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The $1s2s2p^2\ {}^5P_{1,2,3}$–$1s2p^3\ {}^5S_2^0$ Transition in Ne VII

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Abstract

The $1s2s2p^2\ {}^5P_{1,2,3}$–$1s2p^3\ {}^5S_2^0$ Ne VII transitions have been observed in the vacuum-ultraviolet spectrum of a foil-excited neon beam. Their wavelengths and the fine structure follow well the trend recently developed for the isoelectronic series of negative Li through F VI. We compare these results to computations using MCDF-OL and MCDF-EAL methods. We also identify transitions from doubly-excited singlet states in Ne VII and note that some of these have been incorrectly classified in the literature.

1. Introduction

Recent attention to the $1s2s2p^2\ {}^5P$–$1s2p^3\ {}^5S^o$ transition in the beryllium isoelectronic sequence began with the prediction by Bunge [1] that the 348.97 nm line in published beam-foil spectra [2] arose from a transition in Li^- between states metastable against autoionisation. This has now been well verified [3–6]. Additionally, several authors have searched for the analogous transitions along the isoelectronic sequence in Be I [6, 7], B II [6], C III, N IV and O V [8, 9], and F VI [10].

These core-excited states are the lowest energy states of their respective symmetries, and, as such, pose an interesting test of the different variants of Multiconfiguration Dirac–Fock (MCDF) computations. In earlier papers [6, 8], we have compared measurements for some of these elements to MCDF-OL (Optimal Level) calculations, including the Breit interaction as a first order perturbation. The fine structure showed good agreement, but the actual wavelengths showed systematic differences from theory. Subsequently, Hata and Grant [11] performed MCDF-EAL (Extended Average Level) computations [12] on these species. They claim improved agreement in the transition wavelengths. However, for N IV and O V, with the best resolved fine structure measurements then published, the experimental data lay in between the different computations.

In the present paper, we extend the wavelength and lifetime measurements along this isoelectronic sequence to Ne VII. Interest in the $1s2s2p^2$ configuration of Ne VII had previously arisen [13] in the context of plasma diagnostics, where neon is often used as a tracer impurity [14]. We compare the results of our measurements, and the recent fluorine measurements of Martinson et al. [10], to the predictions of MCDF calculations.

2. Experiment

As in previous work on this subject [8], we used a standard beam-foil arrangement to ionize and excite a neon beam. Using the Argonne Physics Division Dynamitron, we accelerated Ne^{+2} ions from an RF discharge source through potentials of up to 4.1 MV to produce beam energies of up to 8.2 MeV. These beams were stripped by carbon foils of 5 $\mu g/cm^2$ areal density. Energies in this range are optimal for foil production of Ne VII [15]. Care was taken to avoid and detect possible contamination of Ar ions in the beam, which would not have been completely removed by magnetic selection after acceleration. (An exception was for wavelength calibration, discussed later.)

The post-foil light was analyzed using a McPherson model 225 one meter near-normal incidence monochromator and was detected using a channel electron multiplier. The monochromator was compensated for the moving light source by an appropriate translation of the grating [16]. Attempts were made to observe the lines of interest in the first three spectral orders, using different gratings of appropriate blaze. Our results include an estimated correction to compensate for a periodic scanning error known to affect such monochromators [17].

Data acquisition was controlled by a PDP 11/45 computer, which recorded photon counts in intervals of equal integrated beam current. At the conclusion of each interval, the computer advanced the monochromator (for spectral measurements) or the foil position (for lifetime measurements). Usually, lifetime and wavelength measurements were made in duplicate under each successful condition, and the results were summed for final analysis.

3. Results

The quintet transitions appear as weak lines among a rich collection of other, unidentified lines of highly ionized neon. Figure 1 shows a spectrum of the region of interest in first order, with a 7.2 MeV incident neon beam and a grating blazed at 80 nm. The wavelengths were referenced to the 52.6457 nm Ar VIII line [18], which appeared when we mixed argon with the neon at the accelerator source. Due consideration was made for second-order Doppler shifts, which significantly differed between the Ne^{+2} and Ar^+ beams.

The quintet state transitions were selected from among these lines using two considerations. Firstly, isoelectronic extrapolation of previous measurements and their variation from theory narrowed the search to within 0.05 nm. In Fig. 2, we show this progression using MCDF theoretical values.

Secondly, decay profiles were taken of all features in this, the central region of Fig. 1. The three quintet state transitions, originating from the same upper state, were matched by their common decay profiles. We find the lifetime of this upper state to be 0.09 ± 0.01 ns, which is somewhat under the value to be expected from the isoelectronic extrapolation of past data and the theory used earlier [8]. We summarize the lifetime data in Table I.

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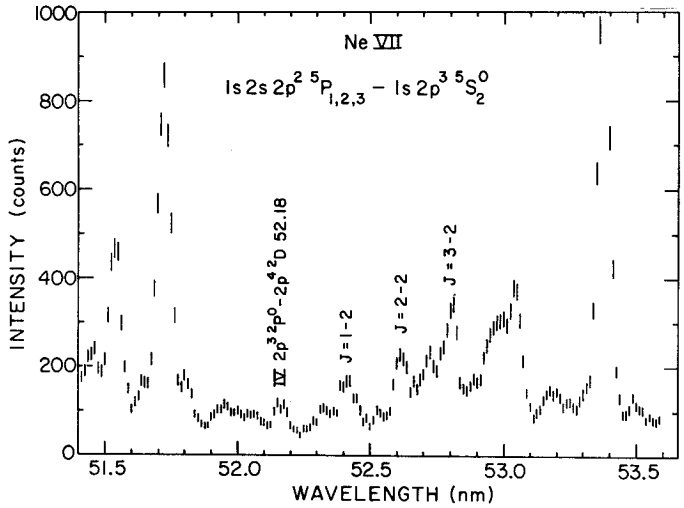

Fig. 1. Beam-foil spectrum of neon at 7.2 MeV, in first order, showing the $1s2s2p^2\ ^5P_{1,2,3}$–$1s2p^3\ ^5S_2^o$ transitions. Most transitions in this wavelength range have not been previously reported.

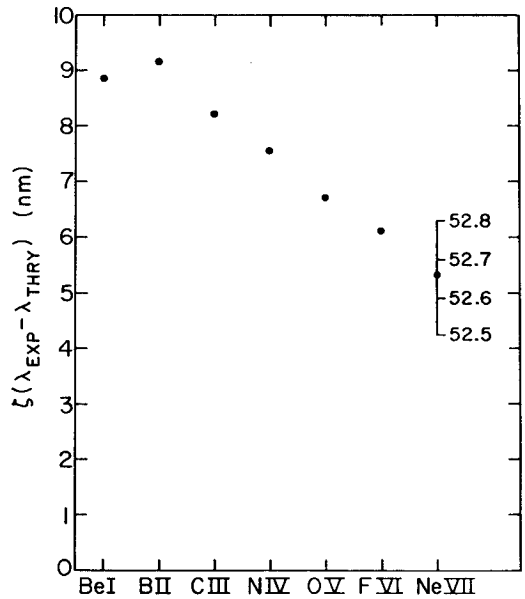

Fig. 2. The difference between experiment and MCDF calculation for the quintet transition wavelengths, scaled by the charge state ζ, along the Be isoelectronic sequence.

Peak locations were found using non-linear χ^2 fits to Gaussian profiles. In Table II, we display our wavelength measurements.

4. Comparison with theory

In response to our earlier papers [6, 8], Hata and Grant [11] claim encouraging improvement in calculation of the transition energies for these systems. Their opinion was based on the published values for C, N and O. We are now in a position to extend the comparison to F and Ne.

In Table III, we compile the available information. As Hata and Grant did not publish values for F and Ne, we used the Grant MCDF program [19] with the Breit interaction post-processor [20] to reproduce and extend their computations. We also used 30 configuration states, the maximum permitted by our program version, consisting of all *jj*-coupled states arising from the $1s^22s2p$, $1s2s2p^2$ and $1s2p^3$ electronic configurations. These included configuration states of total angular momentum J equal to 0, 1, 2 and 3.

However, the MCDF-EAL procedure is block diagonal in J, except for slight interactions in the initial estimation of an average potential, and therefore the $J = 0$ configurations should have no appreciable effect on the states of interest. Rerunning the program, now with only 25 configurations, we see in Table III that in fact the computed transition wavelengths hardly change.

We may now add additional configuration states of the form $1s2s^22p$. In a fully self-consistent MCDF-OL calculation, they would add no new information and would be an unwelcome indeterminancy. However, their inclusion is justified in EAL, as it would be for other CI-type calculations. The final EAL results are quite close to our original OL results and do not appear to represent an improvement in accuracy.

Hata and Grant also computed the fine structure splittings, but for the experimental data then available, they noted that there was not enough information to favour one calculation rather than another. We were unable to reproduce the fine structure splittings exactly as quoted, but these minor differences may only reflect slight differences in the manner in which we ran the program. More significantly, we show in Table IV how the EAL method gives fine structure results which are quite sensitive to the selection of configurations. As a rule, the EAL calculations give larger structures than do their OL counterparts, which is in accord with experiment for the recent F and Ne results. In Fig. 3, we compare experiment to the OL and EAL predictions.

Table I. *Lifetime of the* $1s2p^3\ ^5S_2$ *state*

Ion	Experiment (ns)	Theory (ns)
C III	0.49 ± 0.03[a]	0.39[a]
N IV	0.33 ± 0.06[a]	0.31[a]
O V	0.21 ± 0.02[a, b]	0.26[a]
F VI	0.18 ± 0.02[c]	0.22[d]
Ne VII	0.09 ± 0.01[e]	0.19[d]

[a] Berry et al. [8].
[b] Livingston and Hinterlong [9].
[c] Martinson et al. [10].
[d] Cheng, Private Communication.
[e] This Work.

5. Further remarks on Ne VII

In discussing Fig. 1, we noted that most of the lines in that figure were unidentified. It is appropriate to take a general view of the state of classification of the Ne VII term scheme. While many experiments have been performed to look at the spectra of highly ionised neon below 30 nm [15, 21–25], measurements in the rest of the ultraviolet spectrum for Ne VII [26–29] are incomplete.

Table II. *Wavelengths and energy intervals of the* $1s2s2p^2\ ^5P_{1,2,3}$–$1s2p^3\ ^5S_2$ *multiplets*

Interval	Transition wavelength (nm)	Fine structure (cm^{-1})
$^5P_1$–$^5S_2^o$	52.420 ± 0.020	
$^5P_2$–$^5S_2^o$	52.616 ± 0.010	711 ± 22
$^5P_3$–$^5S_2^o$	52.805 ± 0.010	680 ± 7
$^5P_{cg}$–$^5S_2^o$	52.665 ± 0.010	

Table III. *MCDF computations of mean transition wavelengths (nm)*

Ion	Experiment	OL	H & G[a]	30 C[b]	25 C[c]	28 C[d]
C III	101.606 ± 0.005[e]	98.9[e]	100.37	100.37	100.34	99.07
N IV	82.565 ± 0.005[e]	80.7[e]	81.64	81.64	81.62	80.69
O V	69.475 ± 0.010[e]	68.2[e]	68.81	68.81	68.80	68.08
F VI	59.967 ± 0.010[f]	58.9[g]	–	59.43	59.43	58.86
Ne VII	52.665 ± 0.010[h]	52.0[g]	–	52.26	52.26	51.80

[a] Hata and Grant [11].
[b] This work, all $J = 0, 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$.
[c] This work, all $J = 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$.
[d] This work, all $J = 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$, $1s2s^22p$.
[e] Berry et al. [8].
[f] Martinson et al. [10].
[g] Cheng, Private communication.
[h] This work.

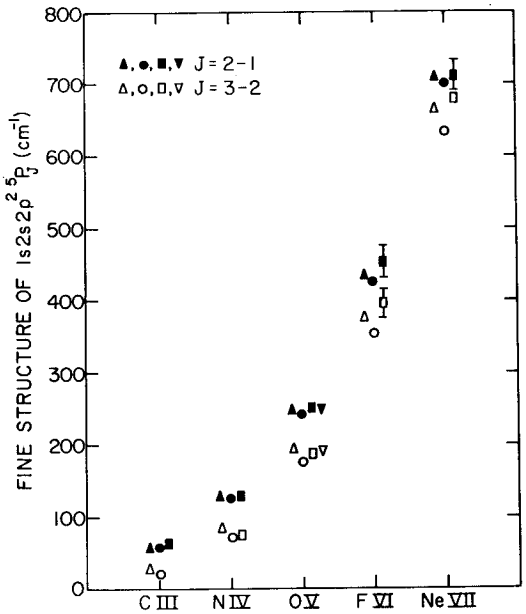

Fig. 3. Experimental and theoretical fine structure intervals of the $1s2s2p^2\ {}^5P$ states. The shaded points represent $J = 2$–1 intervals; the open points represent $J = 3$–2 intervals. The boxes are experimental results of [8], [10] and this work. The downward triangles are the experimental results of [9]. Circles are the MCDF-OL calculations of Cheng [8], the upward triangles are the MCDF-EAL calculations of Hata and Grant [11].

In a recent series of articles [30–32], Edlén reviews the patterns of atomic data along the beryllium sequence. However, data are absent for the $2s2p\ {}^1P_1$–$2p^2\ {}^1S_0$ and $2s2p\ {}^1P_1$–$2p^2\ {}^1D_2$ transitions in Ne VII, which he predicts by interpolation to be found at 56.127 nm and 97.335 nm, respectively [32]. These predictions should be given much consideration. There are no sources of configuration interaction to perturb the states connected by these transitions, and so the interpolation method should be quite good.

However, published classifications of some $2p^2$–$2p3l$ transitions in this system are incompatible with these predictions. In a recent compilation [33], Kelly bases the term system for the $2pnl$ states on the assignments of the 12.1774 nm and 11.1152 nm lines (± 0.001 nm) to the transitions $2p^2\ {}^1S_0$–$2p3d\ {}^1P_1$ and $2p^2\ {}^1D_2$–$2p3d\ {}^1P_1$, respectively [21]. These lines are far from forming a closed loop with the Edlén predictions. Alternatively, one may adopt the classifications of Hermansdorfer [22] who independently assigned the 12.120 nm and 11.100 nm lines (± 0.005 nm) to these transitions. While less precise, these fit well.

In Table III of [22], a line is reported at 110.00 Å. While this agrees with early work of Barrette [15], since revised, its incorrect placement in the table suggests an error in transcription. In this paper, we take that value to be 111.00 Å, which would be consistent with both the placement in the table and another closed loop claimed by Hermansdorfer in his identifications, using the 8.211 nm and 14.129 nm lines.

The $2s2p\ {}^1P$–$2p^2\ {}^1D$ line that Edlén forecasted to be at 97.335 nm we see as a strong line at 97.36 ± 0.01 nm. This agrees with previous observation and identification in a theta-pinch experiment [34] and beam-foil work [35]. However, the $2s2p\ {}^1P$–$2p^2\ {}^1S$ line had not been reported previously. We find this transition at 56.125 ± 0.001 nm. In Fig. 4(a), we show the spectral range of interest, including the corresponding triplet transitions, and in Fig. 4(b), we show a constrained fit to locate the 56.125 nm singlet transition. While this fit presupposed equal peak widths of 0.018 nm, equal to the best fit of the 56.1728 nm line alone, and an intensity ratio of 5 : 1 between the 56.1728 nm and 56.1378 nm lines, the normal branching

Table IV. *MCDF computations of fine structure splittings (cm^{-1})*

Interval	Ion	Experiment	OL[a]	H & G[b]	30 C[c]	25 C[d]	28 C[e]
$J = 2$–1	C III	63.5 ± 1.5[a]	57	59.63	59.51	67.24	60.02
	N IV	127 ± 1[a]	125	129.19	128.94	135.79	128.51
	O V	252 ± 4[a]	242	247.34	246.89	253.15	245.82
	F VI	453 ± 20[f]	426	433.19	432.42	438.28	430.88
	Ne VII	711 ± 22[g]	700	709.46	708.25	713.80	706.31
$J = 3$–2	C III	–	21	30.21	30.16	41.63	30.63
	N IV	79.5 ± 0.8[a]	73	86.72	86.58	96.62	85.48
	O V	188 ± 2[a]	176	194.95	194.66	203.73	192.45
	F VI	396 ± 20[f]	354	378.50	377.97	386.30	374.86
	Ne VII	680 ± 7[g]	633	665.17	664.22	671.95	660.32

[a] Berry et al. [8].
[b] Hata and Grant [11].
[c] This work, all $J = 0, 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$.
[d] This work, all $J = 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$.
[e] This work, all $J = 1, 2, 3$ in $1s^22s2p$, $1s2s2p^2$, $1s2p^3$, $1s2s^22p$.
[f] Martinson et al. [10].
[g] This work.

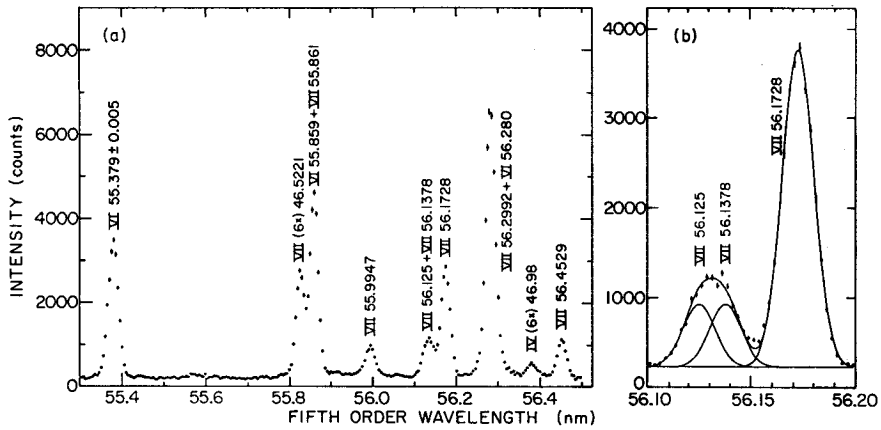

Fig. 4. Fifth order spectra of Ne VII lines from a 3 MeV beam. (a) Prominent transitions, principally $2s2p\ ^3P^o–2p^2\ ^3P$. The strong line at 55.379 nm has been classified as Ne VI $2s2p^2\ ^2D–2p^3\ ^2D^o$ [29, 36]. (b) High resolution scan locating the 56.125 nm $2s2p\ ^1P^o–2p^2\ ^1S$ line. The solid lines represent constrained fits to Gaussian profiles.

ratio, relaxation of these conditions did not significantly alter the results.

6. Conclusions

In this paper, we looked at transitions between doubly-excited states in quintets and singlets. These $\Delta n = 0$ transitions, which are sensitive tests of relativistic effects in this few-electron system, indicate the importance of the Breit interaction and the limits to which it correctly approximates the many-bodied phenomena in the Hamiltonian. We've pointed out before [8] that the fine structure of the ^5P configuration depends largely on the Breit interaction, and the present results seem to indicate a systematic discrepancy with existing calculations at high Z. This is in addition to the systematic difference in the mean transition wavelength, which was noticed earlier.

The results also indicate the need for more classification work in highly ionized neon. It's reasonable to expect that a number of the unidentified lines, some strong, are also in doubly-excited manifolds, and atomic data on neon is of continued importance in its role as a plasma probe. Further work on the term structure of Ne VII is clearly called for, both in light of the sensitivity of the measurements to relativistic effects and because of the spectra available from the beam-foil light source.

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Erratum: In Table I of Reference [8], the $J = 2–3$ fine structure value for Be I should read – 3.

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