Supplementary Information of the paper on

Ordered and disordered solvates of C_{60} and $CBrCl_2H$

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Table 1. Crystal structure parameters and Rietveld refinement data for the monoclinic $C_{60}\cdot CCl_2BrH$ and hexagonal $C_{60}\cdot 2CCl_2BrH$ co-crystals

Chemical Formula	$C_{60}\cdot CBrCl_2H$	$C_{60}\cdot 2CBrCl_2H$
M / g·mol^{-1}	884.47	1048.3
2θ-Angular Range	8 – 50^o	4 – 100^o
Space group	*C*2/c	*P6/mmm*
a /Å	10.140 ± 0.003	10.131±0.002
b / Å	31.233 ± 0.009	10.131±0.002
c / Å	10.122 ± 0.003	10.135±0.002
α / ^{o}	90	90
β / ^{o}	90.214 ± 0.023	90
γ / ^{o}	90	120
V / Å^3	3205.6±0.4	900.9±0.3
Z	4	1
Temperature	300 K	300 K
D_x / g·cm^{-3}	1.833 ±0.001	1.932±0.001
Wavelength (Cu Kα1)	λ=1.540562 Å	λ=1.540562 Å
2θ-shift (zero correction)	0.028± 0.006	-0.025± 0.005
Profile Parameters		
Na		
Reliability Parameters		
R_{wp}	4.80%	3.72%
R_p	3.74%	5.07%
Peak width parameters		
U	12.41 ± 0.74	0.153

V	-5.78 ± 0.32	-0.100
W	0.708 ± 0.034	0.047
Overall isotropic temperature factor, *U* / Å^2	0.0327 ± 0.0030	2.38±0.38
Preferred Orientation (March-Dollase)		
*a**	0.307 ± 0.007	
*b**	-0.851 ± 0.006	
*c**	-0.425 ± 0.009	
R_0	0.736 ± 0.011	

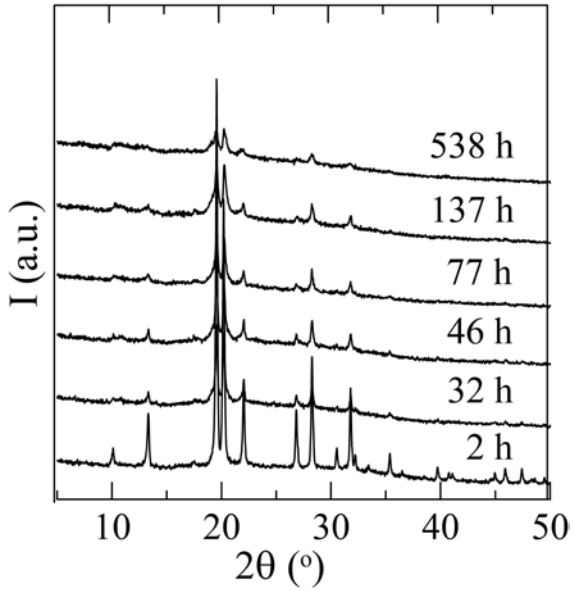

Fig. S1. X-ray powder diffraction profiles as a function of time at 300 K for the hexagonal co-crystals C_{60}·2$CBrCl_2H$ in an open capillary. It is clear that the present structure becomes amorph and the hexagonal co-crystal is not stable under air