

PTI Technical Note

Singlet Oxygen

Singlet oxygen generation and detection are growing fields with applications in such areas as cancer treatment, photosensitized oxidations, and biomolecular degradation. Ground state oxygen is known to exist uniquely as a triplet state. The spin-selection rule reduces its reactivity by forbidding reactions with singlet state species, which comprise the majority of compounds. However, the first excited state of an oxygen molecule is a singlet state, which can readily react with other singlet molecules. Radiative decay to the triplet ground state is a spin-forbidden transition resulting in a long-lived excited state. Excited singlet oxygen emits phosphorescence in the NIR at 1270 nm.

Singlet oxygen is often generated in photochemical reactions and its yield is an important parameter for photochemists who characterize such reactions. There is an emerging research effort to create environmentally friendly photopesticides based on the light-stimulated singlet oxygen action. Singlet oxygen producing photosensitizers are also used to develop antibacterial and antiviral treatments. In addition, singlet oxygen generation and its oxidizing effect is also one of the key interests of the pharmaceutical industry in relation to action and photostability of drugs. Singlet oxygen also plays an important role in environmental protection and photodecomposition of pollutants.

The production of singlet oxygen can be accomplished through the use of photosensitizers (PS). The absorption of light by these compounds leads to an excited singlet state (1PS*) of the sensitizer. Through a process of intersystem crossing, the excited singlet can spin-flip into a lower energy triplet state (3PS*) that reacts in an energy transfer reaction with the ground triplet state of oxygen. This process returns the sensitizer to its singlet ground state while bringing oxygen molecule to the excited singlet state.

Singlet oxygen is a very strong oxidant. It reacts with unsaturated organic compounds typically via cycloaddition or "ene" reactions. It is destructive towards biological systems, causing photoinduced damage in proteins by photooxidation of nucleosides (e.g. guanosine) of DNA and RNA leading to single strand breaks. This photo-induced DNA damage is the basis for Photo Dynamic Therapy (PDT). In PDT, a photosensitizer such as a porphyrin derivative is injected into a patient and selectively accumulates into tumor sites. Upon irradiation, the photosensitizer is excited and ends up in its triplet state. It then reacts with triplet oxygen, leading to excited singlet oxygen. The latter oxidizes DNA in the cancer cell, leading to cell death. Similarly, singlet oxygen, if present, can cause damage in healthy cells, leading to mutations and cancer. Some vitamins (e.g. E and C) are efficient singlet oxygen scavengers.

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