Solvent diffusion through a non-porous crystal 'caught in the act' and related single-crystal-to-single-crystal transformations in a cationic dinuclear Ag(I) complex with 1,3-bis(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and BF_4^- as counterion

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Supplementary Data

Preparative and crystallographic details for $[Ag_2(\mathbf{bitmb})_2](SbF_6)_2$:
crystals of $[Ag_2(bitmb)_2](SbF_6)_2 \cdot 2CH_3CN$ (see L. Dobrzańska, *CrystEngComm*, 2011, **13**, 2303 – 2309) were heated for 40 minutes at 100°C, affording the solvent-free form.

Table S1 Crystal data and details of the refinement parameters for the crystal structures of $[Ag_2(bitmb)_2](SbF_6)_2$

Chemical formula	$C_{34}H_{40}N_8Ag_2 \cdot 2(SbF_6)$
Formula Mass	1247.98
Crystal system	Triclinic
a/Å	8.9070(4)
b/Å	9.6544(4)
c/Å	12.2203(5)
α/°	92.845(2)
β/°	103.284(2)
γ/°	101.842(2)
Unit cell volume/Å^3	995.78(7)
Temperature/K	100(2)
Space group	*P*1
No. of formula units per unit cell, *Z*	1
Radiation type	CuKα
Absorption coefficient, *μ*/mm^{-1}	19.266
No. of reflections measured	9080
No. of independent reflections	3531
R_{int}	0.0381
Final R_1 values ($I > 2\sigma(I)$)	0.0388
Final $wR_2(F^2)$ values ($I > 2\sigma(I)$)	0.0895
Final R_1 values (all data)	0.0471
Final $wR_2(F^2)$ values (all data)	0.0931
Goodness of fit on F^2	1.061

[a] $R_1 = \sum \| F_o | - | F_c \| / \sum | F_o |$.
[b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$.

Table S2 Effect of the counterions on the shape of the formed metallocycles

Compound	Counterion geometry	Counter ion Volume/ Å^3	Metal–metal distance in the metallocycle/ Å	Distance between the least-squares planes of mesitylene rings/centroid–centroid distance between these rings in the metallocycle/Å	N1–Ag1–N19$^{\#}$/°
[Ag_2(**bitmb**)$_2$](SbF_6)$_2$	Octahedral	89	8.07	10.35/10.63	178.8(2)
[Ag_2(**bitmb**)$_2$](PF_6)$_2$	Octahedral	71	7.83	10.39/10.62	179.0(2)
[Ag_2(**bitmb**)$_2$](BF_4)$_2$	Tetrahedral	54	7.17	10.75/11.02	174.1(2)
[Ag_2(**bitmb**)$_2$](NO_3)$_2$	Trigonal	40	6.68	10.93/11.32	169.0(2)

Table S3 Unit cell parameters for **5**

Compound reference	**5**
a/Å	15.381(2)
b/Å	11.818(1)
c/Å	21.410(8)
α/°	90.0
β/°	107.53(2)
γ/°	90.0

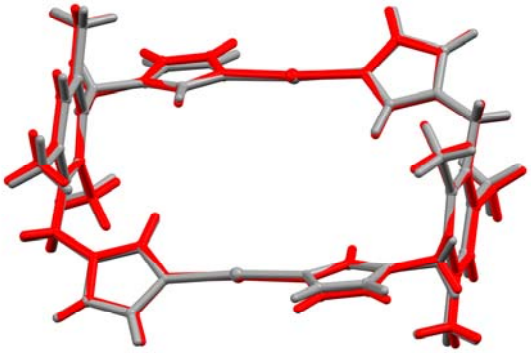

Fig. S1 Overlay of metallocycle **1** (grey) with the corresponding one from **4c** (red); r.m.s. deviation of 0.1437 Å.