Supplementary Information of the

An order-disorder phase transition in the van-der-Waals based Solvate of C_{60} and $CClBrH_2$

Jin Ye[1], Maria Barrio [1], René Céolin[1,2], Navid Qureshi[3], Philippe Negrier[4], Ivo B. Rietveld[5,6], Josep Lluís Tamarit[1,*]

[1] Grup de Caracterització de Materials, Departament de Física, EEBE and Barcelona Research Center in Multiscale Science and Engineering, Universitat Politècnica de Catalunya, Av. Eduard Maristany, 10-14, 08019 Barcelona, Catalonia, Spain
[2] LETIAM, EA7357, IUT Orsay, Université Paris Sud, rue Noetzlin, 91405 Orsay Cedex, France
[3] Institut Laue Langevin, 71 avenue des Martyrs - CS 20156 - 38042 GRENOBLE CEDEX 9, France
[4] LOMA, UMR 5798, CNRS, Université de Bordeaux, F-33400 Talence, France

[5] Normandie Université, Laboratoire SMS, EA 3233, Université de Rouen, F76821 Mont Saint Aignan, France
[6] Université Paris Descartes, Faculté de Pharmacie, 4 avenue de l'observatoire, 75006 Paris, France

Table 1. Crystal structure results of the Rietveld refinement for the monoclinic and hexagonal C_{60}·2$CBrClH_2$ co-crystals

Chemical Formula	C_{60}·2$CBrClH_2$	C_{60}·2$CBrClH_2$
M / g·mol^{-1}	979.41	979.41
2θ-Angular Range	9 – 70^o	4 – 100^o
Space group	*C*2/*m*	*P6/mmm*
a /Å	9.9153±0.0017	10.056±0.003
b / Å	17.412±0.004	10.056±0.003
c / Å	10.0478±0.0017	10.070±0.002
α / ^{o}	90	90
β / ^{o}	101.966± 0.009	90
γ / ^{o}	90	120
V / Å^3	1697.0±0.6	881.9±0.4
Z (Z')	2(1/4)	1 (1/24)
Temperature	295 K	333 K
D_x / g·cm^{-3}	1.916±0.001	1.844±0.001
Wavelength (Cu Kα1)	λ=1.540562 Å	λ=1.540562 Å
2θ-shift (zero correction)	-0.0360±0.0013	0.043± 0.008
Profile Parameters		
Na	0.431±0.015	0.89±0.02

Reliability Parameters		
R_{wp}	5.26%	4.02%
R_p	3.83%	3.09%
Peak width parameters		
U	0.479± 0.035	-0.5 ± 0.3
V	-0.304± 0.020	0.56 ± 0.08
W	0.0677± 0.0028	-0.029 ± 0.006
Overall isotropic temperature factor, U / Å^2	0.0637 ± 0.0013	0.142±0.024
Preferred Orientation (March-Dollase)		
a*	-0.199 ± 0.019	
b*	0.746 ± 0.024	
c*	0.636 ± 0.026	
R_0	0.917 ± 0.007	

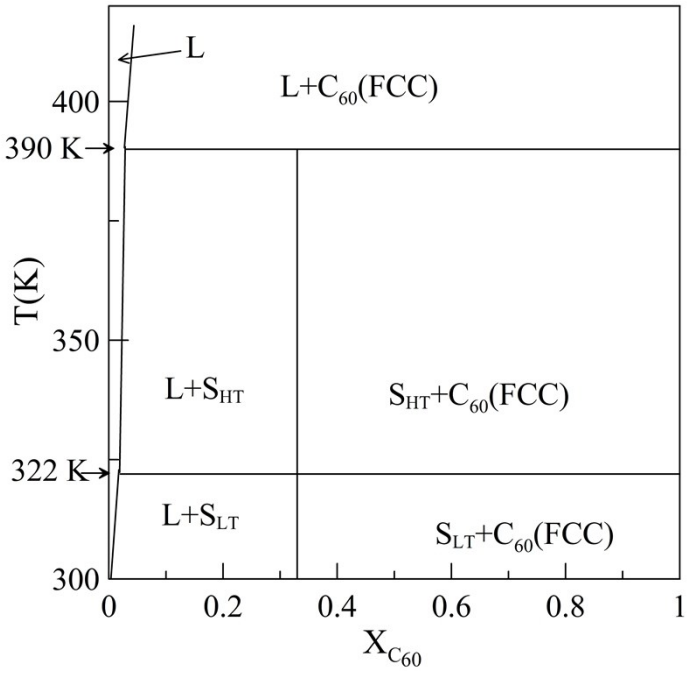

Fig. S1. C_{60} - $CBrClH_2$ phase diagram. L: Liquid phase; C_{60}(FCC): Face-centered cubic phase of C_{60}; S_{LT}: low-temperature monoclinic (C2/m) solvate; S_{HT}: high-temperature hexagonal (P6/mmm) solvate.

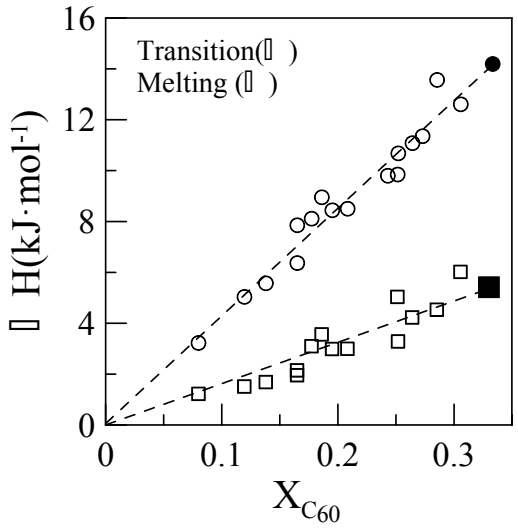

Fig. S2. Tammann diagram for the transition (empty squares) and melting (empty circles) of the C_{60}·2$CBrClH_2$ at 322 and 390 K, respectively. Full symbols are extrapolated values at the co-crystal (X=1/3) concentration.