Supporting Information

Effect of temperature, hydrogen donor, and zeolites on light cycle oil cracking: Thermodynamic, experimental, and DFT analyses

Akshata Vijay Ramteke, Marvi Kaushik, Divesh Bhatia*, K. K. Pant*

Department of Chemical Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi (110016) India

AUTHOR INFORMATION

Corresponding Authors

1. **Dr. Divesh Bhatia**

   Email: dbhatia@chemical.iitd.ac.in

   Phone: +91-11-2659-1456

2. **Prof. K.K. Pant**

   Email: kkpant@chemical.iitd.ac.in

   Phone: +91-11-2659-6172

1.1. Determination of average crystallite size

The Debye-Scherrer equation was used to determine the average crystallite size:

$$t = K\lambda/\beta\cos\theta \quad \text{(S.1)}$$

Here, t is the average thickness of the crystal in the direction normal to the diffracting plane; K is a shape factor, typically close to unity (0.9 is often used as an approximation); λ is the wavelength of the X-ray source; β is the full width at half maximum (FWHM) of the diffraction peak in radians; θ is the Bragg angle. The average crystallite size was calculated by considering at least the five most prominent XRD peaks for each zeolite sample. This method involves identifying the most intense peaks in the XRD pattern, calculating the crystallite size for each peak using the Scherrer equation, and then averaging these sizes. This approach helps mitigate errors associated with individual peak measurements and accounts for any anisotropy in the crystal dimensions. The reliability of this method is supported by numerous studies,[1-4] which used similar techniques to estimate zeolite crystallite sizes and confirmed the effectiveness of using multiple peaks for accurate crystallite size determination. For H-Beta zeolite with a Si/Al ratio of approximately 28, our study measures the crystallite size at 18.9 nm, whereas another study finds it to be 16.7 nm.[2-4] Similarly, for ZSM-5 with a Si/Al ratio close to 30, our study reports a crystallite size of 35.2 nm, whereas another source reports a size of 44.8 nm. [2-4]

1.2. Catalytic activity test

The catalytic activity tests were carried out using the fixed bed micro-activity test (MAT) reactor. The unit has been described comprehensively in our previous works[5,6] and shown in Fig. S1. For both catalytic and thermal cracking tests, quartz wool was used to ensure consistency. By using quartz wool for both thermal and catalytic cracking, it is ensured that any differences observed are only due to the presence of the catalyst (4 g catalyst in the bottom section), while other conditions and any possible interactions between the reactants and the packing material remain the same. The reactor was maintained at 550 °C during the reaction using a split furnace. Nitrogen with high purity (> 99.999 vol. %) was used as the purging gas. The liquid feed was injected into the reactor over a 45 s period using a syringe pump at a mass flow rate of 5.55 g min^{-1}. After the reaction, the vapor products were condensed and collected in a vial, while uncondensed gaseous products were collected using the water displacement method and analysed using a gas chromatography (GC) unit equipped with a thermal conductivity detector (TCD) and flame ionization detector (FID). Liquid species were analysed using gas chromatography by detailed hydrocarbon analysis (GC-DHA) and gas

chromatography by mass spectroscopy (GC-MS). Coke deposited on the catalyst during catalytic cracking was converted to CO_2 during the regeneration step by flowing air at 650 °C for 30 min. The amount of coke produced was measured by the increase in weight of an absorber column containing NaOH pellets that absorbed the CO_2. Experiments were conducted at a weight hourly space velocity (WHSV) of 75 h^{-1}, and a catalyst-to-oil mass ratio of 1.08.

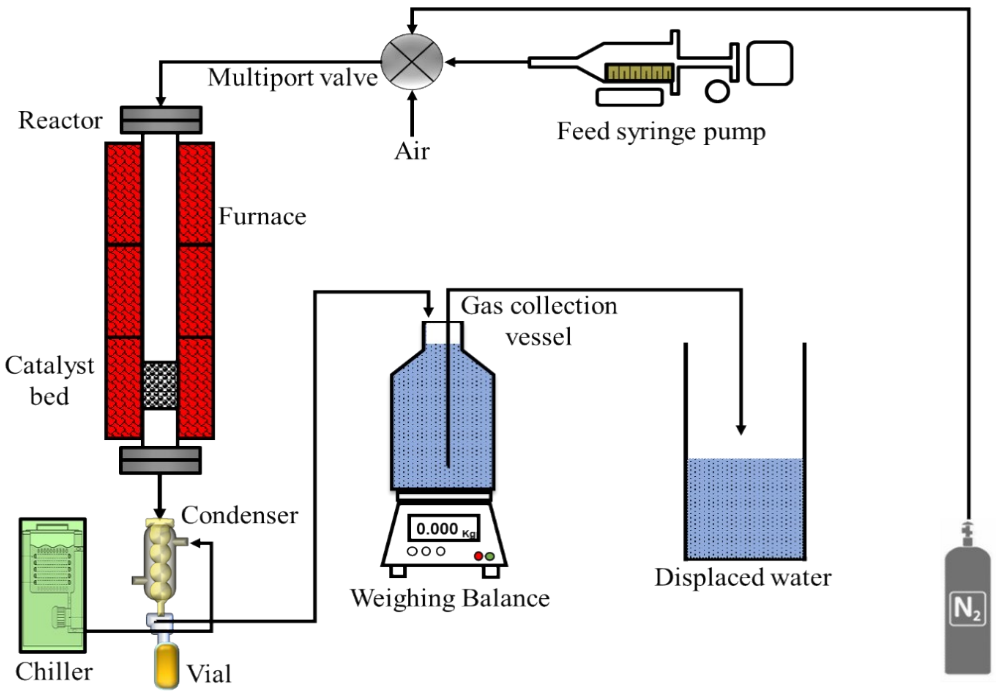


Fig. S1 Schematic of the reactor setup.[5]

The experiments were conducted three times, and the standard deviation is given for each result. For catalytic cracking, the catalyst regeneration process, followed by performance testing, was repeated in a cycle. The catalyst performance was not significantly affected by these cycles of regeneration and reuse, due to which the average performance parameters of all the experimental runs are reported. Equations (S.2), (S.3), and (S.4) were used to calculate the feed conversion, product selectivity, and product yield, respectively. The mass of component j at the reactor inlet and outlet is represents by W^{feed}_{j} and $W^{product}_{j}$, respectively. X_j represents the conversion of component j, while Y_i and S_i represent the yield and selectivity of product i, respectively. The total mass of the feed at the inlet, including n-HD, is denoted as W^{feed}_{T} in Eqs. (S.3) and (S.4). The summation in Eq. (S.3) was performed only for the components that were present in the feed. The conversion of diaromatics was calculated by adding the mass of various diaromatic compounds in the feed and product using Eq. (S.2), which was also used to

calculate the conversion of triaromatics. To determine the selectivity and yield of total monoaromatic hydrocarbons, the selectivity/yield of BTX and 2-ring monoaromatics were added. The light cycle oil (LCO) sample conversion was calculated using simulated distillation analysis (GC-SimDist) according to ASTM D2887. The feed and reaction products were classified based on their boiling point range. Eq. (S.5) was used to calculate the LCO conversion, which was based on the mass of the LCO cut (boiling point > 355 °C) in the feed (W_{LCO}^{feed}) and product ($W_{LCO}^{product}$).

$$X_j = \frac{W_j^{feed} - W_j^{product}}{W_j^{feed}} \times 100 \quad \text{(S.2)}$$

$$S_i = \frac{W_i^{product} - W_i^{feed}}{W_T^{feed} - \sum W_j^{product}} \times 100 \quad \text{(S.3)}$$

$$Y_i = \frac{W_i^{product} - W_i^{feed}}{W_T^{feed}} \times 100 \quad \text{(S.4)}$$

$$X_{LCO} = \frac{W_{LCO}^{feed} - W_{LCO}^{product}}{W_{LCO}^{feed}} \times 100 \quad \text{(S.5)}$$

1.3. LCO properties

The sample is highly aromatic, with aromatics constituting 86.4 wt. % of the LCO feed. The LCO sample is made up of 6.5 wt. % monoaromatics, 65.1 wt. % diaromatics, 12.7 wt. % triaromatics, and 2.1 wt. % polyaromatics (Table S1). The boiling point range of the LCO sample falls between 107 and 370 °C. The low cetane number of 27.9 can be attributed to the presence of polyaromatics, which exhibit poor combustion properties in a compression ignition engine. The CHNS elemental analyzer was used to determine the total sulfur content and nitrogen content, which were found to be 0.54 wt. % and 0.22 wt. %, respectively. The distribution of compounds based on their carbon number is depicted in Fig. S2, revealing that a significant proportion of the total diaromatics is formed by compounds within the C_{10} to C_{13} range, while almost all the triaromatics are contained in compounds within the C_{14} to C_{17} range. Among the diaromatic compounds present in the LCO feed, 1-methylnaphthalene (1MN) and 2-methylnaphthalene (2MN) make up a considerable portion, accounting for 18 wt. % and 15

wt. % of the total diaromatics, respectively. The major triaromatic compounds are anthracene and 9-methylanthracene (9MA), contributing to 37 wt. % and 34 wt. %, respectively, of the total triaromatics. The major tetraaromatic compound observed is benz[a]anthracene (BaA), which contributes 38 wt. % to the total tetraaromatics. Therefore, 1MN, 9MA, and BaA were selected as the representative diaromatic, triaromatic, and tetraaromatic compounds, respectively, for investigating the conversion of higher aromatics into monoaromatics.[5,6]

Table S1 Physicochemical characteristics and composition of the LCO sample.

Density, g/cm^3 (ASTM D 4052)	0.92
Cetane number (ASTM D 976)	27.9
Simulated distillation	
Simulated TBP (D 2887), wt. %	T (°C)
IBP	107
5	194
10	223
30	258
50	277
90	340
95	355
FBP	370
Elemental analysis (wt. %)	
C	82.8
H	11.6
S	0.54
N	0.22
Composition (wt. %)	
n- and i- paraffins	11.2
Naphthenes	2.4
Aromatics	86.4
Monoaromatics	6.5

Diaromatics	65.1
Triaromatics	12.7
Polyaromatics	2.1

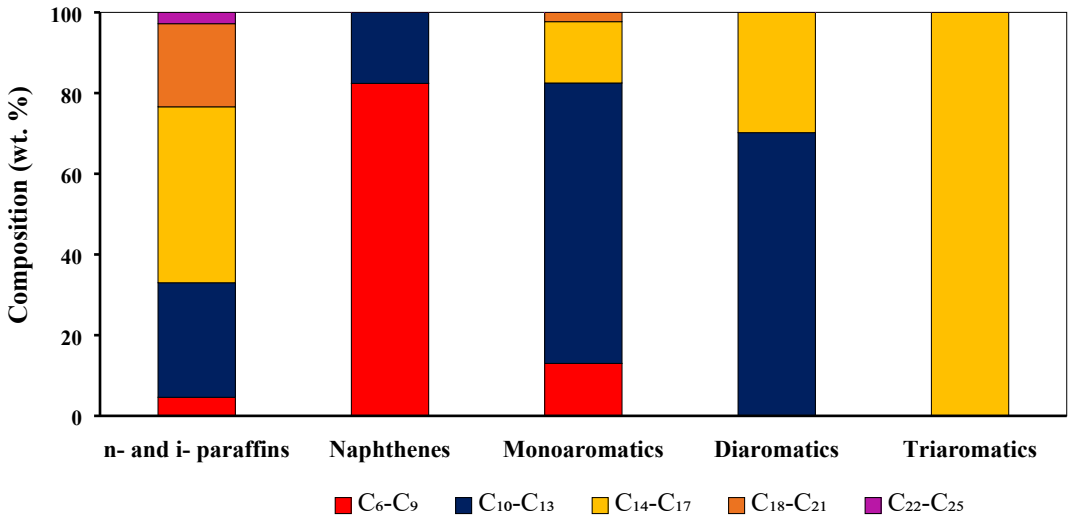


Fig. S2 LCO sample composition based on the number of carbon atoms per molecule.

Table S2 Equilibrium fraction of various diaromatics in the product for cracking of 9MA.

Compound	**wt. %**
Naphthalene	37.8
2-methylnaphthalene	18.9
1-methylnaphthalene	17.5
2,6 di-methylnaphthalene	6.3
4-methylnaphthalene	5.2
2,3 di-methylnaphthalene	5
2-ethylnaphthalene	4.8
1,3 di-methylnaphthalene	4.5

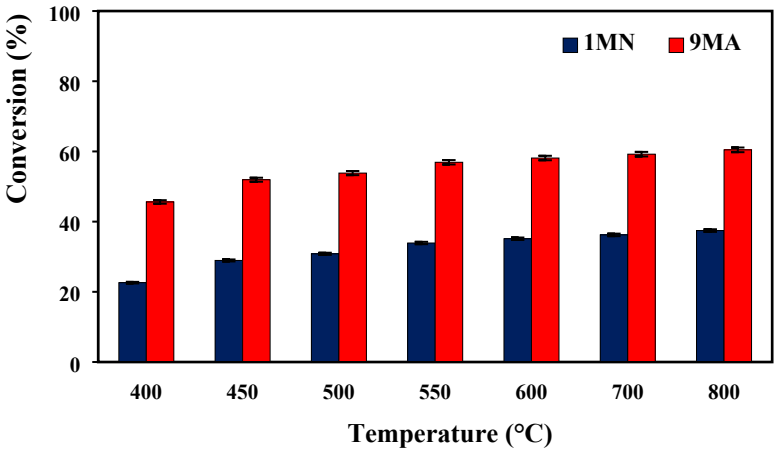


Fig. S3 Temperature effect on individual conversions of 1MN and 9MA (Feed mixture: 50 wt. % 1MN + 50 wt. % 9MA)

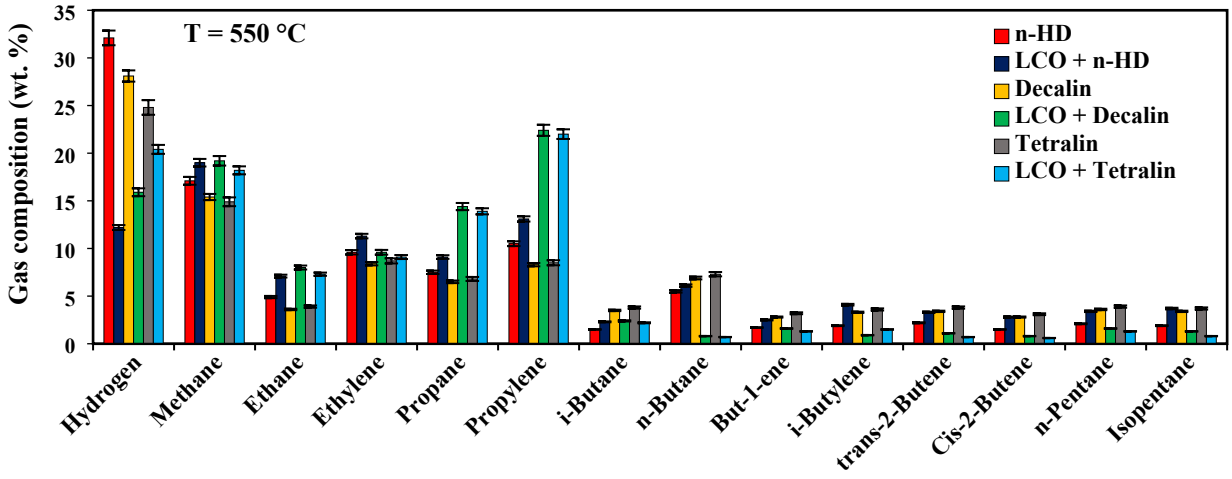
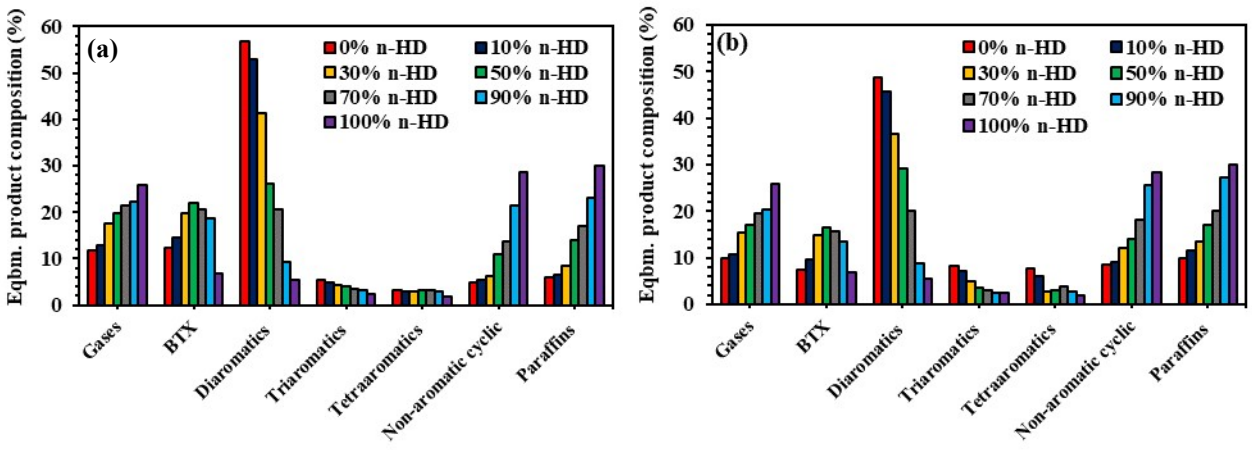


Fig. S4 Composition of the gaseous product for cracking of hydrogen donors and LCO cracking in co-presence of hydrogen donors.



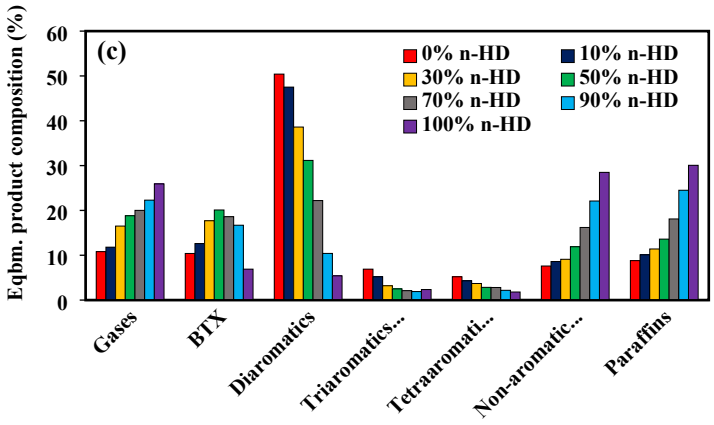


Fig. S5 Equilibrium product composition for cracking of (a) 1MN, (b) 9MA, and (c) 1MN + 9MA with varying n-HD concentrations (T = 550 °C).

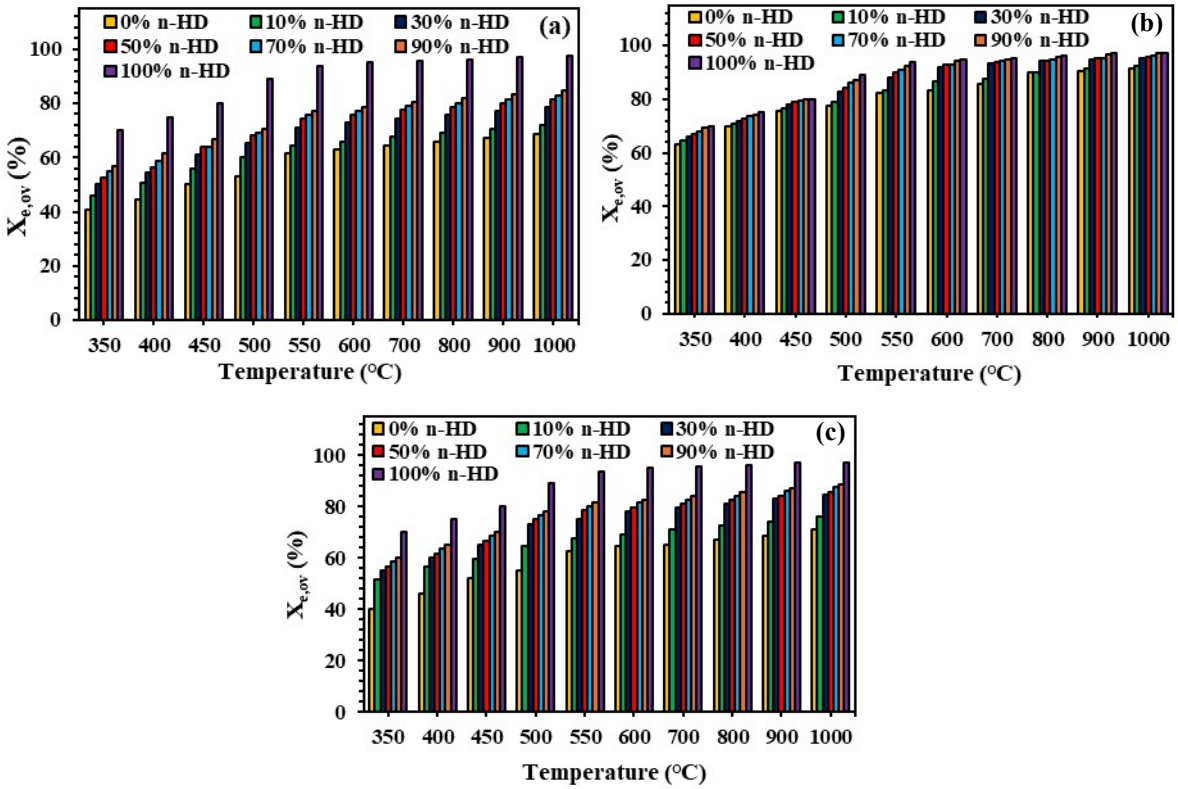


Fig. S6 Effect of temperature on overall equilibrium conversion of feed containing varying proportions of n-HD and (a) 1MN, (b) 9MA, and (c) 1MN + 9MA.

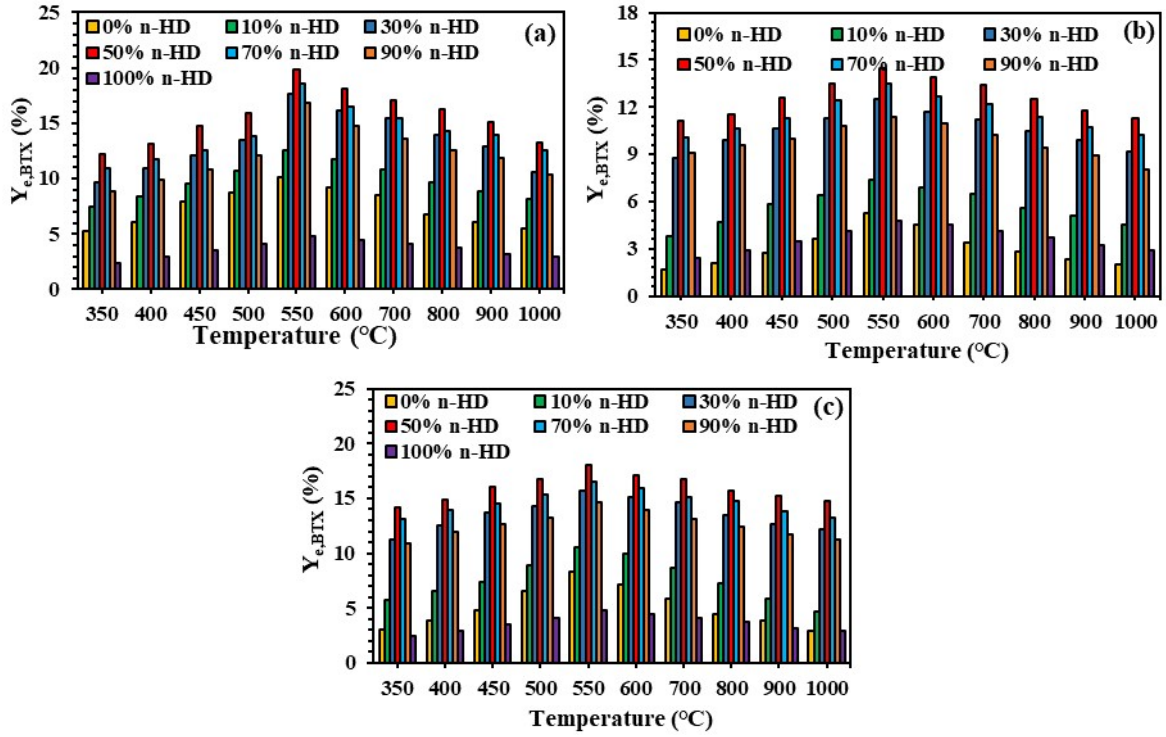


Fig. S7 Effect of different hydrogen donor percentages and temperature on equilibrium BTX yield during cracking of (a) 1MN, (b) 9MA, and (c) 1MN + 9MA.

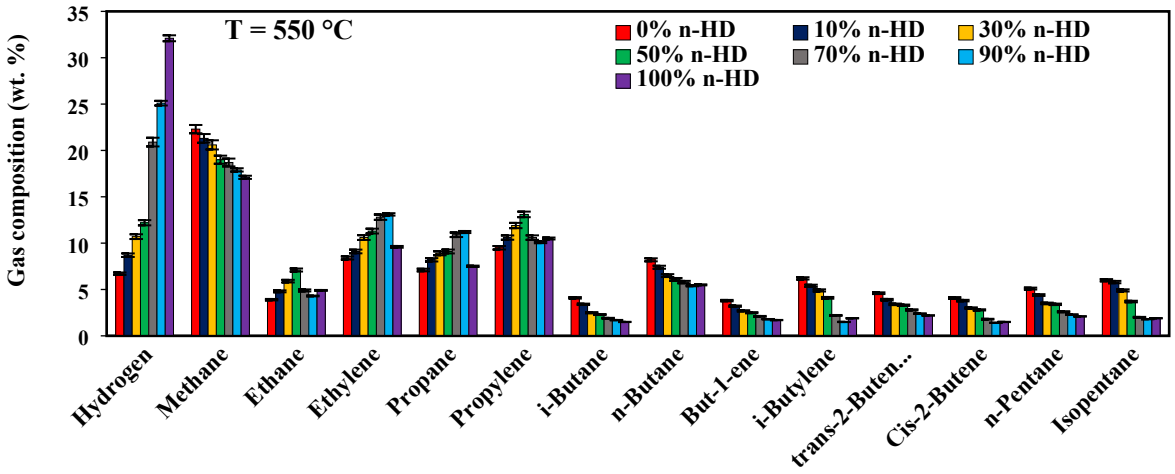


Fig. S8 Composition of the gaseous product during LCO cracking for varying n-HD concentrations.

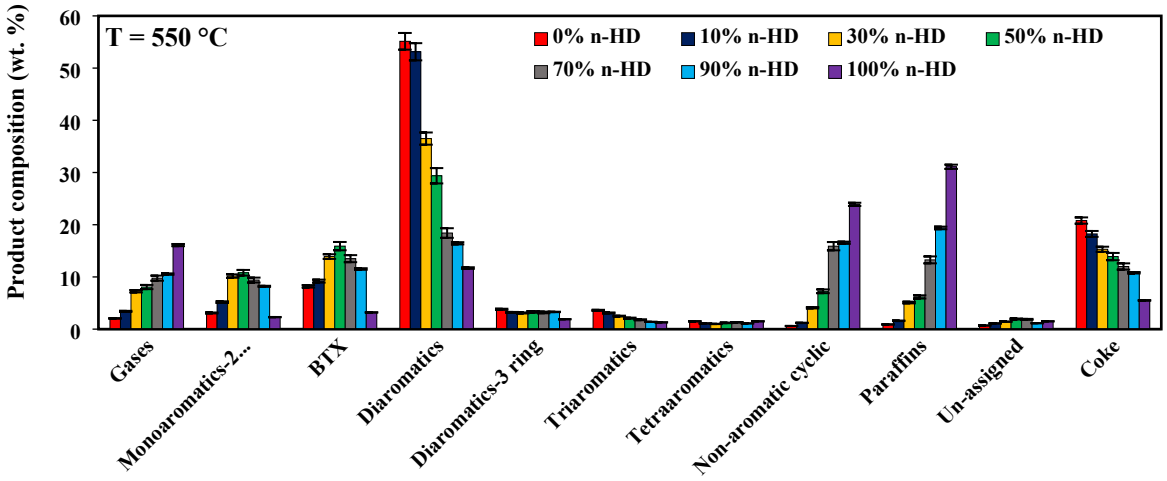


Fig. S9 Product distribution for 1MN cracking for varying n-HD concentrations.

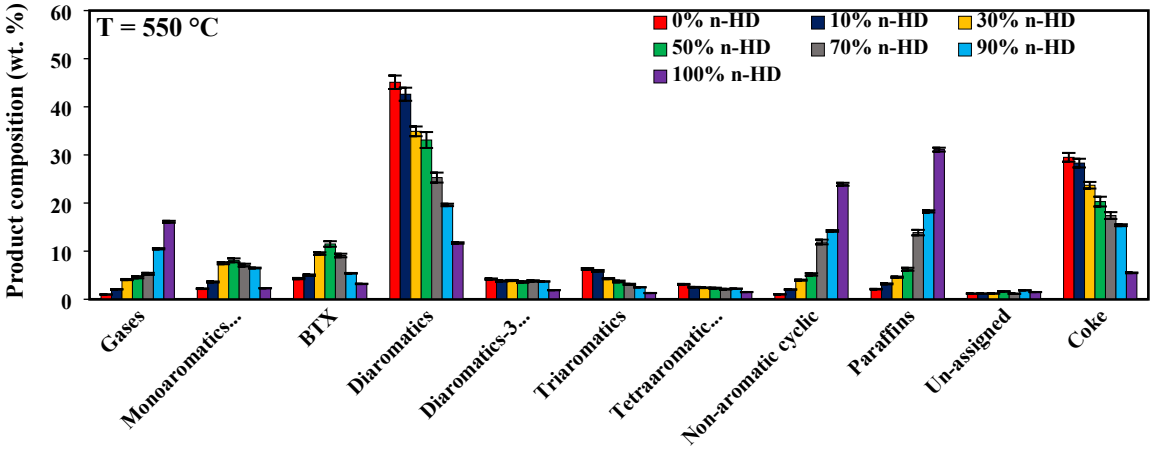


Fig. S10 Product distribution for 9MA cracking for varying n-HD concentrations.

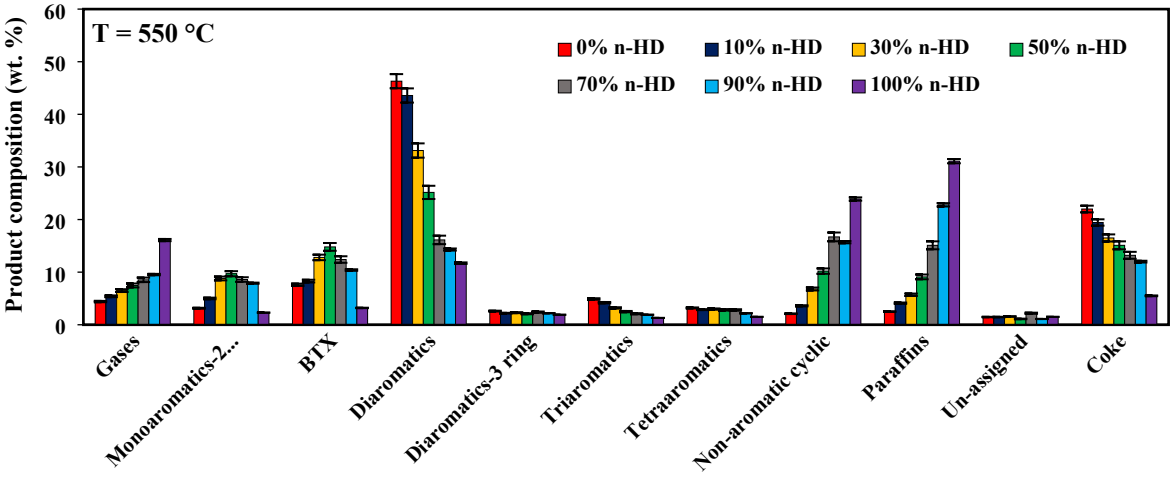


Fig. S11 Product distribution for 1MN + 9MA cracking for varying n-HD concentrations.

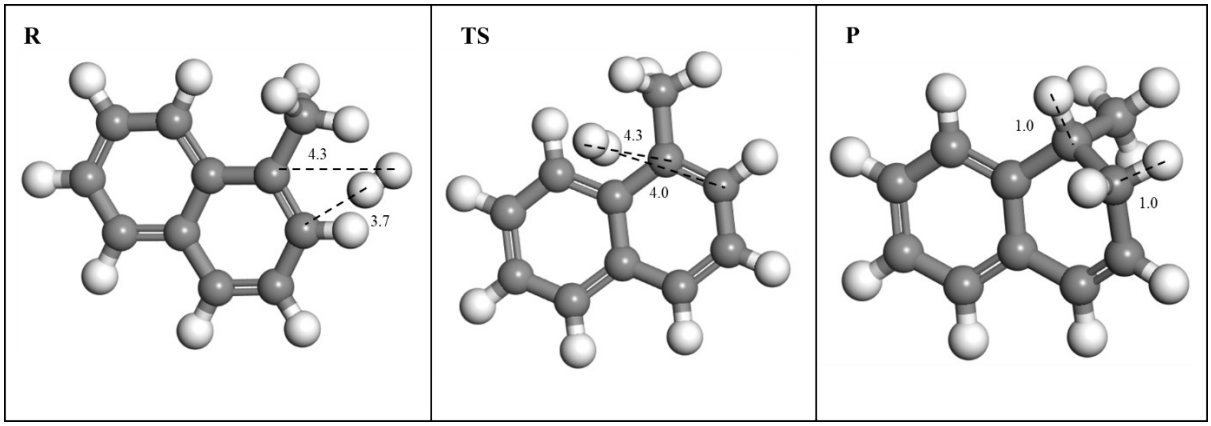


Fig. S12. Optimized structures of reactant (R), product (P), and transition state (TS) for the interaction of H_2 with the closest C-atom of 1MN. Bond distances are in Å.

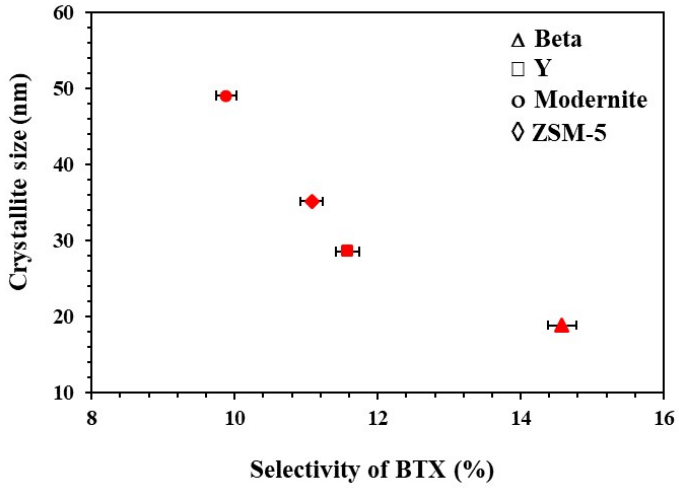


Fig. S13 Correlation between selectivity of BTX and crystallite size.

Table S3 Fraction of BTEX compounds in the product for LCO cracking at 550 °C over various zeolites (B - benzene, T - toluene, X - xylene, EB - ethyl benzene).

Catalyst	**B**	**T**	**X**	**EB**
		(wt. %)		
Mordenite	1.4 ± 0.6	3.2 ± 0.8	4.2 ± 1.0	1.1 ± 0.6
ZSM-5	1.8 ± 0.4	3.8 ± 1.1	5.0 ± 0.9	1.3 ± 0.8
Y	2.1 ± 0.5	4.4 ± 1.0	5.6 ± 1.2	1.7 ± 0.7
Beta	2.3 ± 0.9	4.7 ± 1.2	6.1 ± 1.1	1.9 ± 0.5

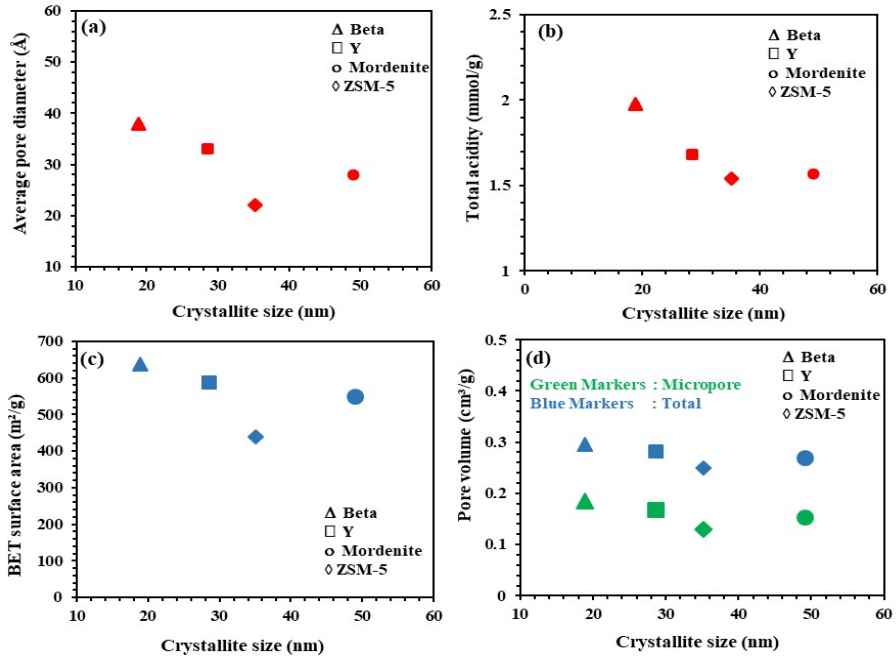


Fig. S14 Correlation between crystallite size and (a) average pore diameter, (b) total acidity, (c) BET surface area, (d) total/micro pore volume.

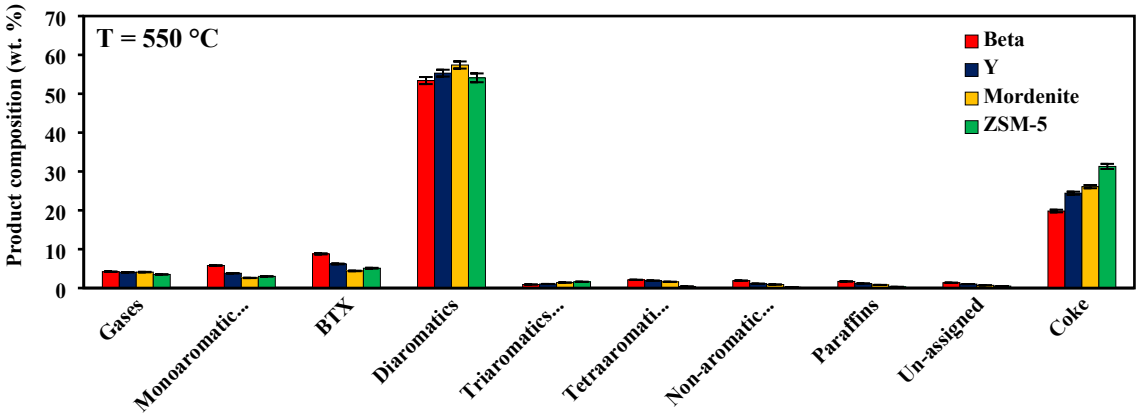


Fig. S15 Product distribution over various zeolites for cracking of LCO.

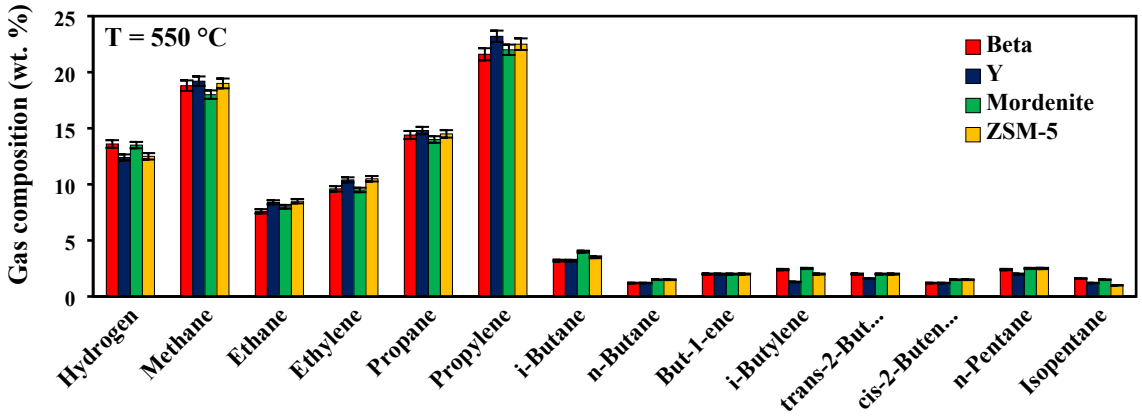


Fig. S16 Composition of the gaseous product for LCO cracking over various zeolites.

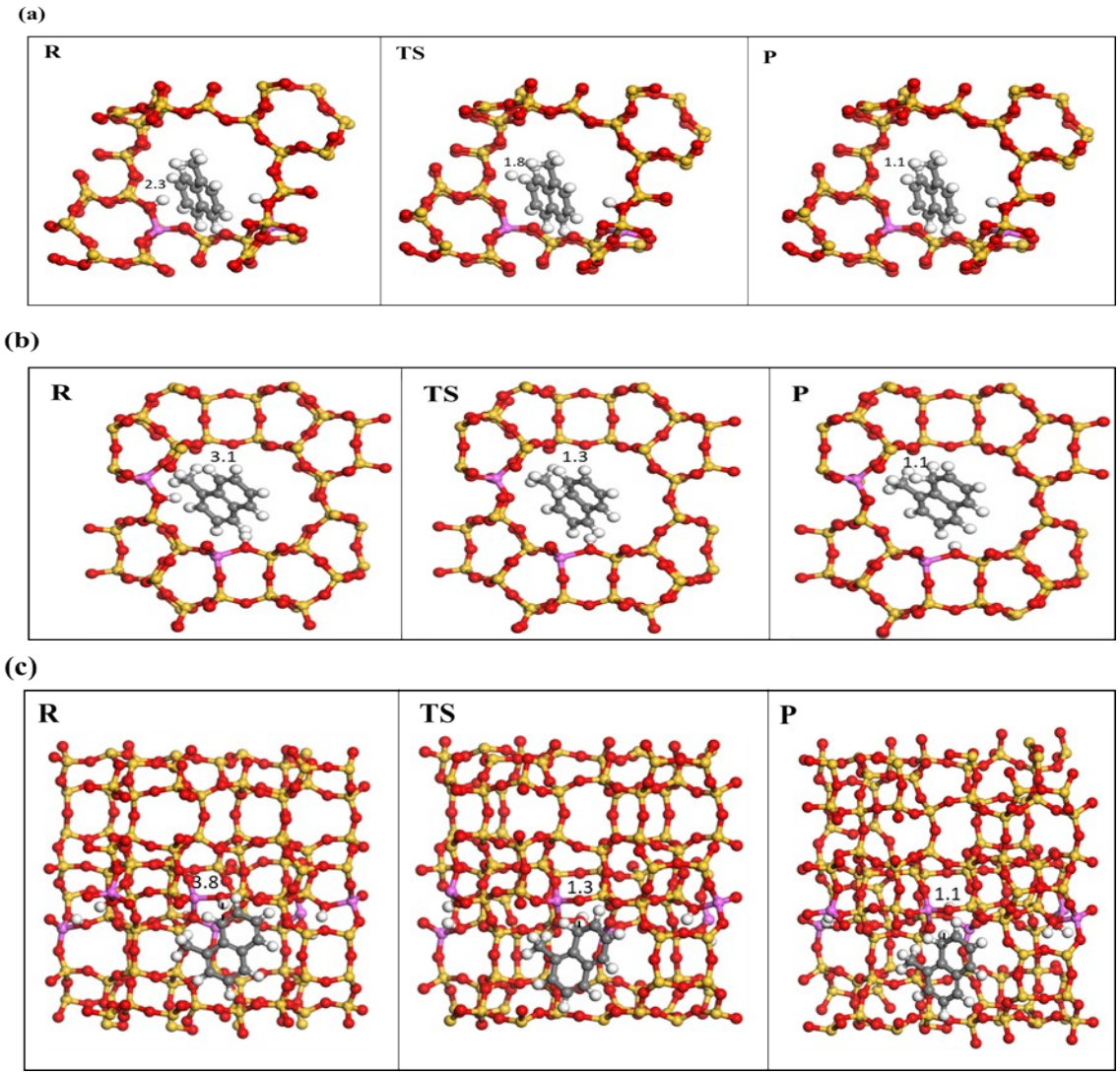


Fig. S17 Optimized structures of reactant (R), product (P), and transition state (TS) for the interaction of BAS with the closest C-atom of 1-MN in (a) Y, (b) Mordenite, and (c) ZSM-5. All bond distances are in Å.

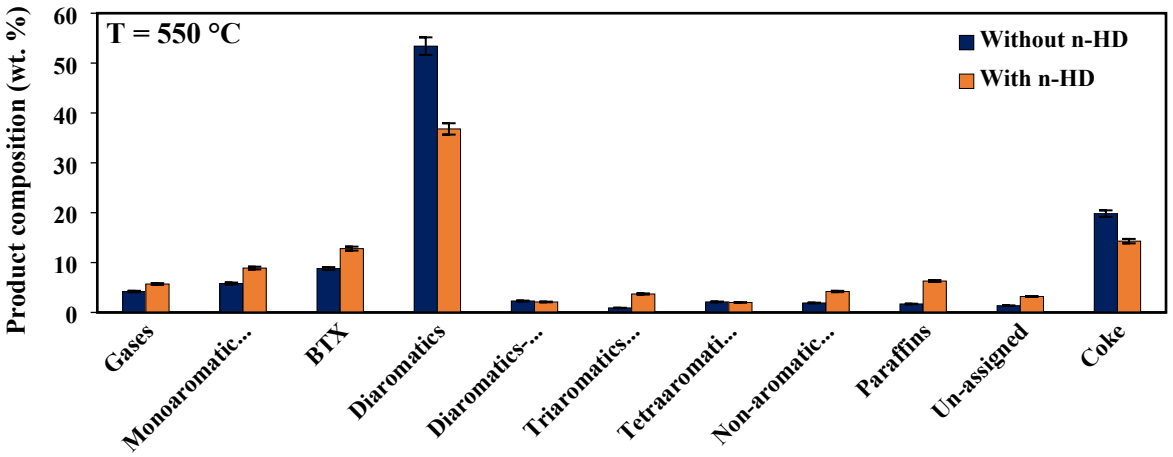


Fig. S18 Product distribution for LCO cracking over Beta zeolite in the absence and presence of 30 wt. % n-HD.

Table S4 H-atoms for hydrogenation and degree of unsaturation of different compounds

Compounds	**No. of H-atoms for hydrogenation of one ring**	**Degree of unsaturation***
Diaromatics	4	7
Triaromatics	2	10
Tetraaromatics	4	13

* Degree of unsaturation = (Maximum number of hydrogen atoms for a given number of C atoms (2C+2) – Actual number of hydrogen atoms in molecule) / 2

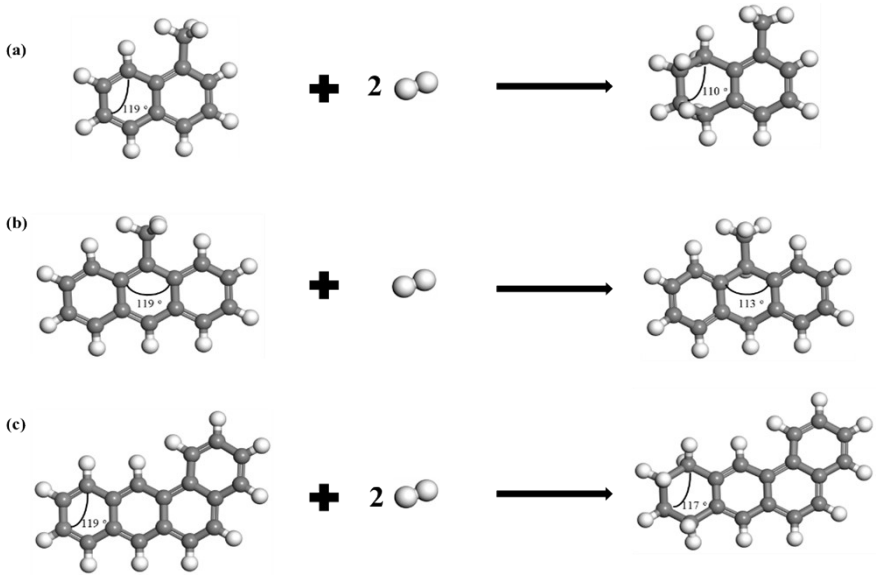


Fig. S19 Optimized structures of (a) 1MN and compound formed by saturation of one ring of

1MN, (b) 9MA and compound formed by saturation of one ring of 9MA, and (c) BaA and compound formed by saturation of one ring of BaA.

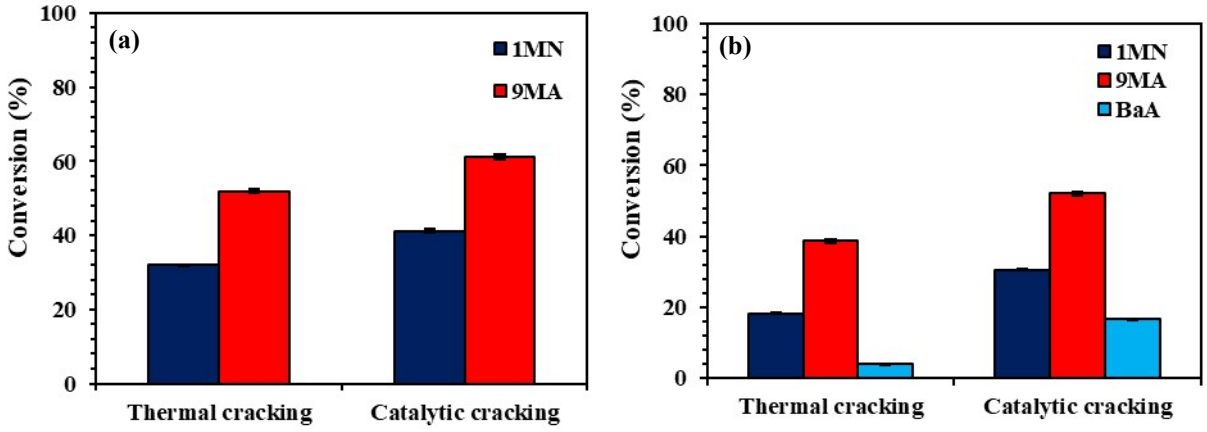


Fig. S20 Individual conversions for the cracking of feed mixtures containing (a) 1MN (50 wt. %) and 9MA (50 wt. %), and (b) 1MN (33.33 wt. %), 9MA (33.33 wt. %), and BaA (33.33 wt. %).

Coordinates of optimized structures of Fig. 9

R (Reactant)

Si O Al H C

1.00000000000000

12.6614000000000004 0.0000000000000000 0.0000000000000000

0.0000000000000000 12.6614000000000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.4060999999999986

60 128 4 12 10

0.33334054 0.790934957 0.059859725

0.341574324 0.539756368 0.057516489

0.713856624 0.789156998 0.062932361

0.729093914 0.539952663 0.06133867

0.95904184 0.792416477 0.057066341

0.968029064 0.539904242 0.056173705

0.527452549 0.844740898 0.131279098

0.651544428 0.204822941 0.562403747

0.643559594 0.455957092 0.559088983

0.278276096 0.200240656 0.559446275

0.272034045 0.451782883 0.56217803

0.034560445 0.195601401 0.555803384

0.028840226 0.448563768 0.555519737

0.458722952 0.131051847 0.629779448

0.194540434 0.32279667 0.307471105

0.19749928 0.706583928 0.310529001

0.448440283 0.707319888 0.315191147

0.196489761 0.949380715 0.309503574

0.450062159 0.949111691 0.311650674

0.130862729 0.518915735 0.375536711

0.792849291 0.658693016 0.807972413

0.540575497 0.649933565 0.80830483

0.797582579 0.276036151 0.808873777

0.544669426 0.270763971 0.819339156

0.795725516 0.033756141 0.803427093

0.541988985 0.028757862 0.806330191

0.856396557 0.46395276 0.874434303

0.672980772 0.787625908 0.947679777

0.672393339 0.534972596 0.947906862

0.286949634 0.791716892 0.946508102

0.281293723 0.537871303 0.944273507

0.043046437 0.795277831 0.946521336

0.037135562 0.541584208 0.944040128

0.475852971 0.843012941 0.878653713

0.322099115 0.204811437 0.443738354

0.322541986 0.458567139 0.446513677

0.701538746 0.199097479 0.446551213

0.703390217 0.44914505 0.443774425

0.944870003 0.194887805 0.446513788

0.947095319 0.448643458 0.444727287

0.52015 0.133052355 0.377842898

0.788806644 0.323062632 0.695846929

0.785071116 0.706573287 0.692207822

0.533374049 0.704639593 0.693122191

0.785138058 0.949821215 0.693144058

0.531403973 0.947868769 0.695973708

0.840238351 0.518861347 0.625030709

0.207022569 0.657688796 0.194745465

0.459933668 0.651508871 0.200176438

0.19954923 0.277703381 0.194208659

0.453133534 0.273377296 0.188413165

0.200023279 0.035676948 0.199279758

0.453492164 0.030818659 0.200882298

0.154019438 0.46359529 0.126408305

0.141527494 0.854783517 0.127232351

0.853006601 0.136415041 0.626128172

0.456797323 0.522878241 0.627402757

0.126113251 0.134698842 0.376308094

0.516781267 0.524030357 0.379876382

0.860696568 0.853307637 0.876594293

0.314318575 0.664900202 0.064152551

0.33711468 0.823915878 0.00058868

0.235089731 0.851405503 0.085629957

0.44226986 0.826834116 0.086243921

0.325794849 0.505307614 0.999219287

0.257819224 0.473216598 0.091456365

0.459174874 0.514962944 0.075565569

0.704514246 0.661267754 0.072242827

0.836614273 0.82192114 0.067056555

0.644724806 0.846518957 0.105886718

0.848740707 0.504921158 0.072778411

0.663369617 0.469934614 0.107008372

0.977157348 0.666099021 0.061862895

0.028315374 0.850056806 0.099426481

0.048686429 0.481523154 0.092986778

0.643584296 0.331063193 0.572563515

0.653145359 0.181088685 0.502647575

0.761175509 0.161593486 0.585817462

0.552386043 0.147020882 0.588141548

0.655103082 0.473857136 0.499275941

0.742758154 0.512570774 0.586609519

0.536039127 0.508915212 0.579253019

0.285879232 0.325855823 0.570995172

0.156252304 0.163650273 0.564071547

0.346015173 0.135679278 0.60065859

0.148491432 0.484492245 0.56767877

0.337049679 0.513575387 0.605561907

0.017883447 0.321982593 0.562402326

0.966692843 0.136395377 0.598850047

0.950827288 0.504820996 0.595563766

0.318700305 0.309669956 0.313088404

0.163907396 0.327319956 0.247452045

0.132557758 0.2227467 0.332113604

0.15012594 0.430581276 0.332572097

0.490304861 0.339957574 0.242638412

0.517998293 0.216668482 0.332892743

0.496059471 0.444052002 0.334449564

0.321971129 0.698993557 0.323103057

0.158681968 0.827951434 0.314593842

0.132367727 0.635127246 0.350019691

0.486375286 0.828268984 0.317107093

0.507673438 0.644478091 0.359400185

0.322990093 0.958149852 0.315417899

0.139666069 0.017816646 0.352740285

0.504776732 0.014400224 0.356176894

0.666467466 0.667932806 0.815951107

0.820330607 0.667603605 0.748412419

0.850046743 0.754115456 0.838040554

0.836008861 0.546802267 0.828432229

0.507198028 0.659369492 0.749269346

0.481059614 0.744829033 0.839019699

0.502763487 0.53431415 0.826050103

0.671316832 0.277507621 0.818931587

0.83588154 0.153925674 0.811132254

0.85613287 0.344746479 0.852266196

0.504540425 0.150770306 0.813098408

0.491751042 0.330480163 0.864654134

0.669110746 0.024322376 0.80973557

0.851935618 0.962665981 0.846076018

0.494172291 0.95492599 0.850655132

0.692363728 0.661956181 0.942954729

0.670129424 0.818991667 0.007172187

0.769972191 0.847338344 0.919797126

0.562690119 0.824709101 0.922701653

0.688696658 0.501941437 0.007532667

0.765759717 0.47597783 0.916858284

0.558907345 0.502919935 0.929804918

0.288942496 0.665858168 0.938217437

0.165294608 0.831605165 0.941747193

0.357826361 0.846796783 0.90261653

0.157704675 0.503866149 0.939970445

0.344549521 0.482796469 0.899585259

0.030808605 0.66893296 0.939428962

0.976615497 0.852471345 0.902208539

0.971094221 0.487085581 0.898930253

0.319981603 0.33202972 0.437030858

0.322206181 0.175644146 0.503365136

0.216572714 0.155756687 0.418464779

0.426935645 0.156533314 0.418948078

0.314490537 0.483376283 0.506505813

0.221832881 0.511409246 0.418543039

0.431693585 0.506867568 0.425629172

0.696565379 0.323655467 0.432677584

0.8228576 0.159007668 0.444126192

0.632743885 0.132657299 0.406980028

0.825711442 0.48674717 0.440787626

0.635259497 0.512540597 0.402711775

0.954468092 0.321615274 0.439812916

0.010443388 0.137773698 0.402121024

0.015458019 0.503562946 0.400650479

0.66486592 0.308791415 0.692167686

0.825896415 0.328129969 0.754917809

0.852007675 0.224283165 0.67065019

0.829195025 0.43135174 0.669191398

0.505003798 0.339461971 0.765512431

0.46493631 0.215350038 0.674502563

0.481836461 0.440588819 0.671518336

0.659624067 0.693954261 0.684262643

0.820822553 0.8281839 0.685166182

0.846116083 0.635043302 0.651158552

0.497626158 0.82613823 0.690246531

0.469277051 0.641529136 0.650511741

0.658232595 0.960083655 0.690149986

0.838170264 0.019650796 0.649517504

0.469814367 0.012864442 0.653353649

0.334264033 0.66125308 0.187168927

0.176564372 0.662925576 0.25367572

0.15440882 0.757095548 0.165887807

0.159515231 0.549673159 0.171543256

0.478807357 0.659208023 0.260224231

0.519537182 0.748921371 0.171606909

0.506283773 0.538829165 0.182127916

0.327119548 0.282716917 0.186825224

0.163249129 0.156006514 0.189838778

0.145943154 0.34573801 0.149292694

0.491235278 0.15300954 0.193787782

0.5102485 0.334058221 0.143583126

0.327020234 0.024393466 0.1934194

0.143823172 0.965210006 0.156592372

0.509774515 0.957761413 0.158437654

0.995038271 0.829764107 0.001020435

0.986660552 0.505786987 0.997974263

0.994976652 0.159984068 0.500449305

0.995786319 0.483378697 0.499078393

0.163482114 0.99515922 0.254354572

0.487307337 0.992209942 0.256452562

0.827362429 0.990292489 0.747917156

0.499143133 0.98696239 0.752550862

0.452738872 0.325728508 0.312077331

0.530750802 0.324699385 0.694758548

0.520713391 0.46538068 0.127319922

0.475328419 0.461356222 0.882682772

0.7072941 0.415730712 0.122723568

0.507609229 0.414273254 0.234324688

0.270525317 0.536684183 0.839953238

0.497813562 0.414730269 0.775728058

0.350082415 0.569990374 0.793439319

0.282633185 0.731638012 0.834184883

0.140784336 0.814798355 0.783062374

0.045638707 0.706904088 0.719331879

0.009911067 0.545077311 0.677761897

0.180366289 0.26374256 0.717632359

0.283917894 0.363821579 0.780651615

0.041088075 0.351683107 0.666903076

0.264213292 0.575076661 0.801905923

0.237284227 0.685453072 0.807201997

0.159613438 0.731722635 0.778603664

0.105774826 0.670199911 0.742968714

0.125709418 0.561939154 0.736014168

0.204583973 0.511102001 0.765673211

0.067977242 0.503283389 0.70012291

0.223463273 0.403692121 0.758504301

0.164959529 0.347505591 0.723143342

0.086597926 0.397178334 0.694045792

TS (Transition state)

0.33503295 0.790581431 0.059785794

0.344365059 0.538383647 0.056324772

0.715079237 0.789444213 0.06308596

0.731160444 0.540552107 0.062009578

0.960298562 0.79323314 0.057010258

0.969776076 0.540963641 0.056372205

0.528651692 0.845156457 0.131423803

0.650220379 0.204853749 0.562730763

0.642060722 0.455465345 0.559112857

0.277276063 0.199145947 0.559461705

0.27117703	0.450352229	0.562601872
0.033713628	0.194304967	0.555430365
0.027978704	0.447223646	0.555543377
0.45773176	0.128486344	0.629420426
0.19409205	0.322269168	0.307494568
0.196928941	0.705786615	0.310551185
0.44793591	0.706657661	0.315476556
0.195775461	0.948948612	0.309292365
0.449448915	0.948533882	0.311757082
0.129942287	0.518466513	0.3757057
0.79539576	0.660041048	0.807214989
0.543712251	0.653159656	0.808869652
0.796550157	0.27690428	0.808725698
0.543375188	0.272443538	0.818620531
0.794521712	0.034112195	0.803515444
0.540866017	0.030460825	0.806226616
0.856086933	0.464910029	0.874076532
0.673133015	0.787710442	0.947586408
0.671161617	0.533659029	0.948617361
0.287773458	0.79385235	0.946717165
0.278815766	0.541134428	0.943941814
0.04364207	0.796421971	0.946329474
0.036027528	0.542563936	0.943994839
0.47700662	0.846286291	0.878763421
0.320264618	0.204624863	0.443522594
0.321140346	0.45805615	0.446758615
0.700512307	0.198600619	0.446673998

0.702386342 0.447925917 0.443715522

0.943527832 0.194178505 0.446315674

0.945906397 0.448040884 0.444855462

0.519023363 0.13241015 0.378110631

0.78848908 0.322728556 0.695567586

0.784782962 0.706730362 0.691377092

0.533250115 0.703426673 0.693629845

0.784017766 0.949792262 0.693194797

0.530275271 0.946654442 0.696323979

0.83919858 0.518550337 0.62457023

0.207812147 0.658268001 0.194772623

0.460473455 0.652481856 0.200321978

0.200403915 0.278042437 0.194394553

0.454174757 0.273343331 0.188948904

0.20052658 0.036040604 0.199363841

0.454015954 0.03081847 0.201166269

0.156397757 0.463563559 0.125924797

0.142492172 0.854975065 0.127352801

0.852476217 0.136756071 0.626059428

0.456220028 0.522327882 0.62746107

0.124582771 0.134238332 0.376017767

0.515505983 0.523431708 0.38028081

0.862203836 0.853265697 0.876057448

0.31735204 0.663751288 0.062840808

0.337997829 0.82552613 0.000773632

0.23655302 0.849549446 0.086010242

0.44383447 0.826240226 0.08625812

0.329857279 0.503510688 0.99689266

0.260113135 0.472552734 0.090405301

0.461325676 0.513199623 0.075032232

0.705020248 0.661639986 0.072606552

0.837881309 0.821785599 0.067564171

0.64572092 0.847221058 0.105858269

0.850911938 0.506627795 0.07401718

0.665230187 0.470301182 0.10749922

0.979677576 0.667081221 0.061769726

0.029793323 0.851497043 0.09902172

0.051373608 0.481811924 0.092304541

0.64011469 0.330827434 0.573487727

0.652157812 0.182482635 0.502851038

0.760271001 0.162576811 0.585998647

0.551876002 0.144859286 0.588037684

0.653328932 0.470926815 0.499148126

0.742538487 0.51155891 0.585627163

0.535492662 0.510485107 0.57909019

0.285456307 0.324452806 0.571599873

0.155333469 0.162210901 0.563876272

0.345540531 0.133416107 0.599947217

0.147661596 0.482626572 0.567680245

0.336567006 0.51269801 0.605663132

0.01683798 0.320572347 0.561759858

0.965383849 0.134799395 0.598161051

0.949865485 0.503108302 0.595536319

0.318192939 0.307788153 0.31270316

0.16362051 0.327787717 0.247413365

0.131487713 0.222343683 0.331829527

0.150709476 0.430294521 0.332718405

0.491027029 0.339597468 0.243226128

0.518052132 0.216011405 0.333094882

0.494274321 0.443659944 0.334793626

0.321416608 0.697940029 0.323192461

0.158414304 0.827331436 0.314246304

0.131074786 0.634650634 0.349880262

0.485566628 0.827666882 0.317203424

0.506854327 0.644038597 0.359821051

0.322299872 0.958056897 0.314980808

0.138525952 0.017217534 0.352470147

0.503427691 0.013776338 0.356418227

0.669491295 0.671363785 0.816447532

0.820484748 0.66738006 0.747511252

0.854344481 0.755025236 0.83694449

0.837415239 0.547969093 0.828188036

0.510099514 0.656903089 0.749906456

0.485169112 0.749938247 0.838466747

0.506463324 0.539323388 0.82908102

0.669936483 0.279967704 0.818955362

0.833995684 0.154560391 0.811260415

0.854995686 0.345462143 0.852345885

0.50377615 0.152618732 0.81238487

0.48869751 0.332488438 0.863795061

0.667858212 0.025217444 0.810052564

0.850531325 0.963376598 0.846462879

0.492487124 0.959202189 0.851427595

0.686365931 0.661030084 0.943083507

0.672465568 0.81880349 0.007136029

0.771931022 0.843452925 0.919437666

0.563811318 0.828798266 0.9230245

0.692594435 0.501838684 0.007999031

0.764647138 0.477842085 0.91634078

0.55640552 0.496748518 0.932715848

0.289717082 0.66739686 0.939364565

0.166097334 0.832573181 0.942214463

0.358890439 0.84689209 0.902780097

0.157198837 0.504205893 0.940584885

0.337821443 0.492252645 0.893318828

0.032022505 0.669743501 0.939154831

0.977775309 0.854042076 0.902148048

0.970592616 0.487002753 0.89926158

0.317946888 0.331825106 0.436413512

0.320736475 0.175915503 0.503111084

0.214870821 0.155364248 0.418182105

0.424972907 0.156306832 0.418598393

0.313471618 0.481656168 0.506784583

0.220577577 0.511742818 0.418858301

0.430355351 0.506382043 0.425931057

0.696234675 0.322707432 0.431915153

0.821591808 0.157881613 0.444159414

0.631175255 0.131421153 0.407563622

0.824433521 0.486411203 0.440925999

0.634049384 0.511648831 0.402817591

0.952242904 0.320976624 0.439921675

0.008755627 0.13751943 0.401601307

0.014265044 0.502393483 0.400490894

0.664788282 0.305026547 0.691927291

0.824992173 0.328549911 0.754774454

0.853551602 0.225156216 0.6703475

0.825812531 0.431936713 0.66897962

0.503790713 0.338607758 0.764238311

0.463728547 0.212767612 0.674177015

0.482876545 0.438769314 0.670817338

0.65921967 0.694185223 0.683781281

0.820171216 0.828512538 0.684672045

0.844829998 0.635338023 0.650007015

0.496545503 0.824755666 0.691668576

0.468214351 0.640251666 0.651433133

0.657042882 0.9593663 0.690552825

0.836308679 0.020496382 0.649765522

0.468933379 0.01036176 0.653107987

0.334931134 0.663580156 0.187105686

0.17656507 0.661942043 0.253592348

0.153802582 0.757619468 0.166333197

0.162074194 0.550019247 0.170817549

0.478894405 0.658868623 0.260406686

0.521014724 0.749622623 0.171940749

0.505867399 0.539730282 0.181880675

0.328056556 0.282852566 0.187025966

0.163825795 0.15645071 0.190168553

0.147692836 0.346064506 0.14909356

0.492092412 0.152951921 0.194222458

0.512035889 0.334116633 0.144275263

0.327560433 0.025107654 0.193834876

0.145546228 0.966041596 0.156099023

0.509860209 0.958227808 0.158332792

0.995096449 0.83022815 0.00076194

0.986251865 0.507141449 0.997975684

0.994424655 0.159058065 0.499938853

0.995140669 0.482728066 0.499038772

0.162784146 0.994578299 0.254041101

0.487622304 0.991329113 0.256585479

0.826106465 0.990077523 0.748120144

0.498156877 0.987717494 0.752681472

0.452081534 0.324818521 0.312575284

0.530760038 0.322031721 0.693368304

0.522242178 0.465273898 0.127645389

0.476971453 0.462608421 0.882734375

0.709352695 0.41627598 0.123191821

0.5086814 0.414010985 0.235420819

0.291643211 0.527690511 0.849773134

0.493336554 0.413943464 0.772503374

0.351788095 0.554466166 0.802535167

0.294098483 0.729098982 0.832013357

0.149112592 0.812885494 0.785185278

0.04655819 0.711205414 0.722644993

0.007700751 0.548308523 0.680315512

0.180491845 0.266585007 0.715015951

0.286629587 0.363532149 0.777824073

0.038557175 0.356771056 0.666746178

0.266368979 0.571859009 0.803096527

0.244006349 0.68064187 0.808169966

0.163856786 0.729465445 0.780800845

0.10690531 0.672260438 0.745648503

0.125475342 0.563630454 0.738218858

0.20542013 0.511075817 0.767006368

0.06736567 0.506763876 0.701821561

0.224773984 0.40406039 0.756999117

0.16572804 0.350020211 0.721511796

0.08567697 0.401167384 0.693944447

P (Product)

0.337246822 0.79127176 0.054545011

0.345488835 0.542272544 0.055263599

0.719279811 0.792850796 0.056084697

0.7346071 0.543650698 0.056300389

0.964678275 0.795734429 0.051257116

0.97410801 0.542034701 0.052120733

0.532723061 0.847529632 0.124438859

0.663014211 0.210698653 0.557741802

0.659918419 0.464703175 0.554087401

0.288076675 0.20558815 0.554657525

0.284380154 0.456500352 0.555799246

0.044238178 0.202207861 0.552812892

0.040646242 0.455442007 0.552888184

0.467131316 0.140922847 0.62560168

0.201083032 0.327735481 0.302821856

0.208061385 0.710203369 0.305655174

0.459491426 0.710845462 0.309736947

0.206862524 0.954981106 0.305667019

0.459731736 0.955048776 0.306748416

0.140975491 0.523168207 0.370731902

0.794122714 0.665101848 0.803915807

0.542767493 0.664583135 0.801874447

0.794105034 0.284684063 0.807238539

0.549201133 0.280591667 0.809640526

0.801457071 0.039577483 0.800706809

0.549658824 0.035211288 0.803948908

0.864383014 0.469307003 0.870088751

0.67818693 0.790026017 0.94071018

0.681035673 0.537321673 0.942806137

0.295792978 0.7867195 0.938507972

0.287114066 0.539042184 0.940711357

0.049398989 0.794689407 0.941462871

0.043363327 0.541655891 0.940336095

0.480458726 0.852315694 0.872034972

0.333640621 0.207061549 0.438706717

0.33579588 0.459776055 0.439669998

0.710648458 0.204230445 0.443667919

0.714051335 0.457164712 0.440285112

0.955500993 0.201713766 0.443478869

0.958352859 0.454891409 0.44199071

0.530705626 0.138153491 0.372814041

0.791630859 0.329615443 0.690322822

0.791502615 0.713447909 0.687279731

0.541537581 0.713587488 0.686322234

0.794288023 0.956959609 0.690362543

0.54025266 0.956504633 0.692925915

0.856848319 0.523967563 0.623233357

0.215623005 0.660298732 0.190348748

0.469783345 0.654855378 0.195282151

0.204801742 0.277972871 0.18966071

0.458534864 0.274975451 0.183192084

0.206664848 0.03575314 0.194786819

0.460237213 0.032156952 0.195508067

0.158891886 0.464892028 0.123319061

0.147654248 0.855762958 0.121263354

0.863155737 0.143854959 0.623693992

0.468287363 0.531022989 0.621961106

0.135794917 0.138824823 0.37281662

0.529516145 0.527822485 0.37379156

0.867725209 0.858692398 0.871353103

0.317499399 0.666296745 0.063980862

0.342757901 0.811024163 0.994059325

0.238432864 0.855381179 0.077811782

0.445937656 0.831092443 0.07980253

0.331414996 0.514180622 0.995776256

0.260363484 0.472497231 0.08633035

0.46332669 0.516343092 0.071831935

0.712055976 0.665300004 0.067019215

0.841913568 0.826994102 0.059386575

0.649264733 0.85098923 0.098372473

0.853873658 0.506434918 0.066671201

0.669455498 0.473488304 0.102054545

0.979907837 0.668778545 0.055166468

0.032716967 0.851104679 0.094819417

0.051740283 0.488201744 0.091860627

0.656274449 0.337925197 0.560578669

0.664708558 0.17416095 0.49913201

0.772205049 0.170729507 0.583232594

0.563139076 0.158863878 0.585664233

0.670195689 0.494652725 0.495007718

0.762883599 0.510739584 0.583049229

0.55451085 0.517270962 0.576586568

0.296118975 0.330911398 0.566920431

0.166140043 0.168421755 0.559068438

0.355835847 0.139201847 0.595113663

0.161639472 0.491045719 0.560965144

0.351114953 0.521175093 0.597236474

0.030506302 0.328689705 0.55881602

0.977692296 0.144838935 0.597088626

0.970120944 0.510930116 0.596266741

0.325761641 0.320302147 0.307522721

0.168812606 0.326903471 0.242925121

0.142936823 0.227293786 0.328935598

0.153121637 0.43523313 0.326795185

0.496464781 0.342396026 0.236917372

0.523289489 0.222327583 0.328232877

0.508141125 0.449589664 0.327660289

0.333071518 0.695779742 0.315481869

0.17477031 0.832479788 0.31224672

0.14263709 0.639468636 0.345185929

0.490664315 0.833242996 0.313543392

0.519758426 0.648902599 0.353908079

0.333056157 0.970903142 0.31071515

0.147268041 0.022523358 0.348260515

0.519533248 0.019764393 0.349942704

0.668624356 0.673000782 0.814067069

0.817253808 0.669431947 0.744005134

0.853529226 0.763207211 0.831062641

0.840741888 0.555690491 0.82617736

0.519621285 0.664180059 0.742068301

0.486579549 0.76782376 0.826495447

0.493218027 0.559967974 0.825562206

0.671881417 0.295130602 0.826353927

0.831035772 0.162421407 0.80871581

0.86534651 0.352219785 0.846350579

0.517140172 0.157233714 0.811728566

0.475454546 0.339812043 0.854962613

0.676024789 0.021656574 0.807907117

0.862676561 0.970970137 0.843012062

0.496583769 0.969386495 0.849654298

0.697901356 0.663841881 0.936228779

0.673701028 0.819687195 0.00036425

0.776159491 0.850830771 0.914285321

0.568372812 0.824549581 0.914770915

0.69128354 0.506986928 0.002784475

0.776497922 0.477833553 0.914166242

0.569381271 0.499431941 0.923314268

0.306683105 0.660458955 0.925143041

0.173365348 0.82212542 0.935143592

0.364075725 0.849836425 0.897286142

0.165503592 0.506280583 0.935003472

0.35366631 0.461560981 0.900634069

0.033602965 0.668278427 0.936687439

0.983419469 0.851917823 0.897218812

0.979604214 0.488620435 0.89464134

0.333667953 0.333581862 0.429362427

0.333075471 0.182465098 0.498623985

0.227739782 0.15729574 0.414312055

0.437396388 0.155269658 0.414499418

0.326374663 0.483055616 0.49951351

0.236156383 0.513046225 0.411203843

0.444971935 0.50899315 0.419496781

0.701578333 0.330473816 0.435008266

0.833075172 0.168918855 0.438976942

0.643643972 0.142612479 0.401487163

0.837041437 0.489619407 0.434330104

0.647597829 0.515074081 0.396634846

0.970166728 0.328052773 0.437198781

0.021350807 0.142935522 0.399592937

0.02884444 0.511073431 0.399062755

0.671125589 0.318006165 0.676692773

0.81053543 0.333100717 0.751537136

0.861258624 0.230125492 0.66930606

0.844480874 0.438149252 0.668641159

0.524730266 0.334608921 0.757410759

0.464572223 0.228354419 0.669087853

0.486916514 0.450020957 0.666901641

0.667238228 0.705482476 0.67535293

0.830278325 0.834940475 0.683608104

0.856056733 0.64167929 0.647817333

0.504950159 0.835324821 0.686325

0.476518936 0.651507095 0.643891258

0.66733019 0.967281123 0.687593694

0.847508508 0.026269853 0.646507939

0.48072086 0.024282569 0.650730604

0.343137175 0.664548638 0.184979795

0.180450098 0.671847159 0.248430605

0.163801883 0.755491252 0.157994853

0.171213769 0.549114497 0.168871525

0.495097969 0.667178149 0.254498679

0.52687196 0.749561422 0.163593954

0.513749967 0.540612867 0.177755358

0.332324672 0.284735781 0.181681095

0.169664799 0.155940778 0.184934231

0.149656225 0.346360879 0.145048907

0.496705172 0.154660701 0.188220671

0.516166714 0.335661744 0.138378375

0.333665437 0.025248542 0.18900276

0.151101485 0.964292019 0.152138479

0.51513432 0.959381779 0.152502052

0.005405544 0.833619527 0.995958134

0.998930598 0.503162472 0.994930095

0.000637072 0.165492422 0.498193503

0.999134586 0.491165629 0.497604213

0.170484412 0.995743392 0.249959696

0.496838815 0.99326811 0.250582584

0.835840501 0.99964773 0.745027307

0.507298372 0.995096537 0.749717658

0.332149624 0.245191192 0.954331185

0.202341878 0.289461268 0.868566891

0.46006429 0.331799416 0.306821149

0.538771045 0.334885703 0.691109669

0.527269198 0.466983544 0.122987527

0.486082789 0.475799411 0.874753456

0.714815049 0.42114566 0.11834266

0.513990431 0.416424361 0.228003773

0.373338818 0.18919533 0.862311228

0.300128609 0.233671087 0.772811234

0.378365857 0.413441166 0.76544892

0.326396272 0.261699735 0.71195017

0.13866915 0.184955473 0.720580185

0.007408019 0.326846325 0.717273923

0.962481419 0.518225028 0.726789883

0.202560211 0.742523644 0.768730182

0.334662103 0.597116689 0.774806776

0.018276545 0.700654112 0.744145904

0.32845865 0.297344047 0.893878294

0.296908938 0.39582775 0.755410156

0.270735329 0.287631924 0.742902936

0.160822622 0.265754668 0.729553901

0.088319154 0.344484824 0.727737792

0.116386662 0.451254511 0.739121311

0.223491785 0.475975138 0.753163384

0.043795334 0.534598519 0.73679853

0.25330546 0.581968997 0.76423565

0.18033672 0.661362985 0.760923465

0.075624076 0.637019316 0.746887195

References

1. T. C. Hoff, D. W. Gardner, R. Thilakaratne, K. Wang, T. W. Hansen, R. C. Brown and J. P. Tessonnier, ChemSusChem, 2016, 9, 1473–1482.
2. A. Kostyniuk, D. Bajec, A. Prašnikar and B. Likozar, J. Ind. Eng. Chem., 2021, 101, 293–306.
3. Kostyniuk, D. Bajec and B. Likozar, J. Ind. Eng. Chem., 2021, 96, 130–143.
4. Kostyniuk, D. Bajec and B. Likozar, Appl. Catal. A Gen., 2021, 616, 118095.
5. A.V. Ramteke, D. Bhatia, K.K. Pant, *Fuel*, 2023, **342**, 127737.
6. A.V. Ramteke, D. Bhatia, K.K. Pant, *Fuel*, 2024, **358**, 130085.