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## ABSTRACT

This paper describes an experimental technique for studying neutral metal complexes using infrared + vacuum ultraviolet (IR+VUV) two-color ionization spectroscopy based on a tunable VUV free-electron laser (VUV-FEL). The preliminary IR spectroscopy results of mass-selected nickel tetracarbonyl are reported in this work. The results demonstrate that the tunable VUV-FEL light allows the selective ionization of a given neutral cluster free of confinement along with the recording of well-resolved IR spectra. As the ionization energies of many neutral clusters are accessible by a broadly tunable VUV-FEL (50–150 nm) and near-threshold ionization can be readily achieved, the proposed experimental method offers unique possibilities for the size-specific study of a wide variety of confinement-free neutral clusters.

## I. INTRODUCTION

Metal complexes are widely used in a variety of reactions in chemical and industrial processes, such as hydroformylation, alkane activation, and the syntheses of hydrocarbons, alcohols, and acids.[1–3] The mass spectrometry and optical spectroscopy analyses of gas-phase metal clusters provide detailed information on their structures, energetics, and dynamics to help uncover the microscopic mechanisms of heterogeneous single-site catalytic processes at a molecular level.[4–6] Numerous efforts have been devoted to the spectroscopic study of charged metal complexes, for which size selection and detection are easy. In contrast, neutral metal complexes present major experimental challenges because the absence of charge makes size selection and detection difficult. Various spectroscopic techniques have been developed to study the structure and dynamics of neutral metal complexes, including matrix isolation spectroscopy,[7] helium nanodroplet spectroscopy,[8,9] far-infrared (IR) spectroscopy,[10] and IR-ultraviolet (IR-UV) double-resonance spectroscopy.[11–16]

Vacuum UV (VUV) one-photon ionization is a powerful method for the ionization sampling of neutral complexes without chromophores (intermediate states). Using this method, neutral clusters can be softly ionized without extensive fragmentation when the VUV photon energy is near the ionization threshold. IR+VUV two-color ionization spectroscopy is widely used for the structural characterization of neutral molecules and clusters.[17–21] However, current IR+VUV spectroscopic methods are limited by the lack of an intense tunable laser that covers the entire VUV region. Recently, we developed the Dalian Coherent Light Source (DCLS) facility,[22] which delivers a VUV free-electron laser (FEL) with a continuously tunable wavelength in the range of 50–150 nm and a high pulse energy. Since clusters with different sizes have different ionization potentials, the tunable VUV-FEL light paves the way for selectively ionizing a given neutral cluster free of confinement, thus facilitating size selection. The unique DCLS VUV-FEL facility makes it possible to study confinement-free, neutral organic and inorganic clusters via IR+VUV spectroscopy.

Metal carbonyl is a prototype for metal–ligand bonding in inorganic and organometallic chemistry and plays an important role in a wide variety of catalytic processes.[1,4,23] Anionic or cationic forms of metal carbonyls have been extensively investigated because of relative ease in size selection and detection. These studies have provided important knowledge on the structures and dynamics of the ionic metal carbonyls. However, fewer efforts were made for neutral metal carbonyls.[4,23] In this work, we describe a VUV-FEL-based IR+VUV spectroscopic method for studying neutral metal carbonyls. Neutral nickel tetracarbonyl was used as an example to demonstrate the capability and resolution of the tunable VUV-FEL light source. Nickel tetracarbonyl [$Ni(CO)_4$], which was the first metal carbonyl to be discovered in 1890,[24] has been studied by Fourier-transform IR (FT-IR) spectroscopy[25] and matrix isolation spectroscopy[26–29] and theoretically.[30–32] However, the IR spectroscopy of mass-selected $Ni(CO)_4$ has not been reported. Preliminary IR spectroscopy results for mass-selected $Ni(CO)_4$ using the VUV-FEL-based IR+VUV strategy are presented in this report.

## II. METHODOLOGY

The experiments were performed at a newly constructed end-station for clusters at the VUV-FEL beam line. The homemade experimental apparatus includes a laser-vaporization supersonic cluster source and a reflectron time-of-flight mass spectrometer (TOF-MS; Fig. 1). Both the source chamber and TOF-MS chamber were pumped using turbomolecular pumps (Edwards, STPA1603C) with a helium pumping speed of 1600 l/s. Sections II A–II E describe this apparatus in detail.

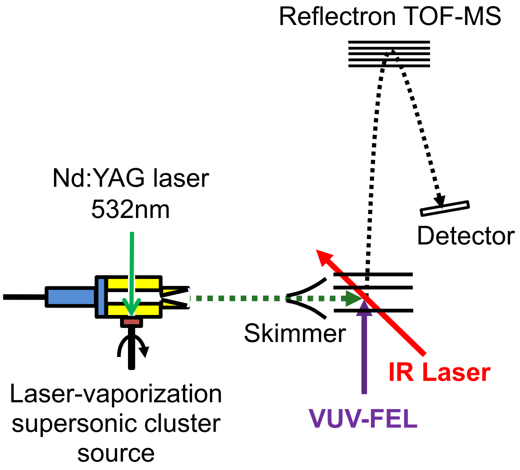

**FIG. 1**. Schematic of the IR+VUV spectroscopy apparatus, which is equipped with a laser-vaporization supersonic cluster source.

### A. Laser-vaporization supersonic cluster source

Figure 2 shows a schematic of the laser-vaporization supersonic cluster source, which is a variant of the sources reported previously in the literature.[33–35] Intense and cold supersonic beams are generated by using a high-pressure pulsed valve equipped with a trumpet-shaped nozzle with a 250-$\mu$m hole (Even–Lavie valve, EL-7-2011-HT-HRR). A typical gas pulse width of 22.5 $\mu$s is used. The gas is directed down a channel and passes over the surface of the sample rod. The 532-nm second harmonic of a Nd:YAG laser (Beamtech Optronics, Dawa-200) is used to vaporize a metal rod ($\Phi$ = 10 mm) with translational and rotational motion. The diameter and length of the waiting room are 5 mm and 16 mm, respectively, and are adjustable for cluster growth. The diameter of the output orifice is 2 mm, and the length of the nozzle is 10 mm. The cluster beams pass through a skimmer (Beam Dynamics, Model 50.8) and enter the reflectron TOF-MS chamber for detection. To produce the given cluster system, the current laser-vaporization supersonic cluster source can be altered for "cutaway" or "offset" type sources[35] based on the influence of cluster composition, temperature, and size.

### B. VUV-FEL facility

The tunable VUV-FEL light used in this study was generated at the DCLS and is described in detail elsewhere.[36] Briefly, the VUV-FEL wavelength is continuously tunable between 50 nm and 150 nm. The VUV-FEL is operated in high-gain harmonic generation mode,[37] in which a seed laser is injected to interact with the electron beam in the modulator. Given the proper optimization of the linear accelerator, a high-quality beam with an emittance as low as ~1.5 mm·mrad, a projected energy spread of ~1%, and a pulse duration of ~1.5 ps can be obtained. The VUV-FEL pulse is currently operated at 20 Hz and can be tuned up to 50 Hz. The maximum pulse energy of the VUV-FEL is ~900 $\mu$J/pulse. To record the spectral characteristics of the pulse, each single VUV-FEL pulse is monitored by using an online VUV spectrometer.

### C. IR laser system

The IR laser beam is generated by using a potassium titanyl phosphate/potassium titanyl arsenate optical parametric

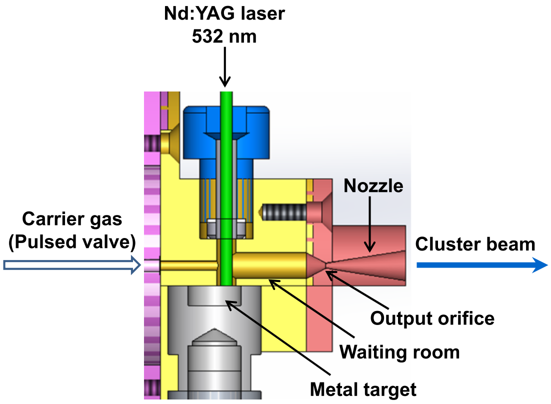

**FIG. 2**. Schematic of the laser laser-vaporization supersonic cluster source.

oscillator/amplifier system (OPO/OPA, LaserVision)[38] pumped by using an injection-seeded Nd:YAG laser (Continuum Surelite EX). The IR output is tunable from 700 cm$^{-1}$ to 7000 cm$^{-1}$ with a linewidth of 1 cm$^{-1}$. The LaserVision system produces 7-ns pulses at 10 Hz. The maximum IR pulse energy is ∼3 mJ/pulse in the region from 700 cm$^{-1}$ to 2000 cm$^{-1}$ and ∼30 mJ/pulse in the region from 2000 cm$^{-1}$ to 7000 cm$^{-1}$. The wavelength of the OPO laser output is calibrated using a commercial wavelength meter (HighFinesse GmbH, WS6-200 VIS IR).

### D. Reflectron TOF-MS

When studying neutral clusters, the extraction plates are powered by a high-voltage direct current (DC) of 2950 V. Charged clusters are deflected out of the molecular beam by the DC electric field of the extraction plates. The remaining neutral clusters are ionized by the VUV-FEL light in the center of the extraction region of the reflectron TOF-MS. The electric fields of the drift tube and the reflector are shielded by using a steel cylinder to avoid interfering with the flight of ions. The ions are detected using a dual microchannel plate (MCP). The transient signals from the MCP are first amplified by using a fast preamplifier (FEMTO, DHPCA-100) and then sent to a dual 1-GHz multiscaler (FAST ComTec GmbH, P7888-2) installed in a computer for real-time data collection. All the timings necessary to trigger the lasers in experiments are generated by using an external delay generator (Stanford Research Systems, DG645). The best resolution achieved for TOF-MS is $M/\Delta M = 10\,000$.

### E. General experimental procedure

Neutral nickel carbonyls were prepared via laser vaporization in expansions of helium seeded with 10% CO using an Even–Lavie pulse valve at backing pressures of 3.5–5.0 MPa. The molecular beams pass through a 4-mm-diameter skimmer and an aperture with a 3-mm opening. Neutral complexes are ionized by the absorption of one photon of the VUV-FEL light and mass-analyzed by using the reflectron TOF-MS. A previous study showed that $\mathrm{Ni(CO)}_n$ ($n$ = 1–4) carbonyls have different ionization potentials.[39] Thus, the ionization signals of a size-specific $\mathrm{Ni(CO)}_n$ carbonyl at a selected VUV-FEL wavelength are not interfered with the signals of smaller and larger clusters. This allows the densities of size-specific nickel carbonyls in a molecular beam to be probed by carefully optimizing the experimental conditions (i.e., the wavelength and pulse energy of the VUV-FEL, concentration of the CO/helium mixture, and stagnation pressure).

The tunable IR light pulse is introduced at approximately 50 ns prior to the VUV-FEL pulse in a crossed manner. The heating of the clusters via the resonant absorption of IR photons can lead to an enhanced ionization efficiency for a given cluster when its ionization potential is just above the VUV photon energy. The IR spectrum of a size-selected neutral cluster can then be recorded by monitoring the enhancement in the signal intensity as a function of IR wavelength. The operating frequency of the pulse valve, the 532-nm laser, and the VUV-FEL is 20 Hz, while that of the IR laser is 10 Hz. The IR spectra are obtained in the differential mode of operation (IR laser on–IR laser off). The IR spectrum is determined by converting the measured relative enhancement of the mass spectrometric ion signal $[I(\nu)/I_0]$ upon irradiation with IR light to relative absorption cross sections $\sigma(\nu)$ using $\sigma(\nu) = -\ln[I(\nu)/I_0]/P(\nu)$. The normalization with IR laser pulse energy $P(\nu)$ accounts for the variations in $P(\nu)$ over the tuning range. Typical spectra were recorded by scanning the IR laser in steps of 2 cm$^{-1}$ and averaging over 900 laser shots at each wavelength.

## III. PRELIMINARY RESULTS

Figure 3 shows the mass spectra of nickel carbonyls ionized at different VUV-FEL wavelengths ($\lambda_{\text{VUV-FEL}}$). At $\lambda_{\text{VUV-FEL}}$ = 143.00 nm, only the $\mathrm{Ni}^+$ cations are observed [Fig. 3(a)]. At 140.00 nm, the $\mathrm{Ni(CO)}_4^+$ cations appear [Fig. 3(b)] along with the $\mathrm{(CO)}_n^+$ ($n$ = 2, 3, 6, 7) cations. At 137.00 nm [Fig. 3(c)], the mass spectral intensities of $\mathrm{Ni(CO)}_4^+$ and $\mathrm{(CO)}_n^+$ ($n$ = 2, 3, 6, 7) increase slightly compared to those at 140.00 nm. The mass spectral peak of $\mathrm{Ni(CO)}_3^+$ begins to appear at $\lambda_{\text{VUV-FEL}}$ = 130.00 nm [Fig. 3(d)]. The $\mathrm{Ni(CO)}_n^+$ ($n$ = 1 and 2) clusters are observed at 120.00 nm [Fig. 3(f)]. For $\mathrm{Ni(CO)}_n^+$ ($n$ = 0–4), the isotopic splitting of nickel is well resolved with relative intensities that match the distributions of natural abundance.

The potentials at which the $\mathrm{Ni(CO)}_n^+$ ($n$ = 1–4) ions from $\mathrm{Ni(CO)}_4$ appear have been extensively studied[39–44] and are not discussed here. The photoionization data are briefly compared with the mass spectra recorded in this study. Photoionization studies[39] indicate that the signals of $\mathrm{Ni(CO)}_4^+$, $\mathrm{Ni(CO)}_3^+$, $\mathrm{Ni(CO)}_2^+$,

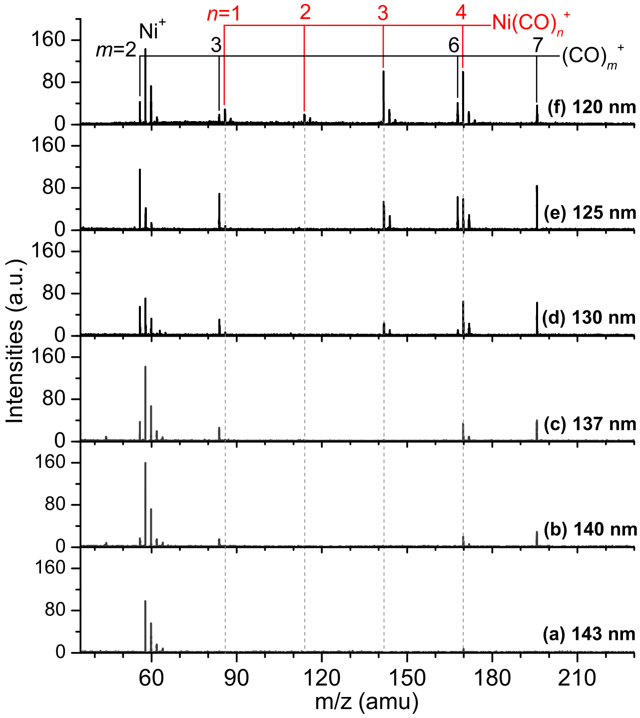

**FIG. 3**. Time-of-flight mass spectra of the cations produced from the VUV-FEL single-photon ionization process at different VUV-FEL wavelengths: (a) 143.00 nm, (b) 140.00 nm, (c) 137.00 nm, (d) 130.00 nm, (e) 125.00 nm, and (f) 120.00 nm. The scale of the mass spectral intensity for each VUV-FEL wavelength is the same.

and $Ni(CO)^+$ from $Ni(CO)_4$ appear at potentials of 8.32 eV (149.01 nm), 8.77 eV (141.37 nm), 10.10 eV (122.75 nm), and 11.65 eV (106.42 nm), respectively. The average bond energy of $Ni(CO)_4{}^+$ was determined to be 1.36 eV.[39] The appearance of $Ni(CO)_3{}^+$ ion originating from the decomposition of $Ni(CO)_4{}^+$ is thus estimated at $\lambda_{\text{VUV-FEL}} \le 128.00$ nm (9.68 eV) when $Ni(CO)_4$ is exposed to VUV ionizing radiation. As shown in Fig. 3(d), the $Ni(CO)_3{}^+$ ion appears at 130.00 nm, indicating that the $Ni(CO)_3{}^+$ ion was generated by the ionization of $Ni(CO)_3$ rather than the decomposition of $Ni(CO)_4{}^+$. At $\lambda_{\text{VUV-FEL}} \ge 125.00$ nm, the $Ni(CO)^+$ and $Ni(CO)_2{}^+$ ions are not clearly observed, consistent with previous photoionization data.[39] These results demonstrate that the tunable VUV-FEL allows for the selective ionization of neutral species.

Figure 4(a) shows the IR spectrum of $Ni(CO)_4$ recorded by monitoring the enhancement in the intensity of the $Ni(CO)_4{}^+$ mass channel at $\lambda_{\text{VUV-FEL}} = 143.00$ nm. The IR power dependence of the signal was measured to ensure that the enhancement intensity was linear with photon flux. The experimental IR spectrum of $Ni(CO)_4$ is dominated by a single peak at 2060 $cm^{-1}$ with a full width at half maximum (FWHM) of 11 $cm^{-1}$. In contrast, the IR spectrum of $Ni(CO)_4$ vapor features a broadband at 2058 $cm^{-1}$ with a FWHM of 20 $cm^{-1}$.[25] In matrix isolation experiments, the IR absorption band was found at 2052 $cm^{-1}$ with a FWHM of 3 $cm^{-1}$ in an argon matrix[26–28] and at 2056 $cm^{-1}$ with a FWHM of 4 $cm^{-1}$ in a neon matrix.[29] The red shifts with respect to the gas-phase values and the narrower bandwidths are attributed to the interaction of the cold rare-gas matrices with the host molecules.[1]

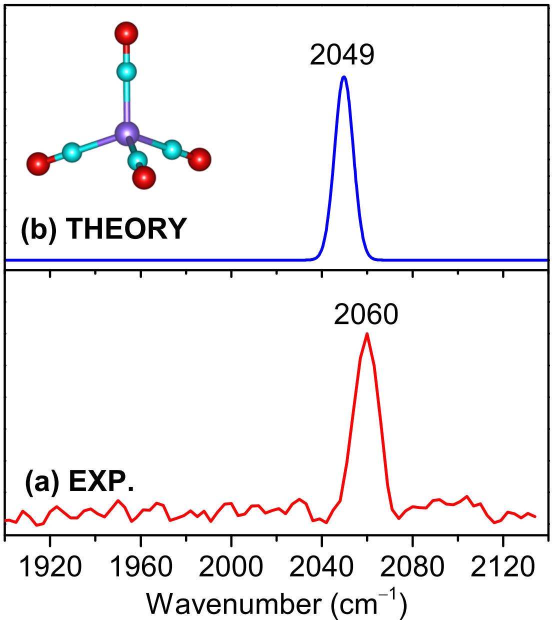

**FIG. 4**. Comparison of the experimental and calculated IR spectra of $Ni(CO)_4$. (a) Experimental IR spectrum measured using the IR+VUV approach with $\lambda_{\text{VUV-FEL}} = 143.00$ nm. (b) Theoretical IR spectrum calculated at the B3LYP/def2-TZVPP level of theory with the harmonic frequencies scaled by 0.968. The inset shows the molecular structure.

Quantum mechanical calculations of $Ni(CO)_4$ with the known tetrahedral ($T_d$) symmetry were carried out at the B3LYP/def2-TZVPP level of theory using the Gaussian 09 program.[45] The carbonyl stretching frequencies were scaled by a factor of 0.968, which was determined as the ratio of the experimental stretching frequency of a free CO molecule (2143 $cm^{-1}$) to the B3LYP/def2-TZVPP one (2214 $cm^{-1}$). The resulting stick spectra were convoluted by a Gaussian line shape function with a FWHM linewidth of 10 $cm^{-1}$.

Figure 4 compares the experimental and calculated IR spectra. The calculated antisymmetric CO stretching vibration of $Ni(CO)_4$ is 2049 $cm^{-1}$, consistent with the experimental value of 2060 $cm^{-1}$. The measured IR spectrum of mass-selected neutral $Ni(CO)_4$ agrees well with the previously reported spectra and theoretical data, suggesting that the VUV-FEL-based IR+VUV two-color ionization spectroscopy technique presented herein is reliable.

## IV. CONCLUSION

We have demonstrated that IR resonance-enhanced photoionization with a tunable VUV-FEL enables the vibrational spectroscopy of neutral metal complexes with high sensitivity and size selectivity. The developed technique does not require the presence of a UV chromophore, a messenger tag, or a host matrix. As the ionization energies of many clusters fall in a range accessible by a broadly tunable VUV-FEL and near-threshold ionization can be readily achieved, IR+VUV spectroscopy based on a tunable VUV-FEL light source offers unique possibilities for the size-specific study of a wide variety of confinement-free neutral clusters.

## AUTHORS' CONTRIBUTIONS

G.L., C.W., and Q.L. contributed equally to this work.

## ACKNOWLEDGMENTS

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