Electronic Supplementary Information

Linear-scaling density functional simulations of the effect of crystallographic structure on electronic and optical properties of fullerene solvates

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Single crystals of PCBM·1-methylnaphthalene (1-MN) were obtained by slow diffusion of 2-propanol into a solution of PCBM in 1-methylnaphthalene. A red prism crystal was mounted on a Rigaku XtaLab SuperNova diffractometer. CuKα X-ray source was used. The structure was solved using direct methods, SHELXTL software was used for the calculations [G.M. Sheldrick. SHELXTL (2013).]. The crystal structure of PCBM·1-MN has been deposited at the Cambridge Crystallographic Data Centre, and the assigned deposition number is CCDC 1519619.

Table S1: Crystal data and structure refinement details for PCBM·1-MN

Empirical formula	$C_{83}H_{24}O_2$
Formula weight	1053.02
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal size	0.350 × 0.250 × 0.100 mm
Crystal habit	Red Prism
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 18.8302(3) Å α= 90°
b = 13.26542(18) Å	β= 105.9578(14)°
c = 18.4305(2) Å	γ = 90°
Volume	4426.37(10) Å^3
Z	4
Density (calculated)	1.580 Mg/m^3
Absorption coefficient	0.731 mm^{-1}
F(000)	2152
Diffractometer	Rigaku XtaLAB SuperNova
Radiation source	SuperNova (Cu) X-ray Source, CuKα
Data collection method	ω scans
Theta range for data collection	8.960 to 74.491°
Index ranges	$-23 \le h \le 18$, $-16 \le k \le 16$, $-17 \le l \le 23$
Reflections collected	26027
Independent reflections	9015 [R(int) = 0.0271]
Coverage of independent reflections	99.5 %
Variation in check reflections	n/a
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.74119
Structure solution technique	Direct methods
Structure solution program	SHELXTL (Sheldrick, 2013)
Refinement technique	Full-matrix least-squares on F^2
Refinement program	SHELXTL (Sheldrick, 2013)
Function minimized	$\Sigma w(F_o^2-F_c^2)^2$
Data / restraints / parameters	9015 / 0 / 768
Goodness-of-fit on F^2	1.032
Δ/σ_{max}	0.000

Final R indices	
8085 data; I>2σ(I)	R1 = 0.0687, wR2 = 0.1817
all data	R1 = 0.0758, wR2 = 0.1921
Weighting scheme	$w = 1 / [\sigma^2 (F_o^2) + (0.1283P)^2 + 3.1947P]$
where P=$(F_o^2+2F_c^2)/3$	
Extinction coefficient	n/a
Largest diff. peak and hole	0.650 and -0.274 eÅ^{-3}

Refinement summary:

Ordered Non-H atoms, XYZ	Freely refining
Ordered Non-H atoms, U	Anisotropic
H atoms (on carbon), XYZ	Idealized positions riding on attached atoms
H atoms (on carbon), U	Appropriate multiple of U(eq) for bonded atom
H atoms (on heteroatoms), XYZ	Freely refining
H atoms (on heteroatoms), U	Isotropic
Disordered atoms, OCC	No disorder
Disordered atoms, XYZ	No disorder
Disordered atoms, U	No disorder

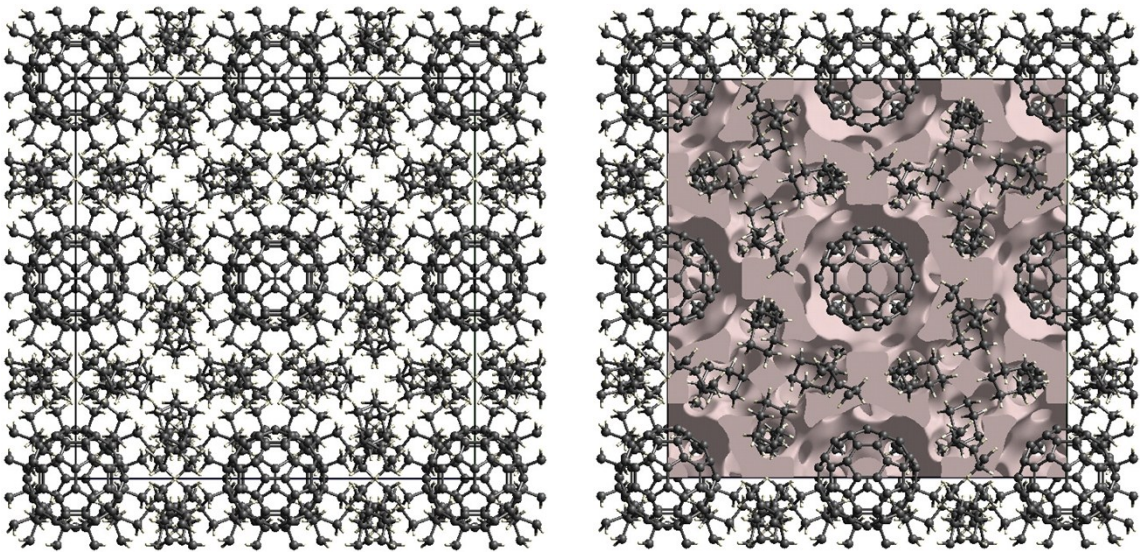

Fig. S1 (a) Unit cell of cyclohexane-solvated C_{60} co-crystal and (b) the isosurface of void in the unit cell.