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Supporting Information

Molecular Recognition and Size-Sieving Adsorptive Separation of m-xylene by Trianglimine Crystals

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1. Experimental Section

Materials. All reagents and solvents were purchased from commercial sources and used without further purification. ^{1}H-NMR spectra were performed at 400 MHz with $CDCl_3$ solutions at 5mg/ml concentration with an Avance III Bruker Corporation instrument.

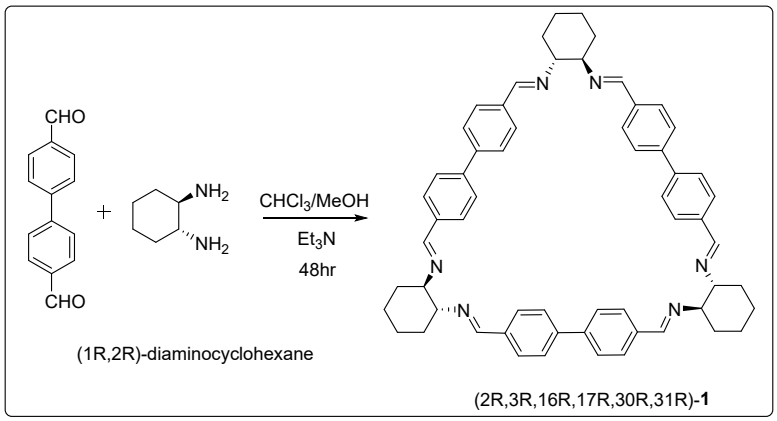
Thermogravimetric Analysis. TGA analysis was carried out using a Q5000 analyzer (TA instruments) with an automated vertical overhead thermobalance. The samples were heated at the rate of 5 °C/min using N_2 as the protective gas.

Powder XRD (PXRD). Powder X-ray diffraction (PXRD) patterns were collected at room temperature on a Bruker D2 Phaser powder diffractometer using Cu Kα radiation (λ = 1.5418 Å, 40 kV and 30 mA). The sample was placed in a zero-background sample holder and normal configuration of the instrument was used.

Gas Chromatography (GC) Analysis. GC measurements were carried out using an Agilent 7890A instrument configured with an FID detector and a Beta DEX 225 column (30 m × 0.25 mm × 0.25 μm). The following GC method was used; the oven was programmed from 50°C, ramped at 10°C min^{-1} increments to 150°C with 15 min hold, the total run time was 25 min; injection temperature 300°C; detection temperature 300°C with hydrogen, air, and make-up flow-rates of 35, 300 and 30 mL min^{-1}, respectively; and the helium (carrier gas) flow-rate 1.2 mL min^{-1} and septum purge flow 3.0 mL min^{-1}. The samples were injected in the split mode (20:1).

Vapor adsorption. Vstar vapor adsorption analyzer from Quantachrome instruments was used for xylenes adsorption. In a typical experiment, 30 mg sample was activated in-situ at 120°C under dynamic vacuum for 8 hours. The temperature was increased to 120°C from room temperature at a rate of 1°C/min. The activated sample was used for the corresponding isotherm measurement. All the adsorption experiments of organic vapors were carried out at 25°C sample temperature.

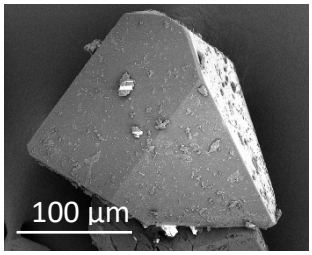
Synthesis of Trianglimine 1. A mixture of (1R,2R)-diaminocyclohexane (0.275 g, 2.38 mmol) and 4,4'-diformylbiphenyl (0.5 g, 2.38 mmol) in $CHCl_3$/methanol (1:10) in the presence of triethylamine (2ml) was stirred at room temperature for 48 h. The white precipitate was isolated and washed with MeOH. Crude product was recrystallized from chloroform/ethyl acetate giving macrocycle **1**.



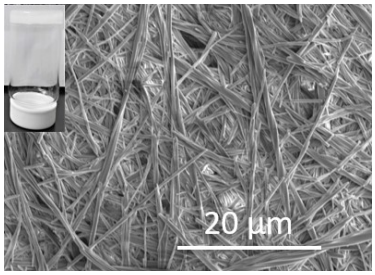
Single Crystal Growth

Crystallization of 1. Macrocycle **1** (10mg) was taken in a vial and dissolved in (2:1) ml of ethyl acetate (EA)/chloroform ($CHCl_3$). Crystals of **1** were obtained by slow diffusion of hexane in a closed vessel with **1** in EA/$CHCl_3$ within 3 days. The apohost (**1A**) was obtained from the activation of **1** (70 °C for 24 h under high vacuum) and it was suitable for SCXRD.

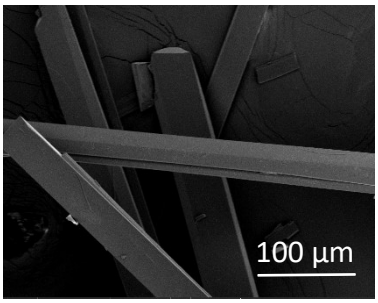
Crystallization of MX@1. 10mg of macrocycle **1** was dissolved in 2 ml of dichloromethane (DCM). To this, 1 ml acetonitrile was added to make system mixed solvent with different polarity. Further, 1 ml m-xylene (MX) was added to that solution and kept for crystallization. After 2-3 days block prism shaped single crystals were found and suitable for single crystal X-ray diffraction. Bulk purities was verified by powder X-ray diffraction (PXRD).



Crystallization of OX@1. 10mg of macrocycle **1** was dissolved in 2 ml of dichloromethane (DCM). To this, 1 ml acetonitrile was added to make system mixed solvent with different polarity. Further, 1 ml o-xylene (OX) was added to that solution and kept for crystallization. After 3-4 days, gelatinous material was formed instead of crystals. We, then, change the conditions where **1** was dissolved in DCM/ethyl acetate (1:1) and further 1ml of OX was added to that solution. Gel was formed from that solution during crystallization.



Crystallization of PX@1. 10mg of macrocycle **1** was dissolved in 2 ml of dichloromethane (DCM). To this, 1 ml acetonitrile or EA was added to make system mixed solvent with different polarity. Further, 1 ml p-xylene (PX) was added to that solution and kept for crystallization. After 2-3 days, needle single crystals were obtained and SCXRD suggests that it was trianglimine crystals with no PX guest. Crystal system- Triclinic, Space group- *P*1, *a* [Å]= 17.0955, *b* [Å]= 5.4229, *c* [Å]= 28.0784, *α* [°]=*γ* [°]= 90, *β* [°]= 91.45, Volume [$Å^3$]= 2602.24.



Crystallization of MX@1 from OX/PX/MX. 10mg (0.0115 mmol) of macrocycle **1** was dissolved in 2 ml of dichloromethane (DCM). To this, 1 ml acetonitrile was added to make system mixed solvent with different polarity. Further, 1 ml each of MX, OX and PX (1:1:1) or 2 ml of C8 aromatic fraction of xylene mixture and ethylbenzene isomer was added to that solution and kept for crystallization. After 3 days block prism shaped single crystals were found and suitable for single crystal X-ray diffraction (SCXRD). Bulk purities were also verified by powder X-ray diffraction (PXRD) which suggested **MX@1** crystals.

Vapor-Phase adsorption measurements

To study the xylene vapor kinetics on activated crystalline materials of **1** (activation was done at 70°C for 24 h under vacuum), samples of 10 mg were exposed to 95% relative pressure of each xylene vapor for different time intervals in different batches. PXRD and NMR were measured at the different time intervals after drying the sample in the fume hood. The amount of uptakes were determined by TGA and selectivity values were determined from the ratio of each isomer peaks using NMR and GC following literature protocols.[1]

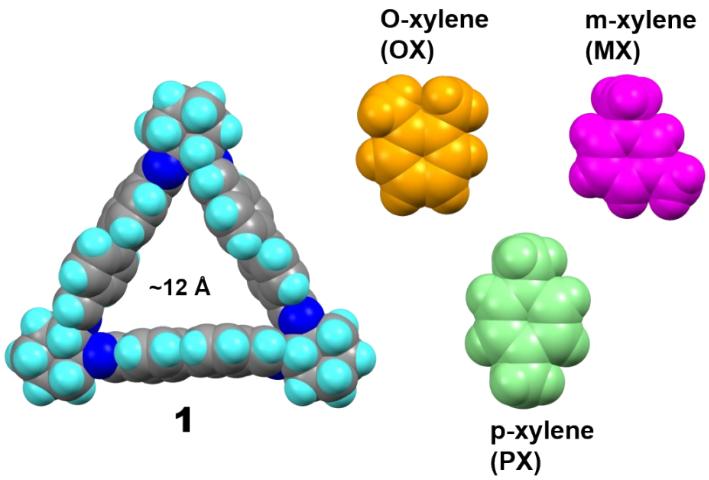


Figure S1. Representation of the host crystalline trianglimine **1** to potential xylene isomers for separations.

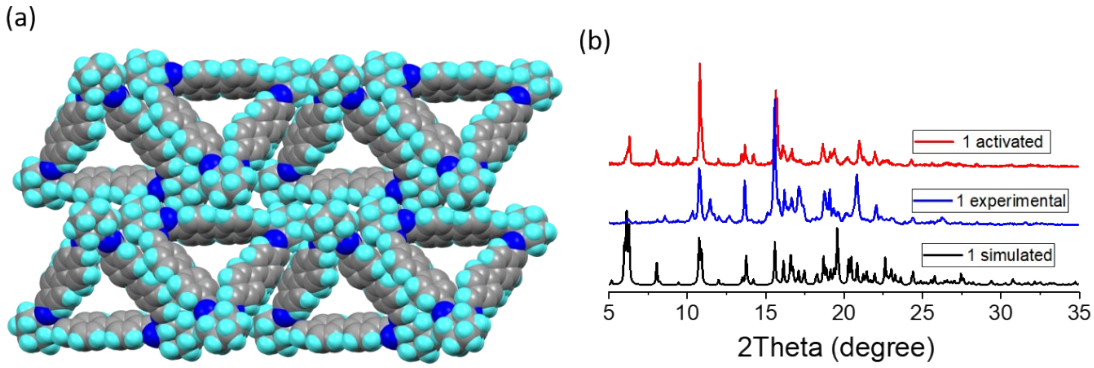


Figure S2. (a) Trianglimine macrocycles (**1A**) are packed in a head to tail fashion that generates layered structure with connecting channels. (b) Comparison of PXRD between experimental and activated (70°C for 24 h under vacuum) materials of **1**.

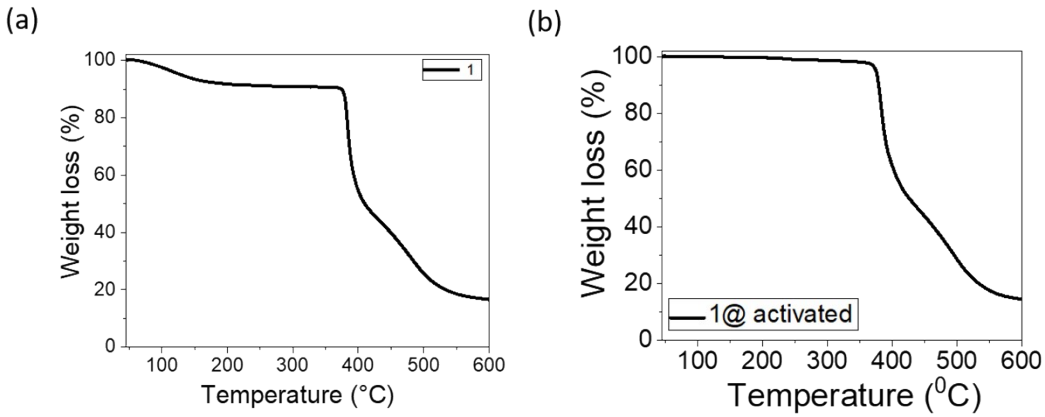
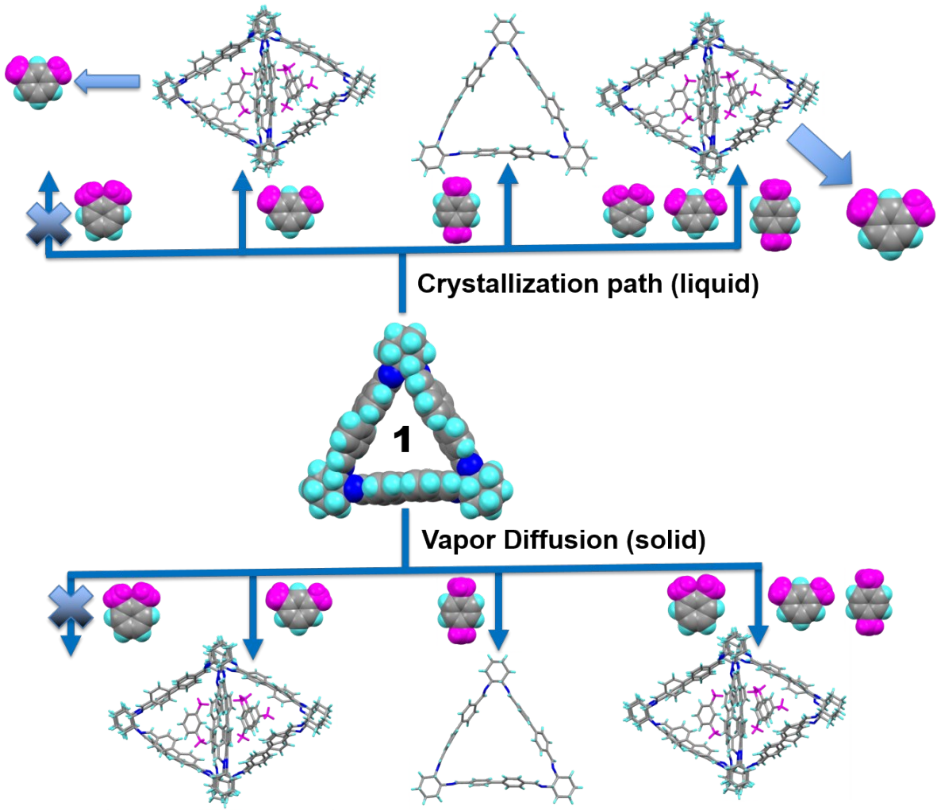


Figure S3. (a) TGA of **1**. (b) TGA of **1A** (activated **1**).



Scheme S1. Schematic presentation of the xylene absorption and selectivity in both liquid and vapor phase by SCXRD.

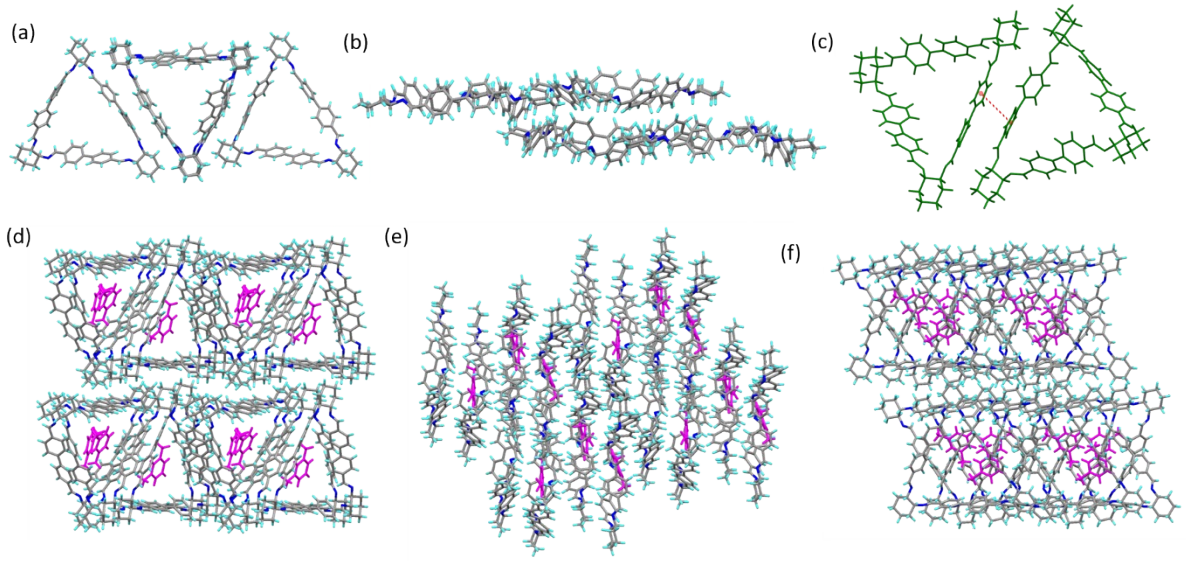


Figure S4. Description of the single crystal structure of **MX@1**: Arrangements of the macrocycles for making the channels in (a) *a*- axis and *b*- axis (b). (c) Two macrocycles are stabilized by π…π interaction in the layer. Packing diagram occupying MX along (d) *a*-axis, (e) *b*-axis, (f) *c*-axis. (Color code: C, grey; N, blue; H, cyan; MX, magenta).

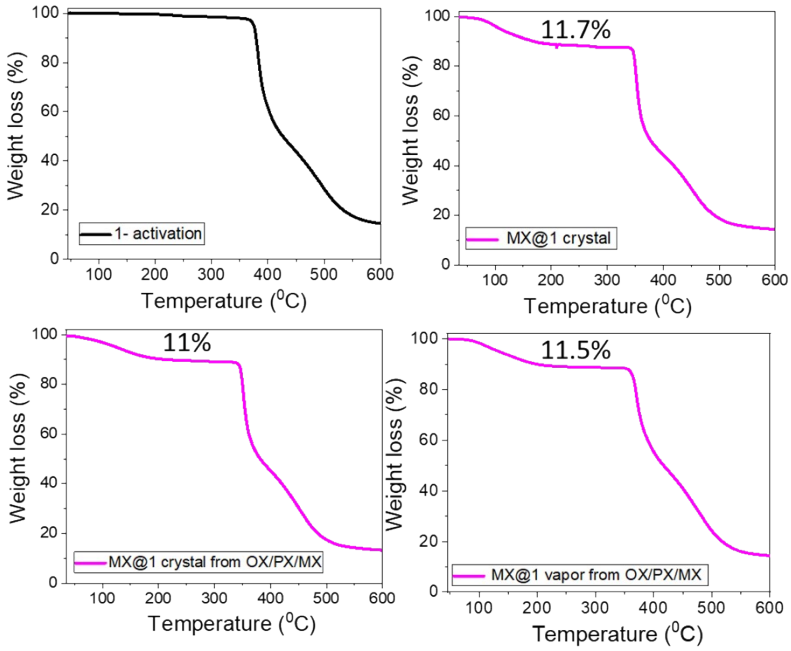


Figure S5. TGA of (a) activated trianglimine crystals **1**, (b) **MX@1** crystals, (c) **MX@1** crystals obtained from OX/MX/PX mixtures, (d) crystalline materials of **MX@1** obtained from OX/MX/PX mixtures vapor.

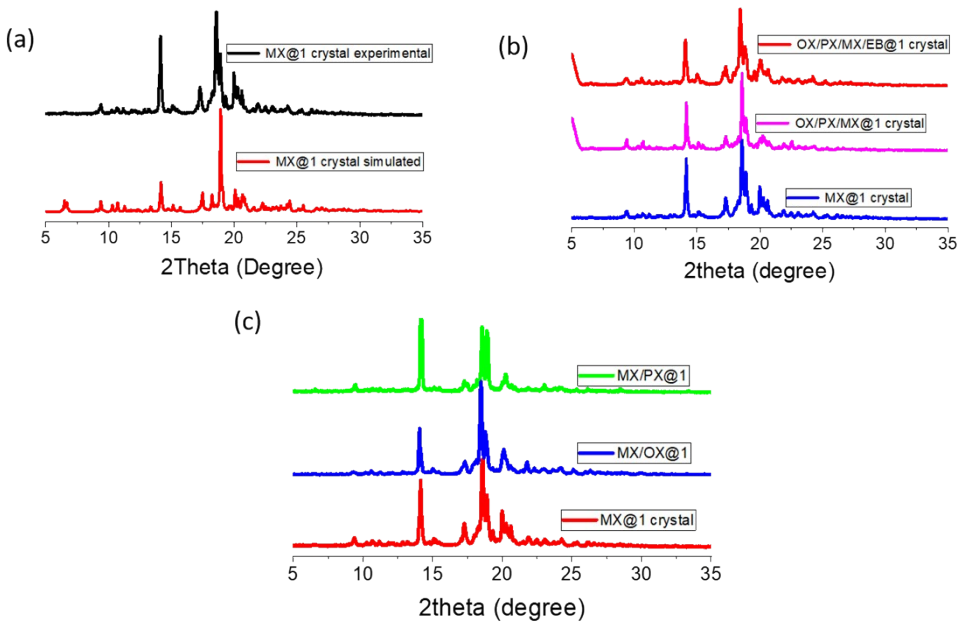


Figure S6. (a) Comparison of experimental and simulated PXRD pattern of **MX@1**. (b) Comparison of PXRD pattern of **MX/PX/MX@1** and **MX/PX/MX/EB@1** with **MX@1** indicates the selectivity towards **MX@1**. (c) Crystal obtained from the OX/PX and MX/PX mixtures matched with the **MX@1** crystal which indicates MX selectivity.

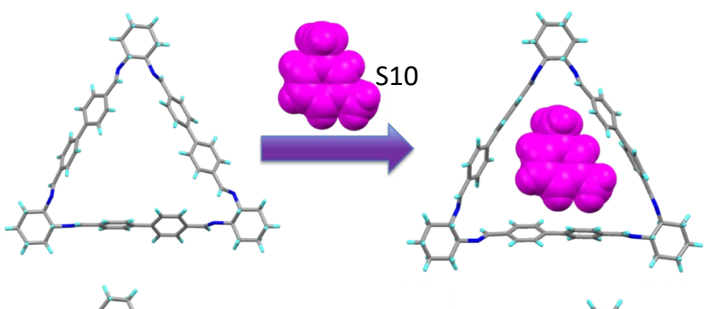


Figure S7. Schematic representation of selectivity of the MX from xylene mixtures by **1**.

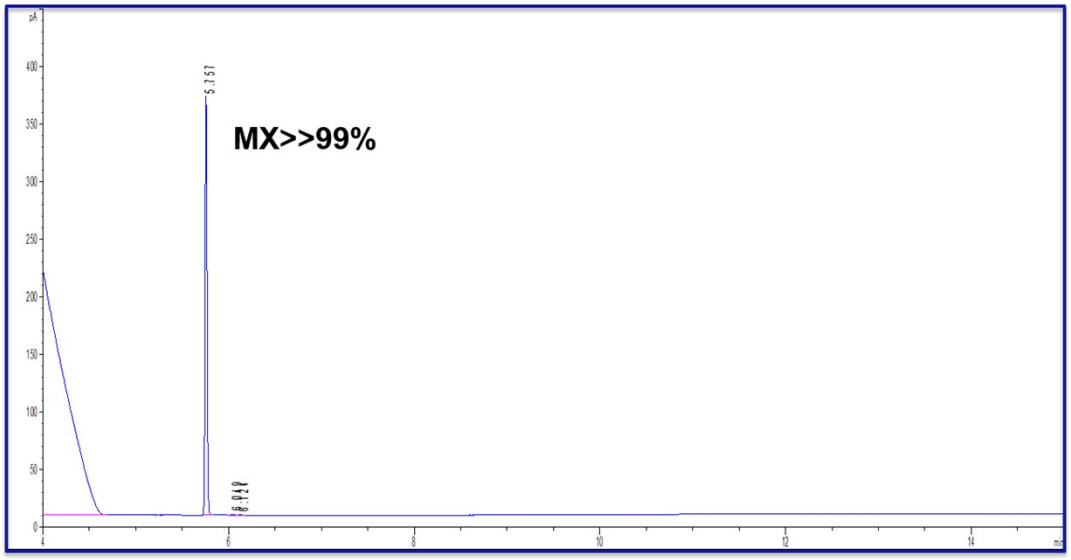


Figure S8. Gas chromatography shows that MX selectivity from the xylene mixtures by **1** in solid-liquid separation.

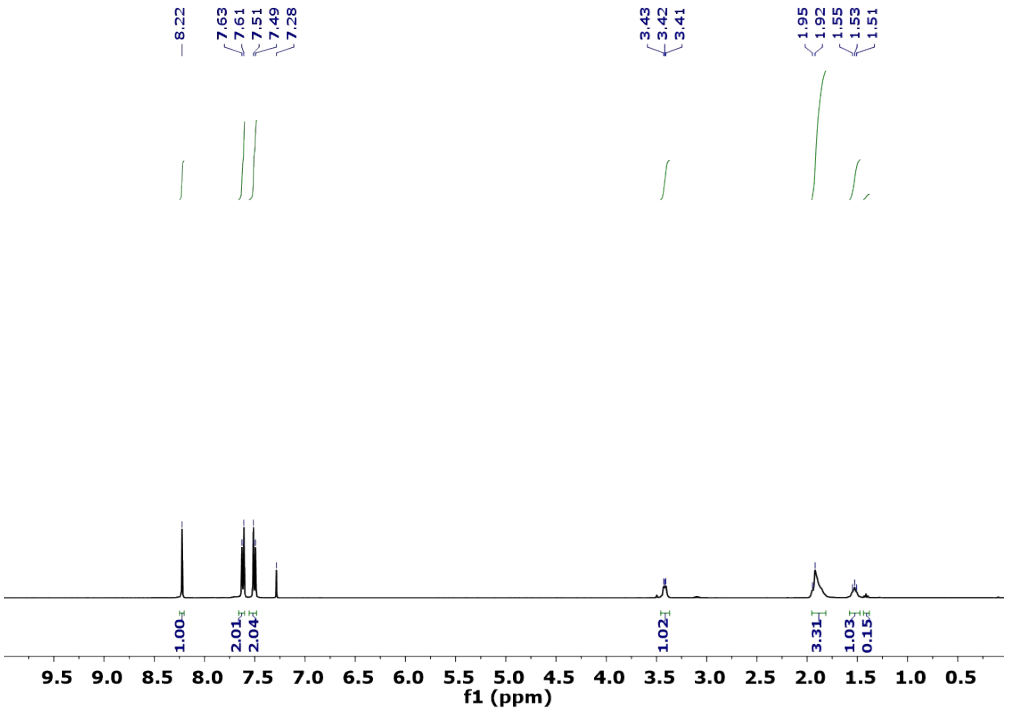


Figure S9. ^{1}H NMR (400 MHz; $CDCl_3$) spectrum trianglimine **1**.

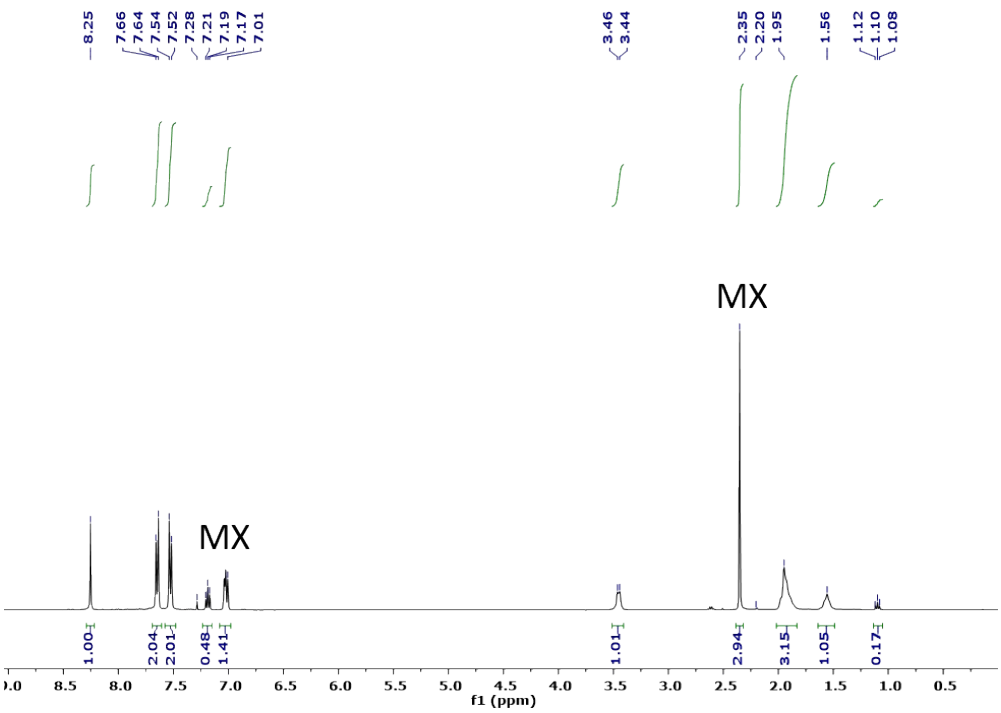


Figure S10. ^{1}H NMR (400 MHz; $CDCl_3$) spectrum of known sample (1:1) host-guest complex of **MX@1**.

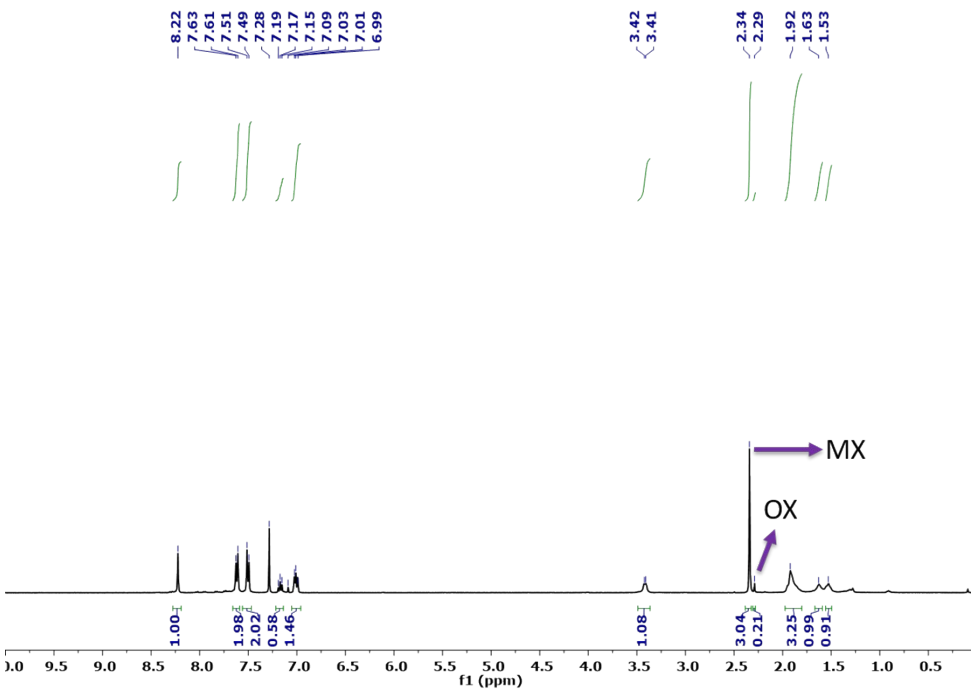


Figure S11. ^{1}H NMR (400 MHz; $CDCl_3$) spectrum of **MX/OX/PX@1** which indicates the selectivity towards MX in vapor.

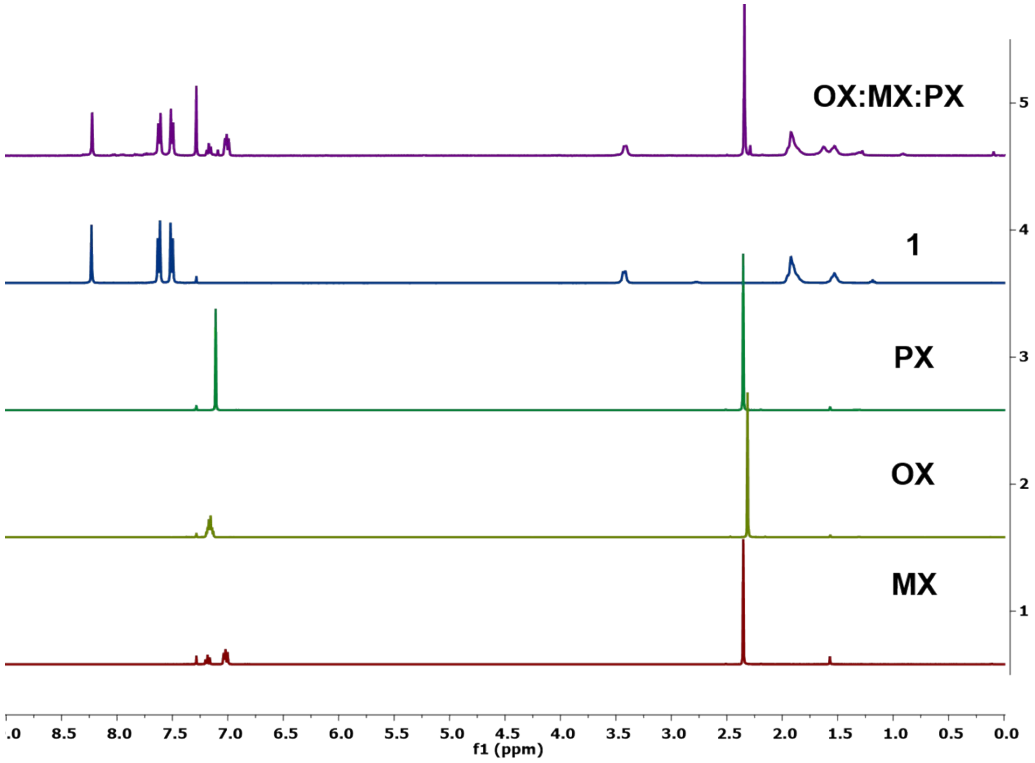


Figure S12. Comparison of ^{1}H NMR spectra (400 MHz, $CDCl_3$, 298K) of individual xylene isomers with separation result in vapor.

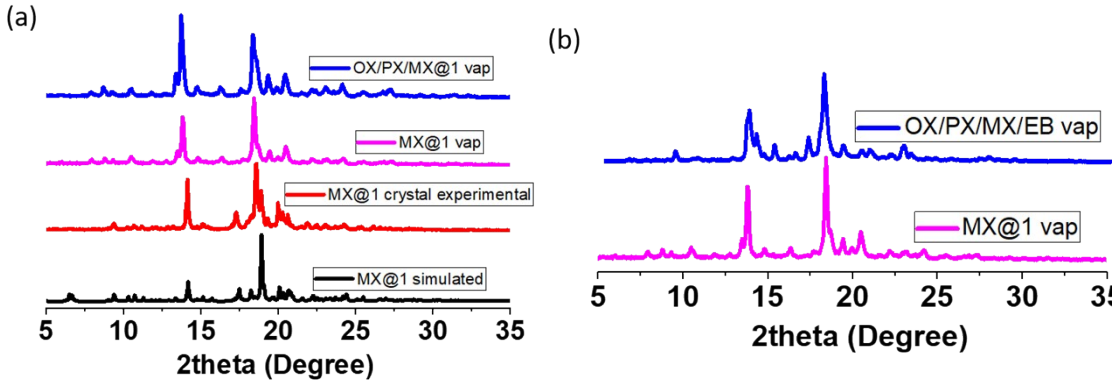


Figure S13. (a) Comparison of experimental and simulated PXRD pattern of the **MX@1** crystal, **MX@1** vapor and **MX@1** selectivity from the mixture of xylenes. (b) PXRD pattern of **MX/PX/MX/EB@1** matched with **MX@1** which indicates the selectivity towards **MX@1**.

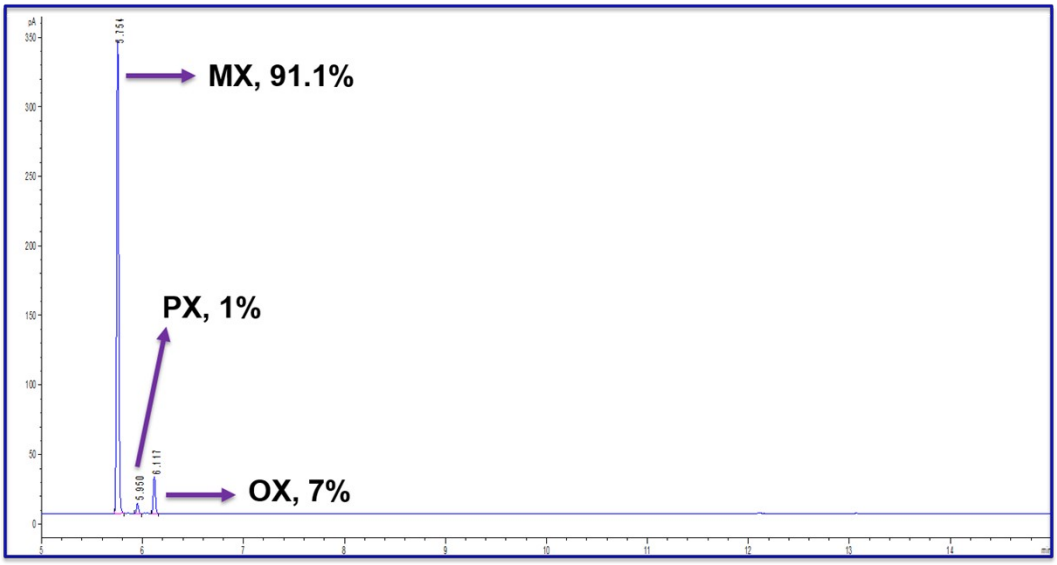


Figure S14. GC analysis of the materials obtained from OX/PX/MX (1:1:1 v/v/v) mixture in the solid-vapor experiment which shows MX selectivity.

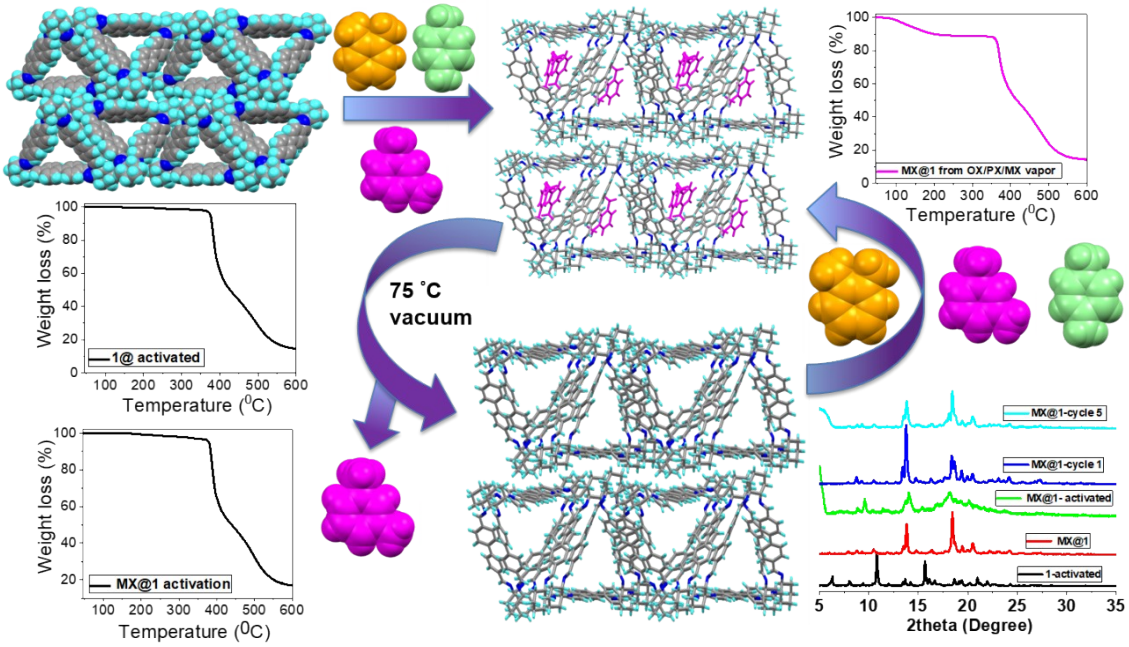


Figure S15. Schematic representation of recyclability and reversibility experiments which shows that it has excellent separation efficiency over multiple cycles in vapor phase.

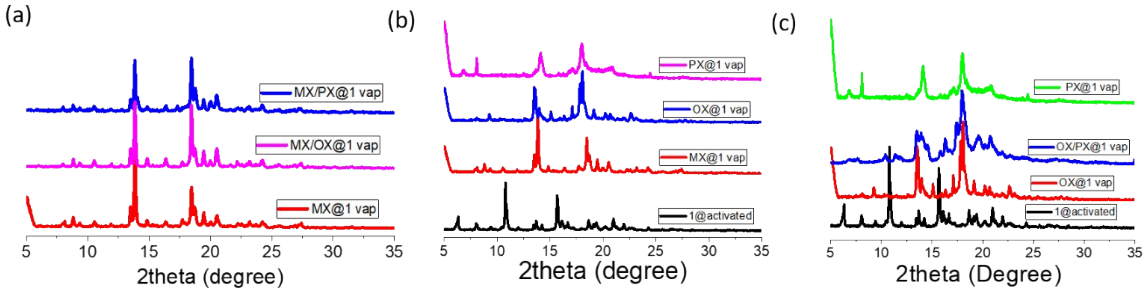


Figure S16. (a) Comparison of PXRD pattern of **MX/OX@1** vapor, **MX/PX@1** vapor and **MX@1** which confirms the MX selectivity from the binary mixture of xylenes. (b) PXRD patterns of individual components of **1A** (activated form), **MX@1**, **OX@1** and **PX@1**. (c) Selectivity of OX from the mixture of OX/PX vapor.

Single Crystal X-ray Diffraction. Single crystals of all the macrocycle trianglimine, were mounted on a Hampton cryoloop with *Paratone*® N oil cryoprotectant. In each case, a suitable crystal of the appropriate size was selected from the mother liquor and immersed in *Paratone*® N oil and then it was mounted on the tip of a glass fiber and cemented using epoxy resin. Single crystal X-ray diffraction (SCXRD) was performed using a Bruker D8-Venture single crystal X-ray diffractometer equipped with a digital camera diffractometer using graphite-monochromated Mo-Kα radiation (0.71073 Å) at 150 K temperature. The linear absorption coefficients, scattering factors for the atoms and the anomalous dispersion corrections were taken from International Tables for X-ray Crystallography. Data integration and reduction were performed using SaintPlus 6.01[2] software. Absorption correction was performed by the multi-scan method implemented in SADABS.[3] Space group was determined using XPREP implemented in APEX-III.[4] Structure was solved using Direct Methods (SHELXS-97)[5] and refined using SHELXL-2014[6] program package (full-matrix least squares on F^2) contained in WinGX.[7] For all the cases non-hydrogen atoms were refined anisotropically. All other hydrogen atoms are geometrically fixed using riding atom model. Attempts to identify the highly disordered solvent molecules failed in some cases. Instead, a new set of F^2 (hkl) values with the contribution from the solvent molecules withdrawn was obtained by the SQUEEZE procedure implemented in PLATON.[8] The crystal data and refinement conditions for all the trianglimines were collected in Table S1 to S4.

Table S1. Crystal data and structure refinements for **1**.

Identification code	**1**
Empirical formula	C_{62} H_{58} N_6
Formula weight	887.14
Temperature (K)	120(2)
Radiation	Mo-Kα
Wave length (λ)	0.71073
Crystal system	Monoclinic
Space group	$P2_1$
a [Å]	17.045(2)
b [Å]	5.436(5)
c [Å]	28.076(2)
α [°]	90

β [°]	91.47(5)
γ [°]	90
Volume [Å^3]	2600.8(3)
Z	2
Density (calculated)[Mg m^{-3}]	1.133
Absorption coefficient [mm^{-1}]	0.067
F(000)	944
Refl. used [$I > 2\sigma(I)$]	9085
Independent reflections	11796
R_{int}	0.0724
Refinement method	full-matrix least squares on F^2
GOF	1.045
Final R indices [$I>2\sigma$(I)]	R_1 = 0.0828; wR_2 = 0.2268
R indices (all data)	R_1 = 0.1057; wR_2 = 0.2440

Table S2. Crystal data and structure refinements for **Activated 1 (1A)**.

Identification code	**Activated 1**
Empirical formula	'C_{61} H_{58} N_6'
Formula weight	875.13
Temperature (K)	150(2)
Radiation	Mo-Kα
Wave length (λ)	0.71073
Crystal system	Monoclinic
Space group	$P2_1$
a [Å]	16.9475(17)
b [Å]	5.4286(5)
c [Å]	28.084(3)
α [°]	90

β [°]	92.011(4)
γ [°]	90
Volume [Å^3]	2582.2(4)
Z	2
Density (calculated)[Mg m^{-3}]	1.126
Absorption coefficient [mm^{-1}]	0.066
F(000)	932
Refl. used [$I > 2\sigma(I)$]	8414
Independent reflections	10608
R_{int}	0.0917
Refinement method	full-matrix least squares on F^2
GOF	1.107
Final R indices [$I>2\sigma$(I)]	R_1 = 0.0702; wR_2 = 0.1849
R indices (all data)	R_1 = 0.0982; wR_2 = 0.2196
CCDC number	2089877

Table S3. Crystal data and structure refinements for **MX@1**.

Identification code	**MX@1**
Empirical formula	'C_{264} H_{270} N_{24}'
Formula weight	3779.02
Temperature (K)	150(2)
Radiation	Mo-Kα
Wave length (λ)	0.71073
Crystal system	Triclinic
Space group	P1
a [Å]	15.711(2)
b [Å]	19.883(3)
c [Å]	20.217(3)

α [°]	80.770(5)
β [°]	68.896(4)
γ [°]	70.524(4)
Volume [Å^3]	5548.9(13)
Z	1
Density (calculated)[Mg m^{-3}]	1.131
Absorption coefficient [mm^{-1}]	0.066
F(000)	2022
Refl. used [$I > 2\sigma(I)$]	40364
Independent reflections	44399
R_{int}	0.0639
Refinement method	full-matrix least squares on F^2
GOF	1.052
Final R indices [$I>2\sigma$(I)]	R_1 = 0.0767; wR_2 = 0.2254
R indices (all data)	R_1 = 0.0856; wR_2 = 0.2394
CCDC number	2089878

One MX solvent molecule is found to be disordered and could not be refined. The final refinement was performed using the PLATON SQUEEZE by removing the solvents.[6,8] The presence of solvent molecules could easily be seen by the residual peaks located in the open channels. Taking into account the number of solvent molecules which were squeezed we determined host to guest ratio as 1:1.

Table S4. Crystal data and structure refinements for **MMX@1** obtained from OX/MX/PX mixture.

Identification code	**MMX@1**
Empirical formula	'C_{264} H_{270} N_{24}'
Formula weight	3779.02

Temperature (K)	120(2)
Radiation	Mo-Kα
Wave length (λ)	0.71073
Crystal system	Triclinic
Space group	*P*1
a [Å]	15.649(8)
b [Å]	19.895(11)
c [Å]	20.237(11)
α [°]	81.409(15)
β [°]	69.174(14)
γ [°]	70.838(14)
Volume [Å^3]	5559(5)
Z	1
Density (calculated)[Mg m^{-3}]	1.129
Absorption coefficient [mm^{-1}]	0.066
F(000)	2022
Refl. used [$I > 2\sigma(I)$]	17554
Independent reflections	43402
R_{int}	0.1431
Refinement method	full-matrix least squares on F^2
GOF	1.051
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0985; wR_2 = 0.2409
R indices (all data)	R_1 = 0.1969; wR_2 = 0.2840
CCDC number	2091064

Computational Details

All the geometries were optimized with Gaussian 16 program packages,[9] using hybrid generalized gradient approximation (h-GGA) DFT functional PBE0.[10] To account for dispersion effects, empirical dispersion-corrected model at GD3 level were applied.[11] The electronic configuration of all atoms were described with the Ahlrichs split-valance polarization basis function Def2-SVP[12] The geometries were optimized without any symmetry constraints. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima or saddle points. For further validation of energetics, single-point calculations were performed on the PBE0-D3/Def2-SVP optimized geometries using the long-range corrected hybrid density functional, ωB97xD, with damped atom−atom dispersion corrections[13] employing a valence triple-ζ-type of basis set Def2-TZVP[14]. The solvent effects [*m*-xylene (ε = 2.3478), *o*-xylene (ε = 2.5454), *p*-xylene (ε = 2.2705)] were evaluated implicitly by a self-consistent reaction field (SCRF) approach using the SMD continuum solvation model.[15] The rigid-rotor harmonic-oscillator approximation was applied for evaluating the thermal and entropic contributions that are needed to derive the enthalpies and Gibbs free energies. The ΔH_{298}^{Sol} value was obtained by augmenting the ΔE_e^{Sol} energy terms at ωB97xD(SMD)/Def2-TZVP with the respective enthalpy corrections at the PBE0-D3/Def2-SVP level in the gas phase. Since the thermal correction to the Gibbs energy of each component depends on its concentration in solution, one can incorporate the concentration terms into calculations. The Gibbs free energy corrections of each component is modified by incorporating its concentration in solution in terms of partial pressure. In the Gaussian program, the concentration can be specified by adjusting the pressure value based on the ideal gas law $p_i = (n_i/V)RT$, where p_i is the partial pressure, R the gas constant (0.082 $L \cdot atm \cdot K^{-1} \cdot mol^{-1}$), T the absolute temperature, n_i the molar quantity, and V the reaction volume. The experimental concentrations of host and guest are approximated by setting the partial pressures as follows:

component	n_i (mol)	V (L)	R ($L \cdot atm \cdot K^{-1} \cdot mol^{-1}$)	T (K)	p_i (atm)
1	1.1×10^{-5}	1.0×10^{-3}	0.082	298.15	0.27
MX, **OX** and **PX**	7.2×10^{-3}				1.76×10^{2}

The Gibbs free energy in the solution phase is a rough approximation, which is not appropriate for association and dissociation processes because there is a significant

degree of denial of the translational degrees of freedom upon moving from the gas to solution phase. As a result, the Sackur–Tetrode equation, which is generally used to calculate the gas-phase translational entropy, cannot be applied directly in the solution phase. Therefore, the solvation entropy (S_{298}^{Sol}) has been estimated as two-thirds of the gas-phase value.[16] Finally, the ΔG_{298}^{Sol} was calculated as: $\Delta G_{298}^{Sol} = \Delta H_{298}^{Sol} - T\Delta S_{298}^{Sol}$. Here, ΔS_{298}^{Sol} represents the solvation entropy, which was estimated as 2/3 of the gas phase value.

Activation strain-distortion/interaction analysis

In this method the bond dissociation energy D_e of a complex AB is divided into the instantaneous interaction energy (ΔE_{int}) and the distortion energy (ΔE_{dis}) according to eq 1.

$$\Delta E\ (= -D_e) = \Delta E_{int} + \Delta E_{dis} \qquad (1)$$

The ΔE_{dis} is the energy that required to promote fragments A and B from their equilibrium geometries in the electronic ground state to the geometries in the corresponding intermediates/complexes, whereas ΔE_{int} is the actual interaction energy between the prepared fragments in the respective intermediates/complexes. The ΔE_{int} can be further divided into different components as explain in the following ETS-NOCV analysis.

Scheme S2. a) Energy values ($\Delta H_{298}^{Sol}/\Delta G_{298}^{Sol}$) are in kJ/mol at ωB97xD(SMD)/Def2-TZVP//PBE0-D3/Def2-SVP level of theory.

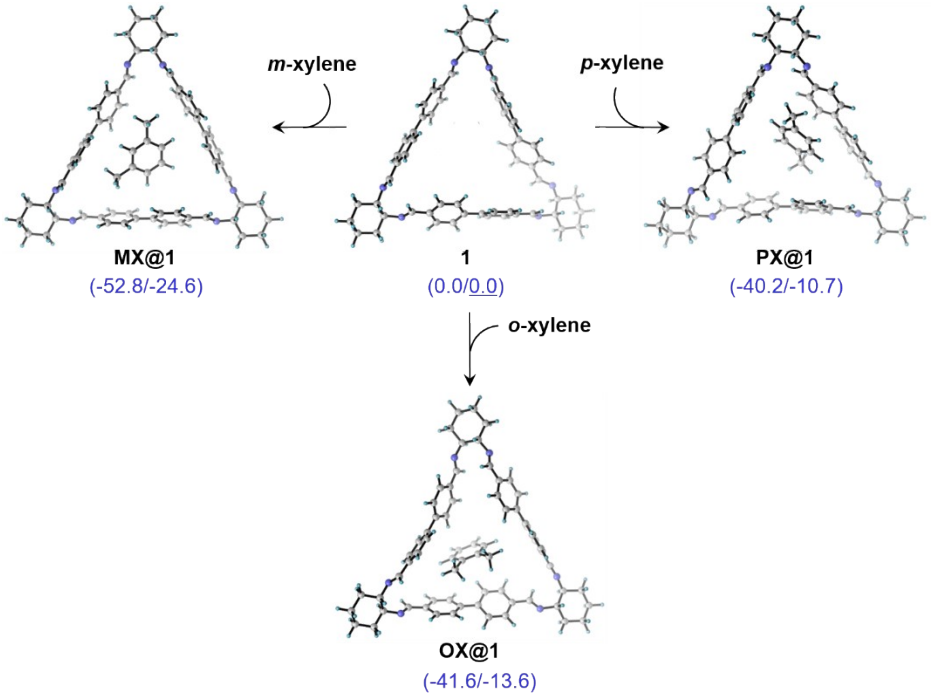


Table S5. Distortion/interaction analysis on **MX@1**, **OX@1** and **PX@1**. The energy terms (in kJ/mol) ΔE_{dis} (distortion energy), ΔE_{int} (interaction energy) and ΔE (ΔE_{dis} + ΔE_{int}) are calculated at the ωB97xD(SMD)/Def2-TZVP level of theory.

	MX@1	**OX@1**	**PX@1**
ΔE_{dis}	4.3(**1**),	21.6(**1**),	20.9(**1**),
	0.1(**MX**)	0.5(**OX**)	0.4(**PX**)
ΔE_{int}	−55.2	−62.4	−59.1
ΔE	−50.8	−40.3	−37.7

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Cartesian coordinates (Å) of the optimized structures of all intermediates and transition states at PBE0-D3/Def2-SVP level of theory. EeS represents the absolute electronic energy in Hartree at M06(SMD)/Def2-TZVP level of theory in EB and ST solvent.

1

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E_e^{Sol}: -2651.15301487 (solvent: *m*-xylene)

E_e^{Sol}: -2651.15399990 (solvent: *o*-xylene)

E_e^{Sol}: -2651.15261348 (solvent: *p*-xylene)

N	12.794862	16.413759	16.311445
N	4.805211	4.884418	19.848494
N	2.222558	15.361760	24.275147
N	13.235562	13.920121	15.003802
N	3.795378	17.614619	23.586627
N	6.951000	4.606036	18.022324
C	13.749864	15.153124	14.477068
H	13.008312	15.665076	13.825654
C	9.451191	10.991331	15.636111
H	8.391280	10.803134	15.449884
C	2.483065	17.767142	24.152112
H	1.699538	17.762638	23.362733
C	10.049342	12.133458	15.114166
H	9.458615	12.827641	14.509352
C	8.034206	6.995699	16.780234
H	7.315301	6.407782	16.205336
C	12.577511	15.946066	17.470945
H	13.336062	15.336276	18.003848
C	3.984883	5.795860	19.523948
H	3.345511	5.706317	18.620519
C	10.183071	10.096761	16.430629
C	14.036228	16.111190	15.655873
H	14.741369	15.580015	16.331863
C	4.917405	3.721599	19.010810
H	4.401766	3.869133	18.036981
C	12.015784	13.626641	14.812992

H	11.344838	14.283862	14.222140
C	9.553637	8.884109	16.994636
C	8.882434	16.542263	19.575055
C	11.397386	12.413933	15.364726
C	9.935983	15.820773	20.155300
H	9.804571	15.378278	21.145469
C	6.406617	3.467451	18.709746
H	6.900540	3.316044	19.694733
C	9.294732	7.296224	18.813269
H	9.553928	6.971555	19.825288
C	11.131196	15.630562	19.469801
H	11.936091	15.051782	19.932201
C	5.167149	17.146083	21.660111
C	9.071943	17.069755	18.284183
H	8.273930	17.657511	17.824049
C	7.606628	16.743241	20.293890
C	2.387022	19.072476	24.939519
H	3.186013	19.076588	25.701140
H	2.599063	19.914413	24.261311
C	8.615170	8.140399	16.255504
H	8.362882	8.455858	15.240132
C	2.181188	16.562700	25.063976
H	2.951842	16.551256	25.865250
C	9.880429	8.440614	18.284607
H	10.584000	9.016627	18.890047
C	3.887486	17.360581	22.346686
H	2.985106	17.284163	21.705220
C	8.368896	6.555762	18.069207
C	6.383703	16.708187	19.607779
H	6.373374	16.498488	18.535734
C	11.312963	16.159746	18.186995
C	15.025617	14.888431	13.677871

H	14.782996	14.222821	12.834045
H	15.723716	14.329559	14.324832
C	10.264258	16.884783	17.602343
H	10.419904	17.300620	16.604468
C	3.501553	9.442280	21.748209
C	7.772937	5.344699	18.646258
H	8.088119	5.107931	19.683662
C	11.537523	10.386433	16.679726
H	12.133019	9.689319	17.274217
C	3.341642	10.704775	22.501993
C	1.022379	19.230848	25.598464
H	0.247752	19.326491	24.816386
H	0.989425	20.164303	26.182932
C	2.581046	13.015839	22.617970
H	2.113132	13.890060	22.160296
C	15.673231	16.178086	13.190766
H	16.600284	15.950437	12.640473
H	14.999854	16.678946	12.471991
C	5.183791	16.903930	20.281649
H	4.239102	16.862342	19.731557
C	7.582242	16.978027	21.681137
H	8.524940	17.031388	22.231248
C	15.956341	17.122162	14.353913
H	16.386918	18.068897	13.990087
H	16.717216	16.667703	15.013819
C	3.821192	7.033933	20.296442
C	2.601418	9.084686	20.732272
H	1.747099	9.728720	20.513870
C	4.719369	7.377368	21.317031
H	5.548002	6.697350	21.525886
C	0.803436	16.724902	25.710365
H	0.615937	15.860855	26.368047

H	0.040322	16.683467	24.913849
C	14.690698	17.398456	15.154964
H	14.902126	18.047741	16.019645
H	13.953875	17.936676	14.533954
C	6.575006	2.202463	17.870487
H	7.647899	2.042269	17.678084
H	6.104013	2.374392	16.887081
C	2.918705	14.383693	24.684734
H	3.480108	14.431496	25.641549
C	2.733776	11.831052	21.915127
H	2.400453	11.782809	20.876202
C	4.307272	2.503955	19.709069
H	3.240516	2.702446	19.901238
H	4.788145	2.393938	20.696570
C	12.135561	11.521746	16.156176
H	13.188916	11.745834	16.338164
C	2.765683	7.907437	20.011551
H	2.053758	7.652692	19.220961
C	5.954562	0.989968	18.553562
H	6.063383	0.098182	17.915674
H	6.506218	0.773977	19.486232
C	4.566014	8.561807	22.020337
H	5.303846	8.827806	22.780372
C	3.797061	10.823011	23.824419
H	4.246615	9.961113	24.321776
C	3.049039	13.127755	23.935070
C	6.385947	17.178427	22.353324
H	6.362892	17.374083	23.427646
C	4.486207	1.234386	18.885170
H	4.061833	0.372378	19.424642
H	3.912593	1.326348	17.945386
C	0.694938	18.033333	26.484158

H	-0.314489	18.133784	26.914446
H	1.396133	18.010984	27.337684
C	3.663598	12.016908	24.523823
H	4.030680	12.086104	25.552036

_m_-xylene (MX)

18

E_e^{Sol}: -310.893602366 (solvent: *m*-xylene)

C	-26.011104	-9.343910	-0.049124
C	-24.907594	-10.086832	-0.482206
H	-23.959786	-9.569733	-0.665317
C	-25.894169	-7.866707	0.199309
H	-25.128395	-7.406939	-0.442586
H	-25.607838	-7.665329	1.245461
H	-26.848035	-7.349747	0.017958
C	-26.192319	-12.116539	-0.447257
H	-26.268901	-13.197111	-0.598406
C	-27.216658	-10.018079	0.177267
H	-28.094251	-9.458051	0.512791
C	-24.975441	-11.469059	-0.688978
C	-27.303935	-11.394245	-0.019141
H	-28.250053	-11.910487	0.163686
C	-23.781071	-12.230204	-1.190625
H	-22.838712	-11.772764	-0.854922
H	-23.760777	-12.247816	-2.293469
H	-23.794961	-13.275449	-0.848442

_o_-xylene (OX)

18

E_e^{Sol}: -310.894236033 (solvent: *o*-xylene)

C	-25.963515	-9.343623	-0.071952
C	-24.826915	-10.084501	-0.459592
C	-25.861000	-7.866082	0.172675
H	-25.516191	-7.329750	-0.726860
H	-25.135593	-7.637146	0.970834
H	-26.829954	-7.439480	0.467107
C	-26.180440	-12.108743	-0.524431
C	-27.184961	-10.006831	0.080310
H	-28.065627	-9.431618	0.380926
C	-24.956943	-11.459120	-0.679616
C	-27.301599	-11.377931	-0.142047
H	-28.268158	-11.872043	-0.016009
H	-24.075202	-12.032760	-0.980136
H	-26.254874	-13.184367	-0.702684
C	-23.499316	-9.405490	-0.632493
H	-23.546578	-8.612571	-1.397177
H	-23.167858	-8.920836	0.300770
H	-22.719928	-10.118356	-0.935717

_p_-xylene (PX)

18

E_e^{Sol}: -310.893310115 (solvent: *p*-xylene)

C	-25.964830	-9.335911	-0.096668
C	-24.867023	-10.126698	-0.454295
H	-23.885146	-9.659138	-0.574642
C	-25.813339	-7.863571	0.159420
C	-26.238476	-12.135308	-0.516376

C	-27.202599	-9.973257	0.045050
H	-28.081433	-9.383476	0.322513
C	-25.000692	-11.497959	-0.658084
C	-27.336268	-11.344531	-0.158741
H	-28.318151	-11.812075	-0.038372
H	-24.121867	-12.087761	-0.935533
C	-26.389935	-13.607652	-0.772458
H	-25.001667	-7.429733	-0.443163
H	-26.739162	-7.315771	-0.070571
H	-25.573448	-7.668602	1.218463
H	-25.464086	-14.155423	-0.542503
H	-27.201571	-14.041519	-0.169845
H	-26.629863	-13.802621	-1.831491

MX@1

144

E_e^{Sol}: -2956.47021617 (solvent: *m*-xylene)

N	-17.416128	-2.392047	-4.833662
N	-8.921695	-2.911933	-12.795166
N	-18.842518	-4.768718	-4.186075
N	-13.734161	-15.190767	-10.624849
N	-8.222869	-5.463371	-13.866156
N	-15.822742	-15.081406	-8.671147
C	-13.211104	-3.285696	-10.604956
H	-14.261127	-3.573207	-10.690877
C	-12.381675	-3.377336	-11.716211
H	-12.793017	-3.710732	-12.673242
C	-16.208466	-2.777187	-4.779563

H	-15.765563	-3.165631	-3.838948
C	-13.861728	-14.407610	-11.614275
H	-14.678277	-14.533076	-12.355963
C	-12.953986	-13.277113	-11.849913
C	-11.020514	-3.065554	-11.621786
C	-10.504846	-2.663997	-10.380646
H	-9.442606	-2.417458	-10.319146
C	-13.129620	-3.188953	-6.911369
H	-12.105312	-3.550094	-6.794156
C	-13.980756	-3.169541	-5.811190
H	-13.613122	-3.499730	-4.835325
C	-14.921780	-2.373660	-8.300723
H	-15.291204	-2.043746	-9.274462
C	-7.292329	-1.822395	-14.234776
H	-6.645102	-1.710070	-13.347635
H	-7.926044	-0.922036	-14.272741
C	-10.167712	-3.152719	-12.813811
H	-10.686563	-3.442275	-13.750672
C	-13.586707	-2.801480	-8.180022
C	-15.311586	-2.756240	-5.942423
C	-13.994008	-17.596375	-10.825117
H	-13.062183	-17.683022	-10.239656
H	-13.694215	-17.556755	-11.884804
C	-15.129953	-16.302175	-8.985596
H	-14.204411	-16.410160	-8.379464
C	-13.040508	-12.535771	-13.033545
H	-13.775056	-12.817148	-13.793620
C	-11.333243	-2.571975	-9.272286

H	-10.921503	-2.232715	-8.318619
C	-17.539148	-9.151124	-6.446618
C	-8.183904	-3.044038	-14.021849
H	-8.864628	-3.153679	-14.894215
C	-15.769005	-2.348876	-7.204205
H	-16.806513	-2.019918	-7.293870
C	-19.133199	-5.337439	-5.282117
H	-19.802520	-4.856699	-6.025812
C	-12.703822	-2.876651	-9.362675
C	-18.226415	-2.485161	-3.650942
H	-17.649767	-2.893432	-2.792071
C	-7.952972	-6.376291	-13.028114
H	-7.054723	-6.322490	-12.377552
C	-5.619097	-3.231787	-15.471279
H	-5.047980	-3.343118	-16.407039
H	-4.874422	-3.166851	-14.657707
C	-8.795358	-7.567080	-12.853106
C	-12.198926	-11.451827	-13.257413
H	-12.268744	-10.906965	-14.201018
C	-12.002745	-12.901390	-10.890152
H	-11.949300	-13.476890	-9.963701
C	-17.663978	-7.314392	-4.855351
H	-17.356822	-6.834722	-3.923599
C	-10.398245	-9.871555	-12.502966
C	-15.198837	-14.182717	-8.027439
H	-14.149174	-14.327655	-7.699963
C	-6.447394	-1.951902	-15.495497
H	-7.108748	-1.963745	-16.380579

H	-5.795182	-1.070977	-15.607659
C	-15.029526	-11.919772	-7.020671
H	-13.967917	-12.108775	-6.837964
C	-17.138993	-8.536555	-5.245505
H	-16.413505	-9.040852	-4.603103
C	-15.804226	-12.897213	-7.656211
C	-10.848244	-8.780460	-13.270748
H	-11.850283	-8.803270	-13.704232
C	-10.060894	-7.654205	-13.450911
H	-10.412298	-6.806983	-14.043464
C	-7.341295	-4.332683	-13.977672
H	-6.657985	-4.258143	-13.104220
C	-19.385107	-3.467025	-3.911622
H	-19.957437	-3.071204	-4.779026
C	-11.177081	-11.809896	-11.107060
H	-10.481170	-11.504833	-10.322756
C	-18.496471	-8.496183	-7.235756
H	-18.808566	-8.939778	-8.184173
C	-18.769316	-1.105996	-3.275292
H	-17.920326	-0.431197	-3.080981
H	-19.300884	-0.694670	-4.150880
C	-15.588425	-10.705932	-6.638684
H	-14.957184	-9.940901	-6.182000
C	-18.604411	-6.654592	-5.660071
C	-14.667352	-16.271069	-10.455636
H	-15.569667	-16.138516	-11.090941
C	-11.254573	-11.059576	-12.296093
C	-19.701227	-1.173598	-2.071849

H	-20.095891	-0.170681	-1.842846
H	-19.128373	-1.492921	-1.182675
C	-6.499415	-4.455775	-15.251288
H	-5.891695	-5.372757	-15.186188
H	-7.184992	-4.594956	-16.105224
C	-16.039941	-17.501203	-8.728535
H	-16.338759	-17.499118	-7.668177
H	-16.966043	-17.360041	-9.312449
C	-17.155838	-12.624535	-7.913323
H	-17.751599	-13.393751	-8.409476
C	-9.128126	-9.778635	-11.913622
H	-8.738418	-10.616291	-11.331538
C	-20.310815	-3.532562	-2.695279
H	-21.136748	-4.227777	-2.915601
H	-19.746339	-3.974080	-1.855732
C	-17.714728	-11.415290	-7.526215
H	-18.777110	-11.231677	-7.704220
C	-20.841479	-2.156529	-2.313070
H	-21.485048	-1.773971	-3.125579
H	-21.482251	-2.234163	-1.420055
C	-16.945318	-10.436004	-6.871627
C	-8.345302	-8.641382	-12.077100
H	-7.359338	-8.590360	-11.606018
C	-15.369259	-18.814979	-9.107453
H	-16.059534	-19.656715	-8.937275
H	-14.500002	-18.987484	-8.447462
C	-14.900652	-18.791211	-10.558053
H	-15.781130	-18.737856	-11.223319

H	-14.374947	-19.725545	-10.812704
C	-19.014867	-7.264046	-6.851188
H	-19.738886	-6.755898	-7.494648
C	-15.236076	-8.149384	-9.180716
H	-16.239757	-8.455025	-8.872627
C	-14.485013	-9.005160	-9.992843
C	-14.740576	-6.918759	-8.735153
C	-12.686737	-7.377376	-9.940368
H	-11.681070	-7.074164	-10.245208
C	-13.199065	-8.600219	-10.368315
H	-12.593473	-9.255343	-10.995750
C	-15.587817	-6.023481	-7.877372
H	-16.144939	-6.596844	-7.122734
H	-16.334803	-5.484576	-8.483774
H	-14.985107	-5.265146	-7.360386
C	-13.448523	-6.543989	-9.123474
H	-13.039445	-5.589805	-8.783592
C	-15.054804	-10.314889	-10.458575
H	-15.736751	-10.166878	-11.313123
H	-15.632923	-10.807324	-9.662411
H	-14.265409	-11.006318	-10.786016

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E_e^{Sol}: -2956.46687387 (solvent: *o*-xylene)

N	-31.830821	-15.125778	2.810536
N	-26.666331	-3.688116	0.926308
N	-32.421304	-12.940926	4.447431

N	-24.342078	-4.000575	-0.924683
N	-22.873822	-16.420604	-4.245666
N	-21.585553	-14.266112	-5.634959
C	-31.129271	-10.510013	3.561476
H	-32.173553	-10.664013	3.281420
C	-25.924759	-2.615957	0.309844
H	-26.438910	-2.421412	-0.651189
C	-21.439431	-18.026167	-5.360408
H	-21.436272	-18.674079	-4.469289
H	-22.334694	-18.304192	-5.942875
C	-29.200840	-14.953897	1.599769
H	-29.244787	-15.125444	2.677581
C	-23.477628	-4.891675	-0.664600
H	-22.790966	-4.796206	0.204856
C	-24.235330	-15.411717	-2.544446
C	-30.499709	-11.494984	4.336360
C	-31.689546	-14.696345	1.625243
H	-32.545172	-14.277510	1.054933
C	-27.995897	-14.984543	0.913354
H	-27.066774	-15.186392	1.451497
C	-28.453994	-10.193865	4.268782
H	-27.409447	-10.073019	4.561661
C	-29.070459	-9.213616	3.477429
C	-24.446007	-2.861492	-0.047719
H	-23.869552	-3.018782	0.892373
C	-26.627793	-15.733494	-2.381392
H	-27.544451	-16.201973	-2.748739
C	-33.119804	-15.018137	3.436703

H	-33.833777	-14.447942	2.802988
C	-30.426220	-9.392114	3.142462
H	-30.923156	-8.657267	2.505005
C	-22.954992	-15.686875	-3.211276
H	-22.062538	-15.204072	-2.763746
C	-24.175980	-10.595290	-3.901504
H	-25.165485	-10.203529	-3.655496
C	-26.230399	-7.060876	2.211974
H	-25.167598	-7.171668	1.976752
C	-28.237886	-5.725823	2.256095
H	-28.726612	-4.766904	2.070471
C	-30.402283	-14.712844	0.917391
C	-31.204730	-12.718207	4.732587
H	-30.591742	-13.468570	5.273593
C	-25.490370	-14.366083	-0.747574
H	-25.515119	-13.714796	0.129904
C	-25.427461	-15.966460	-3.033384
H	-25.374232	-16.600173	-3.921358
C	-28.941731	-6.810914	2.754458
H	-30.001234	-6.696133	2.994751
C	-28.310356	-8.049109	2.979020
C	-22.698402	-13.668487	-5.501004
H	-23.653498	-14.125086	-5.829286
C	-29.157083	-11.316814	4.688556
H	-28.655655	-12.074442	5.298175
C	-24.286773	-14.592784	-1.409570
H	-23.370706	-14.124838	-1.037802
C	-23.349217	-6.138279	-1.426330

C	-27.952329	-14.805936	-0.480520
C	-20.183339	-18.233185	-6.195074
H	-20.111711	-19.285710	-6.513074
H	-19.290367	-18.034118	-5.575283
C	-21.610827	-16.576537	-4.908056
H	-20.758548	-16.285755	-4.256871
C	-26.939504	-8.154259	2.695763
H	-26.428235	-9.112091	2.813112
C	-26.105257	-4.720321	1.404098
H	-25.013398	-4.879016	1.396198
C	-26.677103	-14.949233	-1.214726
C	-23.139334	-8.596373	-2.797819
C	-24.232335	-6.447677	-2.471319
H	-24.998556	-5.714881	-2.733555
C	-23.869695	-1.622196	-0.741889
H	-22.812471	-1.814152	-0.986059
H	-24.394557	-1.493519	-1.704577
C	-21.572818	-15.613107	-6.130484
H	-22.476278	-15.845044	-6.733935
C	-24.014791	-0.369418	0.111996
H	-23.408842	-0.480094	1.029394
H	-23.606457	0.501253	-0.425953
C	-35.038265	-16.303731	4.452036
H	-35.426272	-17.312660	4.665654
H	-35.781897	-15.817670	3.795152
C	-26.868252	-5.836905	1.979341
C	-22.806404	-12.357031	-4.848757
C	-30.359228	-14.489168	-0.463762

H	-31.286526	-14.277507	-1.004155
C	-33.707075	-16.402046	3.715451
H	-33.823774	-16.939671	2.760719
H	-32.976571	-16.976049	4.311394
C	-32.960127	-14.235025	4.757214
H	-32.259884	-14.826162	5.387606
C	-23.031594	-9.886885	-3.507530
C	-22.364697	-7.069619	-1.075994
H	-21.680372	-6.846567	-0.252094
C	-26.068868	-1.357382	1.171469
H	-27.136372	-1.212062	1.397141
H	-25.567097	-1.540422	2.139065
C	-34.301977	-14.123232	5.475211
H	-34.160182	-13.565722	6.414832
H	-34.980443	-13.516448	4.850793
C	-21.658474	-11.654143	-4.454993
H	-20.683937	-12.090857	-4.683694
C	-20.318870	-15.851110	-6.968551
H	-19.447771	-15.544797	-6.363955
H	-20.344298	-15.175952	-7.838901
C	-29.154267	-14.551111	-1.156009
H	-29.137832	-14.385981	-2.236147
C	-24.063941	-11.813309	-4.563763
H	-24.965540	-12.366101	-4.842436
C	-20.173552	-17.302882	-7.402391
H	-21.006672	-17.572833	-8.076374
H	-19.248145	-17.431579	-7.986415
C	-25.470354	-0.130495	0.496435

H	-26.053129	0.103281	-0.412412
H	-25.557959	0.747014	1.157005
C	-22.257929	-8.278622	-1.753483
H	-21.498558	-9.003330	-1.450817
C	-24.128472	-7.656696	-3.142241
H	-24.811258	-7.877312	-3.966261
C	-34.906057	-15.497292	5.740202
H	-34.261287	-16.048380	6.448338
H	-35.886549	-15.392537	6.231783
C	-21.771009	-10.440021	-3.797636
H	-20.868095	-9.890082	-3.521348
C	-26.186813	-10.425331	0.145521
C	-24.812090	-10.380834	0.400202
C	-25.061420	-11.878767	2.271051
H	-24.632917	-12.444205	3.102601
C	-27.013543	-11.222377	0.966214
C	-24.245679	-11.099679	1.452620
C	-26.432827	-11.934791	2.021228
H	-27.079839	-12.541838	2.659560
H	-23.168983	-11.046650	1.633139
H	-24.176099	-9.762573	-0.240104
C	-26.777757	-9.611847	-0.966879
H	-27.505503	-8.881225	-0.576159
H	-26.001973	-9.051365	-1.506628
H	-27.317698	-10.245900	-1.689281
C	-28.489517	-11.298617	0.718969
H	-28.944363	-10.296021	0.701938
H	-28.705236	-11.772300	-0.252927

H	-28.998663	-11.884947	1.495684

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E_e^{Sol}: -2956.46484275 (solvent: *p*-xylene)

N	-31.661775	-15.519701	2.846565
N	-26.682484	-3.925231	0.948757
N	-32.162370	-13.261333	4.491255
N	-24.342815	-4.235088	-0.899491
N	-22.781409	-16.667106	-4.446679
N	-21.395474	-14.471732	-5.591841
C	-30.908424	-10.814634	3.650596
H	-31.931094	-11.011363	3.321515
C	-25.971981	-2.858610	0.287349
H	-26.485626	-2.718419	-0.683010
C	-21.472814	-18.243588	-5.756931
H	-21.536804	-18.997267	-4.955704
H	-22.373035	-18.374827	-6.381898
C	-29.076441	-15.857696	1.623839
H	-29.284889	-16.400650	2.548252
C	-23.477676	-5.113116	-0.598984
H	-22.835475	-5.009106	0.302643
C	-24.019569	-16.105281	-2.466310
C	-30.276355	-11.775577	4.453533
C	-31.357027	-14.851034	1.811808
H	-32.062089	-14.122673	1.360949
C	-27.883711	-16.027973	0.938217
H	-27.134802	-16.725607	1.321152

C	-28.292966	-10.380971	4.495443
H	-27.274479	-10.211276	4.850521
C	-28.910819	-9.423480	3.677200
C	-24.485163	-3.078674	-0.051724
H	-23.911153	-3.194417	0.895754
C	-26.410175	-15.723757	-2.421519
H	-27.364476	-15.656339	-2.949566
C	-32.939582	-15.302317	3.466027
H	-33.595021	-14.658461	2.840054
C	-30.236598	-9.664740	3.269958
H	-30.732692	-8.952235	2.607464
C	-22.783460	-16.382520	-3.210242
H	-21.841987	-16.315155	-2.626365
C	-23.978930	-10.726147	-3.981837
H	-24.967928	-10.283755	-3.840890
C	-26.120615	-7.160144	2.505653
H	-25.043701	-7.223682	2.324956
C	-28.195501	-5.942751	2.367347
H	-28.725462	-5.026478	2.098341
C	-30.065560	-14.996390	1.126209
C	-30.961305	-13.019807	4.822249
H	-30.354918	-13.755539	5.390196
C	-25.156022	-15.697948	-0.362740
H	-25.112551	-15.571824	0.721796
C	-25.249374	-15.989165	-3.130971
H	-25.263890	-16.124730	-4.214649
C	-28.865408	-7.036457	2.892130
H	-29.941554	-6.969202	3.066665

C	-28.183654	-8.226462	3.209552
C	-22.485611	-13.825978	-5.509299
H	-23.425162	-14.212088	-5.953935
C	-28.962007	-11.540079	4.871871
H	-28.457479	-12.277430	5.503133
C	-23.987522	-15.943436	-1.076597
H	-23.032495	-16.014178	-0.547883
C	-23.284819	-6.348162	-1.366049
C	-27.639859	-15.352838	-0.271229
C	-20.214195	-18.439167	-6.592827
H	-20.216875	-19.442942	-7.047290
H	-19.327328	-18.398092	-5.935051
C	-21.531733	-16.850663	-5.128168
H	-20.664308	-16.721933	-4.444428
C	-26.796308	-8.262404	3.013260
H	-26.245069	-9.186054	3.197121
C	-26.085423	-4.884451	1.525600
H	-24.985796	-4.981953	1.562007
C	-26.388666	-15.584309	-1.022079
C	-22.984515	-8.794518	-2.740591
C	-24.008556	-6.597451	-2.541571
H	-24.691528	-5.825646	-2.902463
C	-23.932119	-1.847824	-0.779995
H	-22.868094	-2.021564	-1.007492
H	-24.449856	-1.764978	-1.751513
C	-21.413116	-15.763189	-6.223236
H	-22.305328	-15.887969	-6.874000
C	-24.117533	-0.570401	0.027890

H	-23.521329	-0.633832	0.956101
H	-23.723260	0.290560	-0.535561
C	-34.954032	-16.465931	4.456406
H	-35.416631	-17.448905	4.640282
H	-35.661799	-15.903113	3.821397
C	-26.810199	-5.993385	2.159943
C	-22.598909	-12.542897	-4.804634
C	-29.813830	-14.295024	-0.059119
H	-30.565891	-13.600830	-0.445135
C	-33.635709	-16.639758	3.713632
H	-33.788905	-17.144438	2.746296
H	-32.949456	-17.280265	4.294162
C	-32.728518	-14.543976	4.796477
H	-32.041975	-15.163631	5.414059
C	-22.852764	-10.085721	-3.445183
C	-22.399473	-7.326623	-0.898019
H	-21.835417	-7.147065	0.022013
C	-26.156924	-1.571669	1.098776
H	-27.229939	-1.446302	1.309926
H	-25.659960	-1.705688	2.076849
C	-34.057647	-14.378107	5.532526
H	-33.872871	-13.854567	6.484220
H	-34.700901	-13.713212	4.930549
C	-21.471324	-11.912585	-4.258613
H	-20.499909	-12.395892	-4.383857
C	-20.149479	-15.969719	-7.053559
H	-19.278015	-15.802688	-6.397021
H	-20.105261	-15.191288	-7.831960

C	-28.620820	-14.474040	-0.751822
H	-28.433911	-13.904765	-1.665163
C	-23.851531	-11.936793	-4.653867
H	-24.740514	-12.432089	-5.054839
C	-20.092318	-17.363003	-7.666165
H	-20.917260	-17.479103	-8.392169
H	-19.157989	-17.488577	-8.236460
C	-25.583469	-0.355103	0.385072
H	-26.160226	-0.170911	-0.538865
H	-25.702823	0.543462	1.011486
C	-22.249395	-8.531650	-1.575513
H	-21.579022	-9.297177	-1.178140
C	-23.861194	-7.800849	-3.213339
H	-24.424457	-7.978943	-4.132261
C	-34.750209	-15.714535	5.767453
H	-34.136038	-16.331607	6.447865
H	-35.713677	-15.555539	6.277850
C	-21.597958	-10.704347	-3.591174
H	-20.707485	-10.208966	-3.196158
C	-27.149447	-8.617396	-0.490012
C	-25.878817	-9.188773	-0.337700
H	-25.000356	-8.646976	-0.697835
C	-27.324631	-7.275637	-1.141540
H	-26.467002	-6.615177	-0.949707
H	-28.225413	-6.764726	-0.771897
H	-27.420019	-7.373506	-2.236583
C	-26.812050	-11.145555	0.771623
C	-28.245300	-9.346403	-0.018485

H	-29.250293	-8.924834	-0.115981
C	-25.714928	-10.426689	0.277504
C	-28.081618	-10.586586	0.597559
H	-28.956728	-11.123099	0.975068
C	-26.624612	-12.446812	1.497281
H	-25.926193	-13.108004	0.961605
H	-26.210975	-12.277781	2.506049
H	-27.575119	-12.985154	1.618224
H	-24.707512	-10.841364	0.383672