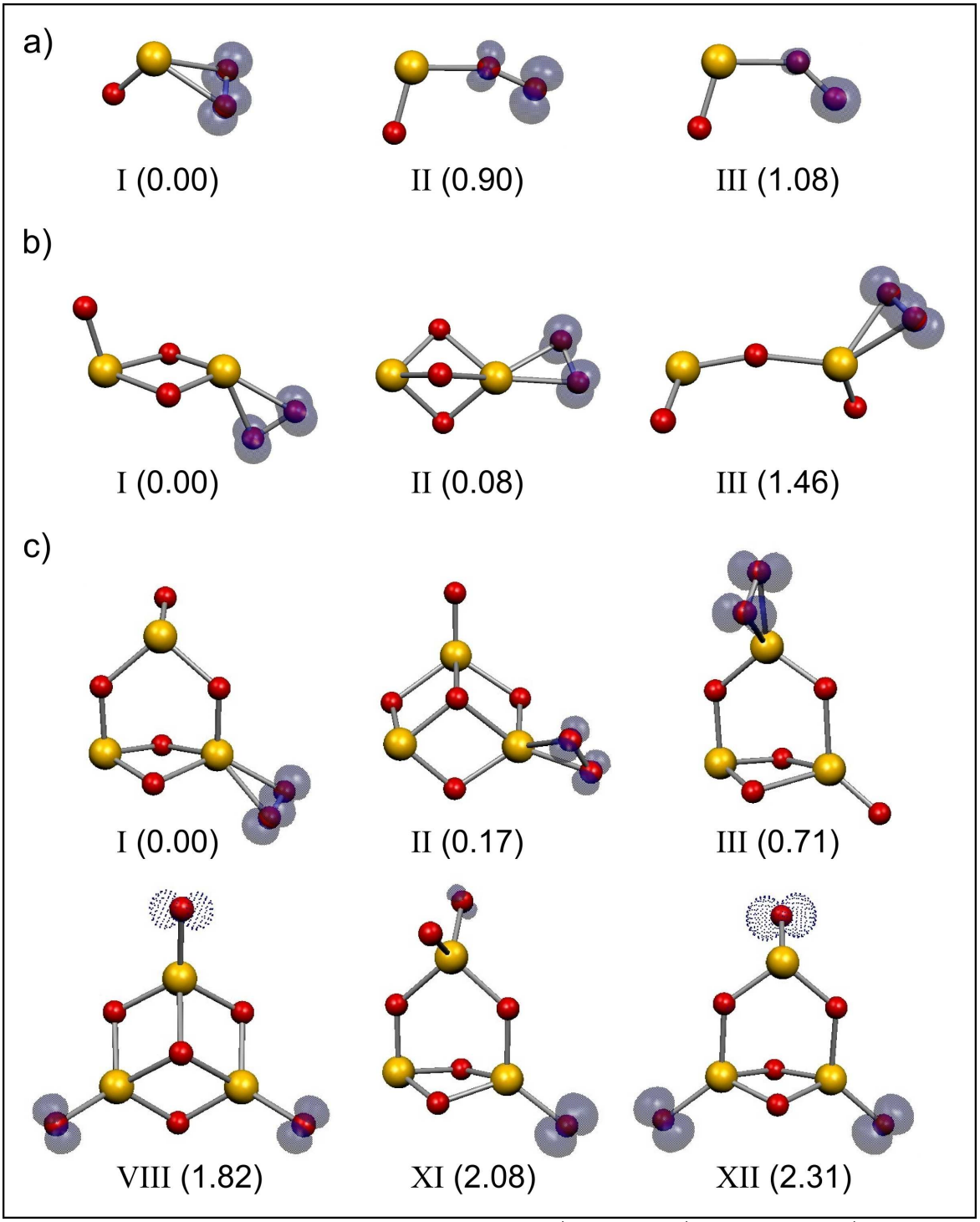
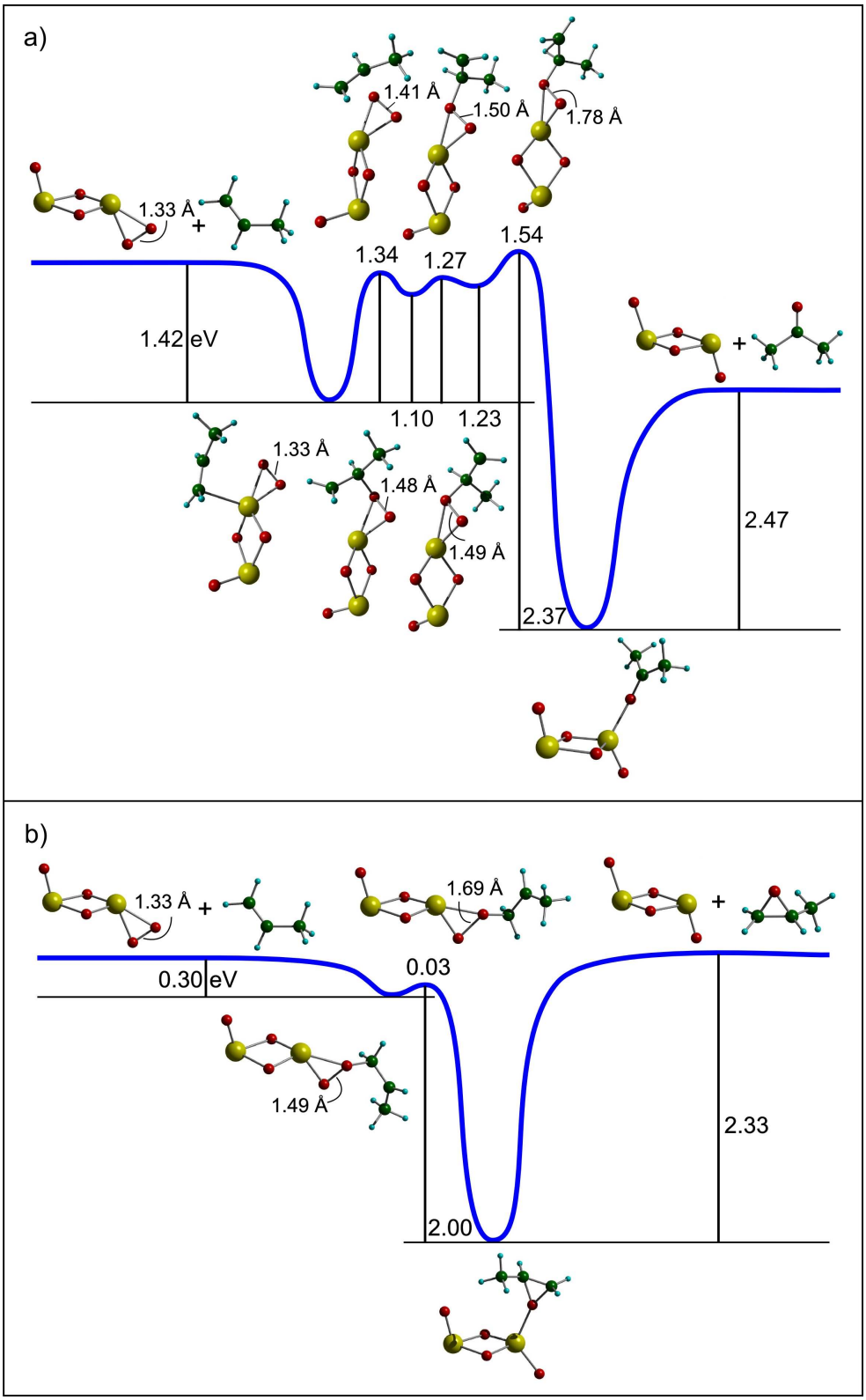
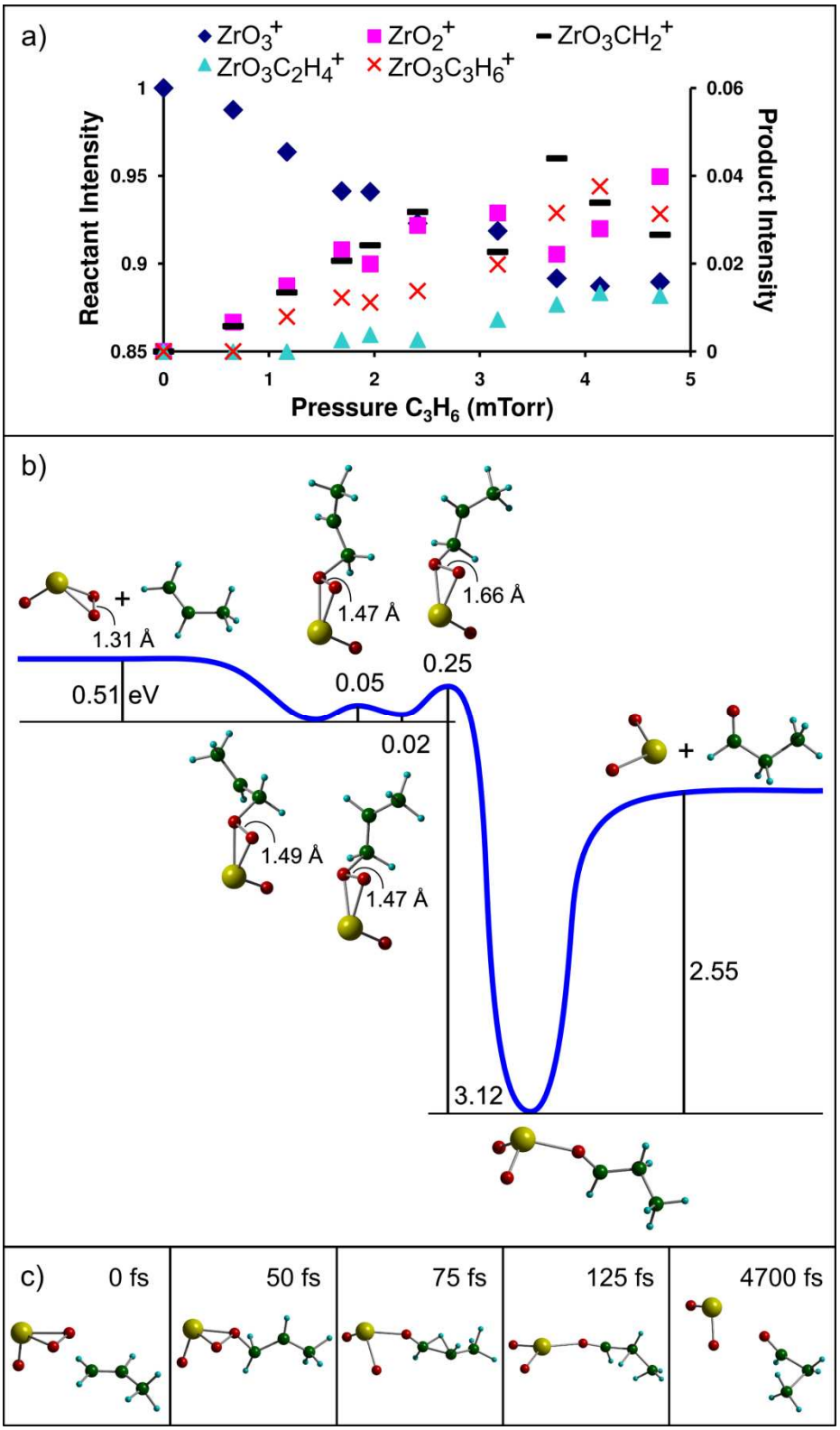


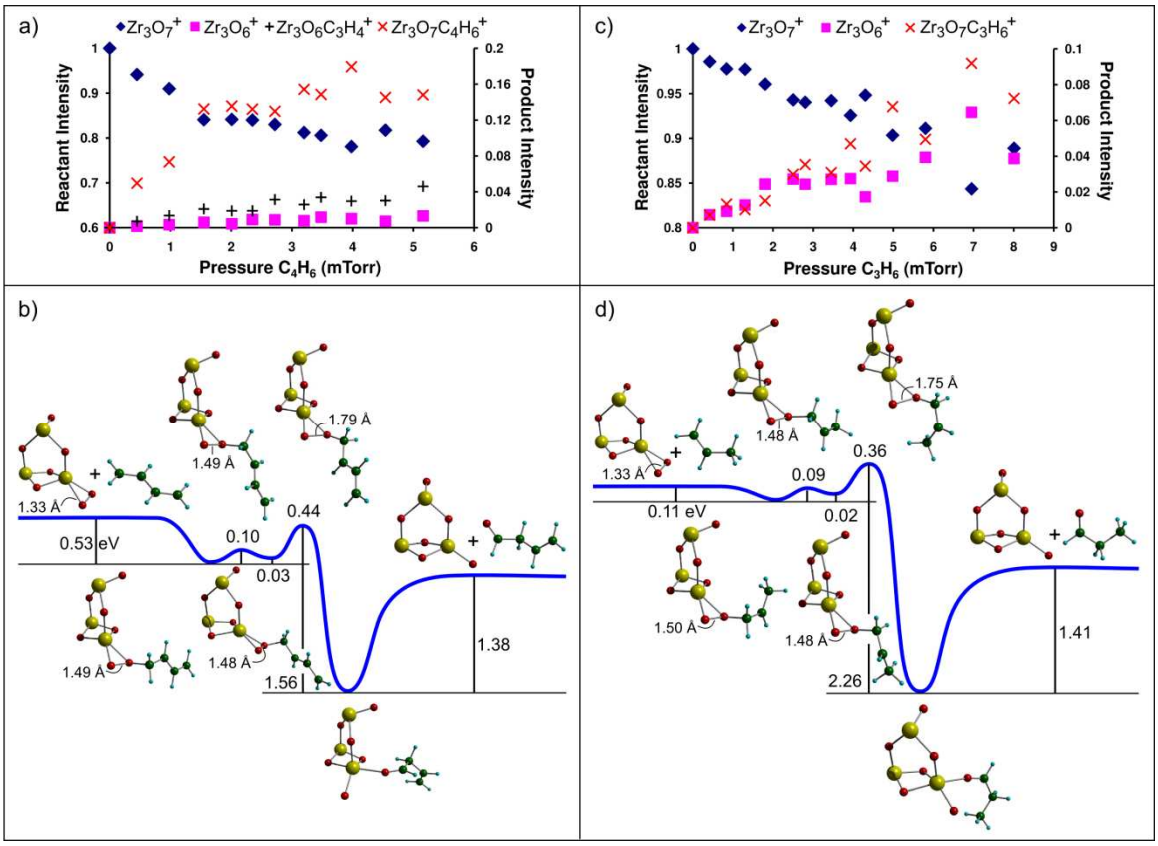
Supp. S1 Calculated structural isomers for (a) ZrO_3^+, (b) $Zr_2O_5^+$, and (c) $Zr_3O_7^+$ given in eV. The gray isosurfaces indicate localized spin density.



Supp. S2 (a) A calculated energy profile given in eV for reaction of $Zr_2O_5^+$ with C_3H_6 forming acetone. (b) An additional calculated energy profile given in eV for reaction of $Zr_2O_5^+$ with C_3H_6 forming an epoxide.



Supp. S3 (a) Branching ratios presented in normalized ion intensities for the reaction ZrO_3^+ with C_3H_6. (b) Calculated energy profile given in eV together with the structures and (c) snapshots from the MD simulations performed at constant temperature (T = 1200 K) for reaction of ZrO_3^+ with C_3H_6 creating propanal.



Supp. S4 Branching ratios presented in normalized ion intensities for the reaction $Zr_3O_7^+$ with (a) C_4H_6 and (c) C_3H_6. Calculated energy profile given in eV for reaction of $Zr_3O_7^+$ with (b) C_4H_6 creating butenal and (d) C_3H_6 creating propanal.