SURFACE DISINFECTANT AND SPACE DEODORANT AEROSOL SPRAY COMPOSITIONS

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The present invention relates to surface disinfectant and space deodorant aerosol spray compositions. This application is a continuation-in-part of our earlier application, Serial No. 167,009 filed January 18, 1962, now abandoned.

Hereinafore various antiseptic aerosol spray compositions have been proposed. However, such formulations have generally been deficient in one or more respects due to the complexities and inaccuracies in compounding satisfactory formulations. For example, some formulations, when sprayed from a pressurized container, form a coarse wet spray or continuous stream rather than the desired aerosol cloud or atomized mist. Other formulations have inadequate germicidal activity, while still others have a germicidal activity which is inconsistent or variable due to the variations in the formulation as the contents of the pressurized can are discharged. Some formulations require shaking of the can prior to use. Many previous formulations have necessitated the utilization of emulsifying agents which not only add to the cost of compounding the formulations, but also leave an undesirable and objectionable film. In addition, many of the proposed formulations are excessively corrosive so that they unduly attack the walls of the pressurized container and hence require the incorporation in the formulation of expensive corrosion inhibitors, the coating of the containers with costly corrosion retardant linings, or the use of fragile, non-corrodible containers. Other proposed formulations are only useful for a single purpose rather than having dual or multifold utility, because of the difficulties encountered in formulating compatible multipurpose formulations.

It is, therefore, an object of the present invention to provide aerosol spray compositions which will function not only as surface disinfectants but also as space deodorants. It is a further object of the invention to provide combination surface and space aerosol spray compositions which will have germicidal activity sufficient to give 100% kill. Another object is to provide aerosol spray compositions which, upon discharge from pressurized cans, will produce aerosol clouds or atomized mists rather than coarse wet sprays or continuous streams. An additional object of the invention is to provide aerosol spray compositions which will have consistent germicidal activity in each discharged portion or dosage of the contents of the pressurized can until the contents of the can are emptied by usage thereof. Another object is to provide aerosol spray compositions which do not require shaking of the can prior to use. A further object of the invention is to provide aerosol spray compositions which are not excessively corrosive to the walls of the pressurized metal cans in which they are housed. A still further object of the invention is to provide aerosol spray compositions which do not necessitate the use of expensive emulsifying agents therein.

It was found that these objects could be achieved provided certain criticalities are carefully observed. The major criticalities are the relative amounts and identities of the components of the solvent system in the aerosol spray composition.

The formulations of the present invention are single phase liquid compositions especially adapted for discharge from a pressurized container or aerosol bomb to thereby form combination surface and space aerosol sprays which will deodorize a room and which, when sprayed on a surface, will leave a continuous wet film that will remain a sufficient time to disinfect and yet not be so wet as to remain wet for an unnecessarily long time under average conditions and thereby cause spotting. The compositions contain five essential components, the identities and amounts of which are described below.

They are, and must be maintained under pressure, e.g., in a nominally sealed pressure vessel until they are released for their intended use, or maintained at a temperature below the boiling point of the lowest boiling component.

The formulations contain from about 0.01% to about 5% by weight active material, the balance being a single phase liquid solvent system.

The active material constitutes about 20% to about 75% by weight of germicide and from about 80% to about 25% by weight, respectively, deodorant. If desired, more than one germicide and more than one deodorant can be used. The identities of the germicide and deodorant may vary greatly and are not particularly critical so long as they are compatible with one another and not too toxic for use.

Suitable germicides or disinfectants include, for example, the conventional phenolic germicides, such as ortho-phenylphenol, para-tertiary-butylphenol, para-tertiary-anisylphenol, ortho-benzyl-para-chlorophenol, secondary-hexylphenol, and secondary-heptylphenol. Other suitable germicides or antiseptic agents include the well known quaternary ammonium compounds, such as alkyl dimethylbenzyl ammonium chloride and paraisobutyl-phenoxethoxyethyl dimethylbenzyl ammonium chloride monohydrate.

The deodorant can be one which functions by desensitizing the nasal passages to odors, by masking the offensive material, or by reacting with odor-causing material to form non-odoriferous compounds. Typical of such well known deodorants are various perfumery materials, e.g., peppermint oil, clove oil and pine oil; the organic peroxides, e.g., cumene hydroperoxide, tertiary-butyl hydroperoxide and tertiary-dodecyl hydroperoxide; the acrylic esters, e.g., lauryl methacrylate; and the quaternary morpholinium alkyl sulfates having an alkyl substituent containing 8 to 24 carbon atoms per molecule, e.g., N-soya-N-ethyl morpholinium ethyl sulfate, N-lauryl-N-methyl morpholinium methyl sulfate, N-myristyl-N-methyl morpholinum methyl sulfate, and N-oleyl-N-methyl morpholinium methyl sulfate.

The single phase liquid solvent system for the active material constitutes from about 99.99% to about 95% by weight, respectively, of the composition.

One component of the solvent system is a saturated monohydric aliphatic hydrocarbon alcohol having from two to four carbon atoms, examples of which include ethanol, isopropanol and butanol. Another component of the solvent system is water. This is necessary in order to have germicidal activity as high as 100% kill in view of the fact that it was found that absolute alcohol solutions of disinfectant agents have no germicidal activity when formulated as aerosols. The remaining component of the solvent system is a propellant capable of generating 30 to 70 psi i.e. (pounds per square inch gauge) at a temperature of about 70° F. Suitable propellants are dichlorodifluoromethane, CCIF₂ (Freon 142), mixtures of dichlorodifluoromethane with dichlorotetrafluoroethane, (CCIF₂₃) (Freon 114) and mixture of dichlorodifluoromethane with monochlorodifluoroethane, CCIF₂CH₃ (Freon 142B). The relative amounts of the components
in these two chlorofluoralkane propellant mixtures are not important to the present invention and can vary greatly, so long as they, and the proportion of propellant in the solvent system, are such that the mixtures are capable of generating vapor pressures of from 30 to 70 p.s.i.g. preferably 30 to 40 p.s.i.g. This is accomplished by use of mixtures of about 30% and 2.5% dichlorodifluoromethane, respectively. Other propellants, such as compressed gases, e.g., carbon dioxide or nitrogen, liquefed lower alcanes, such as propane and butane, and other liquefied halogenated hydrocarbons, such as methylene chloride and trichlorofluoromethane (Propellant II), cannot be used in the formulations of the present invention because of the deleterious properties which they would impart thereto. Dichlorodifluoromethane alone, monochlorodifluoroethane alone, and combinations thereof are not suitable because they cannot generate sufficient vapor pressure at 70° F. to produce an effective spray pattern.

The relative amounts and identities of the alcohol and propellant, and the relative amount of water, are critical to the utility of the solvent system as a vehicle for the active materials. In terms of results desired, the amount of water must be sufficient to provide a 100% kill of bacteria on contact under ambient conditions, but not so great as to cause problems of excessive corrosion within the container or produce and unduly "wet" spray that leaves spots on sprayed surfaces due to slow drying and coagulation into large drops. The amounts of alcohol must be sufficient to dissolve the active ingredients and the propellant, yet not so great as to reduce either the germicidal activity to less than 100% or the effective vapor pressure of the entire composition. The identity of the alcohol must be such as to dissolve the propellant and active materials in sufficient concentration; the amount of propellant must be sufficient, and the identity thereof must be such, as to generate for the composition as a whole a vapor pressure capable of producing a desirable aerosol cloud or atomized mist in a broad spray pattern without requiring agitation of the container, but the amount cannot be so great as to form a separate liquid phase.

In numerical terms, the proportion by weight of alcohol to water should range between 90:10 and 77:23; about 85:15 being preferred, because it makes a 100% germicidal activity combined with minimum spotting. The proportion by weight of propellant to aqueous alcohol should range, for optimum results, between about 15:85, and about 27:73 when the propellant is dichlorodifluoromethane, about 16:64 to about 34:66 when the propellant is a 70:30 mixture of dichlorodifluoromethane and dichlorotetrafluoroethane, between about 23:77 and 60:40 when the propellant is a 35:65 mixture of the same propellants, and between about 18:82 and 45:55 when the propellant is a 50:50 mixture of dichlorodifluoromethane and monochlorodifluoromethane, said range being displaced toward the 15:85 proportion as the relative proportion of dichlorodifluoromethane in the propellant mixture increases.

These guidelines as to critical and preferred proportions are illustrated in the accompanying drawing, wherein:

FIGURE 1 is a graph showing preferred and acceptable areas of proportions of components in the solvent system when dichlorodifluoromethane is the propellant; and

FIGURE 2 is a graph showing preferred and acceptable areas of proportions of components in the solvent system when the propellant is a 70:30 mixture of dichlorodifluoromethane and dichlorotetrafluoroethane.

Referring now to FIGURE 1, indicating preferred and acceptable relative proportions of alcohol, water and the preferred propellant, dichlorodifluoromethane, area P is bounded by lines K-L, L-M, M-N and N-K. The line J-K-L defines solvent systems in which the ratio of alcohol to water is 90:10 and intersects lines L-M and N-K, which define solvent systems generating vapor pressures of 30 and 40 p.s.i.g., respectively, the line L-M also defining the limits above which a usable, uniform spray is not obtainable. The M-N line indicates solvent systems containing the preferred minimum of about 15% by weight propellant, point N also being on line R-N, which indicates solvent systems in which the alcohol-water ratio is 77:23. Thus it will be apparent that at any point within area P, the pressure will be within the preferred range of 30 to 40 p.s.i.g., the alcohol-water ratio will be within the preferred range of 90:10 to 77:23, and the proportion of propellant will be a minimum of 15% (and a maximum of about 27% at point K).

Area G, defined by points J K N R, indicates acceptable, but not preferred, relative proportions in which the amount of propellant, and hence the vapor pressure, are greater than optimum. However, this area is, like area P, generally limited to solvent systems in which the alcohol-water ratio is between 90:10, as indicated by line J-K, and 77:23, as indicated by line R-N. Line J-R, the lower boundary of area G, is the saturation line for dichlorodifluoromethane, beyond which the propellant would form a second liquid phase to form an unacceptable product, not only because of excessive pressure, but also because of the lack of uniformity of spray that would be produced.

Point L, in substantially the center of the area P, corresponds to the solvent system of Example 1, considered to be the optimum for general use in temperate zone conditions.

Referring now to FIGURE 2, which is similar to FIGURE 1 except for the fact that it is based on the use of a 70:30 mixture of dichlorodifluoromethane with dichlorotetrafluoroethane as propellant, area P' designates the preferred area and area G' designates the acceptable, non-preferred area, while line J'-R' designates the saturation line for said propellant mixture below which an undesirable two-phase liquid system would result. Point 2, in the area P', corresponds to the solvent system of Example 2.

It should be evident that the preferred area can readily be determined in a similar manner for any other combination of dichlorodifluoromethane with up to 70% dichlorotetrafluoroethane or up to 97.5% monochlorodifluoroethane. If desired, the formulations can contain various optional materials such as corrosion inhibitors, e.g., silicates, nitriles, phosphates, and borates; coloring materials; and other compatible adjuvants. The compositions are flammable and are not designed for personal or topical application.

The compositions of the present invention may be prepared by mixing together the active material, namely germicide and deodorant, in a miscible mixture of the water and alcohol solvents and then adding the mixture to a pressurized container or aerosol bomb which is subsequently sealed. Then the liquefied propellant, while under pressure, may be admitted to the pressurized container through a valve, the container generally being slightly chilled during this procedure. Alternatively, the formulation can be prepared by pre-chilling the five essential components, either individually or as a mixture, to a temperature below the boiling point of the low boiling propellant and then charging the single phase liquid composition into the pressurized container which is then sealed.

Such pressurized containers or aerosol bombs, of course, contain a dip tube extending from near the base of the container to the neck thereof where it is connected to a discharge and atomizing valve. The filled pressurized container, of course, contains the single phase liquid composition in the major lower portion of the container and also contains above the single phase liquid composition
a gaseous phase which is primarily vaporized propellant with small amounts of vaporized water and alcohol. This upper gaseous phase serves to expel or discharge the liquid composition when the valve of the container is opened. The discharged composition immediately forms into an aerosol due to the extremely rapid vaporization and expansion of the propellant therein.

The compositions of the present invention are illustrated by Examples 1 and 2 and are compared with unsatisfactory similar compositions of Examples 3 through 7 as described by the data set forth in Tables I and II below. The data in Table II constitute an alternative method of calculating the amounts of the various components of the formulations shown in Table I. The solvent systems for Examples 1 through 7 are plotted on the drawing where the numbers in the drawing correspond to the example numbers in Tables I and II.

### Table I

<table>
<thead>
<tr>
<th>Example No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Components</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>Ortho-phenylphenol (germicide)</td>
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<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Alkyldimethylbenzyl ammonium oxide (surfactant)</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
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<tr>
<td>Laurylethylammonium chloride (deodorant)</td>
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<td>11.0</td>
<td>10.0</td>
<td>9.0</td>
<td>8.0</td>
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<td>Water</td>
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<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
</tr>
</tbody>
</table>

**Properties**

- Vapor Pressure (p.s.i.g. at 70°F): 40, 40, 40, 40, 40, 40, 40
- Number of Liquid Phases: 4, 4, 4, 4, 4, 4, 4
- Germicidal Activity (Percent Kill): 100, 100, <100, 100, <100, <100, <100

### Table II

<table>
<thead>
<tr>
<th>Example No.</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Active Material (percent by weight of composition)</strong></td>
<td>0.5</td>
<td>0.5</td>
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<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
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<tr>
<td><strong>Germicide (percent by weight of active material)</strong></td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td><strong>Deodorant (percent by weight of active material)</strong></td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td><strong>Solvent System (percent by weight of composition)</strong></td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td><strong>Water (percent by weight of solvent system)</strong></td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td><strong>Alcohol (percent by weight of solvent system)</strong></td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td><strong>Propellant (percent by weight of solvent system)</strong></td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
</tbody>
</table>

The data set forth in Tables I and II demonstrate the suitability of the compositions of the invention as shown by Examples 1 and 2 and also establish the criticalities discussed above when the data for Examples 1 and 2 are compared with the data for comparative Examples 3 through 7. Thus, the formulations of Examples 1 and 2, whose solvent systems are within areas P or P of the drawing, have a vapor pressure of from 30 to 70 p.s.i.g. at 70°F, while the preferred Example 1, whose solvent system is within area P of the drawing, has a vapor pressure between 30 and 40 p.s.i.g. at 70°F. In addition, the compositions of Examples 1 and 2 are single phase liquid compositions, produce an aerosol spray rather than a coarse wet spray when discharged from a pressurized container, and have satisfactory deodorant activity when used as a space spray. Moreover, the compositions of Examples 1 and 2 have a remarkably high germicidal activity, namely they produce 100% kill, and this germicidal activity is consistent from the first to the last portion or dosage of the compositions discharged from the pressurized container.

On the other hand, the comparative formulations of Examples 3 through 7, whose solvent systems are outside activity is unsatisfactory, and in that their germicidal activity is less than 100% effective and is not consistent from the first portion to the last portion discharged from the container.

The above examples, therefore, clearly demonstrate the complexities and unpredictability of formulating satisfactory surface and space aerosol spray compositions and the necessity for carefully observing the criticalities set forth herein.

It will be appreciated that various modifications and changes may be made in the formulations of the invention in addition to those described herein without departing from the scope of the invention and accordingly the invention is to be limited only within the scope of the appended claims.

We claim:

1. A single phase liquid composition especially adapted for discharge from a pressurized container to thereby form a combination surface and space aerosol spray which will deodorize a room and which when sprayed on a surface will leave a continuous wet film that will remain a sufficient time to disinfest comprising:

   (1) from about 0.01% to about 5% based on the
weight of the composition of active material said active material being:
(a) from about 20% to about 75% of germicide based on the weight of the active material and
(b) from about 80% to about 25% respectively of deodorant based on the weight of the active material, and
(2) from about 99.99% to about 95% respectively based on the weight of the composition of a miscible or single phase liquid solvent system for the active material, said solvent system being:
(c) water,
(d) a saturated monohydric aliphatic hydrocarbon alcohol having from 2 to 4 carbon atoms and
(e) a liquefied normally gaseous propellant selected from the group consisting of dichlorodifluoromethane, mixtures of dichlorodifluoromethane with up to 70% by weight of dichlorotetrafluoroethane and mixtures of dichlorodifluoromethane with up to 97.5% by weight of mono-chlorodifluoroethane.

the relative amounts of said water, alcohol and propellant in the solvent system being such that said composition has a vapor pressure of from 30 to 70 pounds per square inch gauge at 70° F., the propellant is present to the extent of at least about 15% by weight, and the weight ratio of alcohol to water is between about 90:10 and 77:23.

2. A composition as set forth in claim 1 wherein the relative amounts of water, alcohol and propellant are such that said composition has a vapor pressure of from 30 to 40 pounds per square inch gauge at 70° F.

3. A composition as set forth in claim 2 wherein the germicide is a phenolic germicide.

4. A composition as set forth in claim 2 wherein the germicide is a quaternary ammonium germicide.

5. A composition as set forth in claim 2 wherein the deodorant is a quaternary morpholino-alkyl sulfate.

6. A composition as set forth in claim 2 wherein the alcohol is ethanol.

7. A composition as set forth in claim 2 wherein the propellant is dichlorodifluoromethane.

8. A single phase liquid composition especially adapted for discharge from a pressurized container to thereby form a combination surface and space aerosol spray which will deodorize a room and which when sprayed on a surface will leave a continuous wet film that will remain a sufficient time to disinfect comprising:
(a) about 0.1% alkyl dimethylbenzyl ammonium chloride, (b) about 0.035% N-35% N-65% N-ethyl morpholinium ethyl sulfate, (3) about 13% water, (4) about 59% ethanol, (5) about 21% dichlorodifluoromethane, and (6) about 9% dichlorotetrafluoroethane; said amounts being based on the weight of the composition and said composition having a vapor pressure of from 30 to 40 pounds per square inch gauge at 70° F.

9. A single phase liquid composition especially adapted for discharge from a pressurized container to thereby form a combination surface and space aerosol spray which will deodorize a room and which when sprayed on a surface will leave a continuous wet film that will remain a sufficient time to disinfect comprising:
(a) about 0.1% alkyl dimethylbenzyl ammonium chloride, (b) about 0.035% N-35% N-ethyl morpholinium ethyl sulfate, (3) about 13% water, (4) about 59% ethanol, (5) about 21% dichlorodifluoromethane, and (6) about 9% dichlorotetrafluoroethane; said amounts being based on the weight of the composition and said composition having a vapor pressure of from 30 to 40 pounds per square inch gauge at 70° F.

10. A single phase liquid composition especially adapted for discharge from a pressurized container to thereby form a combination surface aerosol spray which will deodorize a room and which when sprayed on a surface will leave a continuous wet film that will remain a sufficient time to disinfect comprising:
(a) from about 20% to about 75% of germicide based on the weight of the active material and
(b) from about 80% to about 25% respectively of deodorant based on the weight of the active material, and
(2) from about 99.99% to about 95% respectively based on the weight of the composition of a miscible or single phase liquid solvent system for the active material, said solvent system being:
(c) water,
(d) a saturated monohydric aliphatic hydrocarbon alcohol having from 2 to 4 carbon atoms and
(e) a liquefied normally gaseous chlorofluorocarbon propellant, the relative amounts of said water, alcohol and propellant in the solvent systems being such that said composition has a vapor pressure of from 30 to 70 pounds per square inch gauge at 70° F., the propellant is present to the extent of at least about 15% by weight, and the weight ratio of alcohol to water is between about 90:10 and 77:23.

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