Beam-gas Spectroscopy of Sextet Transitions in O^{3+}, F^{4+} and Ne^{5+}

Bin Lin, H. Gordon Berry, Tomohiro Shibata, Lanlan Lin
1 Department of Physics, University of Notre Dame, Notre Dame, IN 46556
2 Ames Lab, Ames, IA 50515
(Dated: December 19, 2021)

We present VUV observations of transitions between doubly excited sextet states in O^{3+}, F^{4+} and Ne^{5+}. Spectra were produced by collisions of an oxygen, fluorine and neon beam with a nitrogen gas jet target. Prepared beam-gas experiment yields new and explicit information on doubly core-excited ions. Some observed lines were assigned to the 1s2s2p^2 4S-1s2p^33s, 3d 6P electric-dipole transitions in O^{3+}, F^{4+} and Ne^{5+}. Three lines have been reassigned. Present data are the first explicit measurements on transitions between sextet states in boronlike ions by beam-gas spectroscopy.

PACS numbers: 32.70.-n, 39.30.+w, 31.10.+z, 31.15.Ar

The sextet states of doubly excited boronlike ions are possible candidates for x-ray and VUV-lasers, and have been investigated recently. The lowest terms of this system (1s2s2p^3 6S, 1s2s2p^33s 6P and 1s2s2p^33d 6P) have been studied along the B I sequence. The studies of higher excited sextet states (1s2p^6 3S) have been lately reported. However, the energy level diagrams of these ions are still far from complete. Experimentally, these levels are difficult to observe by conventional spectroscopy techniques, such as the high voltage discharge in gas cell method, because they lie well above several ionization limits of five-electron singlet states. Even though they are metastable against autoionization, they usually de-excite and disappear by collisions with other ions without radiative transitions. The fast beam-foil technique allows straightforward observations of the radiative transitions produced by these sextet states along B I sequence.

In 1992 the beam-foil spectroscopy was used to provide initial data on low-lying sextet states in boronlike nitrogen, oxygen and fluorine. The recent work of Lapierre and Knystautas on possible sextet transitions in Ne VI highlights the significance in this sequence. They measured several excitation energies and lifetimes. The fine structures of individual 1s2s2p^3 6S and 1s2s2p^33d 6P states were resolved and measured in O IV, F V and Ne VI by Lin and Berry et al. There are no further results reported for transitions from sextet states in boronlike system.

In some works on beam-foil spectroscopy of sextet states in B I isoelectronic sequence, their identifications show rather weak lines and overwhelming blending problems. Hence, accurate theoretical studies of sextet states in doubly excited B I isoelectronic sequence are strongly needed to help identifications. However, the theoretical analysis of these five-electron ions is difficult because strong electron correlation, relativistic corrections, and even QED effects have to be included in the calculations. Doublet and quartet transitions in core-excited boronlike ions have been studied successfully using beam-gas collision spectroscopy. Well prepared beam-gas spectroscopy of oxygen, fluorine and neon ions is a possible technique to study the sextet transitions in boronlike O IV, F V and Ne VI. The sextet states in B I isoelectronic sequence are well above several ionization levels and metastable against electric-dipole radiation decay to singly excited five-electron states and against Coulomb autoionization into the adjacent continuum 1s2l'2l''nl^4L due to different spin multiplicities. Thus, the main decay channel is radiation in beam-gas experiments. The lifetimes of the ground quintet states in boronlike ions are long enough (about 10^-5 second for O V) so that the "prepared" beryllium-like ions, excited to metastable quintet states by collisions with nitrogen gas molecular, can reach alkaline vapor target atoms. The spectra obtained have significant features emitted from core-excited ions and very clean background because of, after careful preparation and selection of the ion beam, the dominant core-conserving single-electron pick-up cross-sections of metastable doubly excited ions at low beam energy in alkaline vapor cell.

Presented herein are the first measurements on the 1s2s2p^3 4S-1s2s2p^33s, 3d 6P electric-dipole transitions in boronlike O IV, F V and Ne VI by well prepared beam-gas spectroscopy. Comparison is given with the recent results of measurements from beam-foil spectroscopy, and multi-configuration Hartree-Fock (MCHF) and multi-configuration Dirac-Fock (MCDF) calculations for the transitions.

In this work, the beam-gas spectra of oxygen, fluorine and neon at low beam energy were previously recorded at Lyon using grating incidence spectrometers. The experimental arrangement in Fig. 1 was used. Multi-charged ions extracted from a 14 MHz CAPRICE ECR ion source of the AIM, a joint CEA/CNRS facility at CEA Grenoble with acceleration voltage of 2-20 kV, were mass and charge analyzed by two bending magnets.
FIG. 1: Block diagram of the beam-gas experimental apparatus showing the procedures to be followed to prepare $F^5+$ beam in low (3%) and high (48%) fractions of the metastable states.

and sent into the beam line devoted to UV spectroscopy. A nitrogen gas jet target was placed between the two magnets. After electron capture collisions in a cesium cell, photons emitted were detected at 90 degrees to the ion beam direction by a 2.2 m- McPherson grazing incidence spectrometer equipped with a position-sensitive microchannel plate detector which allows simultaneous recording of spectral lines within a wavelength region of about 50 Å in the range of 60-600 Å.

The spectra of fluorine recorded in above experiments are shown in Figs. 2. In the "direct" $F^5+$ beam (similar for $O^+$ and Ne $^+$ ion beams), the fraction of the ions in the $F^5+$($1s^22s^2$) state is high, about 97%, and that of the $F^5+$($1s^22s3s$) metastable state is low, about 3%. In the upper figure of Fig. 2 one sees that the transitions between doublet terms are dominant. In the "prepared" $F^5+$ beam, the fraction of the ions in the $F^5+$($1s^22s2p^3P_{1,2,3}$) state increases to about 45%, that of the $F^5+$($1s^22s^2$) state decreases to about 50%. The lifetime of the $F^5+$($1s^22s2p^3P_{1,2,3}$) quintet metastable state is long enough for such ions to reach the second excitation region, the cesium cell. The fraction of the ions in the $F^5+$($1s^22s^2p^5P_{2,3,4}$) quintet metastable state is about 5% at the energy (>1 keV/amu). The fraction of transitions between quartet terms increase dramatically, as well as that of transitions between sextet terms. In the lower figure of Fig. 2 the transition labelled as P is identified as the 1s2s2p$^3 6S^o - 1s2s2p^33s 6P$ electric-dipole transition at wavelength of 158.61 Å shows up.

Shown in Fig. 3 are the prepared spectra of oxygen, fluorine and neon obtained in above beam-gas experiments. The 1s2s2p$^3 6S - 1s2s2p^33s 6P$ electric-dipole transitions in O IV, F V and Ne VI have been searched in these clean spectra. The observed 1s2s2p$^3 6S - 1s2s2p^33s 6P$ electric-dipole transitions at wavelength of 120.04 Å for Ne VI [3] is confirmed. The observed 1s2s2p$^3 6S - 1s2s2p^33s 6P$ electric-dipole transitions at wavelength of 106.232 Å for Ne VI [2, 3] are absent. Meanwhile, we have found some notable features were unidentified, which are unable to be seen in direct spectra. Shown in Fig. 4 are the details of the 1s2s2p$^3 6S_{5/2} - 1s2s2p^33s 6P_j$ transition in O IV. Here the transition rates from the fine structure j=7/3, 5/2 and 3/2 of the upper state were the results of single-configuration Hartree-Fock (SCHF) calculation by this work. The wavelengths of the fine structure components were calculated SCHF results plus a fitted shift for all three components. The Gaussian curves of the three components utilized the experimental

FIG. 2: Spectra of F V in the 150-180 Å region for direct and prepared beams. The transition labelled as P is the 1s2s2p$^3 6S^o - 1s2s2p^33s 6P$ electric-dipole transition in F V.
TABLE I: The wavelengths (in Å) of the sextet transitions of O IV, F V and Ne VI.

| Ions   | label | term_{\text{lo}} | term_{\text{up}} | λ_{\text{obs}}(Å) by this work | λ_{\text{obs}}(Å) \text{ by MCHF} | λ_{\text{obs}}(Å) \text{ by MCDF} | λ_{\text{mod}}(Å) |
|--------|-------|------------------|------------------|---------------------------------|---------------------------------|---------------------------------|-----------------|
| O IV   | P     | 1s2s2p^{3} 6S   | 1s2s2p^{3} 6P   | 227.13(4)                       | 228.63 a                        | 228.70 b                        | 230.00 a         |
| F V    | P     | 1s2s2p^{3} 6S   | 1s2s2p^{3} 6P   | 158.61(3)                       | 161.39 a                        | 161.46 b                        | 162.10 a         |
| Ne VI  | P     | 1s2s2p^{3} 6S   | 1s2s2p^{3} 6P   | 119.98(2)                       | 120.04 c                        | 120.33 c                        | 120.20 c         |
| Ne VI  | D     | 1s2s2p^{3} 6S   | 1s2s2p^{3} 6P   | 103.99(3)                       | 106.236 c                       | 106.27 c                        | 106.26 c         |

a Blanke [2] b Miecznik [4] c Lapierre [3]

FIG. 3: The Boron-like 2p-3s and 2p-3d sextet electric-dipole transitions for (a) O IV, (b) F V and (c) Ne VI. P: 1s2s2p^{3} 6S - 1s2s2p^{3} 6P electric-dipole transitions. D: 1s2s2p^{3} 6S - 1s2s2p^{3} 6P electric-dipole transitions. A, B and C: 2s2p\^{2} 4P-2s2p\^{3}(3P)\^{3}d 4P\^{o}, 4D\^{o} and 4F\^{o}. a, b and c: 2s2p^{2} 2D-2s2p\^{3}(3P)\^{3}d 2P\^{o}, 2F\^{o} and 2D\^{o}. d and a': 2s2p^{2} 4P-2s2p^{3}(3P)\^{3}d 4P\^{o} and 2s2p^{2} 2S-2s2p\^{3}(3P)\^{3}d 2P\^{o}. a and b: 2s^{2}2p^{2} 2P\^{o}-2s^{2}3d 2D and 2s^{2}2p^{2} 2P\^{o}-2s^{2}3d 2S.

FIG. 4: Relative intensity of the 1s2s2p^{3} 6S\^{o} - 1s2s2p^{3} 6P transition in O IV. The unit of intensity is arbitrary.

width of 0.6 Å for oxygen spectrum. The summation of the three fine structure components is a least-squared fitting of the measured data. The measured wavelength of the transition of 227.13±0.04 is the weighted center of the fitted profile of experimental data using the above theoretical analysis. After studying the details of the transitions theoretically and experimentally described above, and comparing with the measured results of O IV, F V and Ne VI from beam-foil experiments [2, 3], and multi-configuration Hartree-Fock (MCHF) and multi-configuration Dirac-Fock (MCDF) calculations of F V and Ne VI [2, 3, 4], we assign some unidentified observed lines as the 1s2s2p^{3} 6S - 1s2s2p^{3} 6P electric-dipole transitions in O IV, F V and Ne VI. Results of the identification and measurements of wavelengths of transitions between sextet states by this work and comparison are shown in Table I. Errors of wavelengths are small mainly from calibration and curve fitting. The latter includes experimental and statistical errors.

 Present results on O IV, F V and Ne VI represent the first explicit experimental data on transitions between sextet states in boronlike ions. Well prepared beam-gas spectroscopic experiments have yielded new and explicit information on the system. Using the calculated wavelengths and transition rates by this work and results by others, we were able to assign the observed lines to the 1s2s2p^{3} 6S\^{o}-1s2s2p^{3} 6P electric-dipole transitions in O IV, F V and Ne VI, and measured the wavelengths
with good accuracy.

These measurements are part of a series aimed at understanding optical emissions and energy terms in doubly excited sextet states in boronlike ions. The experiments also lend reliability to the use of MFHD and MCDF approaches in calculating wavelengths and transition rates for the transitions between sextet states in boronlike ions.

We thank J. Désesquelles for helpful discussions.

[1] Bin Lin, H. G. Berry, and T. Shibata, A. E. Livingston, H. P. Garnir, T. Bastin, J. Désesquelles, I. Savukov, Phys. Rev. A 67, 062507 (2003).
[2] J. H. Blanke, B. Fricke, P. H. Heckmann and E. Träbert, Phys. Scr. 45, 430 (1992).
[3] L. Lapierre and E. J. Knystautas, J. Phys. B 33, 2245 (2000).
[4] G. Miecznik, T. Brage and C. F. Fischer, Phys. Scr. 45, 436 (1992).
[5] H. G. Berry, T. Bastin, E. Biemont, P. D. Dumont and H. P. Garnir, Rep. Prog. Phys. 5, 12 (1975).
[6] A. E. Kramida, T. Bastin, E. Biemont, P. D. Dumont and H. P. Garnir, J. Opt. Soc. Am. B 16 (11), 1966 (1999).
[7] K. T. Chung, Phys. Rev. A 29, 682 (1984).
[8] C. F. Fischer, T. Brage and P. Jonsson, Computational Atomic Structure an MCHF Approach (Institute of Physics Publishing, Bristol and Philadelphia (1997).
[9] K. G. Dyall, and I. P. Grant, computer physics communications 55, 425 (1989).
[10] F. A. Parpia, C. F. Fischer, and I. P. Grant, Computer Physics Communications 94 (2-3), 249 (1996).
[11] S. Fritzsche, and I. P. Grant, Computer Physics Communications 103 (2-3), 277 (1997).
[12] K. T. Chung, X. W. Zhu and Z. W. Wang, Phys. Rev. A 47 (3) 1740 (1992).
[13] K. T. Chung and X. W. Zhu, Phys. Rev. A 48(3) 1944 (1993).
[14] G. W. F. Drake and R. A. Swainson, Phys. Rev. A 41 (3) 1243 (1990).
[15] J. Désesquelles, A. Denis, S. Martin, L. Chen, Phys. Rev. A 56, 4317 (1997).
[16] J. Désesquelles, M. C. Buchet-Poulizac, J. Bernard, R. Brédy, L. Chen, A. Denis, S. Martin, H. H. Berry, Phys. Scr. T 92, 290 (2001).