Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

Reversible adsorption and separation of chlorocarbons and BTEX based on Cu(II)-metal organic framework

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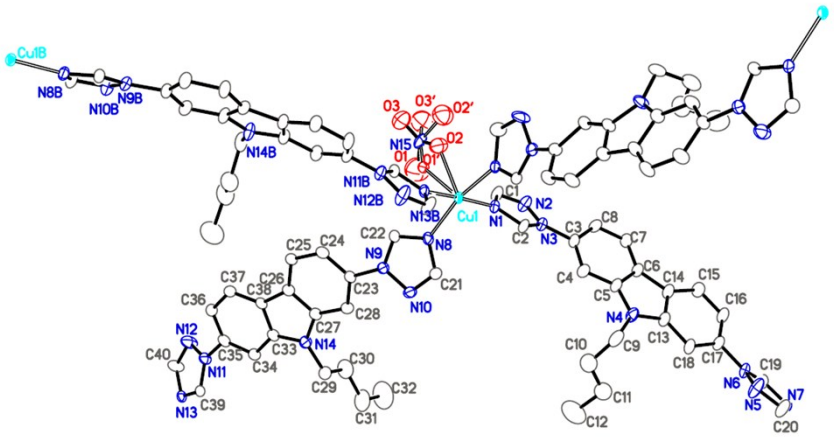


Figure S1. The ORTEP figure of **1**.

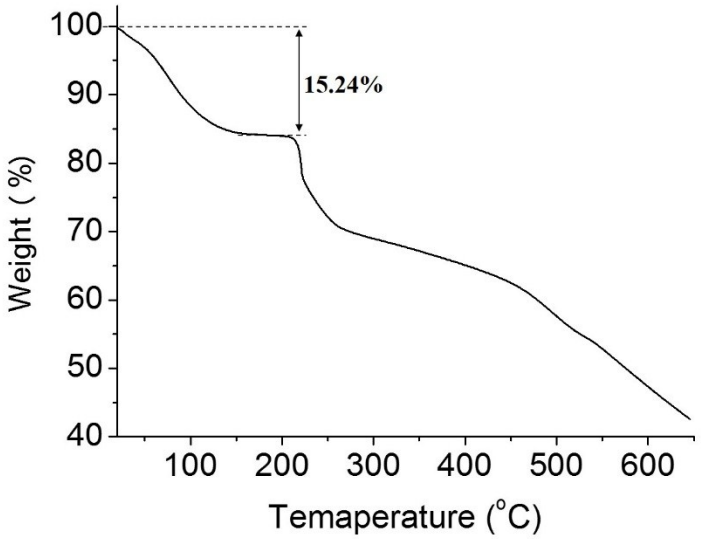


Figure S1. TGA trace of **1** (observed, 15.24 %; calculated 17.24 %).

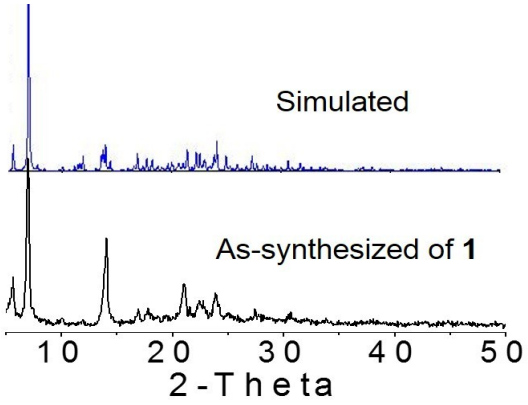


Figure S3. The simulated and measured XRPD patterns of **1**.

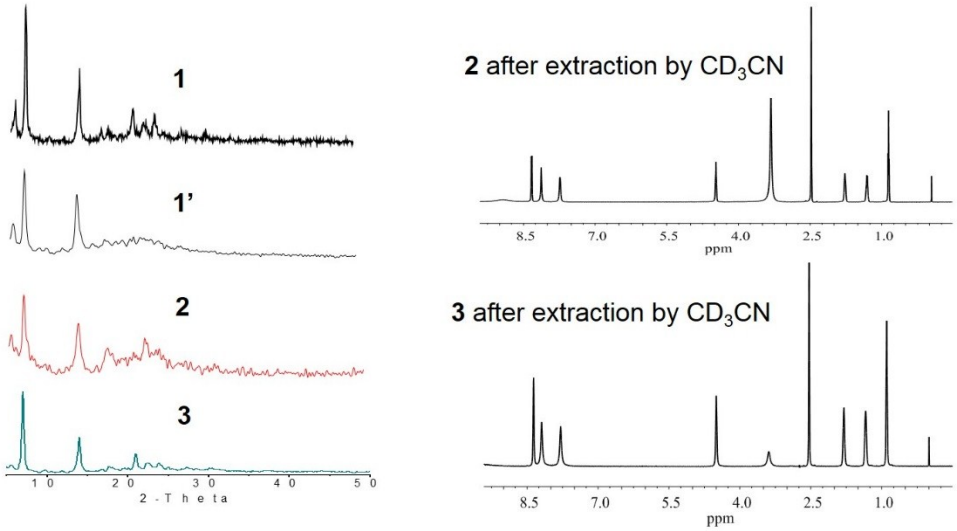


Figure S4. Left: XRPD patterns for **1**, **1'**, **2** and **3**. Right: ^{1}HNMR spectra of **2** and **3** after solid-liquid extraction by CD_3CN. No peaks related to CH_2Cl_2 and $CHCl_3$ guests are found.

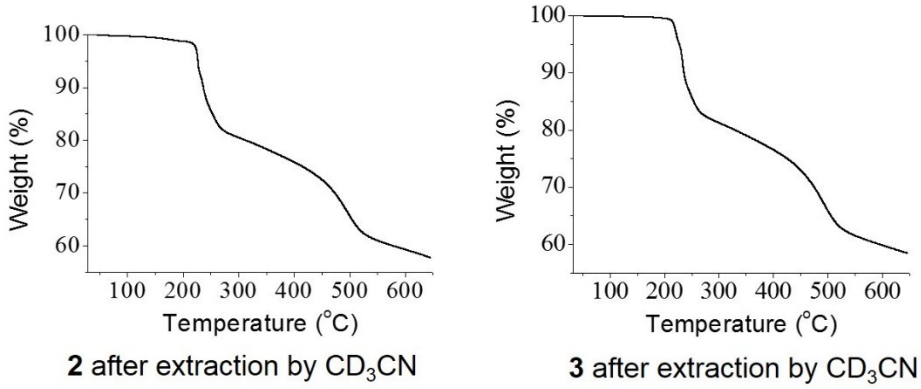


Figure S5. TGA traces of **2** and **3** after solid-liquid extraction by CD_3CN. No guest weight losses are observed, indicating the Cu**L**$_2$ framework is completely desolvated.

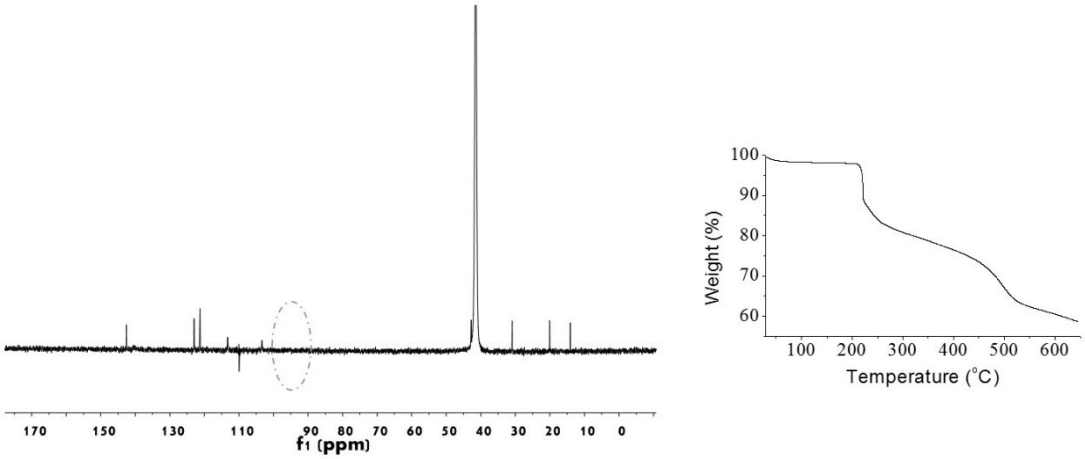


Figure S6. Left: ^{13}C NMR of **1'** soaked in CCl_4 for two days. Right: TGA trace of **1'** soaked in CCl_4 for two days. No effective adsorption for CCl_4 was observed.

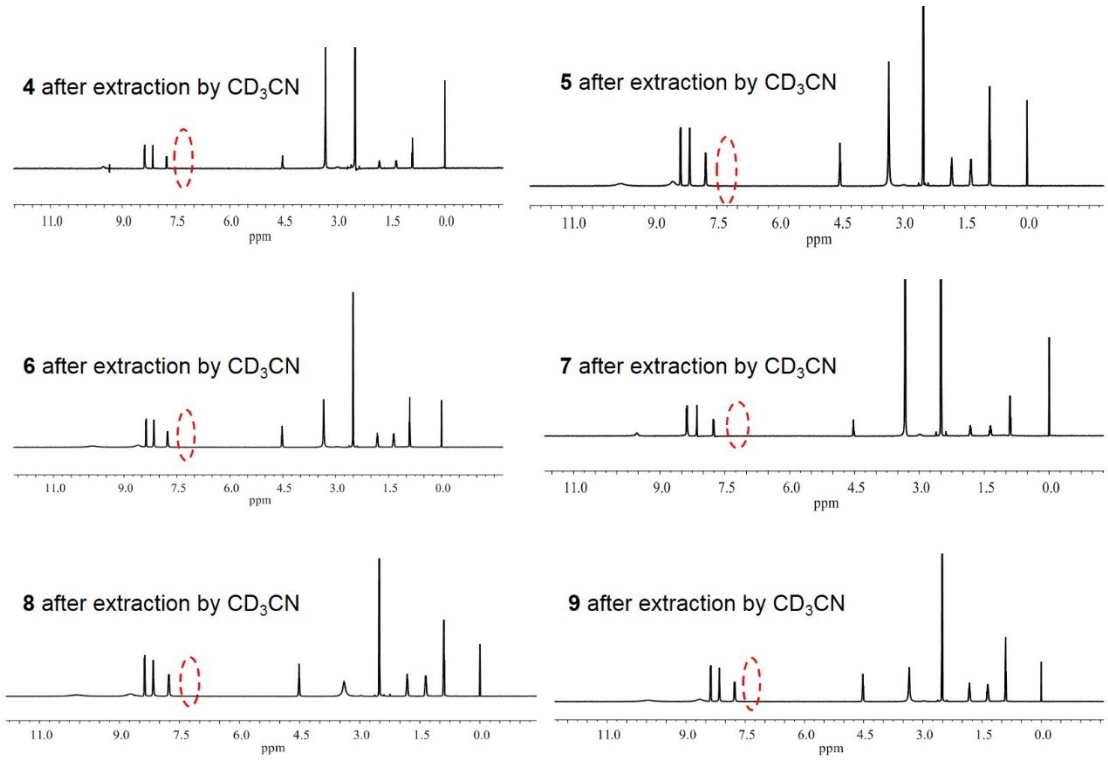


Figure S7. ^{1}H NMR spectra of **4-9** after solid-liquid extraction by CD_3CN, indicating that the encapsulated BTEX can be completely removed by the extraction.

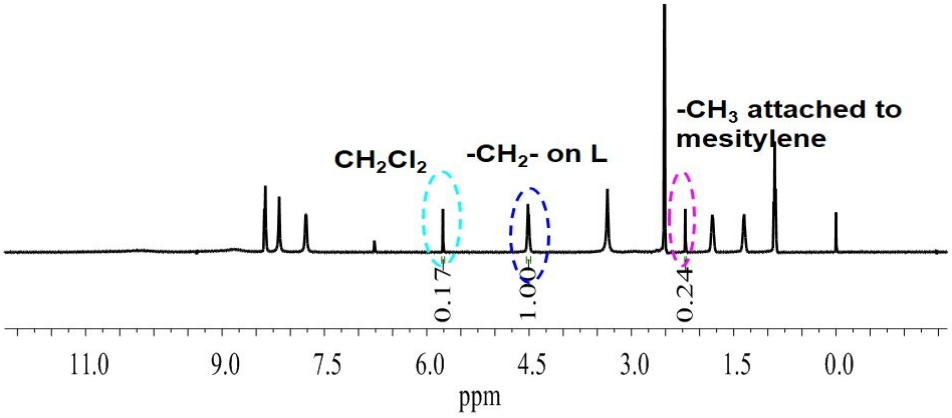
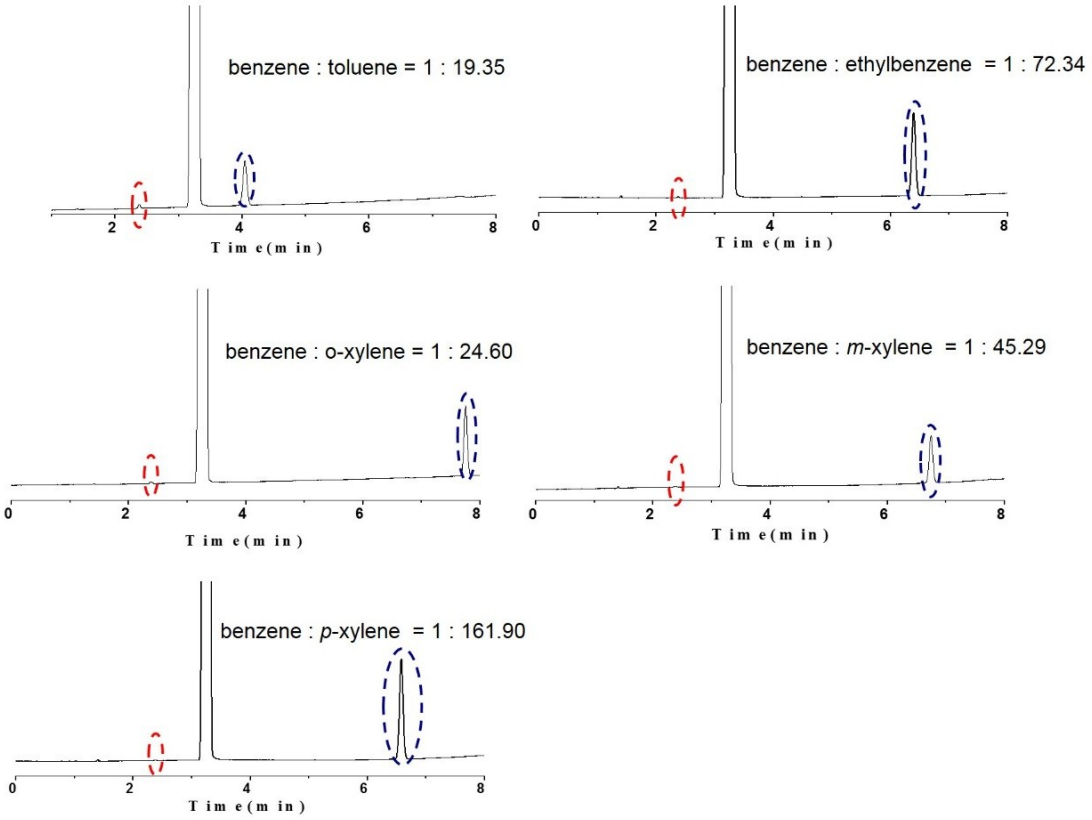


Figure S8. The Cu**L**$_2$ framework can hardly trap C_9-aromatics under reaction conditions. For example, the ^{1}H NMR spectrum indicated that the CH_2Cl_2 guest in **2** can hardly be replaced by mesitylene. When **2** was soaked in mesitylene for 2 days, only tiny amount of mesitylene was uploaded to generate Cu**L**$_2$$(NO_3)_2$·0.34$CH_2Cl_2$·0.11(mesitylene). So it is no significant adsorption for mesitylene based on this Cu**L**$_2$ framework.



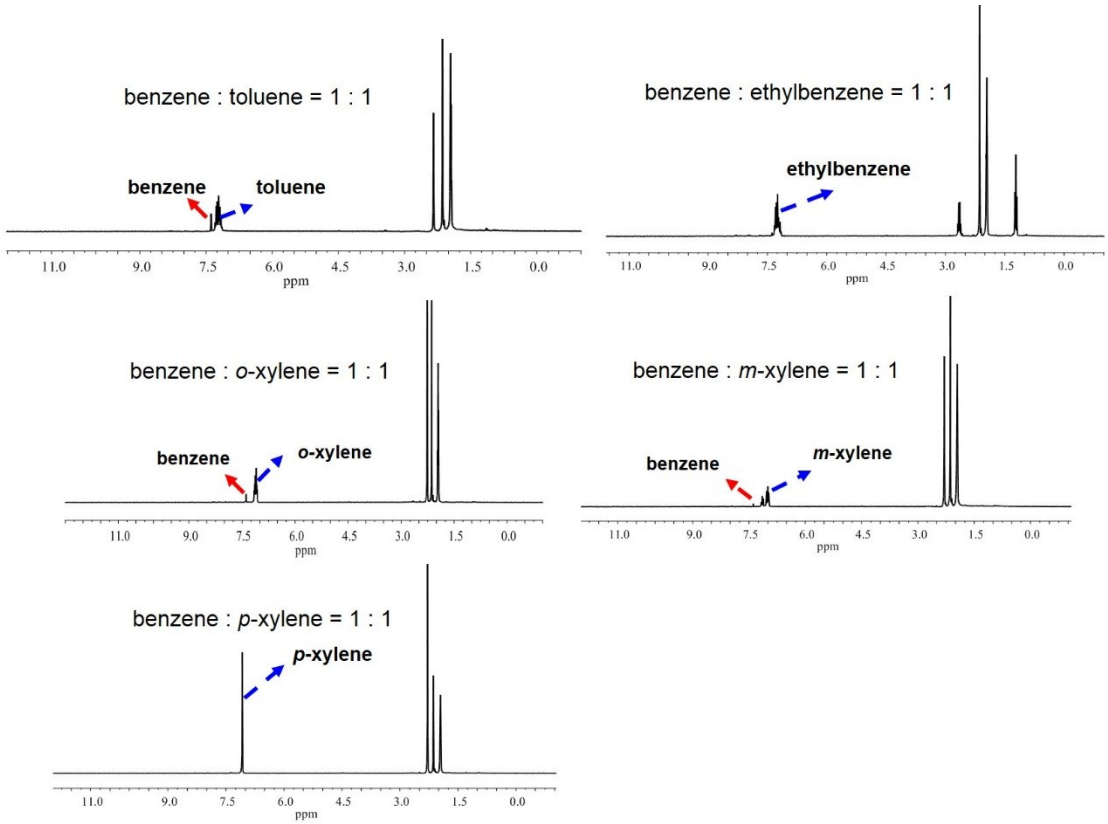
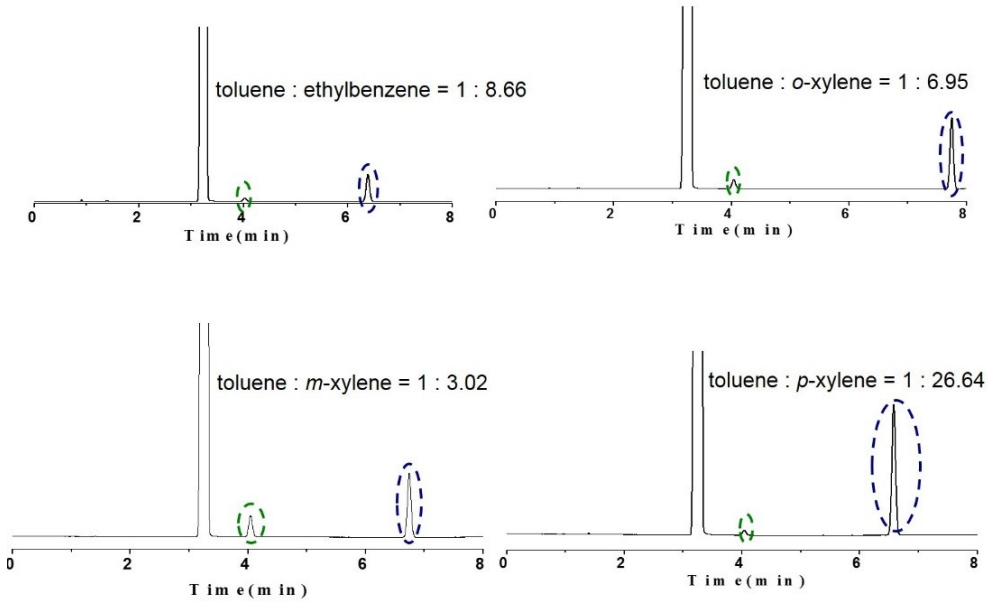


Figure S9. GC analysis results and corresponding ^{1}H NMR (CD_3CN) spectra for separation benzene from its aromatic analogues. For comparison, some characteristic peaks for the encapsulated BTEX are marked in ^{1}H NMR spectra.



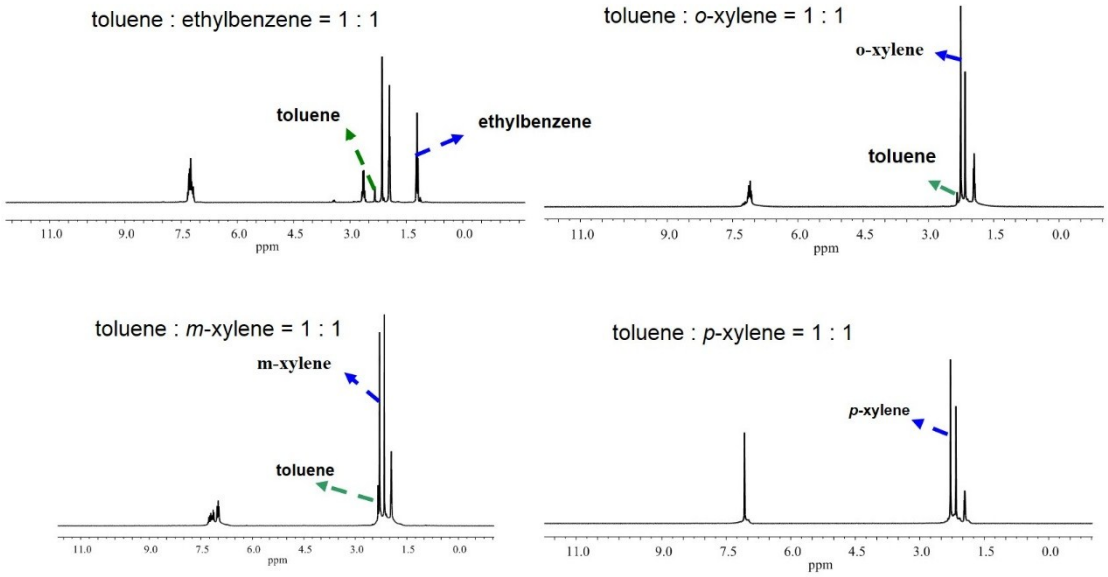


Figure S10. GC analysis results and corresponding ^{1}H NMR (CD_3CN) spectra for separation toluene from its aromatic analogues. For comparison, some characteristic peaks for the encapsulated BTEX are marked in ^{1}H NMR spectra.