Photochemistry and Photophysics of the New $C_{120}O_2$ Isomer formed by Dimerization of [5,6]- $C_{60}O$

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It is found that the newly discovered [5,6]-open oxidoannulene isomer of $\mathrm{C}_{60}\mathrm{O}$ efficiently dimerizes in toluene solution to form a new isomer of $C_{120}O_2$. Excited singlet- and triplet-state properties of the $C_{120}O_2\ product$ have been characterized by various spectroscopic techniques and compared to those of C_{120} , the [2+2]-dimer of C_{60} . The ground state absorption spectrum of $C_{120}O_2$ in toluene is slightly red-shifted relative to that of C_{120} , with a distinctive peak at 329 nm and an $S_1 \leftarrow S_0$ origin band at 703 nm. Its fluorescence spectrum shows two major peaks at 717 and 793 nm. In room temperature toluene, the measured triplet state intrinsic lifetime of this compound is 32 $\mu s,$ a value slightly shorter than that of C_{120} (44 µs). It is also found that $C_{120}O_2$ undergoes dissociation from its triplet state to give back its precursor, C₆₀O oxidoannulene. This oxidoannulene can thus be converted to $C_{120}O_2$ by thermal self-reaction and then restored to monomeric $C_{60}O$ by photolysis. The quantum yield for $C_{120}O_2$ photodissociation has been determined to be several times greater than that for the comparable photodissociation of C_{120} . Further photophysical characteristics of the new $C_{120}O_2$ isomer as well as the results of mass spectrometric and NMR studies will also be presented.