Photophysical Properties of the Triplet State of Deca-Functionalised [70]Fullerenes

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In a previous study of the photophysical properties of the C70Ph2n (n=2-5), using laser flash photolysis and pulse radiolysis techniques, we have observed that the quantum yields of triplet formation (FT) and of singlet oxygen production (FD) diminish linearly with increasing number of attached phenyl groups, from unity for C70Ph4 to 0.5 and 0.18 for C70Ph6 and C70Ph8 respectively. In this series, the C70Ph10 is exceptional and its FT is $\sim$ unity. Most probably, the particular chromophoric structure of C70Ph10 which consists of two cage-centered *-electron systems makes its photophysical properties an exception to those found for the other phenylated C70Ph2n (n=2-4). In order to confirm this peculiar behaviour of the deca-phenylated C70, we have determined the triplet photophysical properties, including absorption spectra, molar absorption coefficients and FT and FD of five other deca-functionalised [70]fullerenes, C70X10, which are C70(fluorobenzene)10, C70(allyl)10, C70(anisyl)10, C70(anisyl)9H and a silyl derivative of C70(Ph)8 with a cyclopentane ring bridging a double bond. We have found that the triplet spectra features of these compounds are rather similar to those of C70Ph10 between 450 and 1050 nm with a lmax at 500nm but have rather different relative absorption intensities between 600 and 1100 nm, in one case being 3.5 times greater around 800 nm. Their FT and FD have, as C70Ph10, a high value between 0.76 and 0.91 ($\pm$15%). A discussion of the dependence of the triplet properties of C70X10 on the nature of the addend is presented. The importance of the nature of the addend for these deca-functionalised [70]fullerenes is in sharp contrast to the negligible effect of the nature of the addend on the photophysical properties of methano[60] fullerenes, which results from the insulating role of the sp3 C atom in the methano-bridges.

Acknowledgements: This work was performed under European contracts ERB FMRX-CT98-0192 and ERB FMRX-CT97-0126. The laser and pulse radiolysis experiments were carried out at the Paterson Institute for Cancer Research Free Radical Research Facility, Manchester, UK with the support of the European Commission through the Access to Large-Scale Facilities activity of the TMR program.