Abstract. Vibrational spectra and geometry relaxation in the core-electron processes of N₂O and CO₂ have been studied by the high-resolution photoelectron spectroscopy and accurate ab initio calculations. We calculated reliable two dimensional potential energy surfaces of the core-hole states of N₂O and CO₂ and performed the vibrational analysis based on these surfaces. We also investigated the geometry changes in the ě and Ļ core-excited states. Theory reproduced the details of the high-resolution spectra providing quantitative assignments and interpretations.

1. Introduction

Vibrational excitation often appears in the photo-ionization and excitation of molecules. This is also the case for core-level photoemission/absorption, even though the core electrons are non-bonding and therefore a significant change in geometry may not be expected. Recent high resolution molecular spectroscopy can observe the fine structure of these vibrational spectra in the core-electronic processes. Theoretical information is valuable to interpret these high-resolution vibrational spectra and to clarify the physics behind the spectra.

Thus, the vibrational spectra and geometry relaxation in the core-hole/core-excited states of various molecules have been investigated by both experiment and theory. For example, for CO₂, the vibrational spectra of the C 1s and O 1s ionized states were measured by Carroll et al. [1] and Kivimäki et al. [2]. Theoretically, Hahne et al. studied the geometry change and vibrational frequency in the O 1s ionized state with the MP2 method [3]. Dobrodey et al. provided the branching ratio in the vibrational levels of O 1s⁻¹ with the SDCI method [4]. Previously, we also investigated the vibrational structure observed in the core-hole states of N₂O [5] and CO₂ [6]. For the inner-shell excited states of these molecules, several experimental and theoretical works have also been performed [7-14]. In the previous studies, we investigated the vibrational spectra in the O 1s excited states of N₂O and clarified the origin of unusual vibrational progression [9] and its thermal effect [10]. We also studied the geometries in the C 1s and O 1s excited states of CO₂ and in the N 1s excited states of N₂O [11]. However, the σ* core excited states have not been focused for these molecules.

The SAC-CI method [15,16] has been successfully applied to wide varieties of chemistry and physics. The method has been established through numerous applications to molecular spectroscopy,
biological chemistry, and surface chemistry [17]. The SAC–CI general-R method [18,19] was developed for investigating complex multi-electron processes like shake-up satellite states and has been successfully applied to those processes [20]. Since the method is designed for the general electronic states, it is also useful for the inner-shell electronic processes. We have investigated various kinds of core-electronic processes using the general-R method [6,9-11,21-27]; for example, core-electron binding energies (CEBE), inner-shell shake-up satellite spectra, vibrational spectra and geometry relaxation of satellites, g–u splitting, valence–Rydberg coupling, and its vibration-induced suppression.

In this article, we present the theoretical and experimental studies on the vibrational spectra and geometry relaxation in the core-electronic processes of N₂O and CO₂. We first explain our ab initio calculations and vibrational analysis using the grid method. Then, we discuss the vibrational spectra in both the core-hole and core-excited states of N₂O and CO₂. Previously, we performed the vibrational analysis of the core-hole states of these molecules. In this paper, we present reliable two dimensional (2D) potential energy surfaces of these core-hole states. We also present the geometry changes in both π* and σ* core excited states of these molecules.

2. Computational details

2.1. Ab initio calculations

We adopted two approaches to calculate potential energy surfaces of the core-hole states. One is the SAC-CI method which calculates the core-hole states directly, while the other is the coupled-cluster singles and doubles with noniterative triples CCSD(T) method within the equivalent core approximation (denoted as ECA CCSD(T)) where the core-ionized atom is replaced by (Z=N+1) atom and the core-hole state is calculated as the ground state. For core-excited states, we directly calculated the excited states by the SAC-CI method.

In the SAC–CI calculations, we adopted the general-R method in which the neutral ground-state Hartree–Fock wave function is used for the reference function. The wave function for core ionization, for example, is given by,

\[ \Psi_{\text{SAC-CI}}^{\text{general-R}} = \sum \Psi_{HF} \exp \left( \sum S_{ij} \right) \Phi_{HF}, \]

where \( \Psi_{HF} \) is the closed-shell ground-state Hartree–Fock wave function. In this method, the higher-R operators such as triples and quadruples are necessary for describing both orbital relaxation and electron correlations of the core-electronic processes. Although the SD-R method is accurate for the one-electron processes of the valence excitations and ionizations, higher-order operators are indispensable for the core-electronic processes.

2.2. Vibrational analysis

We have performed the 2D vibrational analysis based on the ab initio SAC-CI general-R or ECA CCSD(T) potential energy surfaces of the inner-shell electronic states. For calculating the vibrational spectrum, vibrational states were obtained by the grid method, in which Lanczos algorithm was adopted for the diagonalization. Since N₂O and CO₂ have linear structures in the core-hole states, we calculated the symmetric and anti-symmetric stretching modes. Thus, the 2D potential energy surfaces of triatomic molecules were described in the binding coordinates, where the bond distances are \( r_1 \) and \( r_2 \). In these coordinates the kinetic part of the Hamiltonian of the vibrational motion in molecule A-B-C is given by

\[ T = \frac{\partial^2}{2\mu_{ab}\partial r_1^2} - \frac{\partial^2}{2\mu_{bc}\partial r_2^2} + \frac{\partial^2}{m_{\mu}\partial r_1^2}\partial r_2^2 \]
where $\mu_{\text{AB}}$ is the reduced mass of A and B atoms. The coordinates $r_1$ and $r_2$ were represented by the Hermite discrete variable representation (DVR). The potential energy surfaces were fitted by the 2D-Morse expansion,

$$V(r_1, r_2) = \sum_{i,j=0}^{\infty} B_{ij}(1 - e^{-\alpha_{ij}(r_i - r_{i0})})(1 - e^{-\alpha_{ij}(r_j - r_{j0})})$$

(3)

where $r_{i0}$ and $r_{j0}$ are equilibrium distances in each state and were determined by the analytical energy gradients of the SAC-CI or ECA CCSD method. Finally, the vibrational spectra were calculated with the Franck-Condon (FC) approximation. The calculations of 2D vibrational wave functions were executed using the MCTDH program system developed by the Heidelberg group [28].

3. Core-hole states of N$_2$O and CO$_2$

3.1. N$_2$O

N$_2$O is a linear molecule that has two nitrogen atoms, labeled as center (N$_c$) and terminal (N$_t$). We have observed vibrational structures both for the N$_c$ and N$_t$ core-level photoelectron spectra and analyzed the vibrational spectra by calculating the 2D potential energy surface in the symmetric and anti-symmetric stretching coordinates [5]. Relative intensities for vibrationally resolved photoelectron spectra were calculated with the FC approximation. Intensities were also examined using the multi-channel Schwinger configuration interaction method (MCSCI) within the adiabatic approximation.

The N$_c$ 1s and N$_t$ 1s photoelectron spectra of N$_2$O, in the form of $I(0^\circ) + 2xI(90^\circ)$, measured at a photon energy $h\nu = 450$ eV, are shown in Fig. 1. In N$_c$ 1s photoionization, one vibrational progression, quasi-symmetric stretching mode $v'_1$ was enough to fit the spectrum. For N$_t$ 1s spectrum, on the other hand, two vibrational progressions, both quasi-symmetric and quasi-antisymmetric modes were necessary to get reasonable curve fit.

![Figure 1. N$_c$ 1s (left) and N$_t$ 1s (right) photoelectron spectra $I(0^\circ) + 2xI(90^\circ)$ of N$_2$O measured at $h\nu = 450$ eV [5].](image)

The 2D potential energy surfaces of the ground and N 1s ionized states were calculated by the ECA CCSD(T) method. The calculated potential energy surfaces of these states are displayed in Fig. 2 with the equilibrium structures. Geometry change is large in N$_t$ 1s$^{-1}$ state than that in N$_c$ 1s$^{-1}$ state, which explains the vibrational progressions in these core-hole states shown in Fig. 1. The potential energy surfaces of the N$_t$ 1s$^{-1}$ and N$_c$ 1s$^{-1}$ states are flat in comparison with that of the ground state.
The geometrical parameters and the spectroscopic constants of these states are summarized in Table 1 together with the ratios of calculated FC factors and the experimental photoionization ratios. We note that the intensity ratios of the vibrational components are correlated to the ratios of the FC factors when the excitation energy is sufficiently high, that is in sudden limit. We have calculated the FC factors ratios based on the CCSD(T) potential.

The geometry change is sensitive to the level of the theoretical calculations. We present here the results of CCSD(T). According to the CCSD(T) calculation, the equilibrium structures of the ground state and core-ionized states are linear. The optimized bond lengths of the ground state are $R_{NN}=1.133$ and $R_{NO}=1.190\ \text{Å}$, which well agree with the experimental values of $R_{NN}=1.127$ and $R_{NO}=1.185\ \text{Å}$ [29]. The CCSD(T) calculations indicate that both NN and NO bonds are elongated relative to the ground state, $\Delta R_{NN}=+0.010$ and $\Delta R_{NO}=+0.043\ \text{Å}$, in the Ne 1s ionized state. For the Nt 1s ionized state, on the other hand, the CCSD(T) calculations predict both NN and NO bonds shrinks, $\Delta R_{NN}=-0.008$, $\Delta R_{NO}=-0.065\ \text{Å}$; the change in $R_{NO}$ is much larger than that in $R_{NN}$.

The vibrational spectrum of the Nc 1s ionized state calculated by CCSD(T) reasonably agrees with the experimental spectrum. The vibrational excitations are dominantly due to $\nu_1$ mode. The calculated vibrational intensity ratios were 0.47 and 0.11 for $(\nu_1,\nu_3)=(10)$ and (20), respectively, in comparison with the respective experimental values of 0.60 and 0.20. This suggests the underestimate of the geometry change. For the Nt 1s ionized state, on the other hand, the theoretical spectrum by CCSD(T) satisfactorily agrees with the experimental spectrum. The vibrational frequencies are calculated to be 175 and 295 meV for $\nu_1$ and $\nu_3$, respectively, in comparison with the experimental values of 178 and 298 meV. The calculated intensity ratios are 0.84, 0.30, 0.28 and 0.19 for (10), (20), (01) and (11), respectively, and are in reasonable agreement with the respective experimental ratios of 0.82, 0.29, 0.31 and 0.21.
Table 1. Vibrational constants, Franck-Condon factor ratios $R(\nu', \nu')=I(\nu', \nu')/I(0,0)$ and the geometry change for the N$_2$O 1s and N$_2$1s ionized states of N$_2$O [5].

|        | Expt. | ECA CCSD(T) |
|--------|-------|-------------|
|        |       | FCF | MCSCI $^*$ |
| $N_c$  |       |     |            |
| $\omega_1$ (meV) | 136(2) | 125 |          |
| $\omega_2$ (meV) | - | 225 |          |
| $R(1,0)$ | 0.60(1) | 0.467 | (0.472) |
| $R(2,0)$ | 0.20(6) | 0.110 | (0.111) |
| $R(0,1)$ | - | 0.002 | (0.004) |
| $R(1,1)$ | - | 0.000 | (0.002) |
| $\Delta R_{NN}$ (Å) | - | +0.010 |            |
| $\Delta R_{NO}$ (Å) | - | +0.043 |            |
| $N_t$  |       |     |            |
| $\omega_1$ (meV) | 178(1) | 175 |          |
| $\omega_2$ (meV) | 303(2) | 295 |          |
| $R(1,0)$ | 0.82(1) | 0.840 | (0.819) |
| $R(2,0)$ | 0.29(2) | 0.301 | (0.287) |
| $R(3,0)$ | 0.05(2) | 0.061 | (0.057) |
| $R(0,1)$ | 0.31(2) | 0.276 | (0.289) |
| $R(1,1)$ | 0.21(2) | 0.192 | (0.194) |
| $R(2,1)$ | 0.07(2) | 0.055 | (0.054) |
| $\Delta R_{NN}$ (Å) | - | -0.008 |            |
| $\Delta R_{NO}$ (Å) | - | -0.065 |            |

$^*$ Photoionization ratios calculated with multi-channel Schwinger configuration interaction.

3.2. CO$_2$

The vibrational spectra of C 1s and O 1s ionization of CO$_2$ were also studied. This system is of interest since it shows dynamic core-hole localization in O 1s ionization. Theoretically, vibrational frequency and FC factors/geometry relaxation were studied by MP2 [3] and SDCI [4] in the previous works.

C 1s and O 1s photoelectron spectra of CO$_2$, measured at a photon energy $h\nu=500$ and 700 eV, respectively, are shown in Fig. 3 together with a least-squares curve fitting decompositions [6]. The vibrational structure in the C 1s spectrum was assigned to the symmetric stretching vibrations $(\nu', 0, 0)$, whereas the progression in the O 1s spectrum was assigned to the antisymmetric stretching vibrations $(0, 0, \nu')$. Antisymmetric stretching vibration is excited by the vibronic coupling and provides a mechanism of dynamic core-hole localization.

![C 1s photoelectron spectra of CO$_2$](image1)

![O 1s photoelectron spectra of CO$_2$](image2)

**Figure 3.** C 1s and O 1s photoelectron spectra of CO$_2$ measured at 500 and 700 eV, respectively [6].
We calculated the two dimensional potential energy surfaces of the ground, C 1s and O 1s ionized states by using both the ECA CCSD(T) and SAC-CI general-R methods. The calculated 2D potential energy surfaces are shown in Fig. 4. For O 1s$^{-1}$, we show one of the two Jahn-Teller local minima and its diabatic surface; the other surface in which 1s electron in the other oxygen is ionized exists. These two surfaces are relevant in the dynamic localization of core hole of O1s ionized states of CO$_2$. As shown in figure, symmetric mode is excited in C 1s$^{-1}$, while anti-symmetric mode is excited in O 1s$^{-1}$.

![Figure 4. 2D potential energy surfaces of the ground and core-ionized states, C 1s$^{-1}$ and O 1s$^{-1}$ states.](image)

Table 2. Vibrational constants, Franck-Condon factor ratios $R(v'_1, v'_3)=R(v'_1, v'_3)/R(0,0)$ and the geometry change for the C 1s and O 1s ionized states of CO$_2$ [6].

|                  | Expt.       | Theoretical |
|------------------|-------------|-------------|
|                  | SAC-CI      | ECA CCSD(T) |
| C 1s             |             |             |
| $\omega_{e1}$ (meV) | 164(1)     | 175         | 169          |
| $\omega_{e2}$ (meV) | 0.2(1)      | 0.2         | –            |
| $R(1,0)$         | 0.262(4)    | 0.278       | 1.139        |
| $R(2,0)$         | 0.028(4)    | 0.016       | 0.536        |
| $\Delta R_{CO}$ (Å) | -0.0212     | -0.020      | -0.049       |
| O 1s             |             |             |
| $\omega_{e1}$ (meV) | 309(1)     | 330         | 302          |
| $R(1,0)+ R(2,0)$ | 0.553(6)    | 0.956       | 0.534        |
| $R(2,0)+ R(2,1)$ | 0.151(4)    | 0.349       | 0.127        |
| $R(3,0)+ R(2,2)$ | 0.028(4)    | 0.057       | 0.020        |
| $\Delta R_{CO}$ (Å) | 0.0427(3)   | 0.031       | 0.040        |
| $\Delta R_{CO}$ (Å) | -0.0427(3)  | -0.049      | -0.043       |

The calculated spectroscopic constants of the ground state are in good agreement with the well-known experimental values. The calculated spectroscopic constants of the C 1s and O 1s ionized states are summarized in Table 2. We first discuss the SAC-CI general-R results. In the C 1s ionized state, the calculated CO bond length decreases by $\Delta R_{CO}=-0.020$ Å from that of the ground state in very good agreement with the experimental value of $\Delta R_{CO}=-0.021$ Å. The calculated frequency $\omega_{e1}=175$ meV
and anharmonicity $\omega_{e1}^{\perp} = 0.2$ meV are in reasonable agreement with the measurement of $\omega_{e1}=164$
meV and $\omega_{e1}^{\perp} = 0.2$ meV, respectively. The CO* bond length with an O1s ionization was, on the other
hand, calculated to be longer by 0.031 Å than that in the ground state, whereas the other CO bond
length is shorter by ~0.049 Å. The estimated change of the bond length is in fair agreement with the
experimental estimate of $\Delta R_{CO} = 0.043$ Å.

The FC factors were also calculated from the vibrational wavefunctions and the calculated FCF
ratios are listed in Table 2 together with the experimental values. The SAC-CI values are in good
agreement with the experimental values for C 1s while the agreement becomes worse for O 1s. We
also performed the ECA CCSD(T) calculation. The FCFs of the O 1s ionized state by the ECA
CCSD(T) method agree well with the experimental values, though the agreement is worse for the C 1s
ionization. The SAC-CI general-\(R\) method can be applied to wide varieties of core electronic processes
and usually provides reliable results. However, since it uses the ground-state Hartree-Fock for
reference, higher-order \(R\)-operators are necessary for describing orbital relaxation. Therefore, for the
system that exhibits large orbital relaxation, such as O 1s ionized CO2 concerned here, ECA CCSD(T)
method can give better result than the SAC-CI general-\(R\) method.

4. Core-excited states of N\(_2\)O and CO\(_2\)

The equilibrium structures of the core-excited states of N\(_2\)O and CO\(_2\) are characteristic. The core-
excited \(\Pi\) state of these molecules is doubly degenerate in the linear geometry and splits into two
states along the bending coordinate due to Renner-Teller effect. We studied both \(\Pi\) and \(\Sigma\) states of
these molecules.

The N1s-\(\pi^*\) excited states have a bent structure; qualitatively, these states are compared with ONO
and NOO molecules in the equivalent core model for N\(_t\) and N\(_c\) excitations, respectively. The optimized structures of these states are displayed in Fig. 5. For the N\(_t\) 1s-\(\pi^*\) excited state, the
calculated bond lengths and angle were $R_{NN}=1.192$ Å, $R_{NO}=1.198$ Å and 133.9°, respectively, in good
agreement with the ECA experimental values of ONO, 1.1945 Å and 133.9°. The geometry change is
more drastic in the N\(_c\) excited state. The bent structure was also found in the O 1s-\(\pi^*\) excited state. We
also calculated the equilibrium geometry of the N\(_t\) 1s-\(\sigma^*\) and N\(_c\) 1s-\(\sigma^*\) excited states, although they
are located above the respective core-hole states. The geometries of these states are both linear. In N\(_t\)
1s-\(\sigma^*\), the N-O bond length shrink, while in N\(_c\) 1s-\(\sigma^*\), the N-O bond length becomes large.

![Figure 5](image)

**Figure 5.** Calculated equilibrium geometries (Å) of the ground and core-excited states of N\(_2\)O and CO\(_2\).
Next, we discuss the geometry in the C 1s and O 1s excited states of CO₂. The calculated equilibrium structures in these states are also displayed in Fig. 5. The π* core-excited states of CO₂ also have bent structures due to the Renner-Teller effect. Previously, the vibrational spectrum of the C 1s-π* state was observed by XPS and the geometry of this state was experimentally probed [12,13]. In the C 1s-π* excitation, the bond lengths and angle relax to 1.212Å and 134.3°, respectively. Compared with ONO, the equivalent-core molecule, the bond angle is almost the same. The MRSDCI method also calculated the bond distances and angle in accord with the present values [14]. The stable structure of the O 1s-π* excited state of CO₂ is also nonlinear, but asymmetric: the calculated bond lengths of CO* and CO were 1.290Å and 1.176Å, respectively, and the bond angle was 127.8°. The σ* core-excited states also have a minima in the linear structure. The bond lengths are elongated in C 1s-σ* state, while in O 1s-σ* state, C-O* bond shrinks and the other C-O bond length becomes large.

5. Summary
We have investigated the vibrational spectra and geometry relaxation in the core-electron processes of N₂O and CO₂ by the high-resolution photoelectron spectroscopy and accurate \textit{ab initio} calculations. For core-hole states of these molecules, we calculated reliable 2D potential energy surfaces by the ECA CCSD(T) and SAC-CI general-R methods. The calculated vibrational spectra with FC analysis reproduced the experimental photoelectron spectra providing the quantitative assignments. The geometry relaxation in the core-excited states of these molecules was also investigated for the transition to both π* and σ* orbitals. The equilibrium geometries in π* core-excited states are bent, while they are linear in σ* core-excited states.

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