Electronic Supplementary Material (ESI) for Chemical Communications

$Sc_2@C_{3v}(8)$-C_{82} vs. $Sc_2C_2@C_{3v}(8)$-C_{82}: Drastic effect of C_2 capture on the redox properties of scandium metallofullerenes

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(25f) Gaussian 09, Revision A.02; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

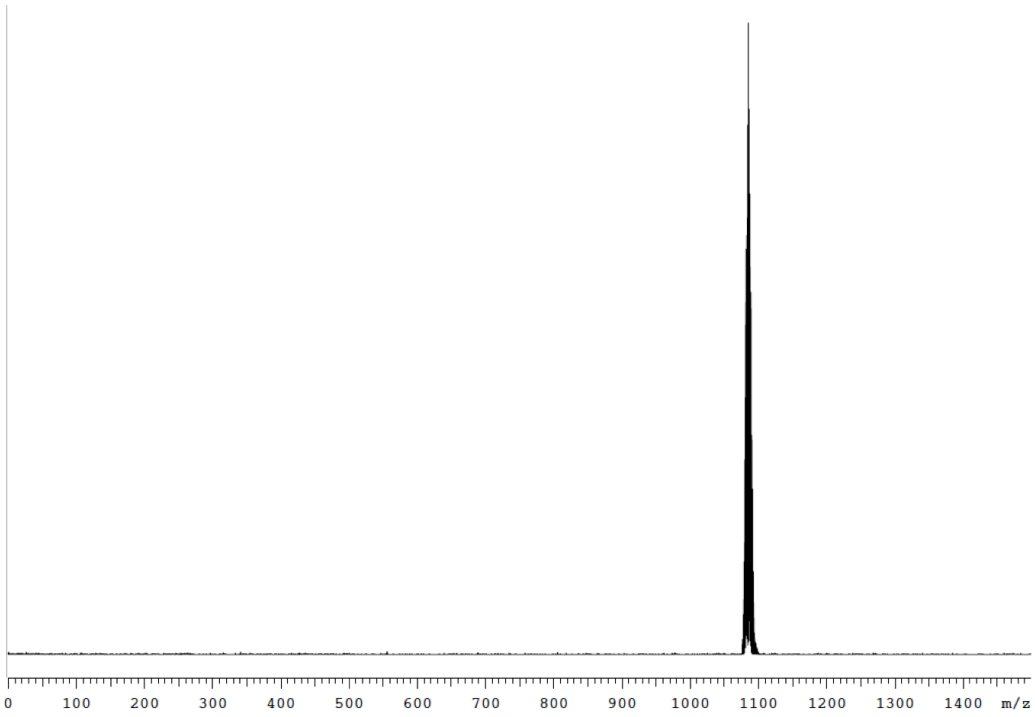

Figure S1 Mass spectrum of $Sc_2@C_{3v}(8)$-C_{82} in a negative reflection mode.

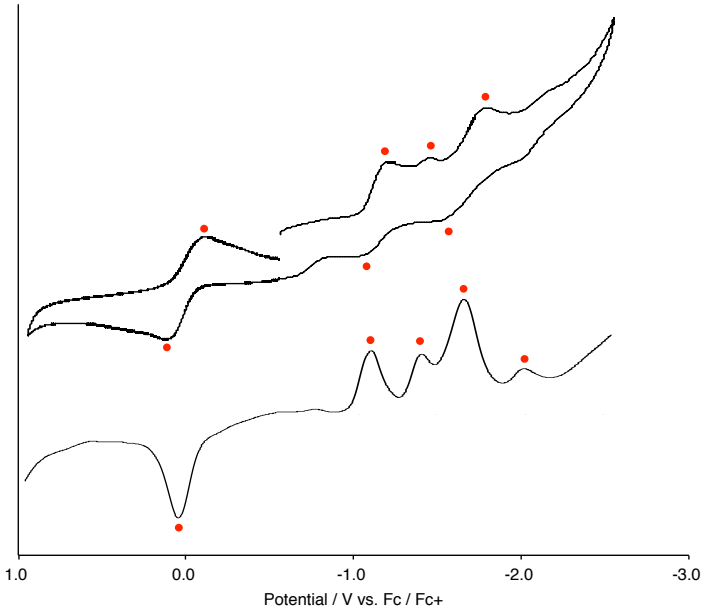

Figure S2 CV and DPV curves of $Sc_2@C_{3v}(8)$-C_{82}.

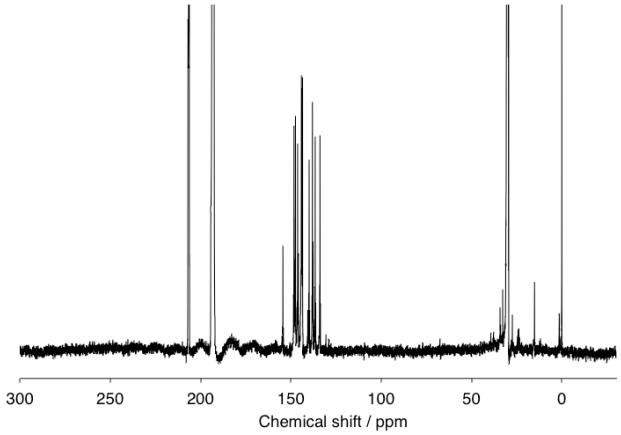

Figure S3 ^{13}C NMR spectrum (125 MHz) of $Sc_2@C_{3v}(8)$-C_{82} measured in CS_2/acetone-d_6 capillary at 298K.

^{13}C NMR (125 MHz, CS_2/acetone-d_6 capillary, 298 K) δ 154.46 (s, 3C), 148.33 (s, 6C), 147.61 (s, 3C), 147.50 (s, 6C), 146.28 (s, 6C), 145.91 (s, 3C), 144.26 (s, 3C), 144.22 (s, 6C), 144.07 (s, 6C), 143.76 (s, 6C), 143.58 (s, 6C), 140.69 (s, 1C), 139.94 (s, 6C), 138.12 (s, 6C), 137.79 (s, 3C), 136.57 (s, 6C), 133.93 (s, 6C).

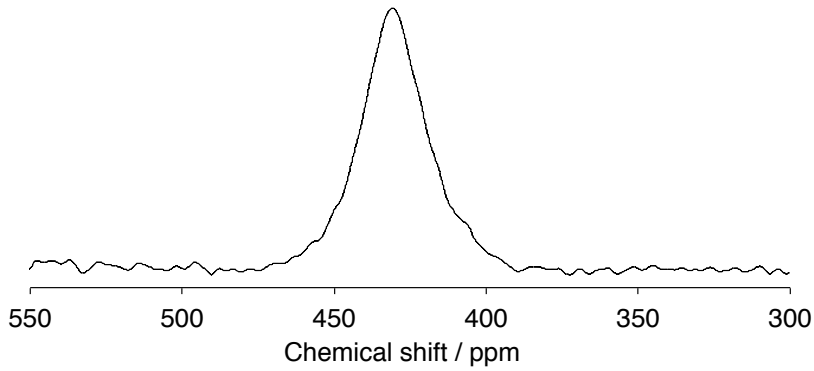

Figure S4 ^{45}Sc NMR spectrum (145.8 MHz) of $Sc_2@C_{3v}(8)$-C_{82} in 1,2-dichlorobenzene-d_4 at 293 K. The chemical shift scale was calibrated using Sc_2O_3 in HCl/D_2O as external reference (0 ppm).

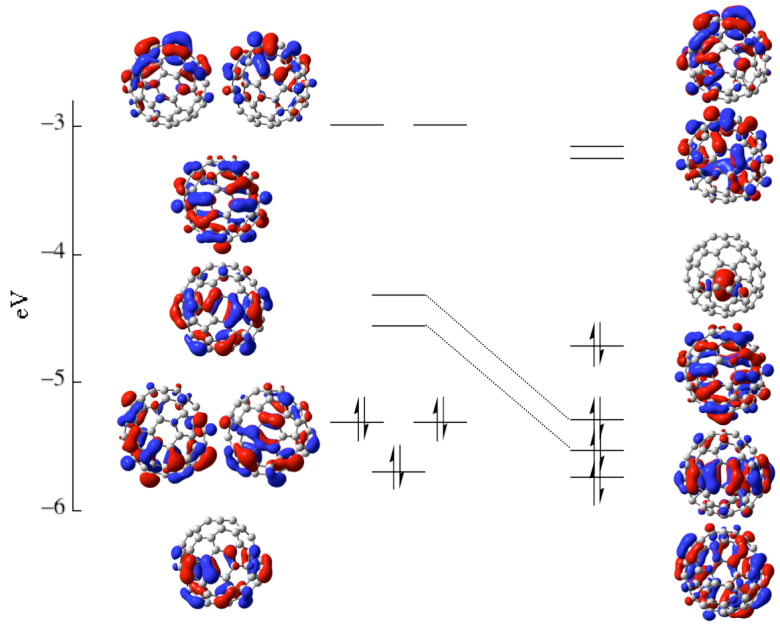

Figure S5 Molecular orbital (MO) diagrams of C_{3v}(8)-C_{82}(left) and Sc_2@C_{3v}(8)-C_{82}(right).

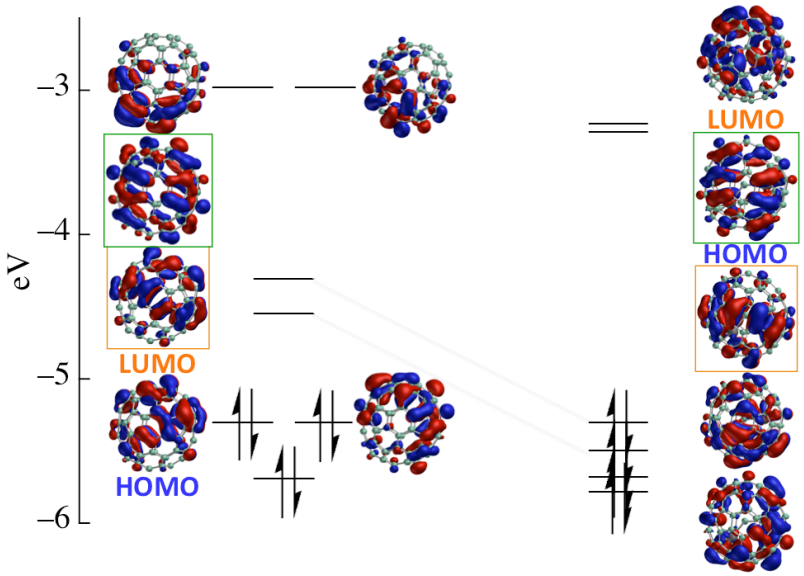

Figure S6 Molecular orbital (MO) diagrams of C_{3v}(8)-C_{82}(left) and Sc_2C_2@C_{3v}(8)-C_{82}(right).

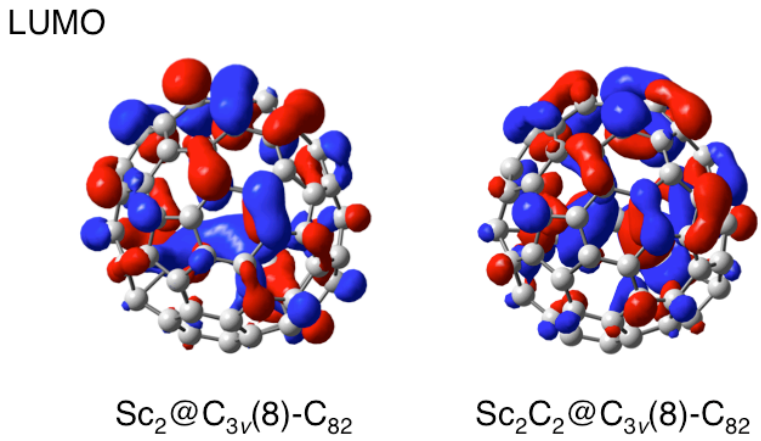

Figure S7 LUMOs of $Sc_2@C_{3v}(8)$-C_{82} and $Sc_2C_2@C_{3v}(8)$-C_{82}.