

Supplementary Information file for the manuscript:

Oxidative Dehydrogenation of Propane over Vanadium-Containing Faujasite Zeolite

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Table S1. Elemental composition of the selected catalyst samples obtained from the energy-dispersive X-ray spectroscopy.

Sample	O [wt%]	Al [wt%]	Si [wt%]	V [wt%]
V _{1.0} FAUdes	76.6	1.2	21.3	0.9
V _{3.0} FAUdes	67.4	0.8	27.1	2.4
V _{5.0} FAU	68.9	0.7	37.7	3.7

Table S2. Results of the catalytic tests for the V_{1.0}FAU sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{1.0} FAU 0.5ml/0.5ml quartz/catalyst	400	30	5.8	34.7	0.8	43.8	20.7
		60	2.7	36.1	0.7	48.8	14.3
		90	4.4	49.1	0.9	36.4	13.6
	450	30	8.6	24.6	1.0	47.9	26.4
		60	7.7	33.7	1.0	42.9	22.5
		90	7.2	41.6	0.9	39.1	18.4
500	30	18.1	14.4	3.0	50.7	31.8	
	60	15.6	22.6	2.2	46.1	29.1	
	90	15.6	22.6	2.2	46.2	29.1	

Table S3. Results of the catalytic tests for the V_{3.0}FAU sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{3.0} FAU 0.5ml/0.5ml quartz/catalyst	400	30	5.1	30.3	0.5	43.2	26.0
		60	21.7	39.9	0.5	38.4	21.1
		90	17.0	46.3	0.4	31.3	21.9
	450	30	11.5	22.0	0.9	47.4	29.8
		60	13.0	29.9	0.6	43.3	26.1

	90	8.8	37.5	0.5	35.6	26.4
	30	27.7	12.1	2.5	51.1	34.3
500	60	26.3	18.9	1.8	46.8	32.4
	90	19.4	24.5	1.3	42.2	31.9

Table S4. Results of the catalytic tests for the V_{6.0}FAU sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{6.0} FAU 0.5ml/0.5ml quartz/catalyst	400	30	12.0	16.7	0.3	59.6	23.4
		60	20.1	28.9	0.3	47.4	23.4
		90	8.0	26.3	0.2	54.4	19.1
	450	30	18.9	10.9	0.8	64.2	24.1
		60	14.7	19.6	0.4	54.8	23.2
		90	12.8	18.9	0.5	58.9	21.7
	500	30	39.1	41.7	1.9	36.9	19.6
		60	40.4	9.9	2.5	61.5	26.1
		90	30.9	13.1	2.5	58.8	26.1

Table S5. Results of the catalytic tests for the V_{1.0}FAUdes sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{1.0} FAUdes 0.5ml/0.5ml quartz/catalyst	400	30	1.7	13.8	0.4	69.2	16.5
		60	4.4	35.8	0	50.5	13.6
		90	10.9	22.5	0	66.7	10.8
	450	30	1.5	13.8	0.5	64.6	21.1
		60	3.7	24.8	0.6	57.4	17.2
		90	3.4	31.0	0.5	57.7	10.8
	500	30	18.1	14.4	3.0	50.7	31.8
		60	15.6	22.6	2.2	46.1	29.1
		90	15.6	22.6	2.2	46.2	29.1

Table S6. Results of the catalytic tests for the V_{3.0}FAUdes sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{3.0} FAUdes 0.5ml/0.5ml quartz/catalyst	400	30	9.4	28.2	0.4	42.3	29.1
		60	6.5	37.1	0.5	37.4	25.0
		90	14.1	34.1	0.2	36.6	29.0
	450	30	16.7	19.1	0.9	47	33.0
		60	5.7	26.7	0.6	41.6	31.1
		90	10.2	41.2	0.9	39.6	57.3

	30	27.0	11.2	2.3	49.4	37.1
500	60	24.2	16.6	1.8	45.4	36.2
	90	25.7	19.5	1.6	41.8	37.1

Table S7. Results of the catalytic tests for the V_{6.0}FAUdes sample.

SAMPLE	T _r [°C]	Flow [ml/min]	Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{6.0} FAUdes 0.5ml/0.5ml quartz/catalyst	400	30	2.6	45.1	0	49.6	6.1
		60	4.2	60.1	0	31.8	8.1
		90	9.5	63.6	0	22.3	14.2
	450	30	6.1	46	0.1	40.8	13.1
		60	4.4	51.6	0.2	35.9	12.4
		90	8.9	65	0.3	19.0	15.8
	500	30	20.2	31.9	0.2	46.3	21.7
		60	11.9	43.5	0.2	39.1	17.3
		90	8.7	56.8	0.3	27.1	15.9

Table S8. Comparison of the initial catalytic performance of the studied samples with their activity after 40h (T = 450 °C, flow 60 ml/min).

SAMPLE		Conv [%]	S _{C₃H₆} [%]	S _{C₂H₄} [%]	S _{CO₂} [%]	S _{CO} [%]
V _{1.0} FAU	1 st run	7.7	33.7	1.0	42.9	22.5
	after 40h	7.5	28.5	0.9	42.8	27.7
V _{3.0} FAU	1 st run	13.0	29.9	0.6	43.3	26.1
	after 40h	8.1	3.2	0.6	43.0	26.2
V _{6.0} FAU	1 st run	14.7	19.6	0.4	54.8	23.2
	after 40h	53.4	4.9	3.5	65.8	25.7
V _{1.0} FAUdes	1 st run	3.7	24.8	0.6	57.4	17.2
	after 40h	4.6	20.0	0.5	63.4	15.8
V _{3.0} FAUdes	1 st run	5.7	26.7	0.6	41.6	31.1
	after 40h	17.1	35.3	0.5	38.9	25.3
V _{6.0} FAUdes	1 st run	4.4	51.6	0.2	35.9	12.4
	after 40h	6.0	47.7	0.1	42.3	9.9

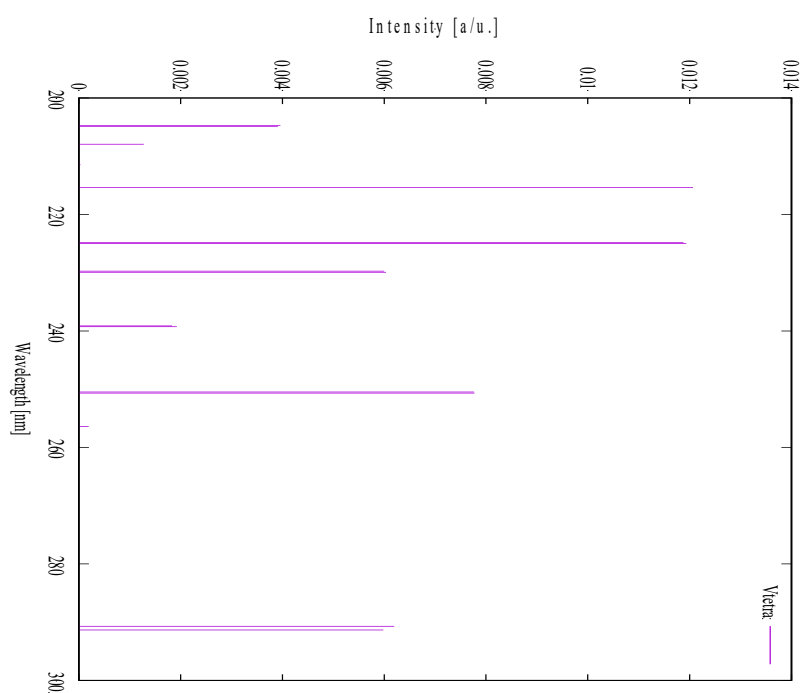


Figure S1. Theoretical (TD-DFT: PBE/def2-TZVP) UV-VIS spectrum of the VO(OH)₃ complex, in which vanadium is located in the tetrahedral environment.

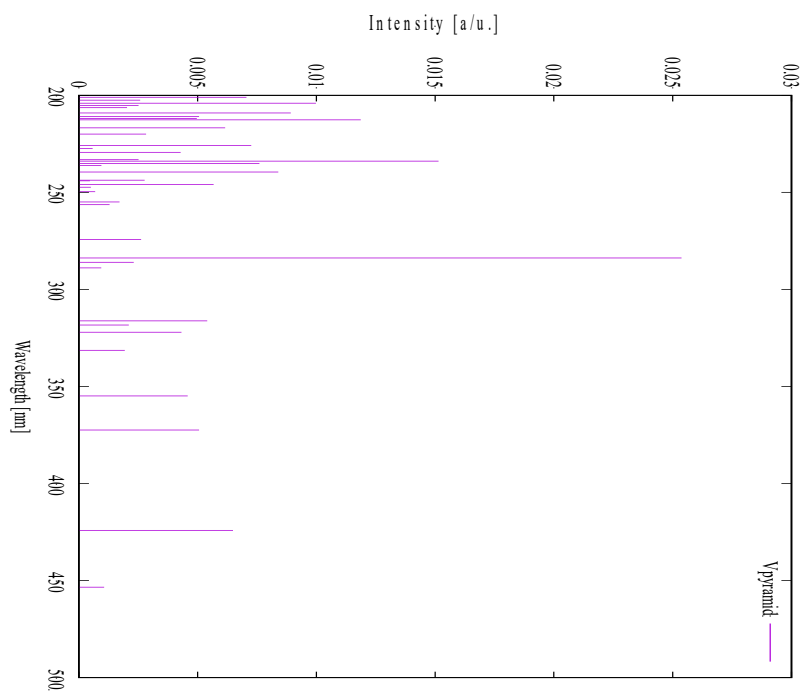


Figure S2. Theoretical (TD-DFT: PBE/def2-TZVP) UV-VIS spectrum of the VO(OH)₄ complex, in which vanadium is located in the square pyramidal environment.

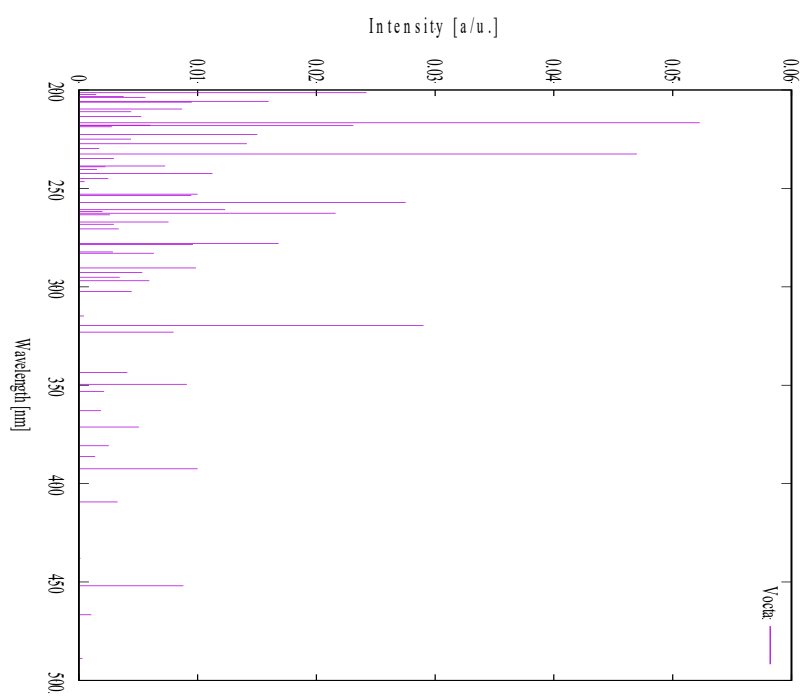


Figure S3. Theoretical (TD-DFT: PBE/def2-TZVP) UV-VIS spectrum of the $\text{VO}(\text{OH})_5^{2-}$ complex, in which vanadium is located in the octahedral environment.

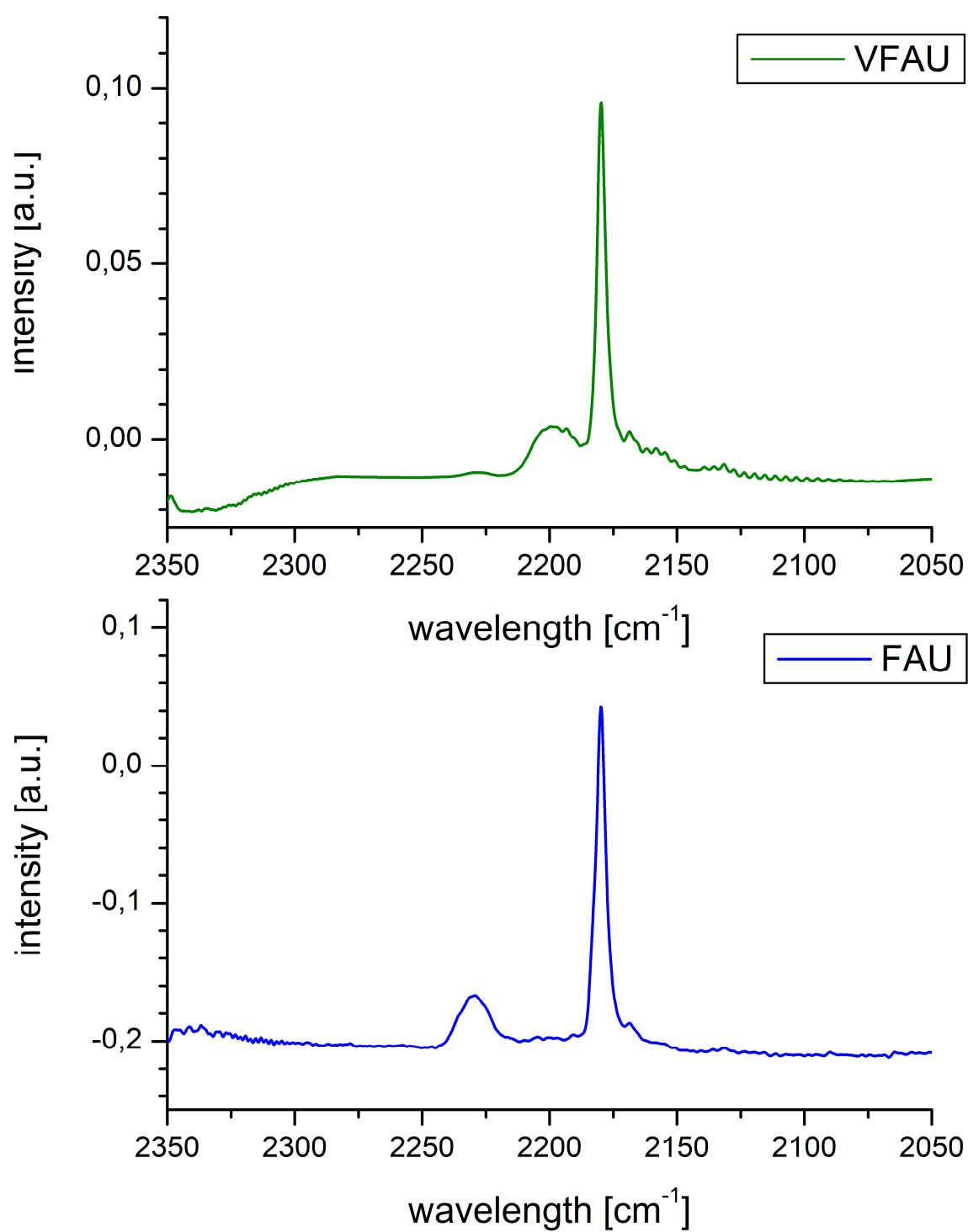


Figure S4. Exemplary IR spectra of the studied samples.

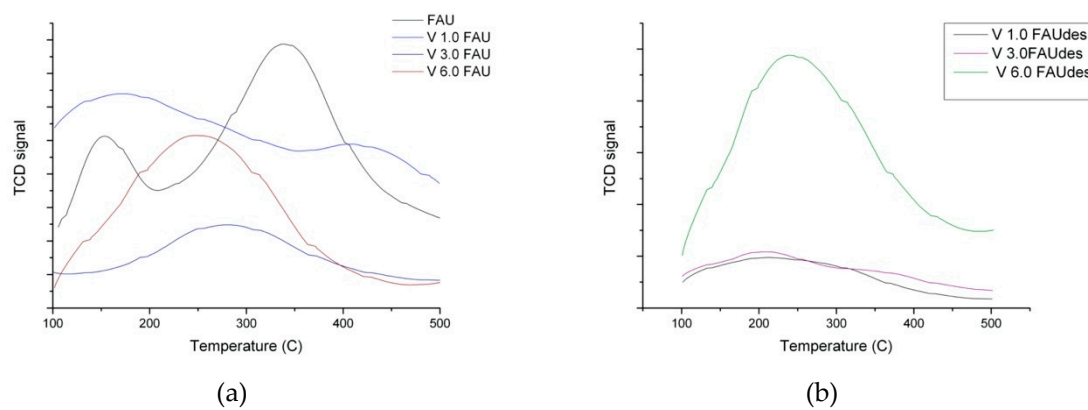


Figure S5. NH₃-TPD profiles for the VxFAU (a) and VxFAUdes (b) series.