Exposure to Commonly Used Disinfectants during the COVID-19 Pandemic, Environ. Sci. Technol. Lett. August 20, 2020. https://dx.doi.org/10.1021/acs.estlett.0c00587
3. Xiaozhi Lim, Quat disinfectants and antibiotic resistance; Chem Eng. News August 30, 2021.
4. PRN 88-2: Clustering of Quaternary Ammonium Compounds | US EPA
5. Setting occupational exposure limits for antimicrobial agents: A case study based on a quaternary ammonium compound-based disinfectant - PMC (nih.gov) September 2020, National Library of Medicine, G Scott Dotson, Jason T Lotter, Rachel E Zisook, Shannon H Gaffney, Andrew Maier, and Jonathan Colvin
6. M.Sommelet, Compt. Rend. 1937, 205, 56
7. W. Kantor, Charles R. Hauser J. Am. Chem. Soc. 1951, 73, 4122-4131.
8. T.S. Stevens, Creighton, A.B. Gordon, and M. MacNicol, 1928, «CCCCXXIII-Degradation of quarternary ammonium salts. Part I» (http://pubs.rsc.org/en/content/articlelanding/1028/jr/j9280003193). J. Chem. Soc. 3193-3197. doi.1039/JR9280003197 (https://doi.org/10.1039%2FJR9280003139).
9. Anti-SARS-CoV-2 Activity of Surgical Masks Infused with Quaternary Ammonium Salts - PMC (nih.gov)
10. Increased Use of Quaternary Ammonium Compounds during the SARS-CoV-2 Pandemic and Beyond: Consideration of Environmental Implications - PMC (nih.gov) June 2020, National Library of Medicine, Priya I. Hora, Sarah G. Pati, Patrick J. McNamara, and William A. Arnold

QUATS product listing

ISO 17034
ISO/IEC 17025
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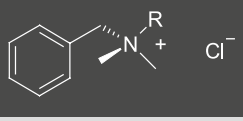
Chiron No.	Name	Synonym / Example Structure	CAS
	Quats **BACs: (Benzylalkyldimethylammonium compounds)**		
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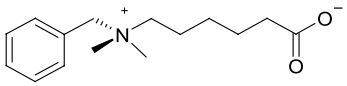
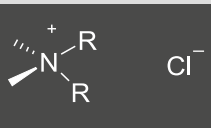
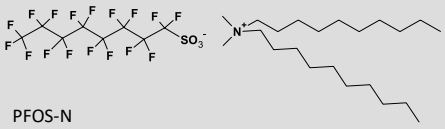
14531.15	Benzyldimethyl-5-carboxypentylaminium hydrobromide (inner salt)		2361417-28-7
14532.17	Benzyldimethyloctylammonium chloride	BAC 8	959-55-7
14533.19	Benzyldecyldimethylammonium chloride	BAC 10	965-32-2
14534.19	Benzyldecyldimethylammonium chloride-d7	BAC 10-d7	1998128-81-6
14535.21	Benzyldodecyldimethylammonium chloride	BAC 12; Zephirol; Benzyllauryldimethylammonium chloride	139-07-1
14536.21	Benzyldodecyldimethylammonium chloride-d7	BAC 12-d7; Zephirol-d7; Benzyllauryldimethylammonium chloride-d7	1998128-83-8
14537.23	Benzyldimethyltetradecylammonium chloride	BAC 14; Benzalkonium chloride; Zephiran chloride;	139-08-2
14538.23	Benzyldimethyltetradecylammonium chloride-d7	BAC 14-d7	1219178-72-9
14539.25	Benzyldimethylhexadecylammonium chloride	BAC 16; Cetaconium chloride; Benzylcetyldimethylammonium chloride	122-18-9
14540.25	Benzyldimethylhexadecylammonium chloride-d7	BAC 12-d7; Cetaconium chloride-d7; Benzylcetyldimethylammonium chloride-d7	1998128-85-0
14541.27	Benzyldimethylstearylammonium chloride	BAC 18	122-19-0
14578.13	Benzyltriethylammonium chloride	BAC-TE; TEBAC	56-37-1
	DDACs: (Dialkyldimethylammonium compounds)		
14542.14	Dimethyldihexylammonium chloride	C6-DDAC	82941-31-9
14543.18	Dimethyldioctylammonium chloride	C8-DDAC; AQ 208	5538-94-3
14544.22	Dimethyldidecylammonium chloride	C10-DDAC; AQ 210	7173-51-5
14717.30	Didecyldimethylammonium perfluorooctane sulfonate	 PFOS-N	251099-16-8
14545.26	Dimethyldidodecylammonium chloride	C12-DDAC; AC 212; Aliquat 204; Dilauryldimethylammonium chloride; Quaternium 47	3401-74-9
14546.30	Dimethylditetradecylammonium chloride	C14-DDAC; Dimethyldimyristylammonium chloride	10108-91-5
14447.34	Dimethyldihexadecylammonium chloride	C16-DDAC; AQ 206; Adogen 436-100; Adogen 436CG; Aliquat 206; Ammonyx D 34	1812-53-9
8375.38	Dimethyldistearylammonium chloride	C18-DDAC; DSDMAC; DODMAC,	107-64-2
8385.38	Ditallowalkyldimethylammonium chloride, techn. Purified	DTDMAC, Adogen 442-110P, Adogen 470	68783-78-8
8384.38	Ditallowalkyldimethylammonium chloride, hydrogenated form	DHTDMAC, Adogen 442, Adogen 442-100P	61789-80-8

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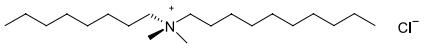
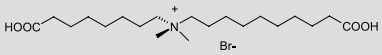
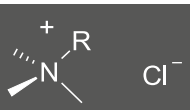
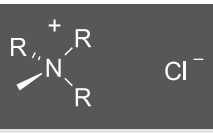
Chiron No.	Name	Synonym / Example Structure	CAS
14547.20	Decyldimethyloctylammonium chloride	 BTC 818; Bardac 2050	32426-11-2
11797.20	9-Carboxynonyl-7-carboxyheptyldimethylammonium bromide		N/A
11798.20	9-Carboxynonyl-7-carboxyheptyldimethyl-d6-ammonium bromide		N/A
	ATMACs: (Alkyltrimethylammonium compounds, ATACs, ATMAs, ATMACs, TMACs)		
14548.9	Hexyltrimethylammonium chloride	ATAC-C6	29801-86-3
14549.11	Octyltrimethylammonium chloride	ATAC-C8	10108-86-8
14550.13	Decyltrimethylammonium chloride	ATAC-C10; Trimethylcaprylammonium chloride	10108-87-9
12716.15	Dodecyltrimethylammonium chloride	ATAC-C12	112-00-5
12717.17	Tetradecyltrimethylammonium chloride	ATAC-C14	4574-04-3
14579.17	Tetradecyltrimethylammonium-d3 iodide	ATAC-C14-d3	N/A
8541.19	Hexadecyltrimethylammonium chloride	ATAC-C16; Cetrimonium chloride	112-02-7
12722.19	Hexadecyl-d33-trimethylammonium chloride	ATAC-C16-d33; Cetrimonium-d33 cholride	112-02-7 (unlabelled)
9137.19	Hexadecyltrimethylammonium bromide	Cetrimonium bromide	57-09-0
12718.21	Octadecyltrimethylammonium chloride	ATAC-C18; Steartrimonium chloride	112-03-8
12719.23	Eicosyltrimethylammonium chloride	ATAC-C20; Arachidtrimonium chloride	15809-05-9
12720.25	Docosyltrimethylammonium chloride	ATAC-C22; Behentrimonium chloride	17301-53-0
12721.27	Tetracosyltrimethylammonium chloride	ATAC-C24	70765-68-3
8542.22	Tallowtrimethylammonium chloride		8030-78-2
13101.5	Chlormequat chloride	2-Chloroethyltrimethylammonium chloride	999-81-5
13100.5	Chlormequat-1,1,2,2-d4 chloride	2-Chloroethyltrimethylammonium-d4 chloride	999-81-5 (unlabelled)
	Methyltrialkylammonium compounds		
14580.25	Methyltri-n-octylammonium chloride	Aliquat® 336 TG	5137-55-3

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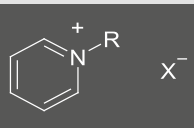
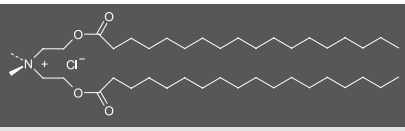
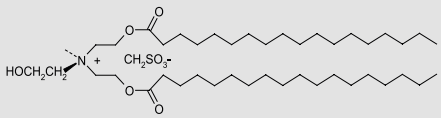
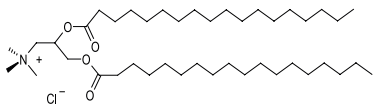
Chiron No.	Name	Synonym / Example Structure	CAS
	Tetraalkylammonium compounds		
2358.4	Tetramethylammonium bromide		64-20-0
2354.8	Tetraethylammonium bromide		71-91-0
2352.16	Tetrabutylammonium bromide		1643-19-2
2357.24	Tetrahexylammonium bromide		4328-13-6
2353.32	Tetraoctylammonium bromide		14866-33-2
14551.40	Tetradecylammonium bromide		14937-42-9
2356.48	Tetradodecylammonium bromide		14866-34-3
14552.56	Tetratetradecylammonium bromide		139653-49-9
14553.64	Tetrahexadecylammonium bromide		139653-55-7
2355.72	Tetraoctadecylammonium bromide		63462-99-7
	Alkylpyridinium compounds		
14581.11	N-Hexadecylpyridinium chloride		74440-81.6
14582.13	Octylpyridinium bromide		2534-66-9
14554.15	Decylpyridinium bromide		2534-65-8
11795.15	9-Carboxynonylpyridium bromide		1279010-77-3
11796.15	9-Carboxynonylpyridium-d5 bromide		N/A
14583.17	Dodecadecylpyridium bromide	Laurylpyridinium chloride; Isothan Q 4; DPB; Laurosept	104-73-4
14584.19	Tetradecylpyridinium chloride		1155-74-4
14555.21	Hexadecylpyridium chloride	Pyrisept; Cetylpyridium chloride	123-03-5
14585.23	Octadecylpyridinium chloride		3165-81-9
	Cathionic Ester Fabric softeners		
14556.42	Dimethylbis[2-[(1-oxooctadecyl)oxy]ethyl]ammonium chloride	 DEEDMAC	67846-68-8
14557.42	Hamburg esterquat	 HEQ	220609-41-6

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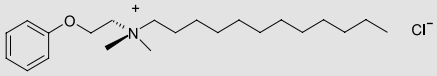
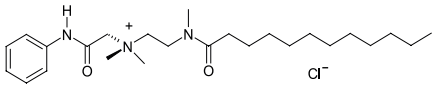
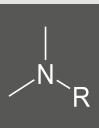
Chiron No.	Name	Synonym / Example Structure	CAS
	Other quats and antiseptics:		
14559.22	Domiphen bromide (antiseptic used in cosmetics)		538-71-6
14566.25	Dofanium chloride (antiseptic)	 Desogen (6Cl); Desocin; Desogen-fest; Dofamium chloride	54063-35-3
	LONZABAC components		
14677.18	Laurylamine dipropylenediamine	Bis(aminopropyl)laurylamine; TA	2372-82-9
14678.15	N-Lauryltrimethylenediamine	Laurylaminopropylamine; DA	5538-95-4
14679.12	Laurylamine	n-Dodecylamine; MA	124-22-1
	Alkylmethylamines **Alkyldimethylamines:**		
14587.8	Hexyldimethylamine	DMA8	4385-04-0
14415.10	Octyldimethylamine	DMA10; Adma 8, DMOA	7378-99-6
14567.12	Decyldimethylamine	DMA12	1120-24-7
14410.14	Dodecyldimethylamine	DMA12; DDA	112-18-5
14412.16	Tetradecyldimethylamine	DMA14; N,N-Dimethylmyristylamine	112-75-4
14411.18	Hexadecyldimethylamine	DMA16; Adma 16; NoKe DMA16; bairdcatb16; Armeen DM 16D; ADMA 16 amine; genamin16r302d; Barlene(R) 16S; FENTAMINE DMA16; Crodamine 3.A16D	112-69-6
14418.20	Octadecyldimethylamine	DMA18; Adma 18; GS-1339; Dimantin; Dimantine; Thelmesan; Dimanthine; Dymanthine; Onamine 18; Amine 2M18D	124-28-7
14494.24	Dodecyldimethylamine	DMA22; Docosyldimethylamine	21542-96-1

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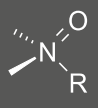
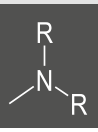
	Alkyldimethylamine oxides:		
14413.10	Octyldimethylamine oxide	N,N-Dimethyl-1-octanamide-N-oxide	2605-78-9
14414.12	Decyldimethylamine oxide		2605-79-0
14409.14	Dodecyldimethylamine oxide	DDAO; LDAO; Lauryldimetylamine oxide	1643-20-5
14492.16	Tetradecyldimethylamine oxide	Myristyldimethylamine N-oxide; TDAO	3332-27-2
14568.18	Hexadecyldimethylamine oxide	Palmitoyldimethylamine oxide	7128-91-8
14569.20	Octadecyldimethylamine oxide	Stearyldimethylamine oxide	2571-88-2
	Dialkylmethylamines:		
14570.33	Dihexadecylmethylamine		16724-61-1
14571.37	Dioctadecylmethylamine		4088-22-6
	Alkyl diethanolamides:		
12307.16	Lauryl diethanolamide, 95% techn.	N,N-Bis(2-hydroxyethyl)dodecanamide	120-40-1
12321.16	Lauryl diethanolamide, purified	N,N-Bis(2-hydroxyethyl)dodecanamide	120-40-1
	Siloxane surfactants **Open chain siloxane surfactants:**		
14310.6	Hexamethyldisiloxane		107-46-0
14311.8	Octamethyltrisiloxane		107-51-7
14312.10	Decamethyltetrasiloxane		141-62-8
14313.12	Dodecamethylpentasiloxane		141-63-9
14314.14	Tetradecamethylhexasiloxane		107-52-8
14392.10	Methyltris(trimethylsiloxy)silane	TMF 1.5	17928-28-8
14405.16	Tetrakis(methylethylketoximino)silane, 50% in toluene	2-ButaneOOOOsilane; OX 30	34206-40-1
	Cyclic siloxane surfactants:		
9684.6	Hexamethylcyclotrisiloxane	D3	541-05-9
13018.8	Volasil 244 (Techn.)	D4	556-67-2
9685.8	Octamethylcyclotetrasiloxane	D4	556-67-2
13924.8	Octamethylcyclotetrasiloxane-13C4	D4-13C4	2086337-19-9
13019.10	Volasil 245 (Techn.)	D5	541-02-6
13020.X	Volasil 344 (Techn.)	D4 + D5	556-67-2/541-02-6
9686.10	Decamethylcyclopentasiloxane	D5	541-02-6
9687.12	Dodecamethylcyclohexasiloxane	D6	540-97-6

For ordering and information about prices and delivery in your country, please contact your local distributor:

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