Supporting Information

Catalytic Effects of Zeolite Socony Mobil-5 (ZSM-5) on the Oxidation of Acoustically Levitated exo -Tetrahydrodicyclopentadiene (JP-10) Droplets

Sahan D. Perera, [a] Stephen J. Brotton,[a] Haylie Shinsato,[a] Ralf I. Kaiser[a,]*

[a] *Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, United States*

Corresponding Author: ralfk@hawaii.edu

Yuyeol Choi,[b] Kyungsu Na[b,]*

[b] *Department of Chemistry, Chonnam National University, Buk-gu, Gwangju, South Korea*

Corresponding Author: kyungsu_na@chonnam.ac.kr

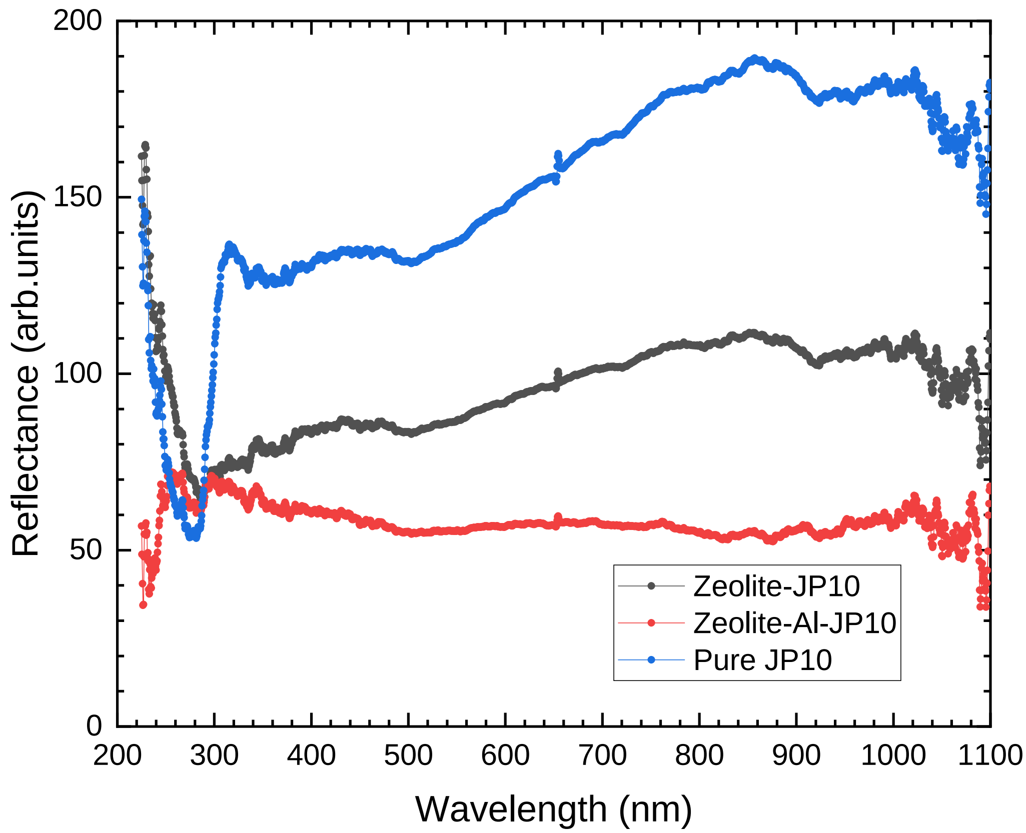


Figure S1. UV-vis reflectance spectral comparison between the droplet of zeolite-JP-10, zeolite-aluminum-JP-10, and pure JP-10.

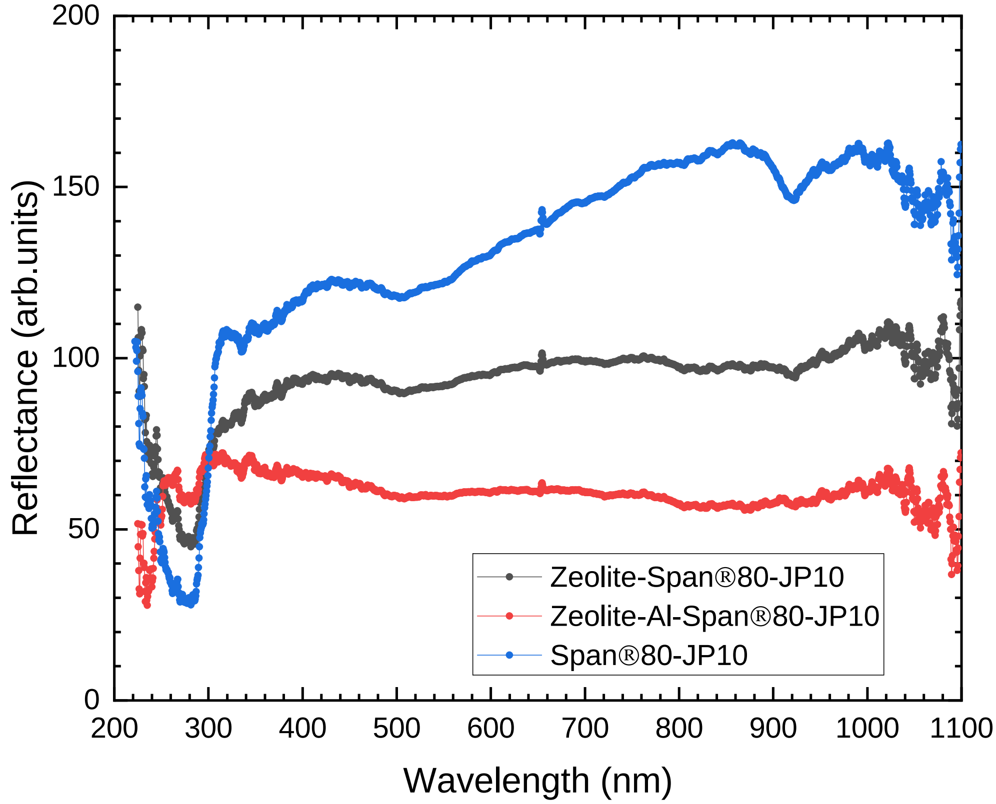


Figure S2. UV-Vis reflectance spectral comparison between the droplet of zeolite-span 80-JP-10, zeolite-aluminum-span 80-JP-10, and span 80-JP-10.

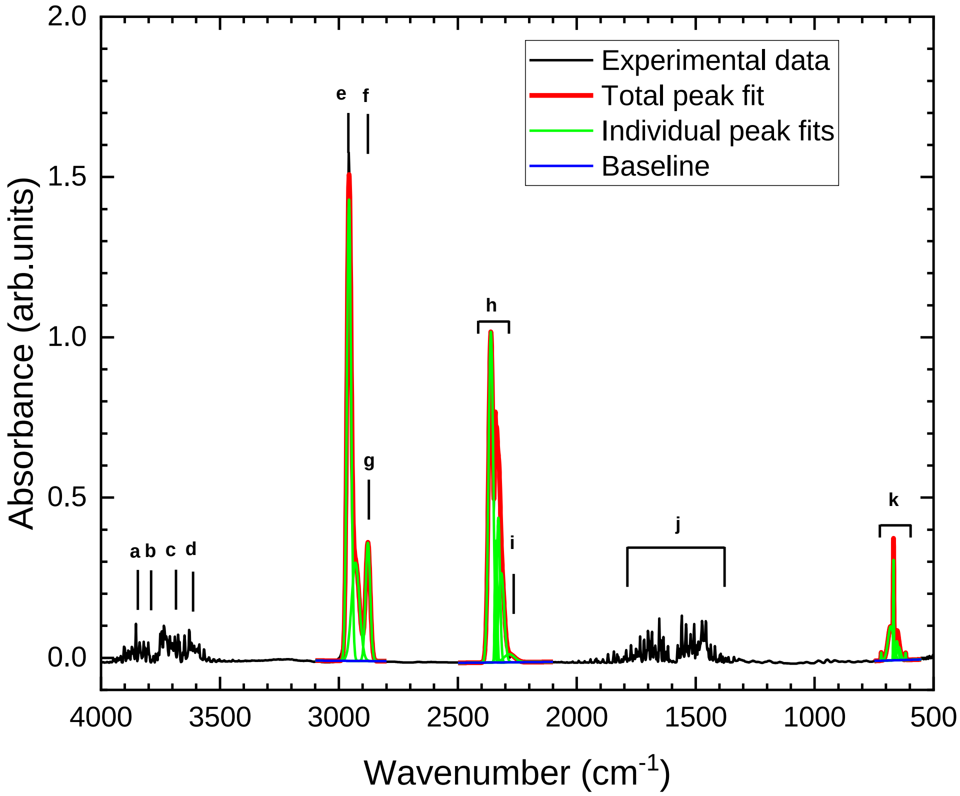


Figure S3. FTIR transmission spectrum following ignition of a JP-10 droplet containing zeolite. The rovibrational peaks/bands of the products and unreacted JP-10 are labelled (a)–(k) and assigned in Table S3. The total fit (red line) and individual peak fits peaks (green lines) are shown.

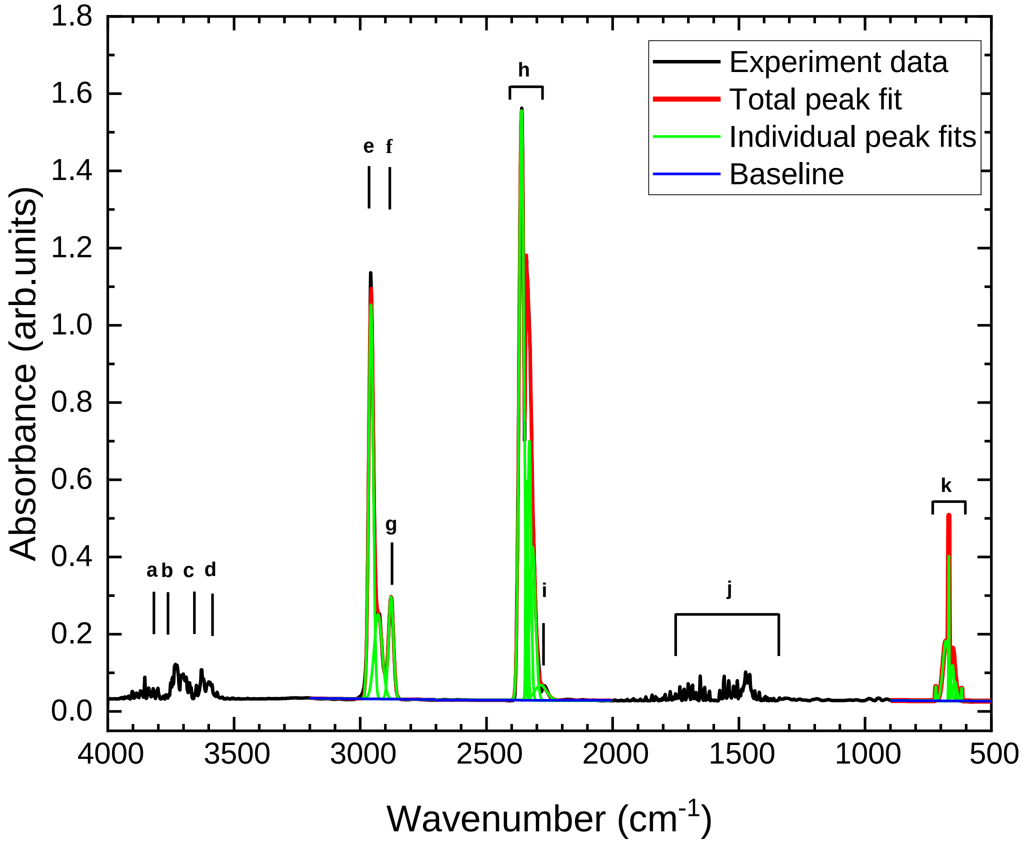


Figure S4. FTIR transmission spectrum following ignition of a JP-10 droplet containing zeolite and aluminum NPs. The rovibrational peaks/bands of the products and unreacted JP-10 are labelled (a)–(k) and assigned in Table S4. The total fit (red line) and individual peak fits peaks (green lines) are shown.

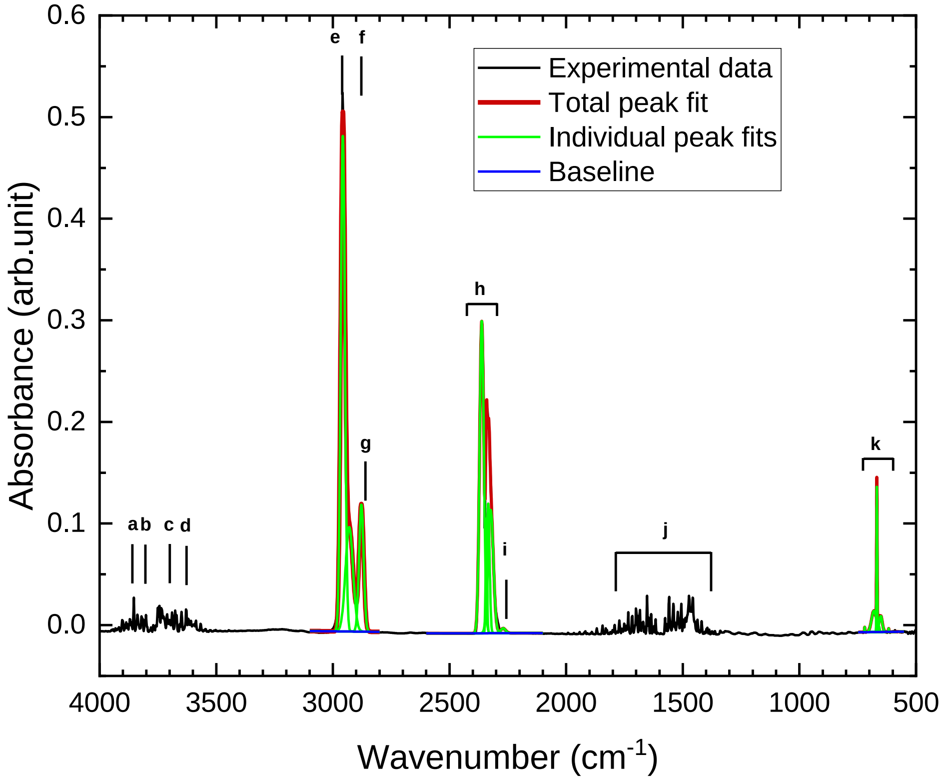
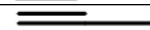
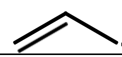
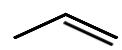
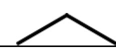
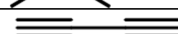
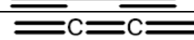
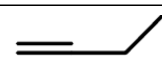
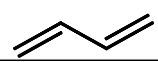
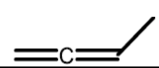
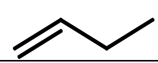
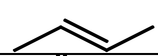
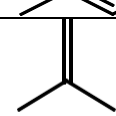
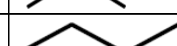
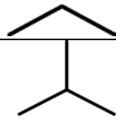
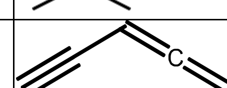
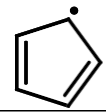
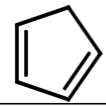
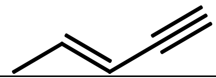
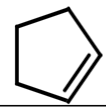
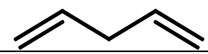
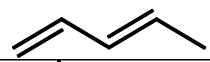
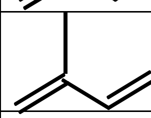
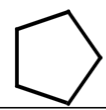
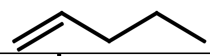
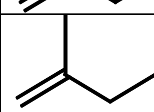
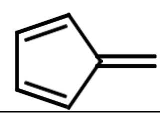
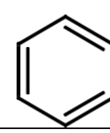
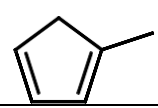
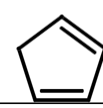
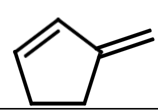
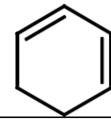
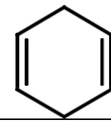
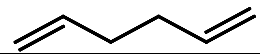
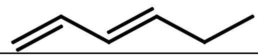
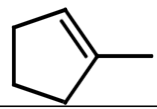


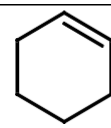
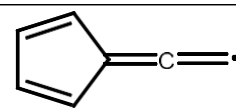
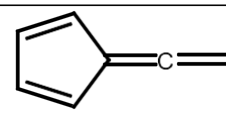
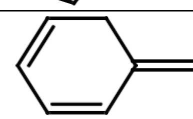
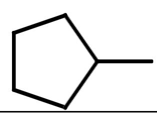
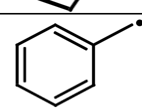
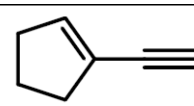
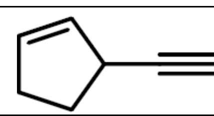
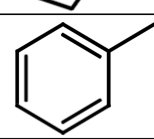
Figure S5. FTIR transmission spectrum following ignition of a JP-10 droplet containing zeolite, aluminum NPs, and span 80. The rovibrational peaks/bands of the products and unreacted JP-10 are labelled (a)–(k) and assigned in Table S5. The total fit (red line) and individual peak fits peaks (green lines) are shown.

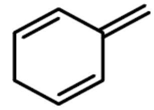
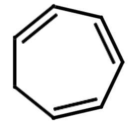
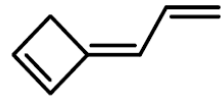
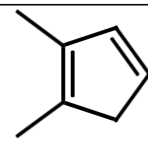
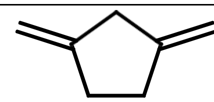
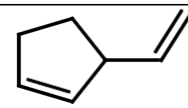
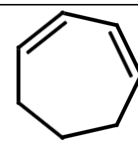
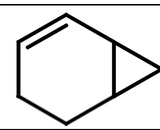
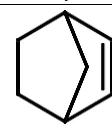
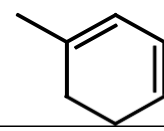
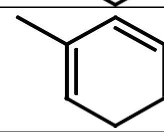
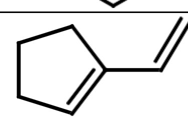
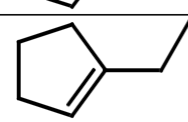
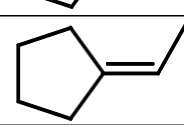
Table S1. Thermal decomposition products reported in the preceding experimental studies on JP-10.

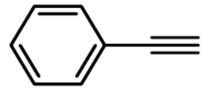
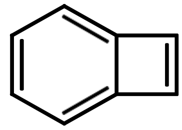
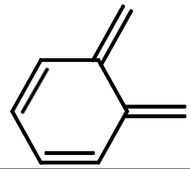
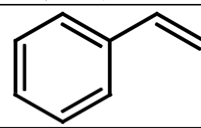
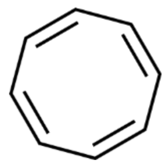
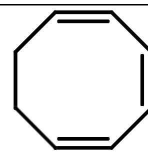
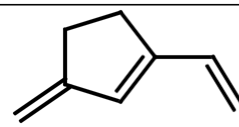
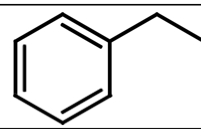
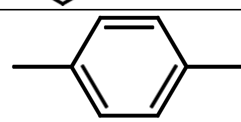
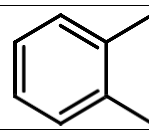
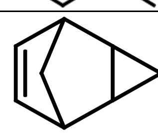
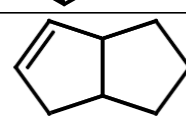
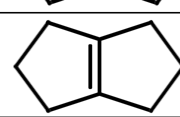
Molecule	**Formula**	**Mass**	**Structure**	**Ref.**
Hydrogen	H_2	2	H—H	10,15,16,17,22, 25,26
Methyl	CH_3	15	$CH_3^{\bullet}$	10,15,26
Methane	CH_4	16	CH_4	10,15-19, 22,24, 26
Acetylene	C_2H_2	26		7,10,14,15,22,26
Ethylene	C_2H_4	28		7,10,14-19,22, 24-26
Ethyl	C_2H_5	29		10,15
Ethane	C_2H_6	30		10,16-19,22
Propargyl	C_3H_3	39		10,15
Methylacetylene	C_3H_4	40		7,10,14,22
Allene	C_3H_4	40		7,10,14,22,24,26
Allyl	C_3H_5	41		10,15
Propene	C_3H_6	42		7,10,15-19,22, 24-26
Propane	C_3H_8	44		3,17,18,19,22
Diacetylene	C_4H_2	50		7,10
1,2,3-Butatriene	C_4H_4	52		10
Vinylacetylene	C_4H_4	52		7,10,15
1-Butyne	C_4H_6	54		7,15
1,3-Butadiene	C_4H_6	54		7,10,18,22,24,26
1,2-Butadiene	C_4H_6	54		7
1-Butene	C_4H_8	56		7,10,18,22,26
2-Butene	C_4H_8	56		7,10,18,22
i-Butene	C_4H_8	56		18,22
n-Butane	C_4H_{10}	56		3,17
i-Butane	C_4H_{10}	56		22
Ethynylallene	C_5H_4	64		10

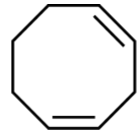
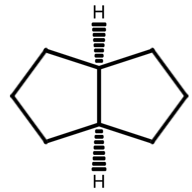
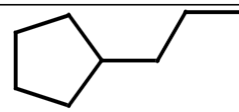
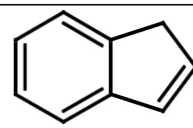
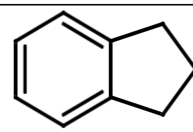
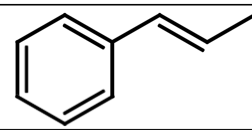
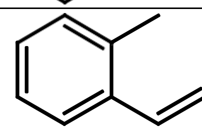
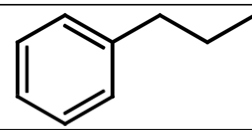
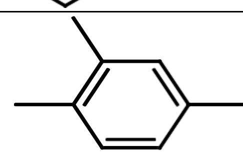
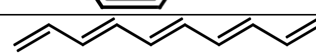
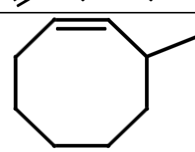
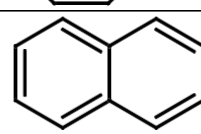
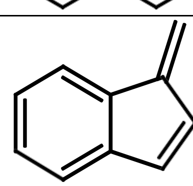
Cyclopentadienyl	C_5H_5	65		10,15
Cyclopentadiene	C_5H_6	66		7,10,14-16,18-20, 24-26
3-Penten-1-yne	C_5H_6	66		7
Cyclopentene	C_5H_8	68		7,10,16-20,22, 25,26
1,4-Pentadiene	C_5H_8	68		7
1,3-Pentadiene	C_5H_8	68		10,15
2-Methyl-1,3-butadiene	C_5H_8	68		22
Cyclopentane	C_5H_{10}	70		10,17,19,25
1-Pentene	C_5H_{10}	70		22
2-Methyl-1-butene	C_5H_{10}	70		22
Fulvene	C_6H_6	78		10,22
Benzene	C_6H_6	78		1,3,10,14,16,18, 19,20,22,24-26
1-Methylcyclopentadiene	C_6H_8	80		7,22
2-Methylcyclopentadiene	C_6H_8	80		22
3-Methylene-cyclopentene	C_6H_8	80		7

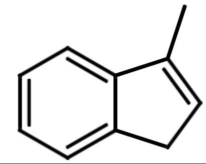
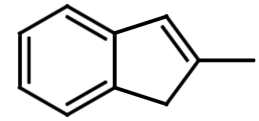
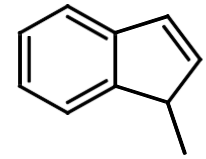
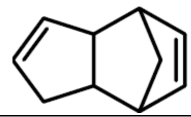
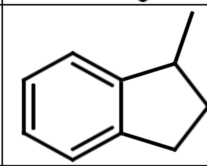
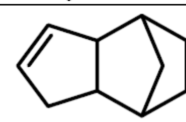
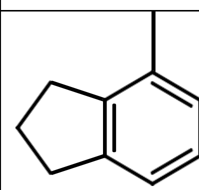
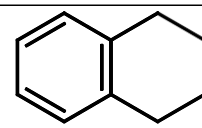
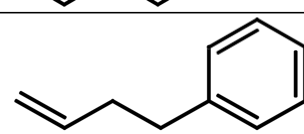
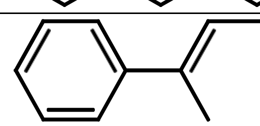
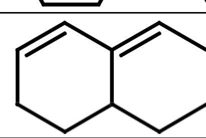
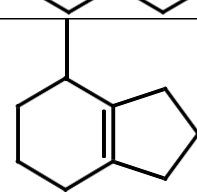
1,3-Cyclohexadiene	C_6H_8	80		10,26
1,4-Cyclohexadiene	C_6H_8	80		10,22
1,5-Hexadiene	C_6H_{10}	82		16
1,3-Hexadiene	C_6H_{10}	82		22,26
1-Methylcyclopentene	C_6H_{10}	82		3

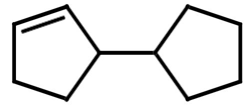
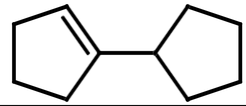
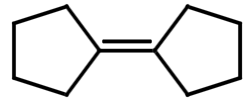
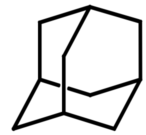
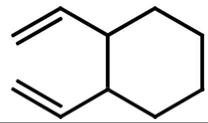
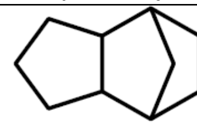
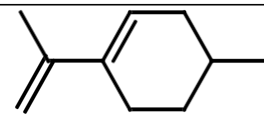
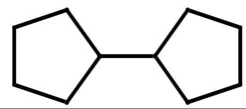
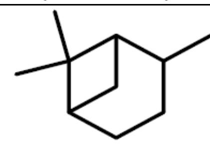
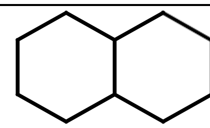
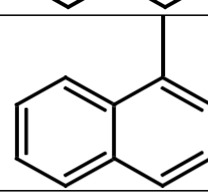
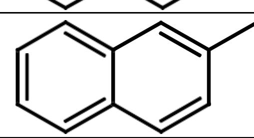
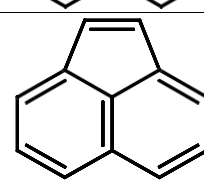
Cyclohexene	C_6H_{10}	82		10,23,26
Fulvenallenyl	C_7H_5	89		10
Fulvenallene	C_7H_6	90		10
5-Methylene-1,3-cyclohexadiene	C_7H_8	92		10
Methylcyclopentane	C_6H_{10}	84		3
Benzyl	C_7H_7	91		15
1-Ethynyl-cyclopentene	C_7H_8	92		19,20
3-Ethynyl-cyclopentene	C_7H_8	92		19,22
Toluene	C_7H_8	92		1,3,7,10,15-20, 24-26

3-Methylidenecyclohexa-1,4-diene	C_7H_8	92		22
1,3,5-Cycloheptatriene	C_7H_8	92		7
2-Propenylidene-cyclobutene	C_7H_8	92		7
1,2-Dimethylcyclopentadiene	C_7H_{10}	94		23
1,3-Bis(methylene)cyclopentane	C_7H_{10}	94		20
3-Ethenyl-cyclopentene	C_7H_{10}	94		7
1,3-Cycloheptadiene	C_7H_{10}	94		7,25
Bicyclo(4.1.0)hept-2-ene	C_7H_{10}	94		7,20
2-Norbornene	C_7H_{10}	94		22,25
1-Methylcyclohexa-1,3-diene	C_7H_{10}	94		22
1-Methylcyclohexa-2,4-diene	C_7H_{10}	94		22
Ethenylcyclopentene	C_7H_{10}	94		22
Ethylcyclopentene	C_7H_{12}	96		3
Ethylidenecyclopentane	C_7H_{12}	96		3

Phenylacetylene	C_8H_6	102		7,10,15
Benzocyclobutene	C_8H_6	102		10
o-Xylylene	C_8H_8	104		10
Styrene	C_8H_8	104		7,10,22,24
Cyclooctatetraene	C_8H_8	104		25
1,3,5-Cyclooctatriene	C_8H_{10}	106		10
1-Ethenyl-3-methylene-cyclopentene	C_8H_{10}	106		7
Ethylbenzene	C_8H_{10}	106		3,7,15,22,24,25
p-Xylene	C_8H_{10}	106		22,25
o-Xylene	C_8H_{10}	106		3,7,10,22,25
Tricyclo[3.2.1.0(2,4)]oct-6-ene	C_8H_{10}	106		22
1,2,3,3a,4,6a-Hexahydropentalene	C_8H_{12}	108		3,7,19,20
Bicyclo[3.3.0]oct-1(5)-ene	C_8H_{12}	108		22

1,4-Cyclooctadiene	C_8H_{12}	108		25
cis-Octahydropentalene	C_8H_{14}	110		3
Propylcyclopentane	C_8H_{16}	112		3
Indene	C_9H_8	116		7,10,15,22,24-26
Indane	C_9H_{10}	118		7,10
Propenyl benzene	C_9H_{10}	118		7,22
1-Ethenyl-2-methylbenzene	C_9H_{10}	118		22
Propylbenzene	C_9H_{12}	120		22
1,2,4-Trimethylbenzene	C_9H_{12}	120		22
1,3,5,7,9-Decapentayne	$C_{10}H_2$	122		15
3-Methylcyclooctene	C_9H_{16}	124		3
Naphthalene	$C_{10}H_8$	128		1,10,7,20,22, 24-26
Benzofulvene	$C_{10}H_8$	128		22

1-Methylindene	$C_{10}H_{10}$	130		22
2-Methylindene	$C_{10}H_{10}$	130		20,22
3-Methylindene	$C_{10}H_{10}$	130		22
Dicyclopentadiene	$C_{10}H_{10}$	130		20,25
2,3-Dihydro-1-methyl-1H-indene	$C_{10}H_{12}$	132		17
5,6-Dihydrodicyclopentadiene (exo-TCD4e)	$C_{10}H_{12}$	132		20,22,25
2,3-Dihydro-4-methyl-1H-Indene	$C_{10}H_{12}$	132		20
1,2,3,4-Tetrahydronaphthalene	$C_{10}H_{12}$	132		20,22
3-Butenylbenzene	$C_{10}H_{12}$	132		22
(1-Methyl-1-propenyl)-Benzene	$C_{10}H_{12}$	132		20
4-Ethyl-3-ethylidene-cyclohexene	$C_{10}H_{16}$	136		7
4-Methyl-2,3,4,5,6,7-hexahydro-1H-indene	$C_{10}H_{16}$	136		17,25

3-Cyclopentylcyclopentene	$C_{10}H_{16}$	136		7,16,19
1-Cyclopentylcyclopentene	$C_{10}H_{16}$	136		17,20
Bicyclopentylidene	$C_{10}H_{16}$	136		17
Adamantane	$C_{10}H_{16}$	136		17,20,22
1,2-Diethenyl-cyclohexane	$C_{10}H_{16}$	136		7
exo-Tetrahydrodicyclopentadiene	$C_{10}H_{16}$	136		1,3,7,10, 14-20, 22,23,24-26
4-Methyl-1-(1-methyethenyl) cyclohexene	$C_{10}H_{16}$	136		20
Cyclopentylcyclopentane	$C_{10}H_{18}$	138		17
2,6,6-Trimethyl-bicyclo(3.1.1)heptane	$C_{10}H_{18}$	138		7
trans-Decalin	$C_{10}H_{18}$	138		17
1-Methylnaphthalene	$C_{11}H_{10}$	142		22
2-Methylnaphthalene	$C_{11}H_{10}$	142		22
Acenaphthylene	$C_{12}H_8$	152		10,22

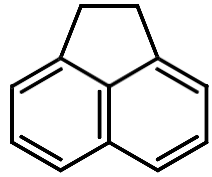
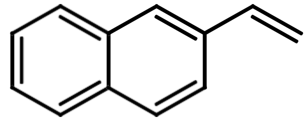
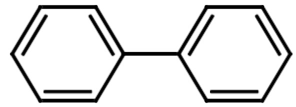
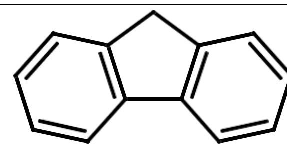
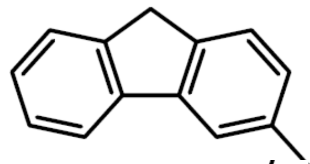
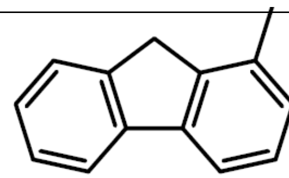
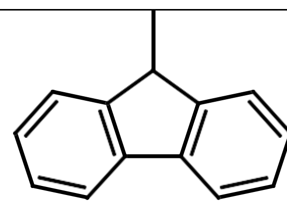
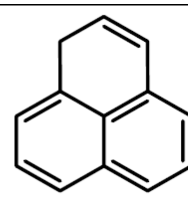
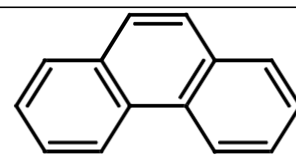
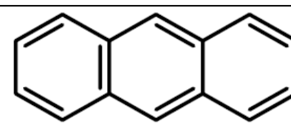
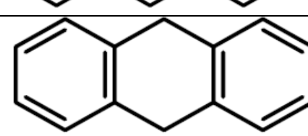
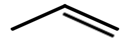
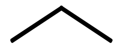
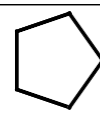
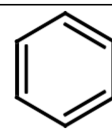
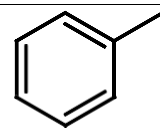
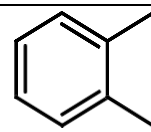
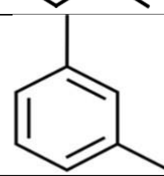
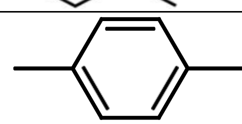
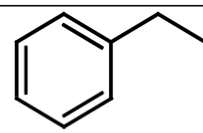
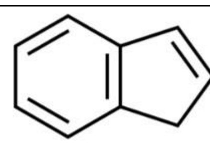
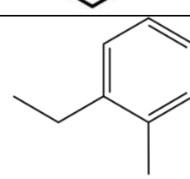
Acenaphthene	$C_{12}H_{10}$	154		22
2-Ethenylnaphthalene	$C_{12}H_{10}$	154		22
Biphenyl	$C_{12}H_{10}$	154		10,22
Fluorene	$C_{13}H_{10}$	166		22
3-Methyl-1H-fluorene	$C_{14}H_{12}$	180		22
1-Methyl-1H-fluorene	$C_{14}H_{12}$	180		22
9-Methyl-1H-fluorene	$C_{14}H_{12}$	180		22
1H-Phenalene	$C_{13}H_{10}$	166		22
Phenanthrene	$C_{14}H_{10}$	178		22
Anthracene	$C_{14}H_{10}$	178		22
9,10-Dihydro-anthracene	$C_{14}H_{12}$	180		22

Table S2. Catalytic decomposition products reported in the preceding experimental studies on JP-10 over HZSM-5 zeolite.

Molecule	Formula	Mass	Structure	Ref.
Methane	CH_4	16	CH_4	34,35
Ethane	C_2H_6	30		34,35
Ethene	C_2H_4	28		34,35
Propene	C_3H_6	42		34,35
Propane	C_3H_8	44		34,35
Butane	C_4H_{10}	58		35
Cyclopentane	C_5H_{10}	70		34
Pentane	C_5H_{12}	72		35
Benzene	C_6H_6	78		34,35
Toluene	C_7H_8	92		34,35
o-xylene	C_8H_{10}	106		35
m-xylene	C_8H_{10}	106		35
p-xylene	C_8H_{10}	106		35
Ethylbenzene	C_8H_{10}	106		35
Indene	C_9H_8	116		35
1-ethyl-2-methylbenzene	C_9H_{12}	120		34,35

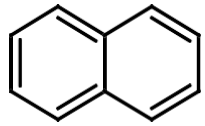
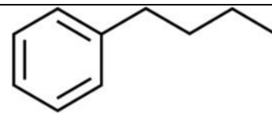
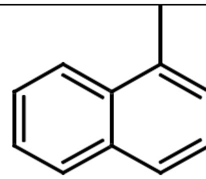
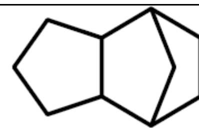
Naphthalene	$C_{10}H_8$	128		34
1-Butylbenzene	$C_{10}H_{14}$	134		34
Methyl naphthalene	$C_{11}H_{10}$	142		34
exo-Tetrahydrodicyclopentadiene	$C_{10}H_{16}$	136		34

Table S3. Vibrational mode assignments for the bands in the FTIR transmission spectrum of JP-10 droplet containing zeolite.

Band	Peak or band wavenumber[a] (cm^{-1})	Molecule	Ref. band (cm^{-1})	Number (symmetry)	vibrational mode[b]
a	3756	H_2O	3756[c]	$3(b_1)$	$\nu_{as}(H_2O)$
b	3714	CO_2	3714.8[d]	$1(\sigma_g^+) + 3(\sigma_u^+)$	combination band
c	3657	H_2O	3657[c]	$1(a_1)$	$\nu(H_2O)$
d	3612	CO_2	3612.8[d]	$1(\sigma_g^+) + 3(\sigma_u^+)$	combination band
e	2956	$C_{10}H_{16}$	2942[e]	68	$\nu(CH)$
f	2929	$C_{10}H_{16}$	2913[e]	62	$\nu(CH_2)$
g	2879	$C_{10}H_{16}$	2865[e]	57	$\nu(CH)$
h	2349 2360	CO_2 CO_2	2349.1[d] 2300 – 2380[f]	$3\ (\sigma_u^+)$	$\nu_{as}(CO_2)$ $\nu_{as}(CO_2)$
i	2279	$^{13}C^{16}O_2$	2283[c]	$3\ (\sigma_u^{+)}$	$\nu_{as}(CO_2)$
j	1600 1455 1467	H_2O $C_{10}H_{16}$ $C_{10}H_{16}$	1595[c] 1456[e] 1468[e]	$2(a_1)$ 54 55	$\delta(OH)$ scissoring (CH_2) scissoring (CH_2)
k	668 649 619, 653, 678, 717	CO_2 $^{13}C^{16}O_2$ CO_2	667.4[d] 649.0[c] 620 -710[f]	$2(\pi_u)$ $2(\pi_u)$ $2(\pi_u)$	$\delta(CO_2)$ $\delta(CO_2)$ $\delta(CO_2)$

[a] Spectral resolution of 4 cm^{-1}.

[b] ν denotes stretch; bend; and as, antisymmetric.

[c] Ref. (61).

[d] Ref. (66).

[e] Ref. (47).

[f] Ref. (67).

Table S4. Vibrational mode assignments for the bands in the FTIR transmission spectrum of JP-10 droplet containing zeolite and aluminum NPs.

Peak or band	Peak or band wavenumber[a] (cm^{-1})	Molecule	Ref. band (cm^{-1})	Number (symmetry)	vibrational mode[b]
a	3755	H_2O	3756[c]	3(b_1)	$\nu_{as}(H_2O)$
b	3714	CO_2	3714.8[d]	1(σ_g^+) +3(σ_u^+)	combination band
c	3656	H_2O	3657[c]	1(a_1)	$\nu(H_2O)$
d	3612	CO_2	3612.8[d]	1(σ_g^+) +3(σ_u^+)	combination band
e	2956	$C_{10}H_{16}$	2942[e]	68	ν(CH)
f	2929	$C_{10}H_{16}$	2913[e]	62	$\nu(CH_2)$
g	2879	$C_{10}H_{16}$	2865[e]	57	ν(CH)
h	2349 2357	CO_2 CO_2	2349.1[d] 2300 – 2380[f]	3 (σ_u^+)	$\nu_{as}(CO_2)$ $\nu_{as}(CO_2)$
i	2278	$^{13}C^{16}O_2$	2283[c]	3 (σ_u^{+})	$\nu_{as}(CO_2)$
j	1600 1455 1467	H_2O $C_{10}H_{16}$ $C_{10}H_{16}$	1595[c] 1456[e] 1468[e]	2(a_1) 54 55	δ(OH) scissoring (CH_2) scissoring (CH_2)
k	668 649 617, 654, 678, 719	CO_2 $^{13}C^{16}O_2$ CO_2	667.4[d] 649.0[c] 620-710[f]	2(π_u) 2(π_u) 2(π_u)	$\delta(CO_2)$ $\delta(CO_2)$ $\delta(CO_2)$

[a] Spectral resolution of 4 cm^{-1}.

[b] ν denotes stretch; bend; and as, antisymmetric.

[c] Ref. (61).

[d] Ref. (66).

[e] Ref. (47).

[f] Ref. (67).

Table S5. Vibrational mode assignments for the bands in the FTIR transmission spectrum of JP-10 droplet containing zeolite, aluminum NPs and span 80.

Band	Peak or band wavenumber[a] (cm^{-1})	Molecule	Ref. band (cm^{-1})	Number (symmetry)	vibrational mode[b]
a	3755	H_2O	3756[c]	$3(b_1)$	$\nu_{as}(H_2O)$
b	3714	CO_2	3714.8[d]	$1(\sigma_g^+) + 3(\sigma_u^+)$	combination band
c	3656	H_2O	3657[c]	$1(a_1)$	$\nu(H_2O)$
d	3612	CO_2	3612.8[d]	$1(\sigma_g^+) + 3(\sigma_u^+)$	combination band
e	2955	$C_{10}H_{16}$	2942[e]	68	$\nu(CH)$
f	2927	$C_{10}H_{16}$	2913[e]	62	$\nu(CH_2)$
g	2877	$C_{10}H_{16}$	2865[e]	57	$\nu(CH)$
h	2349 2356	CO_2 CO_2	2349.1[d] 2300 – 2380[f]	$3\ (\sigma_u^+)$	$\nu_{as}(CO_2)$ $\nu_{as}(CO_2)$
i	2279	$^{13}C^{16}O_2$	2283[c]	$3\ (\sigma_u^{+)}$	$\nu_{as}(CO_2)$
j	1600 1455 1468	H_2O $C_{10}H_{16}$ $C_{10}H_{16}$	1595[c] 1456[e] 1468[e]	$2(a_1)$ 54 55	$\delta(OH)$ scissoring (CH_2) scissoring (CH_2)
k	667 649 617, 655, 681, 719	CO_2 $^{13}C^{16}O_2$ CO_2	667.4[d] 649.0[c] 620-710[f]	$2(\pi_u)$ $2(\pi_u)$ $2(\pi_u)$	$\delta(CO_2)$ $\delta(CO_2)$ $\delta(CO_2)$

[a] Spectral resolution of 4 cm^{-1}.

[b] ν denotes stretch; bend; and as, antisymmetric.

[c] Ref. (61).

[d] Ref. (66).

[e] Ref. (47).

[f] Ref. (67).

Movie M1. Optical high-speed video of the ignition of JP-10 droplet containing zeolite and span 80.

Movie M2. Optical high-speed video of the ignition of JP-10 droplet containing zeolite, aluminum NPs and span 80.