

CHARGE OSCILLATION IN C–O STRETCHING VIBRATIONS: A COMPARISON OF CO_2^- ANION AND CARBOXYLATE FUNCTIONAL GROUPS

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We compare the intensity ratio of symmetric to antisymmetric C–O stretching vibrational transitions in CO_2^- and MCOO^- ($\text{M} = \text{H}, \text{Ag}$ and Bi) using photodissociation spectroscopy. This ratio depends strongly on the bonding partner M , caused by a dynamic change in the molecular charge distribution during vibrational motion. Density functional theory calculations indicate that such charge oscillations can occur for both the symmetric and antisymmetric C–O stretching vibrations in these systems. In the symmetric C–O stretching modes, however, they are at play only if a bonding partner is present, which acts as a reservoir for charge during CO bond compression in the symmetric stretching vibration.