Controlled catch and release of small molecules with cucurbit[6]uril via a kinetic trap

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Supporting information

General Methods. $^1$H NMR spectra were recorded on Bruker Avance 500 BB-ATM (500 MHz) spectrometer. The crystallographic data was collected with a Nonius Kappa CCD diffractometer. Cucurbit[6]uril was synthesized by the reported method. $^1$ Et$_2$O purum grade was purchased from Sigma-Aldrich and used as received. The ionic liquid samples were generously provided by Professor Steven Ley’s lab, Cambridge.

Crystallization procedure. An aqueous solution of CB[6] and 1,3-dimethyl-1H-imidazol-3-ium methylsulfonate (I) was prepared with a slight excess of CB[6]. The solution was stirred for 2 hours at room temperature and was let overnight to decant. The following day, 1 to 2 ml of the clear and saturated solution of CB[6] with I was transferred into a 3 ml sample vial which was without its lid and transferred into a larger vial containing Et$_2$O. The larger vial was then sealed and crystallization occurs within a week in the small vial as Et$_2$O continuously diffuses from the large
to the small vial.

References

(1) Buschmann, H.; Fink, H.; Schollmeyer, E. *DE19603377* 1996.