Electronic Supplementary Information

Synthesis of face-centred cubic Cs$_3$C$_{60}$ in THF

Alec G. McLennan,[a] Alexey Y. Ganin,[a,c] Yasuhiro Takabayashi,[b] Ross H. Colman,[b] Ruth H. Zadik,[b] Matthew J. Rosseinsky[a]* and Kosmas Prassides[b,d]*

[a] *Department of Chemistry, University of Liverpool, Crown Street, Liverpool L69 7ZD, UK.*
Fax: +44 (0) 151 794 3588; Tel: +44 (0) 151 794 3499; E-mail: m.j.rosseinsky@liverpool.ac.uk
[b] *Department of Chemistry, Durham University, South road, Durham DH1 3LE, UK*
E-mail:k.prassides@durham.ac.uk
[c] *School of Chemistry, University of Glasgow, Glasgow G12 8QQ, UK.*
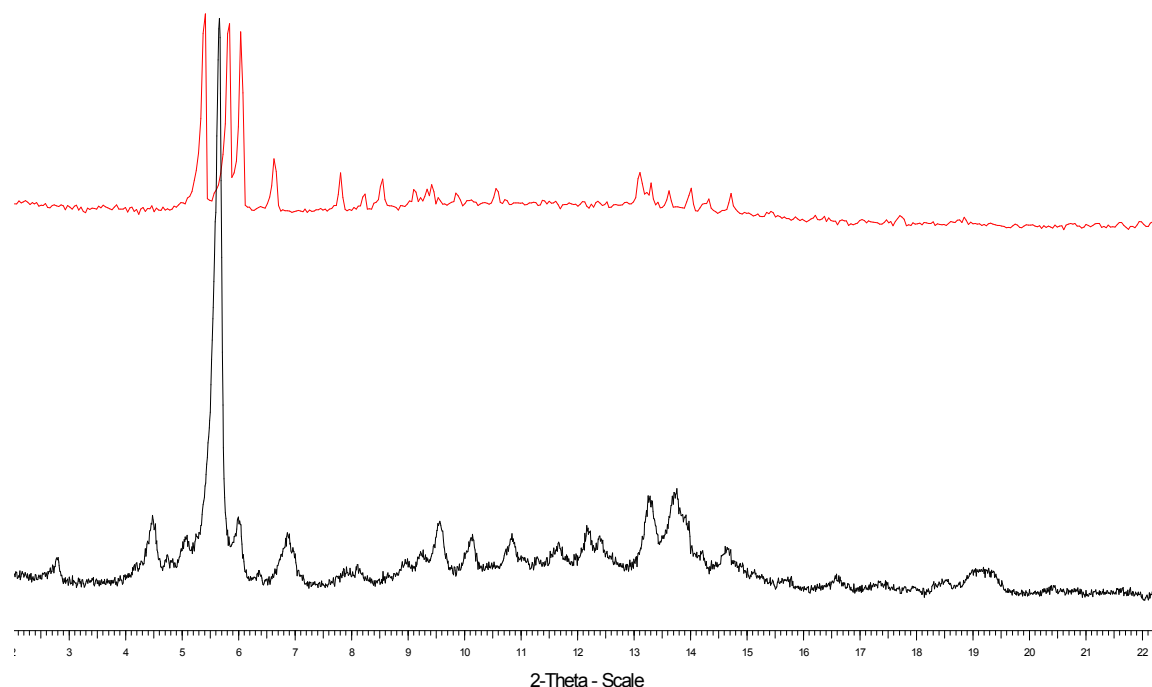[d] *WPI Research Center, Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

Figure S1 X-ray patterns of Mn(cp*)$_2$ (top) and Cs[Mn(cp*)$_2$] (bottom). MoK$_{\alpha1}$ radiation (0.7095 Å)

Table S1. Refined parameters for the fcc (space group $Fm\overline{3}m$) Cs_3C_{60} (**Sample 1**) obtained from the Rietveld refinement of the synchrotron X-ray powder diffraction data at 295 K. Estimated errors in the last digits are given in parentheses. The weighted-profile and expected R-factors are $R_{wp} = 1.14\%$ and $R_{exp} = 0.24\%$. The values of the lattice constant and unit cell volume are: $a = 14.7560(2)$ Å, and $V/C_{60} = 803.24(3)$ Å^3. The positions of the C atoms were adopted from the Ref. [1] and kept fixed in the course of the refinement.

	x/a	y/b	z/c	N	B_{iso} (Å^2)
Cs(1)	0.25	0.25	0.25	0.999(1)	2.67(2)
Cs(2)	0.5	0.5	0.5	0.944(1)	9.63(7)
C(1)	0	0.0491	0.2407	0.5	0.13(8)
C(2)	0.2051	0.0767	0.0978	0.5	0.13(8)
C(3)	0.1764	0.1533	0.0503	0.5	0.13(8)

Table S2. Refined parameters for the fcc (space group $Fm\overline{3}m$) Cs_3C_{60} (**Sample 2**) obtained from the Rietveld refinement of the synchrotron X-ray powder diffraction data at 295 K. Estimated errors in the last digits are given in parentheses. The weighted-profile and expected R-factors are $R_{wp} = 1.78\%$ and $R_{exp} = 0.38\%$. The values of the lattice constant and unit cell volume are: $a = 14.7479(2)$ Å, and $V/C_{60} = 801.92(3)$ Å^3. The positions of the C atoms were adopted from the Ref. [1] and kept fixed in the course of the refinement.

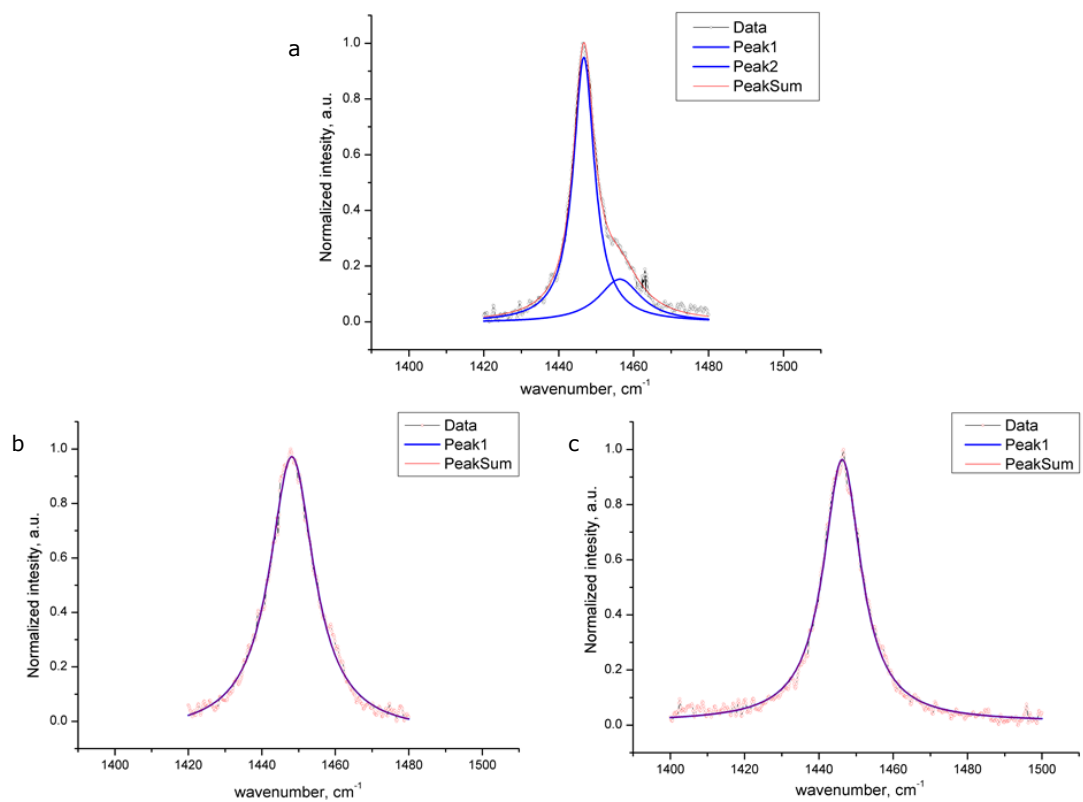|	x/a	y/b	z/c	N	B_{iso} (Å^2)
Cs(1)	0.25	0.25	0.25	0.9859(6)	2.03(2)
Cs(2)	0.5	0.5	0.5	0.975(1)	11.32(5)
C(1)	0	0.0491	0.2407	0.5	0.56(4)
C(2)	0.2051	0.0767	0.0978	0.5	0.56(4)
C(3)	0.1764	0.1533	0.0503	0.5	0.56(4)

Figure S2. Comparison of the Raman spectra and their fit with Lorentzian functions Ref. [1] (a), Sample **1** (b) and Sample **2** (c). The black line/red points correspond to the observed data; the blue line represents the peak contribution to the profile, and the red line shows the overall fit to the data.
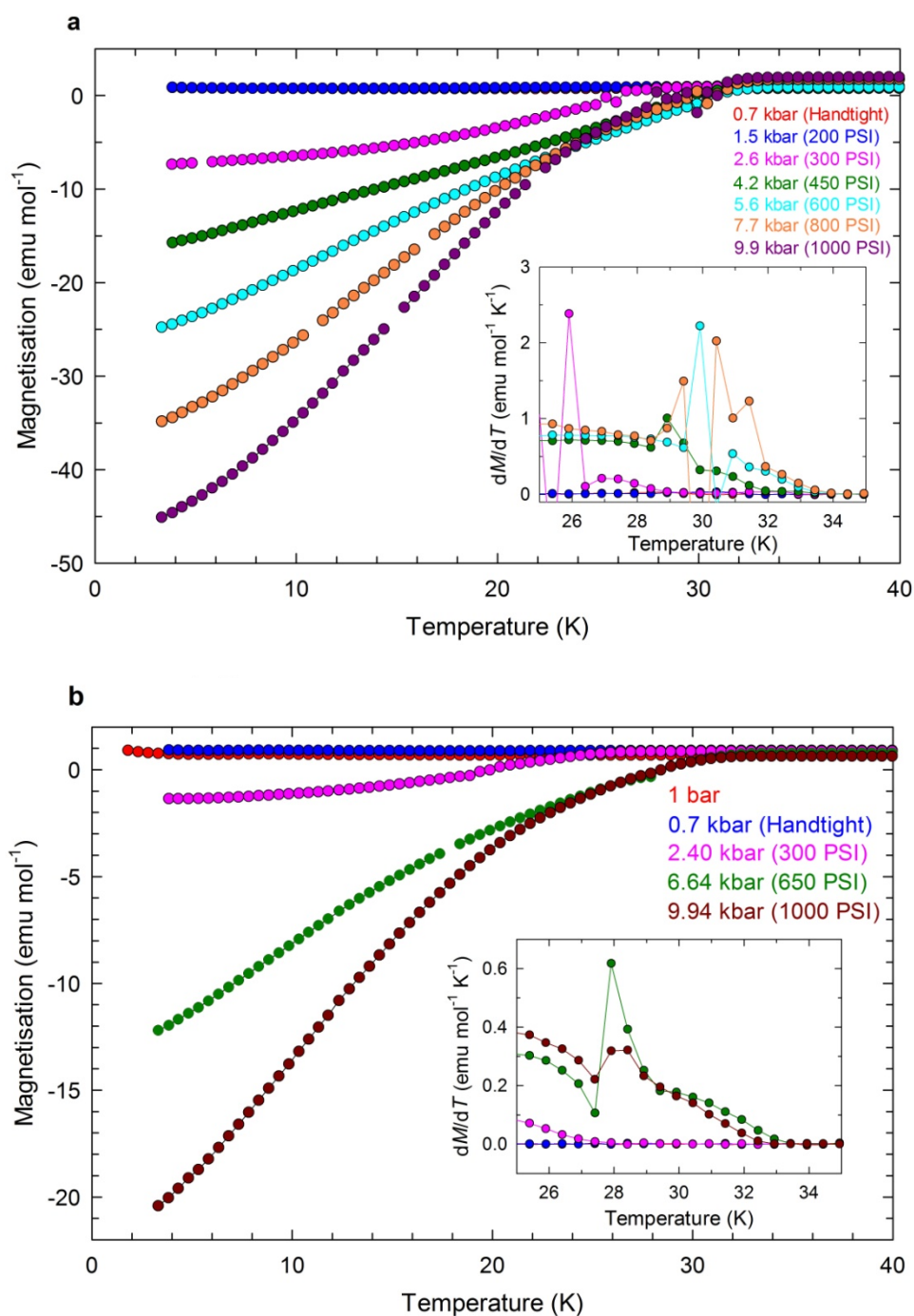
Figure S3. High pressure SQUID magnetic measurements and derivative *dM/dT* of the respective data. **(a)** Magnetisation as a function of temperature for Sample **1**. The onset of superconductivity is at 0.7 kbar with a T$_c$ of 29.5 K. Maximum shielding fraction of 6 % with a T$_c$ of 33.5 K achieved at 9.9 kbar. **(b)** The magnetisation as a function of temperature measurements for Sample **2**. The onset of superconductivity is at 2.4 K bar with a T$_c$ of 29.0 K. The shielding fraction rises to a maximum value of 3 % with a T$_c$ of 33.0 K at 9.9 kbar.

1. A. Y. Ganin, Y. Takabayashi, P. Jeglic, D. Arcon, A. Potocnik, P. J. Baker, Y. Ohishi, M. T. McDonald, M. D. Tzirakis, A. McLennan, G. R. Darling, M. Takata, M. J. Rosseinsky and K. Prassides, *Nature*, 2010, **466**, 221.