
Supplementary information

Zeolite-catalysed olefin carbonylation based on tuning spatial confinement

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Supplementary Information for

Zeolite-catalysed olefin carbonylation based on tuning spatial confinement

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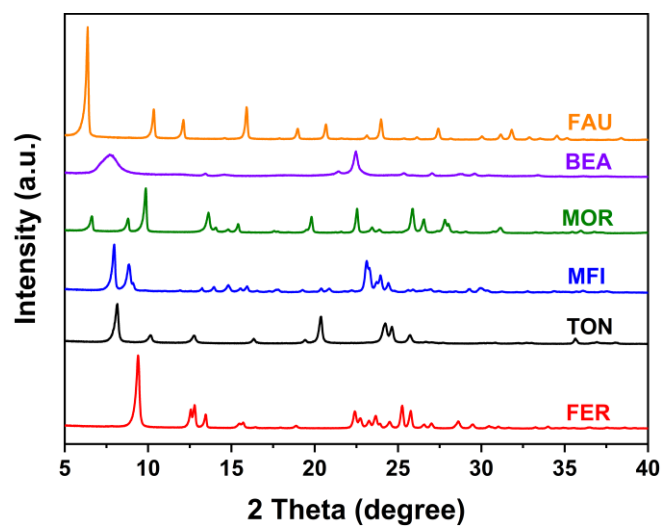
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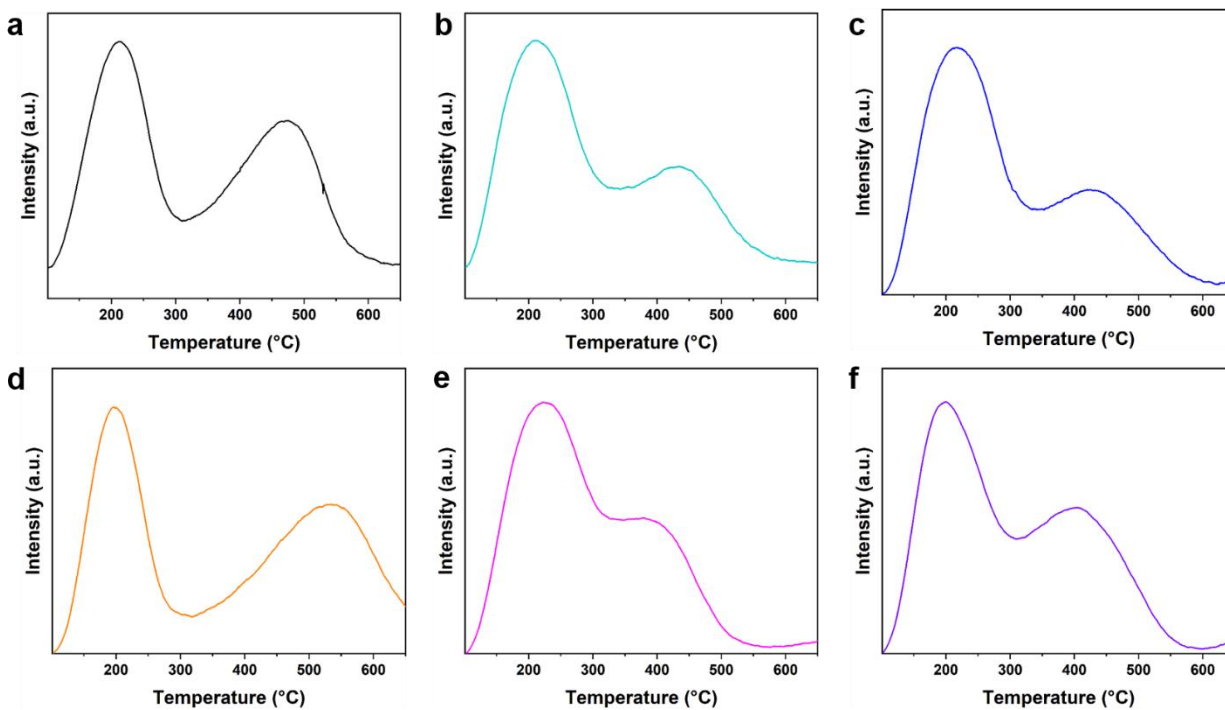
This file includes:

Supplementary Figs. S1 to S28

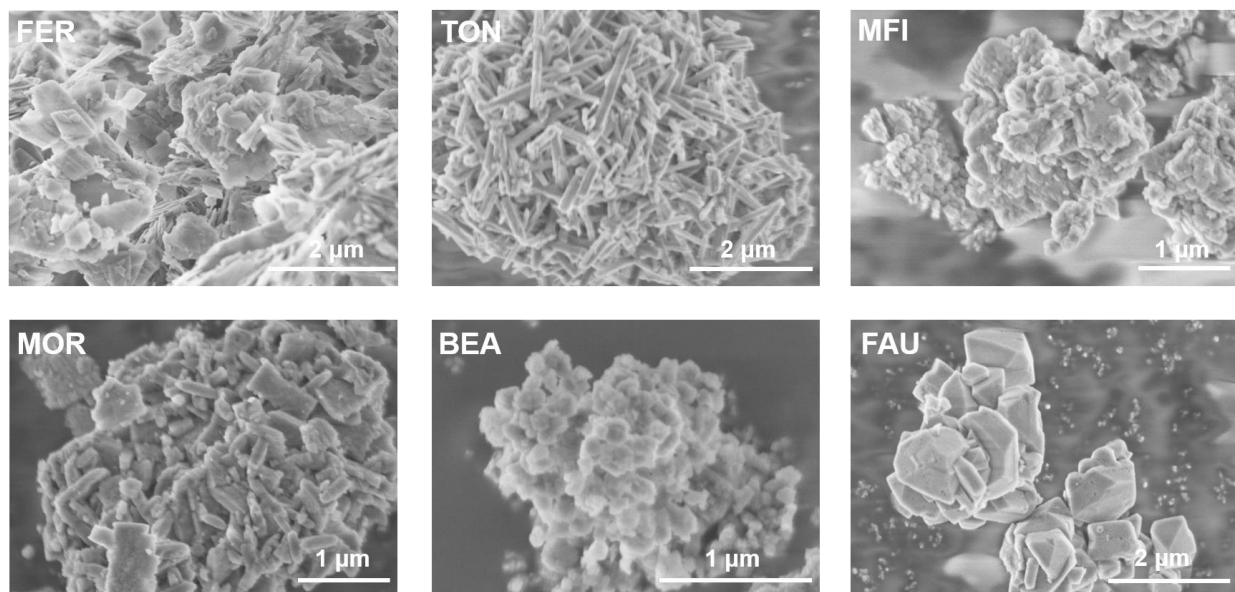
Supplementary Tables. S1 to S18



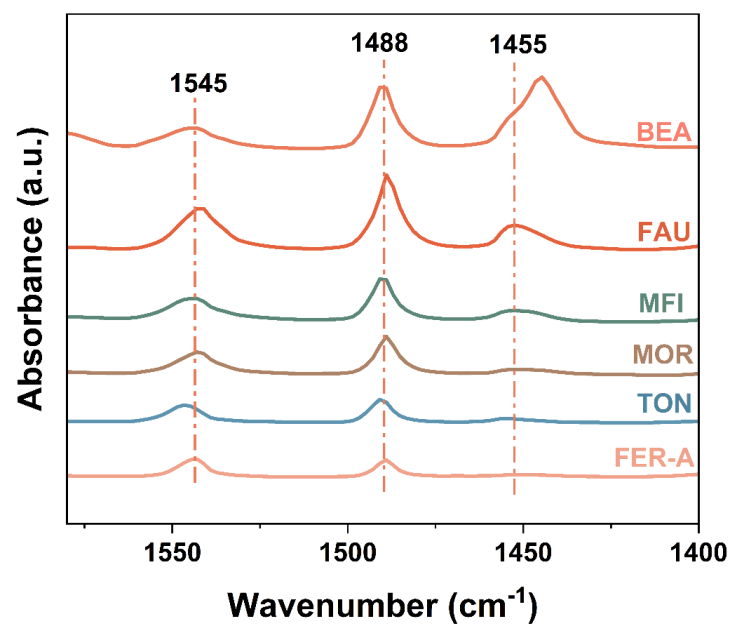
Supplementary Fig. 1. X-ray diffraction patterns of different zeolites. FER is H-FER-A.



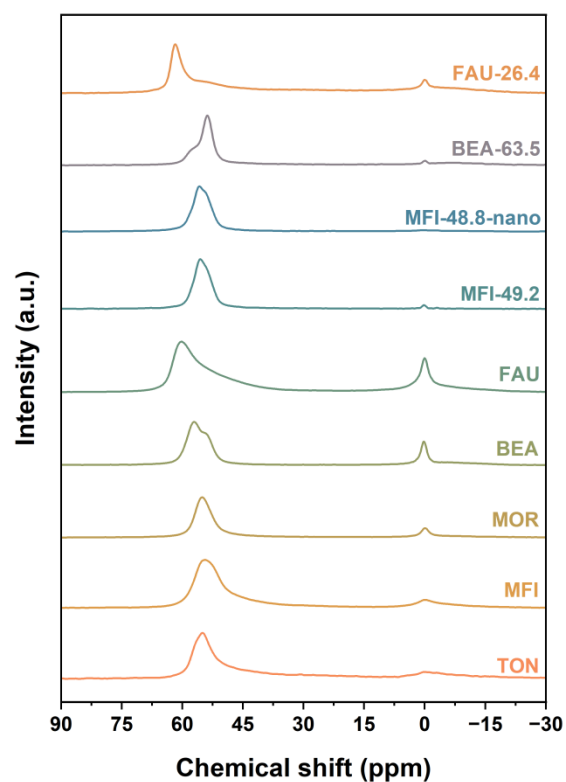
Supplementary Fig. 2. NH₃-TPD profiles of different zeolites. (a) FER (b) TON (c) MFI (d) MOR (e) BEA (f) FAU. FER is H-FER-A.



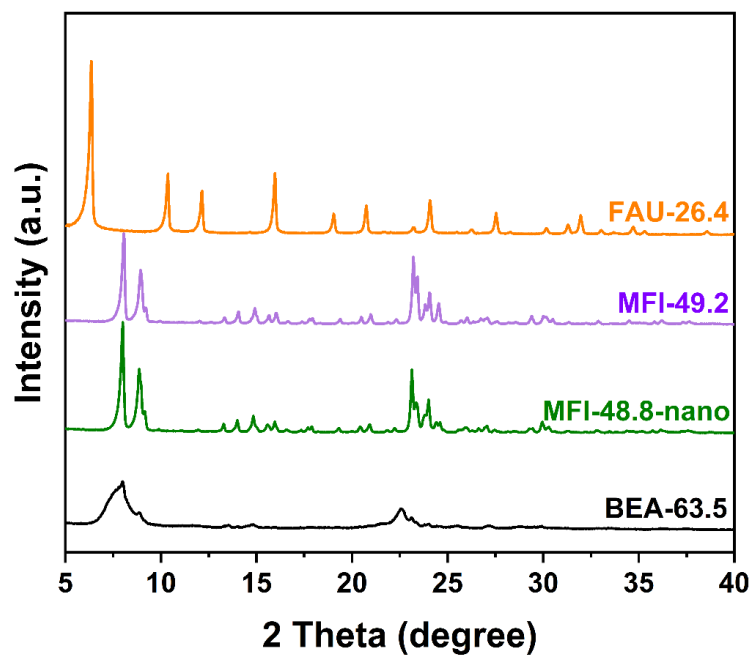
Supplementary Fig. 3. SEM image of different zeolites. FER is H-FER-A.



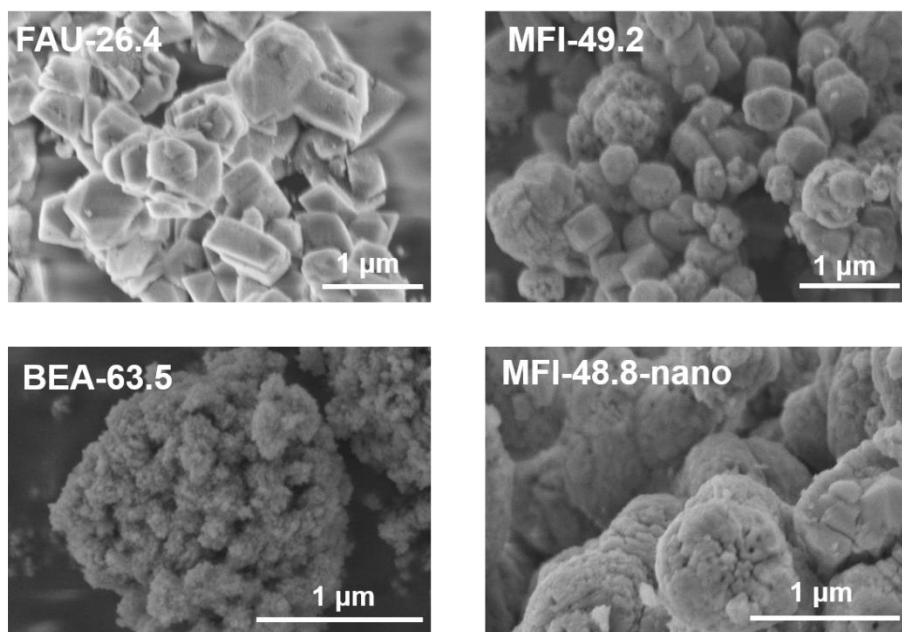
Supplementary Fig. 4. Py-FTIR result of different zeolite topologies.



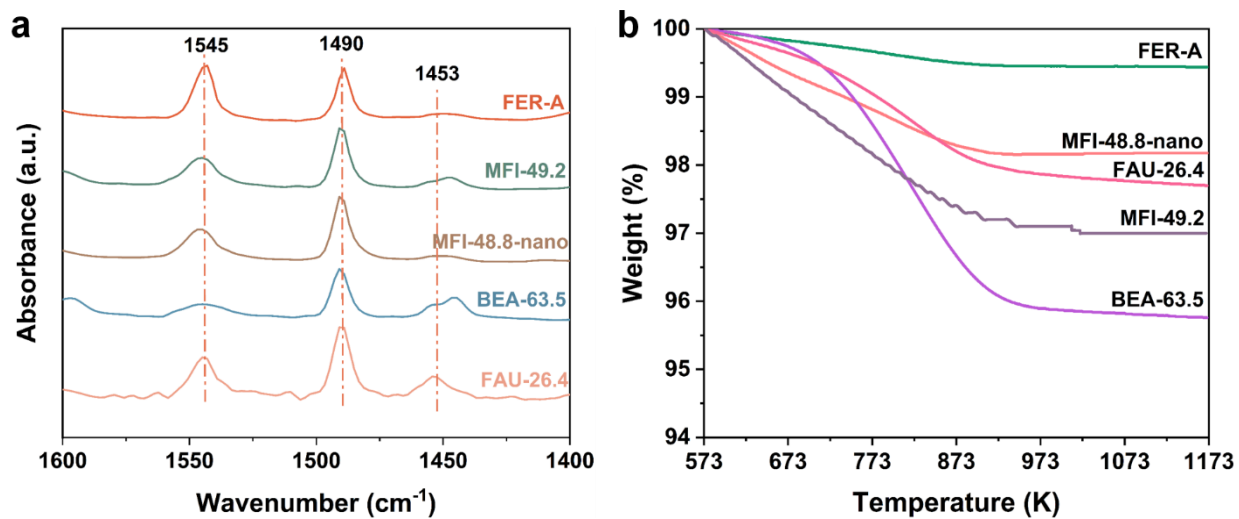
Supplementary Fig. 5. ^{27}Al NMR analysis for different zeolite topologies. Note that MFI-49.2, MFI-48.8-nano, BEA-63.5 and FAU-26.4 are comparative zeolites with high Si/Al ratios.



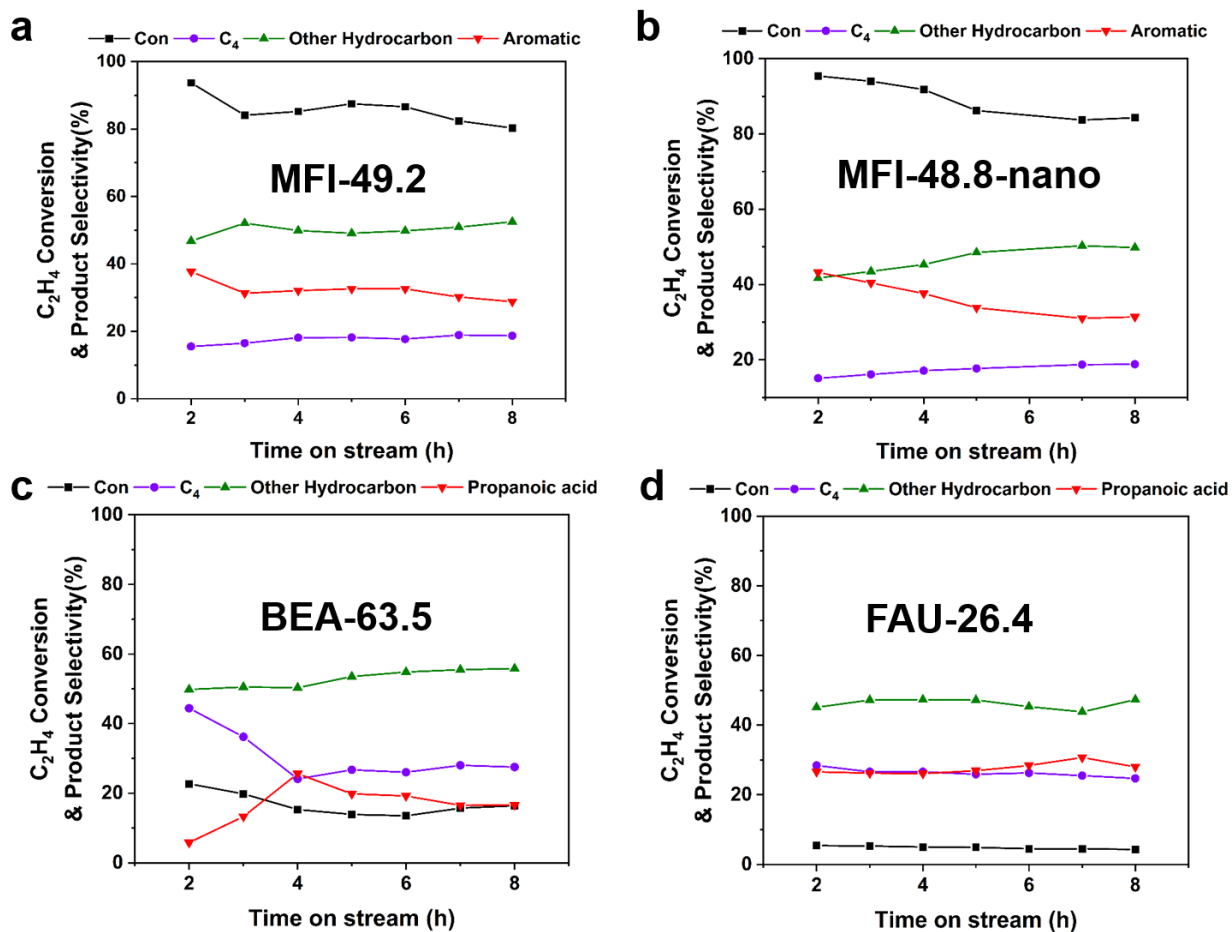
Supplementary Fig. 6. X-ray diffraction patterns of comparative zeolites with high Si/Al ratios.



Supplementary Fig. 7. SEM pictures for comparative zeolites with high Si/Al ratios.

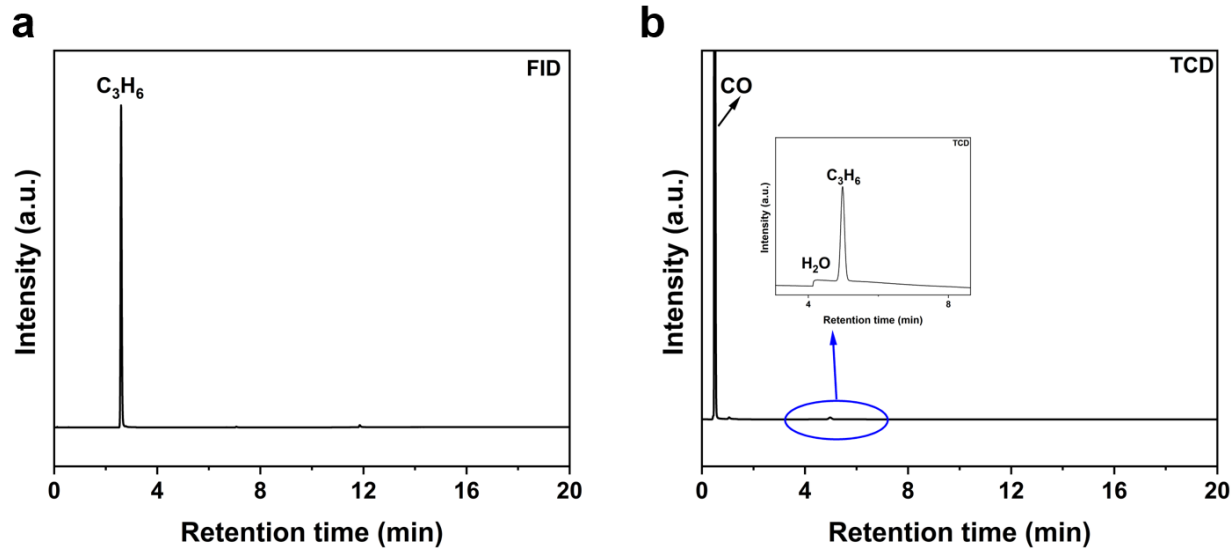


Supplementary Fig. 8. (a) Py-FTIR result of comparative zeolites with high Si/Al ratios; (b) thermal analysis of spent catalysts after ethylene carbonylation reactions.



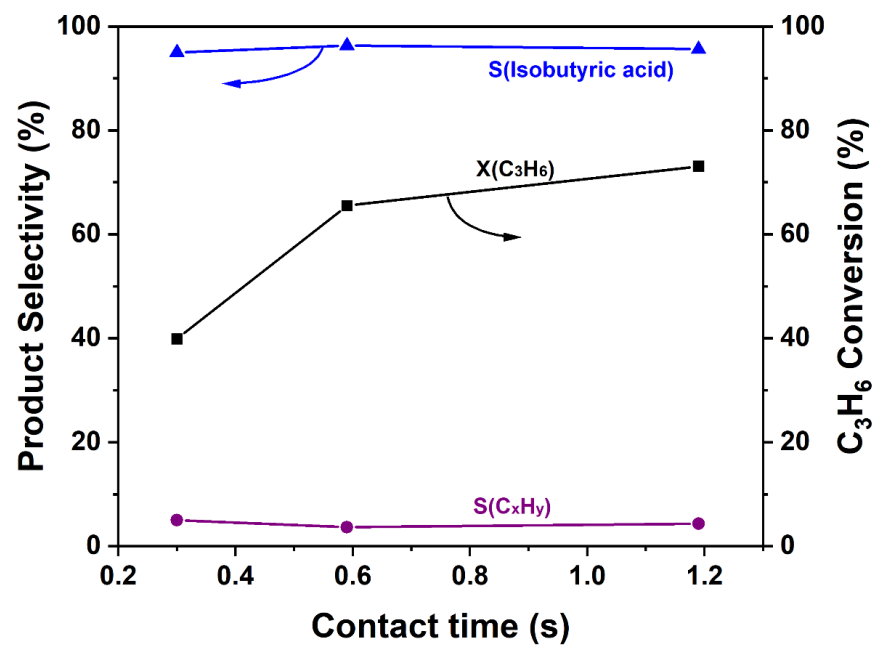
Supplementary Fig. 9. Ethylene carbonylation results over high Si/Al ratios zeolites with different topologies.

Reaction Conditions: 5.1 MPa total pressure, 553 K, $P_{\text{CO}} = 4.62 \times 10^3$ kPa, $P_{\text{C}_2\text{H}_4} = 15.4$ kPa, $P_{\text{H}_2\text{O}} = 76.6$ kPa, WHSV = 0.075 g gcat⁻¹ h⁻¹, N₂ as balance gas.



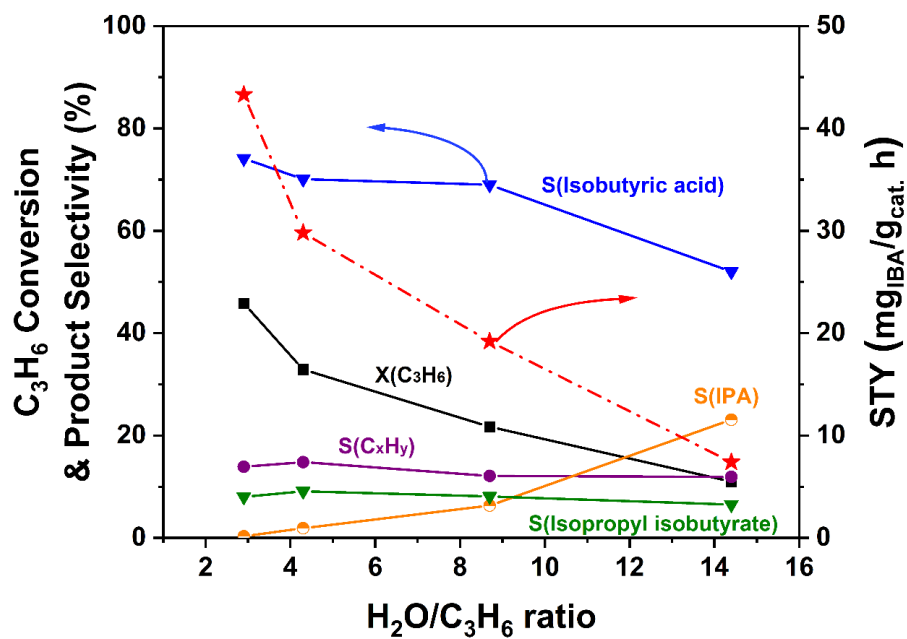
Supplementary Fig. 10. Blank experiments for the carbonylation of propylene under reaction condition.

Reaction Conditions: 5 MPa total pressure, 483 K, $P_{CO} = 4.68 \times 10^3$ kPa, $P_{C_3H_6} = 13.01$ kPa, $P_{H_2O} = 56.2$ kPa, N_2 as balance gas.



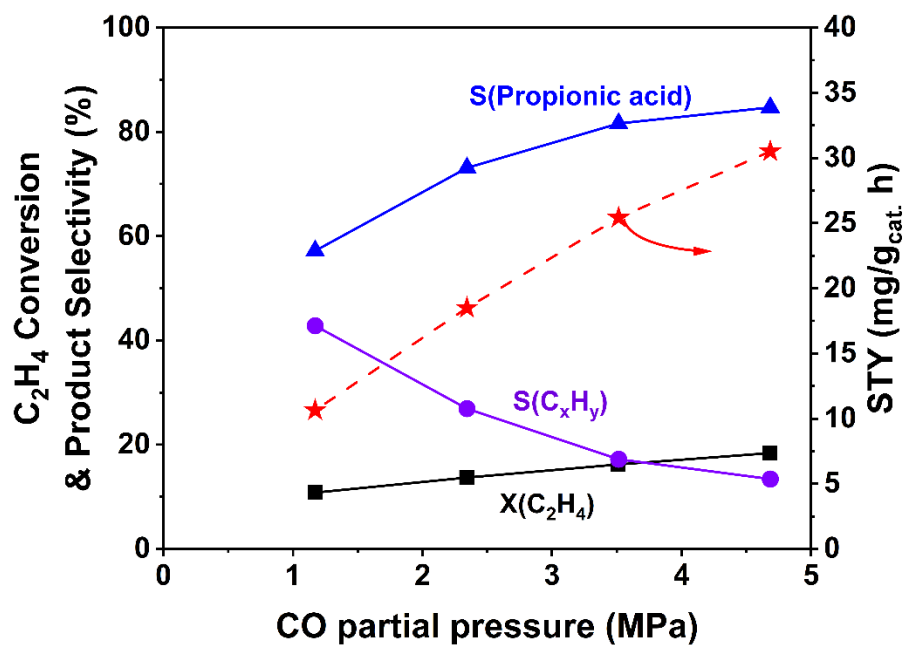
Supplementary Fig. 11. Influence of contact time on propylene carbonylation over FER-A.

Reaction Conditions: 5 MPa total pressure, 493 K, $P_{CO} = 4.68 \times 10^3$ kPa, $P_{C_3H_6} = 13.01$ kPa, $P_{H_2O} = 56.2$ kPa, N_2 as balance gas.



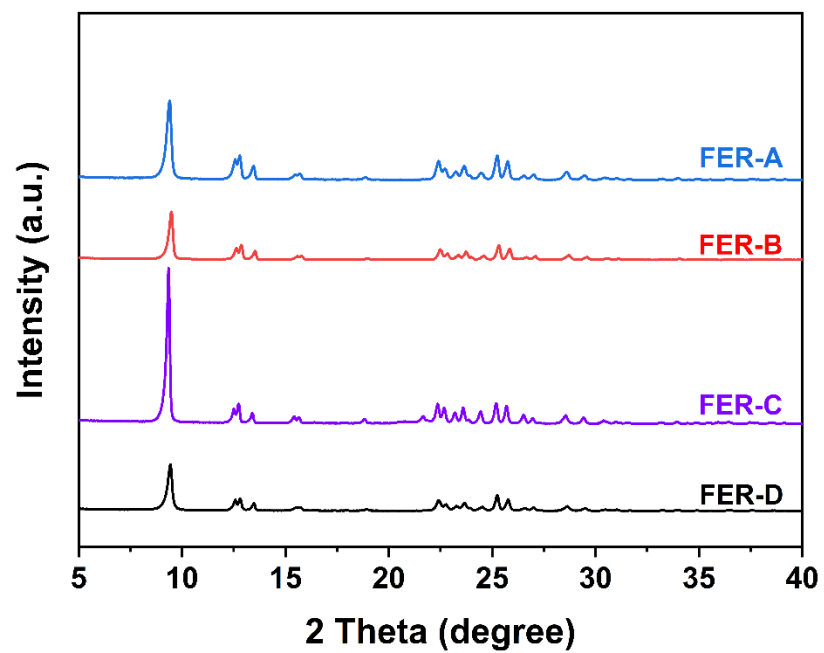
Supplementary Fig. 12. Influence of H₂O partial pressure on propylene carbonylation over FER-A.

Reaction conditions: 5 MPa total pressure, 493 K, $P_{\text{CO}} = 4.68 \times 10^3$ kPa, $P_{\text{C}_3\text{H}_6} = 13.01$ kPa, $P_{\text{H}_2\text{O}} = 37.6\text{--}187.3$ kPa, H₂O/C₃H₆ mole ratio = 2.9–14.4, WHSV = 0.056 g gcat^{−1} h^{−1}, N₂ as balance gas.

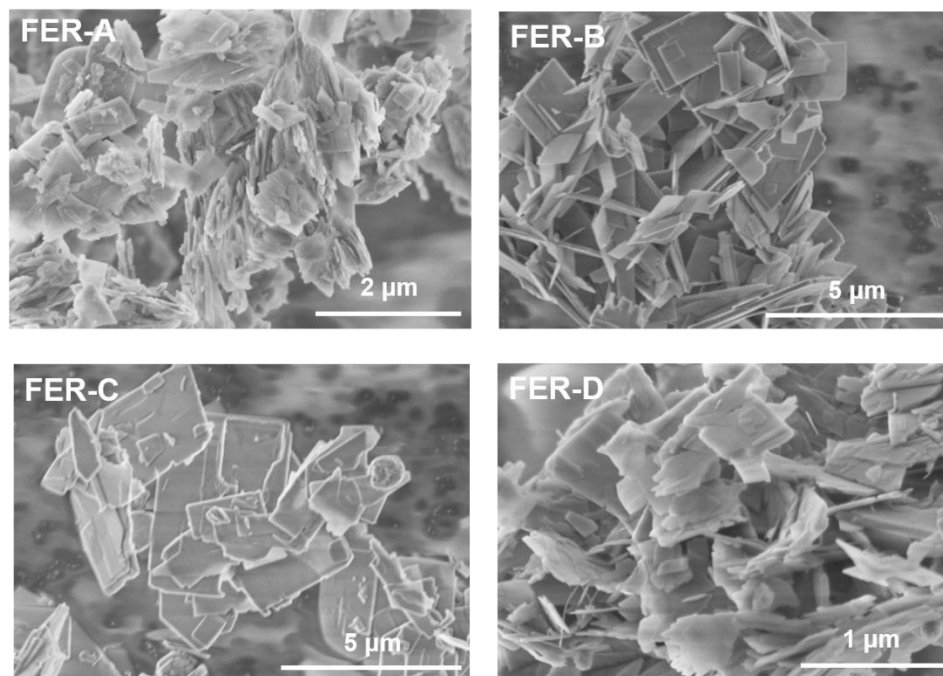


Supplementary Fig. 13. Influence of CO partial pressure on ethylene carbonylation over FER-A.

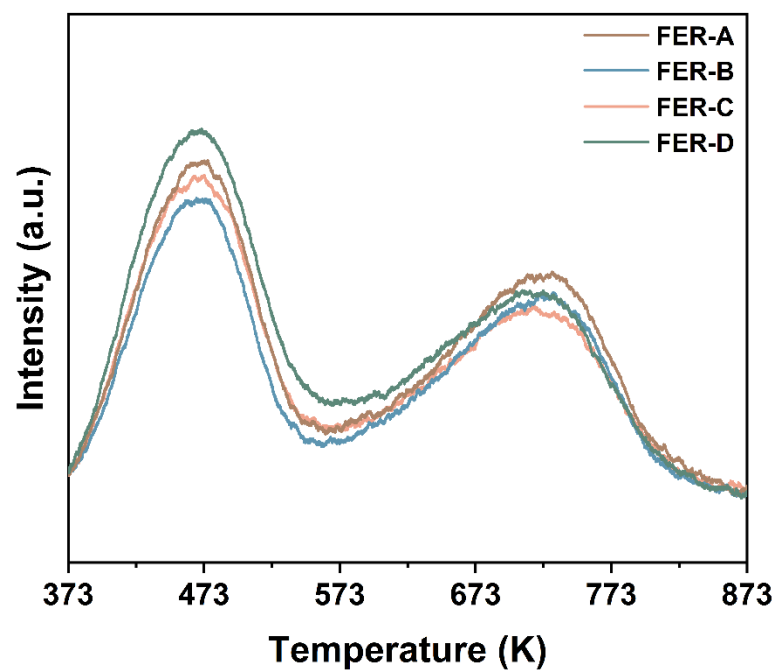
Reaction Conditions: 5 MPa total pressure, 553 K, $P_{\text{CO}} = 1.17\text{--}4.68 \times 10^3$ kPa, $P_{\text{C}_2\text{H}_4} = 13.01$ kPa, $P_{\text{H}_2\text{O}} = 56.2$ kPa, $\text{WHSV} = 0.075$ g g_{cat}⁻¹ h⁻¹, N₂ as balance gas.



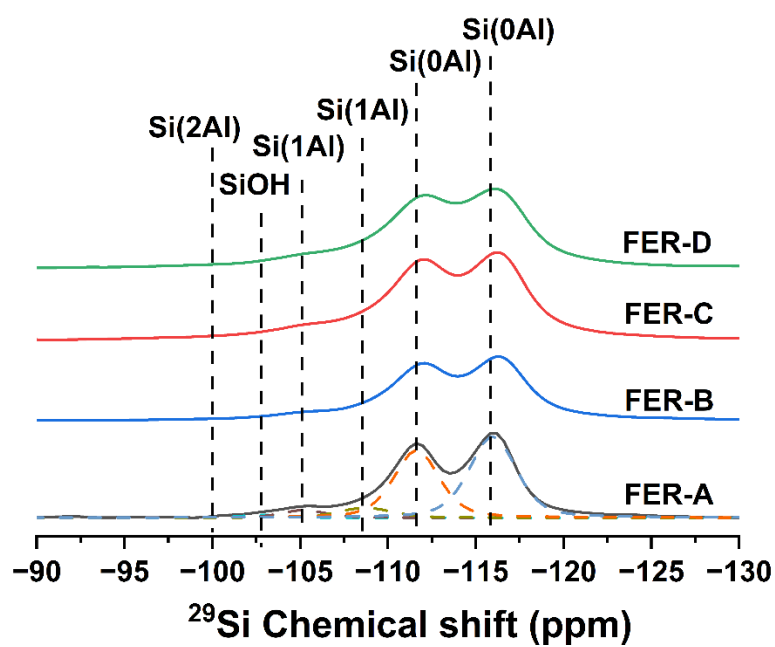
Supplementary Fig. 14. XRD patterns of FER samples.



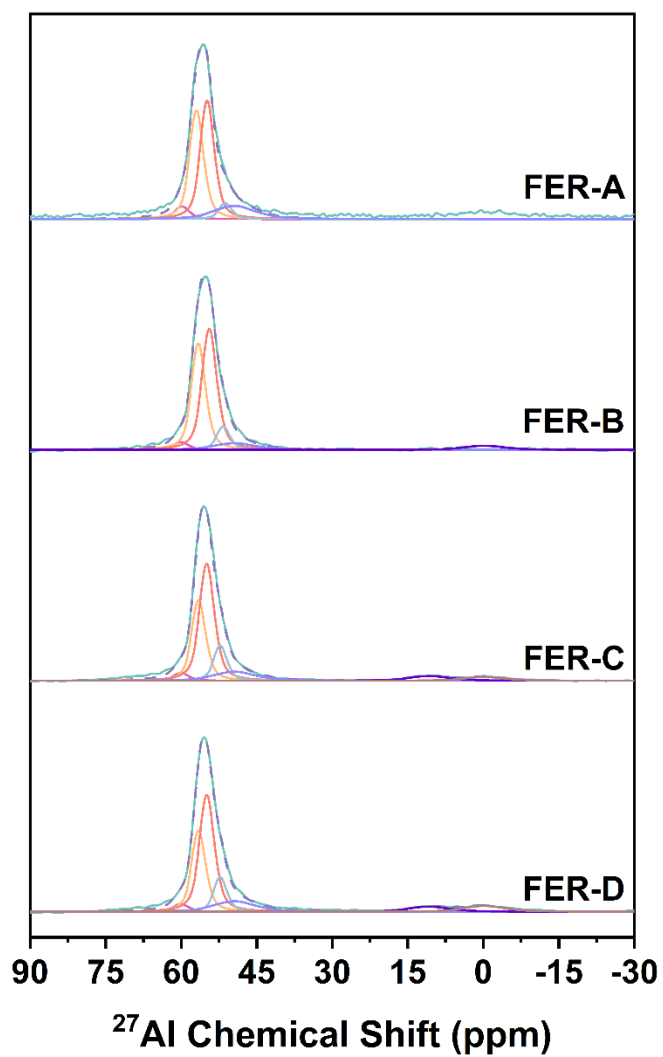
Supplementary Fig. 15. SEM images of FER samples.



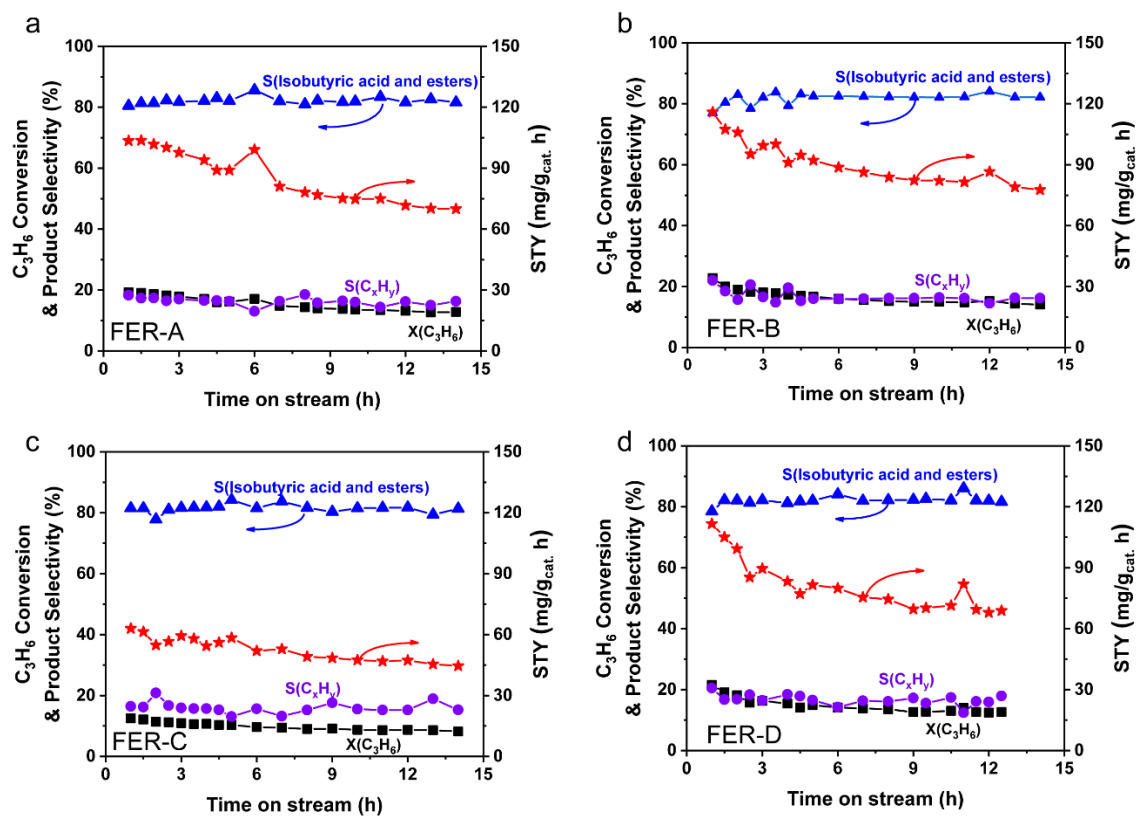
Supplementary Fig. 16. NH₃-TPD result of FER samples.



Supplementary Fig. 17. ^{29}Si NMR result of FER samples.

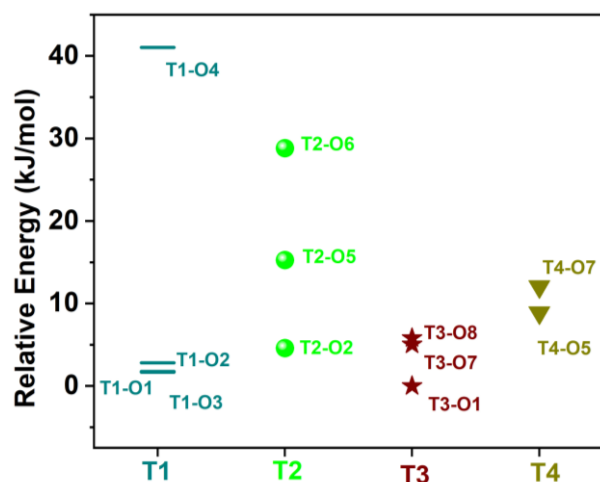


Supplementary Fig. 18. ^{27}Al NMR analysis of T sites distribution for all FER samples.



Supplementary Fig. 19. Comparison of propylene carbonylation reaction on different FER samples.

Reaction Conditions: 2 MPa total pressure, 473 K, $P_{\text{CO}} = 1.52 \times 10^3$ kPa, $P_{\text{C}_3\text{H}_6} = 22.7$ kPa, $P_{\text{H}_2\text{O}} = 29.6$ kPa, $\text{WHSV} = 0.337$ g g_{cat}⁻¹ h⁻¹, N₂ as balance gas.

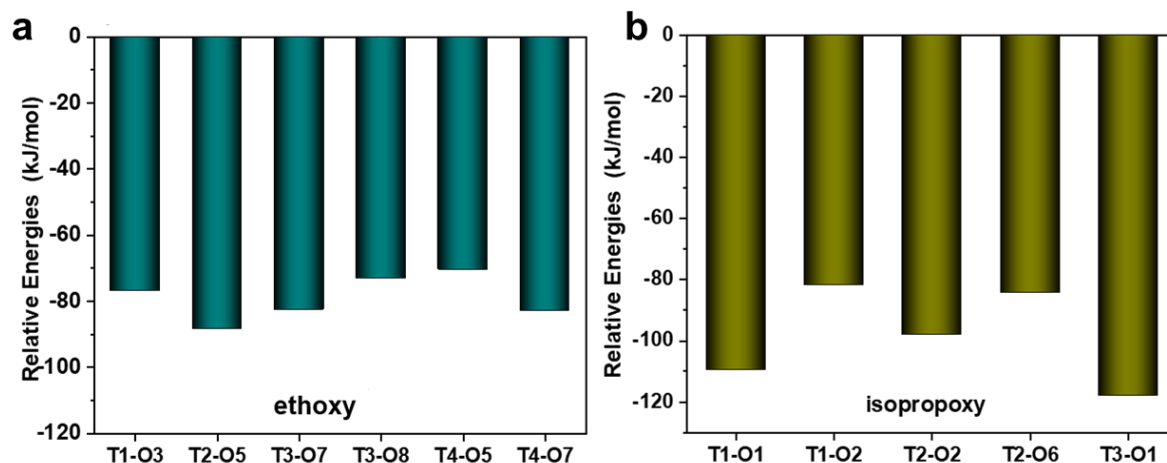


Supplementary Fig. 20. SE (Al substitution energy) of the different Brønsted acid distribution in H-FER framework.

The energy difference (Δ_{SE} in kJ/mol) from the SE of Al3-O1-Si1 (T3-O1) is acquired for comparison. Al substitution energy (SE) is the difference between the energy for the pure siliceous structure and that for the corresponding Al-substituted model. The lower SE associates with a more stabilized corresponding Al-substituted structure.

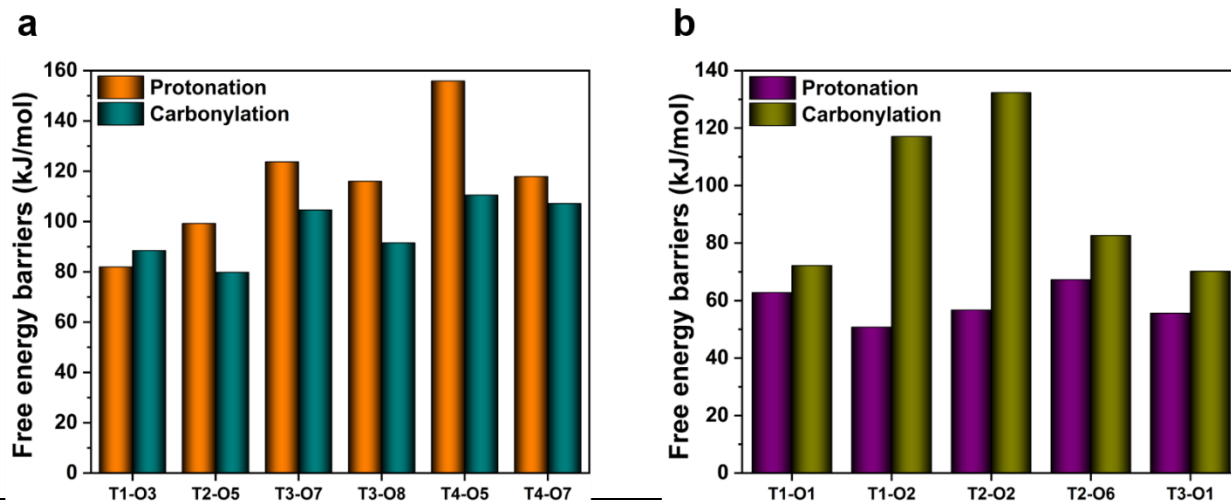
$$SE(Al) = E(Al-OH-Si) - E(Si-O-Si)$$

The energy difference (Δ_{SE} in kJ/mol) from the SE of Al3-O1-Si1 (T3-O1) is acquired for comparison. Al3-O1-Si1 is the lowest one in energy, which indicates that Al3-O1-Si1 (T3-O1) is the most readily to form the Brønsted acid. Owing to the highest substitution energy, Al1-O4-Si1 site is highly unlikely to function as a stable Brønsted acid site.

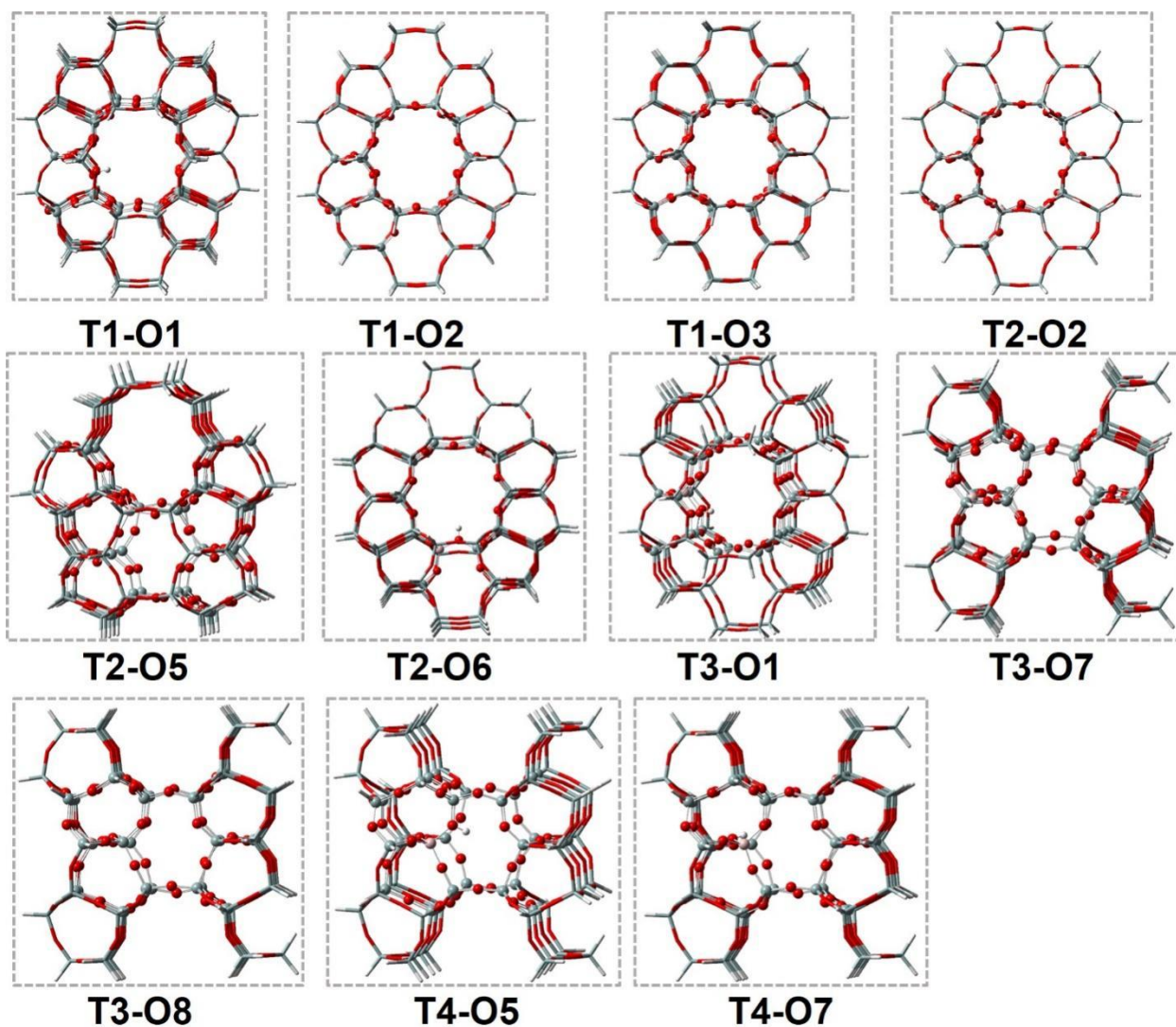


Supplementary Fig. 21. Relative energies (kJ/mol) of the alkoxy species (a: ethoxy b: isopropoxy). Energies of the intermediates are relative to the sum of the neutral species (ethylene and propylene) and the zeolite model.

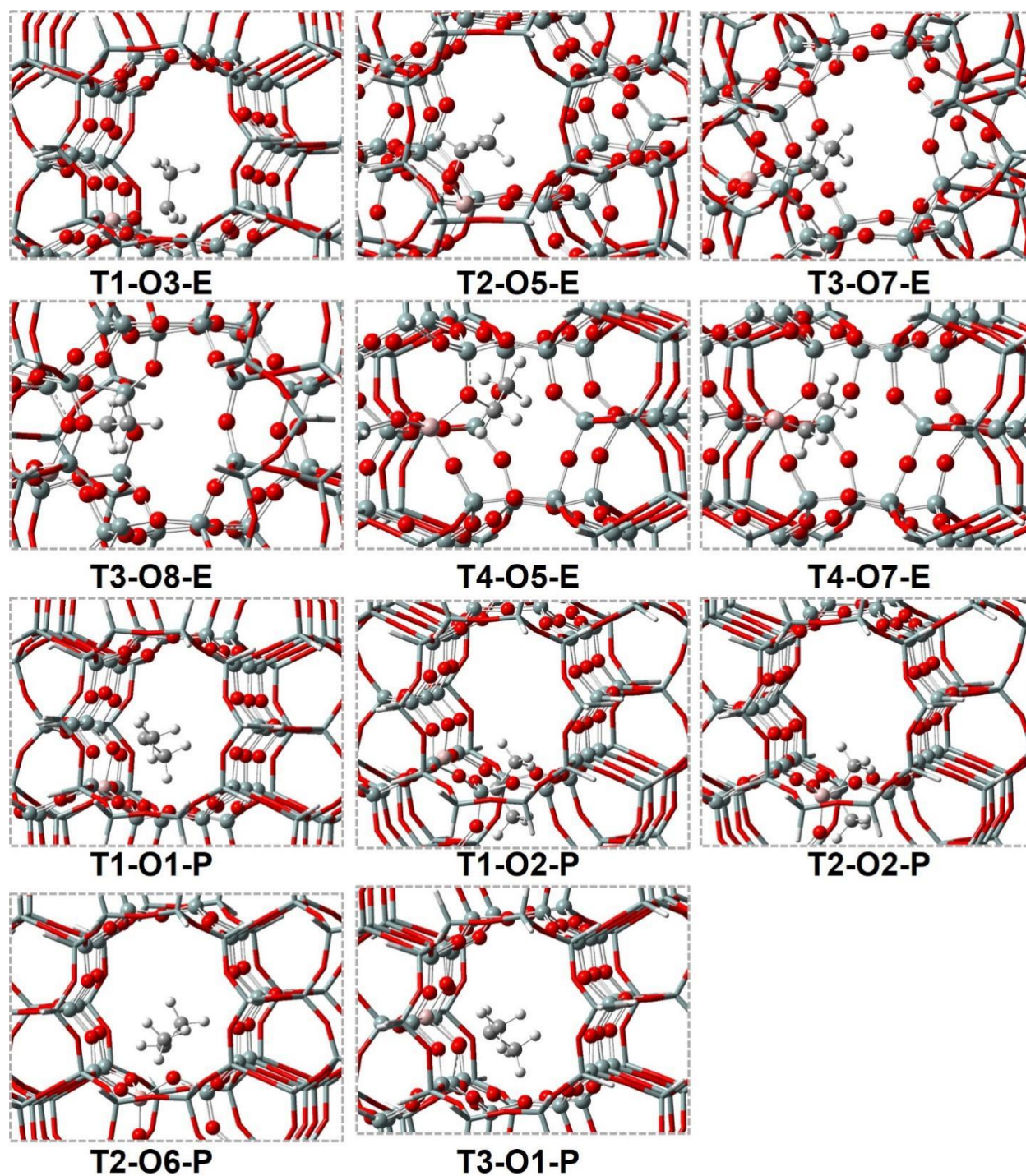
The relative energy of intermediate species represents the stabilization of alkoxy species in the zeolite channel. Lower energy suggests the higher stabilization of adsorption species. For the stability of the alkyl species, ethoxy species shows higher stability over T2-O5 site with the lower energy of -88.4 kJ/mol. For the stability of the isopropoxy species, the isopropoxy species tend to adsorb on T1-O1, and T3-O1 with -109.5 kJ/mol and -118.0 kJ/mol, respectively, suggesting isopropoxy species on the site of T3-O1 are most stable compared to other sites. In addition, the stability of intermediates, along with the stability of the transition state during critical species formation step is critical for elucidating the mechanistic feasibility of this catalytic process.



Supplementary Fig. 22. DFT calculation results for olefin protonation and carbonylation.
 (a) The free energy barriers for ethylene protonation and propionyl cation formation via ethylene carbonylation on different Brønsted acid sites at 553 K.
 (b) The free energy barriers for propylene protonation and isobutyryl cation formation via propylene carbonylation on different Brønsted acid sites at 473 K.

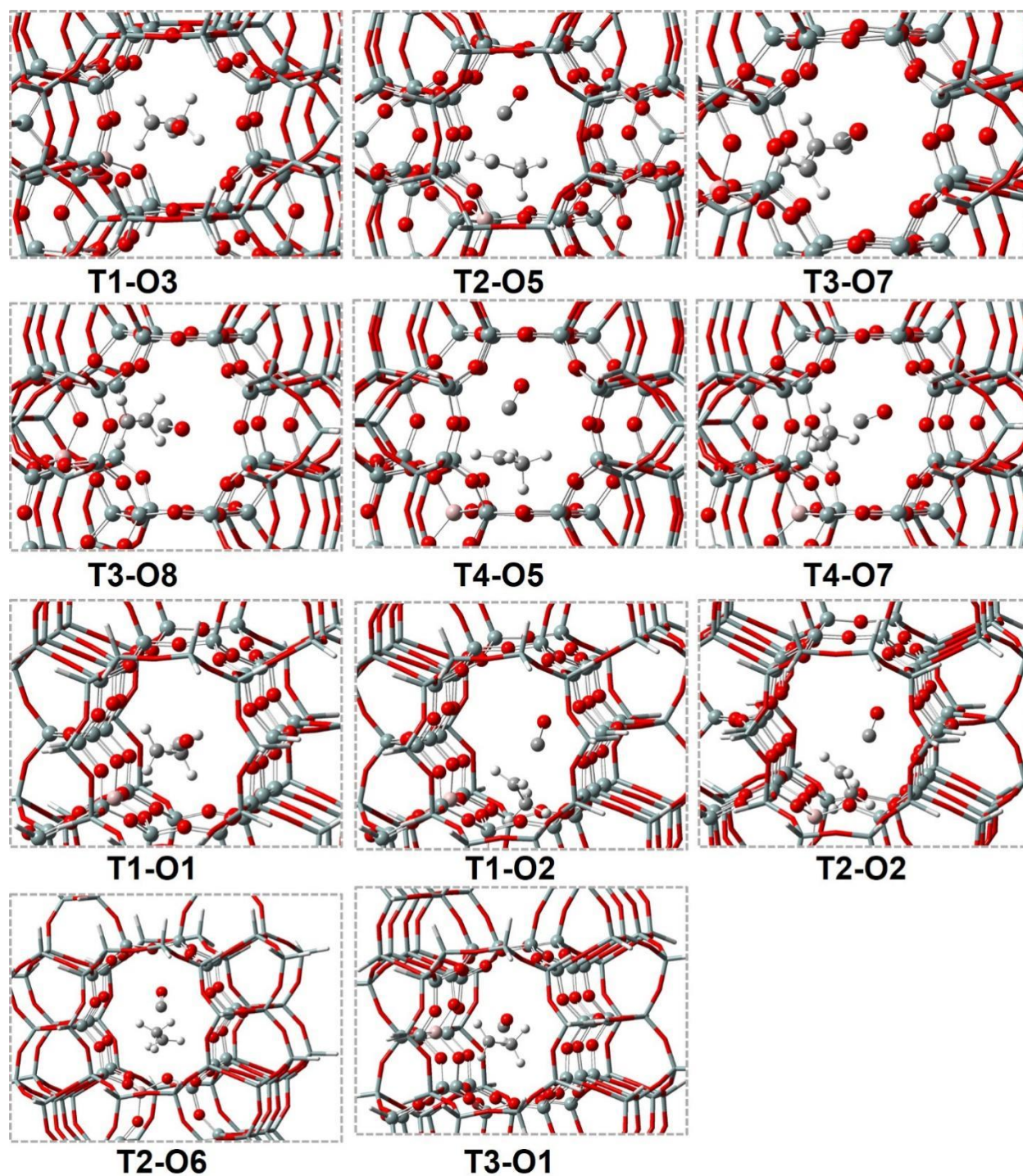


Supplementary Fig. 23. The representative model used in the calculation of the reaction pathway for ethylene carbonylation, propylene carbonylation and olefin dimerization. Considering the existential possibility of T sites, T1-O1, T1-O2, T1-O3, T2-O2, T2-O5, T2-O6, T3-O1, T3-O7, T3-O8, T4-O5 and T4-O7 sites by an extended 96T/96T/96T/96T/100T/86T/96T/74T/74T/74T/74T was selected as the representative pace to study the spatial confinement of the reaction process.

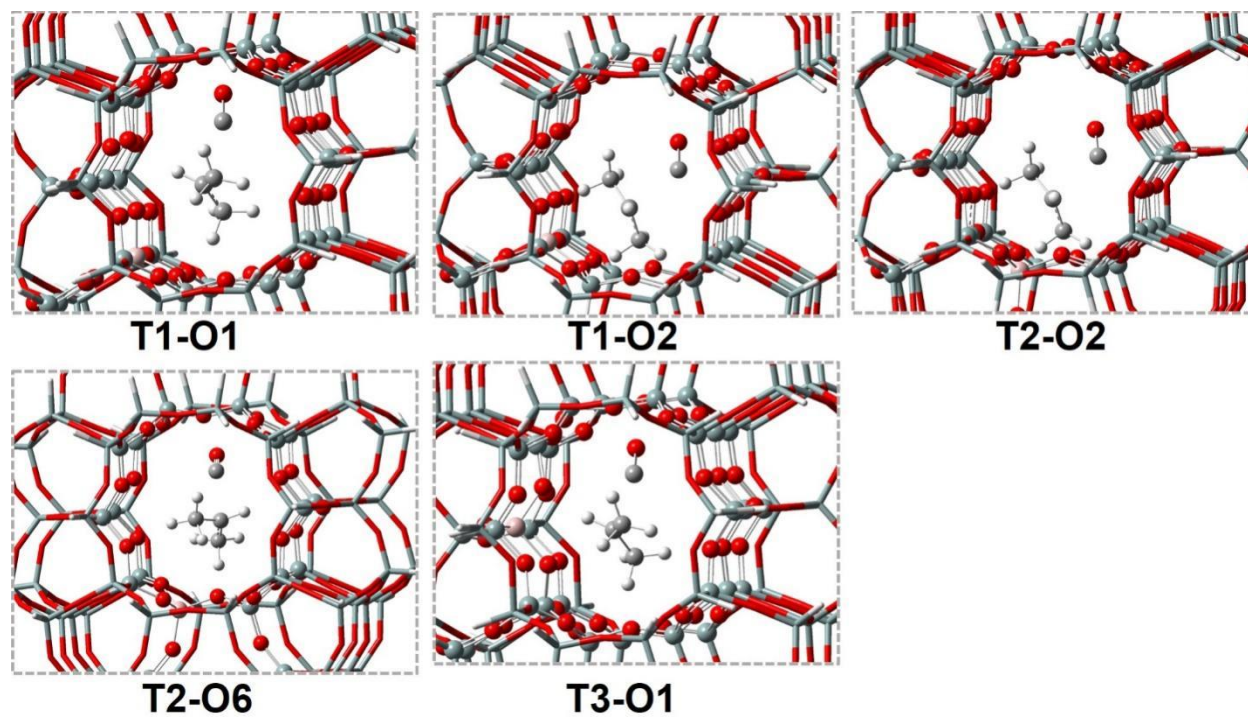


Supplementary Fig. 24. The optimized structures of alkyl species.

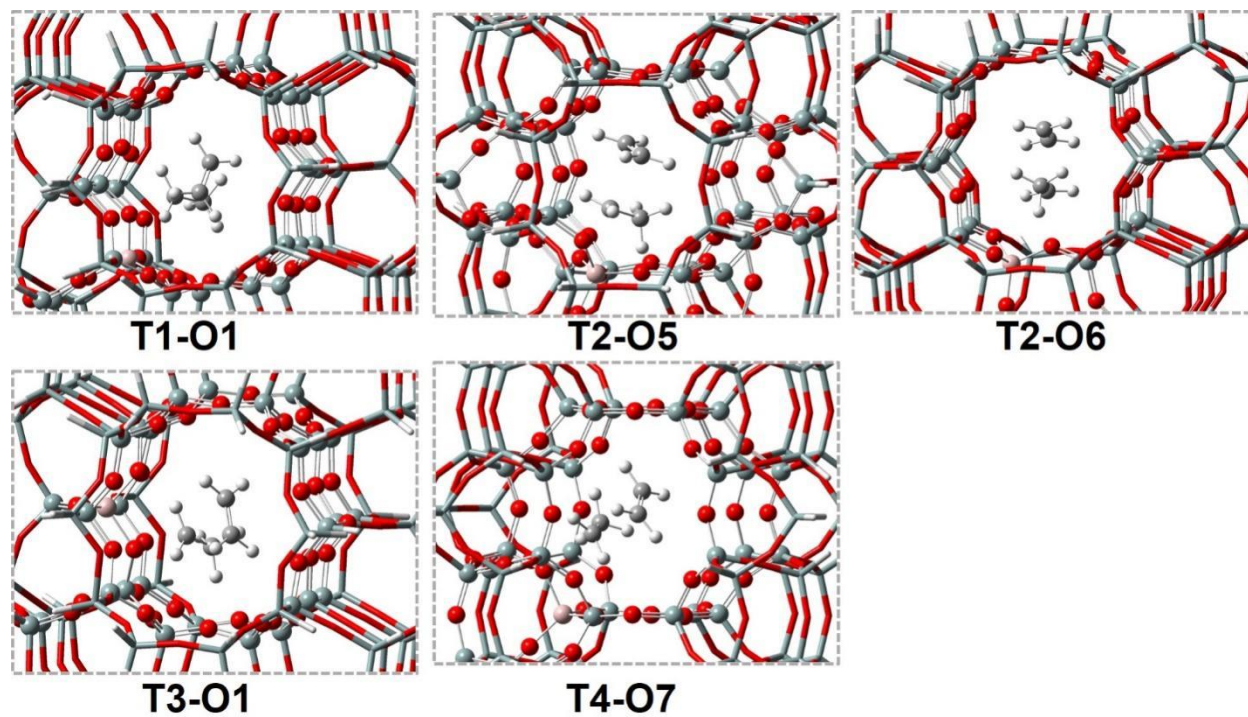
The optimized structures on different Brønsted acid sites (ethoxy on T1-O3, T2-O5, T3-O7, T3-O8, T4-O5 and T4-O7, isopropoxy on T1-O1, T1-O2, T2-O2, T2-O6, T3-O1)



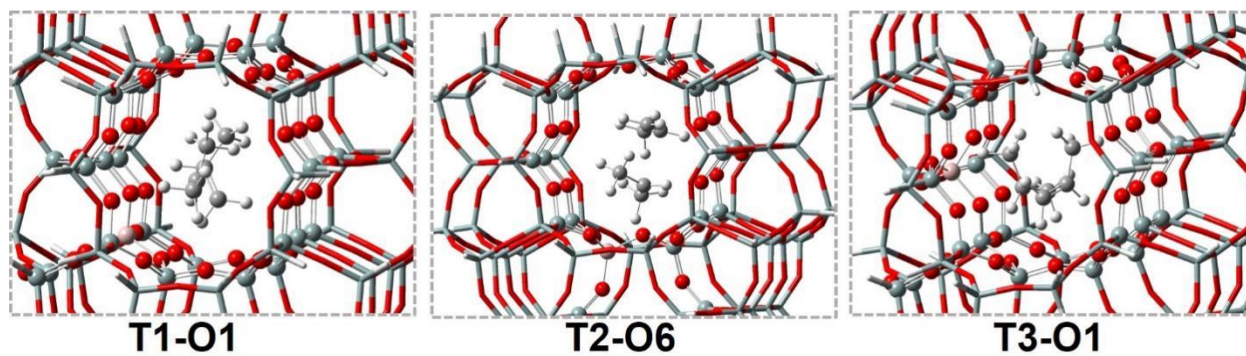
Supplementary Fig. 25. The optimized structures of transition states for propionyl cation via ethylene carbonylation on different Brønsted acid sites. T1-O3, T2-O5, T3-O7, T3-O8, T4-O5 and T4-O7 related to 8-MR cavities, T1-O1, T1-O2, T2-O2, T2-O6 and T3-O1 related to 10-MR.



Supplementary Fig. 26. The optimized structures of transition states for isobutyryl cation formation via propylene carbonylation on different Brønsted acid sites.



Supplementary Fig. 27. The optimized structures of transition states for C_4H_9^+ formation of ethylene dimerization on different Brønsted acid sites.



Supplementary Fig. 28. The optimized structures of transition states for $C_6H_{13}^+$ formation of propylene dimerization.

Supplementary Table 1. Framework information of zeolites with different topology.

Topology	Type material	Channel dimensionality	Channel size	Diameter of maximum included sphere
FER	ZSM-35	2-dimensional	8MR [010] 3.5*4.8 10MR [001] 4.2*5.4	included 6.31 Å diffuse along a:1.56 Å; b:3.4 Å; c:4.69 Å
TON	ZSM-22	1-dimensional	10MR [001] 4.6*5.7	included 5.71 Å diffuse along a:2.31 Å; b:1.56 Å; c:5.11 Å
MFI	ZSM-5	3-dimensional	10MR [100] 5.1*5.5 10MR [010] 5.3*5.6	included 6.36 Å diffuse along a:4.7 Å; b:4.46 Å; c:4.46 Å
MOR	MOR	2-dimensional	8MR [001] 2.6*5.7 12MR [001] 6.5*7.0	included 6.7 Å diffuse along a: 1.57 Å; b:2.95 Å; c:6.45 Å
BEA	Beta	3-dimensional	12MR [100] 6.6*6.7 12MR [001] 5.6*5.6	included 6.59 Å diffuse along a:5.94 Å; b:5.94 Å; c:5.94 Å
FAU	Y	3-dimensional	12MR [111] 7.4*7.4	included 11.24 Å diffuse along a:7.35 Å; b:7.35 Å; c:7.35 Å

Supplementary Table 2. Chemical composition and textural properties of catalysts.

Catalyst	XRF	BET					
	Si/Al mole ratio	S _{BET} ^a (m ² /g)	S _{micro} ^b (m ² /g)	S _{external} ^c (m ² /g)	V _{total} ^d (cm ³ /g)	V _{micro} ^e (cm ³ /g)	V _{meso} ^f (cm ³ /g)
FER-A	32.6	286	234	52	0.213	0.109	0.104
TON	39.8	184.2	147.1	37.1	0.149	0.068	0.081
MFI	14.5	316.2	222.8	93.4	0.231	0.113	0.118
MOR	15.6	366.6	323.5	43.1	0.304	0.165	0.139
BEA	12.5	505.8	385.7	120.1	0.663	0.196	0.467
FAU	5.5	710.9	547.2	163.7	0.421	0.254	0.167

a: BET surface. b:t-plot micropore surface area. c: external surface area. d: total volume absorbed at P/P₀=0.99. e: t-plot micropore volume. f: mesoporous volume.

Supplementary Table 3. Chemical composition and textural properties of comparative zeolites with high Si/Al ratios.

Catalyst	XRF	BET					
	Si/Al mole ratio	S _{BET} ^a (m ² /g)	S _{micro} ^b (m ² /g)	S _{external} ^c (m ² /g)	V _{total} ^d (cm ³ /g)	V _{micro} ^e (cm ³ /g)	V _{meso} ^f (cm ³ /g)
MFI-49.2	49.2	378.7	274.1	104.6	0.237	0.089	0.148
MFI-48.8-nano	48.8	368	135	232.9	0.228	0.061	0.167
BEA-63.5	63.5	527.2	341.1	186.1	0.616	0.165	0.451
FAU-26.4	26.4	761.7	514.2	247.5	0.544	0.258	0.286

a: BET surface. b:t-plot micropore surface area. c: external surface area. d: total volume absorbed at P/P₀=0.99. e: t-plot micropore volume. f: mesoporous volume.

Supplementary Table 4. Carbonylation reaction results over comparative catalysts with high Si/Al ratios.

Catalyst	Si/Al ratios	Conversion & Selectivity		TG analysis (%)
		Conv. (%)	PA Sel. (%)	
FER-A	32.6	14.4	74.4	0.6
MFI-49.2	49.2	82.9	n.d.	3.0
MFI-48.8-nano	48.8	84.3	n.d.	1.8
BEA-63.5	63.5	25.1	17.9	4.2
FAU-26.4	26.4	4.0	28.2	2.3

Reaction Conditions: 5 MPa total pressure, 553 K, $P_{\text{CO}} = 4.62 \times 10^3$ kPa, $P_{\text{C}_2\text{H}_4} = 15.39$ kPa, $P_{\text{H}_2\text{O}} = 76.6$ kPa, WHSV = 0.075 g gcat⁻¹ h⁻¹, N₂ as balance gas.

Supplementary Table 5. Chemical composition and textural properties of comparative FER samples.

Catalyst	XRF	BET					
	Si/Al mole ratio	$S_{\text{BET}}^{\text{a}}$ (m^2/g)	$S_{\text{micro}}^{\text{b}}$ (m^2/g)	$S_{\text{external}}^{\text{c}}$ (m^2/g)	$V_{\text{total}}^{\text{d}}$ (cm^3/g)	$V_{\text{micro}}^{\text{e}}$ (cm^3/g)	$V_{\text{meso}}^{\text{f}}$ (cm^3/g)
FER-A	32.6	286	234	52	0.21	0.11	0.10
FER-B	38.3	302	263	39	0.18	0.12	0.06
FER-C	35.5	273	248	24	0.14	0.12	0.02
FER-D	27.0	314	264	51	0.22	0.12	0.10

a: BET surface. b:t-plot micropore surface area. c: external surface area. d: total volume absorbed at $P/P_0=0.99$. e: t-plot micropore volume. f: mesoporous volume.

Supplementary Table 6. NMR parameters extracted from ^{27}Al MQ MAS NMR.

Magnetic field (T)	Species	δ_{iso} / ppm ^a	C_{q} / MHz	η	P_{Q} / MHz ^b
18.8	Al(IV)-a	62.0 ± 0.2	3.6 ± 0.1	0.60 ± 0.02	3.8
	Al(IV)-b	58.6 ± 0.4	3.5 ± 0.1	0.60 ± 0.02	3.7
	Al(IV)-c	56.2 ± 0.4	3.5 ± 0.1	0.60 ± 0.02	3.7
	Al(IV)-d	53.2 ± 0.4	3.4 ± 0.1	0.60 ± 0.02	3.6
	Al(IV)-2	55.0 ± 0.5	6.0 ± 0.4	0.65 ± 0.02	6.4

^a δ_{iso} value was obtained by fitting the ^{27}Al MQ spectra from F1 slices.

^b $P_{\text{Q}} = C_{\text{q}}(1 + \eta^2/3)^{1/2}$

Supplementary Table 7. Estimated molar amount of T sites of different FER samples.

	T1 (mmol/g)	T2 (mmol/g)	T3 (mmol/g)	T4 (mmol/g)
FER-A	0.024	0.217	0.199	0.027
FER-B	0.012	0.184	0.153	0.031
FER-C	0.013	0.19	0.124	0.051
FER-D	0.016	0.239	0.157	0.063

The distribution of framework Al in each T-sites obtained for each FER sample by combining data from XRF and ^{27}Al NMR.

Supplementary Table 8. Analysis of Brønsted acid site amount and the distribution of FER samples.

	BA concentration (total) ^a mmol/g	BA concentration (10-MR) ^b mmol/g	BA concentration (8-MR) ^c mmol/g	BA concentration (external) ^d mmol/g
FER-A	0.32	0.18	0.14	0.003
FER-B	0.27	0.16	0.11	0.0014
FER-C	0.27	0.18	0.09	0.006
FER-D	0.33	0.14	0.19	0.002

^aThe total acid concentration is determined by using d₃-acetonitrile as the probe molecule. ^bThe acid concentration in 10-MR is determined using pyridine as the probe molecule. ^cThe acid concentration in 8-MR is determined based on difference between total acid concentration and acid concentration in 10-MR. ^dThe external acid concentration is determined using 2,6-di-*tert*-butyl-pyridine as the probe molecule.

Supplementary Table 9. The computed electronic and thermochemical energies for the species in ethylene carbonylation reaction at T1-O3, T2-O5, T3-O7, T3-O8, T4-O5 and T4-O7 sites related to 8-MR cavities at 553K.

T1-O3-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.77692	0.296407	0.481214	0.041107	-39391.2957	-39391.73581	499.4056483
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-39470.38397	0.349907	0.545216	0.078968	-39469.83876	-39470.30501	529.0688053
TS1-Protonation	-39470.35051	0.346274	0.540821	0.076752	-39469.80969	-39470.27376	526.5962137
ZeO-C₂H₅(ads)	-39470.39572	0.354283	0.547187	0.089693	-39469.84854	-39470.30603	519.1353186
CO(g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-39583.71033	0.360641	0.561167	0.081561	-39583.14917	-39583.62877	544.2266207
TS2-Carbonylation	-39583.6769	0.357882	0.557689	0.081831	-39583.11921	-39583.59507	539.9736269
ZeO-propionyl (ads)	-39583.71842	0.363135	0.560887	0.095285	-39583.15754	-39583.62314	528.3357653
T2-O5-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-41374.91827	0.417011	0.685394	0.083908	-41374.23288	-41374.83436	682.5283528
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-41453.535	0.470809	0.749854	0.123338	-41452.78515	-41453.41166	710.9308172
TS1-Protonation	-41453.49545	0.467019	0.744658	0.121613	-41452.75079	-41453.37384	706.9921454
ZeO-C₂H₅(ads)	-41453.54145	0.474874	0.751421	0.133187	-41452.79003	-41453.40827	701.5329263
CO(g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-41566.85766	0.481822	0.765709	0.127877	-41566.09195	-41566.72978	723.7714998
TS2-Carbonylation	-41566.82403	0.478601	0.762196	0.124689	-41566.06184	-41566.69934	723.4027103
ZeO-propionyl (ads)	-41566.88192	0.484193	0.765946	0.136013	-41566.11598	-41566.74591	714.8082131
T3-O7-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-30449.68321	0.308231	0.504687	0.046084	-30449.17852	-30449.63712	520.3937418

C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-30528.29679	0.362053	0.568827	0.085819	-30527.72796	-30528.21097	548.0869956
TS1-Protonation	-30528.25092	0.359199	0.564047	0.087121	-30527.68688	-30528.1638	541.1855259
ZeO-C₂H₅(ads)	-30528.30446	0.366434	0.570478	0.098622	-30527.73399	-30528.20584	535.4324098
CO(g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-30641.62337	0.372321	0.584276	0.088804	-30641.0391	-30641.53457	562.2303562
TS2-Carbonylation	-30641.58488	0.370405	0.581494	0.090177	-30641.00339	-30641.49471	557.5155244
ZeO-propionyl (ads)	-30641.6406	0.375091	0.584462	0.1005	-30641.05614	-30641.5401	549.1695346
T3-O8-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-30449.68567	0.308032	0.50469	0.045334	-30449.18098	-30449.64034	521.2481987
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-30528.30012	0.362298	0.568971	0.08688	-30527.73115	-30528.21324	547.0464419
TS1-Protonation	-30528.2559	0.359349	0.564636	0.086895	-30527.69127	-30528.16901	542.1103364
ZeO-C₂H₅(ads)	-30528.31066	0.366166	0.570623	0.094541	-30527.74003	-30528.21612	540.2278079
CO (g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-30641.62769	0.37352	0.585578	0.085916	-30641.04211	-30641.54178	566.9849038
TS2-Carbonylation	-30641.59085	0.37067	0.582351	0.083953	-30641.0085	-30641.5069	565.5505963
ZeO-propionyl (ads)	-30641.65143	0.375203	0.585104	0.095472	-30641.06633	-30641.55596	555.6034928
T4-O5-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-30449.69478	0.285355	0.465892	0.038357	-30449.22889	-30449.65642	485.1397361
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-30528.30146	0.338387	0.530291	0.072717	-30527.77117	-30528.22874	519.2260976
TS1-Protonation	-30528.2479	0.33574	0.525359	0.078563	-30527.72254	-30528.16934	506.9959034
ZeO-C₂H₅(ads)	-30528.30481	0.343985	0.532304	0.089136	-30527.7725	-30528.21567	502.8790779
CO (g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-30641.62682	0.350484	0.546286	0.082776	-30641.08053	-30641.54404	525.9618957
TS2-Carbonylation	-30641.58377	0.347845	0.542908	0.081849	-30641.04086	-30641.50192	523.1806556
ZeO-propionyl (ads)	-30641.64865	0.352448	0.54616	0.090196	-30641.10249	-30641.55845	517.3991712

T4-O7-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-30449.68625	0.285876	0.466243	0.04044	-30449.22001	-30449.64581	483.1743718
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-30528.30071	0.339282	0.530264	0.078944	-30527.77045	-30528.22177	512.1294531
TS1-Protonation	-30528.25533	0.335902	0.525293	0.078509	-30527.73204	-30528.17882	506.9822865
ZeO-C₂H₅(ads)	-30528.3072	0.343637	0.532117	0.08934	-30527.77508	-30528.21786	502.4353958
CO (g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-30641.6271	0.349906	0.546109	0.079748	-30641.08099	-30641.54735	529.1970306
TS2-Carbonylation	-30641.58803	0.347918	0.543135	0.081502	-30641.04489	-30641.50652	523.8319946
ZeO-propionyl (ads)	-30641.64908	0.352485	0.546282	0.090121	-30641.1028	-30641.55896	517.6227143

Supplementary Table 10. The computed electronic and thermochemical energies for the species in propylene carbonylation reaction at T1-O1, T1-O2, T2-O2, T2-O6 and T3-O1 related to 10-MR at 473K.

T1-O1-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.78639	0.287614	0.426637	0.096359	-39391.35975	-39391.69003	438.1661367
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085
ZeOH-C₃H₆(ads)	-39509.72807	0.37053	0.520248	0.165882	-39509.20782	-39509.56218	470.1226881
TS1-Protonation	-39509.70249	0.366624	0.5155	0.16423	-39509.18699	-39509.53826	466.0153532
ZeO-C₃H₇(ads)	-39509.73338	0.373845	0.522103	0.172566	-39509.21127	-39509.56081	463.7162539
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-39623.03702	0.379875	0.534735	0.165656	-39622.50229	-39622.87137	489.6418155
TS2-Carbonylation	-39623.00692	0.375225	0.529904	0.163075	-39622.47701	-39622.84384	486.6568338
ZeO-isobutyryl (ads)	-39623.06942	0.382822	0.535265	0.176294	-39622.53415	-39622.89313	476.2319508
T1-O2-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.77488	0.296018	0.438659	0.101316	-39391.33622	-39391.67356	447.5389794
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085
ZeOH-C₃H₆(ads)	-39509.7074	0.378911	0.532531	0.170176	-39509.17487	-39509.53723	480.7213634
TS1-Protonation	-39509.68558	0.373759	0.525973	0.167702	-39509.15961	-39509.51788	475.3032898
ZeO-C₃H₇(ads)	-39509.71234	0.383309	0.53445	0.180881	-39509.17789	-39509.53146	469.0653412
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-39623.03392	0.388497	0.546673	0.172322	-39622.48724	-39622.8616	496.6359595
TS2-Carbonylation	-39622.99183	0.385256	0.542342	0.17487	-39622.44949	-39622.81696	487.5098752
ZeO-isobutyryl (ads)	-39623.04635	0.392577	0.547978	0.184512	-39622.49837	-39622.86183	482.195281

T2-O2-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.74252	0.295701	0.438512	0.099754	-39391.30401	-39391.64276	449.4162013
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085
ZeOH-C₃H₆(ads)	-39509.68209	0.379051	0.532611	0.170414	-39509.14948	-39509.51167	480.5117513
TS1-Protonation	-39509.65656	0.374223	0.526471	0.166505	-39509.13009	-39509.49006	477.5519761
ZeO-C₃H₇(ads)	-39509.68583	0.382669	0.534016	0.180629	-39509.15181	-39509.5052	468.8238894
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-39623.00531	0.387852	0.546357	0.16984	-39622.45895	-39622.83547	499.5095019
TS2-Carbonylation	-39622.96073	0.385084	0.541948	0.175715	-39622.41878	-39622.78502	485.8661453
ZeO-isobutyryl (ads)	-39623.02551	0.392272	0.547837	0.183883	-39622.47767	-39622.84162	482.8426904
T2-O6-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-35138.43151	0.211402	0.297396	0.069202	-35138.13411	-35138.36231	302.735524
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085
ZeOH-C₃H₆(ads)	-35256.36313	0.293481	0.390751	0.136136	-35255.97238	-35256.22699	337.7871699
TS1-Protonation	-35256.33686	0.289394	0.3857	0.135519	-35255.95116	-35256.20134	331.9047658
ZeO-C₃H₇(ads)	-35256.36889	0.297632	0.392742	0.147209	-35255.97615	-35256.22168	325.7384568
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-35369.68802	0.30469	0.405755	0.144971	-35369.28226	-35369.54305	345.9713265
TS2-Carbonylation	-35369.65114	0.298912	0.400346	0.139601	-35369.2508	-35369.51154	345.9195868
ZeO-isobutyryl (ads)	-35369.69629	0.306063	0.40521	0.15206	-35369.29108	-35369.54423	335.8436151
T3-O1-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.7763	0.287052	0.426395	0.094056	-39391.3499	-39391.68224	440.90038
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085

ZeOH-C₃H₆(ads)	-39509.72072	0.370246	0.520088	0.165109	-39509.20064	-39509.55562	470.9359298
TS1-Protonation	-39509.69777	0.367161	0.516693	0.163368	-39509.18108	-39509.53441	468.7416365
ZeO-C₃H₇(ads)	-39509.72649	0.373239	0.521501	0.17235	-39509.20499	-39509.55414	463.2041637
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-39623.04373	0.379644	0.534385	0.166313	-39622.50935	-39622.87742	488.3058704
TS2-Carbonylation	-39623.01425	0.376031	0.530421	0.163593	-39622.48382	-39622.85065	486.6555071
ZeO-isobutyryl (ads)	-39623.05863	0.382794	0.535227	0.175707	-39622.52341	-39622.88293	476.9602863

Supplementary Table 11. The computed electronic and thermochemical energies for ethylene carbonylation to propanoic acid over T2-O5 at 553 K.

T2-O5-Ethylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-41374.91827	0.417011	0.685394	0.083908	-41374.23288	-41374.83436	682.5283528
C₂H₄(g)	-78.58320565	0.051597	0.060798	0.007871	-78.52240765	-78.57533465	60.05821936
ZeOH-C₂H₄(ads)	-41453.535	0.470809	0.749854	0.123338	-41452.78515	-41453.41166	710.9308172
TS1-Protonation	-41453.49545	0.467019	0.744658	0.121613	-41452.75079	-41453.37384	706.9921454
ZeO-C₂H₅(ads)	-41453.54145	0.474874	0.751421	0.133187	-41452.79003	-41453.40827	701.5329263
CO(g)	-113.3085872	0.005114	0.011273	-0.034167	-113.2973142	-113.3427542	51.56244427
ZeO-C₂H₅ CO(ads)	-41566.85766	0.481822	0.765709	0.127877	-41566.09195	-41566.72978	723.7714998
TS2-Carbonylation	-41566.82403	0.478601	0.762196	0.124689	-41566.06184	-41566.69934	723.4027103
ZeO-propionyl (ads)	-41566.88192	0.484193	0.765946	0.136013	-41566.11598	-41566.74591	714.8082131
H₂O(g)	-76.42790711	0.021854	0.02896	-0.015212	-76.39894711	-76.44311911	50.12359789
ZeO- propionyl H₂O(ads)	-41643.32728	0.509291	0.798551	0.150811	-41642.52873	-41643.17647	735.0144729
Propanoic acid	-41643.37653	0.511389	0.798566	0.153931	-41642.57797	-41643.2226	731.4911149

Supplementary Table 12. The computed electronic and thermochemical energies for propylene carbonylation to isobutyric acid over T3-O1 at 473 K.

T3-O1-Propylene Carbonylation	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeOH	-39391.7763	0.287052	0.426395	0.094056	-39391.3499	-39391.68224	440.90038
C₃H₆(g)	-117.8990803	0.080065	0.089116	0.037396	-117.8099643	-117.8616843	68.61478085
ZeOH-C₃H₆(ads)	-39509.72072	0.370246	0.520088	0.165109	-39509.20064	-39509.55562	470.9359298
TS1-Protonation	-39509.69777	0.367161	0.516693	0.163368	-39509.18108	-39509.53441	468.7416365
ZeO-C₃H₇(ads)	-39509.72649	0.373239	0.521501	0.17235	-39509.20499	-39509.55414	463.2041637
CO (g)	-113.3085872	0.005114	0.010368	-0.027662	-113.2982192	-113.3362492	50.45282513
ZeO-C₃H₇ CO(ads)	-39623.04373	0.379644	0.534385	0.166313	-39622.50935	-39622.87742	488.3058704
TS2-Carbonylation	-39623.01425	0.376031	0.530421	0.163593	-39622.48382	-39622.85065	486.6555071
ZeO-isobutyryl (ads)	-39623.05863	0.382794	0.535227	0.175707	-39622.52341	-39622.88293	476.9602863
H₂O(g)	-76.42790711	0.021854	0.027893	-0.008903	-76.40001411	-76.43681011	48.81572846
ZeO-isobutyryl H₂O(ads)	-39699.50948	0.408491	0.566433	0.1958	-39698.94305	-39699.31368	491.7034429
Isobutyric acid	-39699.5536	0.406007	0.560908	0.19667	-39698.9927	-39699.35693	483.2194614

Supplementary Table 13. The computed electronic and thermochemical energies for C₄H₉⁺ formation of ethylene dimerization.

T1-O1- ethylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₂H₅ C₂H₄ (ads)	-39549.01589	0.398937	0.609901	0.106004	-39548.40599	-39548.90988	571.7905145
TS-ethylene dimerization	-39548.9833	0.398004	0.60765	0.110048	-39548.37565	-39548.87325	564.6473458
ZeO-C₄H₉ (ads)	-39549.05012	0.405005	0.612266	0.122282	-39548.43785	-39548.92784	556.0029202
T2-O6- ethylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₂H₅ C₂H₄ (ads)	-35295.65491	0.323804	0.462136	0.108955	-35295.19277	-35295.54595	400.7675094
TS-ethylene dimerization	-35295.61628	0.320963	0.45858	0.108294	-35295.1577	-35295.50798	397.4824461
ZeO-C₄H₉ (ads)	-35295.6533	0.321778	0.459859	0.109396	-35295.19345	-35295.54391	397.6832946
T3-O1- ethylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₂H₅ C₂H₄ (ads)	-39549.00944	0.399773	0.610255	0.109888	-39548.39918	-39548.89955	567.7848933
TS-ethylene dimerization	-39548.97558	0.398112	0.607347	0.112687	-39548.36823	-39548.86289	561.3089499
ZeO-C₄H₉ (ads)	-39549.0464	0.403875	0.611487	0.119757	-39548.43491	-39548.92664	557.9841708

T4-O7- ethylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₂H₅ C₂H₄ (ads)	-30606.91231	0.398715	0.609184	0.11496	-30606.30312	-30606.79735	560.8142046
TS-ethylene dimerization	-30606.88121	0.394725	0.605168	0.111419	-30606.27604	-30606.76979	560.2752045
ZeO- C₄H₉(ads)	-30606.95142	0.401579	0.609887	0.121566	-30606.34153	-30606.82985	554.1158527
T2-O5- ethylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(553K) (Hartree)	G(553K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₂H₅ C₂H₄ (ads)	-41532.14245	0.528741	0.831715	0.151495	-41531.31073	-41531.99095	771.8707271
TS-ethylene dimerization	-41532.11883	0.527714	0.830865	0.152314	-41531.28796	-41531.96651	769.9768512
ZeO- C₄H₉(ads)	-41532.18762	0.532727	0.834371	0.158739	-41531.35325	-41532.02888	766.6645543

Supplementary Table 14. The computed electronic and thermochemical energies for $C_6H_{13}^+$ formation of propylene dimerization.

T1-O1- propylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₃H₇ C₃H₆(ads)	-39627.642	0.460343	0.635661	0.227083	-39627.00634	-39627.41492	542.0435021
TS-propylene dimerization	-39627.59966	0.460494	0.633785	0.234589	-39626.96587	-39627.36507	529.5967915
ZeO- C₆H₁₃(ads)	-39627.69798	0.461211	0.635424	0.22854	-39627.06256	-39627.46944	539.7961425
T2-O6- propylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₃H₇ C₃H₆(ads)	-35374.29768	0.380016	0.498617	0.196787	-35373.79906	-35374.10089	400.4253539
TS-propylene dimerization	-35374.26599	0.377506	0.495374	0.19678	-35373.77061	-35374.06921	396.1322868
ZeO- C₆H₁₃(ads)	-35374.32331	0.386484	0.501665	0.211971	-35373.82164	-35374.11134	384.3250256
T3-O1- propylene dimerization	Single Point Energy (Hartree)	Zero-point correction Energy (Hartree)	Hcorr (Hartree)	Gcorr (Hartree)	H(473K) (Hartree)	G(473K) (Hartree)	S_{total} (cal/(mol·K))
ZeO-C₃H₇ C₃H₆(ads)	-39627.61552	0.460558	0.635391	0.228584	-39626.98013	-39627.38694	539.6939898
TS-propylene dimerization	-39627.58497	0.459909	0.633419	0.233071	-39626.95155	-39627.35189	531.1251021
ZeO- C₆H₁₃(ads)	-39627.64047	0.461491	0.635566	0.230818	-39627.0049	-39627.40965	536.9623998

Supplementary Table 15. Calculated Harmonic Vibrational Frequencies (cm^{-1}) for adsorbed species and transition states of ethylene carbonylation reaction at T1-O3, T2-O5, T3-O7, T3-O8, T4-O5 and T4-O7 sites related to 8-MR cavities and T1-O1, T1-O2, T2-O2, T2-O6 and T3-O1 related to 10-MR at 553K.

FileName	Number of Frequencies	Full Frequency List (cm^{-1})	Imaginary Frequencies
T1-O3-ZeOH-C ₂ H ₄ (ads)	231	35.2492, 45.8838, 54.1950, 56.8483, 65.4850, 70.8933, 73.4734, 85.7515, 90.6717, 91.3280, 99.2689, 108.7917, 114.0745, 119.5703, 120.7099, 127.6373, 132.0312, 136.1187, 139.7620, 144.8142, 147.4433, 154.1732, 156.3154, 159.3776, 165.0404, 165.1926, 167.8776, 172.8931, 176.0670, 178.9212, 181.2490, 182.6170, 185.3768, 187.3688, 191.7100, 196.6707, 198.4001, 202.5236, 206.5263, 208.4138, 212.0004, 215.2353, 216.2484, 220.7195, 225.4512, 227.0296, 232.6591, 235.5770, 239.4437, 241.3553, 244.6255, 249.8037, 252.3469, 254.3715, 257.1027, 258.7389, 259.2748, 263.1748, 264.7449, 269.4520, 271.9011, 274.3231, 276.5980, 282.1259, 284.5189, 285.6532, 285.8575, 290.3743, 293.5145, 295.6787, 299.0168, 302.1312, 305.8609, 308.1679, 313.2011, 317.5984, 317.6637, 321.4527, 324.6330, 327.9309, 329.0313, 334.1824, 335.0672, 343.0515, 349.9705, 353.2810, 359.3833, 365.5371, 368.4294, 376.3360, 383.7490, 385.7320, 388.7660, 393.9357, 396.0976, 401.1622, 410.0141, 413.8415, 420.7045, 422.1303, 423.7062, 427.9945, 439.2930, 442.0433, 446.7474, 454.9195, 459.1637, 461.6635, 484.2452, 487.2323, 499.5977, 505.5515, 509.2711, 520.6974, 530.7013, 538.6759, 545.2586, 559.4909, 568.5502, 568.6824, 589.1149, 595.5934, 603.8194, 612.7012, 621.4666, 652.4326, 657.5438, 674.8550, 686.5879, 693.9510, 703.1943, 703.3911, 705.9831, 716.1303, 719.6872, 724.7614, 726.7989, 735.4353, 739.6161, 741.3323, 751.1960, 753.5760, 758.4448, 763.0167, 770.7376, 772.7589, 776.4011, 780.4060, 783.0372, 788.1635, 789.6232, 793.7193, 795.2556, 800.9900, 804.0782, 805.3346, 807.4005, 808.8723, 810.9101, 814.4341, 816.8611, 822.4872, 824.5298, 827.8749, 832.7920, 833.9407, 836.4092, 836.7553, 840.7655, 841.9434, 844.6632, 848.3033, 852.9229, 855.2040, 857.7813, 860.1381, 863.7807, 873.8559, 903.6963, 1044.1615, 1049.0908, 1090.0034, 1101.6502, 1104.0808, 1121.0864, 1124.5783, 1134.6987, 1139.0341, 1142.4840, 1151.9603, 1160.2976, 1165.2329, 1175.2261, 1183.7470, 1189.2898, 1197.8396, 1198.8365, 1205.3691, 1215.3055, 1218.1785, 1220.9707, 1226.5761, 1233.9575, 1238.0570, 1242.1050, 1247.6712, 1253.0563, 1254.2469, 1256.7508, 1258.8014, 1265.6549, 1270.5940, 1276.2309, 1282.4568, 1283.9787, 1296.4085, 1314.9315, 1315.6184, 1342.0061, 1362.1144, 1389.2371, 1398.7888, 1400.1222, 1415.3265, 1493.5736, 1712.0444, 3172.1900, 3184.8979, 3195.2683, 3263.6793, 3286.5063	None
T1-O3-Protonation-TS	231	-355.9244, 38.1301, 50.1550, 52.7968, 55.4512, 64.4058, 77.1156, 77.6157, 89.1588, 93.5206, 95.0464, 103.2858, 110.5278, 115.3789, 122.7507, 124.9792, 130.7861, 132.9963, 135.5927, 138.3168, 140.6727, 149.9800, 155.7713, 159.4907, 162.9704, 164.7346, 166.1237, 170.6771, 174.6146, 176.6917, 180.1199, 180.8009, 183.6880, 187.1322, 188.6599, 193.3894, 197.2748, 198.5467, 202.4687, 204.8042, 207.0173, 210.4770, 214.9424, 218.0063, 222.9036, 225.2147, 225.9716, 229.3914, 234.9040, 237.4439, 240.8555, 244.2763, 245.3915, 251.9171, 255.1845, 256.4160, 258.7272, 261.4896, 262.8970, 265.0908, 266.7370, 272.0670, 273.9347, 276.5897, 277.1964, 283.2726, 285.7108, 289.1429, 291.6428, 295.6546, 297.5485,	-355.9244

		299.7165, 303.2177, 305.5467, 310.8409, 317.0620, 318.9067, 319.6298, 321.5857, 328.1036, 329.7079, 333.1690, 335.8126, 342.9405, 345.8146, 352.1894, 357.5224, 366.6016, 368.4377, 370.3891, 374.9710, 383.3204, 388.0648, 391.8067, 395.6639, 401.5993, 410.1945, 413.5177, 418.1440, 420.9820, 424.7593, 425.2713, 431.4426, 439.2398, 446.6157, 447.1337, 457.0448, 459.6194, 461.5312, 486.0142, 494.9697, 501.9070, 505.0413, 509.8208, 520.7371, 531.9213, 540.3261, 557.4754, 559.4189, 568.3985, 572.0127, 590.6742, 596.3570, 608.4118, 613.9160, 628.2118, 659.7439, 685.7246, 691.6484, 702.7061, 703.1036, 704.1020, 710.9535, 717.7549, 719.1287, 720.0379, 724.4073, 726.5631, 731.2451, 737.9574, 741.1830, 744.1531, 750.7966, 755.0652, 761.2824, 769.2490, 770.1167, 777.0015, 779.4812, 780.3107, 786.3680, 787.8393, 791.4932, 793.2446, 797.5311, 799.0431, 800.6183, 802.6130, 805.8915, 807.6706, 810.0585, 811.6094, 819.6066, 822.0734, 823.6756, 825.7318, 832.2724, 834.2589, 836.7922, 838.7941, 840.7061, 842.2858, 844.5507, 851.3782, 854.3869, 859.0686, 859.7196, 872.5437, 874.0255, 1084.8319, 1091.6899, 1099.8534, 1114.7260, 1122.0720, 1127.1824, 1139.1518, 1145.6122, 1151.8424, 1158.7211, 1170.3932, 1175.9815, 1180.2115, 1185.5520, 1187.2575, 1193.1299, 1195.0459, 1199.7038, 1200.0992, 1203.2520, 1215.3037, 1220.0265, 1224.3179, 1227.1823, 1232.2527, 1233.5408, 1240.4485, 1247.9986, 1253.4384, 1257.0106, 1258.9041, 1263.2619, 1267.7341, 1270.4148, 1278.5012, 1281.2128, 1291.9102, 1299.1109, 1312.5548, 1317.8046, 1336.1593, 1351.7210, 1362.1807, 1395.5793, 1411.1634, 1481.0053, 1578.5226, 2536.9808, 3128.3695, 3159.4096, 3250.1706, 3268.1617	
Tl-O3-ZeO-C ₂ H ₅ (ads)	231	41.0748, 54.5068, 64.3664, 67.5124, 71.0831, 72.6668, 83.9336, 86.6746, 94.6469, 97.1899, 112.1093, 116.3273, 116.9002, 126.9789, 133.3324, 136.0229, 139.8969, 146.8188, 150.4451, 154.3461, 156.8469, 159.8313, 164.0297, 166.5384, 171.0236, 174.9937, 175.8112, 178.5265, 180.2351, 184.4845, 185.6849, 189.9023, 192.1331, 198.9118, 200.7236, 202.7104, 206.2690, 210.4846, 213.7956, 216.6853, 218.6591, 219.7605, 223.9019, 230.1958, 235.5972, 237.9701, 241.0693, 243.1303, 247.2282, 248.3745, 253.1356, 254.2186, 254.8450, 257.8028, 258.9387, 264.0963, 264.7726, 267.7013, 270.9141, 275.4007, 276.1857, 278.9099, 284.7476, 285.3491, 289.6215, 290.4278, 296.3807, 299.3549, 300.6256, 305.2735, 306.7740, 312.0464, 315.6214, 317.3105, 318.8331, 321.4590, 324.6364, 329.2807, 330.5800, 335.6601, 337.1355, 342.4175, 349.7890, 354.2130, 359.2548, 365.2507, 368.7248, 374.2874, 381.4343, 386.3397, 388.0795, 390.8021, 393.9232, 399.2638, 409.8664, 414.5963, 419.2713, 421.8263, 422.5861, 429.7295, 436.9797, 445.1297, 447.0341, 455.0065, 458.9217, 461.7913, 468.7883, 482.5899, 485.6562, 500.8921, 506.3165, 509.2590, 518.9474, 527.2386, 536.3450, 542.7841, 561.8784, 568.7612, 569.4304, 589.7384, 594.9319, 603.2833, 612.8859, 624.0609, 654.9317, 665.0285, 688.1540, 693.7463, 702.4008, 702.7278, 704.7668, 709.3824, 719.3530, 723.1415, 724.6645, 731.0259, 738.5661, 739.5721, 750.8960, 753.6598, 756.2725, 763.5997, 765.5834, 769.8044, 772.9359, 778.6820, 780.4312, 786.1112, 788.0970, 788.9761, 793.3584, 795.4559, 800.6376, 802.8393, 804.6563, 806.7515, 807.1429, 811.3151, 814.4371, 815.7742, 820.2102, 822.8101, 824.8779, 828.8964, 830.2891, 833.7083, 835.9880, 837.2792, 842.4017, 844.0906, 847.0194, 848.5171, 853.7817, 854.4440, 860.3141, 865.0050, 873.3502, 891.2542, 1003.7546, 1088.3412, 1115.2749, 1122.9026, 1126.2695, 1133.4539, 1135.0665, 1144.8454, 1148.0599, 1153.5781, 1160.4829, 1170.7383, 1177.7266, 1184.0027, 1189.4610, 1198.0944, 1199.8353, 1209.8430, 1212.7585, 1216.2483, 1220.0527, 1225.4921, 1228.8198, 1233.5103, 1242.0360, 1247.2366, 1248.2127, 1254.8608, 1258.7527,	None

		1260.2994, 1266.0691, 1271.7802, 1276.2346, 1283.0816, 1286.5847, 1295.6745, 1312.7823, 1313.8561, 1337.8494, 1347.5574, 1352.2939, 1399.6527, 1415.0402, 1419.3007, 1452.2111, 1499.9210, 1533.0021, 1547.2917, 3088.1477, 3162.4575, 3177.6062, 3208.5161, 3235.3486	
T1-O3-ZeO-C ₂ H ₅ CO(ads)	237	33.8395, 38.8988, 48.2502, 53.7517, 56.4143, 60.1462, 74.5648, 78.9927, 86.7981, 91.1663, 96.2378, 99.3773, 102.2021, 112.8295, 114.4502, 116.4298, 119.6665, 126.2718, 130.6110, 135.1358, 140.9152, 144.2226, 149.3934, 151.6798, 156.6389, 159.1609, 161.2358, 165.1430, 168.4050, 171.6874, 174.5532, 176.5406, 179.1057, 181.7612, 184.3543, 186.8709, 188.8878, 193.7664, 201.3246, 202.9040, 205.7305, 209.3377, 213.7324, 214.1299, 217.9361, 221.5874, 225.1545, 227.2328, 233.1161, 236.7646, 241.7695, 244.4921, 247.5351, 250.8855, 252.8425, 255.7203, 258.9097, 259.4284, 260.3817, 261.6550, 264.6580, 265.9722, 268.5057, 272.9109, 275.5132, 278.6084, 279.4647, 285.6903, 286.2959, 289.2075, 292.4691, 297.8523, 299.8730, 303.2704, 304.1792, 307.0989, 313.2226, 318.4321, 319.0939, 322.1594, 322.9594, 328.0432, 330.9445, 331.2524, 336.3725, 338.0214, 345.6402, 350.8391, 355.6559, 360.2470, 365.4193, 368.3314, 368.9484, 379.0735, 386.2329, 389.0962, 394.9406, 398.4594, 400.3061, 412.4694, 414.7188, 418.5590, 422.3071, 423.5274, 428.1797, 437.5404, 444.5420, 447.6674, 450.5911, 459.0363, 460.5397, 467.3899, 481.5838, 487.9688, 503.6756, 506.7356, 509.7557, 519.8691, 528.9653, 537.2785, 543.7000, 559.8033, 569.1436, 569.8104, 590.4100, 595.9673, 605.7616, 613.3532, 622.9097, 656.5578, 670.6560, 688.7503, 689.3477, 702.3322, 703.0027, 707.6785, 711.7287, 718.3973, 721.5246, 724.1472, 733.8685, 738.6844, 739.6875, 751.5527, 752.2735, 756.1494, 763.6603, 767.9905, 771.3754, 774.0992, 776.6225, 780.3766, 786.0060, 787.9388, 790.2185, 792.4799, 794.7262, 799.3890, 803.3808, 804.0226, 806.0027, 807.2211, 810.7533, 813.3208, 815.3048, 821.2212, 822.0666, 823.5292, 827.2929, 829.8524, 832.0676, 836.0350, 836.9621, 839.9956, 842.2592, 846.6230, 848.1632, 853.1161, 855.6560, 859.3071, 862.9275, 871.5438, 892.7048, 1024.3194, 1088.9346, 1110.5195, 1118.8435, 1121.3768, 1130.8932, 1136.3265, 1138.7648, 1143.6930, 1151.3026, 1159.6211, 1165.3446, 1176.9890, 1181.9894, 1187.5751, 1195.1346, 1197.4259, 1207.4057, 1210.6924, 1215.4017, 1216.3437, 1220.4285, 1221.9567, 1229.3097, 1241.8094, 1244.4225, 1245.2757, 1250.8096, 1254.2654, 1258.6005, 1264.2348, 1269.8754, 1275.8336, 1283.8150, 1284.0463, 1295.7051, 1312.0650, 1318.3333, 1340.7665, 1343.9322, 1350.4881, 1389.4005, 1409.1099, 1414.2069, 1438.5953, 1500.7129, 1534.1789, 1554.3361, 2255.2526, 3110.8918, 3160.9701, 3199.2143, 3219.1657, 3237.6569	None
T1-O3-Carbonylation-TS	237	-329.3124, 27.4823, 48.7789, 49.1998, 55.8693, 60.0349, 74.5308, 81.9729, 88.3072, 94.9892, 99.4830, 101.3163, 107.6352, 114.8892, 116.6160, 121.7856, 125.7341, 127.7884, 132.8851, 138.1668, 139.5844, 142.8048, 151.2610, 154.4528, 158.2678, 160.6163, 161.9148, 168.3302, 171.0296, 176.1598, 177.3929, 179.7358, 180.5889, 181.7256, 186.5859, 188.1637, 189.3523, 197.1056, 200.1224, 202.7373, 203.6319, 206.4569, 208.3059, 210.1340, 215.6740, 217.9435, 222.3955, 225.8333, 230.3708, 231.3348, 236.0100, 237.8591, 242.2700, 244.6313, 250.2903, 254.2344, 255.3938, 259.4277, 259.7482, 263.1726, 263.7788, 264.9335, 266.0863, 271.1512, 274.7603, 278.0159, 279.2501, 285.4462, 285.8419, 289.4672, 291.4750, 293.3864, 294.3535, 298.8617, 300.1215, 304.5183, 306.6401, 312.3500, 314.4261, 319.3135, 319.7785, 323.0673, 327.5363, 332.1680, 333.9962, 336.2284, 341.2198, 345.7505, 352.0013, 354.8430, 361.9833, 367.4691, 370.2768, 373.1315, 378.4964, 385.9539, 387.9475, 393.6732, 396.6409, 401.9015, 411.7035,	-329.3124

		414.8699, 419.8433, 421.5022, 423.9112, 424.7037, 429.3621, 440.6744, 446.2849, 447.6697, 457.3493, 460.4730, 461.8731, 484.6558, 490.3757, 499.3556, 504.0237, 510.3339, 519.6926, 532.0829, 539.3127, 555.5847, 558.8019, 570.4219, 570.9619, 591.6549, 596.6329, 610.2083, 614.9372, 623.2683, 661.4790, 677.4348, 691.9470, 703.9349, 705.2149, 708.2599, 715.3868, 716.7919, 719.1210, 721.1290, 726.4537, 727.0255, 736.8321, 740.4460, 745.8052, 751.5732, 753.9378, 759.4361, 771.1801, 772.4805, 777.8414, 779.4860, 780.9715, 786.6233, 789.7624, 793.9095, 795.8844, 800.2401, 800.3395, 801.3785, 803.7360, 805.7240, 808.5074, 809.7283, 811.9748, 818.0428, 821.0141, 823.4202, 827.3839, 828.8887, 832.2049, 833.5863, 834.5648, 835.9417, 838.6434, 840.8412, 847.3150, 852.1755, 854.3723, 858.1762, 859.7375, 873.1164, 934.1314, 1016.5502, 1071.4845, 1082.6110, 1089.4530, 1095.4093, 1114.4266, 1117.7003, 1124.6628, 1135.2498, 1140.0803, 1147.8519, 1158.2849, 1167.2697, 1172.2049, 1180.3756, 1182.1904, 1190.1978, 1192.4387, 1198.0435, 1204.7215, 1206.1573, 1213.3369, 1222.8737, 1225.8490, 1226.0372, 1236.6864, 1241.4089, 1244.2278, 1246.9880, 1248.9426, 1252.3865, 1254.0990, 1260.1178, 1269.1409, 1272.0333, 1277.4362, 1282.6932, 1288.5156, 1309.0006, 1315.8092, 1337.8675, 1362.6691, 1389.2218, 1401.4489, 1410.9983, 1474.3048, 1484.8953, 1528.6635, 2309.3276, 3059.7177, 3156.2322, 3173.7179, 3223.2481, 3318.0528	
T1-O3-ZeO-propionyl (ads)	237	52.1237, 58.6371, 62.7244, 75.9648, 77.9290, 89.1272, 90.8929, 96.8855, 98.4073, 102.3060, 112.2579, 119.4629, 120.8073, 124.4568, 128.8550, 132.4647, 138.2666, 140.3074, 143.6735, 149.3592, 155.3333, 155.7265, 160.7414, 161.4650, 164.1928, 167.4689, 170.9818, 175.8688, 178.8167, 179.8095, 182.9094, 183.5597, 188.6784, 191.3185, 198.0393, 199.4357, 203.4015, 206.6275, 209.2581, 211.1651, 214.8386, 216.9494, 222.0246, 225.5935, 230.4236, 235.4153, 241.3479, 242.3440, 244.8692, 247.5338, 251.9573, 252.9517, 254.3195, 257.4661, 259.6453, 260.3428, 263.7648, 264.7575, 267.7351, 270.8671, 273.0613, 275.3692, 277.0125, 279.1763, 285.4467, 287.6047, 288.8879, 290.3739, 295.8655, 299.9267, 301.7289, 304.0028, 304.3636, 311.1742, 313.5884, 317.2258, 319.2307, 321.8160, 325.9954, 327.6098, 331.2652, 334.3354, 335.0917, 339.4214, 344.1181, 349.0281, 353.9161, 362.8506, 364.9540, 370.6689, 379.0920, 385.3408, 386.6513, 390.0442, 394.7153, 402.8893, 407.2415, 413.6961, 416.3047, 419.0343, 422.6573, 429.3189, 436.2455, 443.5403, 447.2060, 451.0467, 457.6627, 459.7779, 471.1804, 479.5757, 484.0721, 492.6634, 504.5187, 506.4625, 510.3240, 524.3027, 534.4914, 542.0174, 545.7492, 560.6944, 568.4639, 569.6005, 590.5082, 593.4041, 602.0598, 612.4314, 613.8621, 626.9932, 661.3299, 665.2630, 684.5083, 687.2667, 701.5759, 702.7855, 703.5099, 713.1626, 718.5555, 721.0223, 722.3124, 724.9427, 731.7634, 739.3021, 741.2936, 747.8001, 753.5248, 758.7674, 765.1323, 770.0214, 773.2956, 775.8377, 779.4772, 781.5025, 783.9471, 787.9092, 792.3567, 794.7307, 795.8961, 799.9879, 802.0039, 804.1778, 806.7442, 808.6902, 811.1511, 812.9333, 817.1498, 821.1690, 822.4218, 823.9670, 829.2166, 833.0715, 835.3686, 836.3547, 838.9039, 840.4595, 845.2845, 849.2368, 855.0996, 856.2689, 859.5786, 860.5331, 868.1825, 879.4585, 971.8086, 1041.5838, 1084.3947, 1096.0771, 1110.4503, 1114.2829, 1121.8369, 1128.7588, 1133.2817, 1142.0783, 1148.3347, 1152.6763, 1158.9738, 1162.3890, 1173.4270, 1180.6526, 1189.1637, 1197.3058, 1200.2563, 1203.2557, 1207.1184, 1217.6833, 1222.4406, 1225.8133, 1232.4484, 1245.1336, 1246.0351, 1246.8684, 1249.2570, 1255.2183, 1257.4426, 1265.8500, 1274.8388, 1278.1462, 1280.3896, 1286.8362, 1288.2885, 1297.0249, 1309.9402, 1313.4770, 1336.4076, 1352.1442, 1385.8629, 1392.6765,	None

		1413.4108, 1442.1210, 1466.2147, 1516.7444, 1519.3388, 1984.7293, 3075.6042, 3105.4835, 3122.9434, 3179.9043, 3250.9968	
T2-O5-ZeOH-C ₂ H ₄ (ads)	327	63.4528, 64.4801, 67.9724, 71.1481, 76.2876, 81.1334, 83.6176, 89.3763, 90.2253, 93.8300, 97.1826, 99.6586, 103.9872, 109.8761, 111.3480, 112.4795, 115.4984, 117.9684, 120.4241, 122.5722, 125.8012, 127.6674, 130.2997, 133.4703, 136.6261, 139.3805, 140.7478, 143.6012, 144.9555, 145.4973, 148.3488, 148.9759, 149.5745, 150.6816, 154.5224, 155.1895, 159.5562, 161.5078, 162.6441, 163.8632, 166.5382, 170.1972, 171.9109, 174.1283, 177.8305, 179.5068, 181.9469, 183.5865, 186.3558, 190.3405, 197.1979, 199.6496, 201.4877, 202.2389, 202.9268, 203.9096, 207.2512, 210.0845, 211.3746, 213.5281, 215.7193, 222.1503, 223.1770, 225.0166, 227.5567, 227.9984, 229.1039, 233.0356, 234.7538, 236.3742, 238.8985, 239.6727, 242.1676, 245.4222, 247.1005, 248.0983, 251.6975, 253.6943, 257.2615, 259.0116, 261.7088, 263.4059, 267.6302, 268.8314, 271.6451, 273.0263, 275.3990, 276.9696, 277.5894, 279.2975, 281.1170, 282.7041, 284.7226, 288.9668, 289.5972, 291.4716, 292.8068, 293.9574, 296.3935, 298.9160, 300.0101, 302.3523, 302.7870, 305.9084, 306.3402, 307.8334, 310.8493, 313.5756, 316.5983, 318.7449, 326.1041, 326.5170, 330.7958, 334.7550, 336.6447, 342.5977, 346.8005, 352.5836, 355.3419, 360.1090, 362.3274, 365.5425, 369.3535, 375.0285, 376.3459, 378.2711, 381.0340, 385.5669, 387.2062, 388.6733, 391.4296, 391.7254, 393.5564, 396.7179, 397.1661, 399.5734, 400.0695, 401.9335, 404.9507, 407.5563, 410.9370, 414.6584, 418.3207, 421.0496, 425.0829, 427.9665, 430.3375, 435.8006, 436.7526, 440.7470, 444.6772, 446.4591, 454.0083, 458.4512, 462.0475, 466.1159, 472.3664, 474.3705, 482.2637, 487.9710, 488.6600, 491.8340, 495.5391, 497.4109, 499.8884, 504.8134, 509.4050, 512.4276, 521.5473, 529.6501, 540.5467, 543.7253, 555.6509, 556.8955, 569.1207, 574.5998, 577.3306, 590.0322, 606.3334, 612.1993, 624.2326, 636.2528, 643.1383, 646.3199, 652.5620, 661.1933, 666.9221, 670.7453, 671.3402, 674.1319, 677.1924, 687.3309, 688.3739, 692.7172, 696.2062, 697.0960, 705.0756, 706.8923, 709.2213, 712.0641, 715.3160, 719.5410, 724.4033, 726.6683, 728.1732, 729.5990, 741.7552, 748.3849, 749.1651, 751.3615, 754.0175, 756.1013, 758.4443, 759.8069, 760.7126, 761.7281, 762.5439, 768.2400, 771.8498, 774.8761, 778.4045, 782.6225, 783.5180, 784.8121, 786.2638, 789.7320, 793.9413, 795.0117, 795.2630, 796.5661, 798.3018, 800.2027, 801.1309, 804.2691, 807.6646, 809.5322, 812.9383, 814.2986, 815.2114, 818.2030, 818.9115, 820.5599, 823.7205, 825.1525, 830.7066, 832.1023, 835.4232, 837.1065, 838.8746, 842.6849, 843.8799, 845.5467, 850.6040, 853.3708, 863.5687, 1034.9314, 1053.6094, 1070.4181, 1073.9987, 1089.7999, 1092.6359, 1099.0955, 1102.8392, 1105.6775, 1108.8430, 1111.4374, 1115.2641, 1117.1340, 1118.0541, 1124.1076, 1127.7740, 1128.8601, 1133.0225, 1133.7163, 1137.3840, 1139.5467, 1144.5619, 1154.0972, 1156.0500, 1161.7179, 1166.9569, 1171.6784, 1175.1241, 1178.4145, 1182.7921, 1187.1455, 1191.7848, 1193.6055, 1195.9338, 1199.7954, 1201.6646, 1205.5447, 1207.6483, 1209.7373, 1212.1335, 1216.1398, 1219.2649, 1224.3798, 1228.8745, 1231.7320, 1233.9411, 1238.3040, 1240.5133, 1242.0409, 1246.2189, 1247.3229, 1250.5755, 1253.7344, 1255.3138, 1260.1358, 1263.9052, 1265.6092, 1267.3026, 1272.0747, 1274.6048, 1277.4496, 1285.2015, 1288.7749, 1330.3134, 1399.8392, 1488.8772, 1712.7081, 3175.7158, 3190.7801, 3268.1528, 3293.1690, 3331.3059	None
T2-O5-Protonation-	327	-221.2935, 40.6947, 65.3988, 67.2968, 70.9768, 77.3744, 82.6905, 87.3909, 90.6317, 94.2706, 96.2479, 99.5618, 104.9732, 109.1647, 110.7358, 111.2169, 115.9518, 116.9261, 118.2472, 120.5365, 123.2306,	-221.2935

TS		126.6739, 128.2180, 132.0992, 135.5982, 137.1801, 140.1528, 142.6901, 146.4232, 147.2289, 148.0627, 149.5229, 151.8865, 153.6157, 155.1047, 158.9216, 161.5512, 162.8675, 165.4097, 167.4756, 168.9343, 171.4552, 173.1686, 174.7574, 178.0301, 179.4765, 182.7295, 184.3892, 187.5471, 191.9880, 192.6628, 197.6299, 199.1896, 201.3637, 203.2732, 203.4197, 205.9294, 209.9685, 211.5609, 213.3669, 215.4023, 219.1709, 222.2013, 223.5309, 225.5893, 227.9038, 228.9896, 230.2631, 234.5547, 235.0181, 238.5052, 239.1884, 240.6417, 243.3526, 246.0283, 249.0426, 250.7505, 253.0711, 254.6256, 257.0194, 260.9520, 261.9221, 266.8165, 269.2239, 271.2546, 272.1590, 274.6522, 276.2908, 277.8155, 279.2812, 281.8541, 282.9326, 284.0668, 286.5390, 289.1867, 290.5266, 292.4132, 294.0047, 295.1805, 297.2141, 299.1280, 302.6806, 304.1134, 306.0210, 307.4881, 308.7500, 315.2641, 317.0484, 317.7602, 323.8637, 324.5295, 327.2956, 330.1321, 335.1255, 340.3976, 345.0608, 346.9387, 353.5268, 355.5860, 360.0027, 363.2144, 366.5008, 372.8722, 376.4943, 377.5333, 379.2800, 384.7330, 385.8894, 388.0799, 390.8286, 392.4099, 392.7673, 395.1111, 397.0810, 397.9921, 400.6931, 402.1089, 403.4098, 406.1091, 408.9901, 414.7235, 417.8799, 419.2709, 422.8078, 427.2382, 430.2301, 432.7237, 436.6190, 438.5388, 441.1288, 446.0208, 446.8827, 456.2394, 460.2133, 464.2387, 466.3536, 473.1031, 477.6563, 482.1572, 487.2258, 488.8946, 493.4493, 497.5049, 498.7211, 499.9982, 504.5341, 509.6347, 512.6325, 518.4871, 521.9734, 534.4987, 540.6438, 544.8182, 556.4723, 558.2457, 574.0209, 577.1250, 578.1437, 593.6124, 606.5093, 624.0783, 633.4229, 638.1572, 644.2576, 656.6854, 663.8017, 667.8259, 668.5153, 671.8709, 673.2126, 677.2573, 685.4588, 688.6122, 693.2396, 694.0836, 696.7506, 701.6203, 707.0422, 708.8161, 713.9993, 716.8704, 722.4169, 723.2646, 725.7492, 729.3361, 731.1662, 741.5175, 747.1386, 748.8479, 750.5746, 751.6257, 754.2211, 757.1235, 758.7225, 760.2353, 760.5448, 762.0297, 764.3481, 767.8098, 773.0225, 774.3350, 777.3907, 781.3637, 783.1559, 784.9469, 785.9375, 790.1445, 792.2393, 793.0002, 793.6068, 795.5497, 796.4755, 799.8231, 801.9940, 804.6831, 807.5512, 807.6668, 810.0485, 812.2607, 814.6817, 817.0041, 817.9441, 821.9111, 823.0771, 824.9818, 828.9031, 831.9278, 832.3103, 833.4782, 836.7238, 841.6118, 843.9404, 851.4430, 859.2307, 1020.9194, 1047.2364, 1064.1153, 1080.3565, 1083.5685, 1085.6630, 1092.8209, 1095.7561, 1099.7150, 1107.7297, 1108.5869, 1110.6808, 1114.4029, 1120.0790, 1122.9103, 1124.9186, 1131.0450, 1134.0680, 1135.4877, 1141.1065, 1145.2020, 1145.8768, 1149.4388, 1153.2871, 1160.9285, 1161.9936, 1165.3866, 1169.1633, 1169.9833, 1173.1176, 1177.5206, 1180.2119, 1187.5116, 1192.1432, 1194.4155, 1197.1649, 1201.6830, 1203.7717, 1205.7432, 1207.2326, 1210.0306, 1212.7711, 1214.2079, 1221.7579, 1227.3659, 1228.7686, 1229.1716, 1234.5810, 1237.0114, 1238.8616, 1241.1704, 1244.4840, 1246.8785, 1247.9626, 1252.8543, 1254.1479, 1258.6025, 1260.0240, 1262.4226, 1267.6239, 1268.1713, 1274.4557, 1276.6590, 1282.9228, 1286.8646, 1386.0038, 1497.8476, 1615.5398, 2024.2815, 3138.9658, 3176.4134, 3262.5685, 3288.7060	
T2-O5-ZeO-C ₂ H ₅ (ads)	327	63.7906, 64.8488, 69.9654, 71.3788, 76.1606, 83.9624, 87.8336, 90.6444, 93.8494, 97.3630, 99.6016, 104.8613, 109.3664, 113.4908, 114.8502, 118.0678, 118.9554, 121.5742, 125.6474, 129.0476, 135.3209, 136.0940, 138.2630, 139.8341, 141.4390, 144.4677, 145.5498, 147.1475, 148.8483, 150.1015, 150.3425, 154.7242, 158.8171, 159.8927, 160.6871, 161.9843, 163.6857, 167.8232, 170.1928, 171.8168, 173.0470, 177.0917, 178.8874, 180.0425, 183.0040, 186.4292, 190.7414, 196.8467, 198.3195, 201.1827, 202.9023, 203.1183, 205.3102, 206.5818, 210.4661, 211.4209, 214.1988, 216.1638, 219.4641, 223.3251, 225.0473,	None

		226.7594, 227.9465, 229.6747, 231.6278, 232.7337, 235.3949, 239.1033, 239.5257, 242.1371, 243.2759, 245.3306, 247.1215, 248.6298, 253.2802, 255.0026, 258.0821, 259.6507, 262.9568, 266.6596, 268.7076, 269.3573, 271.7350, 273.7703, 275.1735, 277.4650, 279.8419, 281.0369, 283.1746, 283.8317, 285.4475, 289.0800, 289.4022, 291.2051, 291.6409, 294.9849, 295.6593, 297.8270, 299.3579, 302.7343, 304.2695, 306.5813, 307.9140, 309.0313, 314.0735, 316.4233, 320.0178, 324.3613, 326.5855, 329.7337, 334.7197, 336.4770, 342.2260, 343.9760, 347.6684, 352.1385, 356.7213, 359.3400, 361.9376, 364.7091, 370.6316, 373.2024, 375.9345, 378.4465, 381.4005, 384.5156, 386.8942, 388.0030, 390.7532, 391.5739, 392.9136, 395.8946, 396.5850, 398.6037, 400.0037, 401.7612, 404.3795, 405.0688, 410.7484, 414.3871, 418.0668, 421.2074, 424.6450, 426.8728, 429.7570, 434.1424, 435.7728, 440.2914, 444.3306, 446.2262, 451.5547, 455.7028, 459.9790, 465.1062, 468.1008, 472.0633, 473.5051, 482.7532, 486.9687, 488.7003, 493.3330, 495.7336, 498.8887, 500.3935, 504.5049, 509.6974, 512.8788, 521.0721, 528.2612, 540.3930, 544.2783, 556.1508, 557.1467, 570.3114, 575.5636, 577.4678, 589.1766, 606.2490, 619.1309, 627.6253, 638.6940, 645.3292, 654.0260, 659.0301, 664.7276, 670.8267, 671.0962, 673.4929, 674.8059, 687.7563, 688.9136, 692.2688, 695.2187, 697.2223, 705.7714, 706.8389, 709.0037, 712.1252, 714.7451, 719.0420, 724.4343, 726.2085, 728.4171, 729.0878, 741.1171, 747.0671, 748.4505, 749.7153, 753.5704, 754.5670, 756.2292, 758.8631, 760.3278, 761.6810, 763.1417, 764.4780, 768.5498, 772.4649, 774.2584, 776.1274, 782.9034, 783.5979, 784.5011, 786.3919, 789.2706, 794.0107, 794.6845, 794.9758, 796.1854, 797.7036, 800.0596, 801.2566, 804.3213, 805.5120, 808.7678, 810.1351, 812.6295, 814.0352, 816.5032, 818.5652, 820.0903, 820.6102, 823.8645, 825.2827, 830.5016, 832.5255, 835.5875, 836.2294, 837.7817, 839.9763, 843.4002, 845.8105, 853.3393, 868.9759, 1018.8723, 1061.3161, 1074.7194, 1088.7253, 1091.3472, 1100.6676, 1102.2168, 1107.9784, 1110.3803, 1114.3881, 1115.8659, 1119.6259, 1123.1956, 1125.9893, 1128.4263, 1129.3880, 1131.1444, 1133.1870, 1137.2740, 1139.5387, 1144.2619, 1153.0530, 1155.2530, 1156.6476, 1161.8889, 1168.1872, 1174.5565, 1177.3926, 1177.9142, 1183.4437, 1185.5247, 1191.3412, 1195.0601, 1197.3302, 1199.6140, 1200.6464, 1204.9395, 1207.4943, 1209.4884, 1212.4013, 1216.7637, 1217.6931, 1224.1006, 1227.8860, 1230.7795, 1234.1373, 1237.7492, 1240.9585, 1241.7231, 1245.3587, 1247.5522, 1248.4654, 1253.0647, 1259.7285, 1263.1329, 1264.9847, 1269.0672, 1270.9187, 1274.8303, 1277.9949, 1285.0630, 1289.2635, 1348.0115, 1428.8671, 1464.5996, 1510.2265, 1522.8126, 1538.4338, 3084.9597, 3160.1289, 3172.1781, 3194.4163, 3232.4536	
T2-O5-ZeO-C ₂ H ₅ (ads) CO(ads)	333	53.8895, 59.5593, 64.7847, 66.3578, 70.6828, 77.2627, 84.1327, 86.6177, 89.9627, 92.4031, 93.8034, 96.7209, 100.1421, 102.6690, 105.8632, 110.5459, 112.5881, 115.0319, 117.4242, 119.2262, 123.4601, 126.6908, 129.5648, 135.2679, 136.1457, 138.2250, 140.2038, 141.4802, 144.0978, 145.6150, 146.5313, 147.1293, 149.8533, 150.7963, 151.5653, 155.9515, 157.7387, 160.5517, 160.7020, 163.2376, 163.9584, 168.1485, 169.5658, 170.5919, 172.5120, 174.5646, 178.7858, 179.8630, 182.2745, 184.8912, 185.8046, 193.5220, 197.5028, 199.3626, 202.8563, 203.3908, 204.8964, 205.9704, 209.0500, 211.7823, 214.1137, 215.6765, 220.3027, 220.4055, 223.8302, 226.8372, 229.1145, 229.6216, 229.9884, 232.8384, 232.9587, 238.2771, 240.0597, 241.3415, 243.1914, 244.3406, 246.6844, 249.7425, 250.2438, 256.0878, 256.1239, 258.9091, 260.7099, 264.8581, 266.8088, 269.2508, 270.5243, 272.9699, 273.2432, 275.8167, 277.0316, 280.3115, 282.7227, 284.0878, 285.4702, 287.2769, 288.3931, 289.5553, 291.3495, 293.2057, 294.9751,	None

		296.0775, 298.5172, 299.9498, 302.2994, 305.1491, 307.3186, 308.3037, 309.1436, 314.8214, 317.7645, 318.1130, 320.7288, 327.3734, 331.7710, 334.5714, 336.5434, 341.7291, 344.3266, 347.6443, 350.5167, 352.6402, 359.5229, 362.1005, 365.2269, 368.8711, 373.0393, 376.4411, 378.8068, 381.1341, 385.0780, 387.3256, 388.3406, 390.6632, 391.9840, 392.8612, 395.9658, 396.8341, 398.9974, 400.1147, 401.7505, 404.0329, 405.8603, 411.8260, 414.2538, 418.2972, 421.1136, 424.5539, 427.4161, 429.4413, 434.0995, 435.6364, 440.4950, 444.2160, 446.0139, 451.5749, 456.7500, 462.9213, 466.1132, 471.8240, 472.4733, 482.0188, 486.3706, 487.2327, 491.3453, 495.0450, 496.4334, 500.0778, 504.6428, 509.0168, 510.5621, 513.0851, 521.4701, 527.5951, 540.3161, 544.5743, 555.8422, 557.6784, 569.1576, 576.3204, 577.7800, 589.2600, 606.9980, 618.2441, 627.2262, 638.4847, 645.6355, 651.8583, 659.2804, 664.5229, 670.2009, 670.7050, 672.5878, 675.4771, 687.4516, 687.8809, 691.9267, 695.2115, 697.4930, 706.6355, 707.3730, 709.7706, 712.3651, 714.8048, 719.1838, 724.7344, 726.9652, 728.7179, 729.4928, 742.2301, 747.1752, 748.4524, 749.9544, 753.6633, 755.6397, 756.6728, 759.1464, 759.7835, 761.1858, 763.2787, 765.9574, 767.3803, 771.3007, 775.2821, 777.2014, 782.8224, 783.4717, 784.2217, 786.3204, 789.6273, 793.9999, 794.8421, 795.5598, 796.4563, 797.6769, 799.8762, 801.5897, 804.6544, 804.7764, 809.3290, 810.4977, 812.1691, 814.1564, 816.3777, 818.5409, 819.9438, 823.1896, 823.6844, 827.0595, 830.1454, 831.1812, 836.5256, 837.2561, 839.2047, 840.9793, 845.1222, 847.9008, 854.5892, 892.1660, 1038.7540, 1059.0156, 1074.7636, 1090.6848, 1092.9694, 1100.8387, 1103.2727, 1103.6742, 1109.7490, 1110.8140, 1111.4382, 1117.9188, 1119.9589, 1122.9848, 1125.3850, 1130.5088, 1132.1876, 1132.3774, 1135.8552, 1140.8002, 1144.3116, 1152.9092, 1155.2202, 1160.4831, 1163.5140, 1170.4957, 1176.1754, 1178.4928, 1181.1292, 1185.3520, 1186.8241, 1190.8743, 1195.0973, 1196.7893, 1200.7045, 1201.3194, 1204.9946, 1207.8795, 1208.7860, 1212.1930, 1216.6675, 1217.9550, 1224.0215, 1228.0207, 1231.2806, 1235.6751, 1238.5638, 1240.2069, 1243.3482, 1245.4741, 1248.3416, 1250.4039, 1253.6033, 1258.6713, 1263.3615, 1266.3458, 1269.1024, 1273.4984, 1274.9444, 1277.3002, 1284.7519, 1288.6957, 1337.3306, 1418.8216, 1472.5071, 1514.5092, 1530.9380, 1555.8882, 2238.3989, 3108.7594, 3150.1231, 3186.7861, 3213.5387, 3240.3448	
T2-O5-Carbonylation-TS	333	-425.1411, 34.4071, 64.0248, 65.4489, 69.0726, 71.1143, 75.9694, 84.0115, 87.7651, 90.7854, 93.1665, 96.3577, 98.1771, 101.5426, 108.3706, 109.9513, 112.0083, 114.8476, 115.4325, 117.9881, 120.4060, 120.8510, 123.6335, 127.3921, 130.5632, 132.4180, 135.8621, 136.4664, 138.6958, 140.7623, 145.1549, 146.5647, 147.9894, 148.7625, 149.7830, 150.4681, 154.5231, 159.1779, 159.9272, 161.8389, 162.6825, 167.1940, 168.8298, 171.1047, 172.4712, 174.0206, 178.3523, 179.8325, 181.2742, 183.1549, 186.2841, 187.2440, 197.3599, 200.7307, 201.3032, 201.6731, 202.7073, 204.2209, 208.0660, 209.7410, 211.8724, 213.1077, 216.9755, 219.1200, 222.4384, 225.4402, 227.1355, 228.6412, 229.6681, 231.4909, 233.0470, 235.7342, 239.3037, 239.6001, 241.7742, 245.8552, 246.1967, 247.3114, 250.3063, 254.2675, 255.4844, 257.3515, 260.2374, 262.6248, 265.5042, 267.7762, 269.2703, 272.3795, 273.5103, 274.6201, 276.4522, 278.5125, 282.0102, 283.9091, 285.8729, 287.3827, 287.9730, 289.6207, 291.7573, 293.1807, 294.2648, 295.2036, 297.7615, 299.7917, 302.4023, 305.1722, 307.2101, 308.1634, 308.4445, 314.6851, 316.0200, 317.7928, 319.3684, 323.5670, 326.0857, 330.7872, 332.0241, 335.0673, 340.4172, 346.4365, 348.6101, 353.7742, 356.4297, 360.0916, 362.9945, 365.8423, 372.9609, 376.1112, 377.3598, 379.0084, 384.2954,	-425.1411

		385.5813, 388.0394, 388.8698, 391.8510, 392.9887, 394.2158, 396.8421, 397.4935, 400.4202, 401.7970, 403.0202, 404.7772, 406.8420, 414.2619, 415.0914, 417.9563, 419.0837, 421.9901, 426.7379, 430.0483, 432.4971, 436.6121, 437.6000, 440.8577, 445.1483, 446.5880, 455.9293, 459.3673, 463.6014, 466.1814, 472.7220, 476.8451, 482.2131, 487.5934, 490.3202, 493.2574, 496.7354, 499.1858, 499.6484, 504.5257, 509.9422, 512.6474, 521.2116, 532.0814, 540.5092, 544.4624, 556.8730, 557.6485, 575.0816, 576.7870, 577.9122, 593.6379, 608.1786, 622.9450, 632.0737, 639.5087, 645.9408, 657.8784, 660.5470, 666.3069, 669.1400, 671.5751, 673.5441, 675.7930, 686.1307, 688.4061, 692.6436, 694.5504, 696.3471, 703.2454, 706.8833, 708.7052, 713.3702, 715.6594, 720.3947, 723.5488, 726.1536, 728.8829, 729.3673, 741.8306, 747.6844, 749.5963, 750.2428, 752.2861, 754.7295, 757.5318, 758.5477, 759.4281, 760.2768, 762.3390, 763.3043, 769.0088, 771.4195, 773.6676, 775.0906, 781.0703, 782.9579, 784.5923, 786.8848, 790.8205, 792.9224, 793.0932, 793.4280, 795.4255, 796.3023, 800.2869, 802.8426, 803.9835, 806.5592, 808.1693, 810.1411, 812.3563, 814.3307, 816.2776, 818.3050, 821.8622, 821.9288, 824.7514, 828.9755, 830.4991, 832.8722, 834.9121, 836.5419, 840.5886, 843.4822, 844.9334, 851.8667, 943.6606, 1020.2989, 1046.7146, 1057.2917, 1068.3578, 1082.2209, 1084.3856, 1087.3902, 1092.1377, 1095.9790, 1098.3050, 1104.4166, 1109.1491, 1112.6865, 1114.5506, 1121.0237, 1122.5496, 1129.8716, 1131.1660, 1134.4998, 1135.5465, 1140.4532, 1142.2752, 1149.2166, 1153.4371, 1161.4725, 1163.3177, 1168.7636, 1172.0627, 1175.1729, 1178.1482, 1184.4522, 1188.9901, 1191.4527, 1195.0466, 1198.3956, 1199.7592, 1202.3507, 1205.1770, 1207.9718, 1209.6447, 1211.1684, 1212.9494, 1215.4121, 1222.9828, 1226.0377, 1229.0503, 1231.7682, 1235.6766, 1236.6988, 1239.0033, 1241.3186, 1242.2695, 1245.7454, 1249.9038, 1251.8869, 1258.0329, 1260.7578, 1261.8462, 1267.5029, 1268.1267, 1273.4184, 1275.2510, 1282.9753, 1286.2420, 1410.8941, 1477.2564, 1479.0822, 1517.0420, 2297.7079, 3095.3502, 3176.5101, 3193.9453, 3202.8293, 3319.3998	
T2-O5-ZeO-propionyl (ads)	333	59.3103, 65.0646, 67.1930, 71.8799, 76.1618, 81.4601, 83.5192, 88.6091, 90.6611, 94.2022, 97.3583, 99.3414, 103.4218, 110.5098, 111.7968, 114.0494, 116.2918, 118.7727, 122.8739, 125.5090, 130.2912, 133.0689, 135.8953, 138.1097, 139.4855, 141.5177, 143.3307, 145.4902, 146.5840, 148.4837, 150.7503, 152.7610, 153.6696, 155.0422, 159.0541, 161.1659, 162.8202, 165.1721, 167.3660, 169.6283, 171.7667, 173.5866, 175.5824, 177.0724, 179.9704, 183.8123, 185.4886, 189.8820, 195.4590, 197.0295, 197.5078, 201.0337, 201.4325, 203.4763, 204.5580, 205.9576, 210.8180, 211.6435, 213.1373, 215.5801, 221.5868, 222.5222, 224.9397, 225.6970, 227.5852, 228.1134, 229.0811, 232.3595, 233.6765, 235.1724, 238.4611, 240.3446, 241.8452, 246.1546, 247.4090, 248.6332, 252.4913, 254.6221, 256.8449, 258.0846, 262.5390, 264.5966, 268.5292, 268.8904, 270.7768, 271.9444, 272.6800, 275.7006, 277.3910, 279.7156, 281.8260, 282.1531, 285.2847, 286.5298, 287.0789, 289.7314, 291.2073, 293.1281, 294.6282, 295.2326, 297.6754, 299.3246, 301.3645, 304.0085, 305.7310, 306.4220, 308.3057, 312.5479, 315.3190, 318.9643, 320.5850, 326.4022, 330.1719, 333.5690, 334.7697, 339.5467, 342.2960, 348.1660, 351.5206, 358.9659, 362.5810, 364.5104, 366.8810, 371.7113, 375.8672, 377.5098, 379.6911, 383.6803, 385.2635, 387.4505, 389.2293, 390.9329, 392.6361, 396.1400, 396.7373, 398.2196, 399.9723, 401.4062, 401.6910, 404.7030, 408.2806, 414.8604, 418.3957, 420.4204, 421.6372, 425.5379, 427.6124, 431.5332, 435.2355, 439.0194, 442.3213, 443.5634, 446.8044, 453.7290, 459.7577, 463.5678, 467.0545, 470.3483, 473.9891, 482.3589, 485.8356,	None

		488.9436, 493.2963, 495.3904, 498.2880, 500.8055, 504.7812, 509.5360, 512.9927, 520.3957, 523.9152, 539.4478, 542.4512, 549.8331, 556.0678, 556.3348, 564.6843, 575.9016, 577.5206, 584.8833, 598.1044, 606.7319, 615.4170, 628.7908, 639.0429, 645.0644, 653.2822, 659.6793, 665.9138, 670.8554, 671.5564, 674.0597, 675.8795, 687.8274, 689.2568, 692.8237, 697.1570, 697.7817, 706.0850, 707.0515, 708.0196, 710.2822, 714.9756, 719.2541, 722.4276, 726.7557, 728.5796, 729.6490, 741.2036, 746.3662, 748.6289, 749.4784, 752.7857, 753.2822, 756.0163, 758.4596, 760.0724, 761.1234, 762.3552, 763.3562, 771.8759, 772.2078, 772.6487, 777.2994, 779.1537, 783.5894, 784.7091, 786.5630, 790.9990, 793.6497, 794.7149, 795.4397, 796.5109, 797.7526, 800.6620, 801.6690, 803.1203, 806.3576, 808.7275, 810.5368, 812.2759, 814.1799, 816.3140, 817.4748, 819.1696, 821.2718, 824.9354, 825.7645, 830.2304, 830.7914, 834.7816, 836.7745, 839.3516, 842.2025, 844.5377, 846.9364, 853.6394, 863.5520, 960.7462, 1064.2117, 1070.4651, 1087.5160, 1089.6381, 1097.2330, 1099.6366, 1108.5698, 1109.8280, 1110.5646, 1114.2813, 1117.4716, 1117.7841, 1119.3750, 1123.7817, 1129.3213, 1131.4001, 1132.2040, 1132.6378, 1134.5275, 1137.8626, 1140.5160, 1144.1510, 1154.7037, 1157.5244, 1163.1778, 1166.7766, 1170.3701, 1175.5260, 1179.1736, 1181.0426, 1184.3467, 1186.8277, 1195.8081, 1197.6031, 1201.9476, 1202.5087, 1205.2957, 1209.0712, 1211.5843, 1213.6016, 1217.7081, 1220.3424, 1224.6350, 1229.4317, 1231.9528, 1235.3859, 1238.5285, 1241.1202, 1243.4933, 1247.9833, 1248.2271, 1252.2727, 1255.1719, 1259.8471, 1264.0950, 1265.6699, 1269.4554, 1271.2439, 1276.7223, 1278.6651, 1284.9778, 1289.8307, 1304.3534, 1440.4403, 1446.9915, 1496.4195, 1513.1379, 1540.8284, 1975.1221, 3082.8397, 3086.1914, 3176.0262, 3178.2088, 3253.0325	
T2-O5-ZeO-propionyl-H ₂ O(ads)	342	45.9862, 53.0322, 62.6656, 66.8934, 69.7899, 76.5751, 78.6568, 84.2383, 89.1775, 92.5743, 94.7298, 97.8900, 99.5857, 102.9667, 107.9941, 110.9992, 114.3402, 116.3610, 116.9128, 119.2372, 122.5163, 126.9840, 128.8044, 133.2755, 135.6220, 136.6923, 139.8725, 140.8478, 141.8045, 144.8449, 145.8993, 149.4023, 150.3705, 151.5798, 154.4475, 155.4364, 159.1950, 160.1056, 161.6926, 164.5358, 166.0318, 168.4515, 170.7516, 173.3304, 176.0996, 177.6208, 179.6408, 183.3302, 185.2280, 186.7493, 190.9180, 192.0697, 197.1783, 198.3990, 201.3142, 202.5788, 204.1389, 205.9314, 206.6457, 211.3545, 213.5742, 213.7794, 216.8248, 218.1153, 223.2680, 225.2495, 227.7060, 228.9589, 230.3087, 231.7892, 233.2255, 236.2313, 237.4083, 238.5529, 240.0906, 243.2101, 245.8929, 248.1786, 250.3984, 251.0960, 255.0112, 257.2055, 258.7230, 261.7049, 263.4862, 266.1007, 268.0388, 269.9169, 271.1202, 272.5903, 274.4037, 275.8562, 278.4643, 280.4859, 282.2994, 283.2121, 286.2943, 287.4923, 289.6903, 290.0968, 293.6064, 294.4193, 295.0197, 296.7622, 298.5512, 302.8333, 304.1560, 306.1668, 307.2028, 309.7887, 310.8025, 315.6847, 318.3374, 320.0096, 325.9238, 327.0854, 332.2092, 335.1063, 336.6263, 339.6295, 342.8737, 347.3782, 351.4102, 359.2999, 362.6779, 365.0424, 366.1970, 372.4075, 376.0800, 377.7214, 379.5188, 383.3350, 385.0113, 388.0412, 389.7192, 391.2587, 392.7735, 395.6733, 397.4368, 399.5144, 400.5190, 400.8529, 401.7300, 404.8209, 407.7378, 415.0571, 418.0605, 420.7378, 421.8314, 425.3532, 427.6926, 431.0599, 434.3937, 437.5434, 441.9031, 442.9504, 446.3352, 447.9635, 454.5074, 460.1359, 463.8959, 467.2003, 470.8604, 474.6688, 482.2098, 485.9441, 488.9761, 493.5714, 495.6361, 498.7429, 500.6715, 505.3519, 509.6035, 513.5518, 520.0834, 523.8843, 538.9775, 543.6994, 554.1283, 556.9978, 560.2252, 567.6658, 573.6410, 579.4024, 582.8086, 588.9819, 602.3234, 603.7191, 616.0033, 628.2268, 639.0685,	None

		644.8178, 653.0268, 659.0430, 665.8973, 670.8069, 671.5291, 672.6348, 677.0124, 687.5725, 687.8858, 693.0531, 697.0961, 697.7356, 706.6998, 707.0918, 708.3969, 710.7323, 715.0430, 719.5908, 721.5321, 727.3888, 728.8140, 731.0227, 740.3361, 744.0518, 748.7777, 748.9171, 751.9908, 752.8960, 755.9431, 758.1046, 758.9956, 760.1054, 762.1863, 763.5585, 768.6929, 772.1645, 773.1006, 777.5552, 779.9402, 782.5737, 783.5355, 786.4641, 789.6791, 793.1867, 794.0270, 795.3938, 795.7475, 798.2639, 798.5042, 801.6340, 802.0701, 806.0041, 807.9056, 809.5140, 811.7673, 814.3942, 815.7641, 817.8878, 819.2778, 820.0742, 824.1943, 825.9043, 829.7420, 830.3513, 834.9389, 836.7745, 839.3879, 841.5708, 842.9423, 844.6838, 848.8932, 853.8237, 957.4074, 1059.0094, 1069.3337, 1073.3818, 1089.7023, 1094.5678, 1099.0334, 1103.9844, 1108.0826, 1108.8158, 1110.0050, 1114.4054, 1117.3722, 1119.3561, 1121.8756, 1125.8396, 1130.2197, 1131.9585, 1132.9525, 1134.0933, 1135.0380, 1138.7620, 1141.6649, 1154.5766, 1160.7449, 1162.9427, 1165.0041, 1170.4701, 1175.1426, 1180.0404, 1181.4840, 1187.2253, 1187.8717, 1191.7578, 1195.1037, 1200.7521, 1201.6838, 1204.0454, 1207.2077, 1211.1695, 1215.0301, 1216.0583, 1218.2967, 1223.6955, 1228.9067, 1231.1622, 1235.6166, 1236.6211, 1238.5199, 1243.5990, 1246.2303, 1248.5830, 1254.3725, 1255.2803, 1256.7108, 1263.1633, 1265.6449, 1267.5521, 1272.1495, 1273.3645, 1274.4297, 1279.5484, 1287.5516, 1289.6064, 1390.4100, 1432.0158, 1480.5714, 1517.4202, 1524.8265, 1666.0498, 1969.5500, 3095.1518, 3104.8350, 3194.2766, 3206.2574, 3223.0620, 3857.2019, 3973.3346	
T2-O5-Propanoic acid(ads)	342	41.3716, 46.5260, 63.7016, 65.3368, 69.0260, 76.1144, 81.4405, 82.1109, 87.2080, 89.5754, 90.4288, 93.7150, 96.1347, 97.3180, 99.4545, 106.8172, 108.2836, 112.8342, 114.5228, 118.4118, 119.3873, 122.5975, 124.4497, 126.2400, 130.0040, 134.8525, 137.5122, 140.9349, 142.6148, 143.9355, 146.0047, 147.1574, 148.9906, 149.9712, 150.8893, 152.7377, 155.7587, 157.3323, 160.8074, 162.0881, 164.7565, 167.3809, 169.3590, 171.6980, 173.3288, 175.6245, 178.9907, 181.6264, 182.3799, 185.0439, 188.6199, 194.8725, 197.7309, 201.1660, 202.1880, 203.8701, 204.5206, 205.0683, 207.2974, 210.9082, 212.1828, 212.8597, 216.8033, 223.0939, 223.8771, 225.3259, 228.4261, 228.9077, 230.6589, 233.7455, 234.7373, 236.5486, 239.2835, 240.6239, 243.5973, 245.6460, 247.3985, 248.4904, 252.5908, 253.9307, 256.9611, 260.7475, 262.2713, 263.7842, 266.7153, 269.3123, 270.6676, 271.8330, 273.2466, 275.8890, 278.0567, 279.7623, 281.1451, 282.4380, 283.5337, 285.2722, 289.4360, 289.9932, 292.1180, 294.0396, 294.7619, 296.7734, 299.2060, 301.6020, 302.3607, 306.0389, 306.3247, 308.5339, 311.8003, 313.0169, 318.2610, 318.8645, 326.0217, 327.3139, 331.0088, 334.4228, 337.1929, 342.2477, 347.7003, 352.5362, 355.7538, 360.7132, 362.6010, 363.9538, 366.3102, 369.9223, 375.1119, 376.4379, 378.8973, 381.6151, 385.3165, 387.5604, 389.0765, 391.3102, 392.4457, 392.9018, 396.1542, 397.1808, 399.7573, 400.0020, 401.7304, 405.6877, 408.4429, 411.0794, 414.1624, 418.2492, 420.9561, 424.8111, 429.5410, 431.3531, 435.5584, 438.7909, 440.7253, 444.4840, 445.9875, 454.4884, 458.5212, 461.5111, 465.9718, 471.2783, 473.8479, 477.2169, 482.2077, 487.6167, 490.3930, 493.1630, 496.1150, 498.4173, 499.6097, 505.7633, 509.6447, 512.4764, 521.5497, 530.5283, 539.9558, 543.2994, 555.3365, 556.0649, 570.8623, 573.9130, 575.9578, 587.4320, 603.2043, 608.6090, 617.9864, 624.7122, 637.7115, 642.6587, 646.0031, 658.0480, 665.5738, 670.1523, 670.9087, 672.3187, 675.7232, 685.8616, 687.7016, 692.2636, 695.0373, 698.1242, 703.7103, 706.5760, 709.2245, 711.0330, 714.9665, 718.6042, 719.5082, 724.9789, 726.4274, 727.7724, 729.3387, 738.5826, 740.2840, 748.6120, 749.4506, 752.6912, 753.2786, 756.5194, 757.0532, 758.9054, 759.8422,	None

		761.8943, 764.8741, 766.1432, 770.7382, 775.1791, 778.0025, 781.2061, 783.4139, 785.6115, 787.1631, 790.1991, 792.6431, 794.3330, 794.7347, 796.3371, 797.4734, 799.6158, 800.3744, 803.5517, 806.7685, 808.6621, 809.8420, 811.2088, 813.7846, 816.5246, 817.5005, 819.8188, 822.1089, 822.6179, 825.7444, 830.1174, 830.4951, 834.1981, 835.7291, 839.3054, 843.3645, 844.1568, 847.6305, 848.6615, 852.0261, 856.1113, 870.4485, 1013.0674, 1029.7992, 1071.0868, 1089.5016, 1091.4469, 1092.8281, 1100.5129, 1103.4702, 1111.5419, 1113.8741, 1117.2424, 1117.9346, 1119.4829, 1125.9020, 1129.8978, 1131.2242, 1131.9634, 1132.9465, 1134.5189, 1137.8451, 1138.7288, 1149.1427, 1154.3925, 1157.4548, 1161.2281, 1166.2059, 1166.7928, 1173.0383, 1176.7814, 1180.1165, 1181.2600, 1187.0691, 1188.3710, 1196.1891, 1199.6936, 1202.2423, 1204.0254, 1207.7415, 1210.5395, 1214.7055, 1215.6714, 1219.6018, 1225.2365, 1227.3805, 1230.5771, 1232.0660, 1236.4294, 1238.4546, 1240.2007, 1241.9477, 1246.4530, 1247.1467, 1254.2261, 1256.0863, 1261.6279, 1264.2967, 1266.7101, 1269.5537, 1273.4476, 1276.5438, 1280.6190, 1284.8200, 1288.5482, 1305.1845, 1353.8253, 1369.6815, 1408.1404, 1428.1862, 1516.7765, 1526.3122, 1542.8685, 1893.3180, 3094.6046, 3102.7123, 3160.1692, 3182.1650, 3215.9579, 3254.0862, 3609.5392	
T3-O7-ZeOH-C ₂ H ₄ (ads)	243	43.2213, 63.5389, 64.2387, 75.6382, 80.4501, 87.3424, 92.5303, 97.7743, 101.4737, 104.3443, 106.8458, 113.3501, 115.2033, 121.6783, 123.7905, 128.0009, 130.2650, 132.4358, 133.3255, 137.3813, 142.6967, 144.9444, 153.2819, 154.8802, 157.7404, 158.1661, 162.5873, 166.6514, 172.2356, 176.4652, 181.7352, 185.4963, 187.1646, 189.9008, 192.5364, 197.3315, 200.0233, 202.0766, 207.3244, 209.9819, 210.9807, 214.4715, 217.0939, 220.8539, 224.9021, 227.5790, 228.3590, 229.6261, 233.0682, 234.9200, 235.5932, 242.2557, 244.8729, 245.5017, 247.4600, 251.5665, 253.2536, 254.4715, 254.5847, 256.8933, 261.9774, 265.0084, 266.2427, 268.6778, 271.6905, 274.2120, 276.5046, 278.5762, 281.5926, 284.7857, 286.4971, 290.0597, 295.0608, 295.6864, 298.3549, 302.8694, 306.7159, 310.7608, 310.9521, 315.1724, 317.9866, 322.5269, 325.2129, 327.2781, 331.3374, 332.8400, 337.2217, 342.5519, 344.3767, 348.5949, 352.5698, 359.2822, 363.9446, 366.2444, 371.9408, 376.2249, 377.2397, 381.1722, 387.0506, 392.2079, 393.1937, 397.4156, 399.2906, 402.4942, 405.9785, 414.5630, 416.2705, 422.7109, 427.1102, 433.4178, 437.3052, 445.7832, 447.8514, 454.5043, 467.8909, 473.3767, 483.7117, 489.7657, 501.9111, 505.3015, 517.3901, 527.8360, 530.3093, 534.8144, 543.3846, 547.0039, 560.1763, 578.7007, 583.9462, 586.5457, 597.6907, 602.7693, 613.7678, 616.5640, 647.3343, 666.6872, 669.7647, 672.1653, 673.8877, 678.6136, 693.3619, 694.9781, 703.9225, 710.6730, 719.7182, 722.9301, 730.4222, 741.1271, 742.7585, 743.7764, 746.6863, 747.3355, 751.3445, 753.1601, 760.4986, 767.6379, 769.1734, 772.1657, 773.1437, 775.8171, 778.0653, 784.0416, 787.2996, 790.8207, 792.2879, 796.1873, 799.0001, 805.3129, 806.4934, 807.7538, 812.1054, 813.3882, 815.0662, 816.8072, 819.7284, 821.7873, 822.8564, 826.3109, 830.6498, 833.3578, 835.6072, 838.7676, 843.7948, 844.2695, 848.0581, 853.8454, 856.1635, 860.1199, 1040.5598, 1050.9739, 1082.1105, 1090.3523, 1099.1967, 1105.0772, 1110.6119, 1116.4480, 1119.9358, 1123.5055, 1135.5270, 1139.2233, 1142.7688, 1147.9402, 1155.8623, 1163.4145, 1172.0737, 1178.2460, 1180.5980, 1190.9952, 1193.8136, 1199.6502, 1207.6953, 1208.6243, 1214.1947, 1214.5578, 1215.0303, 1219.8059, 1226.8699, 1231.2710, 1236.1000, 1239.5930, 1242.9586, 1246.2086, 1249.4949, 1255.4483, 1258.8429, 1260.2345, 1273.9477, 1275.5734, 1283.4330, 1293.2201, 1295.8030, 1298.9428, 1318.3448, 1324.1815, 1329.7279, 1395.2240, 1488.1719, 1711.3182, 3161.2466, 3182.0607, 3252.9848, 3282.2953, 3437.2281	None

T3-O7-Protonation-TS	243	-181.9765, 60.4271, 66.9997, 77.6167, 81.2533, 83.4913, 92.7854, 99.9828, 103.1503, 106.0077, 112.4371, 112.8049, 118.3126, 119.3804, 124.3137, 126.4325, 128.8482, 131.7663, 133.1751, 137.8580, 140.7456, 147.9872, 149.3904, 154.2722, 155.8172, 161.4394, 164.0419, 168.3426, 169.1817, 177.4764, 178.0231, 180.7760, 186.7573, 189.0449, 189.6457, 194.2846, 198.5088, 199.4573, 206.3861, 207.0056, 210.1698, 212.6765, 214.5163, 218.9514, 221.0219, 224.1131, 227.6962, 229.2895, 234.1849, 235.0860, 236.8588, 239.9843, 242.8563, 244.4794, 247.8398, 249.0767, 251.2178, 253.5545, 254.9034, 257.3999, 258.1192, 262.3907, 266.2347, 268.7577, 270.2237, 274.2154, 275.1744, 275.8927, 280.3622, 285.0910, 287.4595, 291.4526, 292.0685, 297.3626, 299.6834, 304.7107, 307.8312, 311.3832, 313.9030, 317.6352, 321.4556, 324.6962, 327.8141, 329.7559, 333.7000, 334.4852, 338.0978, 342.6929, 343.7763, 348.7151, 355.1935, 362.5125, 365.1110, 367.6777, 375.1520, 377.2513, 379.2883, 386.7004, 391.1938, 393.0923, 395.2215, 398.5014, 402.5099, 405.4240, 410.8312, 416.3192, 420.2114, 428.1462, 431.1483, 443.1251, 446.1165, 447.5011, 451.4693, 456.8378, 468.3397, 477.4303, 487.9143, 490.5279, 501.6367, 504.6121, 515.6261, 527.9732, 530.7651, 539.9225, 547.7253, 551.1806, 560.1436, 582.9248, 586.5834, 589.5441, 598.0216, 606.1331, 611.0921, 644.2327, 653.2491, 668.1543, 674.3070, 676.0287, 691.5126, 696.2752, 700.8420, 706.7815, 712.1271, 715.4896, 721.0749, 722.9954, 729.1521, 739.8827, 742.0079, 743.1708, 747.4642, 750.2725, 750.5020, 753.5512, 756.8194, 763.0234, 768.0792, 772.2740, 774.3138, 776.4966, 778.8629, 782.5194, 783.9960, 786.5692, 792.2312, 794.1993, 795.8283, 799.7525, 801.5233, 803.9654, 806.4516, 810.3251, 812.9255, 814.2197, 815.3110, 818.9583, 821.3590, 824.2043, 827.1007, 829.7100, 830.6372, 836.0131, 842.8730, 846.2842, 851.0809, 861.1708, 866.8941, 1029.1374, 1051.8219, 1081.8641, 1095.0951, 1096.3438, 1104.5986, 1107.8782, 1111.7124, 1117.0366, 1119.3946, 1122.1848, 1132.5250, 1141.7477, 1147.7613, 1150.1577, 1159.2590, 1164.0356, 1171.4047, 1176.1245, 1180.0887, 1193.2527, 1194.6380, 1197.2583, 1205.5587, 1206.5818, 1209.2356, 1211.7966, 1216.9609, 1219.2148, 1224.7677, 1225.5384, 1231.0578, 1232.7069, 1236.5135, 1247.5562, 1248.8633, 1253.7937, 1262.0433, 1263.2590, 1271.0040, 1277.7819, 1281.1087, 1286.4066, 1294.8853, 1298.7689, 1314.8846, 1315.8228, 1330.2290, 1390.7254, 1501.7514, 1619.4634, 2129.2768, 3027.2090, 3174.1705, 3231.1872, 3288.5148	-181.9765
T3-O7-ZeO-C ₂ H ₅ (ads)	243	67.1906, 73.2053, 83.5617, 89.4847, 96.7035, 102.3943, 108.1399, 109.9630, 113.3874, 117.1754, 121.8278, 122.5868, 127.2987, 130.0300, 134.1158, 138.7668, 139.0626, 144.0018, 146.4669, 152.4274, 154.6072, 159.2942, 162.0323, 167.3003, 171.1863, 176.1369, 179.3112, 181.8391, 184.7766, 187.4563, 191.0148, 193.4794, 196.7855, 199.6144, 203.1564, 204.5156, 208.8535, 212.0451, 215.8905, 217.2608, 220.2264, 221.9554, 226.2323, 228.2489, 229.1154, 230.7960, 234.2630, 235.7836, 236.2729, 243.6683, 244.5083, 246.6032, 250.3289, 252.1087, 254.1541, 256.0010, 256.7668, 259.0316, 262.5434, 265.7822, 267.3360, 269.1548, 273.0384, 274.3982, 277.2684, 280.4543, 281.4879, 284.4565, 286.4257, 291.1381, 292.9385, 297.5937, 302.3991, 303.1516, 307.7346, 309.5773, 312.7984, 316.7024, 318.5549, 322.1159, 326.5112, 327.3536, 332.0989, 333.6226, 336.4871, 339.5285, 344.8071, 347.7619, 351.5151, 355.9526, 363.1873, 365.6697, 369.9125, 371.6765, 374.8738, 379.5498, 383.9948, 388.0975, 392.1942, 395.6318, 396.9491, 400.1783, 403.8773, 407.3039, 413.4943, 417.5630, 426.0376, 428.8812, 433.5357, 444.7762, 445.1719, 454.1080, 463.4457, 467.4687, 473.2254, 485.7272, 488.9441, 501.0289, 504.6611, 508.7404, 522.0027, 530.2124, 534.7365, 542.8579, 546.1186, 560.2891, 574.4843, 583.1888, 586.1544, 596.4170,	None

		602.7315, 611.9025, 617.7546, 649.5769, 666.8529, 668.1548, 671.2737, 674.2614, 694.7696, 698.2635, 703.4436, 711.1337, 714.7223, 719.6368, 727.5581, 735.1361, 739.8220, 741.2891, 746.4613, 747.0741, 750.3967, 751.5004, 761.2596, 764.0028, 766.6412, 768.6183, 772.9879, 773.6608, 775.3713, 779.2129, 784.8787, 789.0578, 790.7721, 792.3829, 793.6754, 798.0394, 803.7153, 803.8789, 807.1626, 809.4266, 812.6504, 814.9531, 816.0453, 818.5938, 824.6127, 826.3794, 828.1329, 831.5261, 833.2606, 834.9912, 839.1225, 843.1040, 844.0197, 853.7997, 854.5108, 856.6265, 882.6110, 1028.2484, 1086.9097, 1099.8172, 1101.1239, 1108.1961, 1115.2643, 1116.7846, 1122.0618, 1128.2781, 1131.8845, 1136.7973, 1142.5556, 1146.7161, 1153.4579, 1161.3336, 1170.7261, 1177.5087, 1178.0563, 1188.4839, 1191.9135, 1193.9003, 1197.6438, 1203.7761, 1207.2282, 1209.6845, 1211.6820, 1213.3829, 1217.1427, 1224.2589, 1227.9067, 1234.4095, 1239.7506, 1242.0588, 1247.8235, 1252.3007, 1256.3668, 1257.3767, 1273.4601, 1279.5277, 1285.2642, 1293.4424, 1298.9860, 1314.5166, 1319.7536, 1329.1539, 1377.1615, 1426.6297, 1466.7699, 1499.2921, 1513.4100, 1528.0587, 3096.8144, 3157.1014, 3186.7217, 3217.7966, 3236.2656	
T3-O7-ZeO-C ₂ H ₅ CO(ads)	249	25.6427, 63.7982, 65.1697, 72.0972, 79.6924, 83.6163, 89.2987, 94.6066, 99.0400, 102.3202, 109.0357, 110.5908, 113.8445, 117.6335, 122.0525, 122.8562, 126.6897, 130.8386, 135.5193, 137.5659, 140.0488, 144.3226, 145.1518, 152.2396, 153.1272, 156.5401, 158.5955, 165.6558, 168.7178, 171.2707, 173.2195, 177.9507, 180.0376, 184.5503, 185.8741, 190.5507, 192.3405, 193.3413, 195.8214, 199.3672, 203.9690, 208.8635, 211.8025, 215.5354, 216.7672, 217.5662, 221.8377, 224.3296, 228.2599, 228.9839, 230.8679, 235.8049, 236.0656, 239.9033, 244.6136, 245.6670, 246.3169, 251.1603, 252.9628, 255.7203, 256.8273, 257.0505, 260.6022, 262.6271, 266.0176, 267.4396, 270.0670, 273.2538, 274.7546, 277.7818, 281.6658, 281.9410, 284.5032, 286.3410, 292.0618, 293.4611, 297.3931, 302.3487, 303.9077, 307.3199, 310.0968, 313.7382, 318.3108, 319.8819, 322.0310, 326.3392, 329.0151, 332.4123, 334.4220, 336.1628, 340.2930, 344.7324, 345.9982, 350.8567, 355.8349, 361.8769, 365.9513, 368.6391, 371.0525, 374.8070, 379.1358, 383.4386, 388.2449, 391.7413, 395.1332, 397.0783, 400.2079, 403.5052, 407.0888, 413.1744, 416.6701, 426.0428, 428.1349, 433.1779, 445.1907, 445.6736, 454.1011, 465.1193, 468.0636, 473.3949, 486.1641, 488.8058, 501.3820, 505.0621, 509.9168, 522.1337, 530.1967, 534.4921, 542.9611, 546.1932, 560.7558, 574.4458, 583.0349, 585.9606, 596.4804, 602.3913, 610.8076, 618.1308, 649.5585, 667.6411, 668.6086, 671.8214, 675.3657, 695.4103, 697.4014, 703.2572, 711.9345, 715.7404, 719.4783, 727.9188, 736.6792, 739.5383, 741.3005, 746.2102, 747.3730, 750.3355, 751.2630, 760.8112, 764.6684, 766.4757, 768.2766, 771.0168, 773.5393, 774.4146, 778.2073, 784.4937, 788.9107, 790.0164, 790.6944, 793.8733, 796.1111, 802.5071, 803.1516, 807.2140, 808.9282, 812.8166, 814.6710, 815.6193, 818.2519, 823.7256, 825.2975, 827.5048, 830.8329, 832.2520, 833.6985, 834.9637, 841.0262, 843.2918, 853.3619, 855.1765, 857.5064, 887.1294, 1027.9623, 1086.6076, 1098.1040, 1100.3168, 1107.7916, 1114.1763, 1116.2520, 1121.7235, 1127.1087, 1131.0439, 1136.5303, 1142.7753, 1147.9854, 1153.6541, 1161.9158, 1170.2527, 1176.5730, 1177.7517, 1188.1148, 1192.9633, 1193.0965, 1197.3761, 1203.8680, 1206.9299, 1210.0665, 1211.8195, 1212.7592, 1216.8857, 1224.1716, 1228.3815, 1234.4857, 1238.4292, 1240.0234, 1248.3340, 1252.8220, 1254.9982, 1257.8076, 1271.5001, 1280.5531, 1286.5458, 1296.2043, 1298.3561, 1315.3746, 1318.6799, 1328.7461, 1357.8083, 1410.2295, 1453.4757, 1492.4821, 1506.5156, 1537.3312, 2236.1671, 3104.5105, 3151.2969, 3191.4109, 3217.2447, 3235.2428	None

T3-O7-Carbonylation-TS	249	-409.0160, 51.0798, 56.4851, 73.1665, 78.2569, 82.6830, 90.3199, 98.9355, 102.6376, 105.8487, 107.3158, 112.2041, 113.9725, 116.3811, 120.2406, 121.9916, 125.0013, 128.5278, 134.1461, 135.5093, 137.7143, 139.6223, 142.1725, 151.7684, 153.8769, 155.0090, 158.0631, 161.2203, 165.1549, 165.9513, 172.8626, 179.4310, 181.6426, 185.6940, 187.1392, 188.9015, 193.2134, 194.3853, 198.5797, 201.4146, 207.1362, 209.4173, 210.8863, 213.3704, 216.0356, 218.5295, 220.8330, 224.2363, 226.5730, 230.4041, 233.6814, 235.6074, 236.3263, 240.4096, 242.0721, 244.3326, 247.0682, 248.7372, 250.5457, 252.8160, 255.6628, 257.0171, 257.6275, 259.3408, 263.2772, 266.4443, 269.1806, 269.3889, 275.6902, 276.5818, 277.2088, 282.8040, 285.8528, 286.3277, 292.6855, 294.0084, 296.9995, 301.4472, 304.8819, 308.1370, 310.4213, 313.0099, 314.5081, 315.9589, 319.8182, 322.0060, 324.8467, 327.9368, 331.9052, 334.4393, 336.3725, 339.4088, 344.2186, 347.2277, 349.5571, 353.9801, 362.8004, 366.4549, 369.6109, 375.0926, 378.8473, 379.5018, 385.5531, 392.2451, 393.6827, 395.7726, 400.6475, 402.1793, 405.0981, 411.3279, 416.0326, 418.9623, 426.8423, 434.5883, 441.9198, 445.1534, 447.4497, 451.0386, 456.1193, 468.8062, 478.2462, 487.6779, 490.1522, 502.0243, 504.8827, 516.0592, 527.9964, 531.9896, 538.9730, 544.8632, 549.2141, 560.7406, 580.9776, 586.1021, 587.4864, 600.3561, 606.3225, 612.7072, 637.1357, 652.1907, 669.1251, 674.2039, 677.4981, 692.6028, 697.3496, 700.0468, 703.3386, 713.4402, 717.8037, 721.0845, 728.6229, 738.1436, 741.0274, 744.3158, 746.6766, 747.6534, 752.7050, 753.9861, 754.6881, 763.3181, 767.7630, 772.4228, 774.5079, 775.9729, 778.9051, 782.8681, 785.0639, 787.7925, 791.3446, 792.6962, 797.5003, 800.8035, 802.9265, 805.1129, 807.8143, 810.6467, 811.4915, 813.4076, 816.1408, 820.5209, 822.5609, 825.4997, 827.6584, 830.2342, 830.9009, 835.8801, 836.9589, 841.7585, 848.8932, 850.4386, 860.3048, 924.9625, 1007.2878, 1068.4828, 1087.3092, 1089.7296, 1094.1886, 1097.7545, 1107.2177, 1114.4037, 1117.6020, 1119.5322, 1122.4922, 1130.9403, 1139.8570, 1148.5681, 1149.8002, 1158.1316, 1171.1886, 1178.1581, 1180.0476, 1191.1629, 1193.2764, 1199.0761, 1203.6537, 1205.5121, 1206.9048, 1209.5762, 1211.0618, 1215.6984, 1219.6970, 1223.0752, 1224.9198, 1231.7511, 1232.1521, 1236.6045, 1237.6299, 1244.4696, 1253.5041, 1253.9646, 1258.6418, 1268.8556, 1274.6578, 1283.5888, 1289.0052, 1295.3879, 1311.3000, 1315.6148, 1331.1521, 1385.4570, 1454.4617, 1476.7032, 1506.5114, 2320.8411, 3098.0956, 3178.5932, 3214.4729, 3239.7974, 3374.6502	-409.016
T3-O7-ZeO-propionyl (ads)	249	53.6924, 76.1293, 77.6358, 81.0782, 90.0674, 96.8417, 101.9430, 109.6262, 111.8699, 113.8922, 115.4152, 119.8629, 121.4740, 128.4163, 129.3515, 135.1497, 136.0435, 140.7596, 142.9906, 146.0992, 150.3641, 152.9195, 158.1840, 159.9551, 162.8992, 167.1971, 169.7949, 172.4577, 178.4737, 183.7622, 185.5540, 187.5173, 191.2291, 193.6666, 195.4988, 200.1584, 203.6646, 209.4872, 211.7003, 213.5894, 215.6293, 217.3888, 220.7867, 224.1812, 226.1991, 229.5467, 230.6028, 231.4926, 234.8187, 235.6177, 235.8696, 242.9007, 244.2040, 244.9534, 249.4551, 250.1164, 253.1677, 253.5401, 256.2032, 256.6829, 262.6368, 264.8862, 266.0436, 268.0850, 269.7827, 273.3375, 275.3229, 279.0827, 280.9846, 282.2748, 284.8233, 288.1745, 290.6063, 295.9087, 298.0485, 298.6594, 303.2299, 309.3101, 309.5330, 313.2181, 315.4917, 320.3611, 323.3607, 325.3428, 327.3410, 331.4863, 334.1971, 336.6576, 344.7017, 346.3341, 350.4614, 352.6241, 358.4754, 364.3932, 365.1046, 369.8316, 373.7104, 378.4154, 378.9813, 385.6658, 390.9882, 394.4244, 396.3141, 401.3294, 403.3729, 407.0528, 412.9283, 416.2464, 421.8810, 425.5974, 433.3382, 444.7186, 445.6184, 453.0358, 457.1710, 460.5537, 468.1308, 475.1750, 485.3242, 488.8784,	None

		500.2443, 504.9975, 518.8603, 527.4068, 533.8099, 540.2041, 542.6120, 557.3050, 561.8278, 578.3152, 583.1601, 586.0859, 599.5255, 605.2194, 611.3049, 630.6493, 641.8264, 665.1249, 666.5743, 668.6768, 673.5714, 685.7368, 694.6253, 697.8920, 702.0034, 711.1619, 716.3295, 719.2088, 727.9041, 731.3773, 738.0275, 740.0459, 742.9268, 745.1601, 746.3384, 750.5232, 754.9674, 760.4954, 765.1265, 767.8323, 770.2090, 773.1450, 774.7026, 776.4474, 781.6829, 785.8816, 789.0956, 792.9386, 793.7587, 798.2683, 803.0082, 806.3425, 807.3584, 810.9797, 811.5429, 812.7693, 815.6382, 818.0719, 820.7371, 826.2757, 826.7422, 829.1300, 832.4797, 833.0922, 835.3199, 837.4011, 841.6893, 845.6610, 852.4110, 854.6287, 860.3951, 979.1145, 1069.7350, 1083.3134, 1089.2568, 1098.3349, 1101.9213, 1106.6511, 1112.0559, 1113.1340, 1121.6544, 1125.2812, 1129.1495, 1134.8311, 1142.8555, 1148.6867, 1154.3641, 1160.9322, 1169.0201, 1173.7152, 1176.4858, 1184.8684, 1188.2150, 1192.7698, 1201.3505, 1204.8982, 1207.4891, 1209.7403, 1212.5636, 1214.9710, 1222.6225, 1227.0956, 1234.2701, 1239.9138, 1244.0886, 1245.9838, 1247.7836, 1255.5938, 1259.1843, 1274.4909, 1276.3983, 1288.0487, 1297.4627, 1300.3535, 1309.5250, 1314.7765, 1321.9922, 1332.7170, 1378.2293, 1430.4321, 1483.9948, 1509.5589, 1518.0545, 1944.1759, 3100.1206, 3143.0047, 3188.0110, 3194.4303, 3234.5259	
T3-O8-ZeOH-C ₂ H ₄ (ads)	243	55.8603, 63.3361, 70.1735, 76.8140, 82.7273, 88.1176, 97.2035, 98.9140, 101.3161, 103.2189, 112.7642, 115.2426, 116.5619, 122.4034, 124.0709, 125.8489, 130.0007, 131.5310, 136.2438, 138.9627, 144.2691, 146.4270, 153.2051, 154.2987, 156.9082, 160.6375, 163.7415, 166.0901, 173.0237, 178.4251, 179.5084, 182.5254, 186.5132, 190.0345, 193.9862, 196.4468, 197.6053, 203.7869, 206.0342, 206.5875, 210.1204, 213.8454, 219.1074, 220.3990, 223.6369, 227.0290, 229.2364, 231.6666, 232.8272, 234.2865, 236.7413, 242.2204, 244.7325, 246.5321, 247.2826, 251.1093, 253.0641, 254.5279, 255.5097, 257.1344, 260.6096, 264.4591, 266.8975, 267.9075, 272.4753, 272.8038, 274.2189, 277.0301, 279.5857, 283.1524, 285.3883, 289.8276, 290.9276, 295.5612, 297.9806, 302.7785, 307.3586, 309.6294, 310.5102, 315.0709, 316.9547, 321.3167, 325.2496, 325.8676, 331.4142, 332.6560, 337.4554, 340.4637, 343.9043, 348.0131, 351.3383, 358.3511, 359.9606, 366.1006, 370.9123, 375.1236, 379.1797, 382.7512, 387.7081, 390.2579, 393.7469, 395.2603, 400.1617, 402.1424, 407.4516, 412.9794, 418.0449, 423.1185, 428.9655, 436.0071, 441.4708, 446.2855, 448.6903, 455.7870, 467.9901, 476.2203, 486.9636, 488.2584, 499.0663, 504.8605, 515.8580, 526.8256, 529.4286, 540.7252, 543.7643, 550.1235, 558.2166, 573.8594, 583.6588, 587.1032, 588.6092, 604.5180, 607.1744, 645.4041, 651.1616, 654.0089, 666.8598, 668.0154, 673.7230, 683.9490, 691.1414, 694.6352, 710.1129, 710.9291, 719.5374, 726.4679, 734.3118, 741.6921, 744.9387, 746.3746, 749.9858, 751.2641, 753.9502, 758.1831, 758.9359, 768.4986, 772.5612, 774.4461, 776.2346, 778.0324, 781.4883, 785.0205, 786.5847, 790.1302, 793.3164, 794.2461, 798.1015, 803.1237, 804.3545, 806.4150, 808.9531, 812.9974, 815.3847, 817.2717, 819.2955, 820.9428, 822.8149, 824.2730, 826.2877, 829.7945, 833.5640, 836.0198, 840.6030, 843.0741, 845.2010, 853.3847, 856.0446, 860.5713, 1031.6787, 1049.1909, 1082.9742, 1101.5705, 1102.8491, 1109.1561, 1116.0526, 1122.0158, 1123.9564, 1129.6853, 1131.6068, 1142.3385, 1144.1276, 1147.3995, 1154.1743, 1161.3066, 1168.2327, 1179.1024, 1181.6532, 1194.2579, 1203.2613, 1204.2004, 1206.6001, 1211.1080, 1215.7521, 1217.1991, 1219.4642, 1225.4688, 1228.5240, 1231.7213, 1235.5097, 1239.5747, 1243.5277, 1244.7831, 1248.8207, 1254.5853, 1258.7495, 1262.8139, 1272.2055, 1275.9080, 1284.9917, 1294.9237, 1298.4521, 1301.5776, 1321.2676, 1322.5546, 1333.9612,	None

		1392.3181, 1483.3731, 1711.8832, 3180.2752, 3193.8254, 3270.3274, 3291.7069, 3386.4514	
T3-O8-Protonation-TS	243	-549.9497, 59.4496, 70.1313, 72.9806, 74.2394, 82.1344, 86.9424, 97.1741, 102.7980, 103.4901, 110.1444, 114.2276, 115.2603, 119.4709, 122.9493, 125.8223, 127.2103, 132.5266, 136.9972, 140.7841, 145.6402, 150.9610, 152.9422, 155.1555, 160.1692, 163.9567, 165.4167, 169.5227, 173.5626, 176.1969, 183.4518, 186.1844, 186.9844, 190.2109, 195.5950, 197.5802, 198.9749, 205.3325, 206.7811, 210.4499, 211.5136, 213.2462, 218.6196, 221.1353, 225.9703, 227.3262, 229.6222, 232.4050, 233.7699, 234.7987, 238.3128, 242.0361, 243.6054, 245.3341, 247.6885, 250.7877, 253.2541, 254.8872, 256.8275, 257.5972, 261.9974, 264.0793, 268.5157, 268.7763, 272.6252, 273.8324, 275.5768, 279.9363, 284.1237, 285.7420, 290.1116, 291.2390, 295.7027, 298.4443, 301.7070, 304.1303, 309.7993, 311.7040, 314.0949, 314.6452, 320.7361, 322.1721, 326.4829, 328.8364, 332.1049, 334.5748, 338.1819, 341.0637, 344.4804, 347.8860, 351.5564, 354.0436, 361.8849, 366.3660, 368.8835, 374.8489, 378.4294, 382.9368, 385.6260, 390.6154, 393.3034, 395.2398, 400.0493, 401.4347, 404.7606, 410.5970, 415.6862, 418.8608, 430.0634, 432.0310, 443.6935, 448.0634, 450.5073, 454.7688, 459.7339, 468.3729, 479.7465, 488.2675, 490.4311, 501.7726, 504.2371, 516.4834, 527.2511, 529.9442, 540.8804, 545.5177, 550.5135, 559.9421, 583.5372, 586.9165, 588.9642, 591.7776, 607.3884, 607.9650, 645.3141, 652.0630, 668.2743, 672.1439, 675.5462, 690.5860, 694.6570, 696.0941, 708.6074, 712.3568, 720.7836, 722.0109, 729.7422, 736.5229, 741.1390, 741.8628, 746.4432, 748.0120, 751.3522, 752.3845, 755.9075, 764.8681, 768.1134, 768.6960, 773.6791, 776.4697, 779.6831, 781.1720, 785.3220, 786.6026, 790.9040, 792.5514, 794.0651, 797.0039, 800.3562, 803.4580, 806.3260, 807.5452, 811.0417, 814.1024, 816.6467, 817.6365, 820.2418, 822.8171, 823.9816, 827.4117, 831.7900, 833.6980, 838.6035, 840.8209, 842.9271, 850.6141, 861.0536, 874.0073, 1014.6696, 1088.4310, 1094.9255, 1102.8834, 1104.3935, 1108.6678, 1120.1726, 1125.8123, 1127.4667, 1134.3162, 1140.0911, 1150.8157, 1151.5909, 1155.9160, 1168.7185, 1173.8313, 1176.7147, 1180.1966, 1194.5562, 1194.9928, 1197.7729, 1202.5810, 1204.8350, 1209.8170, 1210.6425, 1212.7173, 1217.6588, 1220.6009, 1226.8841, 1227.9494, 1229.8651, 1237.3787, 1240.7586, 1243.0124, 1248.1551, 1254.0174, 1255.6422, 1260.5676, 1269.8300, 1277.6415, 1289.7565, 1290.9634, 1295.4483, 1302.2742, 1313.8667, 1319.7975, 1333.6310, 1342.4215, 1475.7915, 1573.2690, 2489.0520, 3174.4711, 3179.0001, 3279.8568, 3297.2347	-549.9497
T3-O8-ZeO-C ₂ H ₅ (ads)	243	48.1339, 62.6661, 71.7653, 75.7236, 78.5677, 86.3468, 94.9133, 98.3383, 101.8783, 111.7967, 113.7810, 115.3465, 119.7946, 121.4225, 124.9656, 128.2675, 134.4444, 136.4057, 140.6723, 145.1654, 150.7548, 153.6664, 156.9421, 162.1453, 163.2859, 165.9101, 172.1500, 177.5073, 180.1559, 185.6970, 188.1519, 189.7779, 192.6873, 195.5077, 199.6809, 204.9724, 207.2248, 210.1086, 213.4605, 217.1669, 220.0856, 223.0188, 226.6766, 228.5454, 231.0446, 232.4519, 236.1096, 238.5099, 240.4927, 242.2872, 242.8151, 245.8842, 249.0781, 250.6260, 252.2409, 254.5456, 255.5379, 258.6502, 261.3382, 265.5912, 267.7386, 268.8772, 272.4040, 273.6283, 274.8026, 279.6640, 282.8971, 285.7255, 288.1254, 291.0447, 293.7428, 297.0378, 303.5059, 304.7824, 308.6632, 309.7208, 311.7804, 316.0271, 320.9674, 321.1750, 325.6023, 329.6327, 332.0965, 332.7918, 337.6054, 339.6800, 344.2003, 347.2211, 351.8419, 355.2320, 362.5352, 365.6408, 371.0839, 373.0610, 376.1936, 381.1843, 384.9254, 386.0091, 390.4543, 392.5682, 394.4257, 399.9472, 402.0791, 408.6393, 415.1566, 418.0128, 427.3521, 432.6822, 435.0727, 445.6956, 448.8156, 455.4396, 461.6703, 468.0780, 476.4924, 486.5865, 489.9263, 498.9348, 504.1335, 511.8387, 523.5936	None

		527.0506, 540.0842, 543.5302, 551.2290, 557.1244, 572.6289, 584.5198, 586.6591, 589.1646, 605.1337, 607.8467, 644.2081, 650.9621, 658.8979, 666.9739, 673.7941, 684.6456, 691.6427, 694.5569, 710.4228, 711.9888, 719.8133, 723.0973, 731.6879, 733.0849, 744.7220, 746.7316, 749.2699, 751.4805, 752.2471, 759.5612, 762.8377, 769.0364, 769.5044, 772.2185, 774.9133, 778.5334, 781.5228, 783.5494, 786.1234, 788.8730, 791.1025, 794.0188, 796.9111, 799.0169, 803.1983, 805.9370, 807.4341, 808.3711, 812.5234, 814.4660, 815.7828, 816.6678, 818.4109, 820.9836, 822.1634, 824.0302, 828.1007, 831.7103, 833.7531, 836.7910, 842.5754, 846.5178, 854.9498, 859.0839, 896.2623, 1015.8447, 1094.7317, 1104.9678, 1114.5937, 1118.7434, 1119.9582, 1123.3816, 1129.9070, 1132.4063, 1135.6204, 1141.0798, 1144.6031, 1150.9638, 1155.3672, 1161.4828, 1167.2048, 1180.4421, 1182.9597, 1194.1498, 1195.2164, 1204.4525, 1205.0365, 1210.1276, 1211.7382, 1217.1656, 1218.2578, 1223.1709, 1226.4613, 1228.9481, 1232.7418, 1236.3280, 1237.5644, 1245.2348, 1249.9566, 1253.4979, 1261.2673, 1263.7282, 1274.6820, 1282.9228, 1294.9120, 1297.7907, 1299.1650, 1318.7572, 1319.4420, 1332.0464, 1343.9244, 1405.7459, 1445.8641, 1496.3912, 1517.9140, 1544.4958, 3092.8320, 3144.0099, 3181.1823, 3203.2806, 3221.8420	
T3-O8-ZeO-C ₂ H ₅ CO(ads)	249	33.5478, 36.4811, 49.1369, 61.5747, 68.5689, 68.6400, 80.4812, 85.7312, 86.0588, 87.5504, 96.2478, 98.7336, 102.3792, 108.1303, 109.3485, 112.1569, 118.4537, 124.4563, 129.0266, 130.8124, 136.9058, 138.8537, 139.9653, 145.9943, 148.2867, 150.3741, 153.7019, 155.5648, 163.3003, 164.3763, 167.5016, 171.2900, 175.7283, 177.8732, 185.5793, 188.0951, 192.2123, 194.9847, 199.9362, 200.7942, 202.3579, 206.8938, 210.9073, 214.6074, 217.1515, 222.9856, 225.2768, 225.4389, 227.2986, 232.3857, 234.7493, 236.8460, 239.3282, 243.4033, 244.6369, 245.6875, 246.2140, 248.4073, 249.2745, 252.4201, 255.2475, 255.8183, 257.6447, 261.3794, 262.8656, 264.9528, 266.5056, 269.1944, 273.0554, 278.4243, 281.7777, 284.1140, 285.2971, 288.9491, 290.9065, 294.3561, 296.4708, 301.1674, 304.8506, 308.2010, 311.2289, 313.0568, 316.3016, 321.6276, 323.0930, 326.6911, 329.9386, 332.5586, 337.1818, 340.7509, 343.3997, 344.4614, 347.6938, 348.0603, 357.9886, 360.8887, 367.3287, 371.0722, 375.5285, 378.9755, 380.1104, 384.3439, 386.1799, 391.8731, 395.1005, 395.3957, 399.6383, 406.4913, 413.2127, 415.0760, 421.2767, 427.3540, 436.8966, 437.7335, 447.3746, 453.9978, 459.0117, 460.5289, 467.5578, 478.6051, 482.1045, 487.9103, 494.9207, 503.9588, 508.6123, 522.6624, 532.4878, 539.1781, 549.5082, 550.8160, 560.7856, 579.5781, 585.7467, 587.5661, 590.5410, 606.8057, 609.4171, 641.9901, 650.1051, 660.3852, 667.6820, 674.5943, 684.1217, 689.4248, 694.1342, 705.1788, 710.1408, 720.8632, 724.1779, 736.5748, 739.7542, 742.5350, 745.3370, 747.0225, 753.1656, 754.8074, 763.9671, 767.1554, 770.2714, 771.8829, 774.9108, 777.8450, 780.3948, 783.1290, 784.3680, 786.4534, 787.6400, 793.0470, 795.5432, 798.3531, 801.6291, 802.5903, 805.1644, 806.7428, 810.2515, 812.9446, 814.5548, 817.0351, 818.2409, 821.8401, 824.9226, 826.0917, 828.4349, 829.7526, 834.6871, 838.7186, 839.4659, 849.4429, 853.9968, 857.9123, 859.9985, 900.2986, 1012.5670, 1092.7542, 1110.4491, 1118.4922, 1125.3869, 1126.9943, 1132.2216, 1134.2283, 1138.5231, 1141.1478, 1144.4988, 1151.3324, 1152.7069, 1166.5734, 1167.7423, 1175.8510, 1181.2114, 1184.5946, 1196.5435, 1208.3363, 1210.4849, 1212.1223, 1216.4294, 1217.8627, 1221.9475, 1226.9837, 1231.2471, 1234.4948, 1237.0021, 1242.1099, 1242.3583, 1243.9850, 1247.1451, 1255.3385, 1259.3475, 1263.7891, 1267.0637, 1274.4389, 1288.1502, 1290.1863, 1302.5806, 1310.6488, 1317.4789, 1333.3484, 1344.6210, 1363.4891, 1416.5827, 1456.1194, 1498.3567, 1512.1795, 1605.1143, 2243.7841, 3100.3179,	None

		3178.9209, 3190.9245, 3201.4673, 3259.4973	
T3-O8-Carbonylation-TS	249	-428.6129, 32.4987, 44.4864, 55.9697, 58.2482, 63.5038, 70.4303, 75.0294, 81.8174, 83.6580, 90.7239, 97.8485, 102.9555, 105.1890, 106.9549, 110.0990, 116.4047, 124.4085, 124.6581, 130.7419, 132.6311, 137.8865, 139.9465, 143.0840, 145.6657, 148.1403, 150.4451, 151.9280, 156.6682, 162.3691, 168.4529, 170.3266, 173.9194, 177.6539, 182.4779, 186.0850, 189.8927, 191.9537, 196.6337, 199.0881, 201.9773, 205.0767, 207.4047, 212.1323, 215.2752, 216.2218, 222.0540, 223.3976, 225.5703, 228.5560, 231.6459, 233.6104, 236.7892, 239.7639, 240.7498, 243.6401, 246.3006, 246.5040, 249.3443, 250.6115, 253.6048, 254.8481, 257.1801, 259.1890, 261.6266, 263.2830, 265.4835, 266.5205, 272.7151, 276.8455, 278.5442, 282.5060, 284.7347, 287.2511, 289.1422, 291.8272, 295.1056, 298.8775, 304.5558, 308.2291, 310.1443, 315.7761, 317.7416, 319.0699, 324.1133, 325.9808, 329.2843, 330.7023, 332.6816, 337.4051, 338.4039, 342.3712, 345.4030, 347.9664, 350.9250, 352.0655, 358.2920, 363.9195, 368.3628, 373.0253, 377.6531, 378.8686, 384.1974, 386.8509, 389.6220, 392.9459, 396.0190, 397.3819, 401.0719, 407.8860, 415.9725, 418.1348, 424.6912, 437.7541, 440.1626, 446.6255, 450.4968, 452.2683, 455.1583, 467.6542, 477.8098, 487.0075, 489.7057, 496.2060, 504.2084, 514.3663, 527.0889, 533.5144, 538.9372, 548.2001, 554.8555, 563.9163, 586.3027, 587.8686, 589.7136, 595.9204, 608.2644, 611.1010, 644.5553, 656.6183, 669.5707, 670.1051, 677.3781, 683.6283, 695.1937, 696.3415, 710.4351, 712.2549, 720.9526, 722.1187, 732.5000, 740.3142, 744.5803, 745.3208, 748.3178, 752.0874, 754.2750, 754.9711, 761.6138, 766.6344, 769.8372, 772.8560, 774.9269, 779.9334, 782.4453, 783.7531, 787.8398, 788.5793, 794.6768, 796.9109, 800.6775, 802.2484, 803.9566, 807.3620, 811.1127, 812.5028, 814.5095, 816.6180, 817.1932, 821.9279, 823.4335, 824.7735, 826.7233, 831.4711, 832.0058, 835.5996, 838.3231, 844.2826, 848.7456, 860.5203, 863.3610, 942.8746, 1005.0747, 1076.9182, 1086.2109, 1089.4147, 1109.0870, 1113.5620, 1118.3500, 1122.1727, 1130.1666, 1131.6382, 1134.7223, 1143.7377, 1146.0477, 1152.6567, 1160.4659, 1168.2946, 1177.8040, 1183.8141, 1187.5638, 1193.6805, 1209.4252, 1211.0827, 1211.2265, 1215.2820, 1219.5111, 1220.7467, 1223.2342, 1228.3641, 1231.1472, 1235.4698, 1237.2975, 1240.0049, 1241.8509, 1243.6621, 1248.9315, 1252.4287, 1261.4660, 1262.9126, 1265.4456, 1268.8143, 1278.2388, 1289.0971, 1298.4306, 1310.3132, 1311.4507, 1338.5300, 1344.2698, 1399.4558, 1466.1009, 1486.3257, 1509.3576, 2316.0298, 3105.2215, 3191.2465, 3207.7226, 3225.4089, 3366.9930	-428.6129
T3-O8-ZeO-propionyl (ads)	249	45.8245, 56.2187, 66.7133, 70.6733, 77.1746, 81.4253, 85.3314, 89.6337, 90.2166, 99.9575, 101.3777, 106.9125, 109.5518, 111.7690, 115.7274, 122.7091, 126.2731, 130.3017, 134.8961, 136.9174, 140.9380, 145.8313, 148.6006, 150.6037, 154.9073, 157.3420, 161.6395, 169.2002, 173.8125, 176.0589, 180.0333, 184.8694, 189.3051, 190.4052, 194.6073, 198.9126, 201.1857, 203.7954, 208.2033, 211.8146, 214.3975, 218.7289, 222.2532, 223.5927, 225.1124, 228.4435, 230.5541, 233.7535, 238.5530, 240.9282, 242.1861, 243.7068, 245.0784, 246.5887, 249.9918, 250.8210, 254.2273, 255.1959, 255.6725, 260.3711, 260.8384, 262.3220, 263.6128, 266.6872, 267.8648, 270.6785, 272.5891, 278.4939, 280.4990, 283.3625, 284.4435, 287.8470, 290.8241, 292.6166, 295.0585, 298.9305, 302.8353, 304.7805, 309.0894, 312.9117, 314.1619, 319.5391, 322.3743, 323.6176, 327.5080, 330.4097, 331.1951, 336.7113, 340.6061, 345.0036, 346.4810, 347.8413, 353.3315, 357.9682, 365.4155, 367.1950, 373.6511, 377.8745, 379.8914, 382.1385, 388.0205, 390.8628, 393.8891, 396.1918, 398.1817, 405.7750, 413.1262, 414.2783, 420.8928, 425.2842, 435.4423,	None

		441.1576, 447.8230, 453.5383, 458.7903, 461.7143, 466.4324, 478.9261, 481.8031, 490.2359, 495.8090, 504.3865, 521.2333, 526.5206, 533.3945, 538.8833, 540.5142, 548.9549, 558.3603, 576.9699, 585.5017, 587.5896, 590.1434, 606.4595, 610.4207, 639.0065, 645.2342, 659.3933, 666.4304, 670.7587, 673.6820, 685.4561, 685.9771, 693.5143, 709.6912, 713.1882, 720.5482, 725.5899, 732.8551, 736.2915, 741.8139, 744.6793, 747.5113, 751.9741, 752.6504, 754.9014, 764.4698, 767.8714, 769.9259, 772.2767, 774.3806, 777.4326, 779.0054, 782.3853, 785.5749, 786.9173, 790.0399, 795.3239, 798.0812, 799.8998, 802.1030, 806.0437, 808.8599, 811.8241, 813.9632, 814.6122, 817.2545, 819.0765, 821.9488, 823.4466, 824.2666, 827.6714, 830.1571, 833.8692, 837.0102, 840.3205, 842.8912, 847.8248, 852.2401, 854.7156, 863.4342, 980.9698, 1066.2236, 1089.3265, 1090.7714, 1116.8116, 1117.0043, 1126.4680, 1126.7231, 1128.4209, 1132.0349, 1137.9499, 1142.3045, 1143.6965, 1150.5310, 1158.2277, 1162.5120, 1169.5396, 1176.0652, 1180.6622, 1188.9398, 1198.9592, 1208.8568, 1210.4087, 1212.5649, 1215.2462, 1219.9790, 1228.9268, 1231.7436, 1232.1424, 1237.4103, 1240.8989, 1243.4652, 1247.1340, 1250.8118, 1259.4365, 1259.8113, 1263.6807, 1268.5529, 1276.2776, 1287.9055, 1294.0819, 1300.7684, 1303.2846, 1310.7105, 1326.9650, 1333.5254, 1335.6498, 1397.5538, 1438.1798, 1452.5550, 1515.0869, 1531.3900, 1973.0787, 3082.4163, 3086.2224, 3170.7634, 3175.9167, 3200.6879	
T4-O5-ZeOH-C ₂ H ₄ (ads)	225	26.1321, 42.0122, 44.4158, 61.2863, 71.8411, 76.2019, 81.4603, 86.2477, 94.9730, 97.9466, 102.2963, 108.3887, 114.4485, 122.1936, 124.1602, 129.0948, 133.2137, 141.4887, 142.1788, 144.8699, 149.3499, 154.5170, 155.9549, 158.8302, 165.8865, 167.3802, 171.8282, 173.9535, 179.1969, 183.8055, 188.7562, 193.1208, 197.9488, 199.1716, 203.0922, 205.2516, 210.4541, 215.8645, 220.9374, 223.0153, 224.4675, 226.1964, 230.5685, 231.1749, 234.5105, 238.8836, 239.8965, 240.5762, 244.9827, 246.9380, 248.6708, 250.7234, 253.9519, 256.3212, 259.9483, 262.3502, 263.6180, 267.7544, 270.8945, 272.8538, 276.0404, 278.9502, 281.1937, 283.8403, 288.7690, 290.0682, 291.3853, 297.2765, 299.6308, 302.7686, 305.6882, 309.5476, 313.7961, 316.4613, 318.6567, 321.5051, 322.7588, 326.5161, 329.4214, 330.3670, 334.2334, 339.1364, 339.5559, 345.2463, 352.5420, 355.4305, 361.6060, 364.7448, 370.8617, 372.3477, 378.0620, 382.3954, 389.8688, 396.1086, 397.3296, 402.6211, 402.8782, 411.2727, 413.3705, 425.8860, 429.6489, 430.4307, 441.2797, 446.3298, 449.8077, 466.3737, 469.6858, 480.0454, 489.9440, 503.8300, 507.0994, 514.3220, 524.4754, 540.4269, 544.1840, 547.3240, 561.4768, 573.0347, 583.4494, 585.8338, 594.7556, 605.1789, 620.2191, 645.3631, 659.7458, 669.4895, 673.6037, 675.6198, 677.7861, 684.6229, 687.6007, 697.7077, 714.8485, 717.3119, 720.7196, 727.1346, 735.9988, 737.0457, 742.0297, 748.5130, 750.2805, 752.5843, 756.2272, 762.5858, 764.6806, 768.7225, 775.5579, 780.9957, 785.0495, 789.1911, 790.6516, 792.5791, 799.3466, 801.8841, 803.4508, 806.7694, 810.4787, 811.7071, 813.5190, 818.4822, 818.9600, 819.8841, 825.6953, 826.5180, 828.5697, 833.1944, 835.2069, 837.9241, 840.9346, 842.4052, 849.5948, 851.1856, 861.7646, 864.5401, 1013.8752, 1019.7407, 1086.8786, 1090.9231, 1102.2660, 1108.4214, 1115.3961, 1125.0924, 1130.1385, 1135.7341, 1147.5419, 1151.0448, 1162.3326, 1166.2033, 1173.4447, 1176.7945, 1183.8197, 1184.3733, 1191.8657, 1197.5399, 1215.1619, 1220.9941, 1225.6688, 1228.0437, 1237.4589, 1239.9135, 1242.7577, 1244.2891, 1249.1483, 1254.0039, 1255.0608, 1257.5555, 1261.7697, 1267.2708, 1273.8201, 1275.9317, 1283.8736, 1290.4955, 1296.0085, 1302.6499, 1308.3682, 1336.5553, 1363.8537, 1398.7857, 1487.6134, 1725.0418, 3161.1701, 3181.7154, 3248.1544, 3272.7678, 3721.2604	None

T4-O5-Protonation-TS	225	-213.3197, 59.9446, 67.4347, 71.2279, 74.6525, 79.3820, 88.9643, 96.5251, 98.9293, 104.0722, 109.2333, 117.5409, 120.6620, 128.6851, 132.5153, 133.7414, 138.1453, 140.9115, 148.2809, 153.5249, 156.2300, 158.6056, 161.8367, 163.8452, 167.6405, 174.6225, 175.8725, 180.1003, 183.8663, 188.4318, 191.0705, 191.8958, 198.7939, 201.9910, 205.3331, 211.9202, 213.1565, 215.2702, 218.1305, 221.6745, 225.4216, 229.8570, 233.0525, 236.0438, 238.5353, 240.2673, 243.2061, 243.6944, 246.8963, 247.8583, 249.3311, 251.9734, 253.4595, 257.6573, 261.0294, 261.2924, 265.0040, 267.9732, 269.0540, 273.9839, 275.4980, 279.2431, 282.1333, 287.0164, 287.6031, 290.2755, 294.9546, 296.1777, 302.9541, 305.8894, 308.1168, 312.6959, 318.4594, 318.7839, 322.1762, 324.8828, 325.0105, 330.5620, 332.9071, 335.4012, 338.9844, 340.9942, 341.3626, 348.7783, 351.6213, 360.5475, 364.5737, 368.7214, 372.0603, 374.6676, 379.7839, 381.4940, 384.2478, 388.8736, 394.5909, 400.7347, 403.0899, 406.4500, 413.5746, 417.2174, 431.3707, 439.5796, 442.0371, 448.2154, 452.2788, 457.6237, 466.8158, 480.0791, 490.0461, 499.9228, 508.3950, 513.5808, 526.2386, 539.9817, 549.4861, 555.1341, 572.7246, 579.6256, 587.6085, 594.2691, 599.3765, 606.9225, 624.6512, 647.5037, 666.1661, 667.3065, 674.2127, 676.4534, 681.3063, 692.1172, 695.1313, 708.9568, 709.7980, 714.5254, 722.6017, 723.0753, 734.4125, 742.0477, 747.5981, 750.0376, 751.7083, 754.4928, 756.2357, 764.5119, 765.9150, 769.4551, 775.6592, 779.0796, 784.4840, 784.7176, 788.4571, 789.5725, 794.0164, 798.7406, 801.0844, 801.4306, 803.9279, 804.9887, 808.0881, 812.7617, 815.8326, 817.8101, 820.5511, 822.2658, 824.8411, 826.8941, 831.6902, 833.8224, 838.8951, 843.1704, 844.5175, 845.8897, 860.6620, 868.2187, 1053.8454, 1065.7097, 1082.9996, 1100.4519, 1118.3733, 1121.2154, 1124.7221, 1137.5403, 1141.6666, 1142.2723, 1147.2377, 1150.4539, 1160.0384, 1164.4886, 1175.9568, 1180.9807, 1191.5443, 1203.2536, 1204.9119, 1209.0305, 1211.3685, 1212.2287, 1222.9596, 1225.2549, 1230.6997, 1233.2241, 1234.0320, 1235.3013, 1238.1199, 1242.4046, 1243.8995, 1247.1134, 1254.2000, 1264.2715, 1265.3855, 1272.7138, 1280.2694, 1290.4401, 1298.5954, 1302.4888, 1330.0213, 1333.9300, 1351.2831, 1363.4936, 1453.3761, 1582.9931, 2637.3903, 2925.5475, 3168.1429, 3245.0315, 3293.0165	-213.3197
T4-O5-ZeO-C ₂ H ₅ (ads)	225	41.8586, 63.6295, 70.2281, 76.9486, 88.4114, 90.3383, 92.2261, 102.2488, 108.7262, 112.3837, 117.1747, 125.8493, 125.9830, 129.0750, 138.3805, 141.1969, 146.2299, 151.2666, 154.8659, 156.9171, 161.5373, 168.8232, 171.8688, 173.8747, 180.7462, 184.6679, 186.2180, 192.0826, 195.5113, 198.4761, 198.8509, 205.4691, 208.2303, 214.1454, 219.2671, 220.9142, 222.5631, 230.7561, 231.5387, 234.1751, 235.2125, 239.7665, 241.3857, 242.4108, 244.4139, 247.6056, 247.8040, 250.2769, 251.6527, 256.9657, 259.8171, 260.7151, 263.3906, 265.2127, 269.0531, 270.5983, 273.1107, 276.3452, 279.8654, 283.1498, 285.8251, 288.0021, 290.8441, 294.1910, 296.8506, 300.8741, 304.3691, 306.3935, 311.3538, 313.1544, 315.2318, 318.1771, 322.1605, 324.3169, 324.8606, 328.4798, 332.4894, 334.6296, 336.7413, 339.2038, 342.5728, 348.6910, 351.3201, 357.8270, 359.1492, 366.7109, 369.6324, 372.5961, 373.2439, 379.8008, 388.0930, 391.5229, 398.5007, 399.5025, 405.0692, 408.2337, 413.5729, 420.4570, 427.4627, 431.0674, 443.8359, 446.6245, 455.5553, 458.1385, 465.5335, 477.3773, 488.5544, 499.9922, 507.8680, 513.4171, 516.4297, 536.1646, 544.9558, 551.9700, 565.4507, 576.1419, 587.7974, 593.9208, 599.4847, 606.1667, 618.3115, 646.1024, 657.6852, 666.6763, 671.4839, 674.5251, 678.0578, 681.7528, 691.0007, 695.0947, 709.5972, 713.7330, 723.4070, 727.4807, 736.9031, 737.6065, 746.7651, 748.0700, 750.8991, 754.1486, 756.4631, 764.2912, 768.8891, 771.2502, 775.6800, 776.7480, 784.3491, 787.6664, 789.0813, 792.0705, 797.5081,	None

		800.5979, 803.4077, 804.1422, 806.4681, 809.7850, 813.2401, 815.1734, 815.9407, 817.1703, 819.5929, 821.4228, 824.0034, 826.8051, 832.1728, 834.3951, 835.3760, 836.8568, 840.3585, 850.4114, 853.3236, 863.4388, 894.1348, 1029.7590, 1096.5446, 1110.1038, 1120.4372, 1129.1945, 1132.4919, 1137.2311, 1140.8815, 1142.2886, 1147.5827, 1155.7310, 1163.4122, 1171.7175, 1172.5103, 1178.3174, 1182.7218, 1192.5321, 1200.5557, 1205.4757, 1213.4002, 1216.1791, 1220.3183, 1224.3774, 1230.9818, 1235.1157, 1240.4093, 1241.8738, 1247.3936, 1249.1393, 1250.7223, 1254.3172, 1259.8958, 1262.6465, 1271.0362, 1282.5938, 1283.9205, 1299.0044, 1303.2716, 1329.8282, 1339.8382, 1356.3991, 1365.4826, 1437.3306, 1467.3839, 1510.2740, 1518.7641, 1526.8521, 3090.5890, 3171.2672, 3193.7168, 3209.2080, 3266.4175	
T4-O5-ZeO-C ₂ H ₅ CO(ads)	231	51.5699, 55.0477, 58.7448, 63.8601, 71.4711, 79.1856, 86.1114, 92.6392, 98.2606, 99.4380, 104.3277, 107.7368, 109.1635, 114.1376, 118.0207, 124.8039, 130.2790, 136.6300, 138.4662, 141.2899, 145.7271, 146.9172, 151.3914, 153.9276, 158.9471, 166.5199, 168.6876, 172.5872, 175.5661, 182.0279, 188.8813, 189.3842, 191.8871, 195.8166, 197.3392, 204.2411, 206.0321, 206.9540, 213.6277, 217.0951, 223.7908, 227.2363, 229.9578, 233.8242, 235.4419, 236.0558, 238.9018, 241.0446, 242.6674, 245.1899, 249.1016, 251.0304, 253.0170, 256.0582, 256.5817, 258.5881, 261.3403, 263.5090, 265.9188, 267.0155, 272.0917, 273.1574, 275.7141, 281.0446, 283.6765, 287.3517, 288.8957, 290.6942, 294.5756, 298.7007, 304.3569, 305.5588, 306.9937, 310.4278, 312.8494, 314.9884, 318.1523, 321.6570, 325.0161, 325.8101, 331.0960, 331.3152, 334.2336, 338.0512, 341.0965, 347.8066, 351.0913, 353.5250, 357.3314, 364.1690, 366.8700, 371.6899, 372.1571, 377.9451, 381.8590, 388.1385, 393.9585, 398.0798, 399.6326, 404.8698, 409.8955, 414.4960, 427.5114, 431.7076, 438.9277, 440.8497, 445.6572, 454.6188, 465.3520, 470.2630, 481.2114, 494.9769, 502.3399, 504.7181, 510.2334, 514.7826, 534.0148, 542.2309, 543.9141, 562.2606, 575.0726, 587.9130, 590.9066, 599.2957, 606.8088, 618.1895, 642.9198, 657.4227, 666.8130, 672.4696, 674.7439, 677.0514, 684.8814, 688.0444, 697.0790, 713.7120, 721.7066, 722.3810, 734.7885, 740.5451, 747.1756, 749.6688, 752.6670, 753.5763, 755.6785, 759.3095, 762.0070, 767.4555, 771.4570, 778.8558, 780.1427, 784.0288, 786.9604, 789.0431, 791.1441, 796.5292, 801.1774, 804.5526, 807.1210, 809.5869, 811.3729, 813.3269, 814.7276, 815.8162, 817.3610, 820.0362, 824.4500, 825.0546, 825.4843, 830.4198, 833.8384, 836.8188, 839.7349, 842.6145, 848.4510, 851.4605, 866.6534, 896.1831, 1047.2622, 1091.8624, 1102.9972, 1121.0471, 1122.3863, 1125.3312, 1128.6717, 1135.6738, 1144.1728, 1151.1059, 1159.4971, 1163.0549, 1166.4464, 1170.3947, 1172.9190, 1179.9064, 1194.0327, 1196.9425, 1205.7189, 1209.5607, 1211.4010, 1223.7599, 1228.8986, 1235.2979, 1237.5222, 1238.9333, 1246.6022, 1249.9253, 1252.6617, 1255.5556, 1256.1736, 1258.8423, 1259.6658, 1274.5179, 1283.0056, 1288.3757, 1296.7545, 1304.0217, 1314.7531, 1335.0250, 1347.8456, 1361.3543, 1422.7711, 1469.6291, 1509.6563, 1529.6217, 1556.1858, 2240.1623, 3109.2496, 3135.5193, 3188.0091, 3207.0728, 3254.4686	None
T4-O5-Carbonylation-TS	231	-418.9532, 30.7127, 57.9834, 64.0223, 70.7348, 76.1294, 83.9697, 85.0950, 90.9774, 101.6320, 104.7424, 109.9569, 115.6196, 121.0702, 123.6749, 124.4503, 125.8228, 130.0253, 138.1526, 142.1981, 148.7903, 151.8443, 154.4945, 158.0923, 159.9461, 163.1592, 167.9083, 172.6888, 176.3361, 178.4103, 185.6966, 187.9072, 191.9850, 194.1898, 200.4267, 202.8924, 207.0106, 209.1380, 211.6792, 214.5181, 221.9821, 225.6991, 231.8332, 234.1871, 234.6841, 236.8761, 239.1750, 241.4468, 242.8676, 245.3840, 248.1146, 250.1981, 252.5058, 253.4499, 255.6232, 259.1919, 261.8677, 264.1608, 266.1986, 269.8460, 270.3343,	-418.9532

		272.3066, 277.0600, 279.3700, 280.3258, 286.3281, 287.8140, 290.3924, 292.9400, 295.1581, 300.2265, 304.5102, 305.8813, 308.4011, 312.0288, 318.2026, 319.3659, 322.4410, 324.0513, 325.6700, 329.1990, 333.0388, 335.4836, 337.1808, 340.2340, 343.9029, 348.1298, 351.4735, 354.2734, 363.3753, 364.4473, 368.4534, 373.3796, 376.7008, 377.5959, 383.4402, 387.0827, 392.7117, 396.0297, 399.7802, 403.8689, 406.2703, 412.7724, 417.2881, 430.1957, 440.1823, 442.0693, 449.0466, 450.7714, 458.6891, 466.1121, 479.7883, 490.2661, 499.9453, 508.9426, 514.0264, 528.8925, 540.2416, 549.3189, 554.5078, 574.0700, 579.5607, 588.5834, 597.2139, 600.4063, 608.6449, 622.6702, 647.3953, 665.9466, 667.9234, 673.9896, 675.6922, 679.5055, 690.7494, 695.6576, 708.2947, 710.6094, 718.4315, 723.2337, 723.5107, 727.1177, 738.4733, 747.4619, 750.4586, 753.6044, 756.3257, 757.9752, 766.4134, 766.9516, 775.2928, 776.9798, 781.2110, 786.0536, 788.7333, 789.8875, 795.8454, 800.2684, 801.4231, 804.2063, 806.7117, 808.4615, 811.8293, 812.5051, 814.7502, 818.2710, 819.1313, 822.4468, 825.0206, 829.0046, 831.0647, 831.6456, 833.0593, 836.5423, 840.4145, 845.3909, 847.7923, 865.5130, 941.9547, 1023.5812, 1048.3927, 1096.4256, 1100.9729, 1102.5745, 1118.7232, 1122.8752, 1134.0729, 1139.0485, 1140.6450, 1147.3224, 1150.4984, 1155.6415, 1160.1978, 1167.0219, 1174.3752, 1188.0510, 1195.7565, 1204.7101, 1205.8524, 1209.4429, 1214.9907, 1215.9353, 1220.6318, 1226.7338, 1233.2393, 1235.8762, 1237.5495, 1239.2066, 1244.6728, 1247.5304, 1250.6474, 1254.0578, 1256.8453, 1258.1730, 1268.2859, 1274.9176, 1280.6004, 1295.6405, 1297.6429, 1329.1582, 1334.9432, 1355.8984, 1407.6297, 1476.7012, 1484.1761, 1518.0882, 2300.1918, 3089.4795, 3163.5766, 3176.0582, 3198.6080, 3313.0285	
T4-O5-ZeO-propionyl (ads)	231	37.2227, 56.4127, 60.7250, 74.6212, 77.7065, 89.8044, 92.0083, 98.8393, 102.7769, 105.7711, 109.3443, 112.6761, 117.7213, 125.7102, 128.9158, 136.0683, 140.3979, 143.9494, 147.7475, 148.5171, 152.8552, 160.3752, 166.1449, 170.0480, 171.0271, 173.4092, 179.4065, 185.5136, 188.3998, 190.9309, 193.7185, 196.7445, 204.6824, 205.4603, 207.0611, 212.6774, 218.2650, 220.3121, 226.2518, 227.1993, 230.6282, 232.5658, 235.5526, 236.7391, 239.5230, 240.9714, 243.9640, 247.5565, 249.6770, 250.2135, 253.8479, 256.6204, 258.7228, 260.8987, 263.5391, 265.0274, 267.7875, 269.5638, 272.3417, 273.1242, 278.3366, 281.0943, 283.5342, 286.2523, 290.7423, 291.8255, 294.2487, 298.0657, 303.0724, 303.8901, 307.6058, 308.7249, 310.2626, 314.0014, 317.9281, 322.4069, 325.4706, 326.6440, 327.6183, 332.6847, 334.4417, 338.2328, 340.3253, 345.8241, 351.6484, 355.9422, 359.8422, 363.7993, 368.5444, 370.2779, 371.4795, 374.4094, 378.7708, 382.6314, 393.2453, 396.8921, 399.3190, 403.8659, 408.6172, 413.8858, 421.1379, 431.1277, 435.6644, 442.1014, 444.4591, 451.8754, 463.9764, 467.1084, 475.4392, 494.3833, 499.7024, 507.9778, 515.0543, 529.2632, 538.8631, 541.8865, 557.3505, 569.7932, 575.3910, 585.2668, 590.7034, 600.4388, 605.6218, 614.4091, 639.1008, 641.6025, 659.4104, 666.0545, 675.4211, 676.8954, 679.4887, 687.3947, 696.2731, 697.9352, 714.1689, 720.4848, 722.7869, 734.8711, 737.1832, 742.6113, 747.6846, 751.8959, 752.1530, 754.0341, 758.1447, 760.2771, 761.9448, 769.3377, 774.7849, 778.7556, 782.3850, 784.4264, 787.8858, 789.9207, 794.8174, 799.7650, 801.1628, 804.7090, 807.9843, 809.0141, 811.0406, 813.4509, 816.9489, 818.7293, 822.5517, 824.6449, 825.5292, 826.7952, 832.9752, 835.3322, 837.3820, 838.3844, 847.4590, 849.0973, 850.0663, 859.4875, 870.0749, 1019.2248, 1084.3870, 1088.8345, 1098.6791, 1118.8801, 1120.1136, 1122.9377, 1125.1902, 1133.3990, 1139.0048, 1143.1193, 1149.5799, 1156.3966, 1162.9329, 1167.5438, 1172.4419, 1175.2715, 1182.1725, 1194.9337, 1203.5247, 1208.6448,	None

		1210.5031, 1220.8109, 1232.3229, 1234.5434, 1239.0121, 1243.3369, 1247.2458, 1250.1546, 1251.7476, 1255.1974, 1257.5544, 1259.8765, 1269.1029, 1273.5633, 1274.1684, 1283.0333, 1289.0055, 1295.6898, 1301.3066, 1308.6357, 1336.9191, 1359.1176, 1416.6773, 1455.9822, 1488.7168, 1518.0891, 1526.1675, 1913.8888, 3085.3596, 3109.5261, 3170.3273, 3181.8409, 3215.8933	
T4-O7-ZeOH-C ₂ H ₄ (ads)	225	60.9888, 63.8090, 66.2134, 68.7167, 75.7010, 85.0788, 90.8943, 95.0881, 99.5262, 104.6133, 108.7632, 117.8955, 122.9825, 127.4608, 129.9427, 132.2979, 136.2497, 143.4175, 148.0794, 149.8041, 154.1681, 157.8196, 159.6712, 162.2474, 166.3414, 174.0325, 175.7905, 180.2997, 183.9353, 187.8162, 190.1787, 192.6542, 198.2696, 201.5046, 204.8250, 205.0108, 212.2047, 212.8412, 219.9512, 225.6615, 230.5478, 232.8640, 234.9589, 236.5960, 237.9752, 239.8559, 242.4036, 244.9568, 247.0565, 250.6014, 251.4668, 253.3368, 257.2255, 259.8662, 261.1316, 263.9400, 264.7817, 266.6304, 270.4056, 272.0821, 276.4957, 278.3626, 280.0027, 285.1462, 286.5983, 289.8404, 291.2578, 297.1417, 301.5774, 303.8080, 306.2900, 310.3150, 316.9382, 318.2228, 319.8758, 321.3682, 323.7190, 325.0231, 330.0910, 334.1704, 336.7610, 337.9809, 340.5479, 347.3359, 350.0904, 353.8168, 357.5065, 366.2382, 372.3092, 373.3019, 378.4359, 382.5624, 386.7632, 392.1115, 397.5189, 401.6891, 401.9342, 409.0143, 415.7921, 425.7053, 429.5584, 431.5745, 440.2965, 443.1798, 454.5613, 466.3009, 475.8619, 487.4836, 501.2069, 504.2115, 514.2129, 525.2798, 539.4185, 541.5068, 549.1090, 566.2740, 578.0867, 582.5270, 590.3127, 594.3937, 605.9343, 612.4089, 649.2569, 658.4527, 665.8519, 671.2369, 672.8850, 675.4767, 678.5589, 684.2130, 686.4108, 693.2877, 707.7974, 721.2843, 721.5153, 726.9831, 738.6576, 741.6459, 748.4265, 749.3858, 754.4553, 758.1009, 765.0567, 765.7645, 770.7652, 773.5302, 777.6839, 779.7234, 784.4594, 785.9408, 788.9043, 795.2117, 798.1871, 800.3834, 805.1048, 805.8406, 807.8481, 807.9934, 813.5730, 816.0747, 819.5125, 819.9212, 824.2447, 826.7182, 830.0362, 834.1041, 836.0595, 837.2824, 840.7718, 847.1740, 848.3623, 850.9723, 858.4629, 867.8348, 1027.0531, 1052.2332, 1096.7710, 1100.0989, 1108.7892, 1113.4697, 1125.3354, 1134.0656, 1140.2807, 1144.2684, 1148.7088, 1157.4475, 1160.7766, 1167.9396, 1171.6756, 1177.4132, 1184.0011, 1195.9124, 1212.1309, 1213.3589, 1215.8608, 1218.5566, 1226.0391, 1229.5150, 1231.5868, 1234.8782, 1241.1529, 1244.8729, 1246.4686, 1249.0617, 1250.7163, 1254.3377, 1257.8924, 1269.7356, 1270.2818, 1271.4819, 1283.9274, 1291.6364, 1297.8930, 1300.6271, 1327.4242, 1330.9279, 1356.4725, 1394.7865, 1483.1308, 1711.2000, 3169.9556, 3187.3789, 3261.3272, 3284.6812, 3445.8769	None
T4-O7-Protonation-TS	225	-167.2934, 51.4398, 63.9963, 66.4378, 70.3358, 81.0329, 90.5342, 95.1204, 98.0350, 107.2812, 111.3866, 115.2979, 121.0308, 126.3891, 127.7947, 130.4489, 139.8416, 142.1608, 149.8525, 155.4740, 156.2241, 157.3425, 159.6974, 164.5004, 171.0029, 172.0656, 175.9246, 178.4546, 183.6772, 187.9957, 190.9292, 191.8137, 200.0558, 204.3032, 205.1019, 212.0591, 212.9972, 214.8299, 220.9840, 227.0878, 230.8464, 233.8466, 237.5480, 238.2498, 238.5919, 240.9554, 241.9848, 245.5121, 246.4056, 249.5734, 249.8699, 252.1759, 253.8269, 258.3384, 261.0680, 262.9349, 266.7064, 269.2625, 270.3639, 273.8538, 276.6437, 279.1635, 281.8378, 286.2635, 288.1762, 291.8424, 293.5329, 297.2849, 302.9743, 305.4213, 305.9331, 311.9077, 318.9107, 319.8997, 322.2280, 324.3766, 324.8217, 328.7042, 332.4542, 334.9917, 338.0141, 339.6968, 341.7687, 347.3118, 352.9474, 359.9674, 366.0972, 368.3887, 373.1191, 374.6661, 379.4504, 383.8061, 386.1258, 389.9964, 394.6462, 402.7148, 405.0318, 405.2788, 415.0252, 419.4048, 432.1932, 438.1429, 440.5608, 444.5360, 450.5107, 458.0736, 466.9371, 479.7173, 490.6725, 500.0460, 508.3718,	-167.2934

		513.1973, 527.3367, 540.3516, 549.9416, 553.6174, 570.9256, 578.6498, 588.5783, 593.3560, 601.3279, 607.6074, 624.3436, 648.3069, 667.2319, 667.8177, 674.1094, 675.1145, 680.8132, 691.2146, 695.2476, 701.9802, 709.6286, 711.7389, 722.6420, 722.8377, 734.2908, 742.1676, 749.3449, 750.1369, 754.5514, 754.9429, 755.9707, 765.1885, 765.8660, 772.7908, 777.8307, 779.8987, 786.3862, 788.2184, 789.8634, 795.9633, 796.8620, 799.8316, 801.4988, 803.0301, 804.2505, 808.2081, 812.6542, 815.8237, 817.7834, 819.8306, 821.2539, 824.5506, 827.5864, 832.5675, 833.6874, 837.2809, 840.5856, 844.1237, 845.4826, 864.5502, 877.6320, 982.5025, 1054.2229, 1092.8521, 1096.8161, 1113.5148, 1121.2054, 1125.1048, 1135.3298, 1137.3444, 1141.9258, 1147.0290, 1150.2316, 1154.5917, 1159.9500, 1164.9283, 1176.3116, 1179.4344, 1191.5210, 1197.1051, 1206.8086, 1211.2229, 1211.6887, 1214.1019, 1219.4434, 1227.1964, 1230.6089, 1232.6426, 1235.0219, 1238.4566, 1240.7294, 1242.6283, 1246.4752, 1248.7485, 1252.3742, 1261.0344, 1266.4924, 1266.6188, 1279.2478, 1289.9634, 1292.0759, 1305.0730, 1327.3968, 1337.0751, 1353.7429, 1392.3392, 1499.4382, 1612.1732, 2083.0732, 3138.3238, 3169.1897, 3259.5462, 3287.2051	
T4-O7-ZeO-C ₂ H ₅ (ads)	225	56.1325, 68.7269, 71.1046, 79.2817, 88.8946, 93.1659, 102.8830, 106.8479, 112.0076, 113.3836, 123.0005, 125.1269, 128.0287, 137.8071, 139.0669, 142.9137, 150.0200, 153.6905, 155.7590, 159.4968, 161.8997, 169.2062, 171.3232, 175.5787, 177.8572, 186.1839, 186.6526, 189.9198, 193.3724, 194.6285, 197.1422, 199.8612, 204.1082, 209.0121, 212.5983, 214.3585, 219.9385, 226.1182, 228.9814, 230.7658, 233.9572, 236.7495, 238.1716, 241.3487, 243.3588, 244.1616, 246.7164, 250.4990, 250.9362, 253.1690, 256.8888, 260.1872, 261.4668, 263.3128, 267.8629, 269.9609, 271.9396, 273.8112, 276.9762, 281.7292, 282.6288, 285.2342, 288.2464, 292.1655, 293.0340, 298.4152, 303.2362, 305.6819, 310.4195, 313.4894, 318.3804, 319.3829, 320.9956, 323.3662, 324.1046, 325.2155, 329.8701, 333.5485, 335.2128, 337.6367, 340.8402, 346.5817, 348.1667, 352.8086, 357.2313, 360.8387, 367.5062, 372.3182, 374.0789, 378.6776, 383.2848, 387.4267, 392.2400, 399.7318, 400.9417, 406.3914, 415.6061, 417.2739, 425.0546, 430.6154, 438.6789, 439.6397, 445.0350, 456.7976, 466.1791, 476.6043, 488.2972, 502.1325, 505.9374, 514.1349, 524.3505, 539.0295, 543.4953, 549.2684, 561.6144, 578.0185, 583.5935, 590.7218, 596.7336, 606.7204, 616.9428, 647.8995, 654.8021, 666.6237, 670.7193, 673.9519, 676.4123, 678.9212, 686.5800, 693.8602, 708.6838, 717.5426, 721.3057, 725.2923, 737.6455, 742.7102, 748.3317, 751.7223, 754.5023, 755.8916, 762.2641, 765.4352, 766.3318, 773.4880, 774.9205, 778.3153, 779.2723, 785.7602, 787.4509, 789.4831, 797.8376, 800.1911, 801.9612, 805.5327, 806.7135, 808.4956, 809.0363, 812.2417, 813.8174, 816.5924, 818.7947, 824.1074, 825.2909, 828.3946, 831.7722, 835.1892, 837.4618, 839.4097, 840.4511, 849.8130, 851.0585, 860.1195, 891.2976, 1024.0473, 1091.5411, 1115.8674, 1117.0334, 1124.6801, 1129.8403, 1135.6612, 1142.6833, 1143.2958, 1147.5037, 1152.7108, 1163.0688, 1172.2540, 1179.2626, 1183.9581, 1192.9098, 1195.9943, 1210.0567, 1213.1916, 1218.7183, 1220.8929, 1223.2005, 1229.2690, 1232.8233, 1235.9862, 1240.3873, 1244.1821, 1246.5935, 1250.9549, 1254.1963, 1255.8506, 1261.5531, 1270.2810, 1272.5594, 1285.8030, 1292.3757, 1297.2534, 1305.2736, 1329.4866, 1334.3351, 1355.3188, 1362.9064, 1417.2459, 1456.3108, 1491.6030, 1513.4492, 1531.2584, 3094.1019, 3149.6641, 3185.2627, 3220.7670, 3240.1182	None
T4-O7-ZeO-C ₂ H ₅	231	23.6602, 44.2768, 58.1180, 62.1087, 67.9513, 78.7775, 79.1405, 88.9272, 90.8398, 94.0748, 98.7399, 106.7704, 112.0360, 116.8131, 125.5705, 128.2722, 130.9523, 139.7237, 140.5555, 144.8034, 146.4602,	None

CO(ads)		153.7448, 156.1040, 157.4840, 159.8129, 163.0554, 170.8406, 175.2754, 175.4807, 182.9805, 183.9486, 186.4004, 190.7067, 192.5004, 198.3530, 200.2691, 203.1194, 209.0604, 212.3248, 213.7585, 220.0849, 225.9019, 229.5900, 230.4747, 233.7381, 236.4386, 237.0290, 240.3202, 243.4772, 245.9987, 247.8654, 249.7913, 250.7764, 253.4980, 256.6438, 258.0314, 260.6156, 261.4548, 265.2553, 268.1208, 271.1791, 272.8061, 274.2843, 277.7277, 281.2487, 284.0660, 287.9840, 289.4097, 292.3254, 296.6767, 298.6349, 302.3245, 306.5656, 308.4479, 312.8733, 317.8630, 319.2686, 319.7065, 322.2815, 325.1024, 330.0174, 333.0689, 333.5998, 336.3981, 338.2729, 342.1099, 347.6467, 350.7326, 358.9837, 361.2759, 367.8394, 371.5344, 375.4689, 377.6903, 381.3102, 385.1461, 390.4982, 393.3093, 399.5241, 402.5740, 407.2432, 408.9065, 418.6864, 424.8465, 431.6189, 437.2338, 440.0964, 452.4277, 466.0017, 470.9672, 478.3938, 485.1287, 500.3899, 505.4133, 513.7753, 522.4047, 538.5162, 540.9064, 548.7264, 564.4844, 578.3120, 581.4733, 589.7730, 594.1338, 606.0630, 615.0463, 649.4381, 653.8382, 667.3135, 671.1945, 674.3298, 675.9243, 681.9395, 685.2529, 694.3108, 709.1782, 716.5485, 721.2094, 723.2021, 737.6470, 743.1122, 747.5325, 752.4134, 753.3175, 759.2351, 763.9236, 765.4440, 772.4651, 773.6969, 775.1093, 778.4630, 779.1530, 783.0928, 784.5918, 788.6033, 795.5665, 797.7700, 801.1842, 803.7840, 806.5863, 807.5631, 808.9319, 813.3189, 815.4110, 818.6884, 819.8448, 824.1987, 824.6907, 828.8850, 834.1577, 835.2608, 836.9498, 838.5505, 840.6002, 849.9936, 851.8230, 858.7026, 886.3742, 1026.1764, 1095.9850, 1109.6931, 1114.3361, 1121.6163, 1123.8564, 1132.0833, 1141.2618, 1143.2457, 1149.5616, 1153.8759, 1159.4105, 1170.5665, 1175.3083, 1180.9721, 1193.3592, 1194.7465, 1204.1687, 1210.8571, 1216.6430, 1219.9185, 1220.9136, 1225.2521, 1228.8666, 1231.0153, 1238.1851, 1241.4628, 1246.4718, 1248.4048, 1252.7298, 1254.9390, 1258.2256, 1271.5295, 1273.7707, 1284.1013, 1290.1651, 1298.4776, 1303.9738, 1329.4432, 1331.0297, 1333.0966, 1356.1592, 1410.9219, 1444.1173, 1505.2373, 1517.3017, 1542.7154, 2243.9090, 3111.6724, 3170.6625, 3198.7852, 3225.7748, 3246.2088	
T4-O7-Carbonylation-TS	231	-439.0620, 33.1666, 48.4800, 62.0218, 69.0613, 72.8836, 88.4308, 90.8592, 93.8111, 100.2409, 105.2632, 107.9629, 113.9165, 119.8301, 121.9268, 127.8522, 130.8334, 132.7913, 138.7598, 141.0314, 143.6623, 150.2661, 153.2351, 156.5872, 160.6655, 161.2905, 164.4298, 174.0185, 175.3007, 182.7876, 183.4324, 187.1714, 191.0466, 191.8492, 198.3537, 203.7665, 205.4387, 210.9378, 211.5834, 214.1387, 221.2170, 227.1776, 230.0048, 232.7819, 233.5549, 237.6619, 238.9568, 240.5182, 244.0467, 245.4598, 247.5797, 250.3626, 251.9367, 253.2031, 254.6323, 258.7286, 260.9708, 262.1074, 266.4670, 268.6638, 271.1836, 272.6208, 276.1507, 279.5446, 280.5972, 283.9087, 286.5517, 290.6803, 291.4328, 293.3796, 297.9423, 304.2355, 306.3622, 307.7809, 312.7408, 318.7597, 319.4183, 322.5672, 324.0227, 326.4853, 329.3432, 332.5000, 334.8248, 335.9590, 338.3057, 340.3834, 344.4055, 347.7966, 352.2040, 359.9073, 367.6444, 368.7427, 373.6065, 374.0808, 376.9415, 379.5330, 384.7418, 388.7086, 393.5340, 401.2776, 404.4458, 405.6344, 414.4760, 417.1972, 431.4839, 437.3225, 441.5269, 442.5020, 451.2368, 458.2532, 467.6481, 480.3097, 490.7235, 500.3313, 508.8994, 513.8237, 529.0751, 540.3763, 551.5142, 552.7628, 569.2729, 578.7172, 587.2583, 592.6350, 601.0752, 607.4366, 622.3614, 648.4766, 668.5455, 669.3434, 675.2448, 676.2645, 680.3658, 690.6952, 695.6569, 700.5264, 710.4028, 711.2475, 718.9438, 722.8821, 738.5246, 740.2858, 749.3749, 750.4168, 755.2510, 756.0301, 757.5322, 765.7306, 766.5210, 774.0863, 777.6698, 778.8900, 785.1314, 787.5331, 789.6717, 795.3340, 797.1462, 799.3850, 802.5766, 803.1359, 805.6203,	-439.062

		808.1609, 812.7206, 815.7497, 817.7884, 820.5461, 821.9264, 825.5712, 829.6211, 832.3845, 833.7297, 837.6916, 839.5890, 842.6837, 844.9363, 845.5430, 864.0086, 941.5455, 1018.3496, 1054.2511, 1088.9755, 1096.2616, 1103.6906, 1112.1025, 1120.3672, 1124.3469, 1137.7679, 1141.6139, 1146.0019, 1149.3006, 1152.8235, 1162.5182, 1164.3519, 1176.9114, 1190.4246, 1192.7863, 1206.1630, 1206.7196, 1210.3754, 1212.6203, 1215.5867, 1221.0489, 1224.4964, 1229.6709, 1235.5169, 1237.0300, 1238.5762, 1242.5090, 1245.5290, 1248.6958, 1250.0803, 1258.8830, 1265.3303, 1266.8758, 1280.4673, 1284.3424, 1293.1283, 1303.4968, 1328.5854, 1334.5661, 1353.7304, 1405.8747, 1467.2069, 1497.6037, 1510.7598, 2311.2320, 3112.7573, 3198.4119, 3203.9811, 3219.5928, 3351.3690	
T4-O7-ZeO-propionyl (ads)	231	54.1484, 55.5134, 64.3496, 70.1192, 72.3118, 85.3182, 88.0325, 92.8209, 94.5637, 105.7159, 108.5074, 119.8749, 123.3943, 125.3946, 130.5412, 136.2402, 140.3512, 143.0200, 146.1144, 151.6317, 153.5416, 157.4838, 160.6206, 164.4716, 172.1741, 175.8503, 178.6237, 182.5703, 186.2823, 190.8130, 195.7851, 197.0426, 200.5858, 204.4118, 209.0924, 211.7129, 217.2393, 220.1534, 225.7375, 226.6807, 231.7395, 234.4442, 235.7281, 237.2517, 239.2761, 241.7000, 244.1810, 246.1216, 249.1160, 250.1545, 252.7399, 253.2374, 257.3258, 258.3366, 260.8189, 262.7045, 264.3359, 267.8283, 269.5429, 270.1289, 273.0449, 277.0575, 283.3515, 283.7245, 286.6104, 288.6214, 296.1898, 297.1906, 300.1484, 302.4027, 307.6963, 309.8557, 314.8821, 315.4844, 319.0059, 319.3935, 321.1177, 323.3837, 327.2367, 330.0963, 334.7577, 335.6665, 338.0104, 342.2332, 348.1155, 349.9329, 354.3277, 358.3214, 367.3069, 370.9852, 374.2400, 378.3393, 382.3033, 387.0887, 391.2194, 395.6402, 399.3632, 406.1754, 406.8280, 417.3028, 420.9734, 430.7644, 434.1527, 438.3724, 451.5273, 459.6060, 464.2003, 469.6575, 481.5637, 489.5894, 501.9811, 508.2119, 515.4933, 528.6473, 536.6094, 541.9351, 549.3150, 562.5369, 578.0165, 581.0427, 590.9085, 594.3263, 606.8231, 614.8157, 648.1171, 653.6521, 666.0989, 670.2469, 673.6067, 674.1765, 676.5753, 678.9559, 685.8007, 693.5655, 708.4854, 720.3268, 721.7137, 725.4024, 739.9609, 744.2266, 748.5371, 752.6671, 754.4229, 758.6960, 760.6346, 765.0517, 768.9010, 773.2054, 775.3999, 776.6502, 779.2799, 786.4415, 787.6847, 790.2053, 790.5568, 798.2299, 801.3322, 803.7540, 806.8350, 808.3906, 810.9682, 813.9819, 816.7415, 818.6471, 820.6223, 824.8062, 825.8953, 828.7291, 834.9616, 836.2361, 838.7808, 840.0932, 842.9019, 849.5698, 852.6348, 859.3286, 867.9807, 992.9556, 1062.1038, 1090.9603, 1111.4254, 1120.3782, 1124.2426, 1124.9432, 1126.2557, 1138.0088, 1143.2226, 1144.2139, 1148.6807, 1152.2272, 1166.2761, 1179.2195, 1182.9221, 1187.8324, 1195.9777, 1208.0250, 1213.2664, 1220.8418, 1223.3021, 1224.3777, 1234.0648, 1237.6348, 1241.4390, 1243.5003, 1246.3157, 1248.5205, 1253.1703, 1256.9922, 1260.6993, 1268.4961, 1270.1203, 1272.6258, 1289.6756, 1296.5102, 1298.5826, 1303.9485, 1311.8947, 1329.4756, 1333.8097, 1357.1114, 1395.6966, 1446.4000, 1457.3880, 1514.2904, 1521.1214, 1962.0173, 3085.6497, 3111.1926, 3158.2270, 3174.3432, 3178.3186	None
T1-O1-ZeO-C ₂ H ₅ CO(ads)	231	28.3964, 43.5563, 48.2795, 52.5372, 63.0344, 68.2202, 77.2029, 87.8406, 90.8981, 93.8850, 97.5751, 100.4416, 104.2882, 111.9515, 113.7368, 121.9894, 128.0612, 132.4566, 137.6881, 140.7321, 146.9242, 152.7642, 155.0177, 160.1658, 164.3895, 165.3375, 167.6079, 174.1048, 177.0035, 179.3078, 182.1312, 183.2552, 183.9658, 189.7253, 192.2806, 193.4004, 198.8299, 202.3264, 203.1117, 208.8118, 212.8719, 216.5582, 217.3604, 220.0315, 225.7112, 228.1422, 229.7530, 233.8258, 240.6149, 241.0877, 243.1793, 246.0731, 248.1549, 251.0616, 254.2160, 256.7425, 258.5437, 260.3912, 262.9251, 265.1297, 266.6466,	None

		270.5989, 275.4648, 275.9626, 278.3354, 281.3715, 283.8542, 286.3218, 290.7287, 295.1676, 297.6528, 298.6948, 301.4419, 306.6694, 309.4945, 311.2793, 315.9299, 320.1792, 324.1074, 326.2313, 327.3904, 329.9078, 336.6500, 339.4127, 345.0404, 348.9660, 353.3103, 362.0074, 365.5643, 368.9093, 371.1899, 378.6898, 379.4738, 387.0033, 390.6102, 393.5513, 395.7458, 405.3201, 411.1820, 414.8101, 421.9529, 422.7458, 429.1979, 436.0042, 438.1048, 447.5569, 452.5929, 459.1934, 471.8006, 475.2242, 481.9963, 492.6201, 499.5402, 507.5344, 513.6795, 517.0571, 530.0682, 535.2005, 555.1987, 559.5391, 568.0044, 571.7613, 588.0038, 600.0282, 605.5031, 610.8147, 643.3981, 665.0330, 672.5612, 696.7644, 703.8425, 705.8913, 710.1397, 713.4965, 717.9681, 724.5269, 727.0468, 736.7307, 739.8222, 751.2468, 753.8569, 757.7001, 763.7081, 771.2682, 772.5963, 775.3090, 779.2938, 780.1076, 784.4674, 787.8605, 789.9942, 793.0417, 795.1142, 795.4361, 798.3454, 802.8794, 806.1719, 808.8106, 811.3915, 815.3951, 821.0270, 822.9483, 824.3860, 828.5115, 832.4096, 833.8296, 837.3691, 838.8591, 843.9492, 845.2105, 847.0338, 847.7546, 856.0452, 858.4080, 861.0986, 869.6520, 872.9393, 918.8241, 1029.5020, 1103.0040, 1118.5002, 1121.4463, 1124.7607, 1131.3785, 1137.3712, 1138.7427, 1147.3350, 1147.5913, 1152.6914, 1171.2962, 1181.6992, 1187.6547, 1195.3858, 1196.9545, 1202.7502, 1204.9361, 1210.7722, 1213.0717, 1214.8343, 1222.1106, 1224.6119, 1231.3394, 1232.5115, 1237.0345, 1246.6376, 1252.2476, 1253.3700, 1261.3197, 1263.3336, 1271.0127, 1286.3659, 1287.5327, 1296.6584, 1305.6127, 1318.2671, 1333.7668, 1369.5329, 1369.6735, 1382.1511, 1419.7750, 1437.0079, 1468.6513, 1514.2918, 1520.3763, 1560.5770, 2265.1651, 3081.4355, 3155.7048, 3168.3855, 3184.7203, 3233.6610	
T1-O1-Carbonylation-TS	231	-428.4225, 37.8027, 45.3153, 50.0762, 60.4991, 76.3856, 78.3527, 85.1792, 88.3527, 95.6266, 100.4719, 106.7690, 112.5843, 116.9438, 121.9653, 125.1676, 127.8291, 135.3957, 139.0245, 142.6847, 145.1925, 149.9956, 156.1899, 159.1435, 162.7375, 164.0383, 172.0654, 173.3910, 177.4638, 179.3495, 180.6035, 182.6123, 185.6842, 186.3379, 190.5407, 194.7067, 197.7652, 199.1988, 204.3177, 209.1653, 211.1811, 214.1543, 216.9001, 219.6389, 223.7812, 229.0707, 232.5644, 234.0861, 239.2523, 240.5966, 244.1532, 245.6946, 249.9059, 253.5087, 255.3408, 255.7996, 258.5868, 260.3098, 263.0751, 264.6382, 266.7715, 270.1791, 273.4648, 276.2533, 277.0247, 281.1079, 284.2147, 287.2705, 289.7234, 293.4170, 297.3684, 298.9981, 304.0627, 306.6066, 309.5136, 311.3644, 313.7154, 319.3951, 321.5797, 323.5869, 324.7112, 326.3548, 329.8604, 330.4342, 334.4649, 336.8656, 342.4754, 346.5011, 353.5834, 362.4222, 367.2402, 371.8972, 373.9351, 380.7784, 388.3228, 389.8998, 395.0890, 398.2172, 407.9543, 413.8974, 419.8267, 420.8361, 423.9658, 430.1881, 435.3433, 444.9579, 447.3273, 452.3981, 458.9463, 463.3325, 476.0289, 487.0420, 498.1369, 502.0633, 509.4637, 514.0146, 519.5581, 536.4678, 546.5273, 560.6263, 566.5222, 568.2645, 587.0394, 594.2487, 607.6004, 613.0256, 614.8184, 647.4788, 672.4453, 693.3682, 700.3987, 703.1989, 706.9829, 710.4939, 712.9892, 719.4336, 722.1560, 726.0376, 732.4399, 739.0293, 746.0266, 754.7828, 756.4513, 760.4752, 768.0619, 771.0516, 774.1978, 778.2372, 782.0264, 783.4247, 788.3634, 788.5713, 790.4597, 794.2524, 795.5684, 802.2312, 803.0482, 807.0254, 808.9442, 815.2144, 819.5411, 822.4384, 824.3183, 825.5732, 828.7228, 830.9830, 834.3273, 838.9333, 840.4793, 843.4691, 845.7583, 846.9553, 848.3598, 854.4431, 859.1285, 861.6251, 873.3869, 949.9619, 1023.1311, 1053.9455, 1086.4327, 1086.7181, 1114.4647, 1121.3135, 1127.9996, 1130.2612, 1131.1294, 1135.1763, 1145.3927, 1159.9088, 1167.4764, 1176.8011, 1186.8112, 1189.6707, 1193.6549, 1203.4892, 1210.6535, 1213.6329,	-428.4225

		1217.8398, 1218.9382, 1220.4922, 1225.3154, 1229.1465, 1233.9776, 1237.9353, 1239.3396, 1246.1076, 1248.4188, 1250.5350, 1256.2648, 1264.8797, 1271.3301, 1276.4034, 1286.6413, 1290.2185, 1298.1288, 1305.5008, 1326.6190, 1370.2723, 1394.5507, 1402.5823, 1413.3768, 1480.6217, 1494.8041, 1544.4461, 2319.2074, 3095.6533, 3172.7540, 3216.5389, 3233.6081, 3359.0312	
Tl-O1-ZeO-propionyl (ads)	231	37.5638, 51.4929, 56.8183, 70.9210, 72.0532, 77.2553, 85.4824, 89.1549, 91.3573, 98.0478, 100.8027, 110.9137, 115.4976, 119.4315, 126.8915, 127.3636, 132.8362, 145.1406, 145.7160, 151.5808, 156.7518, 157.5767, 162.3401, 165.3230, 171.7372, 174.1563, 177.6016, 180.2560, 180.7626, 185.6407, 186.9019, 189.7060, 191.2863, 195.2556, 201.1943, 201.6904, 207.1880, 210.2861, 214.2233, 215.3304, 218.5284, 221.9082, 225.5206, 228.5417, 233.9160, 238.1530, 239.3454, 240.8562, 243.6149, 247.0292, 253.0715, 253.3305, 256.3799, 258.8728, 260.5118, 262.0434, 264.7275, 267.3306, 269.9633, 273.7728, 275.3308, 279.7934, 282.3974, 283.6324, 288.2917, 289.5076, 292.7394, 297.0509, 298.2071, 301.4832, 303.0975, 307.6822, 310.5560, 311.4052, 316.0071, 319.0075, 320.9948, 326.6643, 329.2221, 332.3102, 335.8030, 339.4041, 346.4403, 351.1233, 355.8525, 362.2577, 365.2763, 370.6077, 373.3101, 379.7415, 386.8339, 389.0374, 392.1773, 393.6906, 403.0876, 410.5872, 416.5438, 422.2584, 426.3668, 429.3911, 434.4079, 435.6523, 439.9438, 447.3088, 452.7440, 458.6520, 465.1732, 475.0474, 488.3615, 492.6029, 498.5202, 504.6468, 510.7638, 519.9380, 532.1761, 549.1535, 557.1470, 567.6558, 568.6009, 585.9452, 595.7683, 605.0468, 608.1988, 613.4387, 642.9795, 675.0648, 676.1685, 698.5840, 702.9830, 706.9479, 709.6770, 714.4529, 717.7913, 723.0724, 723.4590, 725.5220, 733.0482, 738.3083, 740.4379, 747.9946, 753.8876, 758.1272, 764.6089, 772.0697, 772.5589, 776.6435, 779.7270, 781.3998, 786.9093, 789.8141, 790.8715, 795.6724, 797.2758, 800.2501, 805.0302, 806.7380, 810.2799, 812.0368, 814.7845, 816.7014, 822.1136, 823.5917, 825.2681, 829.4287, 834.2215, 835.7991, 838.8534, 840.1799, 841.7790, 844.9056, 846.2445, 849.6992, 855.5296, 858.5272, 861.4505, 863.3277, 873.8681, 967.9505, 1053.1625, 1109.5890, 1115.8637, 1119.4156, 1121.3867, 1125.6745, 1132.5395, 1146.4687, 1149.5064, 1151.4774, 1158.4200, 1168.4091, 1171.8637, 1182.1833, 1189.6331, 1195.5861, 1203.2123, 1205.1707, 1210.4948, 1213.5201, 1217.6936, 1222.9590, 1229.5908, 1230.6491, 1238.1934, 1242.6387, 1249.6298, 1253.3450, 1256.4083, 1263.0561, 1263.9141, 1270.5777, 1285.4892, 1285.7341, 1296.8557, 1303.4473, 1312.1969, 1318.6100, 1344.8934, 1362.5288, 1370.7893, 1385.0481, 1421.9234, 1441.2932, 1515.2689, 1523.1826, 1577.9502, 1945.3124, 3086.8811, 3120.1397, 3170.3303, 3188.0224, 3198.7705	None
Tl-O2-ZeO-C ₂ H ₅ CO(ads)	237	20.3601, 38.9644, 44.6205, 57.8269, 58.2180, 60.2107, 67.6575, 75.7587, 90.2926, 92.4055, 94.7150, 96.9597, 99.8099, 111.7400, 116.1520, 119.3757, 126.7847, 127.1322, 131.8634, 135.4220, 139.6919, 144.9158, 149.9340, 154.2255, 155.8563, 162.0153, 165.4912, 170.0850, 171.7496, 174.9766, 178.9392, 179.9314, 180.9109, 182.7185, 185.9725, 188.1720, 194.2284, 195.6515, 200.7114, 201.9504, 204.2957, 210.4165, 212.6222, 216.2664, 221.2261, 222.2376, 228.0315, 229.7195, 230.8449, 239.1041, 239.7000, 243.2574, 244.5855, 248.3812, 249.8264, 254.4953, 255.6906, 256.9806, 259.9010, 260.7384, 261.4812, 270.2790, 272.3897, 274.6907, 277.4943, 278.6682, 281.0878, 283.7076, 285.1403, 288.1695, 291.4182, 297.7635, 299.8549, 304.6823, 306.7843, 308.8368, 311.2601, 315.1794, 319.6115, 320.7596, 326.3831, 328.3423, 330.1057, 331.2906, 335.9056, 341.5787, 346.1918, 351.0535, 356.4717, 362.8338, 365.2993, 371.7557, 374.6496, 380.4278, 387.0660, 388.4830, 389.9409, 396.7190, 398.1904, 406.4472, 412.0089,	None

		419.2723, 422.1448, 424.1259, 425.5756, 436.4757, 444.5068, 448.8855, 451.9031, 457.0186, 461.3545, 466.9924, 476.9417, 487.5120, 495.6933, 503.3738, 508.6783, 516.5758, 521.7564, 534.3529, 546.3206, 553.3527, 566.4430, 568.2511, 576.1654, 594.3848, 603.2239, 611.7178, 630.2957, 658.0148, 673.2373, 682.6377, 690.6542, 703.9687, 707.9652, 709.0975, 711.0913, 715.8045, 717.0274, 720.4078, 725.6569, 731.3005, 738.9398, 746.1822, 754.3216, 755.0640, 764.6348, 765.0171, 770.6918, 772.5807, 774.9694, 777.8140, 780.1282, 784.8576, 786.9770, 789.3805, 791.8258, 793.6732, 800.7383, 804.0502, 806.6140, 808.3371, 811.0666, 812.7163, 821.0833, 822.5518, 824.3377, 826.4348, 831.2969, 835.2961, 837.2066, 839.8652, 842.3107, 843.3850, 846.1144, 849.5225, 850.2057, 855.2677, 857.2554, 859.2639, 862.0574, 872.5125, 903.6959, 1011.5387, 1082.7812, 1097.3759, 1122.5735, 1125.6649, 1127.2112, 1135.2699, 1136.0647, 1143.1133, 1149.7772, 1160.5782, 1171.2184, 1182.3304, 1185.7432, 1187.9171, 1197.3437, 1199.1047, 1200.9588, 1203.1558, 1208.8500, 1214.3984, 1215.8963, 1219.1426, 1232.3885, 1235.3706, 1239.1016, 1241.4459, 1246.8093, 1249.0535, 1255.5156, 1262.4547, 1270.7330, 1279.6543, 1287.3747, 1289.2557, 1300.3915, 1311.8136, 1322.2495, 1327.3772, 1337.9027, 1365.8306, 1394.6599, 1415.4321, 1418.8734, 1444.7867, 1496.7722, 1523.5546, 1550.8368, 2246.3740, 3081.7180, 3165.2758, 3175.9482, 3205.3423, 3269.0423	
T1-O2-Carbonylation-TS	237	-379.9259, 38.4442, 47.5989, 57.5095, 66.2271, 66.9868, 75.8184, 85.6226, 90.3272, 92.7427, 94.9431, 98.5401, 111.4840, 115.3109, 121.9123, 125.0348, 125.9330, 133.2643, 135.3559, 138.3742, 145.6860, 150.4027, 154.4754, 157.9620, 160.6481, 167.4715, 169.0527, 173.3887, 174.0571, 177.9066, 181.7099, 182.2376, 184.2652, 186.5528, 187.5988, 192.9081, 195.5132, 199.9346, 201.3789, 202.8995, 205.4222, 210.2338, 216.2016, 217.1631, 220.0209, 220.7755, 223.2194, 230.4497, 232.8873, 239.1127, 239.4459, 241.7584, 246.8792, 248.9146, 251.2066, 252.9429, 255.4325, 258.9864, 260.0419, 261.1034, 263.6343, 269.0481, 271.4741, 273.6987, 276.8610, 279.2250, 281.6118, 284.9140, 287.2136, 287.8996, 293.6078, 298.4419, 300.4498, 305.9208, 307.8560, 310.0648, 313.0839, 315.0229, 315.4058, 320.1367, 321.4495, 326.3752, 327.6696, 331.3537, 333.4915, 339.3361, 344.0184, 345.8437, 350.7317, 354.8497, 364.4545, 365.2472, 371.0361, 374.3385, 376.9697, 384.7557, 387.8922, 392.0906, 395.9543, 398.8017, 411.8194, 415.8704, 418.0015, 423.5489, 425.4551, 429.2843, 435.7655, 440.9869, 444.3051, 450.8602, 453.8421, 461.5946, 462.9770, 479.1860, 489.2863, 503.5058, 508.0298, 510.5502, 518.2556, 525.9899, 545.7502, 549.6104, 561.1298, 569.6003, 574.2193, 594.8699, 599.2774, 609.4583, 615.5863, 631.6534, 666.9298, 680.7211, 682.2758, 703.5005, 704.5567, 707.6315, 707.9806, 716.4481, 719.9373, 721.5491, 726.7151, 728.7603, 740.2228, 741.9507, 742.4364, 746.2997, 755.7704, 757.3693, 765.4656, 772.0265, 774.1189, 775.7532, 779.4022, 783.3972, 787.3206, 788.5085, 790.8954, 793.1365, 798.0402, 799.3132, 801.8783, 805.8146, 808.0204, 810.0863, 812.2512, 818.9043, 821.5862, 824.2074, 825.7619, 829.2945, 831.5697, 834.1165, 837.5785, 841.0382, 844.5858, 849.8519, 851.3519, 853.3008, 855.7736, 856.8199, 861.0798, 873.6169, 922.9862, 1029.8978, 1059.0813, 1090.7718, 1093.6964, 1103.0529, 1108.7563, 1122.7415, 1135.1308, 1141.6343, 1145.5723, 1148.2867, 1153.2486, 1165.9320, 1179.5274, 1181.2704, 1189.6362, 1190.8603, 1194.3615, 1197.9338, 1204.6554, 1210.1493, 1214.6474, 1220.4457, 1231.4944, 1231.7288, 1233.5937, 1237.4496, 1239.3388, 1242.7930, 1248.5373, 1255.7650, 1260.9983, 1263.8127, 1268.8627, 1270.9106, 1276.9309, 1279.4532, 1292.7621, 1308.9247, 1309.6677, 1321.3377, 1352.4493, 1395.1132,	-379.9259

		1402.8949, 1415.7106, 1453.6987, 1484.8702, 1511.6905, 2308.0889, 3105.4610, 3177.3481, 3208.9855, 3258.5139, 3344.9207	
T1-O2-ZeO-propionyl (ads)	237	44.2686, 52.8703, 57.8719, 61.3578, 73.0475, 87.5176, 88.8784, 91.6810, 95.3477, 100.4341, 104.5080, 112.5185, 115.8518, 117.1067, 126.5022, 130.1567, 136.6509, 140.0941, 144.1696, 148.7548, 149.5432, 153.8273, 160.3567, 164.1901, 168.3328, 173.1050, 174.0905, 176.2296, 178.6001, 180.1571, 183.0381, 184.2395, 187.1341, 192.7892, 195.7733, 199.9691, 201.0281, 202.9057, 208.6223, 212.5921, 213.8937, 216.9007, 219.8702, 223.3792, 224.9968, 230.6022, 233.2731, 237.5311, 238.7482, 242.3777, 246.9441, 248.5510, 250.0038, 253.2931, 254.8369, 257.2258, 259.3731, 259.9858, 261.8565, 269.4070, 271.3535, 274.0653, 275.6437, 277.6574, 280.2298, 280.9988, 284.8381, 287.3694, 291.7967, 297.4061, 300.3338, 302.7867, 304.8934, 307.7936, 309.4613, 312.8860, 317.1336, 319.6839, 320.8848, 325.9944, 329.8768, 331.8376, 332.5302, 339.4302, 342.3331, 346.7982, 358.7134, 362.9624, 364.2185, 370.5864, 378.5476, 383.3077, 383.9291, 387.5726, 394.2349, 395.9287, 403.6080, 410.9835, 416.6929, 418.8520, 421.8051, 424.1406, 433.4427, 442.3836, 446.1575, 451.2017, 454.1635, 458.8416, 461.8502, 475.5372, 486.8619, 491.9378, 503.3235, 509.1645, 513.2210, 520.3606, 529.9679, 533.2477, 545.1775, 553.9151, 563.9319, 568.4103, 576.0898, 593.9598, 601.2978, 612.2625, 623.0671, 638.0768, 656.5562, 675.5729, 689.9168, 693.4433, 703.4732, 707.1874, 708.3324, 713.3863, 717.8035, 719.8215, 720.6404, 725.0914, 732.0118, 735.9843, 739.0384, 748.9388, 755.3117, 756.8544, 764.4305, 767.7588, 771.5155, 773.0854, 776.0644, 778.4620, 779.9932, 785.6200, 789.0958, 792.3693, 793.0474, 802.3178, 804.0536, 804.9890, 810.0392, 811.0669, 812.0777, 816.1366, 822.6124, 824.1666, 829.1276, 833.5679, 834.8359, 836.5567, 837.2603, 839.3806, 844.6554, 846.8543, 848.9631, 852.5307, 855.6984, 856.1413, 858.3080, 861.4241, 872.3294, 877.6179, 978.0323, 1050.4186, 1087.0598, 1094.8345, 1124.7736, 1125.4725, 1127.8677, 1137.9687, 1138.7285, 1139.3815, 1144.9036, 1155.0907, 1163.9825, 1174.6514, 1182.1912, 1189.6844, 1190.7450, 1198.1745, 1204.0420, 1206.8993, 1210.4288, 1216.1659, 1219.8315, 1224.8773, 1232.6838, 1237.7839, 1239.4080, 1246.0584, 1250.5606, 1255.8096, 1261.3528, 1264.3051, 1272.3833, 1286.4034, 1288.3621, 1290.2353, 1299.7134, 1300.9346, 1319.0829, 1321.4295, 1333.7043, 1365.2107, 1394.7107, 1400.4327, 1418.9620, 1451.4101, 1473.9402, 1513.6408, 1525.3111, 1991.9412, 3076.8144, 3098.9998, 3130.7192, 3180.0508, 3224.2177	None
T2-O2-ZeO-C ₂ H ₅ CO(ads)	237	23.4572, 29.5949, 40.0618, 58.6667, 60.0232, 63.9172, 67.2412, 75.3973, 83.4408, 88.7239, 92.1414, 92.5556, 95.6342, 101.8803, 110.2250, 116.2569, 117.4432, 120.3960, 124.2199, 129.7272, 136.1611, 142.8883, 147.3092, 150.2621, 153.6069, 155.0049, 161.7123, 167.9530, 172.9073, 176.5291, 179.8822, 181.3358, 182.2347, 183.8466, 186.7550, 190.2740, 191.7216, 195.9798, 201.2045, 205.1808, 206.7917, 208.6466, 215.6216, 216.4542, 218.5802, 221.5912, 224.9796, 227.5575, 233.6220, 237.1926, 238.9943, 240.6356, 247.1954, 249.0829, 250.6756, 252.7188, 254.2871, 259.5005, 260.8736, 261.7702, 265.1839, 267.1657, 268.7184, 272.6922, 275.5697, 277.7116, 280.3665, 283.2237, 287.8317, 289.3763, 294.2410, 297.1335, 299.2551, 303.1365, 305.1029, 309.2602, 312.1390, 315.7393, 319.5821, 322.9617, 326.8240, 327.9142, 328.4420, 330.9725, 335.5273, 339.0088, 343.0301, 349.3349, 351.5314, 362.0511, 366.7570, 367.5535, 371.5623, 375.0976, 378.2537, 383.5736, 387.4097, 394.1460, 394.6894, 398.3359, 412.8907, 414.4946, 421.5061, 424.7444, 427.4917, 432.2561, 446.3149, 447.1636, 451.6276, 455.9899, 460.4023,	None

		468.7589, 478.2076, 487.3834, 494.3784, 501.6189, 505.3576, 517.7042, 523.3356, 533.4649, 546.1371, 552.5194, 560.3862, 567.3248, 571.2177, 591.8751, 602.8035, 609.5671, 629.4255, 655.1330, 664.6413, 675.7435, 687.6607, 701.1665, 703.0921, 704.4510, 705.7948, 714.1798, 716.9807, 721.5721, 724.5742, 734.4756, 738.3289, 747.0432, 748.6700, 757.1448, 763.6290, 768.3789, 770.0112, 770.4768, 773.8962, 777.2518, 779.9427, 781.7213, 783.6760, 789.7266, 791.9368, 792.5766, 799.6539, 801.8283, 802.9184, 806.8262, 807.2357, 811.5221, 816.0770, 819.5550, 822.3912, 825.7411, 828.5118, 831.8410, 833.7670, 835.7424, 838.6575, 839.9640, 841.3527, 846.5294, 848.2138, 853.5439, 857.9466, 860.7671, 867.0272, 872.6469, 909.3079, 1010.5403, 1073.1670, 1104.4143, 1119.2474, 1126.8553, 1129.0674, 1130.1835, 1136.3902, 1143.2905, 1145.0200, 1152.9698, 1173.2275, 1176.3766, 1183.0071, 1189.3185, 1190.9981, 1196.1750, 1196.3291, 1199.2722, 1203.8688, 1207.8399, 1221.7412, 1224.7774, 1227.4607, 1230.8855, 1240.4690, 1246.8761, 1247.2264, 1251.2252, 1255.1248, 1258.7469, 1264.9622, 1279.4503, 1285.5349, 1287.1539, 1297.0997, 1300.9730, 1322.5340, 1326.7689, 1329.8422, 1360.3997, 1363.6622, 1413.3575, 1413.9808, 1444.7896, 1497.8823, 1518.3712, 1536.5853, 2251.4470, 3076.5067, 3157.5547, 3174.2057, 3175.1770, 3235.7317	
T2-O2-Carbonylation-TS	237	-390.4757, 42.1106, 46.7760, 54.7686, 63.5172, 69.8269, 72.7404, 80.4484, 85.0404, 87.4414, 92.3241, 95.0751, 114.1319, 117.3232, 119.8446, 121.9103, 125.9696, 127.5107, 136.8143, 137.4550, 147.6121, 149.0336, 152.9201, 155.3110, 158.2427, 163.4365, 168.6253, 171.1919, 173.3545, 176.6878, 180.0568, 182.9385, 184.8235, 186.0499, 189.4520, 191.7554, 196.1719, 198.5138, 199.5557, 203.9962, 206.5771, 214.1808, 216.6482, 218.1412, 220.7954, 225.7126, 227.5548, 230.8360, 235.6065, 236.9770, 242.5999, 243.0242, 249.5472, 250.2022, 252.6018, 254.2444, 258.3100, 259.2499, 261.6333, 263.5919, 265.0113, 267.4962, 269.6518, 274.7788, 276.7596, 278.2581, 283.0858, 285.1144, 289.6269, 294.1922, 296.9282, 297.1611, 301.7326, 305.5974, 308.5643, 311.9308, 314.6915, 316.7239, 321.3320, 322.5891, 324.4960, 326.1616, 329.7598, 333.9780, 335.0428, 341.0526, 344.1032, 346.7774, 350.7300, 358.3006, 359.2363, 366.0395, 367.5874, 369.9302, 378.0655, 383.6223, 386.1561, 390.8770, 393.7233, 395.3253, 403.6129, 410.4166, 415.5981, 422.2506, 423.8064, 424.8136, 433.4937, 440.6410, 445.9537, 451.2830, 455.8469, 463.3047, 465.3047, 483.4378, 492.6884, 501.2416, 502.8927, 506.6915, 517.3994, 525.6778, 540.3909, 550.4476, 561.9927, 568.2240, 571.8319, 592.7281, 599.0783, 610.0112, 614.8766, 636.2524, 647.8848, 675.3086, 679.3480, 697.9030, 700.6699, 704.1125, 706.5578, 716.2112, 718.4596, 722.0229, 724.2816, 726.0469, 739.9663, 743.0191, 745.2656, 746.9550, 761.5421, 766.7247, 768.0808, 769.0867, 774.8070, 777.0660, 781.5307, 783.2447, 786.0005, 788.6926, 790.2447, 793.1439, 796.9861, 799.2172, 799.4358, 804.1985, 806.6626, 807.9911, 810.1426, 816.9697, 821.1736, 823.5647, 826.2112, 828.4844, 830.8962, 834.0258, 836.3274, 838.7678, 841.1279, 841.5984, 846.9792, 851.9759, 855.8331, 857.2383, 860.2774, 873.8532, 926.2971, 1032.6582, 1069.5463, 1083.4274, 1097.8086, 1102.6141, 1106.5711, 1119.9858, 1132.4809, 1135.6255, 1142.8353, 1148.9712, 1160.1990, 1174.9126, 1179.3532, 1184.8805, 1188.7001, 1190.1112, 1194.5084, 1199.2015, 1209.2910, 1211.4760, 1214.8532, 1216.2209, 1219.4759, 1228.3521, 1234.9190, 1237.1900, 1238.4261, 1239.8592, 1245.2428, 1248.3536, 1251.2066, 1258.3885, 1260.3020, 1266.7179, 1279.6298, 1287.3687, 1294.5888, 1297.3394, 1317.5291, 1318.2183, 1339.9829, 1388.0619, 1398.1142, 1412.9298, 1461.8362, 1497.2803, 1500.3258, 2304.8870, 3106.8486, 3188.3862, 3197.2486,	-390.4757

		3256.2993, 3327.6932	
T2-O6-ZeO-C ₂ H ₅ CO(ads)	159	24.9017, 35.2798, 40.4786, 43.3744, 57.1497, 78.3466, 82.9463, 90.3299, 103.2470, 115.5172, 121.6691, 122.6975, 126.2935, 128.5156, 135.1494, 146.8217, 150.8825, 157.4076, 165.6365, 170.7290, 172.9794, 175.5326, 176.2089, 186.7149, 200.1389, 209.5393, 212.5798, 222.6769, 227.1979, 234.9465, 242.8517, 248.0369, 253.3492, 256.1558, 271.4080, 274.7028, 281.3453, 287.0863, 290.3335, 298.7856, 301.6704, 305.0443, 309.5020, 311.6918, 314.7617, 316.8706, 323.9984, 327.7030, 331.7068, 334.8663, 346.5479, 349.4766, 354.7963, 365.1788, 390.3442, 396.2431, 400.3196, 410.7424, 436.1796, 437.8608, 439.0453, 439.6976, 446.4373, 449.8033, 462.9760, 470.1546, 489.9362, 517.2674, 566.1936, 568.7704, 585.0877, 587.7204, 599.5444, 611.2751, 632.8190, 642.7313, 686.0687, 688.5598, 693.7405, 700.6087, 707.4483, 716.3003, 721.3506, 723.7594, 726.4801, 726.8147, 728.7181, 734.9361, 738.0110, 747.4836, 749.9380, 755.7384, 757.4155, 761.4658, 772.1076, 781.3071, 790.7064, 797.2983, 800.9335, 806.9309, 808.3158, 814.8973, 817.2411, 818.2522, 826.1039, 832.6144, 834.6552, 838.1698, 840.1158, 843.3113, 853.5103, 856.1093, 862.1205, 875.5236, 883.4404, 890.1779, 907.0797, 968.2773, 1040.5577, 1099.7507, 1143.3418, 1149.4159, 1156.3786, 1166.0459, 1170.6786, 1184.3165, 1193.8708, 1206.2911, 1220.0708, 1221.3463, 1228.1372, 1231.8681, 1240.4823, 1246.4989, 1257.9214, 1262.1472, 1280.6116, 1287.2909, 1296.1764, 1318.7891, 1338.2460, 1350.2323, 1404.3626, 1411.5456, 1452.1810, 1505.6696, 1528.0386, 1572.0338, 2219.8781, 2221.7428, 2222.0765, 2235.0500, 2258.5122, 3099.7438, 3160.4983, 3181.6182, 3211.3093, 3232.5334	None
T2-O6-Carbonylation-TS	159	-331.3880, 28.7526, 44.9903, 63.0588, 73.1284, 78.1368, 86.6247, 88.8519, 102.6448, 108.3451, 116.0503, 119.0561, 134.3996, 137.3244, 147.8310, 152.3095, 154.7895, 159.1670, 167.3258, 169.5651, 173.2286, 175.4565, 181.8139, 184.7016, 193.7266, 198.9269, 212.8245, 227.8926, 229.1945, 236.6159, 241.9595, 250.5778, 251.0711, 256.4308, 260.5233, 269.8898, 275.5019, 278.7545, 284.8293, 291.4091, 297.5853, 301.8985, 308.8874, 311.1817, 313.2327, 317.5516, 318.5651, 325.7750, 329.4272, 331.0191, 336.2128, 338.7271, 344.3955, 349.2676, 357.9996, 363.9613, 378.5882, 394.5339, 401.8557, 409.8974, 428.4311, 435.0647, 435.8358, 440.5310, 448.7345, 454.3326, 459.5678, 468.1797, 497.9866, 518.9618, 558.8535, 570.4470, 583.4882, 585.7912, 611.0677, 629.8027, 636.6785, 651.2204, 674.7696, 687.8910, 692.9722, 698.4424, 704.3800, 706.2557, 713.8638, 719.4630, 720.3623, 723.8225, 727.0353, 734.3002, 737.4889, 748.7953, 750.4368, 754.6184, 756.0016, 757.5691, 770.3281, 775.4998, 780.7056, 784.7712, 794.5547, 795.1150, 803.1639, 812.5027, 813.4688, 817.4925, 824.3110, 831.9287, 835.6763, 840.0687, 844.8103, 850.1235, 863.1175, 872.5277, 874.9592, 876.8460, 880.0392, 897.9257, 920.2347, 1000.0661, 1096.1622, 1124.0632, 1131.6090, 1138.7570, 1153.5336, 1163.4883, 1177.6819, 1180.1790, 1191.3318, 1194.2878, 1198.9443, 1212.3654, 1219.2659, 1221.0780, 1226.8139, 1233.5722, 1239.2782, 1240.6725, 1249.9955, 1271.6486, 1284.2801, 1324.6223, 1331.4090, 1342.6239, 1367.1482, 1413.3244, 1478.5147, 1487.5121, 1526.8018, 2220.3383, 2222.5789, 2222.6318, 2236.2996, 2311.9498, 3060.6994, 3148.8178, 3187.5008, 3212.1640, 3332.1035	-331.388
T2-O6-ZeO-propionyl(ads)	159	32.2481, 37.3303, 57.5875, 81.5736, 83.5936, 93.2983, 103.9465, 119.0479, 124.1790, 132.3255, 135.8390, 137.9890, 143.0793, 149.2155, 156.9890, 159.4171, 168.2214, 169.9249, 175.0103, 180.8303, 183.5102, 196.3489, 198.5941, 206.0551, 218.0853, 234.2322, 236.1903, 244.8924, 246.4522, 247.1607,	None

		252.7041, 259.4765, 265.2080, 274.4145, 280.9182, 282.5928, 288.9542, 296.0145, 300.8664, 303.1880, 309.2301, 311.3253, 316.5689, 317.8313, 319.9115, 327.1542, 327.8271, 335.6344, 342.1931, 346.6733, 351.1896, 362.3081, 383.5856, 391.4117, 398.4412, 403.9676, 430.5785, 433.1673, 435.3627, 438.8762, 447.4472, 455.0300, 466.8128, 470.0816, 478.5145, 499.1131, 521.5071, 533.9144, 560.7898, 576.8353, 581.9595, 583.1717, 596.7114, 609.2754, 640.7958, 655.6692, 670.5032, 674.6613, 685.5439, 691.9363, 696.9532, 703.8206, 709.8663, 711.6207, 717.3343, 719.2946, 724.0752, 724.8298, 734.2410, 738.1754, 750.0337, 750.7859, 755.7891, 757.3107, 759.2227, 771.8511, 777.2051, 783.8750, 789.3775, 799.1741, 807.4421, 807.8798, 814.0000, 817.9279, 821.3974, 825.9895, 833.5064, 839.3086, 841.6052, 846.9811, 850.5497, 851.1400, 872.1186, 879.2481, 881.1394, 883.6070, 898.5250, 942.1417, 972.0536, 1048.8480, 1122.2566, 1130.6897, 1132.2313, 1146.0216, 1148.0264, 1155.2962, 1172.2730, 1177.0114, 1181.1387, 1193.1019, 1198.9155, 1214.3224, 1220.0559, 1225.9516, 1226.6170, 1245.3995, 1246.2369, 1255.6867, 1292.6226, 1311.9226, 1325.5652, 1339.9743, 1342.2050, 1373.1019, 1400.2584, 1448.5653, 1464.2273, 1513.9055, 1533.4214, 2022.3805, 2220.1821, 2221.3077, 2221.8352, 2234.9926, 3079.7372, 3089.2695, 3139.0425, 3177.4791, 3190.8005	
T3-O1-ZeO-C ₂ H ₅ CO(ads)	231	21.2760, 24.4258, 36.5467, 44.4178, 60.8977, 65.0125, 69.7202, 74.0741, 81.2284, 84.8181, 90.0467, 96.2342, 107.7965, 111.1638, 115.7024, 117.1066, 122.7098, 125.2834, 127.4983, 137.4703, 140.2499, 147.5601, 151.7063, 152.4589, 160.5421, 161.1284, 168.7778, 173.5880, 176.0717, 177.0875, 179.4947, 180.2135, 181.3675, 183.6872, 187.5318, 190.3317, 196.3257, 197.4790, 202.7555, 203.6020, 207.5238, 210.8077, 211.7719, 218.3085, 222.3078, 224.3890, 232.8301, 235.9401, 237.2585, 241.7326, 244.0986, 244.9598, 249.0554, 251.8778, 253.8423, 257.9398, 260.3798, 260.6568, 264.4014, 265.8328, 272.0845, 272.8480, 274.5142, 276.7835, 281.9247, 283.1940, 284.3600, 289.3082, 290.4242, 295.7061, 297.8033, 298.6134, 302.8932, 307.4610, 311.6430, 314.2623, 315.9099, 317.6439, 324.2471, 324.8269, 328.9409, 330.1170, 334.0117, 336.5091, 344.6527, 349.2513, 350.7169, 359.2717, 363.5218, 368.3814, 372.9511, 377.7880, 383.1612, 385.2359, 388.6261, 393.6075, 393.8087, 406.8995, 413.9948, 415.9586, 420.6382, 421.9746, 431.2415, 437.2339, 439.9987, 445.1547, 450.3671, 455.5441, 459.8148, 471.0985, 490.1387, 491.0546, 498.5512, 501.1024, 515.5425, 520.1346, 535.6445, 546.5229, 562.7845, 567.4376, 569.3980, 577.9721, 595.5000, 609.0649, 612.8135, 614.6220, 647.2872, 663.8868, 675.7638, 692.1968, 696.4734, 699.0330, 700.9734, 715.4735, 720.7637, 723.8545, 727.9396, 737.4901, 738.9422, 747.6213, 755.4180, 758.9862, 764.3346, 771.8525, 772.8687, 776.2123, 777.6695, 781.5734, 783.1208, 787.0172, 789.3622, 791.4580, 793.0855, 795.1405, 799.3762, 800.5423, 805.0818, 809.0413, 811.8560, 812.4071, 818.9443, 820.6426, 825.4721, 826.7036, 829.6129, 830.9701, 832.9006, 833.9251, 835.7187, 842.5051, 845.2750, 846.9142, 851.2416, 857.1990, 859.0495, 863.3626, 874.3077, 903.7607, 1026.5565, 1093.9979, 1119.0265, 1123.6485, 1127.1366, 1130.4782, 1133.9821, 1136.3830, 1136.6921, 1150.0357, 1155.3112, 1161.7209, 1179.6901, 1182.8312, 1193.7075, 1199.0913, 1208.1401, 1212.8490, 1215.0978, 1221.1116, 1223.4982, 1226.4214, 1231.9287, 1234.5692, 1234.8988, 1237.7766, 1240.0049, 1243.9934, 1250.2521, 1252.9042, 1260.9388, 1268.1188, 1269.3030, 1274.7258, 1282.6361, 1295.9494, 1309.4460, 1335.4954, 1345.2553, 1367.8905, 1408.8777, 1416.0081, 1424.3601, 1457.9320, 1507.2355, 1517.5818, 1566.2054, 2226.6485, 3077.9911, 3160.5426, 3173.5717, 3175.6157, 3233.5100	None

T3-O1-Carbonylation-TS	231	-393.1401, 29.3893, 33.7258, 41.3759, 58.7959, 72.1938, 82.9854, 83.7480, 89.5420, 98.3858, 103.0984, 110.6596, 111.8613, 114.7608, 117.1305, 122.2782, 126.0173, 128.8717, 130.0392, 140.5681, 143.4789, 146.5921, 149.1918, 154.8811, 161.7877, 163.1053, 170.5273, 173.9582, 177.0868, 177.8371, 180.1983, 180.8268, 183.4685, 189.6908, 190.5591, 194.2888, 196.2899, 199.4312, 203.3803, 204.9321, 208.6402, 211.1897, 213.0568, 216.1332, 220.8249, 222.5412, 225.3034, 232.3540, 234.3259, 239.0440, 239.4213, 242.9718, 245.8873, 250.7908, 251.7898, 253.4091, 257.9921, 259.4887, 261.5309, 265.4931, 266.5106, 272.0305, 273.0610, 275.7870, 276.9509, 283.2429, 284.4106, 288.5943, 291.2234, 294.9256, 296.8620, 297.9270, 301.1913, 304.2266, 306.0983, 312.1503, 314.4094, 315.0608, 319.8172, 323.7915, 326.5682, 328.4317, 329.8338, 331.2924, 332.9654, 338.8483, 344.2540, 347.1937, 354.2593, 364.0286, 367.5056, 370.0063, 374.5706, 378.5098, 385.9274, 387.5816, 391.4074, 395.4176, 404.1201, 415.2433, 417.3068, 423.6166, 428.6543, 433.5421, 439.5609, 442.7723, 446.2552, 450.6122, 455.9795, 459.8160, 471.0254, 489.2645, 496.0629, 499.9922, 502.4896, 517.5616, 519.2883, 538.1964, 551.5867, 563.0469, 568.2808, 569.3263, 592.6626, 599.6437, 612.8331, 615.8866, 619.1174, 652.3801, 674.0431, 688.7101, 698.5937, 699.6639, 705.7236, 711.4953, 715.9749, 721.4222, 724.2755, 730.2881, 735.6436, 738.5707, 741.1395, 755.7863, 757.4720, 762.6088, 766.3332, 770.4418, 774.2044, 777.0691, 782.1670, 783.3896, 787.0032, 787.8715, 789.8522, 793.7773, 797.7316, 800.1755, 803.2522, 805.4229, 809.0408, 810.7679, 813.9496, 819.6390, 822.3126, 824.9459, 825.5921, 828.3326, 830.7870, 831.9530, 835.0874, 836.7913, 840.3427, 845.4768, 852.0030, 856.3603, 859.1120, 864.9054, 874.8362, 968.8184, 990.1807, 1043.8653, 1067.2514, 1096.0756, 1109.3552, 1117.0296, 1118.8331, 1123.6486, 1129.9102, 1132.8049, 1140.5519, 1148.3149, 1153.0491, 1177.4502, 1177.8163, 1193.4713, 1196.7689, 1205.1166, 1210.2342, 1214.7856, 1218.8186, 1219.7417, 1224.9773, 1225.7543, 1229.9149, 1233.7790, 1235.9312, 1240.6138, 1241.9556, 1245.8785, 1254.9177, 1256.8621, 1263.3323, 1266.0276, 1269.0810, 1275.2954, 1286.9167, 1289.4412, 1303.2086, 1326.8164, 1368.9825, 1393.7403, 1405.0138, 1409.8531, 1473.6810, 1498.9840, 1523.6081, 2318.9635, 3094.9387, 3168.9077, 3182.6968, 3229.3162, 3344.9479	-393.1401
T3-O1-ZeO-propionyl (ads)	231	36.4395, 46.3209, 55.7030, 59.3049, 70.3763, 83.6650, 85.2733, 88.2198, 93.5525, 109.3285, 112.2748, 112.3847, 115.7096, 117.5192, 122.8947, 126.6058, 134.4293, 140.2915, 143.0554, 146.7717, 153.1664, 156.3548, 161.5531, 166.9608, 172.2937, 174.5040, 176.8784, 177.7988, 179.0684, 181.8362, 186.6430, 188.4390, 190.0051, 195.7418, 198.6843, 202.3472, 205.1851, 208.2125, 210.4168, 211.7348, 218.7992, 221.9384, 224.4008, 230.8115, 234.2294, 236.4745, 239.5587, 242.5237, 244.3447, 248.6900, 251.1939, 252.9355, 256.3948, 257.3046, 259.4712, 260.7398, 264.1698, 266.4025, 271.4790, 272.3687, 273.4280, 276.4698, 280.1001, 282.0887, 284.0566, 287.2832, 288.9838, 294.9219, 297.5665, 299.1434, 301.4483, 306.0200, 311.1264, 313.4627, 314.4469, 316.3971, 319.8232, 322.8320, 324.6621, 329.7886, 331.1284, 334.1971, 338.0674, 344.1834, 349.5904, 354.7768, 363.6191, 368.7437, 370.8639, 376.1042, 384.9622, 387.0966, 390.5727, 392.2722, 406.6693, 409.3059, 411.2446, 418.4738, 422.1414, 428.2018, 432.3934, 435.6058, 444.1475, 451.8011, 456.1607, 457.3551, 467.3065, 488.8978, 490.8068, 498.5388, 503.2037, 505.3138, 516.0807, 521.2862, 534.8645, 551.1511, 563.1531, 569.2676, 570.9069, 579.7633, 596.0748, 608.1949, 612.9656, 613.5365, 638.9679, 651.1581, 660.2533, 679.4040, 692.5684, 695.2269, 697.1366, 700.5704, 713.9257, 717.4319, 720.3354, 723.9243, 734.4224, 737.9597, 742.4275, 750.0732, 755.8826,	None

		762.8970, 764.1999, 770.7800, 773.4905, 777.2439, 780.0878, 782.5087, 785.7758, 788.3260, 789.5461, 793.6035, 797.0963, 800.9745, 802.8746, 805.5711, 807.5720, 810.0409, 812.7175, 813.8845, 818.2606, 820.4762, 824.5098, 826.6686, 829.2739, 831.5839, 833.4301, 837.0404, 842.3171, 846.4548, 847.9553, 849.9574, 853.4931, 857.8528, 861.2855, 864.5293, 877.4237, 964.0849, 1056.3390, 1088.1482, 1111.6986, 1115.5223, 1123.9866, 1127.4493, 1129.7734, 1133.2642, 1133.9939, 1139.5980, 1153.8061, 1156.7958, 1167.9724, 1180.8470, 1184.8069, 1195.4614, 1200.8219, 1211.8310, 1219.4411, 1224.6134, 1225.1070, 1230.5535, 1233.6593, 1236.4245, 1239.3104, 1240.0142, 1242.2301, 1248.3932, 1250.7159, 1255.4022, 1264.4002, 1268.9667, 1269.6964, 1279.2230, 1282.9263, 1294.9068, 1300.5936, 1307.4478, 1360.1282, 1370.5815, 1399.6218, 1406.2049, 1411.2868, 1442.6416, 1487.0045, 1520.7210, 1530.5817, 1973.3734, 3085.8481, 3115.3340, 3170.5478, 3182.3807, 3196.1614	
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Supplementary Table 16. Calculated Harmonic Vibrational Frequencies (cm^{-1}) for adsorbed species and transition states of propylene carbonylation reaction at T1-O1, T1-O2, T2-O2, T2-O6 and T3-O1 related to 10-MR at 473K.

FileName	Number of Frequencies	Full Frequency List (cm^{-1})	Imaginary Frequencies
T1-O1-ZeOH-C ₃ H ₆ (ads)	234	38.1575, 40.8718, 47.5696, 65.8849, 73.8236, 77.9802, 84.4749, 88.0724, 94.9557, 96.4981, 101.8894, 111.8594, 116.8788, 120.8396, 125.1637, 127.8637, 139.3966, 140.6528, 146.3126, 149.0482, 155.5170, 159.3165, 162.2685, 164.4788, 170.8896, 174.6098, 176.2231, 178.8483, 179.2515, 182.9924, 185.0831, 186.6066, 189.5465, 191.5499, 194.6816, 200.0173, 201.9443, 205.5946, 207.9571, 211.1424, 216.3147, 217.2449, 220.5571, 224.0159, 228.7364, 231.7166, 234.4029, 239.0314, 241.9863, 243.4982, 247.2904, 248.4168, 253.5255, 255.5494, 257.9228, 259.8411, 261.4659, 264.3018, 264.4088, 267.9809, 273.1070, 275.1871, 278.6709, 281.0663, 283.7086, 286.3379, 289.3585, 295.6345, 297.1364, 298.4237, 302.8165, 306.7897, 308.4786, 309.2953, 311.7013, 316.5639, 319.8327, 325.1116, 326.6181, 329.7015, 331.0693, 337.1440, 340.8648, 345.9129, 350.9687, 356.4579, 364.6531, 366.9383, 370.9306, 379.0891, 385.4016, 388.1099, 392.6309, 394.1889, 399.7064, 405.5050, 414.4847, 422.0640, 422.5609, 424.9394, 430.5551, 436.1548, 445.5206, 446.8409, 453.1760, 456.5455, 458.3799, 474.0355, 484.0887, 494.0100, 498.4652, 504.7963, 512.6495, 519.3738, 533.1608, 544.5650, 557.1005, 564.9764, 567.7643, 576.6882, 588.7472, 601.3260, 606.6617, 609.1130, 613.0471, 644.2776, 660.6491, 674.2354, 691.7111, 697.7169, 704.4966, 705.1902, 707.5270, 714.7170, 718.1896, 724.7649, 727.6655, 738.3206, 739.4058, 750.8576, 754.9170, 763.9571, 766.0709, 770.0566, 772.1920, 774.8995, 778.0368, 780.2421, 783.5128, 789.0327, 792.0892, 795.3297, 797.1006, 799.7899, 802.4402, 805.6197, 808.4819, 809.9695, 817.4010, 817.7842, 822.2693, 824.9124, 828.0983, 831.2938, 833.4431, 837.6923, 838.1314, 842.8062, 844.8414, 845.6374, 848.3552, 854.4892, 858.0599, 861.1190, 871.2358, 878.9956, 934.1425, 976.4764, 984.0156, 1048.9092, 1081.9921, 1103.1897, 1120.4351, 1125.0955, 1127.8713, 1136.7682, 1137.9702, 1145.6939, 1149.9977, 1153.7966, 1171.5835, 1180.5784, 1188.9147, 1192.2666, 1198.2451, 1202.5233, 1204.3217, 1214.7130, 1214.7688, 1217.1119, 1223.7127, 1228.1402, 1230.8440, 1234.6241, 1238.2350, 1242.0814, 1250.2769, 1255.0559, 1259.8287, 1263.5809, 1264.4240, 1277.9250, 1283.0762, 1292.1107, 1295.8463, 1313.0334, 1318.1767, 1342.8390, 1351.5553, 1372.7732, 1390.9236, 1415.8627, 1423.9647, 1465.6941, 1501.6095, 1541.3024, 1732.8519, 3075.1767, 3149.7292, 3172.9235, 3177.4585, 3195.5514, 3278.2733, 3341.1184	None
T1-O1-Protonation-TS	234	-337.2470, 43.3968, 50.3498, 55.7044, 73.8867, 78.3051, 82.3120, 88.1474, 90.9207, 98.2877, 105.1540, 112.0939, 116.1433, 120.5037, 121.5526, 127.4655, 132.7660, 139.1051, 143.4273, 144.5456, 149.5676, 154.9254, 159.2895, 162.8460, 164.1227, 171.7659, 175.0403, 176.5386, 179.5010, 180.9389, 182.4904, 185.7152, 188.1466, 190.1136, 193.9795, 198.7647, 199.4514, 203.4119, 209.1018, 211.6925, 215.1228, 218.5321, 220.1186, 224.2872, 225.8894, 231.4958, 233.2801, 233.8368, 239.5809, 244.6680, 245.4264, 248.6579, 252.2138, 254.0544, 256.7734, 259.8370, 260.2866, 261.1225, 264.7460, 268.1510, 270.6314, 274.9013, 276.1156, 278.8777, 281.9731, 285.0183, 288.1139, 290.7413, 295.6193, 298.6476, 301.9553, 305.8798, 308.7665, 310.8793, 313.2233, 316.0226, 319.4002, 323.0708, 324.6041, 328.3811, 330.3246, 332.3973, 337.4842, 342.4169, 345.6595, 353.5202, 362.8929, 367.0951, 370.3322, 373.9851, 381.1650, 388.3674, 389.5141, 395.5854, 397.6714, 408.5523, 412.9597, 419.5185, 421.0797, 424.3973, 429.8028, 436.2057, 437.6122, 445.9170, 448.0547, 452.7027, 459.2145, 462.4673, 476.0339, 487.1091, 497.6584, 501.2267, 509.8377, 512.2304, 517.9517, 526.7335, 536.1295, 546.2673, 560.5564, 566.3188, 568.5571, 587.2202,	-337.247

		595.1654, 607.6198, 615.0208, 617.5530, 648.4641, 673.4553, 693.9499, 703.7940, 707.5759, 708.3662, 710.0400, 714.3710, 719.6343, 722.0209, 726.2729, 731.1375, 739.6593, 741.0680, 754.2814, 756.2344, 762.4832, 767.8636, 770.6079, 774.3404, 777.7986, 782.0849, 784.5095, 788.1965, 790.3984, 794.0376, 794.6268, 796.7877, 800.8688, 803.7765, 805.6989, 808.9759, 813.3942, 817.5983, 819.7293, 821.8055, 824.8203, 826.6633, 827.8901, 830.6844, 832.9250, 837.4102, 839.1350, 841.7458, 845.7099, 848.4163, 849.7030, 858.3871, 860.7071, 873.6339, 960.0156, 988.3965, 1051.8692, 1083.1900, 1090.7403, 1108.2581, 1119.6494, 1123.1427, 1131.7883, 1133.1168, 1134.8622, 1146.6057, 1156.2918, 1164.9628, 1174.9100, 1184.7156, 1187.2439, 1190.2198, 1198.3263, 1208.0983, 1209.5322, 1215.5568, 1219.2562, 1222.6490, 1224.1275, 1228.7843, 1232.5858, 1238.8137, 1241.7028, 1244.8658, 1248.0565, 1252.8351, 1255.1075, 1261.1743, 1268.3041, 1274.0373, 1285.9902, 1289.2205, 1299.4486, 1303.0836, 1325.6516, 1327.5427, 1342.9367, 1369.3063, 1380.2168, 1391.1587, 1412.4040, 1428.4977, 1474.9850, 1512.8624, 1587.0535, 2385.5512, 3010.2367, 3132.4971, 3147.3791, 3196.0958, 3211.4038, 3249.8478	
Tl-Ol-ZeO-C ₃ H ₇ (ads)	234	46.4303, 50.9189, 52.5178, 66.1090, 70.3524, 78.2891, 84.7075, 91.7481, 93.9581, 98.0895, 113.5718, 117.4500, 122.2262, 125.1886, 127.5202, 137.9206, 142.4502, 149.9924, 152.4431, 156.3438, 160.9804, 164.5365, 168.6772, 171.4607, 172.7716, 178.2118, 179.1960, 180.1441, 184.3457, 186.7390, 189.4829, 195.2290, 197.8167, 202.8494, 206.3589, 209.7951, 212.3515, 213.5736, 216.1353, 222.3323, 224.1598, 228.2886, 232.6032, 235.9289, 240.0382, 240.6370, 243.6536, 244.9545, 247.2829, 251.7847, 253.8601, 255.3358, 257.7268, 260.0125, 261.2966, 262.0666, 266.5722, 268.0760, 272.1360, 273.6352, 276.6490, 279.0714, 281.1586, 284.6678, 285.5939, 289.6079, 296.8449, 298.1411, 299.4344, 302.5550, 305.9335, 307.2189, 310.5745, 312.3974, 317.9145, 319.5520, 321.6618, 327.8754, 328.9679, 331.2049, 334.2658, 340.0608, 345.3116, 349.9404, 356.1361, 362.7263, 366.3524, 370.5784, 375.8843, 381.2352, 385.8032, 388.1786, 394.4541, 395.2178, 407.3556, 413.9337, 416.8263, 419.9684, 422.6344, 427.1985, 432.9351, 441.2960, 444.2604, 449.3534, 451.9517, 457.5417, 472.3598, 477.7841, 484.2717, 496.7501, 499.7835, 507.5242, 513.4532, 517.8652, 533.6777, 536.0499, 557.4700, 561.7675, 568.4495, 571.5003, 590.8812, 600.4735, 609.0335, 614.4727, 647.6532, 663.4145, 676.0523, 693.2385, 701.1762, 703.4161, 705.3787, 714.2503, 716.3835, 721.0987, 724.7148, 727.8992, 735.8923, 739.2211, 750.1841, 755.5764, 757.3615, 760.5821, 769.8731, 772.4294, 776.4524, 779.4491, 781.6824, 785.4719, 790.1862, 793.4966, 795.9102, 797.6255, 801.4007, 802.3387, 806.1438, 809.6572, 811.4056, 816.3506, 817.5747, 824.8500, 825.9461, 830.3020, 831.1140, 832.9073, 838.0393, 840.0866, 843.2946, 844.6555, 847.3613, 849.1960, 853.2479, 854.2122, 860.9971, 864.5330, 876.7658, 916.3245, 957.0686, 969.0102, 1091.9754, 1107.3150, 1121.9743, 1130.1466, 1133.4152, 1134.0064, 1148.4180, 1151.0801, 1154.2430, 1167.2046, 1173.4570, 1185.0969, 1191.3119, 1196.6707, 1198.0417, 1200.8133, 1210.2308, 1215.4282, 1221.3651, 1223.8355, 1227.1465, 1230.1286, 1230.8282, 1236.4334, 1237.3748, 1247.8330, 1253.4323, 1259.0945, 1260.7635, 1262.2495, 1269.9511, 1275.1871, 1282.5924, 1287.0237, 1292.4504, 1307.7385, 1309.6694, 1345.6132, 1373.9897, 1384.8311, 1407.6035, 1413.2818, 1430.6087, 1446.0507, 1457.6037, 1496.4519, 1503.3121, 1516.2484, 1529.3341, 3085.2067, 3090.2981, 3167.2081, 3173.2977, 3206.2587, 3213.3785, 3238.1631	None
Tl-Ol-ZeO-C ₃ H ₇ CO(ads)	240	22.3232, 45.7652, 48.5391, 56.2381, 59.0014, 66.1630, 67.0679, 72.6117, 81.0165, 85.3553, 91.0595, 91.5388, 98.0459, 98.9130, 100.8798, 114.9890, 122.0816, 123.2815, 126.2600, 129.0765, 138.2370, 142.5081, 150.3772, 152.0265, 157.0275, 160.7472, 164.9524, 169.2088, 171.9313, 173.6307, 178.5647, 179.4017, 180.0663, 184.7488, 187.1072, 188.8297, 193.7342, 198.4466, 203.9023, 206.2085, 208.6666, 212.1243, 214.7366, 216.8575, 221.9177, 224.2924, 228.8851, 232.4366, 234.4853, 240.4310, 241.6367, 244.5192, 245.1988, 247.8986, 251.3310, 253.7310,	None

		256.4971, 258.2804, 260.2627, 262.1391, 262.5283, 267.6435, 269.4039, 273.8228, 275.4890, 279.7091, 280.9121, 282.1848, 285.2083, 288.4213, 295.5942, 298.0171, 298.4022, 302.7384, 304.2799, 306.4798, 309.4511, 312.4991, 317.9107, 319.2380, 320.1712, 325.0336, 328.9606, 331.1242, 335.0130, 340.0512, 341.1266, 345.1896, 352.1584, 357.2899, 364.9015, 366.7017, 372.2479, 377.6437, 382.0267, 386.1962, 388.6895, 394.1715, 395.1546, 407.8573, 413.9968, 417.9095, 420.4324, 422.3341, 427.6142, 432.3727, 441.2566, 444.5919, 449.4838, 452.1611, 457.8615, 472.6889, 477.5024, 485.2651, 498.1161, 498.8675, 508.0026, 513.1093, 518.2401, 534.5069, 536.9096, 557.5788, 562.0749, 569.3148, 571.9391, 591.1664, 600.8898, 609.2400, 614.2386, 647.7214, 663.9427, 675.7925, 693.8883, 701.6907, 703.6510, 705.0264, 712.1943, 715.2145, 721.3083, 724.6754, 728.4666, 736.0187, 738.6213, 749.2853, 755.2314, 756.9363, 759.8138, 770.1984, 772.4590, 776.5996, 778.5718, 781.3321, 785.4479, 789.7075, 793.3060, 795.8737, 798.1592, 801.4890, 802.5584, 805.9452, 809.4379, 811.4305, 815.2908, 816.8344, 823.7724, 824.9096, 829.8497, 831.2619, 831.8135, 838.0030, 840.4295, 843.2527, 844.7527, 847.2712, 849.4740, 852.2713, 853.5537, 860.8451, 864.0627, 876.5669, 914.2712, 954.7780, 967.7076, 1092.6144, 1109.8468, 1122.1314, 1128.6138, 1132.2602, 1133.4327, 1148.7962, 1150.2605, 1154.3182, 1170.8710, 1173.2058, 1185.2178, 1190.1820, 1195.4708, 1197.4555, 1200.2053, 1211.7685, 1214.9933, 1220.1197, 1222.3654, 1226.2617, 1229.0845, 1231.3056, 1234.2685, 1236.7459, 1247.2953, 1251.5189, 1258.4064, 1259.9006, 1262.4031, 1269.0748, 1275.0122, 1281.9063, 1285.9818, 1291.5651, 1303.9249, 1307.3585, 1346.0990, 1373.7055, 1395.2921, 1407.8432, 1410.9237, 1412.7425, 1445.0908, 1455.7573, 1492.9776, 1507.0803, 1521.3421, 1529.7550, 2219.1036, 3086.5897, 3102.4094, 3167.4862, 3187.5129, 3195.3162, 3219.6044, 3240.5089	
T1-O1-Carbonylation-TS	240	-286.9834, 43.2623, 61.4306, 63.8802, 72.4516, 73.4064, 78.5658, 80.7195, 86.2952, 97.6618, 98.4605, 102.8299, 103.8738, 112.7616, 118.9176, 120.3677, 125.7222, 126.9591, 136.6785, 138.1502, 140.8113, 145.7362, 154.2155, 158.1876, 161.8920, 162.6164, 167.6803, 174.0736, 175.9007, 177.5787, 180.1895, 181.7452, 182.6231, 187.6408, 190.5089, 191.6300, 194.1241, 195.2565, 198.6678, 201.5125, 204.6924, 212.2913, 214.6430, 216.6550, 219.2625, 221.8291, 226.1498, 230.7873, 233.8340, 235.1319, 236.7347, 242.7557, 245.3638, 246.9952, 250.8843, 253.8648, 254.7855, 257.5424, 259.6546, 261.4323, 262.2750, 269.5631, 270.7720, 273.2836, 275.6639, 278.1446, 280.8584, 283.0406, 286.4312, 290.3001, 293.6509, 296.0179, 298.4375, 300.7025, 305.9448, 306.9581, 309.1402, 311.3567, 313.2505, 315.9414, 320.1083, 321.4786, 326.3254, 328.4724, 329.8761, 332.8314, 337.0065, 343.5468, 345.7939, 352.1306, 362.8559, 367.4404, 370.9649, 374.0563, 381.5463, 386.6304, 388.0508, 394.8223, 395.7105, 398.8778, 409.4807, 411.0913, 416.3786, 420.0515, 423.9436, 428.5561, 433.2329, 438.6498, 444.8426, 446.9032, 453.1126, 460.2810, 465.3641, 476.9822, 488.3538, 497.5080, 502.0255, 509.6252, 513.7377, 519.7448, 535.7132, 547.4324, 561.7163, 567.0368, 569.5451, 587.2566, 597.0215, 607.9363, 617.8271, 620.0803, 651.1935, 674.7944, 699.5642, 704.4042, 705.3576, 708.1451, 714.4589, 715.3998, 723.4655, 724.7704, 730.9446, 731.8645, 739.7936, 742.2669, 755.9469, 756.4222, 762.8234, 769.8784, 772.0207, 775.7025, 780.1399, 781.6468, 782.6969, 787.4838, 790.3882, 795.4175, 796.1036, 797.0463, 801.9563, 803.2428, 806.8731, 809.4898, 813.2126, 819.3376, 820.7630, 823.8363, 824.7902, 826.3479, 829.9755, 831.6255, 836.5938, 838.1337, 840.8367, 842.7001, 845.5443, 848.5202, 852.4106, 857.3707, 858.8632, 861.9164, 874.0344, 952.3688, 978.2668, 1067.7391, 1088.9038, 1100.9573, 1122.3201, 1126.1363, 1129.2716, 1134.9713, 1138.8337, 1146.4901, 1151.3897, 1161.9613, 1167.9291, 1175.5772, 1177.7154, 1183.6426, 1185.8427, 1190.0483, 1202.5684, 1211.3111, 1216.4387, 1219.1759, 1221.8554, 1224.3861, 1226.4453, 1231.7187, 1234.6235, 1244.7436, 1249.4552, 1250.8637, 1254.3031, 1255.9787, 1260.8455,	-286.9834

		1267.7921, 1278.4504, 1284.1147, 1288.5669, 1298.2263, 1304.4212, 1334.8286, 1369.3492, 1371.1821, 1383.7749, 1395.9761, 1416.5519, 1425.1539, 1463.0324, 1467.1673, 1506.0785, 1515.0550, 2291.0292, 3010.8225, 3115.6500, 3161.9637, 3208.1420, 3222.9791, 3227.6708, 3272.2586	
T1-O1-ZeO-isobutyryl (ads)	240	48.7171, 49.5466, 53.3974, 58.1515, 70.3922, 79.9211, 80.3206, 85.2870, 89.2189, 96.9816, 98.8894, 108.7243, 114.0214, 118.2281, 124.4210, 128.0518, 134.9772, 137.0010, 143.0894, 147.1845, 153.4038, 158.3323, 161.1777, 164.5974, 171.4874, 172.8100, 176.9999, 179.2335, 180.7051, 183.9614, 186.3401, 187.9972, 190.5455, 195.8355, 198.6245, 201.0300, 205.3098, 208.1754, 209.4508, 214.7982, 216.7608, 218.5581, 224.4721, 225.6980, 227.6063, 232.6808, 236.7567, 237.9219, 239.3944, 241.1129, 244.8824, 249.6274, 253.9380, 254.8870, 256.4051, 257.9680, 258.9221, 261.9713, 262.4463, 264.1318, 267.1687, 272.7529, 274.2500, 276.1707, 279.6146, 281.4701, 284.2850, 288.5594, 292.4853, 297.5668, 299.0921, 300.0339, 302.6285, 308.6328, 310.5645, 311.5205, 313.3366, 318.5030, 319.3410, 320.2183, 325.8076, 329.2524, 331.0011, 332.3183, 339.8065, 346.4857, 348.6690, 352.8129, 361.3840, 366.1027, 368.6939, 375.6090, 379.4518, 386.7696, 389.2580, 393.8632, 394.1296, 405.9566, 413.0294, 419.6001, 421.6017, 422.6728, 427.6959, 429.8716, 435.2113, 445.9541, 452.2501, 457.7352, 465.2484, 477.2646, 487.1491, 491.2500, 501.3483, 505.6187, 509.9060, 514.2287, 522.7761, 533.8579, 551.3855, 559.6705, 568.6010, 569.0195, 586.9885, 599.2528, 606.9047, 610.9790, 624.5294, 642.6200, 657.6902, 675.1330, 694.2554, 699.6259, 703.3893, 704.2522, 704.7451, 714.7054, 719.0463, 724.5031, 728.7042, 733.1300, 738.3139, 739.0161, 749.9568, 754.4300, 761.2952, 764.5962, 771.4088, 771.9784, 775.7905, 779.4689, 780.8363, 786.8894, 789.6639, 793.3523, 795.8157, 796.7290, 800.1896, 805.7722, 807.1763, 810.2175, 810.7973, 815.5340, 818.1753, 822.1537, 824.7018, 829.8236, 831.8585, 834.4786, 840.2503, 840.6220, 844.7833, 845.4407, 847.7988, 849.7140, 851.0795, 856.2970, 860.4880, 861.6940, 875.0115, 887.6501, 962.8834, 985.9466, 991.0402, 1105.7209, 1115.1972, 1122.7488, 1126.5454, 1130.7237, 1135.2621, 1140.5857, 1147.1463, 1148.6247, 1153.0653, 1156.6598, 1171.8935, 1180.6687, 1188.2206, 1195.2901, 1197.8410, 1202.5931, 1204.6880, 1212.7803, 1216.2203, 1221.8994, 1224.4192, 1230.3077, 1232.0311, 1241.9154, 1247.1801, 1254.0382, 1255.2395, 1260.1146, 1264.0181, 1267.9479, 1276.9474, 1282.6020, 1286.4033, 1294.4758, 1313.1343, 1317.2647, 1337.3062, 1350.8861, 1370.7509, 1393.6139, 1399.5733, 1414.0286, 1421.9775, 1444.9972, 1501.4749, 1506.7691, 1519.0903, 1534.3452, 1978.4385, 3086.0091, 3102.4151, 3132.2063, 3172.5905, 3183.8816, 3193.6808, 3219.2145	None
T1-O2-ZeOH-C ₃ H ₆ (ads)	240	39.6062, 44.8732, 55.7005, 58.1755, 62.6165, 75.5816, 84.9469, 87.2696, 90.0367, 94.0775, 101.6999, 107.7290, 114.5144, 120.4215, 124.3853, 127.6608, 130.6483, 137.4492, 142.6834, 144.1092, 146.5560, 150.5842, 153.2993, 159.2710, 161.3648, 162.4377, 170.9393, 173.3948, 176.7462, 178.0112, 179.6286, 180.2867, 182.7647, 186.4574, 188.7722, 191.3184, 194.8945, 198.3782, 201.3993, 203.2029, 207.7161, 211.0510, 214.0217, 218.4363, 220.4511, 222.8903, 224.9114, 230.7578, 236.9945, 238.3581, 242.1075, 245.0663, 247.9662, 249.2430, 254.0395, 255.2422, 258.4772, 259.4574, 259.9844, 261.6901, 269.2691, 271.2436, 274.2093, 276.9514, 280.8728, 281.0913, 283.4084, 286.2022, 288.8382, 298.0722, 299.3091, 302.2270, 306.0498, 308.4671, 308.5933, 313.3717, 316.2025, 319.3493, 320.7913, 326.3321, 329.6332, 331.6524, 333.9803, 338.2587, 342.8994, 345.9888, 357.8460, 362.7471, 364.5973, 369.1067, 371.3930, 378.5896, 384.6138, 387.6527, 394.3621, 395.2250, 403.7733, 407.5526, 410.5268, 418.6898, 422.1229, 422.3256, 427.8843, 433.7798, 443.3033, 448.1758, 448.5519, 453.3427, 457.8833, 461.9981, 476.2176, 487.7478, 501.1920, 504.2516, 508.9282, 516.6952, 524.0821, 539.5576, 545.8470, 553.3187, 567.8314, 568.4584, 574.9312, 594.6837, 601.4143, 608.1609, 614.7765, 630.1516, 659.2162, 675.7184, 677.7412, 681.1394, 690.5024,	None

		703.4966, 707.4970, 707.6316, 712.9238, 717.0714, 720.1247, 722.0299, 725.9467, 736.3157, 738.8220, 748.5129, 755.3902, 759.8177, 765.4802, 768.0515, 771.0641, 773.8357, 775.3717, 779.1054, 780.7945, 787.6643, 788.8406, 793.7420, 795.3287, 803.4366, 803.6837, 805.2447, 810.2945, 811.5589, 814.7995, 821.0899, 822.3828, 824.5139, 829.8472, 831.4023, 834.1533, 836.2180, 837.0392, 840.1755, 843.6712, 849.0267, 852.9282, 855.5042, 855.8697, 859.9419, 862.6045, 870.4636, 880.3147, 944.8503, 970.6147, 990.7633, 1059.8331, 1090.1264, 1091.1027, 1100.8891, 1119.5890, 1120.5620, 1136.0466, 1139.0809, 1144.1600, 1150.6791, 1157.2814, 1169.3497, 1181.5079, 1185.0423, 1188.7582, 1197.1727, 1199.0360, 1204.5890, 1212.9103, 1215.2230, 1217.3028, 1217.9901, 1222.7688, 1231.2468, 1232.4618, 1235.6763, 1239.4226, 1245.9981, 1253.0904, 1257.2768, 1258.1914, 1263.3780, 1270.6975, 1283.7710, 1285.1829, 1288.0790, 1296.3684, 1316.2460, 1316.9931, 1339.1512, 1343.8470, 1370.5366, 1397.2285, 1416.4616, 1425.5530, 1460.2769, 1484.9206, 1507.4136, 1731.2249, 3062.1623, 3125.5738, 3182.3509, 3185.0979, 3214.7171, 3284.1137, 3474.9855	
T1-O2-Protonation-TS	240	-582.1658, 42.8966, 46.5998, 50.8048, 57.4223, 70.5066, 77.2281, 86.8887, 89.9064, 94.9518, 103.9660, 105.8902, 110.0059, 114.3496, 117.3234, 126.6392, 128.9695, 132.5964, 137.9305, 143.9720, 147.7255, 151.2427, 153.4794, 154.7190, 161.6520, 166.7302, 169.8985, 173.5233, 178.0827, 178.5421, 181.3444, 181.5966, 185.7645, 188.4733, 191.0252, 193.4056, 196.8601, 200.5013, 201.7189, 206.6599, 211.0613, 215.2256, 215.9724, 220.4513, 222.9452, 229.3518, 231.4468, 237.8907, 238.8755, 243.2011, 245.1756, 248.7264, 249.8202, 252.7618, 254.6852, 255.4129, 259.1036, 259.2549, 261.3675, 262.5286, 269.9832, 271.0806, 274.8029, 276.9022, 280.1188, 282.3062, 286.1664, 287.3292, 291.4666, 297.7757, 299.0960, 300.0533, 306.6622, 308.1848, 309.5948, 314.0526, 316.3545, 321.4576, 324.4166, 327.1911, 330.0764, 332.0663, 334.2898, 340.0863, 343.8577, 352.3123, 356.6966, 363.7574, 365.7708, 371.4048, 375.1290, 380.9969, 387.4009, 389.8938, 395.8622, 397.6530, 409.0690, 412.9367, 417.5412, 420.9845, 423.9362, 425.5567, 431.4918, 437.3627, 443.7986, 446.2490, 450.4511, 454.6497, 460.5022, 465.3513, 478.3371, 488.5425, 497.7514, 502.7195, 509.8335, 512.4950, 519.8111, 530.8455, 545.5048, 556.5565, 564.2602, 568.7886, 578.4301, 595.4765, 603.1682, 613.1338, 618.8383, 639.3389, 665.6532, 677.9485, 680.5972, 697.2076, 704.4657, 706.1755, 706.7280, 712.6887, 716.2748, 719.8620, 721.8579, 727.1141, 731.4221, 738.5991, 740.1651, 746.7444, 755.2318, 759.1006, 766.4294, 768.4115, 771.1138, 772.5198, 776.7838, 780.5170, 782.9736, 788.7496, 790.1163, 792.7877, 795.4698, 799.8624, 802.1601, 803.5811, 807.1343, 810.1310, 812.0421, 816.9031, 819.6603, 822.6575, 825.7885, 827.7425, 830.2668, 834.3776, 835.0751, 837.5527, 841.5861, 847.8922, 849.8893, 853.2809, 853.3452, 856.5215, 859.5120, 863.7413, 887.4604, 918.9871, 963.4304, 986.8962, 1061.7301, 1094.4128, 1106.7165, 1109.4462, 1118.0480, 1120.9160, 1134.7731, 1137.7555, 1146.5250, 1149.3595, 1151.1219, 1166.3966, 1179.7240, 1180.1099, 1188.8168, 1190.0499, 1196.1850, 1201.5423, 1205.7454, 1211.9363, 1217.1320, 1224.7781, 1228.3108, 1230.8641, 1231.6162, 1235.3638, 1241.0173, 1245.6682, 1248.2757, 1251.7782, 1256.8826, 1261.0257, 1266.8879, 1273.4820, 1280.6386, 1285.0650, 1291.8489, 1309.8543, 1319.2851, 1333.2020, 1348.2224, 1364.3232, 1369.1302, 1396.1551, 1406.1104, 1413.5794, 1429.8918, 1468.0640, 1507.1994, 1652.7372, 3046.8098, 3127.6463, 3158.6725, 3214.5987, 3233.7626, 3276.0195	-582.1658
T1-O2-ZeO-C ₃ H ₇ (ads)	240	28.3857, 41.4049, 58.3088, 67.9062, 73.6909, 89.6373, 92.8777, 100.1876, 111.7132, 116.8806, 120.0447, 123.0861, 125.4004, 135.9621, 138.5538, 144.0098, 145.4255, 149.4597, 156.4901, 159.0215, 167.9844, 169.5901, 171.0641, 172.8516, 175.9487, 179.1309, 182.0786, 182.6005, 184.1400, 186.6112, 189.4141, 195.2910, 196.7363, 197.8530, 202.6828, 205.8274, 210.6149, 214.5350, 217.0762, 222.0459, 222.4939, 225.4865, 227.8192, 230.6648,	None

		232.4899, 239.3775, 240.7359, 247.6074, 248.7481, 250.3637, 255.1333, 256.3040, 257.8371, 259.2289, 261.7124, 263.9882, 267.4696, 271.8198, 274.1674, 277.3663, 279.2132, 280.4297, 282.7009, 286.4294, 287.9035, 291.6755, 293.4374, 298.1157, 299.8009, 305.0172, 307.4305, 308.9458, 311.7864, 312.8467, 317.2488, 320.5719, 321.1759, 325.9593, 328.7763, 332.1721, 333.1092, 335.3015, 340.8670, 343.0177, 352.6279, 358.8973, 363.5048, 365.6804, 373.2370, 377.0670, 382.2835, 386.9604, 389.2635, 395.3530, 396.7513, 403.4180, 408.3374, 417.1885, 419.3896, 421.4668, 422.3663, 425.3174, 435.0368, 441.4211, 446.8225, 448.0159, 453.2334, 457.1084, 461.2148, 474.7048, 478.8874, 487.9992, 502.2962, 505.6848, 508.8053, 519.0114, 522.4275, 536.4570, 547.1505, 553.5401, 568.6859, 572.3974, 585.2755, 596.3107, 604.7742, 613.0527, 630.3117, 656.4414, 670.6560, 688.0086, 691.1307, 704.2930, 705.9781, 709.3217, 710.1782, 712.5923, 716.9721, 720.2981, 725.6329, 727.7840, 732.5531, 739.0883, 745.7436, 751.8837, 755.2265, 763.5125, 764.6113, 770.1499, 772.3958, 775.8937, 778.1363, 782.3703, 785.1432, 787.9444, 790.7691, 793.1303, 800.2051, 803.9713, 804.0248, 807.5187, 810.6275, 812.4434, 820.6353, 822.7084, 825.1615, 830.0567, 831.9654, 834.3902, 837.0705, 842.1479, 843.7331, 844.5334, 850.1383, 851.7574, 855.7285, 856.3739, 857.1080, 861.6108, 872.3192, 881.9350, 916.0115, 953.0027, 981.5430, 1072.9210, 1096.1312, 1123.2573, 1125.9465, 1129.3761, 1134.5573, 1136.5892, 1140.9066, 1151.4840, 1161.1783, 1169.0741, 1175.5653, 1183.8802, 1187.9856, 1191.8196, 1201.1853, 1202.1737, 1203.8994, 1210.8813, 1213.3312, 1216.9518, 1221.9644, 1227.8709, 1231.7220, 1233.8573, 1234.7985, 1241.6564, 1245.1682, 1253.5505, 1257.1816, 1262.6577, 1269.0180, 1272.9180, 1278.1545, 1288.2405, 1298.3895, 1300.9455, 1314.0144, 1321.0801, 1355.9921, 1385.5089, 1397.8615, 1420.0953, 1426.9103, 1454.0722, 1463.9667, 1488.1686, 1512.9709, 1525.9511, 1530.3336, 3095.7734, 3121.7199, 3171.7260, 3203.0847, 3203.9279, 3247.3609, 3261.7195	
T1-O2-ZeO-C ₃ H ₇ CO(ads)	246	25.8100, 35.8994, 39.3495, 53.7099, 61.6942, 64.4244, 74.4726, 76.1277, 80.9548, 91.2571, 93.1464, 95.3066, 105.1732, 105.7153, 115.4959, 118.6362, 120.6596, 126.7894, 130.6076, 135.6913, 142.6358, 144.5064, 151.7747, 155.7473, 158.0480, 164.3119, 168.8547, 169.8658, 175.0038, 176.5769, 178.7664, 180.4635, 183.0343, 183.3434, 188.3174, 191.2836, 193.5450, 197.5808, 202.3812, 205.4587, 206.6487, 208.8025, 213.3855, 215.1671, 218.1302, 219.9256, 222.7145, 224.9282, 227.1623, 229.5451, 231.6375, 239.1623, 240.8914, 244.8391, 248.6486, 251.2480, 252.6577, 256.3696, 258.4752, 260.2636, 261.4703, 263.7350, 264.8426, 270.3344, 274.1793, 276.6430, 278.4680, 281.0831, 281.5412, 284.5767, 286.8548, 289.9104, 292.3770, 298.5971, 300.4528, 303.4576, 306.8395, 309.3286, 311.0066, 314.4293, 317.1023, 321.2923, 322.6342, 326.5088, 331.6491, 332.0488, 333.9966, 340.6690, 344.4697, 349.5078, 357.5044, 364.2938, 364.7207, 371.0092, 377.8870, 379.8858, 386.3989, 388.4326, 393.9055, 396.1206, 403.2970, 408.0626, 413.0971, 416.8018, 422.6523, 422.8961, 428.0776, 436.7324, 444.6419, 449.2061, 451.9616, 455.0405, 461.4799, 470.5509, 474.8776, 485.8153, 488.5024, 497.2617, 504.9451, 508.3494, 513.5498, 521.6860, 530.6028, 545.2688, 552.1042, 560.5305, 568.4497, 574.3289, 593.8317, 601.8705, 610.6343, 630.7286, 657.1333, 674.9820, 687.6623, 691.4431, 704.8979, 707.4047, 709.5480, 710.6461, 714.2839, 716.4939, 719.3289, 725.1285, 730.8848, 739.2569, 745.4778, 751.6162, 753.7842, 757.1829, 764.8655, 768.9476, 771.0390, 772.6175, 774.0221, 777.7746, 779.5118, 785.5614, 788.4502, 790.9793, 791.3812, 799.6706, 802.0541, 804.8632, 807.1427, 809.9493, 812.1273, 820.9695, 822.3893, 825.8706, 829.7211, 834.6402, 837.6609, 838.9986, 840.9363, 843.4783, 843.7297, 847.6581, 850.0761, 853.5473, 856.6786, 859.1028, 863.1045, 871.3175, 882.3532, 914.8971, 948.5552, 966.5382, 1075.6050, 1097.1610, 1122.0984, 1123.3997, 1131.8160, 1132.8340, 1138.1457, 1143.7733, 1147.1686, 1157.5939, 1171.1774, 1179.7541, 1183.6226, 1188.6111, 1199.0110, 1200.2625, 1203.5552, 1204.4520, 1207.3378, 1207.7998,	None

		1211.4614, 1214.8885, 1219.1958, 1230.8595, 1233.0991, 1237.8512, 1239.8102, 1244.3541, 1245.8926, 1252.8568, 1261.9628, 1268.8766, 1273.5053, 1287.4383, 1288.3081, 1301.1777, 1311.8673, 1325.6081, 1330.1919, 1362.1202, 1376.7097, 1377.6716, 1418.3824, 1420.3328, 1436.3117, 1446.9073, 1491.8295, 1503.5389, 1504.8010, 1527.4918, 2228.8760, 3090.7283, 3125.4792, 3139.0245, 3162.6831, 3203.4287, 3251.9309, 3286.6421	
T1-O2-Carbonylation-TS	246	-81.8892, 47.0304, 48.5131, 63.2429, 66.0976, 75.4299, 77.5960, 78.7396, 88.3949, 96.8364, 97.6308, 104.0883, 109.9165, 117.7411, 122.2128, 126.6067, 130.5046, 131.4147, 133.4039, 135.3164, 142.0640, 148.8687, 150.9051, 152.3344, 156.2506, 159.3334, 164.2541, 168.2710, 171.7483, 175.4130, 176.5984, 182.0155, 183.6107, 183.9178, 185.7349, 188.8327, 194.8100, 195.3424, 199.8542, 202.8074, 205.8371, 207.6738, 213.3941, 216.6917, 219.9185, 221.3324, 223.8860, 227.2633, 231.6684, 234.0011, 238.5409, 241.1695, 243.6406, 245.7412, 250.4026, 254.0095, 254.5721, 258.6453, 259.7787, 261.9602, 262.5717, 266.2197, 269.9652, 272.8799, 275.4797, 280.9374, 281.9884, 282.5217, 286.3267, 289.2510, 293.3003, 294.9168, 299.6349, 303.6093, 306.7039, 308.6681, 309.7104, 314.5131, 318.2649, 318.9254, 321.3780, 322.6948, 328.1983, 329.5346, 333.5972, 338.9902, 343.7217, 347.7997, 348.1593, 351.6791, 354.3813, 357.6887, 366.1500, 366.9570, 371.8591, 377.4732, 382.7348, 387.5946, 388.0000, 391.3076, 395.7848, 400.2135, 412.6052, 415.1693, 418.7586, 422.9898, 425.6150, 428.7941, 434.0435, 435.1953, 442.0083, 443.0553, 449.6306, 454.0377, 461.3754, 464.4270, 478.1958, 489.2088, 504.9087, 507.5394, 509.5002, 517.5307, 524.3873, 545.4362, 546.9690, 562.5250, 572.3955, 575.3658, 596.5640, 600.0307, 613.4846, 617.4585, 634.9468, 662.3762, 674.8346, 677.1286, 679.1857, 703.3315, 703.8881, 704.8846, 707.0712, 712.6338, 716.5539, 721.7129, 728.0958, 728.9836, 738.0386, 742.1998, 743.4076, 754.5644, 756.4769, 766.3714, 769.9000, 771.4472, 773.0246, 774.6013, 779.5920, 780.3399, 784.0167, 786.2666, 790.2233, 790.8565, 792.9108, 797.3990, 800.7456, 802.4791, 805.0841, 809.1860, 811.9228, 813.8224, 819.9287, 820.6910, 824.4621, 827.2571, 829.3613, 832.8629, 835.9648, 837.9177, 843.4432, 850.9023, 851.1628, 853.3866, 855.4757, 856.9652, 860.7856, 874.4763, 948.0992, 979.0594, 1084.6677, 1091.5865, 1107.8335, 1114.9120, 1119.7893, 1125.1956, 1130.3368, 1131.0126, 1143.1331, 1145.6602, 1154.2303, 1164.7958, 1173.0067, 1178.3407, 1182.8575, 1188.5846, 1190.2078, 1192.6364, 1195.1166, 1205.7217, 1210.9288, 1217.8428, 1222.9359, 1229.9626, 1231.9618, 1232.9732, 1237.0018, 1240.1133, 1246.0954, 1250.7098, 1253.1031, 1258.2821, 1260.7634, 1265.6405, 1268.5153, 1274.3390, 1289.1445, 1303.1271, 1305.4326, 1319.2763, 1340.4050, 1347.7991, 1359.3739, 1386.6565, 1400.3138, 1412.9912, 1419.7902, 1432.5318, 1514.2756, 1538.0168, 2275.6653, 2918.2798, 3025.6114, 3164.7962, 3166.2898, 3213.6994, 3251.0665, 3254.5727	-181.8892
T1-O2-ZeO-isobutyryl (ads)	246	29.6023, 48.6335, 58.4543, 61.8898, 78.1230, 78.8497, 87.6122, 90.0564, 94.5385, 99.3439, 105.0116, 114.4312, 121.4459, 122.8453, 125.3841, 132.5877, 137.9803, 140.7479, 145.0465, 149.4720, 151.8906, 153.9100, 160.2847, 165.6406, 168.6370, 172.9196, 175.2555, 177.6116, 179.9693, 183.0782, 184.6202, 187.0279, 193.2585, 195.1985, 196.8293, 200.2800, 202.5487, 203.7981, 210.3620, 214.8196, 217.1555, 219.2924, 221.7623, 223.3662, 224.7649, 232.6032, 234.6435, 238.4783, 240.0458, 243.2932, 247.8865, 250.5242, 251.0249, 252.6164, 255.1323, 257.7066, 260.1902, 262.3044, 265.7560, 270.3654, 271.5068, 274.0722, 276.4450, 279.0148, 280.4297, 281.8439, 284.6664, 288.3301, 294.9510, 296.6440, 301.5011, 304.2435, 306.9318, 309.8107, 311.6508, 312.9534, 315.8894, 317.6304, 320.6893, 323.0647, 325.4329, 328.6440, 330.9027, 334.3889, 335.6804, 341.0143, 346.4566, 355.8850, 362.4638, 364.8496, 369.9405, 373.6180, 377.0286, 381.5724, 386.3091, 394.0048, 395.4357, 396.7291, 401.1108, 405.5703,	None

		414.7626, 417.2432, 421.4620, 425.2940, 426.1927, 434.7357, 441.7143, 445.7294, 450.6349, 455.8361, 460.7038, 468.0643, 474.4593, 483.1304, 491.0647, 502.1262, 507.1054, 511.9771, 519.2111, 529.5413, 545.0350, 553.2405, 566.6703, 569.0573, 577.1074, 595.8544, 602.0515, 604.7393, 613.7669, 621.4894, 656.3847, 663.2750, 678.9297, 683.9372, 690.4280, 703.4013, 704.1883, 705.5958, 709.0760, 714.1356, 720.2622, 720.9158, 721.8725, 726.1112, 735.1277, 738.3412, 747.3567, 756.1779, 757.4331, 762.0205, 768.1608, 770.8540, 772.9307, 776.1701, 781.3299, 783.8308, 787.2981, 789.7066, 793.6751, 799.3760, 801.4117, 802.6886, 805.1720, 811.0203, 812.6601, 815.1879, 821.2144, 823.9766, 826.7099, 830.2028, 831.5740, 832.9014, 837.3497, 840.4713, 843.4296, 844.8288, 847.3340, 853.0996, 854.1175, 855.5602, 858.2706, 858.5601, 861.9310, 873.6671, 897.1489, 960.9113, 985.5236, 1003.2003, 1091.8592, 1105.9072, 1114.0463, 1117.0771, 1132.4438, 1136.6238, 1140.7395, 1144.4859, 1145.0433, 1157.3308, 1169.6611, 1178.2681, 1179.6349, 1181.8453, 1188.0341, 1191.2961, 1196.8828, 1200.3912, 1209.9704, 1215.8523, 1218.3922, 1220.8158, 1228.2979, 1229.9555, 1234.5908, 1237.9864, 1246.8074, 1252.4753, 1253.3551, 1259.5888, 1264.3727, 1272.4453, 1273.5740, 1282.6431, 1289.4496, 1295.0108, 1313.1266, 1329.3220, 1330.4611, 1357.7552, 1369.7546, 1385.9385, 1399.0389, 1416.6996, 1432.2985, 1451.9187, 1509.0723, 1518.1934, 1524.7574, 1556.5476, 1973.0081, 3090.3248, 3128.6149, 3140.5509, 3171.3388, 3201.6843, 3222.5041, 3274.7557	
T2-O2-ZeOH-C ₃ H ₆ (ads)	240	39.7346, 43.6613, 48.5259, 59.6426, 65.5993, 74.5491, 78.5505, 88.1301, 94.1611, 96.8788, 97.5555, 105.7078, 117.4129, 119.1706, 122.7990, 125.0718, 129.1342, 132.0641, 140.3444, 143.4144, 146.3517, 148.6412, 152.8543, 155.0084, 160.7402, 167.3117, 171.4506, 175.2851, 178.7933, 180.4929, 183.2374, 185.3655, 185.8752, 186.9515, 193.2984, 195.7406, 198.4421, 200.1830, 203.9349, 205.6959, 210.2255, 211.7740, 216.3509, 217.7005, 226.2110, 229.6559, 233.5424, 236.6984, 239.4270, 243.1704, 245.3591, 248.3756, 250.5249, 252.0788, 253.5141, 258.2107, 260.0069, 261.3861, 263.1470, 265.2566, 268.0424, 272.4248, 274.0419, 276.3021, 277.6405, 280.2976, 283.1667, 288.0274, 293.7940, 295.6991, 297.2457, 302.0440, 302.7707, 307.3652, 310.6623, 312.7765, 318.4904, 320.6348, 326.0410, 329.0346, 331.0719, 332.3283, 336.8909, 341.4253, 343.1930, 349.6051, 355.3303, 363.5349, 365.6018, 367.7840, 370.5943, 374.5819, 376.1874, 386.0390, 392.1667, 392.7065, 396.3510, 398.5715, 411.9080, 420.6508, 421.3299, 422.5738, 429.9285, 435.0794, 444.5834, 450.9368, 452.5809, 454.5552, 456.8820, 464.5571, 481.4287, 491.0130, 497.2845, 502.6724, 505.8266, 517.8701, 523.0266, 534.6471, 544.9730, 546.3328, 566.4936, 568.0842, 572.7295, 595.8303, 603.9881, 607.7527, 613.9194, 629.7964, 658.5069, 664.9116, 670.3210, 674.8256, 687.3047, 697.0001, 700.7486, 703.1138, 708.9052, 711.8796, 717.0078, 721.8296, 728.5194, 736.8853, 737.7392, 743.5486, 747.6749, 765.4393, 767.3612, 769.3759, 772.6042, 773.7479, 779.3651, 781.6934, 783.0146, 786.2866, 789.7940, 793.8854, 795.8923, 799.8845, 804.0222, 804.4136, 808.1132, 813.0413, 815.7245, 820.2439, 820.9056, 825.4486, 828.7106, 833.5854, 835.3114, 838.0158, 839.3611, 841.7763, 845.8706, 850.6489, 852.0528, 853.5279, 857.7677, 860.6506, 863.6502, 867.0879, 878.2536, 941.8409, 971.8012, 1001.6557, 1068.5504, 1098.7320, 1106.8389, 1108.7041, 1111.8345, 1125.8327, 1128.4810, 1141.0752, 1144.0780, 1147.8229, 1159.3029, 1165.4386, 1178.3160, 1183.7737, 1186.8974, 1192.6787, 1199.0419, 1206.6360, 1208.2257, 1211.7533, 1216.6076, 1219.2402, 1221.3899, 1226.6699, 1231.7416, 1233.2733, 1239.2861, 1242.8565, 1246.5262, 1248.6977, 1257.2760, 1260.5546, 1271.1994, 1279.3779, 1282.9336, 1286.3298, 1290.5814, 1299.7058, 1324.0104, 1326.9355, 1353.5251, 1355.9035, 1380.9231, 1414.0557, 1433.5017, 1465.0118, 1497.3077, 1514.2810, 1739.9756, 3059.1751, 3120.0713, 3184.9200, 3188.6934, 3206.2165, 3282.8341, 3566.1227	None

T2-O2-Protonation-TS	240	-192.4224, 23.0642, 46.9376, 47.5418, 59.0945, 61.9607, 66.3058, 75.9263, 86.0088, 87.5838, 88.4884, 105.5548, 110.5600, 116.0422, 118.3850, 119.9441, 125.2461, 130.1776, 132.2742, 137.7567, 145.5842, 148.6202, 153.0769, 156.3516, 161.1174, 162.7919, 171.8614, 174.4139, 179.2150, 180.7530, 182.2790, 184.5527, 186.6672, 189.0529, 191.7405, 196.2020, 198.9389, 202.8964, 205.7103, 209.4748, 215.2167, 220.0132, 222.1134, 223.7633, 225.9991, 227.9449, 234.5909, 235.5191, 239.3128, 242.7912, 249.7095, 250.9211, 253.1050, 255.0929, 258.8687, 259.7476, 261.6979, 264.6606, 267.3828, 267.6383, 271.2654, 273.2432, 275.5297, 279.5627, 281.7497, 283.2369, 285.5859, 290.9427, 294.0546, 295.8651, 298.7770, 301.1021, 306.9387, 307.5795, 310.3038, 315.7204, 321.3431, 323.5105, 324.2479, 329.9489, 333.2898, 334.6408, 338.9331, 342.6387, 346.9013, 349.8901, 358.9697, 364.1479, 367.2272, 370.8514, 374.0747, 379.4134, 382.1412, 388.5658, 393.2498, 394.7522, 400.9728, 405.9480, 415.8355, 421.5072, 422.4433, 425.9553, 431.2703, 438.4404, 440.7054, 446.9743, 451.6214, 454.5024, 460.8884, 464.5618, 482.8370, 489.8804, 496.7062, 501.6953, 505.5713, 516.9791, 523.0575, 536.8005, 547.4481, 556.9906, 567.0639, 569.6574, 580.3148, 593.8392, 605.4417, 612.2808, 613.8544, 630.0940, 643.6590, 670.1989, 675.5627, 696.3379, 701.7586, 704.8552, 706.9741, 709.1885, 711.3051, 716.2435, 718.8653, 721.7868, 726.2619, 739.9198, 740.5291, 748.0827, 750.0001, 760.5650, 767.4647, 771.3576, 772.1159, 773.4297, 775.5378, 781.1950, 782.5558, 783.6777, 788.2833, 790.4266, 792.1736, 795.8590, 799.9646, 800.6657, 805.7778, 806.3183, 807.7930, 812.5840, 818.9451, 821.2004, 824.0438, 825.3420, 828.6385, 831.0014, 831.9452, 834.8024, 837.7662, 839.0099, 843.2666, 848.7697, 855.6484, 856.0650, 859.9577, 860.3224, 873.9717, 965.1898, 992.2759, 1018.4268, 1087.7728, 1099.6823, 1108.1279, 1110.2008, 1115.0216, 1129.8959, 1133.1102, 1140.5237, 1144.7271, 1146.7744, 1170.0923, 1175.4128, 1181.6335, 1186.8903, 1189.4874, 1192.4617, 1199.0025, 1207.4855, 1210.7471, 1212.0941, 1214.3227, 1221.4598, 1224.8599, 1227.7480, 1232.7647, 1238.3850, 1239.2863, 1239.8098, 1247.4866, 1253.9939, 1259.3163, 1263.1905, 1275.6338, 1281.1138, 1285.4905, 1289.1029, 1294.5522, 1301.7732, 1315.5090, 1326.6601, 1339.8580, 1357.3030, 1382.9671, 1395.9949, 1411.0437, 1445.5308, 1467.9178, 1500.9720, 1537.9904, 1724.4742, 3031.3147, 3135.9608, 3171.8585, 3190.0111, 3204.0463, 3279.8187	-192.4224
T2-O2-ZeO-C ₃ H ₇ (ads)	240	41.8639, 64.9630, 67.0994, 73.5659, 76.0503, 82.3402, 90.5669, 91.4612, 93.5079, 109.7009, 116.5030, 119.1872, 123.2453, 126.7641, 130.7771, 138.9669, 142.8832, 150.4167, 153.0039, 155.4958, 159.3496, 163.3134, 170.4228, 175.7846, 177.8757, 180.5958, 180.8958, 183.5169, 185.2551, 187.2781, 189.6940, 192.5909, 199.5149, 199.9908, 206.6004, 209.1461, 212.8052, 216.5194, 216.8175, 219.6353, 220.6629, 227.8403, 228.0900, 233.0204, 234.4989, 238.1717, 241.1075, 245.9656, 249.6671, 252.8693, 254.4373, 259.0799, 259.4138, 262.2001, 262.7046, 264.7534, 266.8966, 267.8946, 270.1755, 273.0515, 275.3347, 279.5112, 281.2511, 284.5546, 286.4542, 290.0190, 291.4363, 295.5255, 298.1040, 300.3027, 304.3699, 305.2667, 308.0493, 311.4463, 313.7019, 319.6767, 322.7655, 325.5942, 327.8129, 331.2523, 335.5972, 338.6986, 341.2675, 347.2794, 353.0984, 356.8059, 365.2378, 366.6581, 371.8677, 373.7441, 376.9433, 381.5345, 387.0109, 393.8243, 394.6116, 396.0798, 401.3066, 413.2360, 416.2406, 420.7014, 421.6278, 422.7986, 433.8940, 439.1260, 447.0036, 452.8559, 454.1054, 460.8962, 463.0819, 479.5844, 487.7849, 493.1464, 498.9828, 503.2200, 507.7189, 517.9674, 524.0135, 532.5739, 546.5728, 551.4521, 557.4325, 567.5639, 571.4880, 594.6593, 604.1550, 610.9308, 632.7818, 659.4295, 668.3095, 676.1357, 690.0483, 700.8762, 701.1895, 703.0601, 705.1671, 713.2990, 716.4774, 720.1204, 723.7762, 728.3911, 738.3697, 743.1691, 745.4010, 749.2915, 761.0989, 766.4727, 768.1108, 771.3491, 775.1878, 777.0778, 782.8142, 784.0185, 786.6117, 789.6241, 791.7566, 792.6687, 798.1634, 802.2544, 805.2198, 805.9459, 808.5829, 812.9421, 818.6541, 821.8836, 826.1108, 826.6288,	None

		830.1089, 833.0255, 834.5443, 838.7909, 840.2533, 840.7149, 847.6248, 848.8093, 854.3017, 857.8284, 860.3852, 867.6613, 870.1510, 872.7093, 919.5926, 953.9007, 979.8813, 1060.9921, 1106.6972, 1120.4166, 1128.4620, 1129.4083, 1132.9172, 1137.6128, 1144.1113, 1147.8658, 1158.2740, 1175.2060, 1178.7831, 1182.5352, 1192.8521, 1194.7122, 1196.4087, 1203.5135, 1204.6171, 1208.2609, 1209.4249, 1221.0414, 1224.3048, 1228.2737, 1230.4514, 1233.6337, 1241.4481, 1243.4905, 1249.0001, 1252.1677, 1256.3562, 1258.5894, 1266.1312, 1274.8432, 1286.2318, 1286.8059, 1295.7751, 1301.4585, 1314.9024, 1330.4101, 1353.1543, 1361.6797, 1387.4065, 1412.5577, 1418.1819, 1435.1743, 1467.8975, 1483.8105, 1509.3759, 1512.9015, 1526.2591, 3094.2894, 3101.6870, 3175.3020, 3180.5175, 3212.7274, 3228.0117, 3246.8994	
T2-O2-ZeO-C ₃ H ₇ CO(ads)	246	22.6826, 32.3113, 41.8211, 46.9760, 59.8152, 63.4601, 67.7397, 69.3332, 73.7671, 83.3762, 90.7310, 91.6046, 93.6913, 106.0114, 109.9368, 114.7089, 115.2643, 122.9074, 125.4855, 130.1916, 136.2869, 142.0492, 147.5870, 153.0356, 154.6383, 158.0237, 164.6243, 165.9741, 172.1026, 175.2415, 177.0582, 182.1371, 182.8061, 185.6381, 187.1874, 190.4045, 192.9174, 197.0403, 199.4216, 204.9580, 206.5052, 209.4045, 210.2511, 215.9844, 217.1404, 219.2746, 222.1364, 223.6427, 227.3133, 228.8517, 233.8239, 239.0958, 240.4587, 248.1825, 249.2173, 252.5110, 254.3758, 255.4854, 259.6965, 260.5691, 262.3364, 265.6183, 266.3675, 268.8073, 270.3507, 273.1586, 278.0964, 279.7033, 283.8628, 286.6898, 289.1762, 292.2283, 297.4690, 298.1681, 300.2007, 301.7405, 305.6244, 308.3166, 314.4926, 316.0256, 319.7987, 323.2015, 325.7753, 328.1947, 330.0840, 333.2677, 339.0572, 341.2953, 347.1532, 350.9563, 360.9380, 365.8453, 367.0653, 370.7948, 374.0254, 375.4009, 379.3363, 386.8330, 393.6932, 395.4105, 397.7150, 404.0756, 412.3173, 414.4490, 422.6283, 423.9831, 425.1413, 439.8965, 443.1588, 448.3199, 451.4706, 454.6862, 460.0715, 468.9786, 474.1119, 478.2461, 489.6684, 496.4846, 503.0031, 507.0801, 517.8729, 521.7504, 534.4080, 545.6449, 552.5088, 567.6950, 570.0199, 582.6225, 592.8899, 604.7583, 609.3736, 637.0155, 655.7847, 671.2417, 680.5634, 688.1471, 700.1284, 701.7490, 702.6918, 705.6143, 713.3374, 714.8309, 717.0770, 722.8328, 728.4267, 737.9183, 741.9590, 746.4130, 749.3414, 760.1018, 767.1163, 768.2069, 769.6543, 770.8380, 774.4348, 777.8075, 781.2664, 784.1441, 786.7919, 790.2472, 791.4940, 798.1223, 800.5979, 803.9884, 806.2896, 807.5301, 811.6260, 818.9125, 821.3662, 822.3770, 824.8258, 829.3436, 831.5303, 835.7933, 838.9345, 839.3339, 841.4438, 847.2561, 848.4893, 853.3432, 857.8365, 860.9543, 867.5771, 872.2688, 876.4861, 923.4441, 953.4211, 959.8083, 1062.9701, 1101.7697, 1116.4697, 1121.6978, 1126.4619, 1129.8858, 1135.9424, 1144.3400, 1149.0499, 1151.8556, 1172.4296, 1174.7386, 1185.1038, 1187.4627, 1192.7287, 1193.7469, 1198.6776, 1205.8690, 1210.6548, 1212.0618, 1213.9784, 1219.2043, 1225.9914, 1226.9805, 1230.6315, 1238.5794, 1244.9846, 1246.6107, 1251.7096, 1253.4716, 1257.5858, 1263.5297, 1277.2280, 1284.6666, 1286.3995, 1299.3203, 1302.5024, 1328.4191, 1329.9869, 1358.6244, 1359.6579, 1370.4389, 1412.5453, 1433.3212, 1441.1490, 1451.9394, 1492.6981, 1502.6541, 1509.3670, 1526.7345, 2239.6330, 3091.7669, 3121.1047, 3142.4453, 3165.7892, 3198.4947, 3234.7529, 3261.9886	None
T2-O2-Carbonylation-TS	246	-115.4234, 48.9500, 54.3713, 65.2445, 69.8966, 73.2659, 77.2446, 81.5267, 90.9192, 93.1873, 95.4736, 104.2856, 105.5324, 119.0816, 122.2806, 124.8164, 130.3457, 133.3054, 136.5093, 139.3945, 145.2677, 151.2127, 152.3625, 156.0014, 156.9840, 160.8497, 166.4657, 169.3288, 174.1363, 176.0096, 179.1649, 182.2887, 185.7467, 187.1624, 187.6377, 189.8904, 196.8072, 198.5775, 201.2120, 203.3024, 205.1443, 208.0774, 213.4767, 219.2635, 220.5283, 223.5481, 228.4476, 231.8443, 233.7914, 238.8802, 244.3172, 245.2381, 247.4713, 249.9569, 254.3806, 256.1803, 259.2865, 261.3320, 263.6505, 265.8839, 267.3852, 269.3230, 272.0741, 275.1849, 279.7806, 280.8410, 283.0342,	-115.4234

		284.3062, 287.2114, 291.6453, 296.8144, 301.0460, 301.7492, 306.1068, 307.0532, 309.3976, 312.8451, 316.3185, 318.3762, 322.2776, 323.9008, 327.4096, 331.7625, 334.7482, 339.1951, 341.2740, 343.3104, 345.3185, 351.8986, 357.3934, 360.0735, 365.1852, 367.8759, 370.1532, 374.7924, 380.2504, 384.9988, 386.1488, 389.2508, 394.7603, 395.8263, 401.2729, 409.1619, 411.8258, 416.4641, 421.5499, 424.2046, 426.0942, 433.3051, 435.8923, 441.6633, 447.4085, 451.9624, 455.0272, 464.0320, 469.1424, 482.8897, 493.4602, 501.2015, 503.7772, 506.4180, 517.3259, 524.7899, 539.4127, 548.5875, 564.4084, 568.8850, 574.8938, 592.2957, 600.3969, 612.2173, 617.6092, 633.3832, 644.8108, 656.8357, 673.2484, 676.4268, 691.0097, 699.1364, 704.0759, 706.6590, 713.7897, 717.7792, 721.3602, 727.5038, 729.2465, 739.6718, 742.9649, 744.6547, 749.8178, 759.7893, 764.5802, 767.7281, 769.1664, 773.2964, 775.3059, 777.4136, 778.8117, 784.4124, 785.7801, 788.0125, 790.3460, 793.3705, 795.0464, 797.8531, 800.6114, 803.6422, 807.1236, 807.6677, 808.8607, 811.7277, 819.6513, 822.6277, 823.1780, 827.5426, 829.0933, 831.6535, 837.6981, 841.2859, 843.3410, 843.9288, 852.1113, 854.2367, 854.6843, 858.2761, 873.9072, 941.8653, 983.3699, 1056.3298, 1092.8730, 1107.1166, 1111.3456, 1119.5377, 1124.8514, 1129.6980, 1130.7738, 1146.6158, 1147.9314, 1165.0466, 1167.2751, 1178.9249, 1181.6497, 1184.8713, 1187.5884, 1190.8353, 1192.1477, 1196.5126, 1208.5322, 1212.8371, 1216.4507, 1217.3607, 1222.2330, 1229.3877, 1231.4605, 1235.1677, 1238.2788, 1241.2248, 1244.2278, 1246.8983, 1257.4552, 1257.9236, 1267.1847, 1270.6523, 1274.2082, 1283.5262, 1292.0677, 1293.2289, 1312.4598, 1335.0109, 1345.1479, 1353.3215, 1387.7908, 1391.3960, 1410.7018, 1429.1078, 1447.6035, 1519.7499, 1540.8173, 2273.7942, 2803.3039, 3106.7872, 3148.6843, 3178.6049, 3190.7664, 3244.6461, 3246.6095	
T2-O2-ZeO-isobutyryl (ads)	246	41.6767, 48.5619, 54.9896, 63.9232, 67.9898, 75.7737, 83.6628, 90.8173, 91.8322, 105.3150, 111.2137, 116.1750, 119.8493, 121.6678, 125.2415, 127.7274, 134.5633, 139.7629, 141.3332, 143.9562, 152.1808, 152.7064, 158.1845, 160.4765, 162.6531, 166.3046, 173.7823, 176.2070, 180.4761, 182.4210, 183.6456, 184.9320, 187.1649, 188.7230, 195.1118, 198.2947, 202.3217, 203.2540, 206.1376, 208.5634, 215.6867, 216.7282, 217.7967, 222.1912, 223.9639, 227.7264, 236.0215, 238.1561, 239.9787, 241.6336, 246.1092, 248.5495, 250.9622, 252.6087, 254.4928, 257.9305, 259.5244, 261.2748, 264.8244, 267.4203, 271.9119, 273.2979, 273.8011, 276.4007, 280.3671, 283.2427, 285.8369, 288.3900, 290.2820, 295.6207, 298.4189, 300.9879, 305.2907, 307.0615, 309.3589, 311.2903, 315.3486, 320.6992, 324.7230, 327.5156, 328.5505, 331.5219, 333.1088, 338.6665, 346.3091, 349.7865, 350.4047, 359.8342, 366.0724, 366.6943, 369.2132, 370.8526, 374.0935, 380.4328, 384.3310, 387.3617, 390.6114, 394.3387, 395.8636, 400.8384, 413.4248, 420.0502, 422.5478, 422.9065, 428.5165, 435.4300, 444.9925, 448.2276, 450.5256, 455.9049, 459.6442, 477.8413, 487.2383, 491.5968, 495.1354, 502.3266, 512.8742, 518.5336, 524.3248, 537.7729, 543.7857, 555.1724, 562.7617, 567.0790, 569.6468, 574.5949, 594.0983, 603.5509, 611.7806, 624.3933, 632.0205, 654.2234, 669.3860, 673.6592, 689.4674, 703.3208, 703.9940, 706.4860, 707.7478, 710.2490, 713.3529, 718.2569, 723.2905, 726.6399, 738.4910, 741.1346, 749.6339, 751.2719, 768.7267, 771.1445, 773.0110, 774.2362, 775.1676, 780.2467, 782.4008, 784.1374, 787.2964, 792.9560, 793.2001, 796.2046, 801.4293, 803.3867, 805.7766, 807.9075, 808.5332, 813.1194, 818.7408, 820.4424, 823.7280, 827.0857, 830.4597, 832.3794, 834.7226, 837.9801, 838.5878, 841.1323, 845.9044, 848.8450, 851.1349, 854.7038, 859.0926, 862.6448, 864.8464, 877.6145, 892.9124, 971.8783, 987.8805, 995.9718, 1106.8170, 1115.5541, 1116.4581, 1128.0949, 1130.5312, 1145.1402, 1146.6035, 1148.9555, 1152.2374, 1156.5367, 1165.4988, 1178.5382, 1182.4459, 1189.8515, 1193.3830, 1195.6667, 1205.4223, 1206.0997, 1210.8951, 1212.2653, 1220.6840, 1224.3238, 1229.0120, 1231.3405, 1234.7284, 1242.3656, 1245.2812, 1247.3415,	None

		1252.6474, 1259.5835, 1261.2170, 1273.5853, 1282.2668, 1284.1694, 1292.5055, 1299.9276, 1308.4552, 1323.2766, 1329.6074, 1354.4008, 1360.2904, 1372.8632, 1378.1119, 1414.1311, 1424.4105, 1451.4353, 1512.6302, 1521.2780, 1527.6075, 1544.6405, 1981.1368, 3096.5378, 3102.9880, 3165.8103, 3174.5045, 3193.9072, 3212.7716, 3229.8903	
T2-O6-ZeOH-C ₃ H ₆ (ads)	162	32.4922, 35.7573, 41.0470, 59.2030, 75.6376, 80.1039, 91.0434, 103.0464, 113.3231, 114.0895, 120.7283, 122.9864, 131.4430, 137.4465, 143.2079, 144.2920, 157.2922, 164.7450, 168.8261, 170.8490, 174.3513, 177.3380, 180.9625, 190.9885, 196.4522, 215.1523, 223.8027, 228.7114, 233.2306, 239.7588, 248.3011, 251.9557, 255.5723, 264.1429, 276.4565, 276.7233, 282.1766, 289.3998, 295.7019, 300.8219, 307.9880, 309.7431, 311.4433, 315.0569, 319.5637, 324.9009, 328.0073, 330.6127, 333.7479, 340.5815, 347.1684, 359.0731, 372.1630, 387.4939, 396.7575, 399.3010, 419.5477, 432.2114, 435.0950, 437.3873, 444.9217, 445.7046, 450.1440, 456.9270, 467.9710, 488.9204, 523.2429, 562.6492, 572.3457, 585.1274, 586.8637, 608.0975, 610.8213, 623.5629, 645.5356, 661.5642, 674.6928, 687.4862, 688.7232, 690.3618, 696.0342, 701.8821, 707.1448, 710.2329, 715.5983, 720.1352, 724.0751, 729.7920, 734.1203, 737.4242, 749.0312, 749.4940, 755.7450, 757.2639, 761.8198, 770.9748, 781.8235, 784.8817, 789.2715, 797.8608, 806.0940, 815.1609, 817.0507, 819.7474, 828.2310, 834.5152, 840.5822, 842.2686, 846.1823, 850.1794, 853.1284, 877.1062, 878.2951, 881.3707, 883.2692, 897.9228, 938.0483, 967.7673, 986.9350, 1019.0253, 1050.5084, 1091.6429, 1141.4019, 1144.4141, 1152.0585, 1167.1004, 1178.3948, 1192.8631, 1194.0274, 1200.4989, 1206.1666, 1215.2086, 1216.7646, 1225.4404, 1229.0767, 1231.1167, 1248.2662, 1252.4387, 1266.4250, 1283.9153, 1295.2915, 1319.5777, 1342.8744, 1349.1649, 1353.2649, 1372.5434, 1420.8726, 1457.8214, 1492.9482, 1514.8552, 1735.6730, 2219.6345, 2221.6345, 2221.7996, 2235.2250, 3068.8604, 3140.1398, 3171.3919, 3185.8031, 3228.1534, 3246.6123, 3290.8460	None
T2-O6-Protonation-TS	162	-132.4876, 38.3951, 49.7785, 51.9057, 79.4313, 85.8462, 87.9360, 92.2484, 103.3409, 117.3741, 125.4109, 130.0086, 132.9252, 136.6120, 147.7036, 157.6834, 159.2849, 163.6812, 168.7928, 169.2361, 175.1325, 182.3147, 184.0785, 191.4276, 194.9469, 198.3904, 208.4661, 226.3057, 236.3446, 238.7041, 243.2008, 248.9585, 262.9520, 268.0794, 272.9328, 278.2236, 284.2874, 292.2278, 298.1499, 304.4600, 309.7183, 311.0948, 316.0336, 317.6738, 323.4817, 329.1439, 330.9445, 335.6223, 339.2443, 348.3473, 360.3242, 363.5181, 367.9451, 385.3954, 396.5326, 401.4618, 404.9700, 425.8513, 429.3664, 432.6311, 436.8500, 441.3084, 451.3845, 454.9684, 460.5717, 467.3034, 493.4571, 519.1353, 544.0875, 556.6316, 569.7845, 585.1645, 587.6549, 609.7243, 626.7732, 641.3218, 650.9443, 671.9938, 687.6006, 691.8773, 695.1819, 701.7758, 707.0931, 713.4467, 718.0890, 718.2371, 723.3805, 724.6123, 734.3253, 737.2599, 748.1142, 748.7126, 754.7666, 755.8442, 760.1765, 770.1601, 774.8447, 777.5109, 782.7032, 794.4513, 798.7102, 803.0370, 811.0761, 813.7683, 816.4917, 820.0079, 831.2760, 835.2446, 839.1146, 844.6235, 849.5054, 864.7816, 868.2908, 872.6944, 877.5052, 880.4139, 894.6910, 924.3821, 972.1251, 1107.1774, 1125.0857, 1128.2604, 1132.1137, 1146.3200, 1156.6203, 1173.3971, 1176.7725, 1185.2337, 1187.1340, 1202.6220, 1209.1525, 1212.0784, 1219.9812, 1226.2939, 1230.0067, 1232.1428, 1238.4899, 1244.5130, 1262.7624, 1282.1427, 1296.6086, 1318.1726, 1330.0556, 1337.0597, 1354.6556, 1365.2427, 1373.4283, 1415.5616, 1455.7751, 1501.7323, 1588.4272, 2220.5216, 2222.3223, 2222.9761, 2236.2332, 2268.5915, 3041.3074, 3106.9039, 3153.4889, 3204.0246, 3251.1253, 3263.1405	-132.4876
T2-O6-ZeO-C ₃ H ₇ (ads)	162	36.3388, 49.0742, 70.6070, 78.1121, 84.5774, 113.6164, 117.8123, 124.2439, 127.6426, 134.5478, 137.0391, 150.7493, 154.0575, 156.4019, 162.8512, 167.3285, 170.2099, 173.7975, 176.8151, 177.9816, 199.2992, 200.4892,	None

		216.6991, 219.6597, 221.9592, 225.7539, 237.0522, 244.6085, 245.3335, 254.2835, 259.2682, 274.8172, 278.5754, 285.9611, 287.6206, 293.9297, 300.8791, 301.9529, 305.5361, 309.9691, 315.0859, 317.2250, 318.9578, 325.6497, 331.5352, 334.7904, 336.1695, 342.5103, 353.8379, 355.6210, 360.6829, 370.1344, 392.9560, 396.6470, 397.1796, 421.4582, 432.2363, 436.6748, 438.7341, 440.8585, 442.0738, 448.5987, 461.4149, 466.9937, 481.3340, 490.7526, 520.8289, 567.5681, 571.2111, 583.8980, 590.7324, 602.3823, 610.4644, 629.1838, 636.3145, 682.0866, 688.7197, 693.1928, 697.4148, 700.9188, 705.7328, 718.2956, 722.0105, 724.3904, 725.6749, 731.0543, 733.9442, 735.0735, 737.5329, 746.1628, 749.1891, 755.7107, 757.0354, 763.0037, 771.4242, 776.3171, 789.6845, 796.2515, 799.7505, 806.9370, 811.0596, 817.2196, 817.6576, 821.0491, 829.2763, 831.7743, 835.4023, 840.5940, 845.0126, 853.2462, 863.9414, 875.7380, 880.1774, 880.6854, 896.1000, 911.6257, 957.3915, 968.4408, 974.4215, 1128.5512, 1140.9795, 1148.6889, 1150.2936, 1157.0316, 1161.4551, 1177.0361, 1189.5518, 1192.4223, 1207.5258, 1214.5088, 1216.6576, 1225.4029, 1232.2970, 1235.0054, 1243.8280, 1252.5346, 1261.6024, 1278.8179, 1290.4179, 1298.5041, 1323.2629, 1344.4434, 1371.4929, 1389.0555, 1432.8211, 1441.1930, 1490.8956, 1504.6153, 1509.2451, 1518.9086, 1532.8864, 2220.1410, 2221.6022, 2222.2331, 2235.1323, 3089.6679, 3095.7780, 3171.4765, 3174.9770, 3207.6198, 3229.2230, 3246.9396	
T2-O6-ZeO-C ₃ H ₇ CO(ads)	168	43.4816, 53.2072, 59.0615, 64.0694, 65.9300, 73.4723, 80.0488, 88.5087, 109.6460, 116.8923, 122.7796, 132.0156, 135.4416, 138.6120, 147.7021, 156.1521, 160.1542, 161.1916, 162.4506, 167.4571, 173.0390, 177.6244, 181.2799, 182.0974, 199.5526, 203.8607, 211.9713, 213.0642, 220.2491, 230.4013, 236.0578, 251.0456, 255.2260, 257.8579, 258.1128, 263.2092, 277.5735, 277.9360, 288.4730, 292.4827, 297.8029, 301.8827, 308.3844, 311.8092, 312.3818, 316.9951, 318.9055, 325.9856, 327.8898, 329.5810, 335.2606, 338.1215, 345.5276, 353.0943, 355.8591, 364.9668, 371.5903, 389.7823, 396.4161, 402.5927, 423.7953, 435.7184, 436.5251, 438.9142, 443.6814, 446.3442, 447.7386, 463.0759, 467.8995, 487.9429, 513.6832, 522.2085, 554.0513, 567.5182, 585.3548, 587.3562, 592.0443, 610.2378, 628.5657, 641.4719, 688.4458, 689.9574, 693.9096, 700.6941, 707.4773, 713.6257, 718.0440, 723.0851, 723.8807, 726.1604, 727.0494, 731.5599, 734.8556, 737.8879, 749.6589, 755.0075, 756.0165, 756.8081, 758.4547, 771.7231, 781.4382, 789.9785, 794.8609, 799.4994, 806.3608, 815.4953, 816.7999, 817.1038, 825.8240, 831.2277, 833.6083, 837.4608, 840.2377, 843.4195, 851.9797, 860.1697, 874.5124, 878.9762, 881.0056, 897.5003, 911.3803, 957.6925, 976.9359, 993.5247, 1129.4568, 1139.3041, 1146.6144, 1153.9221, 1167.4957, 1173.1511, 1179.8928, 1189.4354, 1193.8158, 1215.9207, 1216.8173, 1220.0073, 1225.3866, 1231.2974, 1237.9584, 1238.6105, 1250.9192, 1253.9657, 1264.5601, 1298.4198, 1305.9314, 1330.0259, 1341.5592, 1386.1593, 1397.5044, 1435.8168, 1440.2982, 1477.2100, 1498.6743, 1512.2427, 1528.1651, 1530.9094, 2219.7341, 2221.9289, 2222.0183, 2235.1694, 2254.7245, 3098.0026, 3101.0080, 3179.2175, 3183.6684, 3187.3150, 3208.3304, 3251.2418	None
T2-O6-Carbonylation-TS	168	-117.4396, 50.2130, 61.2208, 68.8678, 76.0416, 80.3893, 84.9159, 90.5575, 93.4277, 104.8171, 110.7076, 117.6223, 118.0176, 133.6506, 137.7902, 142.4349, 150.5740, 158.4562, 161.4565, 164.2481, 165.8206, 168.3527, 176.0411, 176.5431, 184.4491, 189.0566, 196.1042, 198.2418, 205.8197, 212.4756, 227.1084, 236.3855, 244.4152, 247.1736, 256.1703, 261.7537, 268.1636, 271.6283, 276.5682, 279.3844, 285.8211, 295.2940, 297.0580, 304.2262, 306.4190, 309.5890, 315.1296, 319.0487, 323.2655, 325.7423, 329.5654, 332.3293, 340.8880, 349.3002, 351.4779, 360.6820, 361.2536, 378.3274, 397.1739, 402.3856, 411.3923, 416.4926, 424.7111, 428.6941, 432.9513, 439.9704, 447.1423, 448.8229, 457.1822, 463.8263, 469.3119, 500.9960, 516.7200, 552.8325, 567.0010, 585.0479, 587.6295, 610.6017, 624.5284, 642.3557, 660.0809, 671.4600, 687.3365, 688.7985, 693.3293, 698.9036, 702.8350, 710.5797, 714.2958,	-117.4396

		717.1875, 718.1215, 722.9914, 724.2298, 734.1768, 737.5916, 743.1371, 748.9796, 753.7162, 754.0959, 756.7396, 759.4025, 769.9650, 772.6293, 776.6471, 782.4628, 794.4981, 801.7913, 808.1110, 809.7839, 813.4230, 816.1654, 823.4510, 831.5360, 834.2525, 841.3052, 844.5333, 850.2459, 860.8598, 869.9692, 873.6688, 875.6278, 892.7648, 937.2291, 987.3530, 1119.4241, 1122.9232, 1130.2197, 1140.0628, 1154.2814, 1161.1168, 1165.6205, 1171.8861, 1178.7532, 1186.5194, 1205.3790, 1207.6915, 1215.5547, 1218.2769, 1225.3390, 1238.8679, 1240.5496, 1252.9211, 1257.9511, 1272.3417, 1282.7951, 1307.9915, 1326.5085, 1329.0850, 1343.8850, 1366.7442, 1371.4130, 1395.8556, 1440.7788, 1450.0065, 1522.0802, 1534.8282, 2219.8668, 2222.4210, 2223.0999, 2236.6849, 2301.1617, 2855.9311, 2980.8891, 3124.7672, 3161.9405, 3204.0641, 3242.5031, 3269.4994	
T2-O6-ZeO-isobutyryl (ads)	168	48.0439, 57.8422, 67.3695, 73.1455, 86.3668, 89.8663, 107.7362, 117.6256, 120.7480, 125.2777, 137.3339, 142.9979, 148.5927, 151.9147, 156.9672, 164.1461, 167.4058, 168.4149, 173.2788, 183.9070, 185.6383, 197.0493, 204.4489, 208.2322, 223.1058, 234.8559, 237.3176, 240.7683, 245.6451, 248.1329, 257.1046, 262.1291, 265.4906, 270.2523, 276.5494, 281.4970, 287.0981, 293.0662, 295.1660, 299.4787, 303.9210, 310.2100, 311.2326, 313.3170, 316.7030, 322.0186, 326.0102, 328.8329, 336.8255, 341.6411, 345.4342, 349.4382, 356.9274, 363.2768, 384.2511, 394.5330, 396.1631, 402.6844, 410.5201, 427.5919, 428.2365, 433.5685, 437.7713, 451.7977, 454.5950, 465.5036, 467.9049, 489.2063, 516.1640, 529.1270, 552.6212, 557.4347, 573.8496, 583.2480, 585.6175, 603.8394, 608.7848, 642.2223, 657.2183, 668.6891, 685.7266, 688.2786, 690.2999, 698.5112, 705.9190, 710.3437, 711.7834, 715.0369, 720.2100, 721.1376, 723.9859, 734.0375, 737.3686, 748.9014, 753.1270, 755.3711, 757.0914, 762.6192, 770.8647, 778.5891, 780.7959, 785.0096, 798.1951, 805.8349, 807.0602, 813.2306, 816.2106, 826.0609, 835.3811, 838.6955, 842.9123, 847.1753, 850.4088, 852.1366, 855.1489, 865.2183, 875.7444, 879.6424, 881.9480, 897.1812, 951.8607, 959.2905, 990.9438, 1005.1010, 1126.0671, 1132.9367, 1141.3606, 1146.0771, 1152.7407, 1171.2192, 1172.5840, 1179.4895, 1182.9214, 1189.2095, 1192.9184, 1211.1244, 1215.2518, 1224.6317, 1228.3190, 1231.2553, 1242.2169, 1242.9552, 1253.5407, 1288.4406, 1294.0592, 1304.4882, 1334.0165, 1336.1231, 1364.3345, 1368.0193, 1429.2046, 1459.6844, 1499.1977, 1515.7460, 1526.3227, 1535.2527, 2019.6536, 2219.5271, 2221.8963, 2221.9799, 2235.5545, 3082.0890, 3084.8937, 3106.5071, 3174.1965, 3181.5954, 3184.1625, 3241.0534	None
T3-O1-ZeOH-C ₃ H ₆ (ads)	234	25.1870, 43.1086, 51.8350, 66.6431, 74.5747, 81.2353, 91.3733, 97.5395, 99.9499, 104.5142, 106.8329, 108.5150, 113.4270, 117.3348, 121.1044, 126.9620, 128.9700, 137.7005, 141.4646, 144.2818, 151.6714, 156.0264, 159.9104, 162.1537, 169.4984, 172.7346, 175.2304, 177.4197, 178.6901, 180.0771, 181.2897, 187.3323, 188.3691, 193.3372, 197.1970, 199.0896, 201.7340, 204.9814, 207.5965, 210.2160, 212.3479, 213.2389, 218.5916, 222.5416, 224.0157, 232.6684, 234.8475, 237.8251, 240.6600, 243.6041, 246.6954, 250.9058, 251.5850, 255.3636, 258.2040, 259.2829, 264.0557, 264.7922, 269.9311, 271.2886, 271.8394, 273.6527, 276.0633, 282.4348, 283.1126, 286.0092, 289.6504, 293.8790, 296.7763, 297.4801, 301.4085, 302.1351, 310.7957, 312.8884, 313.5343, 315.9313, 319.6262, 323.8367, 325.1294, 329.1901, 331.3710, 335.0198, 340.5439, 343.3835, 348.2733, 357.4721, 363.1158, 367.9677, 370.0456, 375.7378, 384.9487, 386.2816, 387.3686, 392.9160, 402.3517, 410.0048, 414.4710, 420.8482, 422.2513, 425.7074, 433.8517, 436.8352, 438.1323, 443.5806, 453.2858, 454.1374, 457.0257, 468.1473, 487.0599, 492.0684, 499.3006, 500.5520, 515.5401, 519.4660, 535.7527, 550.5450, 562.2408, 568.3886, 569.3567, 583.1355, 594.0789, 605.5948, 610.8871, 613.7642, 614.6756, 647.9445, 660.5930, 676.1032, 678.1785, 693.3551, 697.9275, 700.8457, 702.1363, 716.5134, 719.7096, 724.4999, 734.2267, 738.3800, 740.9581, 750.0759, 757.3300, 761.3226, 765.5718, 771.6841, 771.7859, 777.3095, 778.4226, 782.0762, 787.7029, 788.6581, 791.4558, 794.5726, 796.0186, 800.7197, 801.8412,	None

		806.3424, 809.6630, 811.2294, 812.6790, 818.7578, 821.2783, 824.7788, 827.5394, 829.2907, 830.3490, 831.2726, 833.6699, 839.7011, 843.3054, 844.0994, 845.2324, 850.5049, 857.7180, 860.6501, 864.5295, 876.8943, 941.7674, 961.9924, 986.4568, 1053.9455, 1092.7948, 1098.2629, 1121.8435, 1129.6287, 1131.7491, 1131.9399, 1137.4218, 1139.5870, 1152.7390, 1157.0684, 1163.7417, 1179.4739, 1184.7735, 1191.4883, 1205.5484, 1208.6086, 1210.9059, 1215.5090, 1223.4621, 1223.7816, 1226.4145, 1231.6760, 1235.8896, 1236.4966, 1238.0994, 1238.3329, 1243.3872, 1249.7422, 1252.7183, 1254.3085, 1262.7775, 1267.7765, 1269.0805, 1279.5320, 1290.5204, 1293.5662, 1305.6866, 1352.3601, 1361.7631, 1371.0522, 1401.7624, 1414.5613, 1424.3641, 1469.0932, 1503.1021, 1520.6861, 1731.7030, 3076.0667, 3153.5826, 3174.7413, 3176.8273, 3202.9487, 3276.5436, 3337.7100	
T3-O1-Protonation-TS	234	-181.4632, 32.6566, 35.3208, 58.4706, 73.3899, 80.9881, 84.1425, 89.5764, 95.8531, 101.4545, 107.8698, 109.3693, 112.4341, 115.6900, 119.2777, 121.8764, 129.2432, 135.6693, 140.4851, 144.4044, 146.6778, 150.3297, 154.4797, 157.6049, 161.9834, 170.0075, 174.3387, 176.4533, 178.3573, 179.6148, 181.2579, 183.5716, 186.8190, 191.7763, 192.6134, 196.3836, 198.3817, 202.2016, 203.6011, 209.1750, 211.8067, 213.2103, 216.6635, 220.7290, 224.7023, 226.4891, 233.7003, 234.6615, 239.9345, 242.6952, 245.2490, 248.1768, 252.1289, 253.1458, 257.5161, 258.3661, 261.4368, 265.3626, 266.5461, 272.1230, 272.7889, 275.4326, 277.5494, 282.4417, 284.9304, 289.1087, 289.9900, 294.9309, 297.8656, 298.5069, 300.4127, 304.8629, 311.2190, 313.0241, 314.0824, 318.4952, 320.3112, 325.0528, 327.0806, 328.4762, 330.7432, 333.5049, 338.2081, 344.4749, 346.9840, 352.6068, 362.8297, 366.6777, 370.3654, 375.1167, 378.4101, 386.2469, 386.8239, 391.5192, 395.2949, 406.9371, 411.3102, 418.1753, 423.4953, 427.9338, 432.1699, 437.3291, 440.1303, 445.0843, 449.6418, 452.5577, 456.0325, 458.8293, 471.3128, 487.9390, 496.2455, 499.5855, 501.3794, 513.3234, 518.6923, 530.5599, 537.6215, 549.6118, 562.9240, 568.2251, 569.3190, 586.7321, 596.9743, 611.6326, 614.2940, 617.4335, 638.8593, 662.0006, 674.2855, 689.0821, 698.7674, 700.4111, 703.9243, 708.9881, 716.2421, 721.0733, 724.7102, 731.0604, 736.9718, 738.7999, 739.9717, 754.3845, 757.9672, 760.7720, 766.9404, 771.2431, 777.7342, 778.5454, 782.0407, 783.9344, 786.7255, 788.6649, 789.1925, 790.6839, 795.5736, 797.4149, 800.4018, 803.6451, 807.2843, 808.9985, 812.0250, 814.4791, 818.3806, 822.0249, 823.5945, 826.1005, 827.5845, 829.7718, 834.3989, 835.6359, 839.4120, 840.7405, 846.6691, 855.4804, 859.0483, 863.7315, 874.8058, 979.5278, 1001.0218, 1016.1795, 1085.9460, 1107.0672, 1118.5604, 1122.4125, 1127.1768, 1130.9850, 1133.1350, 1140.0698, 1149.0599, 1156.6756, 1157.1200, 1172.1222, 1179.3956, 1194.7416, 1196.3913, 1203.6914, 1211.7552, 1214.3640, 1218.5426, 1221.1072, 1222.4762, 1226.1812, 1229.5430, 1233.6821, 1235.1534, 1238.8143, 1240.7599, 1242.7300, 1254.4948, 1256.0100, 1257.5104, 1261.8913, 1268.8746, 1273.8097, 1282.9362, 1291.1836, 1299.9920, 1319.4399, 1337.1544, 1344.9518, 1370.0909, 1379.4143, 1382.7807, 1408.3643, 1443.1225, 1458.1599, 1530.3813, 1570.9479, 2051.6675, 3043.4874, 3137.2008, 3140.8341, 3204.4599, 3227.0208, 3242.9191	-181.4632
T3-O1-ZeO-C ₃ H ₇ (ads)	234	29.3583, 53.5722, 64.4697, 73.8938, 80.7601, 82.8154, 92.5338, 93.4289, 108.6341, 112.0278, 113.4499, 114.8469, 119.0024, 122.5555, 128.7218, 134.1776, 140.9205, 143.6968, 151.1864, 154.0913, 156.6601, 161.7449, 167.6570, 173.4430, 175.8258, 177.0038, 178.2792, 180.8275, 186.5276, 187.2000, 192.1542, 194.4436, 197.7010, 201.7181, 203.4046, 207.7930, 208.6722, 211.6110, 212.4372, 219.1910, 223.4667, 230.0559, 234.3727, 235.1575, 238.2697, 241.0246, 242.6159, 245.7334, 248.6919, 251.6219, 252.2260, 258.3106, 258.8729, 263.2189, 264.8237, 265.8460, 270.1483, 271.2669, 273.4012, 275.2804, 277.8650, 281.7817, 282.3224, 284.7920, 288.9987, 291.9009, 295.2192, 297.1601, 299.1685, 302.4703, 307.1159, 311.2371, 313.2651, 314.7886, 315.9483, 318.7350, 324.2229, 327.0782,	None

		329.3021, 330.8829, 336.1563, 339.8069, 342.7740, 348.8420, 353.7533, 362.9357, 368.7475, 371.7151, 375.3847, 380.4761, 385.2906, 389.2456, 391.1920, 394.2168, 405.1133, 413.8329, 416.3010, 421.2120, 422.6845, 428.5043, 433.3074, 436.5326, 440.9396, 445.2004, 454.6888, 456.9379, 466.4712, 472.2671, 488.0751, 493.6170, 499.2099, 503.0986, 514.6361, 521.2362, 535.4216, 551.6467, 563.7593, 568.7112, 570.4887, 580.8621, 597.0195, 609.8234, 613.3283, 614.3666, 649.3615, 666.1836, 678.8578, 680.6737, 694.4174, 695.5907, 699.2899, 700.4953, 717.2567, 720.1774, 724.2930, 731.4948, 738.7076, 742.7142, 747.1204, 756.6696, 758.9482, 764.7442, 769.1042, 772.8232, 777.0039, 778.0704, 783.2833, 786.1849, 788.6788, 791.0296, 792.1501, 795.2226, 800.1024, 802.5609, 806.7657, 809.1732, 811.2011, 813.3770, 817.9908, 819.3239, 820.1779, 825.8301, 827.9968, 829.4702, 830.6374, 832.2614, 839.1340, 841.0236, 844.2616, 848.4766, 854.0106, 858.2187, 862.2777, 866.1500, 878.4286, 909.6432, 948.5630, 963.6034, 1089.5849, 1098.1886, 1123.8071, 1124.2181, 1126.9130, 1133.6686, 1135.7972, 1136.3360, 1151.7946, 1156.8170, 1171.1150, 1178.4115, 1180.1501, 1191.9094, 1196.4445, 1201.6722, 1209.9605, 1214.8521, 1217.5467, 1224.1654, 1226.7107, 1228.5264, 1233.2776, 1235.6908, 1238.4762, 1239.8791, 1242.4439, 1245.5261, 1248.5216, 1255.5529, 1257.8757, 1267.7162, 1272.0475, 1276.5076, 1288.2522, 1295.7322, 1306.1206, 1335.6679, 1374.7311, 1393.8749, 1404.9439, 1412.7278, 1420.9061, 1438.5646, 1452.8006, 1491.2052, 1505.1463, 1518.9765, 1522.0258, 3085.1279, 3097.9267, 3169.0886, 3175.6028, 3195.0731, 3206.5883, 3221.5546	
T3-O1-ZeO-C ₃ H ₇ CO(ads)	240	23.9875, 31.4662, 52.2985, 56.4063, 64.7008, 71.0491, 74.3856, 80.7814, 83.5836, 88.8952, 93.9471, 102.3664, 108.6102, 109.3050, 114.4253, 114.8651, 116.7465, 122.8429, 123.8487, 132.6167, 136.2680, 141.5526, 145.9644, 152.6735, 155.0323, 159.0491, 161.6909, 169.0326, 174.1931, 176.8056, 177.3125, 178.7055, 181.2147, 187.0624, 188.0710, 193.7946, 195.1728, 199.5048, 202.1613, 205.1501, 208.7618, 210.1105, 212.3339, 213.4924, 219.7826, 223.4741, 232.5275, 235.1650, 236.6362, 238.4575, 242.2165, 243.3126, 246.8669, 249.6229, 253.0182, 255.4804, 258.5662, 258.8736, 263.0661, 264.6129, 265.4641, 270.6598, 271.6795, 273.6479, 276.9247, 281.2993, 282.4359, 284.9102, 288.5699, 292.1914, 295.2214, 298.0600, 299.4116, 302.5875, 304.6953, 309.1488, 311.5661, 314.2663, 316.4493, 318.9281, 322.8705, 325.1836, 330.4565, 331.0308, 334.4802, 336.6933, 340.6421, 344.4511, 349.7256, 354.9112, 362.7834, 368.1167, 372.7792, 375.4376, 383.0494, 385.3594, 390.9092, 392.0946, 394.4061, 405.0805, 413.7848, 418.3463, 421.8613, 425.8440, 428.5752, 434.0245, 436.6008, 441.8681, 446.5169, 454.7744, 457.6745, 466.6653, 473.2948, 488.4964, 493.6112, 499.0545, 503.1531, 514.8733, 521.5723, 535.3581, 552.3381, 563.8260, 569.4503, 571.3696, 581.8899, 597.1143, 609.8593, 613.2710, 614.3225, 649.6574, 666.3747, 678.8682, 682.4667, 694.5033, 696.5801, 698.8616, 700.6278, 717.0251, 720.0020, 723.8209, 732.1696, 737.9120, 743.0435, 747.1196, 756.1574, 758.7709, 764.6369, 768.7390, 771.5480, 776.8098, 778.3019, 783.1690, 784.9808, 788.3020, 791.1043, 792.2938, 794.8317, 799.9561, 802.1181, 806.1742, 809.0547, 811.1573, 813.2136, 817.7245, 818.4409, 820.2393, 825.7342, 827.5988, 829.6978, 831.1053, 832.0570, 839.7028, 840.9965, 844.3411, 849.4184, 853.8209, 857.9821, 862.0826, 866.1757, 878.6251, 911.6593, 950.7615, 966.1660, 1091.3288, 1099.9433, 1123.5782, 1126.7297, 1129.2540, 1133.4867, 1136.1568, 1136.6687, 1151.6603, 1156.3169, 1170.5080, 1178.3050, 1180.6461, 1192.4898, 1198.6687, 1201.8246, 1209.4965, 1214.2748, 1217.2223, 1223.1989, 1226.2103, 1228.5478, 1232.7210, 1235.1814, 1236.5652, 1238.9245, 1242.0068, 1245.1419, 1248.6868, 1255.3907, 1260.9788, 1266.6740, 1272.0843, 1276.0353, 1286.9742, 1294.2332, 1304.4832, 1334.6125, 1374.0694, 1395.8451, 1405.5894, 1412.0391, 1436.3047, 1448.8109, 1457.9684, 1491.2664, 1513.1921, 1522.0351, 1527.9675, 2227.4115, 3087.9647, 3103.2427, 3171.1370, 3179.5785, 3200.9373, 3215.1225, 3229.9956	None

T3-O1-Carbonylation-TS	240	-118.2862, 22.7513, 37.4667, 39.2258, 56.8324, 62.2082, 66.1190, 78.6961, 83.5294, 87.0600, 96.8315, 107.4108, 111.7693, 111.8636, 114.1514, 115.9448, 121.0938, 125.3555, 127.2488, 131.5154, 138.6394, 140.1493, 143.2410, 147.4228, 153.3964, 157.5641, 160.9172, 169.1511, 171.7022, 174.0871, 176.3957, 178.2668, 178.9223, 184.4366, 185.7120, 189.7366, 191.6369, 194.7927, 197.1487, 199.4787, 203.4443, 207.9144, 209.7498, 211.5663, 214.0762, 221.1661, 225.8677, 226.5452, 229.3412, 234.4335, 235.5678, 240.1913, 245.1515, 247.3437, 251.0557, 252.1854, 256.9032, 259.3262, 260.1391, 261.8239, 264.7705, 267.9153, 270.1457, 272.7242, 274.8755, 276.0091, 278.4290, 283.1680, 284.8673, 288.3908, 289.8772, 296.1083, 298.3265, 300.7520, 301.1686, 304.1164, 312.5642, 315.1640, 316.3748, 318.8357, 323.7358, 325.4488, 327.4500, 331.7175, 333.6242, 334.4467, 338.0173, 345.7981, 348.5548, 353.1566, 364.1820, 365.4158, 366.2870, 370.1361, 374.9392, 380.0815, 386.1621, 387.2134, 390.8567, 395.0327, 406.6884, 414.4006, 415.7216, 422.2419, 424.3782, 428.4666, 433.8209, 438.9606, 440.8687, 444.8434, 446.5505, 455.4850, 459.3537, 471.7721, 489.2677, 493.7522, 498.2608, 500.9528, 516.6896, 519.7635, 537.4017, 551.0916, 563.0508, 568.8090, 571.3364, 592.2557, 599.0241, 612.0096, 616.6829, 618.9962, 654.0811, 675.6163, 688.7316, 698.0193, 701.1509, 701.8837, 716.9820, 719.7674, 721.9212, 725.2099, 729.7246, 738.0390, 739.3612, 742.0773, 746.2562, 756.1116, 757.2236, 766.1492, 772.7251, 776.9401, 778.2673, 783.6444, 786.3482, 787.8457, 789.8288, 792.2934, 794.0860, 795.5764, 799.5244, 802.8529, 804.2289, 807.6001, 807.8931, 812.4481, 813.1936, 816.2366, 820.4567, 823.2431, 823.9822, 827.2306, 828.4753, 832.0897, 834.9891, 836.7465, 840.9368, 845.1586, 845.8971, 854.7742, 857.4186, 859.3317, 874.1329, 949.4779, 990.2452, 1054.7489, 1092.6188, 1108.6501, 1111.2865, 1116.8026, 1125.5294, 1131.5118, 1136.3605, 1143.9511, 1146.4884, 1149.7208, 1166.1009, 1168.8295, 1175.2547, 1180.9174, 1190.6955, 1195.3214, 1206.2867, 1208.9387, 1215.6524, 1220.3421, 1223.5459, 1230.3462, 1231.3335, 1232.4246, 1233.2222, 1238.2211, 1240.9006, 1244.3499, 1247.6896, 1252.9468, 1254.3205, 1262.5938, 1269.9419, 1272.1380, 1284.3440, 1287.9959, 1298.5994, 1326.0418, 1363.4952, 1366.2769, 1386.9648, 1390.0314, 1407.9178, 1416.2537, 1452.5581, 1475.2642, 1519.5998, 1522.4831, 2307.6814, 3014.8775, 3028.6889, 3137.6595, 3144.2608, 3207.8669, 3212.9735, 3248.9079	-118.2862
T3-O1-ZeO-isobutyryl (ads)	240	26.3073, 50.0474, 52.8391, 57.8293, 74.0461, 79.6416, 83.3498, 85.9240, 93.6034, 94.2916, 109.6522, 113.6788, 114.4134, 120.4778, 121.4353, 124.0108, 126.3124, 137.1671, 141.4513, 142.1510, 152.2487, 155.0562, 160.2874, 164.3581, 172.3874, 173.2489, 176.1102, 176.7931, 178.4859, 180.7286, 183.6586, 187.0076, 191.1769, 195.1578, 198.1795, 201.1240, 204.1492, 206.1406, 207.9624, 209.4962, 212.4232, 218.0971, 220.6458, 222.6047, 229.9843, 233.8960, 236.9154, 238.4060, 239.9147, 241.3568, 247.9091, 248.9766, 251.5263, 254.4868, 259.5114, 259.7975, 264.2739, 265.9978, 267.3000, 271.7887, 272.7585, 275.6050, 279.7710, 281.8742, 284.6311, 286.2600, 289.0575, 294.5944, 296.2847, 298.4512, 300.0838, 304.0555, 308.0546, 311.5923, 315.4823, 316.1585, 317.5147, 318.4697, 323.4263, 325.5698, 328.1010, 330.7592, 333.1892, 336.1563, 343.9331, 348.1072, 354.9109, 360.0300, 363.9121, 365.8001, 368.7205, 374.5254, 376.7708, 385.6905, 387.1409, 391.7387, 393.5836, 406.2938, 410.6319, 413.0654, 418.3609, 422.4527, 428.8480, 433.0272, 433.9445, 442.4315, 453.4817, 455.7976, 466.0314, 483.1933, 490.9633, 496.1689, 498.5768, 501.6722, 516.3490, 524.2328, 534.5000, 556.4348, 560.3879, 566.4233, 569.5984, 570.8132, 576.6934, 592.3392, 601.9117, 613.2834, 614.5540, 622.1856, 647.3108, 660.8660, 678.5935, 693.1042, 694.1323, 699.2907, 701.0399, 715.5913, 717.7984, 719.6094, 724.4906, 730.3042, 738.5247, 742.9769, 745.8353, 756.6919, 759.8307, 765.2653, 769.3624, 772.4975, 777.5358, 781.5540, 783.7333, 786.9493, 788.9528, 790.2830, 795.4001, 798.8586, 801.3901, 803.4429, 807.2733, 808.5743, 810.3371, 813.8114, 816.7908, 818.6160, 820.3258, 824.9000,	None

		827.0033, 829.8726, 831.9753, 833.8470, 837.4298, 840.5375, 843.8583, 846.1004, 854.1027, 858.4937, 860.8737, 864.9097, 877.3012, 893.1761, 950.5440, 983.4451, 995.1019, 1090.5859, 1104.6493, 1122.5314, 1126.3762, 1131.7990, 1137.3765, 1141.8570, 1143.5644, 1155.2735, 1162.3277, 1166.4411, 1170.6979, 1179.0425, 1180.4320, 1195.0841, 1201.9098, 1210.8346, 1216.1519, 1220.5809, 1223.9809, 1225.3595, 1228.4360, 1232.1212, 1237.1161, 1238.7034, 1244.3809, 1246.6533, 1248.5701, 1250.9066, 1254.9654, 1257.0723, 1267.5633, 1273.4565, 1278.0558, 1287.7531, 1299.3670, 1305.8002, 1338.7998, 1358.0483, 1372.8376, 1389.2700, 1403.5530, 1414.0965, 1417.2175, 1448.0419, 1498.6661, 1510.7329, 1523.8614, 1531.1763, 1969.6188, 3088.4068, 3113.3445, 3131.0512, 3175.1874, 3209.6375, 3210.8182, 3248.8395	
T3-O1-isobutyryl H ₂ O(ads)	249	34.6589, 47.7475, 61.2843, 62.6889, 70.6407, 73.5620, 79.6114, 85.8143, 87.8736, 93.3277, 95.1724, 109.7277, 112.1759, 113.5905, 117.2783, 118.2159, 124.6398, 126.8205, 132.1790, 136.7744, 140.8479, 148.3074, 153.8327, 156.3803, 162.1049, 165.3093, 170.0514, 174.8273, 177.4134, 178.3722, 180.4664, 183.0090, 183.2070, 186.1707, 190.6167, 191.6124, 194.5206, 198.0550, 201.9198, 204.3740, 205.6083, 207.1628, 213.7416, 216.7210, 218.4675, 222.8389, 228.6648, 232.1013, 234.2197, 234.5020, 241.1904, 242.9675, 244.9960, 250.2419, 252.8698, 253.8555, 256.6113, 259.7153, 261.2968, 262.1411, 264.6451, 266.2856, 271.7546, 274.5717, 275.2322, 276.7954, 281.4767, 283.3603, 285.2646, 292.5985, 294.9402, 296.7115, 298.5691, 302.3250, 307.7072, 310.2364, 311.6077, 314.7487, 315.4946, 317.4063, 323.1630, 325.2142, 326.1265, 329.4361, 332.6271, 336.8606, 343.2792, 347.6449, 349.8787, 356.9178, 360.3535, 362.2539, 368.2521, 372.5301, 374.5999, 376.8189, 384.7936, 386.2284, 391.6058, 392.3320, 403.1828, 407.6875, 411.9461, 415.4880, 420.3598, 426.4884, 431.6110, 434.3438, 437.0863, 441.8615, 445.6573, 455.1131, 460.1328, 467.6403, 483.5676, 490.0316, 497.0512, 497.4776, 500.9939, 511.6082, 515.6210, 524.5725, 536.0749, 548.8480, 559.1880, 562.9305, 568.8295, 571.0237, 580.3234, 592.5554, 603.3405, 608.7532, 613.5048, 640.2584, 644.8600, 674.3668, 678.4619, 695.7583, 698.4312, 701.0524, 702.1892, 716.8779, 722.4812, 727.5033, 727.9661, 736.0857, 737.4984, 743.6057, 748.5250, 750.7912, 760.0646, 766.7796, 770.0732, 770.7596, 774.5469, 780.6312, 781.7504, 786.4811, 787.8774, 789.7612, 795.3765, 797.9865, 798.8473, 802.2429, 807.1842, 809.8356, 810.9591, 815.6286, 817.1947, 820.3540, 824.6723, 826.7738, 827.2956, 832.5536, 834.1690, 834.9998, 842.7896, 843.7472, 848.2011, 852.1258, 852.9795, 860.3664, 861.1120, 865.4601, 877.6733, 902.5464, 970.5287, 980.1002, 1014.8851, 1095.3040, 1106.9081, 1126.6784, 1129.9508, 1132.7988, 1138.8245, 1139.3101, 1146.9230, 1148.0547, 1163.2526, 1165.5885, 1170.2423, 1180.4052, 1181.9241, 1194.7982, 1204.4994, 1209.7508, 1215.8730, 1220.8429, 1222.1160, 1225.8839, 1229.2793, 1231.3025, 1237.6794, 1239.1914, 1240.0933, 1244.0178, 1250.6784, 1252.6403, 1256.2985, 1260.7546, 1271.0413, 1272.4535, 1276.7181, 1284.7026, 1299.8658, 1310.4072, 1313.8512, 1344.1324, 1372.1931, 1384.1897, 1408.4413, 1420.0320, 1423.2747, 1446.1034, 1499.7835, 1505.0310, 1526.2370, 1558.4346, 1650.8348, 1915.6469, 3086.8701, 3098.1684, 3103.8770, 3174.5383, 3185.3607, 3203.4816, 3208.0403, 3834.6348, 3949.9222	None
T3-O1-isobutyric acid(ads)	249	22.2582, 33.7383, 42.7141, 55.4607, 61.4449, 70.8041, 77.7808, 83.3539, 88.3239, 94.3461, 99.0312, 103.3311, 108.2465, 109.7176, 116.9488, 118.9245, 120.8042, 126.2466, 131.6641, 133.5336, 141.2306, 144.2561, 152.9659, 154.9536, 159.9373, 163.5815, 170.6018, 174.3168, 175.2257, 178.0186, 180.1771, 182.3754, 183.4217, 187.3777, 189.0458, 195.0530, 199.1009, 201.2569, 203.0967, 206.2842, 210.4596, 213.2518, 214.6278, 221.9361, 223.1571, 224.1228, 231.5007, 233.6300, 238.5333, 240.4862, 244.0174, 245.8892, 248.3485, 252.2142, 254.3812, 256.3490, 258.4915, 258.9312, 262.0411, 264.0811, 265.6916, 267.7510, 271.1346, 273.5736, 274.2811, 277.7889, 282.1042,	None

		283.9912, 285.2245, 287.4891, 293.5659, 295.9700, 299.8576, 301.4245, 302.0747, 310.7601, 312.8766, 313.2079, 315.2774, 316.4443, 320.1244, 324.2221, 325.6046, 329.1959, 331.4380, 335.0195, 339.9608, 343.2047, 348.3868, 357.0034, 362.2886, 368.2330, 370.4341, 376.1402, 385.3785, 386.1806, 386.9979, 389.6103, 392.4442, 402.8985, 411.1669, 413.7693, 419.4676, 422.6958, 426.2433, 432.9332, 437.0163, 438.8900, 444.4594, 454.4135, 458.5492, 468.8105, 488.3016, 491.7146, 498.8895, 501.3896, 507.4963, 515.3538, 520.6477, 533.8197, 551.4814, 558.4133, 563.7396, 568.9046, 570.8488, 586.2383, 594.4577, 604.4186, 611.0089, 613.1008, 617.6521, 649.5502, 662.1573, 675.3989, 694.7059, 697.3977, 700.4086, 701.0749, 715.3834, 717.5784, 719.1138, 723.5099, 736.8688, 738.0853, 740.7137, 749.0684, 753.1337, 760.7460, 762.2189, 768.1934, 770.9566, 775.7654, 776.9852, 780.1711, 785.2024, 786.9344, 788.4353, 789.0913, 791.7639, 795.6554, 797.8264, 800.0706, 803.7413, 808.3911, 809.6288, 812.5469, 818.0017, 820.5066, 824.0420, 827.1980, 829.3570, 833.0782, 835.7847, 836.7155, 841.4027, 842.8623, 846.8830, 852.3384, 857.4064, 857.7836, 862.3690, 863.0265, 876.3195, 894.7857, 933.8327, 973.6984, 988.6707, 1088.9882, 1112.8487, 1113.7078, 1124.0854, 1125.6418, 1129.9175, 1133.2261, 1138.9311, 1140.2369, 1146.7384, 1156.9874, 1162.0907, 1172.2076, 1181.0149, 1186.0034, 1197.7345, 1202.5389, 1209.5773, 1213.9568, 1221.6747, 1223.4624, 1225.6811, 1229.4299, 1234.0587, 1236.0378, 1238.6349, 1241.2115, 1242.1902, 1247.1397, 1251.7422, 1254.8172, 1255.7094, 1268.7728, 1272.5461, 1276.4305, 1282.6895, 1285.0434, 1297.4747, 1299.2625, 1311.9594, 1341.7977, 1349.9907, 1366.7347, 1405.4171, 1413.0405, 1416.6050, 1428.7095, 1448.6180, 1502.6346, 1512.1471, 1523.7393, 1538.1771, 1914.2176, 3079.2594, 3087.4637, 3118.3941, 3139.2881, 3161.0207, 3171.2830, 3182.1849, 3188.4349, 3819.3917	
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Supplementary Table 17. Calculated Harmonic Vibrational Frequencies (cm^{-1}) for adsorbed species and transition states of C_4H_9^+ formation of ethylene dimerization.

FileName	Number of Frequencies	Full Frequency List (cm^{-1})	Imaginary Frequencies
T1-O1-ZeO- C_2H_5 $\text{C}_2\text{H}_4(\text{ads})$	243	31.3388, 38.4473, 50.2576, 56.8702, 65.2155, 72.8352, 76.7296, 84.8399, 87.6422, 92.7257, 94.5876, 102.1372, 103.1881, 115.1243, 121.6892, 123.8270, 126.9783, 130.0440, 138.4438, 139.4638, 146.7059, 150.7123, 153.6496, 160.5103, 162.9797, 164.7197, 168.0271, 172.1539, 176.1787, 177.8972, 180.7240, 181.9946, 182.6409, 189.2850, 189.8931, 192.3082, 197.2350, 201.3677, 202.4441, 208.5759, 212.0822, 213.7347, 215.8613, 219.0713, 225.3605, 227.2141, 229.4431, 233.1953, 237.4245, 239.7964, 241.0705, 242.0525, 243.6910, 246.9887, 248.6175, 253.9695, 256.6463, 258.2611, 260.1346, 262.8335, 263.9980, 266.4694, 270.0142, 274.4939, 275.8801, 278.5762, 281.9557, 283.7969, 286.1998, 290.8479, 294.4505, 297.6951, 299.3593, 302.5992, 306.2544, 309.3389, 311.5926, 316.4284, 319.7808, 322.4023, 325.8182, 327.1559, 329.7305, 336.2528, 337.1767, 344.0333, 348.0368, 352.8014, 360.6290, 365.5160, 367.3056, 368.9114, 374.5150, 379.5455, 386.7056, 390.2695, 393.2596, 395.2451, 405.3368, 410.6624, 414.3455, 421.6880, 422.8435, 429.0853, 435.3468, 437.9244, 447.4084, 452.1489, 458.8197, 469.9302, 475.2047, 481.8732, 492.2000, 498.6683, 507.2251, 512.9843, 516.9740, 530.5899, 535.7713, 555.3774, 559.6842, 568.3105, 571.6452, 588.3083, 600.0676, 605.6833, 611.4033, 643.3864, 664.9106, 672.6282, 698.0131, 701.4793, 706.0492, 709.7915, 713.2677, 716.8378, 724.8870, 727.2489, 736.9997, 740.0442, 751.0583, 755.3248, 758.2078, 764.3089, 771.5920, 772.2245, 775.3708, 779.5283, 780.0848, 784.5555, 787.4618, 788.5042, 792.8571, 794.3878, 796.2249, 797.9045, 803.5796, 803.8307, 808.7814, 810.2330, 815.1628, 819.5383, 820.6241, 824.6317, 827.8605, 831.3527, 832.8895, 835.7879, 837.9829, 839.0656, 843.9829, 845.1170, 847.9135, 848.6909, 851.4931, 854.9603, 859.2662, 861.0158, 871.0306, 914.0315, 982.9683, 1021.2201, 1027.9618, 1089.7740, 1105.7056, 1119.5224, 1121.3661, 1125.3929, 1131.4635, 1132.5160, 1141.7563, 1148.7106, 1151.9124, 1154.3753, 1172.2739, 1182.5020, 1187.6243, 1195.8842, 1196.5958, 1198.5379, 1203.3506, 1208.7703, 1213.1304, 1213.7614, 1222.8374, 1226.0151, 1232.0721, 1233.3101, 1239.9312, 1245.8746, 1250.7476, 1254.0907, 1254.7082, 1261.0983, 1263.6688, 1272.2135, 1285.4718, 1286.0151, 1295.7080, 1302.3375, 1316.0267, 1333.1634, 1347.5113, 1369.3088, 1383.6722, 1401.2218, 1419.9007, 1421.2110, 1458.7965, 1486.8493, 1501.1998, 1517.2054, 1527.3066, 1731.9757, 3077.1385, 3159.0920, 3163.6469, 3167.7718, 3177.3493, 3182.0633, 3249.1208, 3249.5582, 3272.6087	None
T1-O1-ethylene dimerization-TS	243	-389.9175, 35.9778, 45.0244, 54.9622, 74.2423, 75.1048, 80.8122, 84.8316, 87.2120, 99.3208, 105.2774, 107.7417, 111.7351, 119.4684, 122.4272, 125.4460, 127.2604, 131.1658, 137.9086, 141.6797, 145.2417, 155.8657, 159.5450, 162.1987, 163.3298, 169.1170, 171.2279, 175.1505, 177.0725, 180.2806, 181.0856, 182.4916, 187.4558, 188.3118, 190.7800, 194.7138, 199.0975, 199.7723, 204.1115, 205.8009, 211.1541, 213.4522, 216.3889, 218.9120, 220.0031, 225.2509, 226.4956, 232.7378, 233.9580, 235.3589, 240.0367,	-389.9175

		243.9874, 245.3141, 249.2236, 252.0159, 253.1461, 256.1051, 258.7036, 260.2489, 261.5544, 265.6005, 267.4265, 271.3522, 274.4284, 274.6578, 276.9381, 282.1297, 285.9115, 287.4749, 288.9084, 293.7071, 297.3951, 299.2857, 303.7798, 306.6412, 309.2051, 310.1434, 312.8025, 319.4790, 321.6643, 323.7930, 326.3732, 328.3799, 330.0633, 332.3298, 335.7488, 342.3744, 345.9830, 353.0567, 361.9835, 367.0733, 370.6979, 373.4722, 380.5712, 387.3071, 389.3800, 394.8999, 398.1106, 407.8771, 412.4026, 418.8095, 420.7307, 423.2812, 429.5535, 434.2259, 443.4995, 445.3821, 452.0943, 457.3978, 460.5031, 462.6639, 476.4102, 486.9122, 497.9769, 501.3321, 509.7543, 513.9573, 518.6819, 537.0519, 545.7362, 561.1189, 566.3029, 567.9958, 586.4798, 593.6621, 607.5357, 611.8601, 615.1462, 647.8918, 673.2348, 694.1274, 700.1770, 703.3414, 706.7973, 709.6248, 713.8467, 720.0889, 721.8035, 726.2400, 733.2014, 739.7231, 745.6326, 756.2080, 758.1135, 761.5921, 768.7388, 769.4696, 774.5950, 778.8973, 782.1112, 784.7123, 788.4476, 790.1526, 791.4522, 794.0830, 795.2599, 802.5880, 803.0497, 807.0690, 808.8143, 815.2252, 818.9074, 821.8458, 824.4156, 824.9723, 827.1609, 830.3069, 833.5070, 836.1743, 839.4282, 842.3919, 843.5631, 846.2514, 847.6536, 850.7096, 858.8926, 861.3862, 863.5441, 873.6288, 941.4938, 1012.9794, 1038.5352, 1065.3161, 1068.5130, 1085.7282, 1089.4854, 1095.1991, 1116.3194, 1122.9106, 1131.9434, 1132.8249, 1133.3097, 1137.7692, 1150.3022, 1162.4878, 1168.5481, 1177.5839, 1188.2265, 1190.8818, 1193.7341, 1201.6255, 1207.9687, 1212.4524, 1218.2750, 1220.9147, 1222.5527, 1226.0198, 1229.2193, 1232.9069, 1237.8325, 1243.6459, 1245.6707, 1249.5633, 1252.8634, 1257.1312, 1257.6554, 1265.1531, 1270.4153, 1276.8576, 1286.9156, 1290.1804, 1296.9621, 1302.5930, 1327.4368, 1371.2801, 1392.9779, 1399.4776, 1405.4783, 1413.2583, 1488.2975, 1493.2577, 1496.7781, 1530.6144, 1694.3093, 3093.1587, 3173.0259, 3181.4705, 3194.6714, 3228.4726, 3256.5813, 3280.1660, 3301.4019, 3389.9683	
Tl-O1-ZeO-C ₄ H ₉ (ads)	243	41.5406, 53.9698, 56.7512, 70.9046, 80.3021, 89.0501, 93.3051, 97.1610, 99.2096, 100.4280, 106.7420, 112.8688, 120.6731, 124.2996, 127.5794, 132.7156, 134.0198, 138.8841, 152.4749, 155.8104, 157.0396, 158.9632, 162.7193, 165.5492, 171.3283, 174.3852, 178.4471, 178.5993, 180.6130, 181.8080, 187.6190, 189.0501, 191.9660, 196.6717, 198.5101, 203.2289, 206.5938, 209.6619, 213.5256, 215.9657, 218.7913, 224.7385, 225.8859, 228.8195, 230.1073, 239.0361, 240.8497, 243.0610, 246.6912, 250.1152, 251.5318, 254.6606, 256.9491, 258.3164, 261.3832, 262.3537, 264.3303, 266.3596, 270.9209, 273.4044, 274.5197, 277.8885, 281.7641, 282.0481, 286.5831, 290.1539, 297.1714, 298.1988, 299.6176, 302.3409, 305.3514, 308.0653, 310.1895, 313.0657, 317.5464, 318.7603, 320.2213, 324.4967, 329.0752, 331.1281, 332.6978, 337.1543, 343.7109, 347.8720, 349.2276, 361.9279, 365.0279, 366.4498, 371.0031, 378.0561, 380.0484, 383.3689, 386.8873, 392.4013, 396.9061, 403.2682, 407.5843, 413.1371, 417.6690, 425.1117, 426.5784, 431.3355, 436.7496, 442.7645, 446.6438, 451.3958, 455.1587, 472.8151, 482.5762, 490.5662, 499.8907, 503.6728, 510.4663, 512.7901, 525.1586, 537.9885, 553.7291, 560.4257, 565.7472, 567.5774, 574.2292, 591.2361, 601.3983, 609.3681, 615.0168, 645.6541, 658.8953, 674.6212, 695.8626, 700.9379, 703.0126, 705.0875, 713.7472, 719.1169, 725.8642, 728.6009, 736.0985, 741.0224, 750.7090, 754.6226, 759.5688, 760.1205, 769.3831, 770.6531, 774.0641, 774.7933, 779.7374, 781.3851, 784.0451, 790.5878, 791.7257, 793.8869, 795.8322, 798.5698, 804.4137, 806.0338, 807.2476, 810.7025, 814.8110, 817.6468, 820.8645, 823.7824, 825.7625, 830.3559, 831.5962, 832.8029, 835.5649, 841.3383, 843.2409, 844.0035, 846.1522, 849.2577, 851.6934, 854.5489, 859.5715, 862.5791, 872.4811, 932.0726, 934.3430, 990.9133, 1019.9433, 1097.1029, 1114.6206, 1115.3171, 1127.5404, 1134.1382, 1136.4830, 1144.6587, 1151.7285, 1154.1725, 1156.9047, 1159.1164, 1172.0081, 1181.2233, 1193.7773, 1194.5014, 1196.3489, 1199.7048, 1205.8293,	None

		1217.1807, 1222.1158, 1227.8687, 1231.6347, 1233.0451, 1240.5381, 1241.4909, 1249.7717, 1256.3911, 1257.5467, 1262.5104, 1264.9286, 1266.3019, 1274.8028, 1279.8299, 1283.4185, 1284.9060, 1287.8595, 1300.0058, 1313.0648, 1320.1247, 1343.6731, 1345.5542, 1368.7898, 1370.2583, 1403.2081, 1408.2721, 1410.9369, 1439.4678, 1450.3949, 1509.4221, 1516.4221, 1519.7487, 1525.8474, 1541.0554, 3055.0711, 3089.0546, 3102.2329, 3143.1576, 3153.6141, 3168.3027, 3206.7601, 3212.2734, 3228.4494	
T2-O5-ZeO-C ₂ H ₅ C ₂ H ₄ (ads)	345	49.1709, 63.3123, 65.5542, 70.0687, 78.4865, 84.2259, 86.5979, 87.9104, 89.2772, 93.3988, 96.8666, 98.4399, 101.0844, 106.1150, 110.5601, 112.0792, 112.9867, 116.9723, 117.9952, 121.8802, 124.2608, 126.6542, 130.0287, 134.3890, 136.0169, 137.8823, 140.4061, 141.6182, 144.8641, 145.8035, 146.8563, 147.4790, 150.3106, 150.4027, 154.3522, 156.8078, 160.4353, 161.4336, 162.8379, 164.2882, 166.0952, 168.6735, 170.0105, 172.3472, 174.2933, 177.8560, 179.3326, 180.7642, 184.0127, 185.6023, 187.0461, 189.4413, 198.7513, 200.4071, 202.3112, 202.7768, 203.5334, 205.6243, 208.2267, 211.7539, 212.9130, 215.4298, 217.1271, 221.0272, 221.6513, 226.1131, 226.6171, 228.4390, 229.5759, 231.4222, 233.5041, 236.2359, 239.8689, 241.5022, 242.8843, 245.5534, 247.9136, 249.6706, 252.6360, 254.4592, 257.9271, 259.2560, 260.1273, 265.0127, 266.9353, 268.4341, 270.1101, 271.9358, 273.0300, 274.7839, 276.1879, 278.7353, 281.1899, 283.4274, 284.1368, 286.6854, 288.8186, 289.9011, 292.2325, 293.0560, 294.5403, 296.4411, 297.4545, 299.4589, 301.7031, 304.9725, 306.7793, 307.2990, 309.3942, 315.3519, 317.3119, 320.1461, 324.0158, 327.5848, 330.2881, 333.4809, 335.6145, 341.5369, 343.6103, 346.5214, 352.5933, 353.5376, 359.9479, 363.2503, 365.1898, 369.4033, 372.7990, 377.2054, 379.0170, 382.0664, 385.4277, 387.3368, 389.2963, 390.8751, 392.9094, 393.1724, 395.7780, 397.1569, 399.4258, 399.9276, 401.8694, 404.7373, 406.0004, 412.7942, 414.3470, 418.3834, 421.0215, 424.5757, 428.0214, 429.7371, 434.1885, 436.1219, 441.2706, 444.3597, 445.9129, 451.7198, 457.2754, 462.5922, 465.9435, 471.4058, 472.4728, 482.8020, 486.7767, 488.3556, 491.3131, 495.8183, 496.3986, 499.8840, 504.4915, 509.6449, 513.1123, 520.9077, 525.3307, 529.4235, 541.0411, 544.4831, 556.4945, 557.4101, 570.4549, 577.1117, 577.8599, 589.5371, 606.9628, 618.6539, 626.2503, 638.1095, 645.2822, 652.5398, 659.2571, 664.6204, 669.6656, 669.9902, 672.3180, 675.8976, 686.9735, 687.5896, 691.7667, 695.3110, 697.7583, 706.4095, 707.6151, 710.0332, 712.3474, 714.5887, 719.3165, 724.6140, 727.5243, 728.8774, 729.9600, 743.6960, 746.2339, 748.0309, 750.2188, 753.7400, 756.5579, 757.5037, 758.8646, 760.3109, 761.4093, 762.8548, 766.3038, 768.7247, 771.5554, 774.8862, 777.4412, 782.4989, 783.1189, 784.9623, 786.7106, 790.7761, 794.6668, 794.8646, 796.2579, 796.5593, 797.7279, 799.6518, 800.9574, 804.3831, 805.7308, 808.8528, 810.5032, 812.6416, 814.5596, 816.1113, 817.9463, 820.5061, 822.5632, 823.1755, 827.5457, 830.2197, 832.0595, 836.1304, 837.3899, 837.7688, 839.8428, 843.9568, 844.4081, 846.6727, 853.1429, 896.1328, 978.0372, 1015.9726, 1047.0546, 1057.8633, 1072.3436, 1077.9869, 1090.2953, 1092.7959, 1099.8410, 1103.1988, 1108.4665, 1109.8210, 1111.4402, 1112.6068, 1119.2136, 1119.6379, 1122.7072, 1125.3769, 1129.6199, 1132.2589, 1132.9305, 1136.4166, 1143.0789, 1145.6171, 1152.6194, 1154.9049, 1164.4302, 1165.1524, 1173.7137, 1176.3849, 1178.9867, 1182.9725, 1186.4161, 1187.8790, 1190.6136, 1193.4396, 1197.0098, 1200.8525, 1201.4553, 1205.5431, 1208.4625, 1208.8378, 1212.8366, 1216.4623, 1219.0326, 1223.2611, 1227.7163, 1231.8858, 1236.2760, 1239.0072, 1239.8976, 1242.7349, 1243.9017, 1247.3716, 1249.3242, 1252.7189, 1254.9340, 1259.6813, 1263.2748, 1265.5395, 1267.1929, 1272.6060, 1275.0354, 1276.9779, 1284.6865, 1286.8162, 1325.0864, 1399.7430, 1412.7992, 1470.0326, 1481.8053, 1501.8615, 1519.4253, 1553.3682, 1731.0550, 3119.8733, 3152.4346, 3174.2663, 3191.5895, 3213.0317, 3228.6473, 3262.4811, 3266.3926,	None

		3285.0150	
T2-O5-ethylene dimerization-TS	345	-356.5794, 63.9527, 66.9725, 69.1523, 70.9034, 76.8362, 81.8326, 86.4443, 88.2890, 90.0549, 95.2565, 97.6407, 100.1854, 105.9932, 110.2414, 112.6931, 113.8870, 117.1152, 117.4991, 122.2924, 123.6970, 128.4841, 129.1638, 132.4153, 136.7939, 138.0605, 139.9328, 142.6170, 145.1820, 145.8927, 146.4720, 148.7814, 149.4131, 150.5525, 152.5720, 154.8265, 158.4504, 160.2036, 162.7110, 164.2239, 167.0854, 168.7954, 171.7160, 172.6688, 173.7438, 177.8296, 179.8549, 181.7502, 183.1205, 185.8583, 186.1685, 197.2514, 197.5874, 201.7397, 202.4208, 203.7822, 204.6269, 206.5728, 210.9094, 211.9751, 212.8952, 213.9834, 218.3901, 221.0209, 224.3511, 225.0479, 227.8990, 229.5101, 230.0770, 233.5039, 235.1971, 239.4019, 240.0355, 241.5739, 242.2766, 245.7131, 246.4436, 250.0666, 250.8745, 253.7467, 256.5497, 257.6008, 262.9339, 263.2126, 267.8370, 269.6437, 271.8257, 272.9620, 274.0665, 275.7896, 276.4155, 279.5904, 282.9574, 284.5202, 285.3490, 286.6746, 289.0327, 290.3538, 291.5777, 292.8928, 294.2169, 295.0016, 297.1746, 299.0707, 300.2021, 304.3698, 304.6200, 307.5699, 308.1765, 311.0348, 317.2386, 318.1928, 320.5279, 325.9668, 327.4667, 330.4576, 333.7227, 335.5570, 340.8873, 346.6828, 349.0001, 354.2326, 357.0407, 360.0910, 363.3105, 366.1618, 372.7970, 375.5065, 377.2941, 378.9259, 384.2695, 385.4785, 387.9869, 388.8695, 391.7819, 393.1906, 394.2445, 395.7419, 397.6550, 400.6481, 401.6683, 402.6120, 405.5975, 408.2193, 414.3407, 414.4735, 418.8590, 421.4031, 423.2200, 426.2962, 429.9578, 432.9079, 436.9425, 437.9648, 441.6723, 445.5751, 446.4350, 449.2820, 456.7075, 459.4514, 463.5173, 466.1314, 472.7329, 476.6819, 482.4446, 487.9993, 490.1433, 492.9365, 496.5189, 498.8129, 499.5375, 504.6170, 509.5115, 512.3496, 521.7541, 532.0403, 540.7080, 544.2035, 556.5044, 557.8897, 575.7599, 577.5147, 577.8531, 592.9512, 607.8070, 622.0976, 631.2592, 638.3598, 645.6482, 657.4679, 660.1988, 666.1087, 668.8752, 671.3938, 673.6057, 675.9883, 686.1764, 688.3304, 693.4858, 695.5341, 697.3920, 704.1366, 707.1670, 708.9110, 713.9397, 715.9148, 720.6578, 723.6419, 726.3903, 729.3614, 729.5496, 742.8322, 746.9829, 749.6108, 750.8801, 752.0793, 755.1755, 757.0319, 758.2980, 759.3631, 759.8774, 761.9967, 763.6240, 766.7099, 771.3993, 774.3409, 775.5571, 781.5386, 782.9233, 784.9610, 785.7560, 791.5532, 792.9507, 793.3825, 793.8679, 795.3880, 796.5185, 799.9410, 802.3109, 805.4586, 807.3221, 808.5353, 810.9293, 812.2132, 813.8048, 816.1632, 818.4696, 821.0019, 822.8810, 825.3467, 828.4982, 829.7039, 833.4961, 833.7070, 836.0070, 836.9838, 839.6067, 841.8051, 846.9144, 852.0752, 957.2704, 1015.0293, 1020.5064, 1050.5738, 1064.8011, 1068.0404, 1078.4861, 1082.4286, 1088.9269, 1090.3026, 1092.6636, 1097.5949, 1102.7742, 1105.6495, 1110.4596, 1113.8000, 1115.4734, 1116.5524, 1122.7895, 1123.6089, 1131.1373, 1131.3609, 1132.3899, 1134.9108, 1141.3124, 1143.1534, 1150.2481, 1155.4188, 1163.5035, 1165.0651, 1172.3064, 1172.7925, 1178.0642, 1180.2543, 1185.7363, 1190.4419, 1195.0747, 1196.2892, 1199.6601, 1200.3730, 1203.1139, 1205.8444, 1208.1837, 1210.7680, 1211.3561, 1213.7161, 1215.6517, 1224.6956, 1228.1370, 1229.4701, 1234.5545, 1236.7183, 1239.1967, 1239.6087, 1242.8021, 1244.2222, 1247.1792, 1249.6491, 1251.1126, 1254.7743, 1258.5786, 1261.8533, 1263.0084, 1266.6410, 1269.6071, 1274.0022, 1276.2153, 1283.4168, 1285.6385, 1392.1283, 1420.1033, 1486.5079, 1489.4459, 1502.7911, 1523.3733, 1694.5196, 3113.2896, 3193.2794, 3201.1927, 3209.2901, 3215.7670, 3225.8816, 3291.1125, 3321.4622, 3351.4602	-356.5794
T2-O5-ZeO-C ₄ H ₉ (ads)	345	56.5424, 64.7288, 67.2072, 67.6882, 70.7329, 75.0299, 85.6055, 87.5615, 90.6862, 91.0131, 96.0680, 97.4006, 102.4466, 105.8414, 110.9852, 113.0861, 114.5854, 117.5111, 119.2412, 123.8707, 124.9811, 128.9184,	None

		135.6977, 136.5746, 138.3908, 139.4064, 140.5078, 144.6772, 145.5858, 146.5768, 148.4607, 149.9128, 150.7819, 152.7460, 155.5677, 159.6391, 162.0557, 162.6215, 164.0521, 167.7884, 169.6051, 171.5494, 172.6317, 175.2080, 178.8040, 179.9877, 183.2787, 186.0759, 187.4033, 197.2401, 198.3547, 201.3957, 202.0019, 203.2585, 204.8679, 206.4553, 207.3884, 211.5047, 212.2318, 215.9888, 217.4909, 221.8688, 223.7146, 225.1916, 227.9676, 229.1628, 229.9884, 232.7056, 236.4710, 236.8818, 239.1670, 240.2074, 242.2562, 244.9843, 246.0977, 248.3170, 253.4662, 254.6549, 258.1542, 259.2904, 262.7669, 265.0571, 268.4064, 268.9866, 271.3566, 272.2059, 274.6852, 277.4625, 278.4550, 281.4344, 281.7955, 283.9895, 285.9883, 288.6974, 289.3970, 291.4261, 292.3245, 293.4784, 295.3543, 296.4112, 298.2868, 299.5237, 303.2571, 304.0905, 307.1154, 308.9061, 309.8814, 315.5840, 317.2915, 319.6567, 322.0974, 326.3495, 329.8970, 334.5620, 336.5690, 340.0278, 342.5039, 348.2910, 352.0456, 357.7507, 359.2424, 362.2253, 364.0211, 367.4455, 373.0132, 376.1398, 378.1965, 379.4247, 384.8339, 386.4078, 388.1108, 389.7971, 391.1231, 392.6296, 395.4516, 396.2872, 397.1306, 399.9652, 401.4690, 403.5513, 405.3133, 406.9526, 414.3594, 417.6562, 419.4464, 421.1669, 424.6092, 428.6548, 431.9673, 434.5405, 436.1274, 440.5981, 444.4600, 445.9413, 451.5523, 457.8986, 462.7334, 466.2590, 471.7814, 473.2734, 482.4234, 486.4688, 488.6529, 492.8053, 495.7381, 497.6675, 499.8101, 504.3543, 509.3330, 512.4527, 513.7708, 521.1688, 528.4346, 540.2767, 544.0737, 556.0108, 557.0855, 569.6654, 575.6577, 577.2677, 588.8116, 606.2471, 617.8674, 626.7992, 638.2575, 645.2057, 652.6925, 658.9201, 664.5262, 670.4185, 670.8072, 673.0432, 675.0556, 687.5677, 688.2083, 691.7751, 694.9726, 697.2461, 706.0526, 706.9089, 709.1988, 712.0218, 714.5598, 719.0015, 724.1494, 726.1814, 728.2451, 728.8793, 741.4482, 746.6181, 748.4776, 749.6895, 753.2236, 755.0428, 757.7015, 759.3029, 759.5607, 762.1016, 762.9828, 765.7991, 768.2981, 771.7640, 773.6443, 776.3630, 779.9048, 782.8594, 784.0635, 785.5423, 787.9339, 791.6783, 793.9430, 794.5390, 795.6407, 796.2749, 798.4297, 800.2221, 801.2618, 804.1215, 807.2414, 809.7297, 810.3932, 813.2111, 813.9585, 815.8325, 818.4754, 820.0375, 822.5329, 823.4680, 826.5556, 829.7075, 832.2378, 835.7616, 836.4371, 838.3130, 839.6178, 842.0897, 845.0522, 852.4357, 886.2475, 902.5761, 984.8476, 1012.7781, 1060.5337, 1074.3750, 1088.9729, 1091.8781, 1098.0325, 1100.3780, 1102.5131, 1108.9560, 1110.0695, 1115.7362, 1116.7122, 1119.4983, 1122.7151, 1126.5922, 1129.8766, 1131.5010, 1132.4936, 1136.7979, 1139.6362, 1140.9653, 1144.0833, 1152.4034, 1154.3255, 1158.3081, 1162.6619, 1169.2964, 1175.1432, 1177.6454, 1179.6554, 1183.9398, 1186.2532, 1191.1241, 1192.8564, 1196.2998, 1200.1469, 1200.5508, 1204.6027, 1207.5007, 1209.2331, 1211.6395, 1216.6909, 1218.2100, 1223.5652, 1227.3920, 1230.8844, 1234.4867, 1237.9871, 1240.0027, 1242.5563, 1244.6989, 1247.5676, 1248.8245, 1252.5756, 1258.6584, 1262.5542, 1265.0943, 1267.7744, 1270.7111, 1273.3760, 1275.2814, 1278.1261, 1284.1009, 1287.9456, 1299.6854, 1346.3320, 1377.7760, 1404.8272, 1433.6567, 1453.2718, 1507.6277, 1511.1865, 1524.1945, 1531.8341, 1540.3517, 3057.6763, 3066.6004, 3100.7263, 3113.7764, 3133.6441, 3145.2150, 3168.1363, 3185.2065, 3217.5648	
T2-O6-ZeO-C ₂ H ₅ C ₂ H ₄ (ads)	171	43.6571, 57.5803, 67.0679, 70.3676, 77.9489, 84.7615, 100.4040, 110.3046, 118.2556, 118.7697, 121.4921, 130.1684, 137.7068, 143.0583, 153.1292, 160.9402, 165.1891, 168.2120, 171.9215, 173.1154, 178.5914, 180.6241, 187.6850, 190.3022, 204.7353, 212.1564, 215.2734, 218.9217, 226.7964, 237.7455, 243.2259, 247.8938, 251.8058, 255.2802, 258.4266, 269.1882, 276.7159, 282.3226, 289.4340, 292.6235, 298.5386, 302.0732, 308.3480, 311.4231, 312.1766, 313.9768, 318.0182, 319.6764, 328.3989, 330.3516, 333.0049, 335.9791, 346.5495, 350.1147, 356.9208, 368.2911, 391.5341, 396.5970, 400.2892, 411.0085, 434.6216,	None

		435.8632, 438.2599, 438.9781, 446.7137, 451.2157, 463.7757, 473.4225, 492.1892, 525.9841, 567.0821, 569.9477, 583.5812, 586.7341, 603.1250, 610.4154, 634.5378, 646.2079, 686.1888, 688.7104, 690.7858, 697.8154, 703.4815, 715.0238, 719.3032, 721.7818, 723.8384, 725.4910, 727.0235, 734.5574, 737.4724, 746.4829, 749.0738, 755.7231, 757.0904, 763.0191, 771.4967, 782.8762, 789.3930, 793.2528, 798.9733, 805.3790, 810.0153, 811.5366, 814.5848, 817.3799, 824.0162, 829.8545, 833.0608, 837.8478, 842.4227, 845.0555, 847.1984, 855.4164, 857.3549, 862.3233, 879.6702, 881.5981, 890.1071, 906.0916, 978.3904, 1014.2186, 1039.0427, 1048.6594, 1090.5739, 1114.2762, 1141.8872, 1144.0851, 1152.3409, 1161.4037, 1169.2770, 1185.7360, 1191.9091, 1198.4293, 1208.6237, 1217.1920, 1219.9257, 1227.1628, 1229.1191, 1240.0903, 1246.9416, 1249.0473, 1259.6037, 1277.9660, 1284.6776, 1298.6288, 1316.9807, 1337.9262, 1343.7524, 1390.1227, 1400.3031, 1413.2944, 1462.0601, 1484.9584, 1520.9141, 1526.7851, 1545.7495, 1730.9882, 2219.9884, 2221.5881, 2222.0648, 2234.9538, 3103.1284, 3167.4793, 3176.2597, 3187.8687, 3189.4002, 3201.3707, 3250.2107, 3254.3224, 3282.5046	
T2-O6-ethylene dimerization-TS	171	-319.4915, 41.1712, 49.6738, 64.0691, 84.5365, 89.4488, 92.9353, 98.5061, 118.5540, 121.6615, 128.5557, 133.8067, 137.5632, 143.4422, 150.0214, 157.9005, 163.0222, 165.3725, 170.7185, 173.9438, 180.4431, 181.8637, 187.8401, 191.1145, 195.3700, 201.1906, 211.2435, 224.7082, 230.6408, 236.9299, 242.0040, 251.6877, 254.8531, 259.9256, 269.2884, 270.9834, 276.8780, 277.2711, 283.8585, 294.0669, 298.5907, 304.4842, 308.3036, 311.6990, 313.8554, 317.6890, 320.5041, 321.8840, 331.4814, 332.5770, 336.5232, 337.5025, 347.2795, 352.3763, 361.3709, 365.5202, 376.4496, 396.5543, 401.2179, 406.9745, 429.3307, 431.7888, 433.6105, 439.9244, 450.2882, 453.8368, 459.8775, 467.0042, 467.2342, 492.7618, 523.7197, 557.9255, 570.1459, 583.1322, 585.3861, 610.7862, 623.9122, 640.0818, 652.5783, 671.2280, 687.7083, 690.4251, 696.6258, 701.1132, 708.1608, 711.5142, 716.8745, 718.4482, 723.4179, 728.4009, 734.2218, 737.0960, 748.1396, 751.8756, 754.8966, 755.9733, 761.3061, 770.3851, 777.7848, 778.1524, 781.7659, 793.4557, 795.2696, 802.2046, 809.4748, 812.2117, 817.0513, 823.9942, 829.5868, 833.5868, 836.6957, 842.5534, 844.5032, 865.1087, 867.3966, 868.7674, 870.7534, 875.0765, 880.1775, 894.2822, 918.0653, 957.5067, 1056.1485, 1066.1634, 1088.0710, 1113.3585, 1125.3176, 1129.5446, 1135.6447, 1151.1711, 1153.5760, 1174.5229, 1176.0420, 1183.3240, 1186.4948, 1192.2791, 1206.1445, 1208.2113, 1220.8856, 1224.2604, 1228.8975, 1235.1756, 1238.7476, 1239.6635, 1258.6432, 1262.5073, 1278.3012, 1307.4766, 1323.7384, 1343.3527, 1364.5844, 1394.9060, 1406.2503, 1479.3687, 1487.4802, 1490.9038, 1525.4488, 1697.4859, 2220.3453, 2222.2483, 2222.5933, 2235.9423, 3058.5386, 3154.6885, 3176.4757, 3192.6085, 3217.2993, 3226.3515, 3275.1791, 3297.4535, 3366.0954	-319.4915
T2-O6-ZeO-C ₄ H ₆ (ads)	171	37.0518, 70.3484, 79.8148, 90.0748, 92.3242, 98.5773, 106.2949, 108.6232, 119.8076, 123.5725, 126.8854, 139.2269, 141.0330, 145.9966, 155.2657, 159.2411, 162.9574, 168.1319, 168.5373, 173.1222, 176.7290, 180.3003, 187.5537, 188.7386, 196.7035, 199.4557, 210.6752, 226.7064, 237.0904, 244.6122, 246.3743, 251.3139, 266.5735, 270.8016, 273.8039, 276.3402, 279.8866, 286.7091, 292.7924, 298.6649, 307.5208, 309.9974, 310.5336, 316.9288, 320.7382, 324.1670, 326.1967, 332.6153, 335.6599, 340.1411, 348.9891, 358.9647, 362.0147, 374.6994, 395.6658, 398.3252, 402.0825, 409.6603, 416.2188, 425.4553, 430.8253, 434.2051, 440.1831, 446.5244, 454.4228, 462.5617, 465.3695, 468.6527, 500.8121, 518.3147, 552.8324, 568.0046, 584.7868, 586.7750, 605.2808, 611.0137, 625.7985, 640.7258, 657.6873, 666.7118, 686.3418, 687.6798, 691.3204, 700.2180, 703.4370, 711.4719, 714.4758, 717.0920, 721.1684, 723.5326, 734.5145,	None

		737.1531, 742.9031, 748.4698, 754.2634, 755.6357, 757.7846, 769.7961, 775.0724, 775.9428, 780.5222, 793.2905, 800.4698, 805.8971, 808.8275, 811.0550, 813.7410, 820.0867, 829.9286, 834.3192, 841.0631, 841.5261, 846.9205, 858.4945, 864.6525, 869.4482, 873.9886, 888.9368, 895.1484, 939.8246, 954.1736, 974.2850, 1026.6544, 1101.1853, 1113.8110, 1122.2853, 1131.8803, 1146.9646, 1148.9607, 1154.3620, 1157.3201, 1164.5325, 1171.2169, 1183.9893, 1192.9209, 1205.4400, 1211.7714, 1216.2023, 1222.3322, 1229.0329, 1233.3895, 1242.1386, 1250.4281, 1269.8270, 1276.8800, 1301.1910, 1306.2055, 1323.4324, 1328.3630, 1362.5160, 1396.4327, 1410.6269, 1434.8962, 1457.6347, 1462.7391, 1475.7869, 1511.6199, 1580.7631, 2220.3441, 2222.5268, 2222.8504, 2236.6220, 2786.1977, 3055.9973, 3140.9151, 3162.4210, 3196.2196, 3218.5479, 3247.6490, 3258.0125, 3298.3380	
T3-O1-ZeO-C ₂ H ₅ C ₂ H ₄ (ads)	243	36.6940, 52.6707, 58.3614, 66.1383, 67.0071, 74.7611, 81.7827, 84.1316, 93.8759, 96.5002, 109.0614, 111.3150, 114.6892, 115.4891, 121.7995, 126.3404, 129.4869, 136.7155, 138.9681, 142.8745, 147.9288, 152.2466, 156.1953, 159.8776, 161.7830, 170.2013, 173.3239, 175.5392, 176.0433, 177.5531, 180.7307, 181.5602, 186.8157, 188.2060, 192.3101, 196.3184, 196.8659, 201.9633, 202.8720, 208.3243, 211.6762, 212.3524, 213.9341, 218.5035, 224.3448, 225.1508, 228.9844, 233.8299, 237.1333, 238.6764, 242.2454, 245.8489, 246.1441, 251.5567, 252.8172, 256.0268, 260.0640, 260.3626, 264.9723, 265.7653, 271.5314, 272.8903, 274.5417, 277.4081, 281.0258, 282.8971, 284.1892, 288.6389, 290.1060, 294.2897, 296.8866, 297.9408, 301.2587, 304.8378, 307.7291, 314.0537, 314.7578, 316.1703, 320.1126, 323.9986, 325.4826, 328.9365, 330.3868, 333.8636, 336.4136, 343.6500, 348.8503, 351.4436, 358.0864, 363.4758, 368.5641, 372.7958, 374.1011, 380.5200, 385.4175, 386.9213, 392.7011, 393.3736, 407.0702, 413.4978, 416.7486, 419.6165, 421.8865, 431.3494, 436.7342, 439.4147, 444.1124, 451.8678, 455.6656, 459.4261, 471.2925, 489.7433, 491.7655, 498.7404, 499.8398, 515.6828, 520.8345, 534.8835, 546.9486, 562.7041, 567.5508, 569.3749, 577.7960, 595.0182, 608.7485, 613.3214, 614.4570, 647.7609, 663.6590, 676.4624, 693.2468, 698.7475, 701.0026, 701.9525, 716.6674, 720.6848, 724.3661, 731.0538, 738.1214, 739.9389, 747.4998, 755.0325, 760.0279, 764.9093, 770.9533, 771.9810, 776.6858, 777.5766, 781.0160, 784.5156, 787.2572, 788.8675, 791.8458, 793.4314, 794.9302, 799.4073, 802.6083, 805.7931, 809.2627, 811.0096, 812.0605, 818.4374, 819.5849, 819.9731, 824.3870, 828.2638, 829.8355, 830.5383, 832.3189, 836.2992, 838.9000, 843.8032, 843.8941, 849.1772, 856.3621, 859.4422, 863.4905, 874.4679, 895.8885, 898.9330, 1001.4271, 1006.1421, 1027.5039, 1084.5316, 1094.9366, 1123.8184, 1127.1375, 1128.0375, 1130.7307, 1133.6724, 1137.2046, 1138.4941, 1154.4580, 1160.4976, 1164.6812, 1178.4181, 1184.8139, 1195.3676, 1201.5342, 1202.3686, 1210.5137, 1215.5364, 1223.1382, 1223.3530, 1225.8666, 1233.2726, 1236.2172, 1236.9594, 1237.6471, 1239.6426, 1250.3533, 1251.8035, 1253.0363, 1256.0580, 1266.0802, 1267.8457, 1270.4184, 1276.3385, 1288.3349, 1293.9633, 1306.3667, 1331.3728, 1337.1141, 1370.9727, 1404.1138, 1416.5656, 1417.8914, 1422.8776, 1457.0115, 1506.6489, 1508.4894, 1516.8434, 1519.5019, 1739.5919, 3079.9034, 3167.2340, 3173.7981, 3174.1359, 3191.3190, 3192.3476, 3255.6201, 3264.7780, 3287.0022	None
T3-O1-ethylene dimerization-TS	243	-382.4153, 41.3653, 58.0241, 63.0074, 72.4797, 84.0832, 88.4167, 92.5457, 100.2998, 101.6475, 110.5310, 112.8948, 114.8438, 115.8076, 120.0712, 127.6979, 128.8440, 132.5043, 138.2737, 144.6762, 147.3413, 154.4322, 159.3090, 160.2493, 162.8317, 168.6620, 171.7978, 174.9721, 176.6126, 178.6039, 180.3163, 184.1660, 188.8710, 189.6818, 193.5706, 196.0295, 199.5860, 201.5109, 204.2211, 207.3334, 210.3230, 213.3699, 215.3510, 222.3500, 225.2906, 225.7106, 232.5279, 234.5976, 239.7058, 240.0562, 243.5537,	-382.4153

		245.6884, 250.2023, 252.2509, 252.8018, 258.3603, 259.0115, 261.1570, 265.4435, 266.3767, 272.3366, 272.9727, 275.9615, 276.8248, 278.2107, 283.3023, 283.6485, 287.7710, 290.6639, 294.7764, 297.4136, 298.1441, 300.8390, 303.4056, 308.2222, 313.7270, 314.8162, 315.5434, 319.1043, 323.8042, 326.5398, 328.0819, 329.1380, 330.6497, 332.9027, 338.3631, 344.7732, 347.2629, 354.3735, 363.8352, 367.3328, 369.9843, 375.3745, 378.8428, 385.9095, 387.5333, 391.1753, 395.0531, 404.6768, 415.8159, 416.6000, 421.9001, 428.8551, 433.6355, 438.5475, 441.0520, 445.5911, 449.0547, 455.6472, 459.5758, 471.0774, 485.5844, 489.2702, 495.8234, 499.8632, 502.0566, 517.0627, 519.9800, 538.0403, 551.5893, 563.5836, 568.4172, 569.4320, 590.9056, 598.4154, 612.3420, 615.4857, 617.5691, 653.3178, 675.3961, 688.4069, 697.9654, 699.9596, 705.7460, 709.0949, 716.5710, 721.2504, 724.3288, 731.8707, 737.3368, 738.6217, 740.4841, 756.6564, 756.8842, 761.5842, 766.6522, 770.1076, 777.0842, 778.5974, 782.3085, 784.7427, 787.4557, 788.1105, 789.4642, 794.2619, 797.7723, 800.5731, 803.1808, 805.5793, 808.6450, 810.8194, 814.0333, 817.8237, 821.6171, 823.9312, 824.4350, 826.7716, 829.9908, 832.3194, 833.8335, 836.2428, 839.4539, 844.8755, 848.9743, 856.1384, 858.6868, 863.7843, 874.5180, 880.9192, 991.1626, 998.2264, 1036.6350, 1044.6613, 1073.4507, 1083.5926, 1094.5917, 1102.7611, 1111.9077, 1114.8801, 1123.8783, 1127.6887, 1130.3048, 1132.9010, 1142.5417, 1151.7126, 1155.1841, 1175.6426, 1178.8757, 1193.6223, 1194.6293, 1199.3706, 1208.0139, 1210.8757, 1218.9430, 1221.4895, 1223.6891, 1225.4801, 1227.2738, 1231.7365, 1235.2556, 1237.5759, 1239.2788, 1242.6924, 1247.8157, 1250.7786, 1256.9710, 1260.9908, 1264.3613, 1269.5509, 1274.8238, 1285.6973, 1287.8170, 1303.2432, 1326.4484, 1370.0481, 1393.0162, 1402.1030, 1411.2238, 1422.1561, 1488.4759, 1498.2281, 1511.1865, 1528.9465, 1690.5339, 3091.3872, 3166.6373, 3178.3345, 3197.6328, 3205.6295, 3214.0815, 3277.6752, 3304.8087, 3362.4527	
T3-O1-ZeO-C ₄ H ₉ (ads)	243	37.8615, 39.3573, 58.3591, 66.4559, 70.2505, 83.7751, 85.2055, 94.9047, 108.5777, 110.2761, 112.2365, 115.8789, 122.4849, 123.9782, 128.0870, 135.1427, 139.4332, 142.1057, 146.2156, 147.7641, 153.0927, 154.8919, 160.2243, 167.4085, 171.1385, 174.0287, 175.5258, 177.3156, 179.1630, 181.8975, 185.4210, 188.3552, 190.9734, 195.7574, 196.7517, 201.1920, 202.7448, 207.9785, 210.1855, 212.0316, 213.7659, 219.8497, 224.1815, 232.1284, 232.5763, 235.8851, 238.9964, 242.6888, 245.3529, 247.9643, 251.9833, 253.8285, 258.1341, 259.0925, 260.6415, 265.0452, 266.0182, 270.9923, 273.1764, 274.0819, 276.7634, 277.9974, 282.1679, 283.8121, 286.6369, 287.6750, 290.5293, 295.2522, 297.5292, 300.7856, 302.1956, 306.9840, 310.8444, 315.0061, 316.5347, 317.5903, 323.8554, 324.3620, 329.3371, 331.6137, 332.5873, 333.6684, 337.3601, 341.8200, 349.1258, 350.5249, 363.0360, 363.6965, 368.1567, 373.8149, 378.9698, 384.7888, 386.7378, 392.2879, 392.9083, 405.3004, 412.8601, 417.8660, 421.1612, 422.3709, 429.4958, 435.2676, 437.1952, 442.1381, 445.0275, 454.1629, 458.0710, 465.0009, 481.2729, 491.6769, 496.0252, 498.9325, 502.4189, 517.8747, 523.7191, 536.1259, 548.9541, 563.3770, 566.1942, 570.2764, 574.9744, 595.1347, 606.6448, 612.9628, 614.3973, 648.7890, 658.1911, 676.1304, 691.3482, 697.2544, 699.3114, 700.4004, 716.3011, 720.0440, 724.0641, 730.0442, 737.9225, 739.8816, 747.1160, 755.1529, 757.2835, 759.6433, 764.9481, 769.8222, 772.7300, 776.2014, 779.4328, 781.4263, 785.2494, 787.8038, 790.4157, 792.2585, 792.9065, 795.6407, 799.3694, 802.7466, 806.9633, 809.7900, 811.7714, 813.8606, 818.3997, 819.1511, 824.5841, 826.4599, 829.4330, 830.5020, 832.0234, 836.2730, 841.9625, 842.3720, 844.6701, 846.0550, 850.7155, 856.5046, 859.0881, 863.3853, 874.8929, 929.0985, 943.5392, 982.4088, 1054.7526, 1092.2848, 1095.0314, 1121.3217, 1126.2036, 1127.9681, 1133.2096, 1134.7450, 1138.0795, 1142.6547, 1151.3111, 1156.2634, 1162.5518, 1180.7653, 1183.5359, 1193.8164, 1198.2735, 1201.4713, 1208.6661,	None

		1214.3858, 1221.9358, 1224.4752, 1228.0858, 1232.5303, 1235.4506, 1236.1825, 1237.6015, 1240.2950, 1246.2513, 1250.5820, 1254.2084, 1260.7846, 1267.4325, 1268.1657, 1276.2727, 1285.0374, 1288.0059, 1294.8086, 1307.6052, 1318.3705, 1333.5602, 1337.2119, 1362.7098, 1369.6599, 1404.2250, 1406.6805, 1412.0391, 1437.4899, 1446.8666, 1516.1302, 1518.3195, 1525.9755, 1533.9884, 1537.8269, 3066.8921, 3073.5541, 3086.1386, 3113.2907, 3146.0704, 3157.3398, 3160.6098, 3200.7800, 3223.3915	
T4-O7-ZeO-C ₂ H ₅ C ₂ H ₄ (ads)	243	40.9270, 61.3492, 71.0508, 77.8790, 79.3999, 89.0106, 93.5350, 98.2600, 105.3070, 106.8314, 109.4792, 116.2214, 120.9522, 126.6073, 128.2259, 132.2503, 137.7403, 140.4683, 143.3797, 146.7734, 154.2528, 156.8624, 158.1563, 163.0659, 165.5742, 168.5674, 172.5588, 175.7515, 179.8107, 183.9749, 186.3374, 188.6261, 193.8300, 199.1445, 200.6249, 202.3227, 204.0253, 210.0821, 213.1282, 214.8838, 221.8631, 226.9246, 230.9000, 232.7482, 235.0663, 237.2715, 237.4768, 239.8787, 243.4922, 247.6723, 249.6698, 251.1445, 254.1769, 254.9502, 257.9211, 260.6301, 262.0017, 264.2682, 268.2277, 269.2311, 271.7814, 273.1861, 278.3595, 280.5220, 283.3257, 285.5008, 289.2043, 289.8439, 294.6427, 299.7269, 301.8755, 302.5456, 308.4416, 309.8098, 312.6870, 318.8607, 319.2850, 320.7184, 322.9630, 326.2338, 329.8537, 333.3589, 334.3087, 338.0488, 339.3962, 343.6336, 347.6363, 351.3857, 359.6007, 360.4724, 367.6080, 371.3765, 373.7566, 376.9839, 379.1755, 383.5322, 385.5365, 391.3935, 396.7963, 399.0326, 406.1529, 407.7752, 409.7234, 419.6337, 426.5847, 431.7036, 437.9968, 440.6470, 452.3775, 466.2192, 471.0238, 483.4693, 485.8539, 500.6765, 506.3014, 513.7592, 524.2400, 539.0217, 541.6378, 549.4293, 564.8598, 578.0949, 581.9379, 590.0223, 594.8281, 606.1254, 615.3132, 649.8592, 655.0405, 667.4155, 671.2074, 674.5348, 676.2716, 681.4314, 685.6907, 694.1130, 709.0988, 716.7644, 720.9162, 723.4101, 737.2300, 742.9480, 747.1450, 752.9123, 753.6135, 759.0077, 763.9022, 765.7236, 772.5437, 773.8791, 777.4539, 778.7437, 781.2019, 783.3808, 784.3350, 786.8191, 795.7313, 797.3596, 800.8715, 803.5744, 806.6320, 807.3592, 809.0090, 813.2670, 814.3719, 818.3526, 820.1472, 823.0682, 823.8974, 829.8418, 833.4093, 836.5647, 837.1032, 839.5582, 847.2229, 849.2066, 850.8113, 857.2555, 868.7409, 887.5181, 1014.8424, 1033.0863, 1038.1722, 1096.3027, 1107.5052, 1108.7903, 1113.6241, 1119.5518, 1123.3849, 1131.4749, 1141.2422, 1143.2552, 1149.8739, 1155.3779, 1159.2833, 1169.2660, 1174.1413, 1181.1854, 1194.2489, 1200.4800, 1206.5740, 1211.2569, 1216.0814, 1219.7394, 1220.8896, 1224.7398, 1229.5993, 1231.1918, 1238.1794, 1240.0936, 1246.4740, 1248.1634, 1250.5402, 1252.9960, 1255.3512, 1258.7304, 1269.6079, 1270.8799, 1285.7030, 1293.9421, 1296.2264, 1304.5787, 1333.3492, 1333.9078, 1337.7211, 1354.4868, 1403.0955, 1412.8160, 1451.3604, 1493.9806, 1522.5092, 1546.5006, 1561.9463, 1732.9530, 3127.9448, 3168.1916, 3177.6688, 3190.4042, 3214.0471, 3222.8893, 3246.6137, 3255.6734, 3282.9114	None
T4-O7-ethylene dimerization-TS	243	-315.4737, 62.5615, 68.4929, 72.1026, 75.0840, 79.8204, 89.6374, 93.3408, 98.2034, 99.8591, 104.9234, 107.3078, 114.5145, 120.2987, 123.8470, 126.2916, 130.4888, 132.3723, 140.5056, 142.8675, 148.6176, 151.5229, 154.0359, 160.4395, 161.7004, 162.6417, 172.1437, 175.1425, 175.5600, 178.2607, 182.2951, 184.8929, 188.1465, 191.8860, 195.5589, 199.5460, 202.6421, 204.4782, 212.0002, 213.5115, 214.0036, 220.8450, 227.0675, 231.2284, 233.4733, 235.8139, 239.3138, 239.5803, 241.7673, 244.4923, 247.3995, 248.9179, 251.1953, 252.6042, 254.0134, 255.6963, 258.9091, 261.6254, 263.3661, 267.1278, 269.7572, 271.0984, 271.9864, 277.7269, 279.2386, 280.6381, 282.3535, 287.6148, 289.3853, 290.9922, 294.7220, 298.3057, 305.6224, 306.0058, 309.2357, 314.1410, 319.1444, 319.6079, 323.8260, 324.6523, 325.9727, 330.6817, 332.1538, 334.9600, 336.9575, 338.1611, 342.4158, 347.3267, 349.6372, 356.0487, 360.6946,	-315.4737

		366.0629, 369.1422, 372.4812, 376.2888, 379.0286, 380.6634, 385.0062, 389.4090, 394.0655, 401.4215, 404.3158, 405.3399, 414.0042, 417.3796, 431.0647, 437.0987, 440.9872, 441.9772, 451.1756, 457.8928, 467.1850, 479.8547, 490.4100, 500.4099, 508.7915, 513.9177, 528.3655, 540.3506, 550.8712, 553.4228, 568.7290, 578.1508, 587.1800, 592.9963, 601.4584, 606.8522, 622.9671, 648.5679, 667.9248, 669.1268, 674.6100, 675.4964, 680.8955, 691.9895, 695.3067, 701.7221, 709.7401, 711.0283, 717.0099, 722.2353, 738.4661, 740.3316, 748.4005, 749.8221, 754.4653, 755.3362, 757.7012, 765.1328, 765.7884, 771.9081, 776.8858, 778.0555, 784.1608, 786.7243, 788.0550, 794.0611, 796.4608, 798.1934, 800.9316, 802.3722, 805.2125, 806.2805, 812.0595, 814.2092, 816.4347, 819.3265, 821.4516, 825.1866, 829.1340, 831.5892, 832.6924, 837.0533, 838.2086, 842.9910, 843.5872, 846.1653, 847.6302, 863.7268, 903.9350, 944.7488, 1020.7728, 1034.7503, 1048.9621, 1058.5599, 1095.2096, 1096.9397, 1103.5493, 1111.6551, 1119.4346, 1123.2003, 1136.6095, 1141.5371, 1145.3431, 1147.9246, 1153.4443, 1160.3813, 1164.4893, 1175.0004, 1188.2263, 1191.0771, 1195.5322, 1205.3080, 1208.8332, 1211.1137, 1214.6444, 1217.0141, 1222.0289, 1224.9573, 1229.9577, 1233.1083, 1236.4235, 1237.0304, 1241.4080, 1245.0259, 1247.1843, 1249.2206, 1251.0384, 1262.2456, 1265.5224, 1278.9812, 1283.8092, 1291.6045, 1302.6908, 1327.2210, 1333.4337, 1351.8996, 1388.4970, 1394.8697, 1476.1370, 1480.3656, 1486.6467, 1519.1108, 1693.2148, 3111.2898, 3183.7627, 3191.7366, 3202.1345, 3219.7836, 3222.1393, 3277.3308, 3305.1487, 3363.4008	
T4-O7-ZeO-C ₄ H ₉ (ads)	243	57.0782, 65.9279, 68.0500, 75.0416, 80.5516, 89.4442, 93.0297, 94.1052, 98.7885, 103.7004, 109.8705, 114.4501, 119.0241, 125.2345, 129.8662, 135.5610, 138.8165, 143.2704, 147.7073, 149.9512, 153.9766, 155.8830, 159.5278, 162.3028, 166.0753, 172.3620, 176.0290, 182.4925, 186.6658, 188.2431, 190.8812, 198.1221, 199.5660, 201.7064, 206.7991, 210.2373, 214.0513, 220.4460, 222.6030, 227.0628, 229.2866, 232.1697, 234.4758, 236.5084, 237.6986, 239.2896, 243.0788, 246.2163, 248.4060, 250.3286, 251.9609, 253.4197, 257.3981, 259.6932, 262.3080, 263.1767, 267.7164, 269.6960, 270.1193, 271.1526, 273.1768, 277.3799, 281.6309, 282.4123, 286.7997, 289.7936, 292.4640, 293.4713, 298.7085, 304.9310, 305.8375, 307.8705, 315.5509, 316.6120, 318.2047, 320.3526, 322.2153, 325.4173, 326.6098, 329.7470, 332.7670, 334.8196, 337.6797, 341.8261, 345.7455, 348.0356, 353.0554, 360.9781, 363.2403, 369.8199, 373.7408, 376.2127, 378.8843, 385.1801, 388.7872, 391.9315, 399.5063, 401.1949, 406.9936, 409.8341, 418.0655, 421.4960, 429.4266, 435.7612, 438.2318, 439.5788, 453.3398, 465.3762, 472.0436, 483.9228, 488.5317, 501.0411, 504.4328, 514.0474, 530.0730, 539.0989, 545.5007, 550.5591, 564.1578, 577.9537, 582.1195, 590.1743, 594.5619, 606.1722, 615.9710, 648.3736, 653.7793, 666.5093, 671.1571, 673.5772, 675.1472, 682.7456, 684.5658, 693.4330, 708.2457, 714.3515, 720.5992, 721.6166, 735.3722, 743.0863, 745.3352, 747.5749, 752.6662, 753.7686, 759.3235, 763.4081, 765.4960, 772.4565, 773.5160, 777.3326, 778.1791, 780.8501, 783.5190, 785.2861, 787.9046, 797.0570, 797.9511, 800.8456, 803.6542, 806.1707, 807.2866, 809.0531, 813.2574, 815.5713, 818.4579, 823.5319, 823.8763, 824.6522, 827.5702, 828.8062, 833.8877, 836.8877, 838.6376, 839.3434, 849.4307, 851.0303, 859.7206, 924.0202, 948.4358, 966.4187, 1064.0538, 1090.6833, 1094.2535, 1112.8548, 1114.5294, 1123.5065, 1131.7642, 1140.3007, 1142.6789, 1147.9121, 1151.2207, 1158.4203, 1159.8003, 1169.2055, 1176.4991, 1179.8210, 1191.1894, 1194.5261, 1203.0089, 1212.3356, 1215.0725, 1218.8748, 1220.0542, 1224.0623, 1230.2978, 1230.5446, 1237.3159, 1241.9398, 1245.7844, 1248.5781, 1251.8334, 1254.4172, 1258.0138, 1270.1658, 1272.8043, 1274.1526, 1284.3494, 1290.1145, 1297.0051, 1302.3706, 1313.8233, 1328.5567, 1330.0270, 1343.3834, 1354.0778, 1355.6938, 1408.6556, 1441.0989, 1443.2703, 1496.1438, 1508.6139, 1512.2960, 1516.9538, 1529.4267, 3052.3239,	None

		3073.9473, 3096.7263, 3118.0829, 3149.8044, 3173.7341, 3182.2362, 3192.1409, 3271.2369	
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Supplementary Table 18. Calculated Harmonic Vibrational Frequencies (cm^{-1}) for adsorbed species and transition states of $\text{C}_6\text{H}_{13}^+$ formation of propylene dimerization.

FileName	Number of Frequencies	Full Frequency List (cm^{-1})	Imaginary Frequencies
Tl-Ol-ZeO- C_3H_7 $\text{C}_3\text{H}_6(\text{ads})$	261	39.4486, 60.0105, 62.4215, 70.3442, 76.9970, 81.9058, 83.6666, 96.0873, 101.7936, 102.3470, 110.0310, 113.5089, 115.1465, 118.4257, 121.0650, 124.3231, 127.5058, 133.7777, 139.6440, 146.5505, 152.6808, 157.5247, 160.0931, 161.4483, 162.1131, 167.0151, 173.7815, 174.6745, 179.3025, 180.6850, 182.9311, 184.8948, 187.0723, 190.8899, 191.7804, 195.2489, 200.1057, 202.6181, 205.1294, 210.0075, 214.2336, 216.1157, 218.7337, 219.8152, 226.0008, 227.6825, 229.1129, 232.6867, 236.4359, 238.9950, 241.6727, 244.4283, 246.1205, 250.2410, 252.9826, 257.1637, 259.7774, 261.3170, 261.9824, 266.0719, 268.8561, 270.9504, 275.3838, 276.5269, 278.1141, 279.3564, 281.2914, 283.5699, 289.0821, 292.1571, 295.3930, 296.3617, 299.4923, 301.1628, 305.7841, 306.6831, 310.6173, 313.2932, 318.4159, 320.9052, 327.0543, 328.7019, 330.9455, 333.1985, 336.4390, 342.7960, 345.9854, 350.9871, 355.7623, 362.5098, 364.2628, 367.5697, 372.2221, 379.3479, 383.4812, 389.2947, 392.4056, 395.9430, 400.3067, 403.0451, 405.3166, 412.7520, 414.0922, 416.5048, 424.3283, 428.6440, 435.0110, 441.2769, 443.8002, 450.8389, 456.7483, 460.3942, 468.8601, 474.3796, 482.0532, 490.6987, 491.8183, 493.1538, 497.6921, 510.3645, 512.0554, 520.6422, 531.3577, 548.0290, 559.4767, 565.5663, 569.3879, 584.0719, 590.6629, 596.8654, 604.0778, 611.9717, 635.3613, 642.9921, 675.2512, 678.2620, 697.9177, 702.1126, 710.5052, 717.0241, 718.7504, 721.0867, 725.7383, 729.9259, 735.7571, 741.3630, 743.8702, 749.8961, 756.9433, 757.4203, 764.2851, 769.4826, 770.6026, 777.1907, 778.0626, 782.5463, 786.5402, 788.7690, 791.6513, 795.3337, 796.9777, 799.4088, 805.5059, 808.3078, 808.9975, 812.2172, 813.7418, 818.7473, 819.7018, 822.4223, 826.0620, 828.9042, 831.6694, 834.0891, 834.7333, 842.1698, 844.7310, 847.8409, 849.7548, 853.6844, 859.3540, 864.8009, 871.0588, 881.9901, 929.1342, 942.7176, 961.4938, 970.7677, 975.8764, 985.7755, 1067.5349, 1106.2682, 1109.8886, 1115.8862, 1121.9247, 1131.8921, 1135.8960, 1138.4679, 1141.1140, 1146.7820, 1150.7915, 1156.7322, 1173.0516, 1180.6076, 1188.6927, 1197.3984, 1198.1376, 1201.4210, 1204.7069, 1206.6542, 1207.9468, 1209.6458, 1213.0587, 1216.3435, 1221.5988, 1225.7052, 1231.9375, 1234.9789, 1237.7833, 1247.1582, 1255.0090, 1258.0715, 1258.7910, 1260.7160, 1267.1733, 1283.8243, 1292.8757, 1304.4701, 1306.2472, 1314.4466, 1331.0044, 1368.1383, 1376.5636, 1379.9960, 1384.8394, 1416.0604, 1428.2862, 1431.0815, 1441.2902, 1462.9132, 1475.6008, 1497.4637, 1509.7267, 1513.6238, 1548.3793, 1562.9751, 1572.2093, 1754.0733, 3091.0657, 3120.4936, 3158.4842, 3164.1986, 3177.9810, 3189.4326, 3198.4733, 3213.3798, 3223.0597, 3245.8961, 3258.5245, 3287.5441, 3310.3193	None
Tl-Ol-propylene	261	-300.0920, 69.0867, 78.5559, 82.3290, 88.1013, 93.8240, 99.2948, 107.8716, 109.5297, 111.6614, 114.3908, 118.1044, 123.8231, 126.7670, 132.4823, 135.3116, 139.7734, 141.9743, 150.8522,	-300.092

dimerization-TS		151.3765, 160.4790, 161.2340, 163.1609, 168.7774, 170.8696, 176.7799, 177.1992, 179.2156, 182.1815, 185.7519, 189.0295, 191.5396, 193.7291, 197.7454, 197.8939, 199.5363, 200.9877, 207.9638, 213.1671, 216.4563, 220.3788, 222.2263, 223.6868, 226.5421, 230.1108, 232.8381, 234.8273, 236.8280, 241.4880, 242.7410, 244.5644, 247.8467, 250.4333, 251.4226, 256.7227, 258.2306, 260.6795, 261.8618, 265.9915, 268.4363, 274.6503, 277.1490, 278.2635, 278.7294, 280.4308, 284.0798, 286.4026, 289.1334, 292.7540, 295.8895, 296.6607, 299.6331, 301.0766, 307.6448, 308.9870, 310.9153, 312.3350, 315.4281, 320.1797, 324.5566, 327.7843, 329.0431, 330.2922, 331.5749, 333.6155, 339.8403, 344.1271, 349.2209, 353.0610, 357.8998, 363.5830, 367.9962, 371.3225, 376.5151, 382.6484, 388.1558, 390.9936, 391.9467, 395.5559, 399.1283, 408.2430, 411.0175, 413.8188, 418.8405, 426.0652, 427.4160, 434.8939, 447.5311, 448.7458, 454.6729, 456.7923, 461.0541, 467.9318, 479.1759, 484.0094, 490.5093, 494.3627, 497.9890, 505.2537, 514.0086, 515.5832, 521.3610, 534.0705, 538.8605, 552.0132, 561.1287, 566.8442, 572.3285, 588.3357, 591.2288, 600.7999, 611.2374, 619.6827, 651.1341, 656.3823, 671.9351, 698.6918, 711.1364, 711.4561, 712.9787, 713.7547, 719.8125, 724.6641, 725.4947, 737.5307, 738.3365, 742.1576, 744.5152, 755.5868, 756.8506, 764.2315, 769.3805, 770.4472, 775.1930, 776.7403, 778.0374, 780.9012, 788.2328, 790.3972, 793.2084, 794.5860, 795.1867, 798.8770, 801.3196, 806.1744, 810.4687, 814.1603, 815.5130, 817.6305, 820.5063, 822.7780, 824.5225, 825.9039, 831.0782, 832.7395, 840.1953, 844.2044, 846.2857, 849.9139, 853.0014, 856.2274, 862.8033, 871.5947, 880.6467, 931.4869, 957.8214, 973.4513, 997.0655, 1008.4442, 1046.4537, 1052.5300, 1061.2823, 1088.6153, 1092.5980, 1110.5601, 1114.6383, 1117.2521, 1127.7399, 1132.5989, 1138.1693, 1143.8533, 1150.6857, 1163.0799, 1165.5259, 1168.2791, 1176.2459, 1186.7680, 1188.7987, 1189.5174, 1199.1857, 1201.6095, 1207.3724, 1211.2026, 1215.3984, 1217.3549, 1222.6680, 1223.3161, 1226.2599, 1230.2208, 1240.9998, 1242.7966, 1246.9978, 1249.7964, 1250.8170, 1254.2943, 1267.3696, 1282.2679, 1284.2565, 1287.8285, 1289.8206, 1308.1997, 1325.1844, 1347.3823, 1348.8245, 1368.8539, 1398.7586, 1433.2258, 1438.1840, 1446.4220, 1453.2502, 1478.0562, 1485.0495, 1497.4609, 1514.4453, 1523.9146, 1532.8487, 1553.8827, 1717.1802, 3079.0578, 3139.3057, 3151.9623, 3171.3913, 3192.4821, 3215.9159, 3239.7187, 3278.0863, 3281.1812, 3298.1863, 3328.5190, 3334.0509, 3380.1807	
Tl-Ol-ZeO-C ₆ H ₁₃ (ads)	261	37.6016, 46.0713, 58.3849, 68.5928, 74.9893, 80.7790, 85.6617, 91.9523, 94.5555, 95.0954, 99.2280, 108.6341, 115.6955, 126.0619, 126.4877, 128.1154, 132.9525, 135.9039, 141.6556, 149.0640, 153.5800, 158.0369, 159.6480, 164.0509, 165.5199, 170.9275, 173.8529, 178.8643, 180.4958, 182.5676, 184.8318, 187.4938, 192.1535, 193.0932, 197.7925, 200.2128, 202.1801, 204.8807, 210.0460, 213.0825, 215.2094, 216.5175, 221.3852, 222.6714, 228.5320, 229.1635, 236.3335, 238.7010, 239.8455, 243.5110, 244.6982, 246.6652, 250.2344, 254.1231, 255.6150, 257.2863, 259.2504, 261.6825, 263.6383, 264.9719, 267.8236, 270.7414, 273.9427, 275.5840, 278.0684, 282.2874, 283.0621, 286.2100, 289.6888, 293.7213, 298.6446, 299.1587, 301.7967, 303.8738, 307.9447, 310.4766, 313.3665, 316.5795, 318.6375, 320.0643, 323.4890, 328.1322, 329.5582, 331.5590, 335.6523, 344.1150, 346.5487, 349.6721, 355.2382, 357.7071, 364.3094, 367.0824,	None

		371.5101, 379.0357, 381.0154, 387.2512, 389.0645, 395.6172, 399.1806, 405.2137, 414.2331, 416.7626, 419.4461, 425.5274, 427.8299, 432.6425, 437.3014, 443.2832, 450.5437, 451.9791, 456.3652, 460.7559, 471.7529, 478.2116, 488.0896, 498.3313, 501.6396, 504.4130, 510.1001, 514.3660, 523.4330, 538.4105, 552.9900, 560.9442, 567.1271, 569.0662, 590.8228, 597.7015, 609.4566, 611.2174, 615.8595, 645.2759, 674.2111, 674.7621, 695.9929, 701.4909, 702.1694, 703.5608, 712.7278, 718.7182, 725.8440, 729.4385, 734.9914, 737.8936, 740.7170, 750.3553, 759.5866, 759.9032, 765.3212, 769.5590, 771.6702, 774.3800, 779.4698, 781.2077, 782.8197, 790.3933, 791.5085, 794.7522, 795.8588, 799.4454, 801.5521, 805.4689, 809.8761, 810.7188, 817.8353, 818.8954, 824.1723, 825.4662, 828.5208, 829.9876, 832.2847, 835.2163, 840.2956, 842.5120, 843.5505, 847.0614, 848.4893, 852.2421, 856.8397, 858.7009, 861.4589, 867.9939, 878.9227, 885.0636, 921.2449, 956.6776, 995.9772, 1004.1501, 1044.3469, 1071.5271, 1095.6273, 1117.0872, 1123.2764, 1132.2051, 1135.6293, 1148.9521, 1152.3448, 1153.8821, 1157.8656, 1163.9434, 1172.3290, 1180.2481, 1185.8439, 1191.8278, 1197.4806, 1200.0563, 1204.8918, 1211.2810, 1212.2972, 1218.6889, 1220.7361, 1225.8849, 1229.0600, 1231.0895, 1238.9307, 1239.6363, 1246.9933, 1253.7909, 1256.2826, 1261.1575, 1262.1013, 1265.3756, 1271.7127, 1276.7476, 1277.4968, 1286.2779, 1289.7269, 1302.3097, 1307.2760, 1330.1448, 1340.6803, 1369.3496, 1379.2062, 1395.4853, 1408.0766, 1412.3356, 1415.1370, 1426.0276, 1428.5981, 1445.3580, 1451.0794, 1483.4958, 1498.9075, 1507.5928, 1514.8314, 1519.8691, 1527.2819, 1546.8647, 3052.1727, 3059.9328, 3089.1989, 3095.3628, 3117.4964, 3134.2073, 3157.1679, 3180.9352, 3183.9443, 3188.4126, 3190.0595, 3200.8601, 3224.6630	
T3-O1-ZeO-C ₃ H ₇ C ₃ H ₆ (ads)	261	34.1746, 51.7825, 58.8853, 70.1903, 75.9499, 85.0585, 89.6147, 100.3155, 107.7794, 109.3173, 117.5352, 117.7628, 121.0630, 122.8157, 128.1448, 128.5315, 131.5946, 140.2938, 143.3004, 150.9748, 152.2704, 155.8734, 164.6051, 166.2559, 171.5889, 175.3305, 176.7782, 178.2222, 182.0667, 182.5323, 187.4345, 188.1969, 190.4452, 191.8072, 194.1503, 198.6660, 201.2540, 201.9698, 204.7967, 209.1735, 214.1366, 217.2926, 218.4689, 219.8876, 225.3470, 227.6583, 233.4518, 234.5914, 237.9453, 242.8812, 243.9182, 247.2079, 248.8196, 250.3315, 253.6783, 256.1904, 259.0266, 262.5135, 266.0430, 267.5692, 270.1727, 273.7093, 276.2340, 277.7587, 279.8020, 283.0176, 286.6175, 289.2547, 292.2034, 293.7253, 296.4078, 297.9181, 299.0436, 306.2758, 307.0964, 310.5497, 313.6537, 314.2854, 316.3128, 322.9233, 326.0672, 327.0522, 328.3226, 333.1889, 337.0629, 341.5990, 346.7951, 349.6797, 355.0202, 361.0736, 365.0707, 370.3410, 372.4186, 378.7378, 386.5730, 388.2859, 390.0580, 392.4740, 397.1813, 403.3154, 406.1774, 414.3047, 420.4653, 421.7028, 431.9872, 438.5754, 443.5385, 446.3939, 450.5997, 453.8748, 460.2973, 468.5193, 472.8301, 482.4203, 490.2016, 491.5199, 497.1539, 502.2784, 510.2849, 519.8962, 529.4713, 539.6542, 546.0496, 561.7199, 564.9967, 571.5626, 576.7962, 591.2729, 605.1078, 607.1738, 609.0688, 613.8954, 631.7322, 652.6596, 668.9009, 672.9829, 694.7875, 697.6166, 709.9726, 712.7040, 714.0066, 723.4841, 728.0942, 729.8794, 734.7187, 738.4548, 742.3111, 751.0822, 756.2729, 761.5764, 771.2952, 772.2708, 774.8162, 776.7881, 780.5099, 781.0113, 786.1403, 790.1885, 792.5078, 795.5643, 796.4894, 798.1092, 801.0220,	None

		802.8835, 805.7795, 809.4369, 815.8458, 817.6975, 819.8419, 822.7191, 826.2123, 828.2301, 831.7483, 835.6023, 838.1683, 842.2695, 843.0582, 847.1973, 849.7907, 852.6064, 860.0285, 867.9909, 870.4109, 877.0307, 932.3065, 944.8849, 955.9288, 977.0393, 991.4618, 1009.8314, 1045.4776, 1086.0403, 1109.8265, 1116.5347, 1120.5155, 1123.6961, 1126.9493, 1129.8298, 1132.4596, 1139.6288, 1151.6305, 1153.4504, 1155.5879, 1174.7933, 1179.3530, 1186.8270, 1193.3070, 1194.0567, 1199.4488, 1203.8847, 1205.9385, 1208.8516, 1211.6301, 1216.4604, 1219.9962, 1221.1298, 1225.3241, 1227.0020, 1231.2762, 1232.7067, 1242.5288, 1243.8841, 1250.3452, 1254.0227, 1258.4875, 1269.4474, 1275.9899, 1278.9206, 1289.1999, 1308.9992, 1324.9546, 1336.2100, 1363.4232, 1364.1349, 1367.6217, 1402.4007, 1433.9872, 1440.4188, 1449.3604, 1468.9266, 1476.4364, 1493.7201, 1502.4779, 1510.1287, 1512.5221, 1554.6442, 1622.1307, 1753.1784, 3082.1347, 3123.4962, 3164.6347, 3171.0240, 3171.9318, 3181.0492, 3190.3965, 3207.1387, 3258.4545, 3272.9100, 3278.5671, 3286.1698, 3305.2934	
T3-O1-propylene dimerization-TS	261	-273.1083, 60.2012, 64.1000, 77.8540, 91.9486, 94.4416, 100.5426, 110.0066, 110.6820, 113.6286, 118.7240, 122.0976, 124.1579, 126.7747, 130.6481, 131.2616, 140.2259, 140.8202, 144.5971, 148.8245, 151.4726, 156.9789, 159.7764, 166.8539, 169.9751, 173.1483, 176.0886, 180.0539, 180.7173, 183.4731, 187.0357, 189.6245, 190.2971, 191.1457, 195.5373, 198.7827, 199.8235, 206.2348, 207.6736, 209.2915, 215.6371, 220.8649, 221.5412, 223.2499, 225.5461, 229.0169, 230.2516, 235.4487, 238.4622, 245.2657, 247.2545, 250.1679, 251.3390, 252.7527, 256.8876, 258.7922, 261.0467, 264.1168, 264.5259, 269.6335, 271.8640, 274.7835, 275.2944, 278.3040, 280.5532, 285.5393, 286.6497, 290.6241, 293.9209, 296.5438, 297.6548, 299.3324, 301.0161, 303.4861, 309.2004, 310.4964, 313.8548, 317.2772, 323.4254, 325.9977, 328.7042, 328.8768, 329.4655, 334.3234, 336.1185, 339.5142, 346.9855, 347.4459, 350.7581, 358.5650, 363.6160, 367.4295, 367.9625, 375.7177, 382.5236, 384.3540, 388.0090, 389.5886, 393.7570, 397.5761, 407.9075, 409.6222, 412.5260, 420.0374, 423.8709, 433.8463, 439.6066, 445.4001, 449.3089, 450.2173, 455.8024, 457.1110, 468.7781, 487.3799, 489.1768, 491.7400, 494.6828, 496.5428, 502.1503, 518.6727, 523.1027, 535.8180, 538.9775, 543.3737, 560.9896, 568.2319, 572.2207, 580.8654, 590.4984, 591.6951, 599.7789, 610.7150, 618.4586, 651.4795, 654.2651, 671.2547, 693.1973, 705.5822, 710.1581, 712.1686, 714.4815, 718.7888, 725.1033, 736.0979, 736.9392, 738.2813, 740.6300, 744.9286, 756.4760, 758.8437, 760.8928, 766.4227, 770.6042, 775.6165, 778.5351, 779.6415, 784.9885, 786.6387, 791.4983, 794.7838, 795.4865, 796.7431, 798.9599, 800.9298, 804.1958, 806.6409, 809.1249, 814.6509, 817.4399, 819.0958, 821.2641, 823.3292, 826.4939, 828.6852, 831.4566, 836.4128, 840.5731, 843.9799, 848.1528, 851.8559, 860.6590, 864.4039, 871.0762, 876.8472, 920.8672, 957.8394, 979.9069, 989.0476, 997.5137, 1033.5513, 1036.5545, 1047.5262, 1089.0932, 1102.7590, 1108.7277, 1110.1113, 1116.4894, 1120.6580, 1128.3435, 1129.9916, 1133.9665, 1147.0376, 1149.0924, 1151.8006, 1153.7880, 1173.3324, 1186.2578, 1190.8637, 1191.3276, 1197.3330, 1200.5724, 1205.9120, 1208.3054, 1214.8634, 1218.0931, 1224.6736, 1227.8259, 1228.5197, 1230.5728, 1232.4737, 1238.0890, 1240.4523, 1244.2613, 1247.1006, 1251.5477, 1262.6601, 1266.2813, 1281.0809, 1283.6910, 1287.1988,	-273.108

		1306.9159, 1317.5362, 1357.2710, 1363.0683, 1369.7836, 1378.8673, 1420.4848, 1444.3271, 1446.2462, 1459.4599, 1478.1954, 1489.6890, 1500.3879, 1517.7522, 1528.5584, 1563.7295, 1575.9228, 1720.9040, 3080.5431, 3140.2093, 3153.8829, 3177.4675, 3187.2958, 3218.2735, 3235.5883, 3259.9736, 3283.0223, 3300.5379, 3302.3592, 3316.7197, 3373.5302	
T3-O1-ZeO-C ₆ H ₁₃ (ads)	261	44.3753, 59.1643, 61.3542, 71.7295, 76.0630, 85.9404, 92.1196, 94.5468, 103.7192, 105.4745, 107.2785, 116.1732, 118.9427, 119.0986, 124.4379, 127.1423, 133.7083, 137.1169, 144.6331, 148.4969, 149.9432, 158.2901, 161.8111, 168.7204, 173.4853, 175.2205, 176.8303, 177.1322, 179.6737, 182.5968, 185.7368, 190.0582, 192.6537, 194.7245, 196.8726, 200.1384, 206.0903, 209.4612, 213.1021, 214.1518, 218.3478, 222.2999, 223.1005, 227.3631, 230.6985, 232.9058, 237.6018, 240.0630, 240.4932, 244.4525, 247.9683, 248.4687, 251.2677, 254.0654, 256.3095, 257.8967, 261.2637, 264.9617, 268.1021, 270.2791, 272.5535, 275.2799, 277.1605, 279.3255, 282.6584, 283.8786, 289.4988, 290.9950, 292.7657, 295.8776, 297.9911, 300.3679, 305.1120, 309.5828, 311.4308, 313.4682, 317.6073, 318.9861, 320.3019, 326.4301, 327.3868, 328.5927, 329.9564, 335.1433, 344.5124, 348.5145, 349.6981, 355.6265, 363.3707, 364.1861, 365.5628, 370.3916, 373.4459, 380.2459, 385.2884, 388.3802, 390.7537, 393.9791, 399.2137, 400.5558, 404.7112, 414.4144, 415.7460, 421.7265, 430.5183, 436.0971, 441.8065, 446.9454, 449.2531, 456.8780, 458.6390, 463.3218, 471.8895, 473.1733, 490.8609, 495.9318, 497.7527, 502.6748, 514.2423, 519.2875, 519.8031, 538.9504, 548.1959, 563.5457, 566.8029, 569.8709, 585.8892, 595.5249, 603.1923, 611.8159, 612.4174, 617.4346, 644.0772, 651.3622, 671.7686, 683.1712, 700.7473, 708.1253, 709.7990, 714.1041, 721.7043, 726.8782, 728.8255, 731.3890, 737.0802, 741.3849, 744.7148, 752.6689, 756.5609, 759.4395, 765.7617, 768.5137, 771.9331, 775.2181, 776.7289, 784.6976, 786.0333, 786.9354, 791.4214, 794.7862, 798.7207, 800.7657, 805.0437, 808.2409, 813.5896, 814.1660, 820.0796, 822.2281, 825.9474, 827.1149, 829.3466, 831.1434, 832.0454, 834.6440, 835.6108, 840.7779, 843.8510, 845.8817, 853.3349, 858.1383, 859.9188, 868.2710, 872.1966, 887.5038, 932.1169, 957.4567, 1000.3438, 1020.4906, 1034.5210, 1078.1444, 1091.4830, 1116.3382, 1126.0362, 1129.8043, 1134.8675, 1137.4409, 1141.2706, 1146.6632, 1155.4009, 1157.7774, 1170.3869, 1178.1674, 1179.5241, 1181.7512, 1198.7269, 1200.3044, 1204.0581, 1207.5037, 1214.5503, 1216.5844, 1220.5480, 1226.5519, 1230.4353, 1235.0610, 1236.1285, 1241.4691, 1243.0535, 1247.1519, 1251.1028, 1253.6481, 1258.2413, 1260.2105, 1260.5519, 1278.6811, 1287.0168, 1288.3920, 1290.3994, 1295.6139, 1308.7013, 1310.1112, 1343.6139, 1369.7188, 1375.8312, 1386.7057, 1392.8579, 1404.6069, 1417.8619, 1423.7000, 1431.5389, 1446.3871, 1453.3000, 1494.0051, 1502.1474, 1503.9265, 1512.2757, 1520.3914, 1535.8235, 1541.3543, 3071.9936, 3080.8091, 3084.3457, 3096.8266, 3142.0084, 3171.6982, 3175.3671, 3179.2243, 3183.5799, 3210.5514, 3246.2925, 3272.7214, 3279.0377	None
T2-O6-ZeO-C ₃ H ₇ C ₃ H ₆ (ads)	189	37.3588, 43.4594, 53.6772, 55.8640, 66.0032, 70.3352, 72.5454, 89.3240, 94.7624, 110.8710, 118.7287, 125.7363, 127.7895, 132.3002, 135.1096, 138.6772, 149.8373, 151.0793, 157.3605, 163.9397, 167.1194, 168.7608, 175.2048, 176.7624, 180.1876, 188.8026, 201.5209, 207.3185, 214.3103, 216.9560, 232.2088, 236.3277, 241.1743, 242.3726, 248.2110, 253.4750, 256.7230, 265.0690,	None

		275.9035, 278.3628, 287.6245, 292.5493, 296.7307, 300.4680, 306.1957, 308.3725, 311.0603, 314.4013, 316.6078, 322.8993, 325.6141, 330.1091, 334.4948, 336.2148, 346.5621, 353.0847, 358.9707, 365.2834, 373.6196, 390.3638, 396.8745, 403.2218, 423.1848, 434.5132, 435.3956, 439.5163, 443.6086, 444.9497, 445.5480, 448.4279, 461.3506, 466.3589, 487.0238, 510.0369, 517.5401, 554.1309, 567.8415, 585.8079, 587.9596, 592.0329, 609.4915, 613.2676, 628.2370, 640.7169, 686.4050, 687.8210, 692.3268, 699.3314, 706.1720, 710.6002, 714.5379, 719.9279, 722.2722, 724.5943, 724.9946, 728.6268, 734.2381, 738.4387, 750.4621, 753.0334, 755.9547, 756.4734, 757.5496, 772.3539, 779.5395, 789.9749, 796.1021, 799.6704, 807.1262, 815.3020, 816.4573, 817.2258, 825.2428, 830.0935, 832.3544, 835.0750, 839.0537, 843.0983, 852.9907, 858.7113, 872.2744, 876.1178, 881.5800, 896.8832, 911.3380, 940.4163, 952.8003, 957.6025, 965.6536, 970.9200, 974.9091, 1055.6189, 1085.6463, 1132.8748, 1139.4199, 1151.6325, 1155.8963, 1168.9792, 1171.1957, 1179.3391, 1186.2972, 1194.1292, 1203.5317, 1206.0880, 1216.7940, 1219.3748, 1225.2996, 1227.1185, 1234.3625, 1237.3663, 1249.0489, 1254.3608, 1257.9177, 1295.3601, 1316.6503, 1338.3408, 1340.7977, 1347.5544, 1371.8246, 1390.4943, 1426.8490, 1429.9366, 1437.4298, 1467.0944, 1469.3160, 1495.1988, 1501.6252, 1506.6344, 1508.5909, 1513.2550, 1532.0078, 1757.4602, 2220.2103, 2221.4181, 2221.9365, 2234.8150, 3045.9783, 3094.9271, 3106.8762, 3110.5402, 3144.3878, 3168.5990, 3170.9120, 3173.1692, 3206.3210, 3218.5063, 3227.8742, 3258.0081, 3280.1261	
T2-O6-propylene dimerization-TS	189	-181.8507, 17.1501, 46.1757, 72.8665, 75.0888, 79.3783, 85.1218, 90.5019, 102.2664, 110.6602, 118.8502, 125.8111, 132.4035, 138.8982, 144.0245, 148.8457, 151.0457, 156.4969, 159.5332, 164.4507, 169.5769, 171.8406, 177.4090, 178.3594, 187.4484, 189.3029, 195.2284, 200.8507, 206.1251, 224.4774, 228.1977, 232.1562, 236.0693, 242.1948, 247.5888, 254.4388, 259.6529, 265.7998, 270.7474, 275.2453, 284.0662, 288.9842, 292.9821, 299.6501, 301.3007, 305.1730, 312.7517, 314.6241, 316.5537, 318.7994, 321.8934, 323.8596, 330.2428, 335.7846, 340.5922, 345.7015, 348.7640, 352.1932, 360.1993, 372.0504, 383.1253, 393.7889, 400.5926, 412.7917, 423.9780, 435.0914, 438.4233, 440.7594, 445.9983, 449.2535, 451.6158, 455.8839, 460.1362, 467.3468, 501.9208, 513.9484, 561.2079, 570.4264, 586.2695, 588.5795, 613.4883, 623.0846, 631.4438, 655.4098, 675.8285, 680.2817, 687.8810, 690.1020, 698.1036, 701.7469, 706.4921, 719.6342, 720.9128, 724.1305, 725.4596, 727.0649, 733.0004, 738.0039, 738.3630, 749.8135, 752.3288, 755.3739, 757.1046, 762.1406, 771.5810, 779.7027, 781.0493, 791.1925, 794.6979, 796.5412, 805.1593, 813.9859, 814.8047, 818.1238, 821.5679, 829.4562, 836.7322, 840.1663, 842.1307, 843.6667, 852.8169, 870.7862, 877.1042, 877.8770, 882.1373, 897.0495, 925.2499, 948.6431, 968.9837, 988.1582, 992.7381, 1064.6140, 1098.5316, 1122.7825, 1134.3873, 1136.8124, 1147.3600, 1159.4039, 1168.1443, 1174.7544, 1180.8919, 1193.1242, 1206.1883, 1211.6595, 1212.5345, 1218.2168, 1220.0899, 1228.2558, 1230.9556, 1235.3065, 1242.9774, 1247.0269, 1256.0042, 1267.5205, 1285.9891, 1316.0532, 1329.9688, 1337.3107, 1363.8767, 1367.2899, 1386.5341, 1398.1680, 1422.4689, 1427.7771, 1455.8498, 1467.7486, 1481.4786, 1488.1325, 1505.7785, 1521.1375, 1532.9943, 1750.5533, 2220.0990, 2222.5432, 2222.6208, 2235.7287,	-181.851

		3043.0638, 3045.7443, 3060.4914, 3114.7953, 3140.7319, 3145.3373, 3147.7496, 3187.4892, 3200.7225, 3228.7560, 3272.5659, 3285.8788, 3326.2358	
T2-O6-ZeO-C ₆ H ₁₃ (ads)	189	37.3011, 48.3644, 55.0925, 79.7363, 83.9240, 92.5782, 110.3202, 114.1935, 124.0529, 129.1529, 131.6981, 136.8913, 147.7492, 150.6738, 156.8496, 160.0679, 164.3892, 165.7783, 170.6628, 178.3161, 182.3500, 193.7624, 200.2106, 201.7297, 212.5452, 225.4262, 228.0585, 238.0330, 241.2612, 248.4697, 253.0984, 256.9247, 260.3020, 264.7494, 272.7634, 275.6288, 281.6741, 287.1147, 290.3660, 292.1347, 300.5875, 305.6927, 311.6888, 313.5619, 314.5833, 318.9133, 321.8795, 326.6497, 330.6634, 333.2711, 338.6390, 341.0342, 346.1634, 353.4654, 359.3966, 366.8928, 377.6789, 393.0993, 395.6715, 398.9234, 415.2592, 429.6250, 433.7022, 436.3457, 441.3239, 445.0285, 453.8604, 465.9443, 467.3567, 476.2751, 487.5677, 502.1366, 522.8378, 526.5445, 563.2453, 578.2660, 582.9526, 588.6835, 614.0889, 630.8236, 634.3374, 650.6245, 677.3148, 687.9526, 693.0295, 697.4412, 700.8155, 705.6447, 717.8468, 718.8595, 724.5384, 727.6180, 734.4085, 735.3251, 738.1174, 743.6552, 750.1009, 752.9874, 756.0363, 757.4414, 767.1657, 772.5313, 780.5058, 786.4676, 793.7317, 795.7753, 805.0325, 808.6441, 812.8913, 815.1714, 820.0214, 826.5027, 828.7824, 837.0010, 840.6094, 846.2242, 851.4859, 868.6944, 873.2047, 875.2199, 876.9820, 883.7043, 894.2936, 904.7279, 944.0149, 967.6130, 985.4200, 988.5386, 1006.8011, 1071.4903, 1090.9997, 1129.1874, 1142.4945, 1151.1364, 1158.7833, 1161.1509, 1175.8508, 1184.1408, 1188.6190, 1195.8192, 1200.9825, 1206.5824, 1211.3956, 1215.9846, 1227.8606, 1229.7592, 1232.3854, 1240.9261, 1246.9006, 1249.0846, 1252.1842, 1281.5399, 1290.0469, 1295.8376, 1335.9074, 1341.5576, 1358.0092, 1392.1480, 1401.1104, 1408.4882, 1425.4267, 1431.9807, 1433.7992, 1459.5154, 1493.1991, 1503.5783, 1511.3311, 1515.3596, 1524.1880, 1536.5879, 1542.4808, 1551.6121, 2219.8018, 2221.7924, 2222.2221, 2234.8374, 3074.6020, 3087.7504, 3098.3357, 3112.1347, 3137.4638, 3154.7208, 3171.4391, 3179.5291, 3185.7112, 3208.3901, 3219.1721, 3247.1698, 3257.8192	None