Photophysical Properties of Selected C₈₄ Isomers

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The photophysics of higher fullerenes remain poorly characterized, in part because they may exist in several isomeric structures that can be difficult to isolate for study. This project addresses the properties of C₈₄ isomers. Using recycling HPLC methods, a sample of purified C₈₄ has been separated into three fractions. The first contains a mixture of the three most abundant isomers — $D_2(IV)$, $D_{2d}(II)$, and $C_s(a)$. UV-vis absorption spectroscopy confirms that the second and third fractions contain predominately the C_2 and $C_s(b)$ isomers, respectively. A kinetics-based method has been used to find the effective molar absorptivities of these fractions. Sensitive time-resolved absorption measurements following 532 nm excitation reveal a surprisingly wide range of triplet state lifetimes among these isomers. Using samples dissolved in a solid polymer film to suppress bimolecular triplet decay processes, kinetic components have been observed with exponential lifetimes ranging from 5 to 710 μ s. The species with the 710 μ s triplet lifetime shows a T_n \leftarrow T₁ absorption peak at 740 nm. Quenching studies indicate that one C_{84} isomer has a triplet state energy below that of oxygen's ${}^{1}\Delta_{g}$ state, while the others have energies above this level. Further results, including luminescence spectra and variabletemperature triplet decay kinetics, will also be presented.