Sub-Natural-Width Resonant Auger Electron Spectra of CO_2

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The C and O 1s excitation spectra of CO_2 exhibit rather broad structures at the $2\pi_u$ resonances. This is due to unresolved vibrational components whose separation is less than the lifetime width of the core-excited state.
We have investigated nuclear motions in the C and O $1s^{-1}2\pi_u$ excited states using resonant Auger electron spectroscopy.

The experiment was carried out on beamline 27SU at SPring-8 in Japan. The photoemission spectra were recorded with a high-resolution electron spectrometer (SES-2002 Gammadata-Scienta) under the *sub-natural-width* conditions, i.e. with overall linewidth smaller than the lifetime widths of the core-excited states.

Strong enhancements of the photoemission channels to the $A^2\Pi_u$ and $B^2\Sigma_u$ states by the C 1s $\rightarrow 2\pi_u$ excitation and to $X^2\Pi_g$ by the O 1s $\rightarrow 2\pi_u$ excitation are observed, illustrating that the participator Auger decay occurs.
The difference in the participator Auger decay channels at the different excitations can be explained from the fact that the O lone-pair orbital $1\pi_g$ participates in the O 1s hole decay whereas only the $1\pi_u$ and $2\sigma_u$ bonding orbitals which have C 1s atomic population can participate in the C 1s hole decay.

We find that symmetric stretching vibrations (n,0,0) in the $B^2\Sigma_u$ and $X^2\Pi_g$ states are enhanced at the C 1s and O 1s $\rightarrow 2\pi_u$ excitations, respectively.
The resonant photoemission shows unresolved quasi-continuous structure at higher binding energy. This quasi-continuous emission can be attributed to unresolved bending vibrations.
The reason why the stretching and bending vibrations are caused in the Auger-final states is that the core-excited state is unstable at the stable point of the ground state along these stretching and bending coordinates.

As a consequence the nuclear motions along these coordinates are caused in the core-excited state and then these motions are transferred to the Auger-final states.