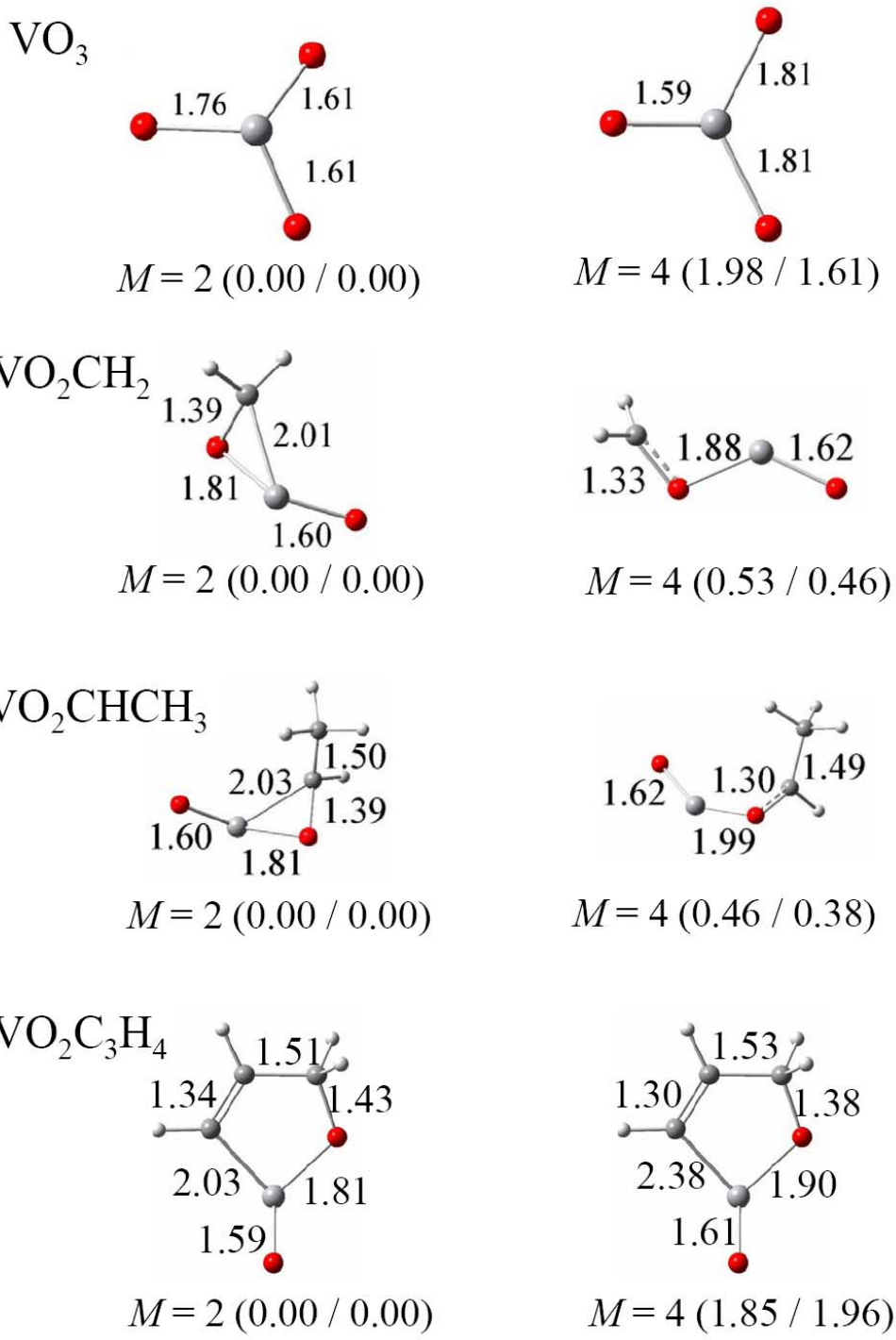

Figure S1: Optimized structures and relative energies of VO_3, VO_2CH_2, VO_2CHCH_3, and $VO_2C_3H_4$ in the doublet (M = 2) and quartet (M = 4) spin multiplicities. The energies (in eV) are given as ($\Delta H_{0\,K}$ / $\Delta G_{298\,K}$) below each geometry. The bond lengths in 0.1 nm are given.

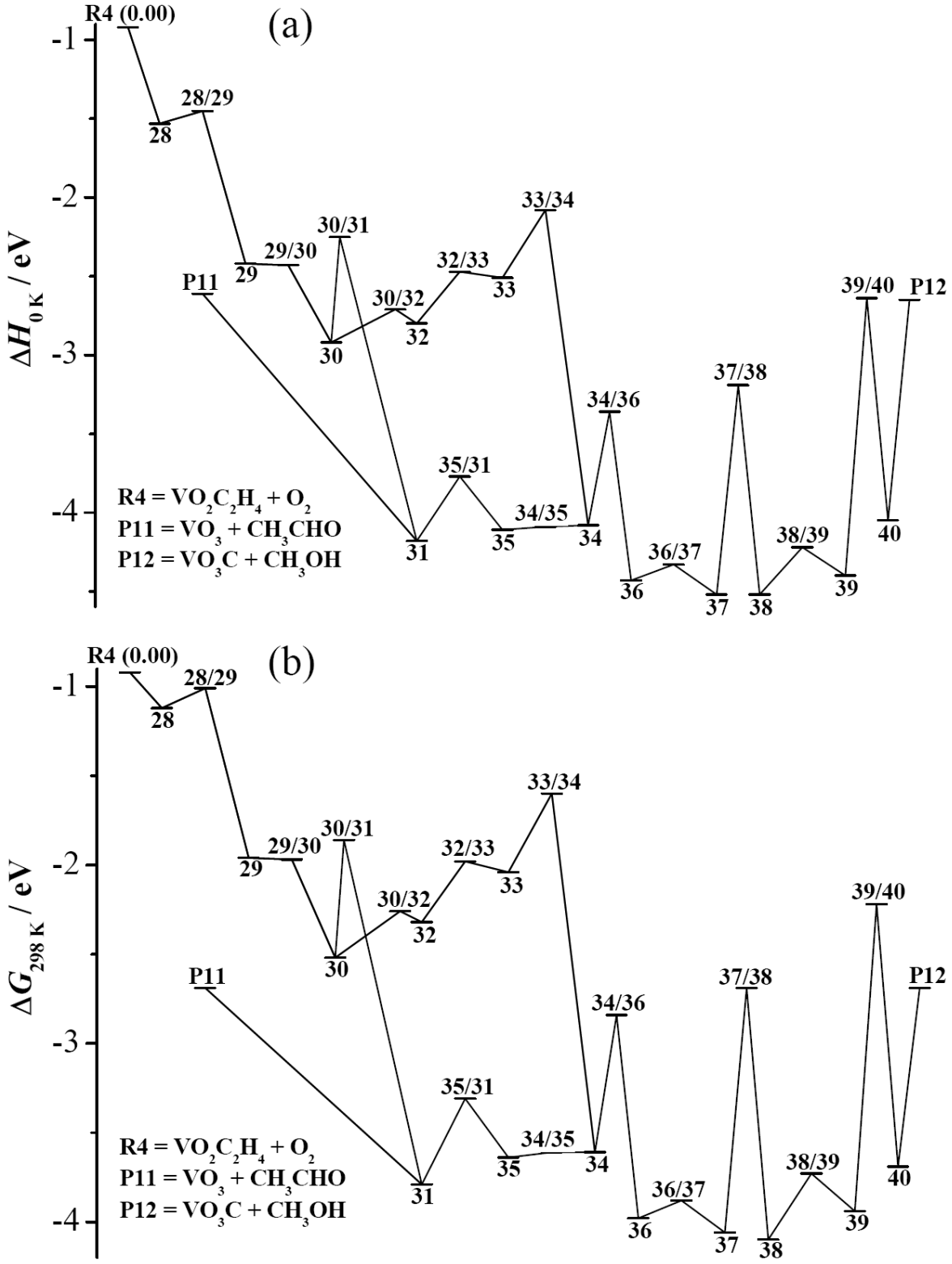

Figure S2: Potential energy profiles for the reaction of VO_2CHCH_3 with O_2. The profiles are plotted for zero-point vibration corrected energies (a) and Gibbs free energies at 298 K (b) relative to the separated reactants $VO_2CHCH_3 + O_2$. The reaction intermediates and transition states are denoted as n and n_1/n_2, respectively.

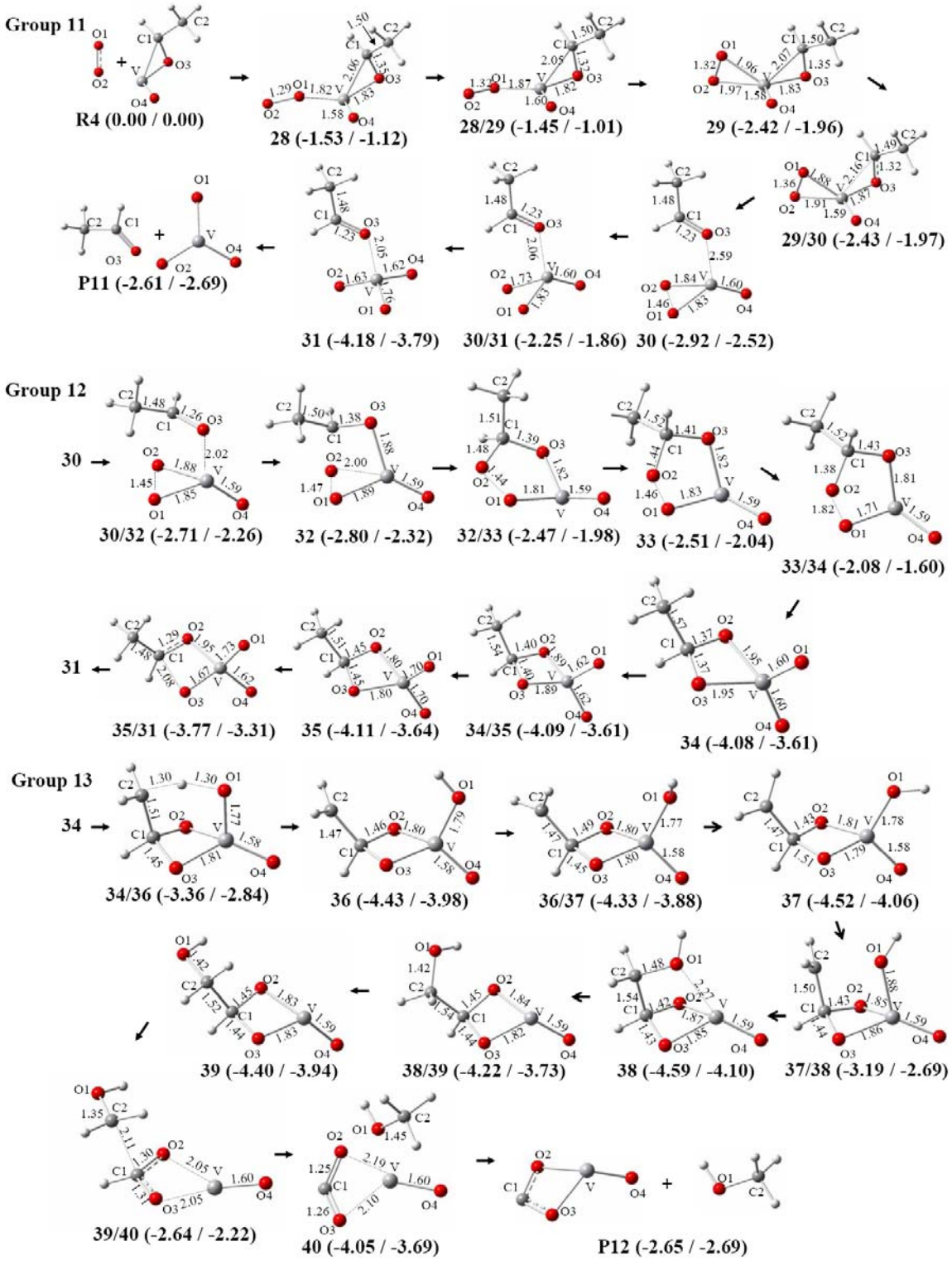

Figure S3: Optimized structures and energies of the species in Figure S2. The energies (in eV) are given as ($\Delta H_{0\,K}$ / $\Delta G_{298\,K}$) below each geometry. The bond lengths in 0.1 nm and some bond angles in degree are given.