

Supplementary Information: Electronic structure, bonding and stability of fumarate, maleate, and succinate dianions from X-ray spectroscopy

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Supporting figures

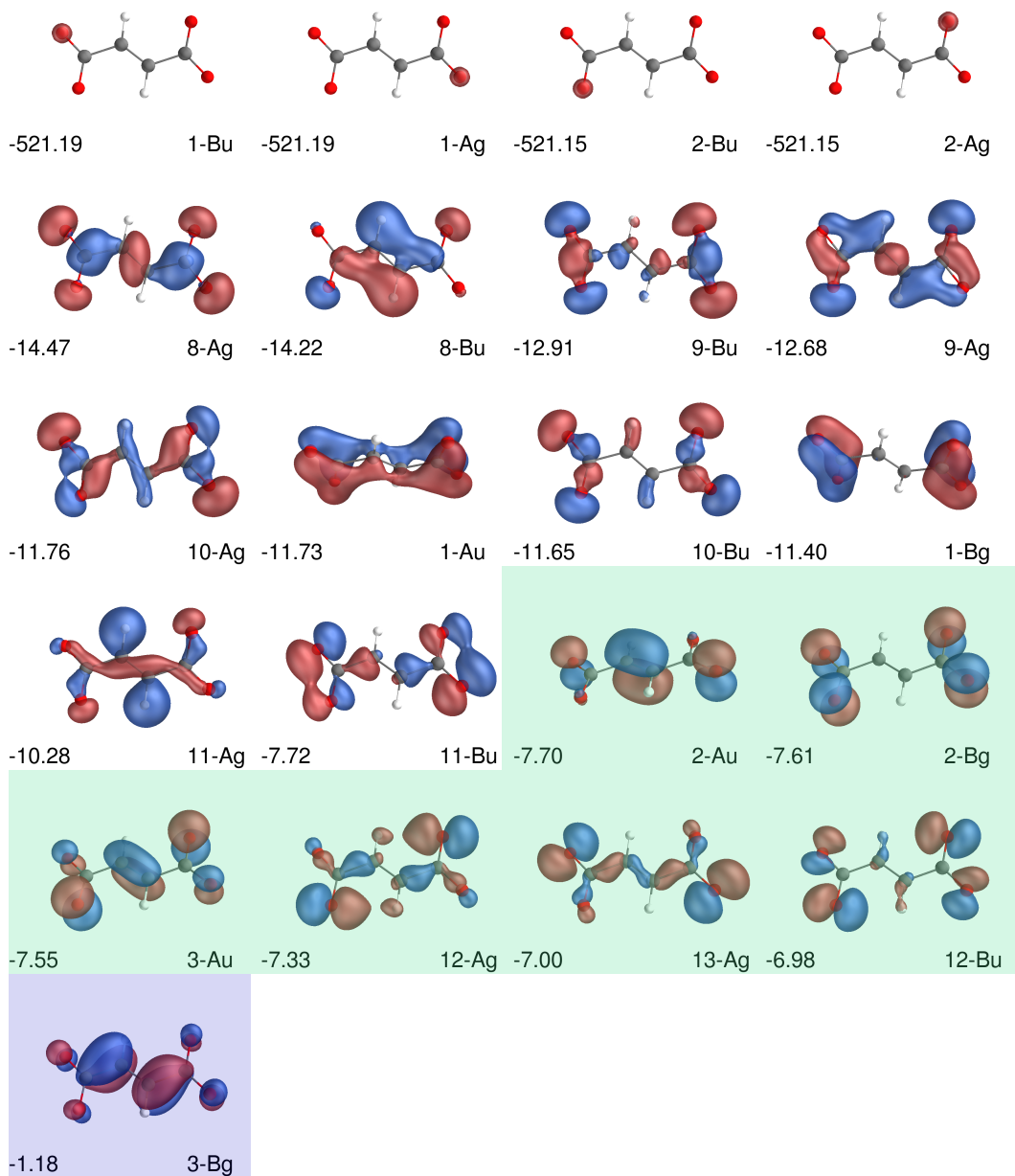


Figure S1: Molecular orbitals of fumarate which are involved in the electronic transitions in XAS and RIXS. The orbital energy (eV) and orbital symmetry are specified on bottom on the left and right side of each orbital, respectively. The first 4 presented orbitals are localized oxygen core orbitals, the next 16 occupied orbitals give the main contribution in the RIXS profile in the energy-loss up to 17 eV. Molecular orbitals involved in the RIXS in the energy-loss up to ≈ 6.5 eV are highlighted by green shading. LUMO orbital is highlighted by purple colour.

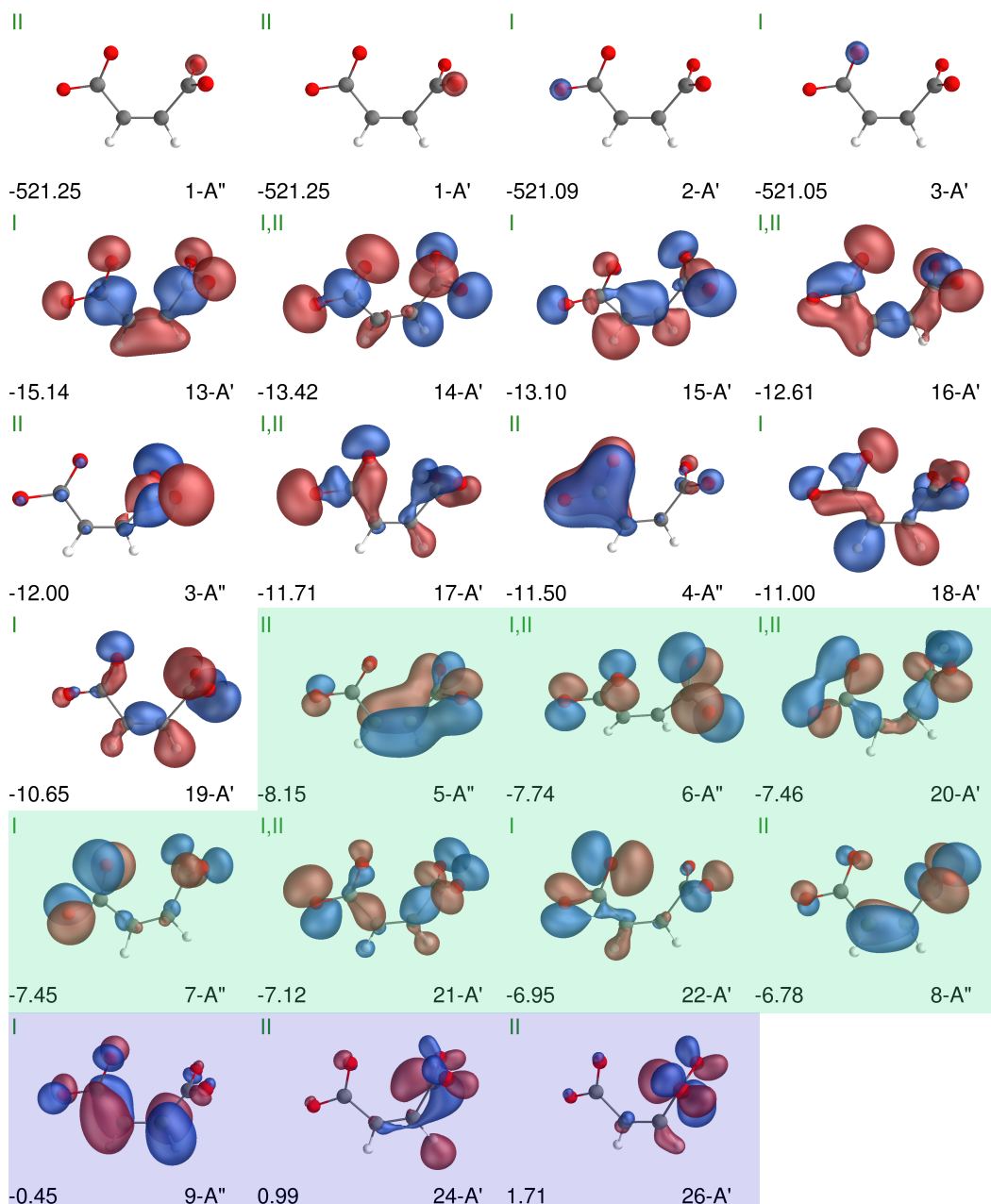


Figure S2: Molecular orbitals of maleate which are involved in the electronic transitions in XAS and RIXS. The orbital energy (eV) and orbital symmetry are specified on bottom on the left and right side of each orbital, respectively. The orbital contribution to the first or/and second resonance is noted in the top left side of the each orbital. The first 4 presented orbitals are localized oxygen core orbitals, the next 16 occupied orbitals give the main contribution in the RIXS profile in the energy-loss up to 17 eV. Molecular orbitals involved in the RIXS in the energy-loss up to ≈ 8 eV are highlighted by green shading. Unoccupied π^* orbitals are highlighted by purple colour.

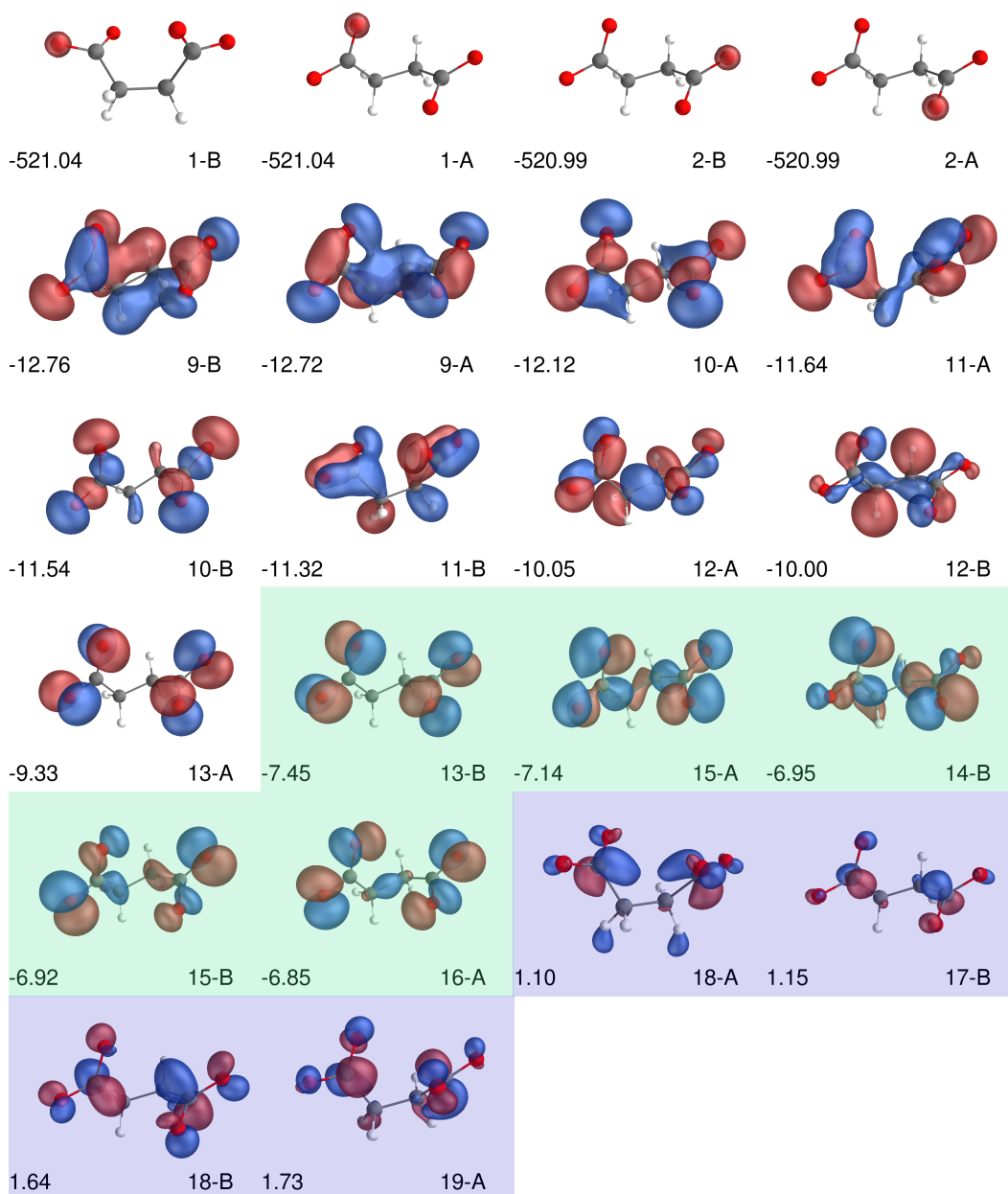


Figure S3: Molecular orbitals of succinate which are involved in the electronic transitions in XAS and RIXS. The orbital energy (eV) and orbital symmetry are specified on bottom on the left and right side of each orbital, respectively. The first 4 presented orbitals are localized oxygen core orbitals, the next 14 occupied orbitals give the main contribution in the RIXS profile in the energy-loss up to 17 eV. Molecular orbitals involved in the RIXS in the energy-loss up to ≈ 8 eV are highlighted by green shading. Unoccupied π^* orbitals are highlighted by purple colour.

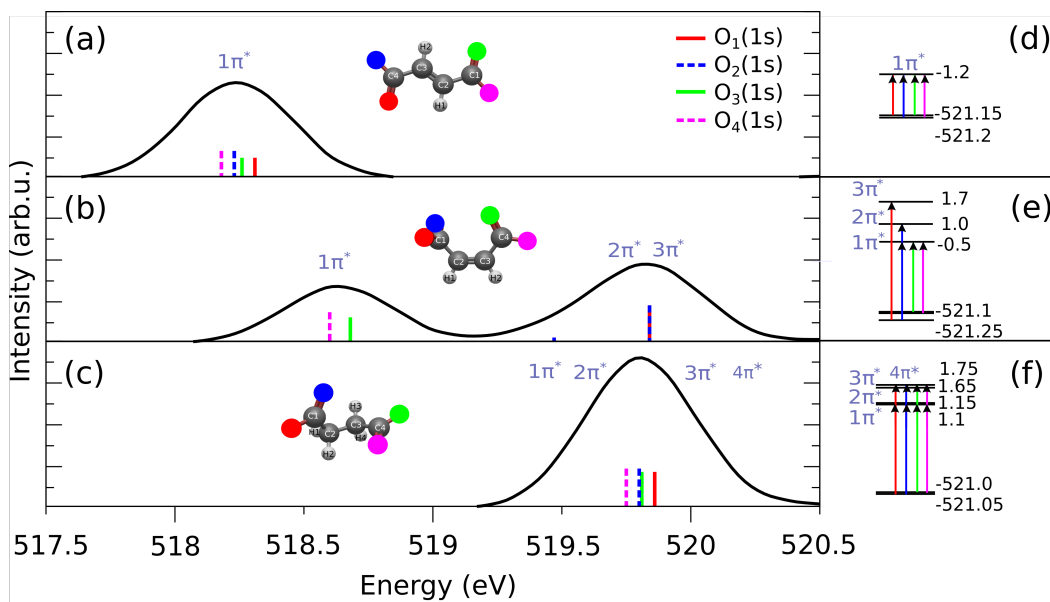


Figure S4: The simulated XAS spectrum of fumarate (a), maleate (b) and succinate (c). Transition amplitudes of electronic states are depicted as sticks, with each stick's color matching an oxygen atom in the molecular structures shown in (a), (b), and (c). Transitions at the O K-edge in the XAS, corresponding to each molecule, are illustrated on Kohn–Sham orbital-energy diagrams in (d), (e), and (f). The color of each transition arrow corresponds to the color of electronic states in XAS to which the transition makes contribution.

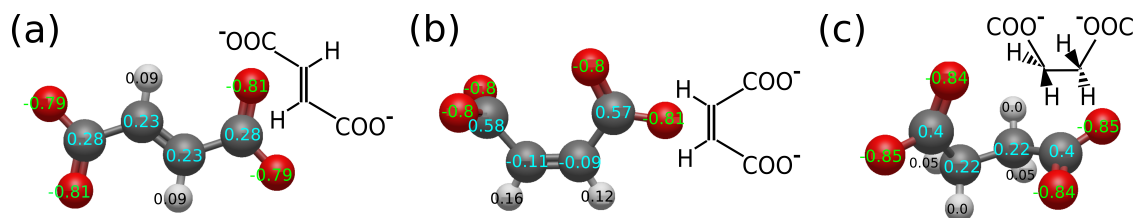


Figure S5: Mulliken charge populations and molecular structures of fumarate (a), maleate (b) and succinate (c).

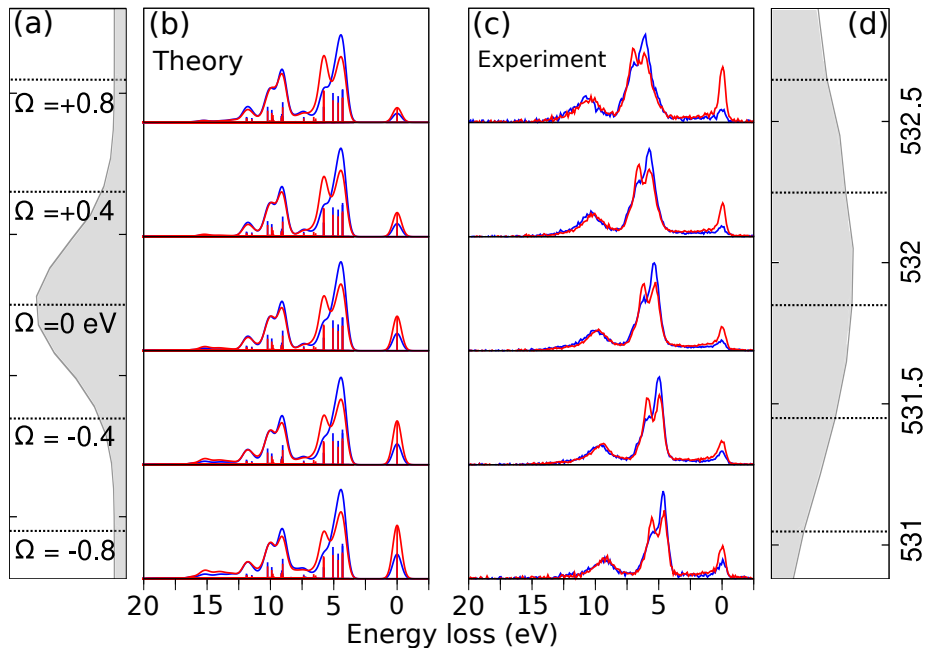


Figure S6: Comparison of theoretical (b) and experimental (c) normalized RIXS spectra of fumarate for different excitation energy values. Panels (a) and (d) show the theoretical and experimental XAS, respectively, with dashed lines indicating the energy excitation and the corresponding detuning Ω .

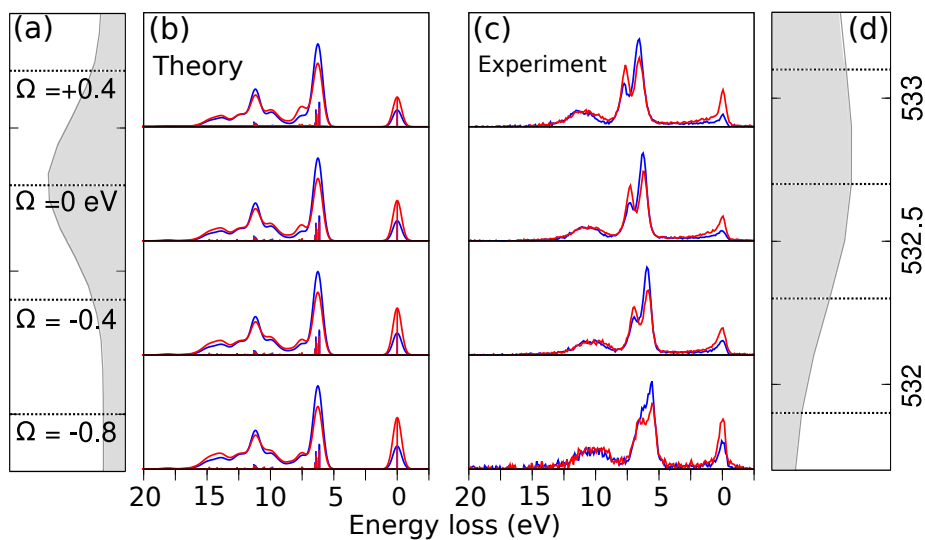


Figure S7: Comparison of theoretical (b) and experimental (c) normalized RIXS spectra of succinate for different excitation energy values. Panels (a) and (d) show the theoretical and experimental XAS, respectively, with dashed lines indicating the energy excitation and the corresponding detuning Ω .