

## Supporting Information for

# First Kinetic Evidence for the CH/ $\pi$ and $\pi/\pi$ Solute-Solvent Interaction of C<sub>60</sub> in Diels-Alder Reaction with Cyclohexadiene

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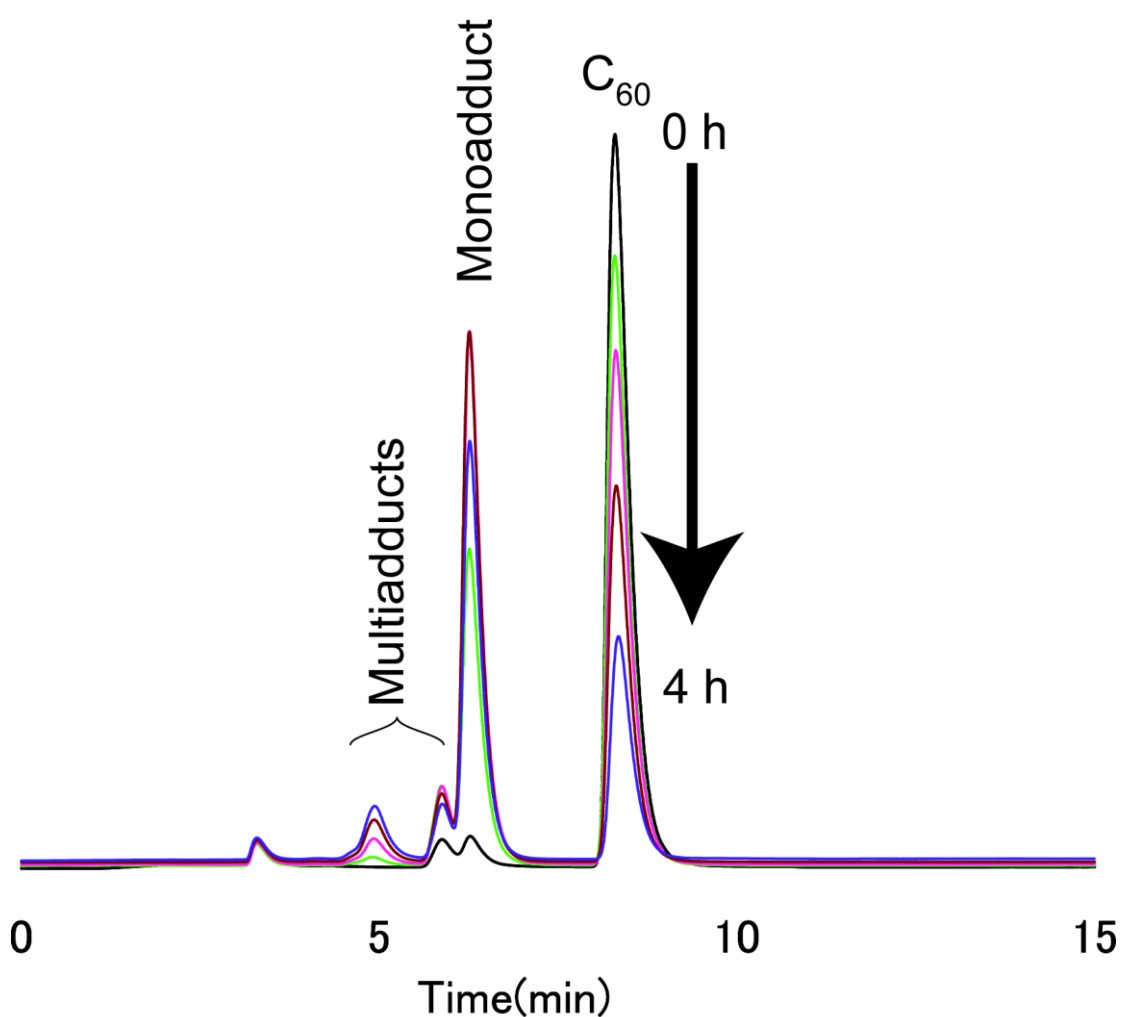
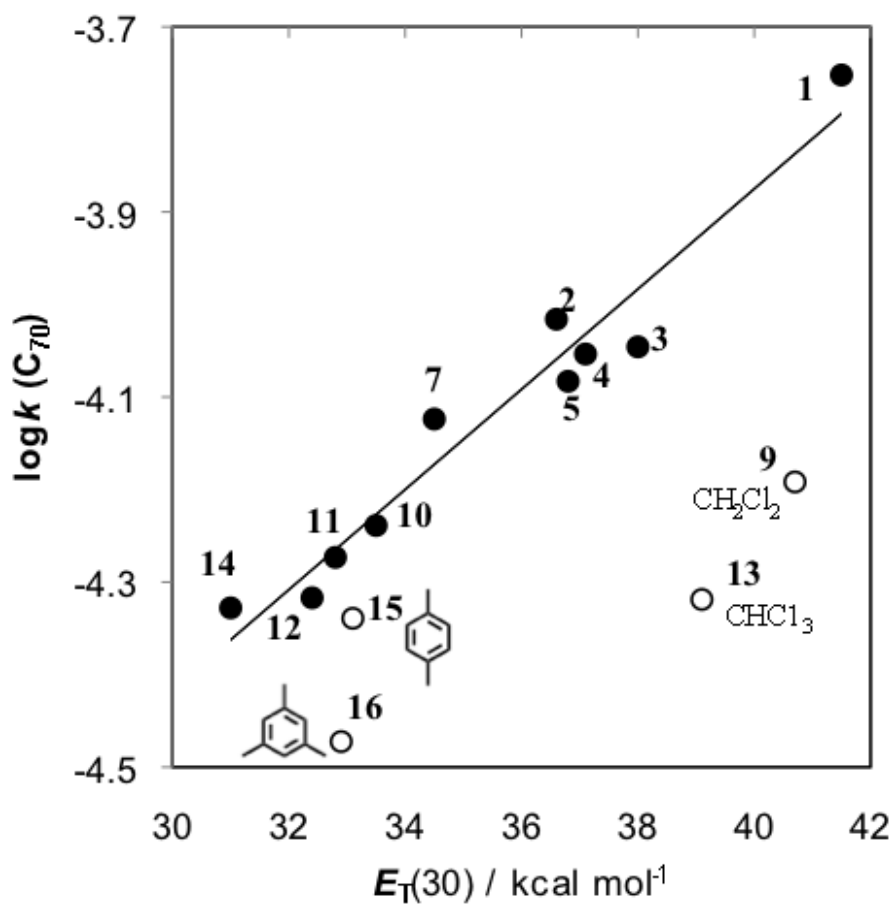
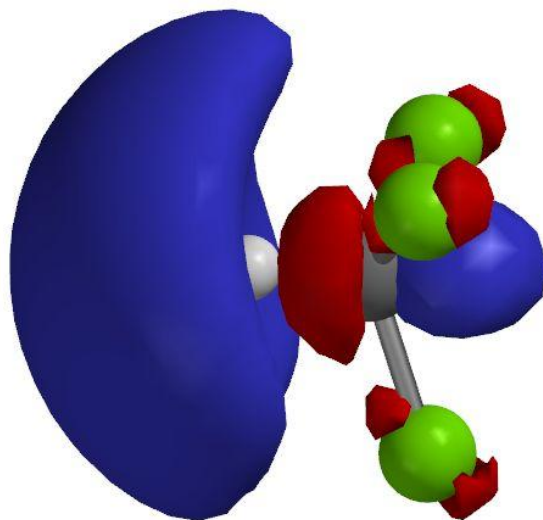


Fig. S1 Representative HPLC chart (buckyprep, toluene 1 mL/min) of the DA reaction of C<sub>60</sub> in toluene.



**Fig. S2** Plots of  $\log k_2(C_{70})$  vs  $E_T(30)$  in various solvents. 10 solvents included in the correlation; 4 outlying solvents (open circle) were excluded from the correlation. For point numbers, see Table 1.



**Fig. S3** LUMO+3 orbital of CHCl<sub>3</sub> (Iso value is 0.032), in which  $\sigma^*$  orbital of C-H bond is well distributed.

**Full citation of SPARTAN' 08**

Spartan'08, Wavefunction, Inc. Irvine, CA. Y. Shao, L.F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S.T. Brown, A.T.B. Gilbert, L.V. Slipchenko, S.V. Levchenko, D.P. O'Neill, R.A. DiStasio Jr., R.C. Lochan, T. Wang, G.J.O. Beran, N.A. Besley, J.M. Herbert, C.Y. Lin, T. Van Voorhis, S.H. Chien, A. Sodt, R.P. Steele, V.A. Rassolov, P.E. Maslen, P.P. Korambath, R.D. Adamson, B. Austin, J. Baker, E.F.C. Byrd, H. Dachsel, R.J. Doerksen, A. Dreuw, B.D. Dunietz, A.D. Dutoi, T.R. Furlani, S.R. Gwaltney, A. Heyden, S. Hirata, C-P. Hsu, G. Kedziora, R.Z. Khalliulin, P. Klunzinger, A.M. Lee, M.S. Lee, W.Z. Liang, I. Lotan, N. Nair, B. Peters, E.I. Proynov, P.A. Pieniazek, Y.M. Rhee, J. Ritchie, E. Rosta, C.D. Sherrill, A.C. Simmonett, J.E. Subotnik, H.L. Woodcock III, W. Zhang, A.T. Bell, A.K. Chakraborty, D.M. Chipman, F.J. Keil, A. Warshel, W.J. Hehre, H.F. Schaefer, J. Kong, A.I. Krylov, P.M.W. Gill and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, **2006**, 8, 3172-3191.