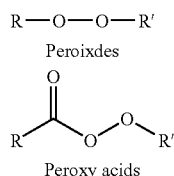


oxide and peroxyacetic acid. These two compounds represent entirely different groups of chemical compounds. A peroxide is a compound containing an oxygen-oxygen single bond, while peroxy acids (also known as peroxyacids and peracids) are acids in which an acidic —OH group has been replaced by an —OOH group. Peroxides and peroxy acid have the general structures:



[0105] Peroxides tend to decompose easily and can sometimes initiate explosive reactions. Peroxy acids are generally not very stable in solution and decompose to ordinary oxyacids and oxygen. One novel discovery of the present invention is that dry sources of the peroxides, and separately, dry sources of the peroxy acids, such as TAED, are stable when dissolved in the organic/aqueous solutions of the invention, and require activation for maximum efficacy and speed against chemical and biological agents, including, but not limited to, aromatic hydrocarbons, mustards, environmental mutagens, organophosphate pesticides, nerve agents and bacteria.

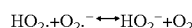
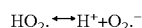
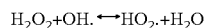
[0106] Hydrogen peroxide decontaminates chemical warfare agents (CWAs) more efficiently in alkaline solutions that generate HOO^- . In some instances, the alkaline perhydrolysis process is considerably faster than analogous alkaline hydrolysis or neutral oxidation processes. This is attributed to an increased nucleophilicity of HOO^- due to the presence of a lone pair of electrons on the oxygen atom adjacent to the nucleophilic centre. This phenomenon is referred to as the 'α-effect'. Although not fully understood, α-effects are historically considered not to occur in the absence of solvent. However, the observed chemistry of modified vaporous hydrogen peroxide (mVHP) is analogous to the alkaline perhydrolysis chemistry observed in solution. Some of the many difficulties observed using modified vaporous hydrogen peroxide as a CBW decontaminant are: (i) the rapid outgassing of H_2O_2 under alkaline conditions, resulting in a short effective pot life; (ii) the caustic character of the alkaline solutions needed to create mVHP; (iii) mVHP can only be used in enclosed spaces in which heated dry air must be circulated to reduce the relative humidity and avoid condensation of hydrogen peroxide and water during decontamination, and, (iv) the production of toxic by-products produced when mVHP is the primary reactive oxygen species.

[0107] Peroxy-oxidizers, including but not limited to, peroxycarboxylic acids such as peroxyacetic acid, and dry sources thereof, can dissolve in the isotropic organic/aqueous solutions of the polar amphipathic organic components of the present inventions. When appropriately activated, these compounds can generate oxidizing agents which (i) overcome the limitations of mVHP; and (ii) accelerate the hydrolysis of phosphate esters, mustards, as well as the phospholipids, proteins and oligonucleotides of bacteria, spores and viruses.

[0108] As discussed above, a molecule of the reactive oxygen species tetraacetylenediamine (TAED) is perhydrolyzed at the appropriate pH by activators such as hydroper-

oxide anions, and will generate 2 moles of peroxyacetic acid, which, in turn, form percarboxylate anions and/or singlet oxygen. These oxidizer molecules can react with a threat load of toxant, and neutralize/remove the toxant without the production of toxic by-products.

[0109] In the present invention, hydroperoxide anions, which perhydrolyze the reactive oxygen species, are produced by the chain propagation reaction to generate percarboxylate anions and singlet oxygens:



The desired percarboxylate anions and singlet oxygens cannot be generated from either hydrogen peroxide alone and cannot be generated using sodium hypochlorite, but only from the generation of peroxyacetic acid and its oxidizers from TAED. Moreover, these compounds react with organophosphates, mustards, bacteria, spores, and viruses via very different reaction pathways and mechanisms from those generated by activation of hydrogen peroxide or sodium hypochlorite. These different reaction pathways can be exploited to increase the efficacy of the decontamination solutions of the invention and to avoid the creation of hazardous by-products.

[0110] In order to be most effective in a decontaminant made from the organic/aqueous solutions of the present invention, the reactive oxygen species should be able to dissolve in sufficient amounts to achieve stoichiometric hydrolysis and/or perhydrolysis of the toxants. The term "reactive oxygen species" ("ROS") refers to peroxides or peroxyacids, whereas the term "oxidizers" refers to reactive oxygen which may be in the form of hydroxyl radicals (from peroxides) or peroxycarboxylic anions and singlet oxygen (from peroxy acids). As a group, reactive oxygen species include, but are not limited to, hydrogen peroxide, hypochlorite ion, and peroxyacetic acid (PAA). These compounds require some type of activation process during which one or more molecules are split to generate the oxidizing agents. Such oxidizing agents include, but are not limited to, hydroxyl radicals, or peroxyacetic anions and singlet oxygens, which may go on to participate in further chemical reactions with toxants.

[0111] The term "radical" or "free radical" refers to a cluster of atoms, one of which contains an unpaired electron in its outermost shell of electrons. The term "hydroxyl" describes a molecule consisting of an oxygen atom and a hydrogen atom joined by a covalent bond. The neutral form is known as a hydroxyl radical and the singly-charged hydroxyl anion is called hydroxide. Hydroxyl radicals are an unstable configuration, and such radicals generally quickly react with other molecules or other radicals to achieve the stable configuration of four pairs of electrons in their outermost shell (or one pair for hydrogen).

[0112] Other embodiments of the invention are organic/aqueous solutions comprising one or more reactive oxygen species, further comprising one or more chemical activators to generate the oxidizer(s). When dissolved, the peroxycarboxylic acids require activation to generate the peroxy anions or singlet oxygen atoms which are the actual oxidizers of the toxants. Methods of activation include, but are not limited to: (i) changing the pH of the solution by adding an alkaline base such as sodium hydroxide to the decontamination mixture; (ii) changing the pH by employing buffering systems that