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# $C_{60}(C_6H_4Me)_4Ph_4$: a fully substituted derivative of the pentagon-fused $C_{60}Cl_8$

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1 The $^1$ HNMR spectrum of $^{\#\,1809}C_{60}Cl_4Ph_4$ and the UV-Vis spectra comparison of $^{\#\,1809}C_{60}Cl_4Ph_4$ and $^{\#\,1809}C_{60}Tol_4Ph_4$.

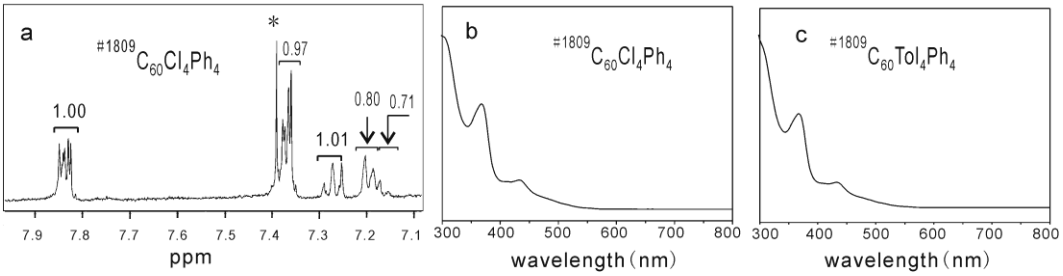


**Figure S1** a) $^1$ HNMR spectrum of $^{\#\,1809}C_{60}Cl_4Ph_4$ where asterisk represents the impurity; UV-Vis spectra of: b) $^{\#\,1809}C_{60}Cl_4Ph_4$ and c) $^{\#\,1809}C_{60}Tol_4Ph_4$ in toluene.

The $^1$ HNMR and UV-Vis spetra of $^{\#\,1809}C_{60}Cl_4Ph_4$ are in accordance with those in the literature and have better signal to noise ratio.[S1] The comparison of its UV-Vis spectrum with that of $^{\#\,1809}C_{60}Tol_4Ph_4$ indicates they are isostructural.

2 The electron density plots of $^{\#\,1809}C_{60}Cl_4Ph_4$ and $^{\#\,1809}C_{60}Tol_4Ph_4$.

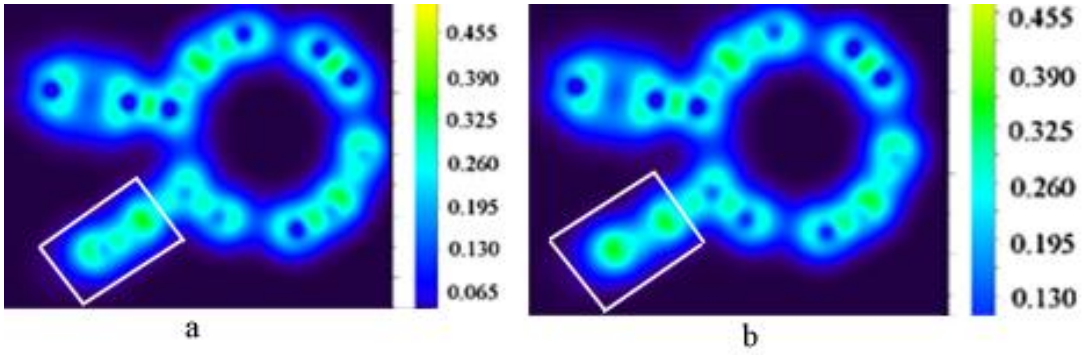


**Figure S2** The electron density plots of a) $C_{60}Cl_4Ph_4$ and b) $C_{60}Tol_4Ph_4$ along xz plane. The white rectangle area represents the obvious transformation of electron density.

**References**

S1 Y. Z. Tan, Z. J. Liao, Z. Z. Qian, R. T. Chen, X. Wu, H. Liang, X. Han, F. Zhu, S. J. Zhou, Z. P. Zheng, X. Lu, S. Y. Xie, R. B. Huang and L. S. Zheng, *Nat. Mater.*, 2008, **7**, 790.