Long-Lived States of CO^{++} Formed by Photoionization of CO^{+}.

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Data concerning the life-times and the structure of double-charged molecular ions has been restricted to low-resolution type experiments [1,2]. Precise experimental data is needed in order to compare with refined energy calculations. In this work we present a high-resolution ($\Delta E = 15$ meV) energy-spectrum of long-lived states of CO^{++}. The details of the experiment will be publish elsewhere [3], briefly: The experiment was conducted at beamline 10.0.1 using the ion-photon beam end station. A CO^{+} ion-beam was extracted from the CIGA (Cuernavaca Ion-Gun Apparatus) at 6-keV acceleration energy. After being collimated and focused, the ion beam was merged with the photon beam. The double-ionized CO is separated by means of a magnetic analyzer and counted after a TOF of about 6 μs. The background signal due to collisions with the residual gas has been subtracted. The resulting spectrum is shown in figure 1.
An appearance voltage of CO^{++} at 27.155 eV indicates that most of the CO^{+} originates from $^2\Sigma^+$ vibrationally relaxed. The subsequent structures are due to the vibrational resonances of single-photon absorption into long-lived states of CO^{++} and the observed intensities are mainly associated to their lifetimes. In order to explain the present spectrum a calculation using the methods of MRCI (multi-reference configuration interaction) and ACPF (averaged coupled pair functional) was performed. The potential energy curves used in this calculation are shown in figure 2. The first series of structures, below 28.5 eV, correspond to the overlap of the vibrational sequences of the $1^1\Sigma^+$, $1^3\Pi$ and $1^1\Pi$ states as inicated in figure 1.
A series of resonances appear in the energy range from 28.6 to 29.3 eV. No metastable states of CO^{++} are identified in this energy range. These resonances do not resemble a vibrational sequence since their separation does not narrow at higher energies. Their origin is still unknown. The spectrum shows a deep at 30.130 eV in the background signal, we believe that this is due to intersection of a dissociative $^3\Sigma^-$ state with $^3\Pi$ metastable state, this value can be used for calibration purposes in future calculations.

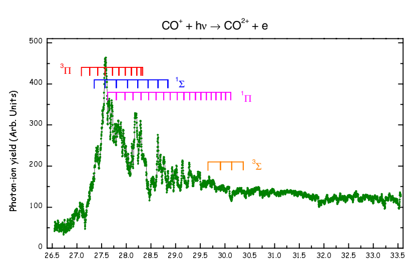

Figure 1. CO^{++} spectrum taken with a resolution of 15 meV.

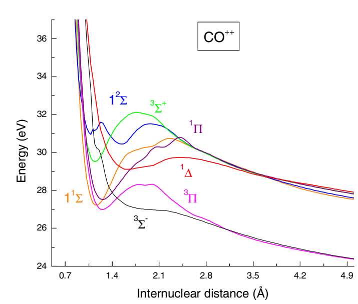

Figure 2. Potential energy curves used for the present calculation.

In conclusion, we present a high-resolution experiment for the formation of metastable doubly charged molecular ions, the state of the art theoretical calculation partially explains the features observed. These data present a unique opportunity to understand the structure of the metastable doubly-charged molecular ions.

REFERENCES

1. M. Larsson, B.J. Olsson and P. Sigray, Chem. Phys. 139, 457 (1989).
2. F. Penent, R. I. Hall, R. Panajotovíc, J. H. D. Eland, G. Chaplier, and P. Lablanquie. Phys. Rev. Letters, 81, 3619-3622 (1998).
3. On the Photoionization of O^+, A.M. Covington, I.R. Covington, A. Aguilar, G. Hinojosa, M. Sant'Anna, I. Alvarez, C. Cisneros, A.S Schlachter, and R. Phaneuf.

Work supported by the Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy contract DE-FG03-97ER 14787 with the University of Nevada, Reno; by the Nevada DOE-EPSCoR Program in Chemical Physics, by the DOE Facilities Initiative, by CONACyT and DGAPA through the CCF-UNAM.

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