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Using photoexcited triplet states to probe small-molecule endohedral fullerenes by ESR VASILEIA FILIDOU, London Centre for Nanotechnology, University College London, London WC1H, UK, SALVATORE MAMONE, School of Chemistry, University of Southampton, SO17 1BJ, UK, ALESSANDRO BAGNO, FEDERICO RASTRELLI, Dipartimento di Scienze Chimiche, Universita di Padova, via Marzolo, 1 -35131, Italy, YASUJIRO MURATA, KOICHI KOMATSU, Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan, XUEGONG LEI, YONGJUN LI, NICHOLAS J. TURRO, Department of Chemistry, Columbia University, New York, New York 10027, US, MALCOLM H. LEVITT, School of Chemistry, University of Southampton, SO17 1BJ, UK, JOHN J.L. MORTON, London Centre for Nanotechnology, University College London, London WC1H, UK — Ortho to para conversion of molecular hydrogen H_2 can be catalyzed by the use of a coupled paramagnet such as a fullerene in its triplet state. The recently synthesized endohedral fullerenes $H_2@C_{60}$ and $H_2@C_{70}$ were photoexcited to their long lived triplet state (S= 1) and probed by electron spin resonance (ESR) and electron nuclear double resonance (ENDOR) spectroscopic techniques. With these techniques we characterized both spin systems by extracting the hyperfine interaction the kinetic parameters of the triplet state and the spin relaxation times. The observed variations of the linewidths and the lineshape are discussed in the context of a dynamic Jahn-Teller effect. Irradiation of the $H_2@C_{70}$ at different temperatures reveals that the fullerene triplet state can serve as a spin catalyst for ortho to para interconversion while for the triplet $H_2@C_{60}$ no appreciable interconversion is observed

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