

A combined experimental and theoretical
spectroscopic protocol for the determination of
the structure of heterogeneous catalysts:
Developing the information content of the
resonance Raman spectra of M1 MoVO_x

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Supplementary Material

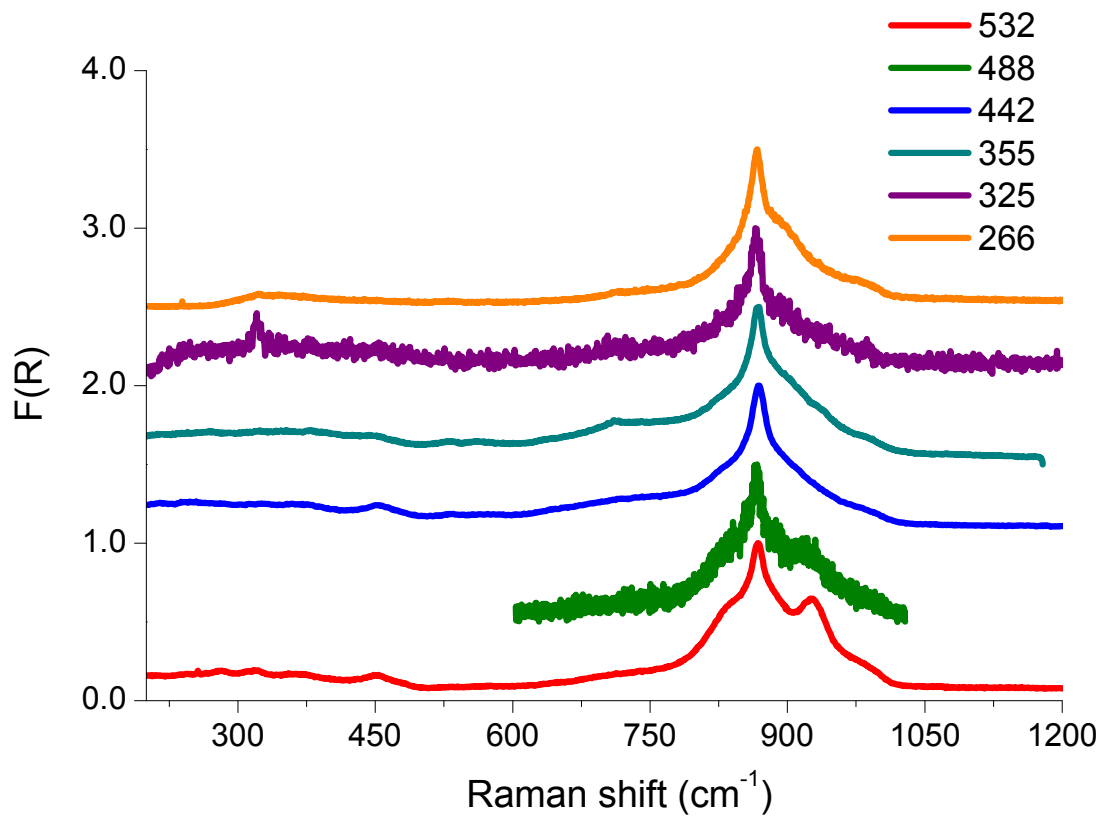
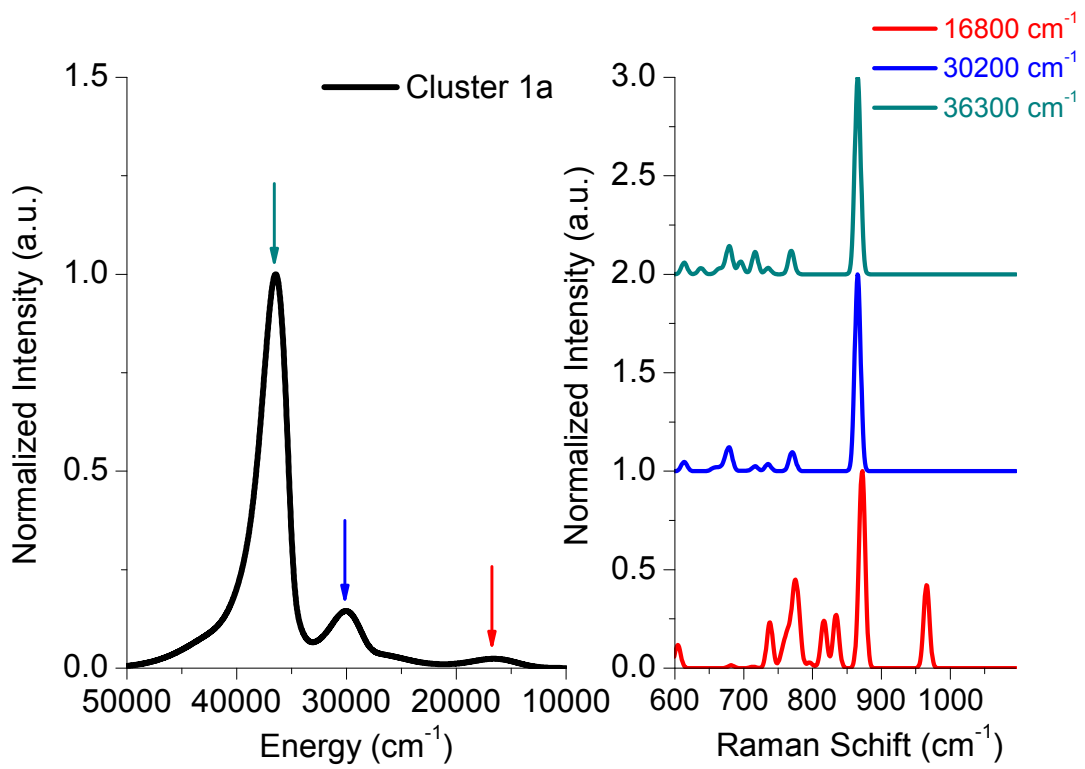
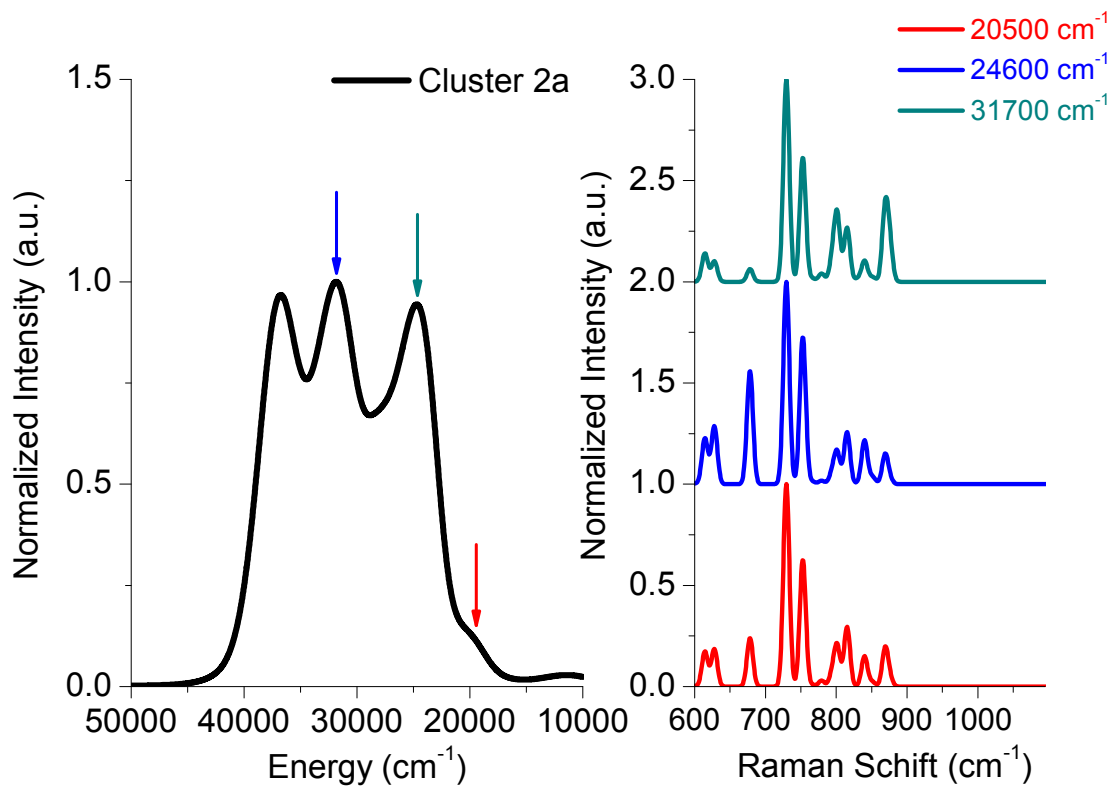


Figure S1. Experimental rRaman spectra of MoVO_x recorded at laser frequencies 532 (red), 488 (green), 442(blue), 355(cyan), 325(purple) and 266 nm (orange). The spectra are presented in $F(R)$ normalized units.

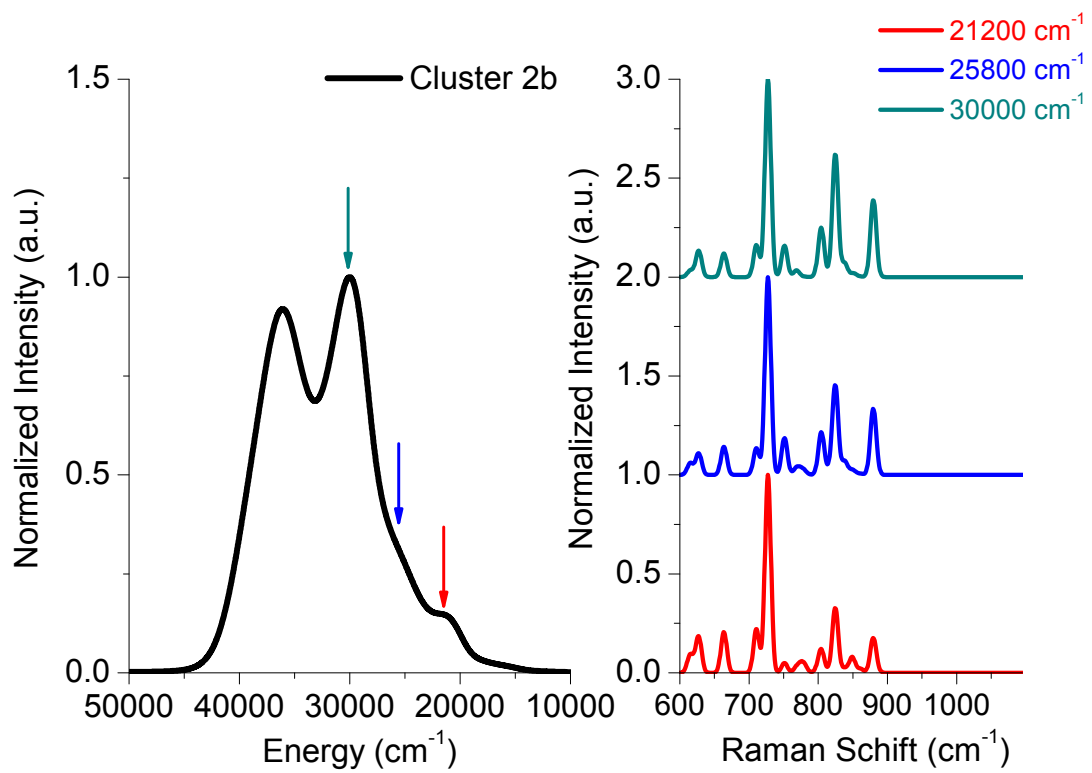
a)



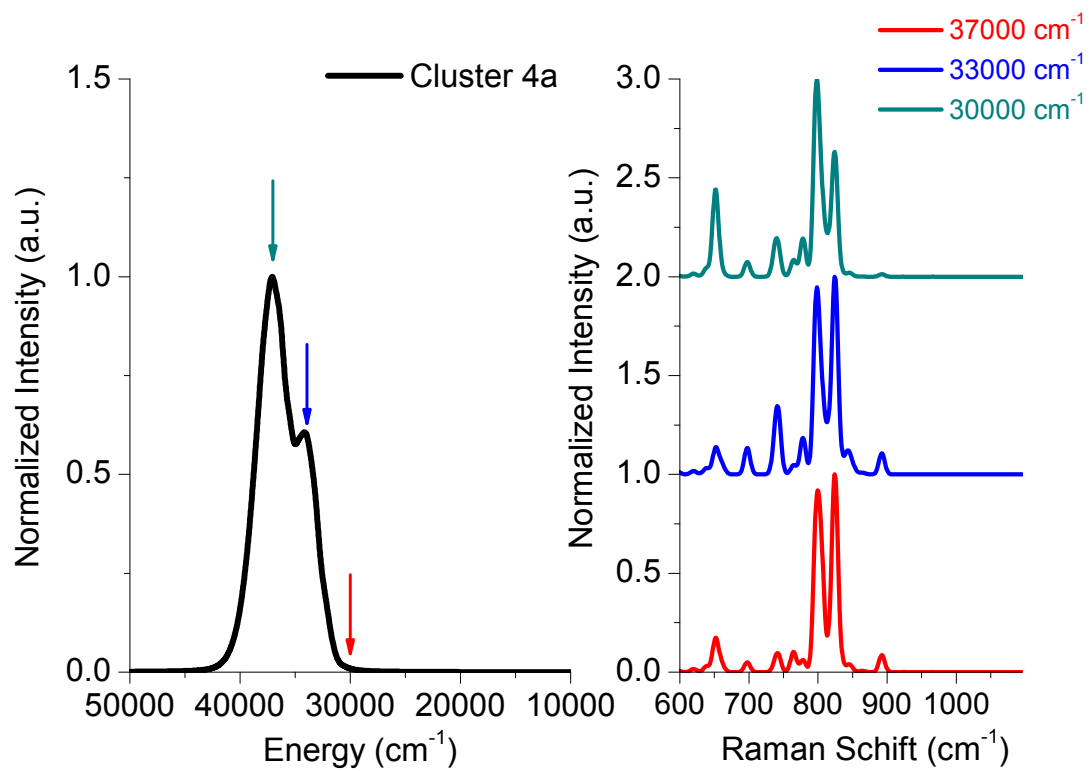
b)



c)



d)



e)

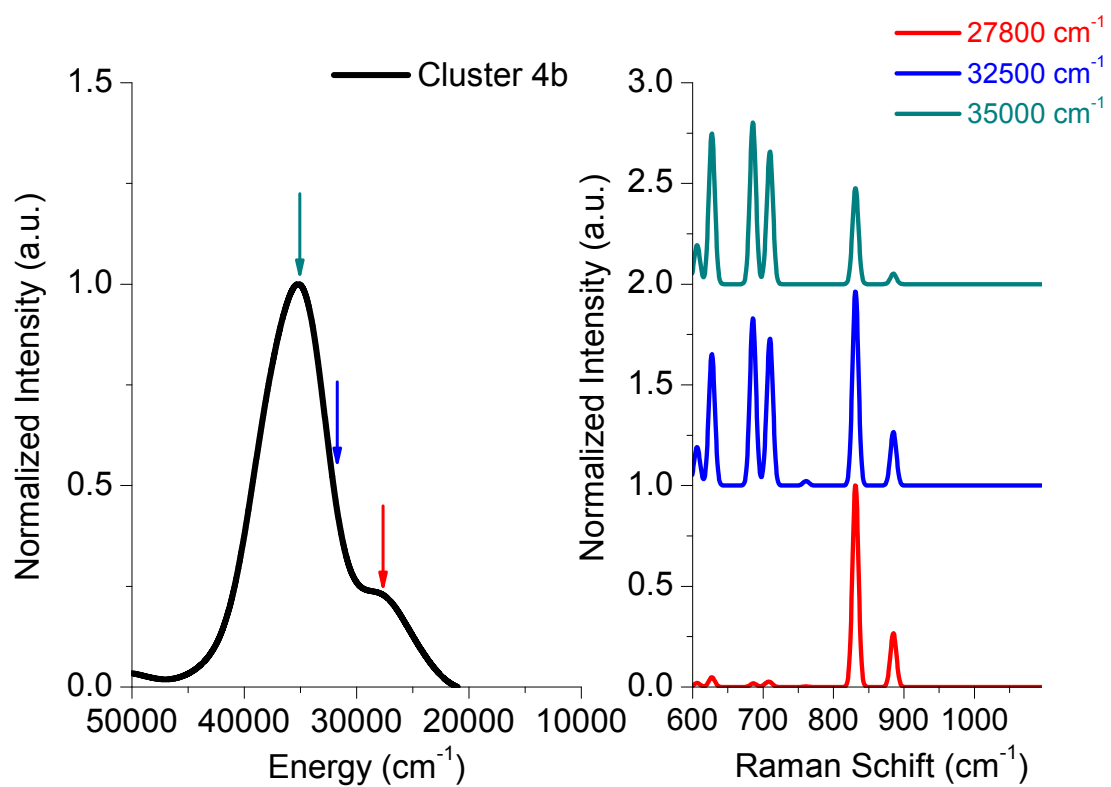


Figure S2. Calculated Absorption and rRaman spectra for a) cluster 1a, b) cluster 2a, c) cluster 2b, d) cluster 4a and e) cluster 4b. Red, blue and cyan arrows indicate the energies at which the rRaman spectra were generated.