1s2s2p3d 6L - 1s2p3d 6D, L=F, D, P Transitions in O IV, F V and Ne VI

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(Dated: March 1, 2019)

We present observations of VUV transitions between doubly excited sextet states in O IV, F V and Ne VI. Spectra were produced by collisions of an O+ beam with a solid carbon target. We also studied spectra obtained previously of F V and Ne VI. Some observed lines were assigned to the 1s2s2p3d 6L - 1s2p3d 6D, L=F, D, P electric-dipole transitions, and compared with results of MCHF (with QED and higher-order corrections) and MCDF calculations. 42 new lines have been identified. Highly excited sextet states in five-electron ions provide a new form of energy storage and are possible candidates for VUV and x-ray lasers.

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

I. INTRODUCTION

Highly excited sextet states in five-electron ions provide a form of energy storage. The research for stimulated VUV- and x-ray emission from highly excited sextet states in five-electron ions has attracted attention in recent years. This new form of energy storage and potential VUV-ray lasers could have many applications in basic science, technology, medicine, and defense. In a proposed VUV and x-ray laser system, one seeks a probability to trigger a release of K- and L-hole energies of sextet states in boron-like ions. Although K- and L-hole energies are not as high as energies released in nuclear fusion, capacity of highly excited sextet states in five-electron ions to store energy is significant (several hundred electron volts per atom shown in Fig. 1). Such a system involves long-lived "storage" metastable states, and there nearby are short-lived higher excited sextet states, from which transitions are emitted with photon radiation, and quintet continuum. An ideal system where VUV and x-ray lasers may be implemented would be among heavy and highly excited ions that have metastable sextet states with long lifetimes. However, structure and transition properties of these sextet states are currently very known.

In 1992 beam-foil spectroscopy [1,2] was used to provide initial data on low-lying sextet states in doubly excited boron-like nitrogen, oxygen and fluorine. Recent work of Lapierre and Knystautas [2] on possible sextet transitions in Ne VI highlights the significance in this sequence. They measured several excitation energies and lifetimes. Fine structures of individual 1s2s2p3d 6P_J states were resolved and measured in O IV, F V and Ne VI by Lin and Berry et al [2]. There are no further results reported for transitions from highly excited sextet states.

In his work, fast beam-foil spectra of oxygen were recorded at Liege using grading incidence spectrometers [2,3]. Spectra of fluorine and neon were previously recorded at the University of Lyon and the Argonne National Lab, The 1s2s2p3d 6L - 1s2p3d 6D, L=F, D, P electric-dipole transitions in O IV, F V and Ne VI have been searched in these spectra, and compared with results of MCHF (with QED and higher-order corrections) and MCDF calculations.

II. THEORY

Energies, lifetimes and relevant E1 transition rates of the doubly excited sextet states 1s2s2p3d 6L, L=F, D, P and 1s2p3d 6D in boron-like O IV, F V and Ne VI
were calculated with Multi-configuration Hartree-Fock (MCHF) method (\textit{\textsuperscript{3}} \textit{\textsuperscript{4}} \textit{\textsuperscript{5}}) (with QED and higher-order relativistic corrections \textit{\textsuperscript{6}} \textit{\textsuperscript{7}}), and Multi-configuration Dirac-Fock (MCDF) GRASP code \textit{\textsuperscript{8}} \textit{\textsuperscript{9}} \textit{\textsuperscript{10}} \textit{\textsuperscript{11}}.

For a sextet state in a five-electron system (β, LS=5/2JM_J)=(n_1l_1^{\nu_1}n_2l_2^{\nu_2} n_3l_3^{\nu_3} n_4l_4^{\nu_4} n_5l_5^{\nu_5} 6L_J, M_J ), where \( \nu=0,1, ..., \) or \( \min (2l_i+1), i=1,2, ..., 5 \), the wavefunction is

\[ \Psi(\beta, LS=5/2J)=\sum_{i=1}^{N} \sum_{M_J=-J}^{J} c_i(\beta_i, LS=5/2JM_J), \] (1)

where \( c_i \) is a configuration interaction coefficient. \( N \) is a total number of configurations with the same LSJM_J and parity, and \( \phi(\beta_i, LS=5/2JM_J) \) is a configuration state function (CSF).

In single-configuration Hartree-Fock (SCHF) calculations only the configurations corresponding to the desired levels, 1s2s2p\textsuperscript{3}d or 1s2p\textsuperscript{3}d, were considered. After updating MCHF codes we performed relativistic calculations with an initial expansion of up to 4000 CSFs and a full Pauli-Breit Hamiltonian matrix. For a five-electron system a CI expansion generated by an active set leads to a large number of expansions. To reduce the number of configurations, we chose configurations \( n_1n_2n_3n_4n_5 \), where \( n_i=1, 2, 3, 4 \) and 5, \( l_i=0, ... \min (4, n_i-1) \). We did not include g electrons for \( n=5 \) shell.

For MCHF calculations of the lower states 1s2s2p\textsuperscript{3}d \( 6L, L=F, D, P \) we chose 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d and 5s electrons to compose configurations. For the 1s2p\textsuperscript{3}d \( 6D \) state we chose 1s through 4d electrons. Fine structure splitting is strongly involved in the experiments and identifications. After determining radial wavefunctions we included relativistic operators of mass correction, one- and two-body Darwin terms and spin-spin contact term in both SCHF and MCHF calculations; these were not included by Miecznik et al. \textit{\textsuperscript{8}}.

We used the screened hydrogenic formula from \textit{\textsuperscript{9}} \textit{\textsuperscript{10}} \textit{\textsuperscript{11}} to estimate quantum electrodynamic effects (QED) and higher-order relativistic contributions for sextet states in five-electron oxygen, fluorine and neon.

In MCDF \textit{\textsuperscript{4}} \textit{\textsuperscript{10}} \textit{\textsuperscript{11}} calculations, firstly we used single-configuration Dirac-Fock approach (SCDF). A basis of j\textsuperscript{ij}-coupled states to all possible total angular momenta J from two non-relativistic configurations, 1s2s2p\textsuperscript{3}d and 1s2p\textsuperscript{3}d, was considered. For convergence we included the ground state 1s\textsuperscript{2}2s\textsuperscript{2}2p\textsuperscript{2} of the five-electron systems. After calculating all possible levels for all J, eigenvectors were regrouped in a basis of LS terms. To obtain better correlations of energy levels of the doubly excited sextet terms 1s2s2p\textsuperscript{3}d \( 6L, L=F, D, P \) and 1s2p\textsuperscript{3}d \( 6D \) in O IV, F V and Ne VI, improved calculations included 1s\textsuperscript{2}2s\textsuperscript{2}2p, 1s\textsuperscript{2}2s\textsuperscript{2}2p\textsuperscript{2}, 1s2s\textsuperscript{2}2p\textsuperscript{3}, 1s2s\textsuperscript{2}2p\textsuperscript{3}3s, 1s2s\textsuperscript{2}2p\textsuperscript{3}3p, 1s2s\textsuperscript{2}2p\textsuperscript{3}3d, 1s2p\textsuperscript{3}3s, 1s2p\textsuperscript{3}3p, 1s2p\textsuperscript{3}3d, 1s2p\textsuperscript{3}4s, 1s2p\textsuperscript{3}4p and 1s2p\textsuperscript{3}4d mixing non-relativistic configurations.

In GRASP code \textit{\textsuperscript{4}} \textit{\textsuperscript{10}} \textit{\textsuperscript{11}} QED effects, self-energy and vacuum polarization correction, were taken into account by using effective nuclear charge \( Z_{\text{eff}} \) in the formulas of QED effects, which comes from an analogous hydrogenic orbital with the same expectation value of \( r \) as the MCDF-orbital in question \textit{\textsuperscript{4}} \textit{\textsuperscript{10}} \textit{\textsuperscript{11}}.

### III. EXPERIMENT

The experiments were performed with a standard fast-ion beam-foil excitation setup at a Van de Graaff accelerator beam line at the University of Liege \textit{\textsuperscript{2}} \textit{\textsuperscript{12}} \textit{\textsuperscript{13}} \textit{\textsuperscript{14}} \textit{\textsuperscript{15}} \textit{\textsuperscript{16}} \textit{\textsuperscript{17}} \textit{\textsuperscript{18}}. To produce spectra of oxygen in the wavelength region near 660-710 A a beam current of about 1.3 \( \mu \)A of \( ^{32}O^{+} \) and \( ^{16}O^{+} \) ions accelerated to energies of 1.5 and 1.7 MeV were yielded at the experimental setup. Such energies were expected to be an optimum for the comparison and production of \( O^{+} \) ions by ion-foil interaction \textit{\textsuperscript{19}}.

The beam current goes through a carbon exciter foil. The foils were made from a glow discharge, had surface densities about 10-20 \( \mu \)g/cm\(^2\) and lasted for 1-2 hours under the above radiation.

VUV radiation emitted by excited oxygen ions was dispersed by a 1m- Seya-Namioka grating-incidence spectrometer at about 90 degrees to the ion beam direction. A low-noise channeltron (below 1 count/min) was served as a detector. Spectra were recorded at energies of 1.5 and 1.7 MeV with 100/100 \( \mu \)m slits (the line width (FWHM) was 1.1 A) and 40/40 \( \mu \)m slits (the line width (FWHM) was 0.7 A) in the wavelength range of 660-710 A.

We have reinvestigated unpublished beam-foil spectra of \( ^{16}O^{+}, ^{19}F^{+} \) and \( ^{20}Ne^{5+} \) ions recorded previously by accelerating \( ^{16}O^{+}, ^{20}(FH)^{+} \) and \( ^{20}Ne^{+} \) ions to beam energies of 2.5 MeV, 2.5 MeV and 4.0 MeV at the University of Lyon and the Argonne National Lab. The line width (FWHM) was 0.3 A, 0.8 A and 0.3 A in the wavelength range of 660-710 A, 567-612 A and 490-555 A in the spectra, respectively.

### IV. RESULTS

Fig. 2(a) -2(c) display three typical spectra of oxygen at beam energies of 1.5, 1.7 and 2.5 MeV in the wavelength range of 660-710 A. In the wavelength region of 660-710 A transitions between the sextet states 1s2s2p\textsuperscript{3}d \( 6L, L=F, D, P \) in O IV were expected. At an \( O_{2}^{+} \) beam energy of 1.5 MeV, \( O_{2}^{+} \) ions are mainly excited to terms of \( O^{2+} \) and \( O^{3+} \). There are no lines emitted from sextet states in O IV in Fig. 2(a). At an \( O^{+} \) beam energy of 1.5 MeV, \( O^{+} \) ions are mainly excited to terms of \( O^{3+} \) and \( O^{4+} \). New and unidentified emissions appear in the spectrum in Fig. 2(b). Fig. 2(c) shows a spectrum with better resolution to see details of lines.

For the 1s2s2p\textsuperscript{3}d \( 6L, L=F, D, P \) transitions we expected to resolve fine structures of the lower states 1s2s2p\textsuperscript{3}d \( 6L \) in the experiments, whereas fine
structures of the upper states 1s2p3d6D are close and less than resolution of the experimental spectra. O V 3p-4d, O IV 2s2p3d-2s2p5s, O V 2s3d-2s4f and O III 2s2p2p3d-2s3p transitions are at 659.589 Å, 670.601 Å, 681.332 Å and 703.854 Å, respectively, close to the neighborhood of the doubly excited sextet transitions. The four wavelengths have been semi-empirically fitted with high accuracy ±0.004 Å by [21, 22, 23] and provide a good calibration for the measurements. Standard error for wavelength calibration is ±0.01 Å in the wavelength region of 660-710 Å. Nonlinear least square fits of Gaussian profiles gave values for wavelengths, intensities and full widths at half maximum (FWHM) of lines. Uncertainties of wavelengths are related to intensities of lines. Through the use of optical refocusing we achieved spectroscopic line width of 0.3 Å. Precision of the profile-fitting program was checked through several known transition wavelengths.

Most of new identifications have been obtained by searching in the spectra for sets of unidentified lines and by comparing energies and relative intensities of the 1s2s2p3d6L1s2p3d6D0 transition with results of calculations by MCDF and MCDF approaches. A promising candidate for the 1s2s2p3d6F11/2-1s2p3d6D9/2 transition appears at the wavelength of 666.99±0.06 Å in the spectra in Fig. 2(b) and 2(c) recorded at 20O+ ion beam energies of 1.7 and 2.5 MeV, which does not appear in the spectrum in Fig. 2(a) recorded at 20O+ ion beam energy of 1.2 MeV. Shown in Fig. 3 are details of the 1s2s2p3d6F0-1s2p3d6D transition in O IV recorded at an O+ ion energy of 2.5 MeV. The curve SCHF is convoluted theoretical profile of fine structure components with a Gaussian function. The experimental width of 0.3 Å for the oxygen spectrum was utilized. The transition rates to fine structure j=11/2 to 1/2 of the lower state were results of single-configuration Hartree-Fock (SCHF) calculations by this work. The wavelengths of fine structure components were calculated SCHF results plus a fitted shift for all five components. Measured wavelength of a component is the weighted center of the fitted profile of experimental data. Experimental transition rate is proportional to area of a peak (fitted intensity×FWHM of experimental data). The curve "Sum" is summation of fitted fine structure components of experimental data. Ratio of measured transition rates for J=11/2-9/2, 9/2-*, J=7/2-*, J=5/2-*, J=3/2- and J=1/2- components at an ion energy of 2.5 MeV in Fig. 3 is about 67.4×0.3:56.3×0.3:45.5×0.3:46.2×0.28:20.9×0.3:11.3×0.3 = 5.96:4.98:4.02:3.81:1.85:1.00. * represents all possible J’s of the upper state 1s2p3d6PJ allowed by electric-dipole transition rules. The ratio is slightly different from theoretical ratio of E1 GF values (in length gauge) of SCHF calculations of 1.188:0.990:0.793:0.595:0.397:0.198 = 6.00:5.00:4.00:3.00:2.00:1.00. Based on above analysis we assign the set of lines as the 1s2s2p3d6F-1s2p3d6D0 transition in O IV [20].

FIG. 3: Relative intensity of the 1s2s2p3d6FJ - 1s2p3d6DJ transition in O IV in the experimental spectrum of oxygen at a beam energy of 2.5 MeV. Unit of intensity is arbitrary.
$^6D^0$ transition in O IV, and determine their wavelengths with good accuracy of $\pm 0.06$ Å.

Similarly, after studying details of transitions theoretically and experimentally described above, and comparing with multi-configuration Hartree-Fock (MCHF) and multi-configuration Dirac-Fock (MCDF) calculations of O IV by this work, we were able to assign these unidentified observed lines as the $1s2s2p^33d$ $^6L-1s2p^33d$ $^6D^0$, $L=F, D$ and P electric-dipole transitions in O IV. Results of the identification and measurements of wavelengths of the transitions are listed in Table I. Errors of measured wavelengths of $\pm 0.06$ Å are small mainly from calibration and curve fitting. The latter includes experimental and statistical errors. In Table I average theoretical transition energy AV is the center of gravity of the $1s2s2p^33d$ $^6L-1s2p^33d$ $^6D^0$ transition energies (computed from fine structure lines calculated by this work) with results of theoretical analysis. Experimental transition energy $E^+$ is the center of gravity of the $1s2s2p^33d$ $^6L-1s2p^33d$ $^6D^0$ transition energies (computed from observed lines) with results of experimental transition rate analysis. $AV^+$ is summation of above average transition energy (AV), QED effect (QED) and higher-order correction (HO). Errors for calculated transition energies in Table I are the root mean squared differences of calculated and experimental transition energies as given below in the table. We also list calculated relativistic transition energies (N-REL) by SCHF method. In Table I we present measured fine structure wavelengths and theoretical values for O IV. The measured and calculated results are consistent after considering experimental and theoretical errors. Fourteen lines are new observations with wavelength accuracy of $\pm 0.06$ Å.

It is noted that in Fig. 2 the line for the $1s2s2p^33d$ $^6F_7/2-1s2p^33d$ $^6D^0_{3/2}$ transition in O IV is much stronger than the SCHF result. The line is a blend of the $1s2s2p^33d$ $^6F_{j=7/2,1}1s2p^33d$ $^6D^0_{j=3/2}$ transition in O IV and a line at the wavelength of 666.27$\pm 0.06$ Å. The latter was identified as the $1s^22p^3p$ $^1D_2-1s^22p^4d$ $^1F_3$ transition at the wavelength of 666.819$\pm 0.03$ Å [21, 22, 23]. In this work we could resolve the set of lines and improve the wavelength accuracy of the $1s^22p^3p$ $^1D_2-1s^22p^4d$ $^1F_3$ transition to 666.27$\pm 0.06$ Å. We list results in Table II. For the $1s^22p^3p$ $^1D_2$ state there are two couplings, $1s^22p(j=1/2)3p(j'=3/2)$ $^1D_2$ and $1s^22p(j=3/2)3p(j'=1/2)$ $^1D_2$. For the $1s^22p^4d$ $^1F_3$ state there are two couplings, $1s^22p(j=1/2)4d(j'=5/2)$ $^1F_3$ and $1s^22p(j=3/2)4d(j'=3/2)$ $^1F_3$. Their energies are different. MCHF and MCDF methods handle it in different ways and give different results. MCHF calculation gives the minimum energies among both configurations. In Table II are listed wavelengths of SCHF and SCDF calculations. We studied the spectrum in the wavelength range around 590 Å and found a strong unidentified line located at 599.85$\pm 0.06$ Å. After studying its details, we assign it as the $1s^22p^3p$ $^1D_2-1s^22p^4d$ $^1F_3$ transition in O IV.

We obtained spectra at a $^{20}$HF$^+$ beam energy of 2.5 MeV for fluorine. Through the use of optical refocusing we achieved spectroscopic line width of 0.7 Å. Using similar experimental analysis as described above we obtained the wavelength accuracy of $\pm 0.10$ Å for the $1s2s2p^33d$ $^6L-1s2p^33d$ $^6D^0$ transitions in the wavelength region of 570-620 Å [24, 25]. In Table III all observed lines for the $1s2s2p^33d$ $^6L - 1s2p^33d$ $^6D^0$, $L=F, D$, $P$ transitions in F V are reported. Fourteen lines are new observations. The strongest fine structure component is the $1s2s2p^33d$ $^6F_{11/2}-1s2p^33d$ $^6D_{9/2}^0$ transition at the wavelength of 574.05$\pm 0.10$ Å.

We obtained spectra at a $^{20}$Ne$^+$ ion beam energy of 4.0 MeV for neon. Through the use of optical refocusing we achieved spectroscopic line width of 0.4 Å in the second order spectrum. Similarly, we obtained wavelength accuracy of $\pm 0.05$ Å for the $1s2s2p^33d$ $^6L - 1s2p^33d$ $^6D^0$ transitions in the wavelength region of 490-550 Å [26, 27]. In Table IV we present measured fine structure wavelength values and theoretical values for the $1s2s2p^33d$ $^6L_{j=1}1s2p^33d$ $^6D_{9/2}^0$ transition in Ne VI. Fourteen lines are new observations. The strongest fine structure component is the $1s2s2p^33d$ $^6F_{11/2}-1s2p^33d$ $^6D_{9/2}^0$ transition at the wavelength of 503.45$\pm 0.05$ Å.

We have studied differences between experimental and theoretical transition energies of the $1s2s2p^33d$ $^6L - 1s2p^33d$ $^6D^0$ transitions along B I isoelectronic sequence. In Fig. 4, 5 and 6 are plots of differences between theoretical and experimental transition energies of the $1s2s2p^33d$ $^6L-1s2p^33d$ $^6D^0$ transitions.

![FIG. 4: Difference (in cm⁻¹) between theoretical and experimental transition energies for the 1s2s2p^33d 6F - 1s2p^33d 6D^0 transitions.](image)
### TABLE I: Energies $E$ (in cm$^{-1}$) and wavelengths $\lambda$ (in Å) for the 1s2s2p$^3$3d $^6L_J$ - 1s2p$^3$3d $^6D_{J'}$ transitions in O IV by this work. We list differences $dE$ between theoretical and experimental transition energies for the transitions.

| J-J' $\lambda$ | $E_{\text{exp}}$ | $E_{\text{mpchf}}$ | $E_{\text{mpcf}}$ | $\Delta E_{\text{mpcf}}$ | $\lambda_{\text{scdf}}$ | $\lambda_{\text{schf}}$ | $\Delta \lambda_{\text{schf}}$ | $\lambda_{\text{nrel}}$ | $\Delta \lambda_{\text{nrel}}$ |
|----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 1s2s2p$^3$3d $^6D_J$, 1s2p$^3$3d $^6D_{J'}$ | ±0.06 | ±0.167 | ±0.385 | ±0.783 | ±0.167 | ±0.385 | ±0.783 | ±0.167 | ±0.385 | ±0.783 |
| 1/2$^a$ | 655.38 | 150290 | 665.83 | 150188 | -102 | 666.07 | 150134 | -156 | 663.74 | 150661 | 371 | 661.98 | 151062 | 772 |
| 1/2$^b$ | 655.65 | 150229 | 666.08 | 150132 | -97 | 666.25 | 150094 | -135 | 663.93 | 150618 | 389 | 662.18 | 151016 | 787 |
| 5/2$^a$ | 655.92 | 150168 | 666.32 | 150078 | -90 | 666.56 | 150024 | -144 | 664.25 | 150546 | 378 | 663.49 | 150946 | 777 |
| 7/2$^a$ | 666.27 | 150089 | 666.69 | 149995 | -95 | 666.74 | 149984 | -106 | 664.65 | 150455 | 366 | 663.88 | 150857 | 768 |
| 9/2$^a$ | 666.63 | 150008 | 667.10 | 149903 | -106 | 667.35 | 149846 | -162 | 665.08 | 150358 | 350 | 663.31 | 150759 | 751 |
| 11/2$^a$ | 666.99 | 149927 | 667.47 | 149819 | -108 | 667.73 | 149761 | -166 | 665.51 | 150261 | 333 | 663.72 | 150666 | 739 |
| AV | 666.41 | 150058 | 666.86 | 149957 | -101 | 667.06 | 149911 | -147 | 664.83 | 150415 | 357 | 663.06 | 150817 | 759 |
| QED | -23.2 | -23.2 | | | | | | | | | | | |
| HO | 270.8 | 84.6 | | | | | | | | | | | |
| AV$^T$ | 665.76 | 150205 | 147 | 666.79 | 149972 | -86 | | | | | | | |
| nonrel | 670.72 | 149094 | -964 | | | | | | | | | | |

1s2s2p$^3$3d $^6D_J$, 1s2p$^3$3d $^6D_{J'}$ transitions with nuclear charge $Z = 8, 9$ and 10.

### TABLE II: Wavelengths $\lambda$ (in Å) for the 1s$^2$2p$^3$3d $^1$D$_J$ - 1s$^2$2p$^4$d $^1$F$_J$ transitions in O V.

| $\lambda_{\text{obs}}^a$ | $\lambda_{\text{obs}}^b$ | $\lambda_{\text{scdf}}^a$ | $\lambda_{\text{schf}}^a$ |
|-----------------|-----------------|-----------------|-----------------|
| ±0.06 | ±0.03 | | |
| 666.27 | 666.819 | 651.12 | 589.09 |

$^a$ this work. $^b$ Elden [23].

$^6$L - 1s2p$^3$3d $^6D^o$, L=F, D, P transitions in boron-like ions. Here theoretical transition energy is the center of gravity of the 1s$^2$2p$^3$3d $^6L_J$, 1s$^2$2p$^3$3d $^6D_{J'}$, transition energies (computed from calculated fine structure lines by this work) with results of theoretical analysis, and experimental transition energy is the center of gravity of the 1s$^2$2p$^3$3d $^6L_J$ - 1s$^2$2p$^3$3d $^6D_{J'}$, transition energies (computed from observed lines) with results of experimental analysis. In Fig. 4 MCDF, SCHF and SCDF differences are constant for the 1s$^2$2p$^3$3d $^6F$ - 1s$^2$p$^3$3d $^6D^o$ transitions with nuclear charge $Z = 8, 9$ and 10. Non-relativistic differences (N-REL) are linear. MCHF differences for oxygen and fluorine are small, just 106 and 249 cm$^{-1}$.

In Fig. 5 SCHF, SCDF and MCDF differences are constant for the 1s$^2$2p$^3$3d $^6D$ - 1s$^2$p$^3$3d $^6D^o$ transitions with nuclear charge $Z = 8, 9$ and 10. Non-relativistic differences are linear. MCHF differences for oxygen and fluorine are small, just 235 and 104 cm$^{-1}$.

In Fig. 6 SCHF and MCDF differences are constant for the 1s$^2$2p$^3$3d $^6P$ - 1s$^2$p$^3$3d $^6D^o$ transitions with nuclear charge $Z = 8, 9$ and 10. SCDF and non-relativistic differences are linear. These linear or constant energy differences can be used to predict easily and with high accuracy transition energies for the 1s$^2$2p$^3$3d $^6L$ - 1s$^2$p$^3$3d $^6D^o$, L=F, D, P transitions for boron-like ions with...
TABLE III: Energies $E$ (in cm$^{-1}$) and wavelengths $\lambda$ (in Å) for the 1s$2s2p^23d$ $^6L_J$-$1s2p^33d$ $^6D_J$, $L= F, D, P$ transitions in F V by this work. We list differences $dE$ between theoretical and experimental transition energies for the transitions.

| $J\rightarrow J'$ | $\lambda_{Exp}$ | $\lambda_{Exp}$ | $\lambda_{MCHF}$ | $\lambda_{MCHF}$ | $\lambda_{QED}$ | $\lambda_{QED}$ | $\lambda_{HO}$ | $\lambda_{HO}$ | $\lambda_{AV}$ | $\lambda_{AV}$ | $\lambda_{N-REL}$ | $\lambda_{N-REL}$ |
|-----------------|----------------|----------------|----------------|----------------|----------------|----------------|--------------|--------------|--------------|--------------|----------------|----------------|
| $1s2s2p^33d$ $^6D_J$ - $1s2p^33d$ $^6D_J'$ | ±249 | ±156 | ±596 | ±1041 |
| 1/2-* | 571.76 | 174899 | 511.40 | 175009 | 110 | 572.27 | 174743 | -156 | 569.83 | 175491 | 592 | 568.94 | 175765 | 867 |
| 3/2-* | 572.01 | 174822 | 571.64 | 174935 | 113 | 573.52 | 174666 | -156 | 570.07 | 175417 | 595 | 568.17 | 176004 | 1182 |
| 5/2-* | 572.41 | 174700 | 571.05 | 174810 | 110 | 572.92 | 174544 | -156 | 570.48 | 175291 | 591 | 569.59 | 175565 | 865 |
| 7/2-* | 572.91 | 174547 | 572.55 | 174675 | 110 | 573.42 | 174392 | -155 | 571.02 | 175125 | 578 | 570.13 | 175399 | 851 |
| 9/2-* | 573.48 | 174374 | 572.58 | 174648 | 274 | 573.99 | 174219 | -155 | 571.62 | 174941 | 567 | 570.75 | 175208 | 834 |
| 11/2-9/2 | 574.05 | 174201 | 573.15 | 174474 | 274 | 574.56 | 174046 | -155 | 572.23 | 174755 | 554 | 571.37 | 175018 | 817 |
| AV | 573.16 | 174471 | 572.52 | 174668 | 196 | 573.67 | 174316 | -155 | 571.28 | 175044 | 573 | 570.31 | 175343 | 871 |

QED and higher-order corrections for the $1s2s2p^23d$ $^6L - 1s2p^33d$ $^6D$, $L=F, D, P$ transitions in O IV, F V and Ne VI are up to -220-370 cm$^{-1}$ (see Table I, III and IV) and can’t be ignored in careful comparison with experiments. Here QED and higher-order corrections were calculated from effective nuclear charge $Z_{eff}$ obtained from MCHF and SCHF calculations. In Fig. 11 are plots of the above corrections to weighted mean transition energies. The results show that weighted mean wavelengths for the $1s2s2p^23d$ $^6L - 1s2p^33d$ $^6D$, $L=F, D, P$ transitions in O IV, F V and Ne VI are sensitive to QED and higher-order corrections to 0.27 Å, 0.26 Å and 0.18 Å, respectively. They are larger than estimated experimental precision of ±0.06 Å, ±0.10 Å and ±0.05 Å. Transition energies are strongly related to electron correlation. We could not get exact electron correlation. QED and higher-order corrections of sextet states in boron-like systems are large enough to be seen experimentally. This
TABLE IV: Energies E (in cm⁻¹) and wavelengths λ (in Å) for the 1s2s2p²3d ⁶L_J-1s2p³3d ⁶D_J, L= F, D, P transitions in Ne VI by this work. We list differences dE between theoretical and experimental transition energies for the transitions.  

| J-J' | λexp | λexp | λmchf | λmchf | λschf | λschf | λescf | λescf | λmchf | λmchf | λschf | λschf | λescf | λescf | λescf | λescf |
|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

TABLE V: Lifetimes (in ps) of the 1s2s2p²3d ⁶P-J-1s2p³3d ⁶D_J states in N III, O IV, F V, Ne V, and Na VII.  

| Ion      | MCHF | SCHF | MCDF | Expt | Theory |
|----------|------|------|------|------|--------|
| 1s2s2p²3d ⁶P-J | | | | | |
| N III    | 45.37 | 40.65 | 47.42 | 66±12\(^a\) | 42.8±18\(^b\) |
| O IV     | 15.32 | 15.29 | 16.01 | 12±3\(^a\) | 14.95±4\(^b\) |
| F V      | 6.82  | 6.90  | 7.02  | 11±4\(^a\) | 6.689±4\(^b\) |
| Ne VI    | 3.57  | 3.54  | 3.61  |      |        |
| Na VII   | 2.10  | 2.04  | 2.07  |      |        |
| 1s2p³3d ⁶D_J | | | | | |
| N III    | 275.3 | 286.2 | 255.3 |      |        |
| O IV     | 225.7 | 238.7 | 213.1 |      |        |
| F V      | 196.7 | 204.3 | 183.3 |      |        |
| Ne VI    | 170.1 | 178.1 | 153.0 |      |        |
| Na VII   | 150.8 | 157.4 | 140.0 |      |        |

\(^a\) Blanke [1]. \(^b\) Miecznik [6].

work could provide a good test for QED and higher-order corrections if electron correlation were known.

V. CONCLUSIONS

We performed MCHF (with QED and higher-order corrections) and MCDF calculations to get energies, lifetimes and relevant E1 transition wavelengths and rates for the 1s2p³3d ⁶L - 1s2p²3d ⁶D_J, L=F, D, P electric-dipole transitions in five-electron O IV, F V and Ne VI. Present beam-foil study of oxygen, fluorine and neon led to observations of 42 new lines in the sextet system of O IV, F V and Ne VI. We measured wavelengths with good accuracy. Identifications are mainly obtained by comparing transition wavelengths and rates with results of MCHF and MCDF calculations. Theoretical and experimental transition energies are consistent in errors.
FIG. 5: Difference (in cm$^{-1}$) between theoretical and experimental transition energies for the 1s2s2p$^2$3d $^6$D - 1s2p$^3$3d $^6$D$^o$ transitions.

FIG. 6: Difference (in cm$^{-1}$) between theoretical and experimental transition energies for the 1s2s2p$^2$3d $^6$P - 1s2p$^3$3d $^6$D$^o$ transitions.

Differences between theoretical and experimental transition energies are in reasonable range. For lifetimes of the 1s2s2p$^2$3d $^6$P states in O IV and F V there remain large discrepancies of about 20% between results of MCHF and MCDF calculations and experiments from [1].

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FIG. 7: Reduced experimental transition energies $E/(Z-1.86)$ (in cm$^{-1}$) for the $1s2s2p^23d\ ^6F_J-1s2p^33d\ ^6D_J^o$ transitions.

FIG. 8: Reduced experimental transition energies $E/(Z-1.86)$ (in cm$^{-1}$) for the $1s2s2p^23d\ ^6D_J-1s2p^33d\ ^6D_J^o$ transitions.

FIG. 9: Reduced experimental transition energies $E/(Z-1.86)$ (in cm$^{-1}$) for the $1s2s2p^23d\ ^6P_e-1s2p^33d\ ^6D_J^o$ transitions.

FIG. 10: Lifetimes (in ps) for the $1s2s2p^23d\ ^6P_e$ states in B I isoelectronic sequence. Experimental values are taken from Table V.

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FIG. 11: Lifetimes (in ps) for the \( 1s2p^33d^6D^o \) states in the boron sequence.
FIG. 12: QED and higher-order corrections (in cm$^{-1}$) for (a) the 1s2s2p$^2$3d$^6$F - 1s2p$^3$3d$^6$D$^o$, (b) 1s2s2p$^2$3d$^6$D - 1s2p$^3$3d$^6$D$^o$ and (c) 1s2s2p$^2$3d$^6$P - 1s2p$^3$3d$^6$D$^o$ transitions in B I isoelectronic sequence.