Supplementary Information

Isomers recognition by dynamic guest-adaptive ligand rotation in a metal-organic framework with local flexibility

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1. Materials and Methods

Materials and reagents

All chemicals were used directly without further purification. *N*, *N*-dimethylformamide (DMF) and methanol were bought from Tianjin Damao Chemical Reagent Factory. PX, MX, and OX were purchased from Tianjin Guangfu Fine Chemical Industry Research Institute. EB was obtained from Alfa Aesar (China) Chemicals Co., Ltd. N-propylbenzene (N-PB), and ethyltoluene isomers including p-ethyltoluene (P-ET), m-ethyltoluene (M-ET) and o-ethyltoluene (O-ET) were purchased from Aladdin Co. Ltd (Shanghai, China). 1,4-diazabicyclo [2.2.2] octane (TED) and 1,4-benzenedicarboxylic acid (H₂BDC) were procured from Shanghai Bepham Science & Technology Co., Ltd. Nickel (II) chloride hexahydrate (NiCl₂·6H₂O) was purchased from Fuchen (Tianjin) Chemical Reagent Co., Ltd. 9,10-anthracenedicarboxylic acid (H₂ADC) was obtained from Shanghai Tengsai Biotechnology Co., Ltd. Chloroform-d (deuterochloroform, CDCl₃) was purchased from J&K Scientific Ltd.

Methods

Pawley refinements were performed on the Reflex module of Materials Studio, using 2 theta data from 5° to 50°. The integrated intensities were extracted with the Pseudo-Voigt profile and the Finger-Cox-Jephcoat method was used to correct the peak asymmetry. For all structures, the unit cell parameters a, b, c, FWHM parameters, U, V, W, profile parameters NA, NB, and zero point were refined. The background was also refined with 20th order polynomial.

The Hirshfeld surface was calculated through the program Crystal Explorer¹, and it was constructed on the basis of the calculated electron distribution as the sum of spherical atom electron densities.²,³ The Hirshfeld surface is implicitly defined by the equation w(r) :
\[ w(r) = \frac{\sum_{i \in \text{molecule}} \rho_i (r)}{\sum_{i \in \text{crystal}} \rho_i (r)} \]  

(S1)

Where \( \rho_i (r) \) is a spherically-averaged atomic electron density located at the \( i \)th nucleus.

**Calculation of Thermodynamic Parameters.**

The adsorption enthalpy and adsorption entropy of the analytes on the stationary phase were determined by gas chromatography and calculated by van’t Hoff formula:

\[
\ln k' = \frac{\Delta H}{RT} + \frac{\Delta S}{R} + \ln \Phi
\]

(S2)

Here, \( k' \) was the retention factor, \( R \) was the gas constant, \( T \) was the absolute temperature, \( \Phi \) was the phase ratio, \( V_s \) was volume of the stationary phase, and \( V_m \) was the mobile phase.

It was worthy noting that \( V_s \) was calculated from the thickness of stationary phase on the capillary column according to SEM images, while \( V_m \) was calculated from the column internal volume subtract the \( V_s \). Then, we could calculate \( \Phi \) according to the following equation. Finally, we obtained the \( \ln \Phi \) for \( \text{Ni(ADC)(TED)}_{0.5} \) columns were -0.874.

\[
\Phi = \frac{V_s}{V_m}
\]

(S3)

\( k' \) was obtained based on:

\[
k' = \frac{t - t_0}{t_0}
\]

(S4)
2. Supplementary Figures

**Figure S1.** PXRD patterns of Ni(ADC)(TED)$_{0.5}$ (a) and N$_2$ adsorption and desorption isotherms at 77K (b).

**Figure S2.** TGA curves of Ni(ADC)(TED)$_{0.5}$.

**Figure S3.** PXRD patterns of the sample and C8 aromatic-included materials.
Figure S4. The structure of EB-included for Phase_1 (a) and Phase_2 (b).

Figure S5. PXRD patterns of simulated the framework with different configurations of anthracene rings.
Figure S6. Pawley refinement of MOF structures: (a) EB@Ni(ADC)(TED)\(_{0.5}\), (b) PX@Ni(ADC)(TED)\(_{0.5}\), (c) MX@Ni(ADC)(TED)\(_{0.5}\), (d) OX@Ni(ADC)(TED)\(_{0.5}\).

Figure S7. PXRD of Ni(ADC)(TED)\(_{0.5}\) and the regenerated sample.
Figure S8. Ni(ADC)(TED)$_{0.5}$ coated capillary column ((a): 2.5 μm thickness; (b): 1.6 μm thickness)

Figure S9. The van’t Hoff plots of xylene isomers and ethylbenzene on the Ni(ADC)(TED)$_{0.5}$ GC column.
**Figure S10.** The kinetic adsorption isotherms of the sample.

**Figure S11.** TGA patterns of the C8 aromatic-included sample.
Figure S12. FT-IR patterns of the C8 aromatic-included sample and original one.

Figure S13. Separation performance of Ni(ADC)(TED)$_{0.5}$ in binary vapor phase experiments (a) and multi-component vapor phase experiments (b).

Figure S14. Adsorption cycles for the separation of an equimolar mixture of C8 aromatic isomers (vapor phase).
**Figure S15.** $N_2$ adsorption and desorption isotherms at 77K (red: the activated sample; black: the regenerated sample).

**Figure S16.** Multicomponent liquid phase breakthrough measurements for an equimolar mixture of C8 aromatics of Ni(ADC)(TED)$_{0.5}$. 
**Figure S17.** The adsorption configurations of the edge-to-face (a) and face-to-face configurations (b) by taking EB@ Ni(ADC)(TED)₀.₅ as an example.

**Figure S18.** Optimized configurations of EB (a), PX (b), MX (c), OX (d) on the framework.

**Figure S19.** Molecular shapes of C₈ aromatic isomers ((a) green: EB; (b) blue: PX; (c) brown: MX; (d) pink: OX).

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Figure S20. Relative contribution to the Hirshfeld surface area for various molecular contacts in guest-included Ni(ADC)(TED)_{0.5}.

Figure S21. GC chromatograms on the Ni(BDC)(TED)_{0.5} capillary column for the separation of C8 aromatic isomers.
Figure S22. GC chromatograms on the Ni(ADC)(TED)$_{0.5}$ capillary column for the separation of ethyltoluene isomers and n-propylbenzene.
3. Supplementary Tables

Table S1. Crystallographic and refinement information for Phase_1.

| Identification code          | Phase_1          |
|------------------------------|------------------|
| Empirical formula            | C_{38}H_{28}N_{2}Ni_{2}O_{8} |
| Formula weight               | 758.03           |
| Temperature/K                | 100(2)           |
| Crystal system               | orthorhombic     |
| Space group                  | I222             |
| a/Å                          | 13.770(3)        |
| b/Å                          | 16.220(3)        |
| c/Å                          | 18.220(4)        |
| α/°                          | 90               |
| β/°                          | 90               |
| γ/°                          | 90               |
| Volume/Å³                    | 4069.4(14)       |
| Z                            | 8                |
| ρ_{calc} g/cm³               | 1.451            |
| F(000)                       | 684.0            |
| 2Θ range for data collection/°| 0.118 to 2.072   |
| Index ranges                 | -19 ≤ h ≤ 19, -22 ≤ k ≤ 21, -25 ≤ l ≤ 25 |
| Reflections collected        | 90373            |
| Independent reflections      | 6198 [R_{av} = 0.3369, R_{sigma} = 0.1230] |
| Data/restraints/parameters   | 6198/920/141     |
| Goodness-of-fit on F²        | 1.328            |
| Final R indexes [I>=2σ (I)]  | R_{f} = 0.1590, wR_{f} = 0.3742 |
| Final R indexes [all data]   | R_{f} = 0.1801, wR_{f} = 0.3858 |
| Identification code | Phase_2 |
|---------------------|---------|
| Empirical formula   | C38H28Ni2Ni2O8 |
| Formula weight      | 758.03  |
| Temperature/K       | 100(2)  |
| Crystal system      | orthorhombic |
| Space group         | Pca21   |
| a/Å                 | 21.220(4) |
| b/Å                 | 10.730(2) |
| c/Å                 | 18.190(4) |
| α/°                 | 90      |
| β/°                 | 90      |
| γ/°                 | 90      |
| Volume/Å³           | 4141.7(14) |
| Z                   | 4       |
| ρ_calc g/cm³        | 2.121   |
| 2Θ range for data collection/° | 0.134 to 2.052 |
| Index ranges        | -25 ≤ h ≤ 27, -14 ≤ k ≤ 13, -25 ≤ l ≤ 23 |
| Reflections collected | 71469  |
| Independent reflections | 10318 [Rint = 0.2575, Rsigma = 0.1777] |
| Data/restraints/parameters | 10318/945/172 |
| Goodness-of-fit on F² | 1.085  |
| Final R indexes [I>=2σ (I)] | R₁ = 0.1391, wR₂ = 0.3241 |
| Final R indexes [all data] | R₁ = 0.1645, wR₂ = 0.3447 |
**Table S3.** Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for Phase_1.

| Atom   | x    | y    | z    | U(eq)  |
|--------|------|------|------|--------|
| Ni1    | 5000 | 5000 | 5698(2) | 16.7(9) |
| Ni2    | 10000 | 5703(2) | 13.4(8) |
| O19    | 4122(5) | 5925(5) | 4435(4) | 11.3(15) |
| C15    | 3833(9) | 6180(8) | 4996(6) | 33(3) |
| O17    | 1119(5) | 9224(5) | 4358(4) | 12.6(14) |
| O20    | 3881(7) | 5694(6) | 5534(5) | 22.8(18) |
| O18    | 778(7) | 8963(6) | 5562(5) | 24.5(19) |
| C16    | 1257(6) | 8922(5) | 4624(4) | 9.5(17) |
| C5D    | 8120(13) | 4061(9) | 6808(7) | 58(3) |
| C6D    | 8369(13) | 4389(7) | 7488(9) | 58(3) |
| C1D    | 8320(14) | 3900(10) | 8113(7) | 58(3) |
| C2D    | 8021(13) | 3083(9) | 8059(7) | 58(3) |
| C3D    | 7772(12) | 2756(7) | 7380(9) | 34(2) |
| C4D    | 7822(13) | 3245(10) | 6754(7) | 58(3) |
| C1A    | 2937(10) | 8877(9) | 5878(7) | 21.7(15) |
| C2A    | 3771(11) | 8616(10) | 6273(8) | 34(2) |
| C3A    | 4375(12) | 8178(9) | 6300(9) | 34(2) |
| C4A    | 4113(11) | 7470(10) | 5935(9) | 21.7(15) |
| C14A   | 3274(10) | 7486(8) | 5497(8) | 14.3(12) |
| C5A    | 1942(12) | 6048(10) | 4320(9) | 21.7(15) |
| C6A    | 1040(13) | 5974(11) | 4025(12) | 34(2) |
| C7A    | 466(13) | 6681(10) | 3959(11) | 34(2) |
| C8A    | 756(12) | 7387(10) | 4292(10) | 21.7(15) |
| C11A   | 1623(11) | 7451(9) | 4674(9) | 14.3(12) |
| C9A    | 1895(11) | 8187(9) | 5006(10) | 19.2(16) |
| C13A   | 2651(10) | 8171(8) | 5491(8) | 14.3(12) |
| C10A   | 3086(11) | 6815(9) | 5052(9) | 19.2(16) |
| C12A   | 2217(11) | 6756(10) | 4701(9) | 14.3(12) |
| C5B    | 1902(14) | 5954(12) | 4519(7) | 21.7(15) |
| C6B    | 965(15) | 5822(14) | 4290(9) | 34(2) |
| C7B    | 315(15) | 6494(12) | 4276(9) | 34(2) |
| C8B    | 621(14) | 7271(12) | 4487(8) | 21.7(15) |
| C11B   | 1581(13) | 7409(11) | 4725(7) | 14.3(12) |
| C1B    | 3123(13) | 9138(11) | 5387(7) | 21.7(15) |
| C2B    | 4067(14) | 9240(13) | 5615(9) | 34(2) |
| C3B    | 4701(15) | 8561(11) | 5620(9) | 34(2) |
| C4B    | 4435(12) | 7773(11) | 5414(7) | 21.7(15) |
| C14B   | 3464(11) | 7667(9) | 5179(7) | 14.3(12) |
| C10B   | 3176(13) | 6875(11) | 4966(7) | 19.2(16) |
| C12B   | 2231(13) | 6738(12) | 4740(7) | 14.3(12) |
| C9B    | 1881(12) | 8195(12) | 4942(5) | 19.2(16) |
| C13B   | 2825(11) | 8344(9) | 5173(6) | 14.3(12) |
| N1C    | 5000 | 5000 | 6805(7) | 25(3) |
| C3C    | 5337(16) | 4189(9) | 7049(9) | 31(2) |
| N2C    | 5000 | 5000 | 8175(6) | 17(2) |
| Atom     | x        | y        | z        | U(eq)  |
|----------|----------|----------|----------|--------|
| Ni2      | 2476.7(12) | -490.1(18) | 4932.5(15) | 6.9(3) |
| O20B     | 6577(4)   | 245(5)   | 628(3)   | 14.1(9) |
| O20C     | 2373(4)   | 1340(6)  | 5126(3)  | 13.7(13) |
| C15B     | 3667(4)   | -316(6)  | 5686(3)  | 5.3(13) |
| O16C     | 2345(4)   | 7699(5)  | 6252(4)  | 13.9(9) |
| O19B     | 6583(4)   | 823(5)   | 5156(3)  | 14.1(9) |
| O17B     | 3406(4)   | -755(5)  | 508(13)  | 14.5(9) |
| C15C     | 3366(4)   | -189(5)  | 508(13)  | 14.5(9) |
| O16B     | 2571(4)   | 7614(6)  | 5060(3)  | 13.9(9) |
| C18B     | 6315(4)   | 559(6)   | 5715(3)  | 4.4(13) |
| C18C     | 2505(5)   | 1796(7)  | 5716(4)  | 15.0(16) |
| O19C     | 2665(4)   | 1191(6)  | 6241(4)  | 15.2(13) |
| C8B      | 4212(5)   | 1316(6)  | 668(3)   | 21.2(9) |
| C7B      | 4482(4)   | 2202(6)  | 7130(4)  | 24.8(9) |
| C6B      | 5117(4)   | 2470(7)  | 7097(4)  | 24.8(9) |
| C5B      | 5512(5)   | 1733(7)  | 6693(4)  | 21.2(9) |
| C14B     | 5247(4)   | 953(7)   | 6152(4)  | 21.0(9) |
| C4B      | 5778(5)   | -1316(7) | 4754(4)  | 21.2(9) |
| C3B      | 5538(4)   | -2126(8) | 4252(4)  | 24.8(9) |
| C2B      | 4887(4)   | -2300(8) | 4196(5)  | 24.8(9) |
| C1B      | 4520(5)   | -1756(7) | 4728(4)  | 21.2(9) |
| C11B     | 4724(4)   | -757(7)  | 5171(4)  | 21.0(9) |
| C9B      | 4348(4)   | -112(6)  | 565(4)   | 10.8(10) |
| C13B     | 4605(4)   | 661(7)   | 618(1)   | 21.0(9) |
| C10B     | 5632(4)   | 338(6)   | 566(7)   | 10.8(10) |
| C12B     | 5389(4)   | -566(7)  | 5207(4)  | 21.0(9) |
| N1A      | 2508(3)   | -549(5)  | 387(7)   | 11.7(9) |
| C5A      | 3026(5)   | -1272(9) | 358(1)   | 38.5(11) |
| N2A      | 2458(3)   | -604(5)  | 247(6)   | 11.7(9) |
| C8A      | 2978(3)   | -1341(9) | 273(5)   | 38.5(11) |
| C3A      | 1939(5)   | -1024(10) | 359(5)   | 38.5(11) |
| C6A      | 1913(5)   | -1178(9) | 2760(5)  | 38.5(11) |
| C4A      | 2536(6)   | 688(9)   | 356(6)   | 38.5(11) |
| C7A      | 2574(6)   | 630(9)   | 272(6)   | 38.5(11) |
| C1C      | 1431(4)   | 3144(9)  | 605(4)   | 35.2(11) |
| C2C      | 901(6)    | 3820(10) | 617(9)   | 63.1(18) |
| C3C      | 905(6)    | 510(10)  | 613(5)   | 63.1(18) |
| C4C      | 1397(4)   | 5734(9)  | 583(6)   | 35.2(11) |
| C14C     | 1977(4)   | 5109(6)  | 575(4)   | 13.7(7) |

**Table S4.** Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for Phase_2 squeeze.
| MOFs              | Pore size* |
|------------------|------------|
| Ni(ADC)(TED)0.5  | 0.569      |
| EB@Ni(ADC)(TED)0.5 | 0.510    |
| PX@Ni(ADC)(TED)0.5 | 0.519    |
| MX@Ni(ADC)(TED)0.5 | 0.519    |
| OX@Ni(ADC)(TED)0.5 | 0.514    |

*Calculated by Zeo++ 4

**Table S6.** Selectivity of C8 aromatic isomers for the Ni(ADC)(TED)0.5 packed column.

|        | EB    | PX    | MX    | OX    |
|--------|-------|-------|-------|-------|
| EB     | -     | 1.13  | 1.36  | 4.77  |
| PX     | 0.88  | -     | 1.21  | 1.47  |
| MX     | 0.73  | 0.83  | -     | 1.22  |
| OX     | 0.60  | 0.68  | 0.82  | -     |
Table S7. Values of $\Delta H$ and $\Delta S$ for structural isomers of xylene isomers and ethylbenzene on the Ni(ADC)(TED)$_{0.5}$ GC column.

| Analytes | o-xylene | m-xylene | p-xylene | Ethylbenzene |
|----------|----------|----------|----------|--------------|
| $\Delta H$ (kJ·mol$^{-1}$) | -56.27   | -65.36   | -68.68   | -69.16       |
| $\Delta S$ (J·mol$^{-1}$·K$^{-1}$) | -132.70  | -151.31  | -155.33  | -154.52      |

Table S8. The weight loss temperature of the guest molecules in the framework.

| Aromatics | Temperature($^\circ$C) |
|-----------|-----------------------|
| EB        | 196.34                |
| PX        | 192.71                |
| MX        | 182.10                |
| OX        | 176.59                |

Table S9. The binding energy of C8 aromatic isomers on the framework by the edge-to-face configuration and face-to-face configuration, respectively.

| Adsorption configuration | Adsorbate molecule | Binding Energy (kJ·mol$^{-1}$) |
|--------------------------|--------------------|-------------------------------|
| Edge-to Face configuration| EB                 | -90.70                        |
|                          | PX                 | -85.32                        |
|                          | MX                 | -81.14                        |
|                          | OX                 | -71.80                        |
|                          | EB                 | -82.85                        |
| Face-to Face configuration| PX                 | -84.80                        |
|                          | MX                 | -74.70                        |
|                          | OX                 | -69.14                        |
**Table S10** Molecular sizes of C8 aromatic isomers.

| Aromatics | a (Å) | b (Å) |
|-----------|-------|-------|
| EB        | 6.7   | 9.6   |
| PX        | 6.6   | 9.2   |
| MX        | 7.3   | 8.9   |
| OX        | 7.5   | 7.6   |
**Table S11.** The sum of the minimum distances of various guest-host contracts in guest-included sample.

| Aromatics      | The minimum distances (Å) |   |   |   |
|----------------|---------------------------|---|---|---|
|                | H···H | H···C | C···H | C···C |
| ethylbenzene   | 2.00  | 2.67  | 2.9  | 3.6 |
| p-xylene       | 2.27  | 2.7   | 2.8  | 3.6 |
| m-xylene       | 2.43  | 2.95  | 2.8  | 3.4 |
| o-xylene       | 2.37  | 3.2   | 2.8  | 3.5 |

**Table S12.** Selectivity of ethyltoluene isomers and n-propylbenzene for the Ni(ADC)(TED)0.5 packed column.

|        | N-PB | P-ET | M-ET | O-ET |
|--------|------|------|------|------|
| N-PB   | -    | 1.10 | 1.22 | 6.37 |
| P-ET   | 0.91 | -    | 1.11 | 1.40 |
| M-ET   | 0.82 | 0.90 | -    | 1.26 |
| O-ET   | 0.65 | 0.72 | 0.80 | -    |

**Table S13.** Column resolution for ethyltoluene isomers and n-propylbenzene on the Ni(ADC)(TED)0.5 packed column.

| Rs                               | R_{P-ET/M-ET} | R_{M-ET/O-ET} | R_{N-PB/M-ET} |
|----------------------------------|---------------|---------------|---------------|
| Ni(ADC)(TED)0.5 column           | 1.32          | 0.79          | 0.85          |
Table S14. Comparison of separation of C8 aromatic isomers on the Ni(ADC)(TED)\textsubscript{0.5} and the reported columns.

| Materials                | Elution order    | References |
|--------------------------|------------------|------------|
| co-pillar[4+1]arene     | MX < OX < PX < EB| 5          |
| MOF-5                    | EB < MX ≈ PX < OX| 6          |
| Zr-BTB-C\textsubscript{14} | EB < MX < OX < PX| 7          |
| UiO-66                   | PX < MX < EB < OX| 8          |
| MIL-47                   | EB < PX ≈ MX < OX| 9          |
| CD-MOF\textsuperscript{a} | PX < MX < EB < OX| 10         |
| MIL-101                  | PX < MX < EB < OX| 11         |
| MIL-53(Fe)\textsuperscript{a} | EB < PX < MX < OX| 12         |
| MIL-53(Al)\textsuperscript{a} | EB < PX = MX < OX| 13         |
| Untwisted Zr-BTB-FA     | EB < MX < OX < PX| 14         |
| VF-WAXMS                 | EB < PX < MX < OX| 14         |
| HP-5MS                   | EB < PX = MX < OX| 14         |
| Ni(ADC)(TED)\textsubscript{0.5} | OX < MX < PX < EB| This work |

\textsuperscript{a}: liquid chromatographic separation
Table S15. Summary of separation selectivity of C8 aromatics in various materials.

| Materials          | Separation selectivity | References |
|--------------------|-------------------------|------------|
|                    | EB/PX  | EB/MX  | EB/OX |       |
| Zn$_2$(aip)$_2$(bpy) | 0.33  | 2      | 2      | 15    |
| Zn$_2$(aip)$_2$(bpe) | 0.312 | 0.526  | 0.769  | 15    |
| Co$_2$(dobdc)      | 3.21  | 2.05   | 1.21   | 16    |
| MIL-53(Al)         | 0.32  | 0.26   | 0.092  | 22    |
| MIL-101(Cr)        | NG    | 1.1    | 0.714  | 17    |
| MOF-5              | 0.51  | 0.427  | 0.241  | 6     |
| H/ZSM-5            | 0.148 | NG     | NG     | 18    |
| Li/ZSM-5           | 0.251 | NG     | NG     | 18    |
| Na/ZSM-5           | 0.498 | NG     | NG     | 18    |
| K/ZSM-5            | 0.908 | NG     | NG     | 18    |
| UiO-66             | 1.03  | NG     | 1.77   | 19    |
| MIL-125(Ti)-NH$_2$ | 0.625 | NG     | NG     | 20    |
| Cu(CDC)            | 0.2   | NG     | NG     | 21    |
| MIL-47             | 0.55  | 0.71   | 0.72   | 22    |
| Sql-1-Co-NCS       | 0.14  | 0.26   | 0.017  | 23    |
| [Ce(HTCPB)]        | 0.42  | NG     | NG     | 24    |
| AZO-cage           | 0.15  | 1.11   | 1.83   | 25    |
| [Zn(o-phen)(2,6-NDC):DMF] | 1.5  | 0.017  | 0.09   | 26    |
| Ni(ADC)(TED)$_{0.5}$ | 1.86 | 2.68   | 3.75   | This work |

Note: NG refers to not mentioned.
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