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2-ALKYL QUATERNARY AMMONIUM COMPOUNDS

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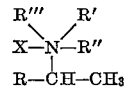
No Drawing. Continuation-in-part of application Ser. No. 595,349, Nov. 18, 1966. This application Feb. 5, 1968, Ser. No. 703,191

Int. Cl. C07c *87/00*

U.S. Cl. 260—567.6 1 Claim

ABSTRACT OF THE DISCLOSURE

This invention relates to germicidal quaternary ammonium compounds having the formula:

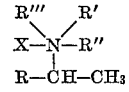


wherein R is a straight-chain alkyl having an even number of carbon atoms between 12 and 14, R′ and R″ are lower alkyls, R‴ is a member of the group consisting of benzyl, alkyl-subsituted benzyl wherein the alkyl contains 1 to 5 carbon atoms, halo-substituted benzyl, and menaphthyl, and wherein X is a halide.

This invention relates to quaternary amonium compounds, and it particularly relates to such compounds wherein the nitrogen is directly linked to the penultimate carbon atom of the starting hydrocarbon.

This is a continuation-in-part of co-pending application Ser. No. 595,349, filed Nov. 18, 1966 now abandoned.

The quaternary ammonium compounds embodying the present invention have the structure:



wherein R is a straight-chain alkyl having an even number of carbon atoms between 12 and 14, R′ and R″ are lower alkyls, preferably either methyl or ethyl, R‴ is a member of the group consisting of benzyl, alkyl-substituted benzyl wherein the alkyl contains 1 to 5 carbon atoms, halo-substituted benzyl, and menaphthyl, and wherein X is a halide.

It has now been discovered that when R contains an even number of carbon atoms, between 12 and 16, these compounds form unexpectedly potent germicidal quaternary compounds.

These quaternary ammonium compounds, which are prepared from 2-alkyl amines, are unexpectedly far superior to those prepared from 1-alkyl amines insofar as concerns their microbiocidal properties. Furthermore, the C_{14} and C_{16} 2-alkyl quaternaries are more biocidally active than other adjacent homologs.

The following examples are illustrative of the present invention but are not intended to limit the invention except as claimed:

EXAMPLE 1

1 gram equivalent weight of dimethyl-2 amino hexadecane was reacted with 0.98 gram equivalent weight of benzyl chloride, in an equal weight of 20% isopropanol in distilled water by agitating and heating to 80° C., under

reflux in a round-bottom flask for about 1 hour, or until no further reaction occurred, as measured by argentometric titration of the ionic chlorine. Reaction was about 95% complete as dimethyl benzyl 2-hexadecyl ammonium chloride, and also present was about 3% of dimethyl 2-hexadecyl amine hydrochloride. Sufficient sodium hydroxide was added to liberate the amine, and an amount of benzyl chloride sufficient to quaternize the latter was added. The reaction was then continued for about one-half hour at the end of which time the quaternization was essentially completed.

EXAMPLE 2

Using the same procedures as in Example 1, but substituting equivalent amounts of the dodecyl, tetradecyl and octadecyl amine homologs, the corresponding dimethyl benzyl 2-alkyl ammonium chlorides were prepared.

The 2-alkyl quaternary ammonium chlorides of Examples 1 and 2 were tested for microbiocidal activity in comparison with the corresponding 1-alkyl quaternary ammonium chlorides, using the standard "Phenol Coefficient Method" as described in the "Official Methods of Analysis of the Association of Official Agricultural Chemists," 9th Edition, pages 63–65, against *Staphylococcus aureus* and *Salmonella typhosa.*

Using, as examples of the respective 2-alkyl and 1-alkyl compounds, the 2-hexadecyl quaternary, as prepared above, and the corresponding 1-hexadecyl quaternary, the microbiocidal results, expressed as phenol coefficients, were as follows:

Dimethyl benzyl 2-amino hexadecyl ammonium chloride:	Dimethyl benzyl 1-amino hexadecyl ammonium chloride
S. aureus 1330	580
S. typhosa 777	640

The same procedure was used to compare the corresponding 2-dodecyl, 2-tetradecyl, 2-hexadecyl, and 2-octadecyl quaternaries, with the following results:

	C-12	C-14	C-16	C-18
S. aureus	160	916	1,330	160
S. typhosa	110	666	777	110

From the above, it can be seen that there is a spectacular and most unexpected jump in biocidal activity between the dodecyl and the tetradecyl compounds. The hexadecyl compounds are even more germicidally active than the tetradecyl.

The above results make it clear that quaternaries prepared from the 2-alkyl amines are unexpectedly far superior to those prepared from the 1-alkyl amines. Furthermore, the C_{14} and C_{16} 2-alkyl quaternaries are so much more biocidally active than the C_{12} homolog that it amounts to a difference of kind, especially in view of the rapid decline between the C_{16} and C_{18} homologs.

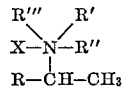
In addition to using benzyl chloride to form the quaternaries, it is also within the scope of the present invention to use substituted benzyl chlorides wherein the benzyl ring may be substituted in any one or all positions by an alkyl group having from 1 to 5 carbon atoms, or by a halogen such, as chlorine or bromine; or a menaphthyl compound such as a halomethyl naphthylene, exemplified by alpha-chloromethyl naphthylene, may advantageously be used.

Obviously, many modifications of the present invention are possible in the light of the above teachings. It is,

therefore, to be understood that within the scope of the appended claim, the invention may be practiced otherwise than as specifically described.

The invention claimed is:

1. A compound having the formula:



wherein R is dodecyl or tetradecyl, R′ and R″ are methyl, R‴ is benzyl, and X is chloride.

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U.S. Cl. X.R.

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