Supporting Information

for

Synthesis of C\textsubscript{70}-fragment buckybowls bearing alkoxy substituents

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\textsuperscript{1}H and \textsuperscript{13}C NMR data of 3a, 3b, 4a, 4b and 5a–c, simulated UV–vis spectra of 5a, 5b and 5c
Figure S1. $^1$H and $^{13}$C NMR spectra of 3a.
Figure S2. $^1$H and $^{13}$C NMR spectra of 3b.
Figure S3. $^1$H and $^{13}$C NMR spectra of 4a.
Figure S4. $^1$H and $^{13}$C NMR spectra of 4b.
Figure S5. $^1$H and $^{13}$C NMR spectra of 5a.
Figure S6. $^1$H and $^{13}$C NMR spectra of 5b.
Figure S7. $^1$H and $^{13}$C NMR spectra of 5c.
2. Computational data

All the theoretical calculations were conducted by Gaussian09.s1 Calculation of UV-vis spectra of 5a, 5b and 5c was performed by TD-DFT (time dependent density functional theory) at the CAM-B3LYP/6-31G+(d,p) level of theory with using the optimized structures from single crystal X-ray analysis data.

Figure S8. Simulated UV-vis spectra of 5a, 5b and 5c.
Reference

S1. 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. Maricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, I. 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, 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, N. J. 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian09, Revision B.01; Gaussian Inc.: Wallingford, CT, 2010.