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On the 3s–3p and 3p–3d Transitions in Ne-like Ni XIX*

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Abstract

An experimental and theoretical study has been made of the 3s–3p and 3p–3d transitions in Ni XIX. The method of beam-foil spectroscopy, using 30–64 MeV Ni ions from a tandem accelerator, has been combined with theoretical calculations using the multiconfiguration Dirac–Fock (MCDF) program.

1. Introduction

The first experimental investigations of energy levels in highly ionized members of the Ne I isoelectronic sequence were carried out more than 50 years ago. In 1936 Edlén and Tyrén [1] thus reported the wavelengths of the $n = 2$–3 resonance transitions in Ne-like K X–Cr XV. Somewhat later Tyrén [2] presented additional data for Cr XV and further extended the analyses to Mn XVI–Co XVIII.

Much interest has in recent years been focussed on the ions of the Ne I sequence. A major impetus for their study was provided by Vinogradov *et al.* [3] who found these systems to be suitable candidates for lasing action in the far UV and X-ray regions. This amplification of radiation has been demonstrated in recent years [4, 5].

Transitions in Ne-like Fe and Ni have been identified in the far UV-spectrum of solar flares [6, 7]. The applicability of transitions in Ne-like ions in connection with the diagnostics of tokamak plasmas has also been emphasized recently [8].

Laboratory measurements of the 3s–3p and 3p–3d transitions in the Ne I sequence have been reported for several ions, e.g., Ca XI [9], Sc XII [10], Ti XIII [11, 12], V XIV [10], Cr XV [10, 13], Mn XVI [10] and Fe XVII [14]. These experimental studies, performed using the laser-plasma and beam-foil light sources, have been complemented by a number of theoretical investigations. For example, the relativistic multiconfiguration Dirac–Fock (MCDF) code has been successfully applied to the calculation of wavelengths in Ne-like ions [15].

In the present paper we have extended the beam-foil spectroscopy technique to Ne-like Ni XIX. The experimental investigation has also been combined with a theoretical study of transition wavelengths and oscillator strengths for several members of the Ne I sequence.

2. Experimental and data analyses

The experimental work was carried out at the Brookhaven National Laboratory. Beams of Ni ions, obtained from the MP-tanden Van de Graaff accelerator, were sent through a thin (20 μg/cm^2) carbon foil. The spectra were analyzed with a Minuteman 322G, 2.2 m grazing-incidence spectrometer, the exit slit of which was replaced by a 25 mm microchannel plate, coupled to a resistive anode encoder. For details of the experimental arrangement the reader is referred to Ref. [16].

Spectra were taken at four ion energies, 30, 40, 49 and 64 MeV and in the wavelength region 200–450 Å. To cover this wavelength range the microchannel plate had to be placed at several positions on the Rowland circle.

Spectra were further recorded at various distances on the downstream side of the foil. In this way information was obtained about decay curves and lifetimes of the various transitions, as discussed in Ref. [16]. The lifetime results will be reported in a forthcoming paper [17].

In the determination of wavelengths for Ni lines not reported earlier we used transitions in Ni XVIII (Na-like) and Ni XVII (Mg-like) with accurately known wavelengths from previous work [18, 19] as standards. The wavelength accuracy for the new transitions is estimated to about ± 0.1 Å.

3. Dirac–Fock calculations

A number of calculations have been performed for the Ne I isoelectronic sequence. Previous work thus includes non-relativistic calculations [20, 21], applications of relativistic perturbation theory [22], as well as multi-configuration Dirac–Fock calculations [15]. To obtain a consistent set of wavelengths and transition probabilities we have performed additional theoretical studies. Thus multiconfiguration Dirac–Fock (MCDF) computations of the energy levels and transition probabilities were performed for the neonlike isoelectronic ions Ti^{+12} through Ni^{+18}. The calculations were carried out by network using the National Magnetic Fusion Computer Center CRAY X-MP E computer in Livermore, California. The code used was an improved version [23] of the

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Table I. *Multiconfiguration Dirac–Fock (MCDF) calculations for Ti XIII–Ni XIX*

Transition		Ti XIII	V XIV	Cr XV	Mn XVI	Fe XVII	Co XVIII	Ni XIX
$3s(3/2,\ 1/2)_2$–$3p(3/2,\ 1/2)_1$	λ	550.07	507.21	469.95	437.31	408.50	382.93	360.12
	τ	440	391	349	313	283	257	235
	B	.86	.88	.90	.92	.94	.96	.98
$3s(3/2,\ 1/2)_1$–$3p(3/2,\ 1/2)_2$	λ	506.35	470.67	439.59	412.25	388.02	366.38	346.95
	τ	243	221	202	186	173	161	150
	B	.56	.56	.55	.55	.55	.54	.54
$3s(3/2,\ 1/2)_2$–$3p(3/2,\ 3/2)_3$	λ	472.91	435.99	403.60	374.89	349.23	326.12	305.17
	τ	207	183	164	147	132	119	107
	B	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$3s(3/2,\ 1/2)_1$–$3p(3/2,\ 3/2)_1$	λ	477.06	441.22	409.78	381.90	356.93	334.37	313.84
	τ	234	210	190	172	156	142	129
	B	.88	.90	.92	.93	.95	.96	.98
$3s(3/2,\ 1/2)_2$–$3p(3/2,\ 3/2)_2$	λ	435.55	401.70	372.04	345.79	322.34	301.24	282.12
	τ	220	196	175	156	141	126	114
	B	.54	.54	.54	.53	.53	.53	.52
$3s(3/2,\ 1/2)_1$–$3p(3/2,\ 3/2)_2$	λ	458.27	422.94	391.88	364.30	339.60	317.33	297.11
	τ	220	196	175	156	141	127	114
	B	.43	.44	.45	.45	.46	.46	.47
$3s(3/2,\ 1/2)_1$–$3p(3/2,\ 3/2)_0$	λ	413.70	377.94	346.56	318.81	294.12	272.05	252.23
	τ	229	203	181	161	143	127	112
	B	.77	.78	.79	.81	.82	.84	.87
$3s(1/2,\ 1/2)_1$–$3p(1/2,\ 1/2)_1$	λ	504.57	468.61	437.38	409.99	385.78	364.20	344.85
	τ	243	221	202	186	172	161	150
	B	.51	.53	.54	.56	.57	.58	.59
$3s(1/2,\ 1/2)_0$–$3p(1/2,\ 3/2)_1$	λ	453.30	419.30	389.35	362.70	338.70	317.12	297.40
	τ	231	206	185	166	150	136	123
	B	.48	.51	.54	.56	.58	.60	.61
$3s(1/2,\ 1/2)_1$–$3p(1/2,\ 3/2)_2$	λ	471.18	433.97	401.41	372.62	346.94	323.86	302.95
	τ	216	192	171	153	137	123	111
	B	.96	.97	.98	.98	.99	.99	.99
$3p(3/2,\ 1/2)_1$–$3d(3/2,\ 3/2)_0$	λ	351.61	327.25	305.88	286.91	269.88	254.47	240.39
	τ	112	103	95	88	81	75	70
	B	.88	.90	.91	.93	.95	.96	.98
$3p(3/2,\ 1/2)_1$–$3d(3/2,\ 3/2)_1$	λ	346.18	321.75	300.32	281.32	264.29	248.89	234.86
	τ	27	21	16	13	10	8	7
	B	.18	.15	.13	.11	.10	.09	.08
$3p(3/2,\ 3/2)_3$–$3d(3/2,\ 5/2)_4$	λ	368.76	343.01	320.60	300.89	283.40	267.75	253.66
	τ	97	90	84	78	73	69	65
	B	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$3p(3/2,\ 1/2)_2$–$3d(3/2,\ 3/2)_3$	λ	358.15	331.33	307.87	287.13	268.62	251.97	236.88
	τ	91	83	77	71	65	60	56
	B	.86	.86	.86	.86	.86	.87	.87
$3p(3/2,\ 3/2)_1$–$3d(3/2,\ 3/2)_2$	λ	361.56	335.32	312.53	292.54	274.87	259.13	245.03
	τ	94	87	80	74	69	64	60
	B	.64	.63	.63	.62	.62	.61	.61
$3p(3/2,\ 3/2)_2$–$3d(3/2,\ 5/2)_3$	λ	364.99	338.99	316.43	296.64	279.12	263.48	249.42
	τ	100	92	86	80	75	71	66
	B	.82	.82	.82	.82	.82	.82	.82
$3p(1/2,\ 1/2)_1$–$3d(1/2,\ 3/2)_2$	λ	353.90	327.53	304.46	284.05	265.83	249.42	234.54
	τ	93	85	78	72	66	61	57
	B	.87	.87	.87	.87	.87	.87	.87
$3p(1/2,\ 3/2)_1$–$3d(1/2,\ 5/2)_2$	λ	365.95	340.13	317.69	297.99	280.53	264.92	250.87
	τ	104	97	90	85	80	75	71
	B	.80	.81	.82	.83	.84	.85	.86
$3p(1/2,\ 3/2)_2$–$3d(1/2,\ 5/2)_3$	λ	364.23	338.52	316.19	296.58	279.20	263.67	249.69
	τ	99	91	85	79	74	70	66
	B	.99	.99	.99	.99	1.00	1.00	1.00

λ = transition wavelength (Å).
τ = lifetime of upper level (ps).
B = branching ratio (B = 1.00 implies that there are no other allowed decay modes).

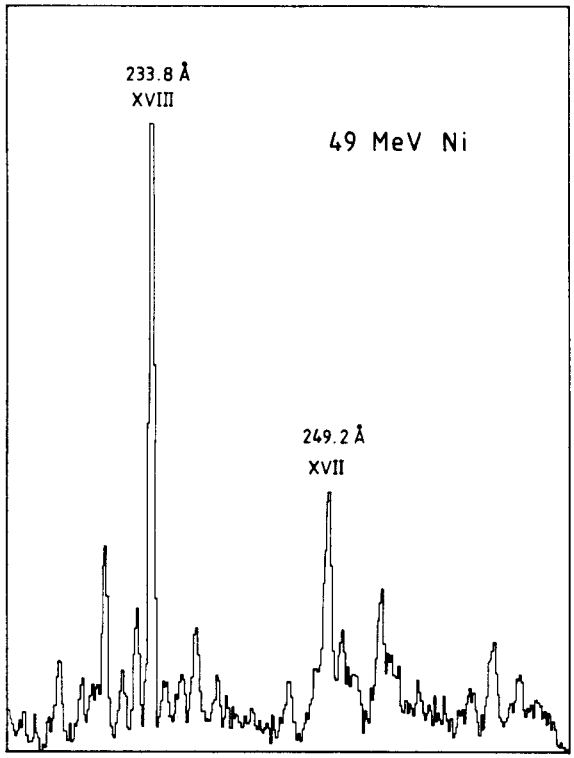

Fig. 1. Partial spectrum of Ni, recorded using 49 MeV ions. The strongest lines belong to Ni XVII and Ni XVIII, whereas several of the less intense ones are transitions in Ni XIX.

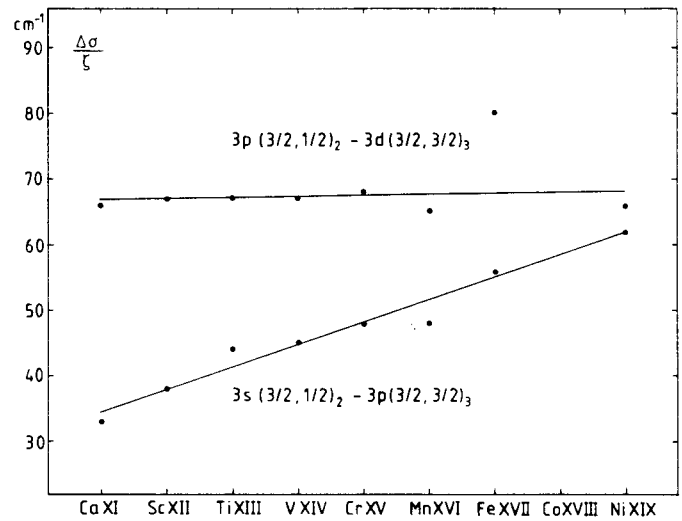

Fig. 2. Isoelectronic study of the difference between theoretical and experimental wavenumbers for two transitions in the Ne I sequence.

program MCDF developed by Grant and coworkers [24]. Computations were made using the MCDF-EAL option of the code, and included the desired configurations $2s^2 2p^5 3s$ (4 levels), $2s^2 2p^5 3p$ (10 levels), $2s^2 2p^5 3d$ (12 levels) and, to provide a balanced set of orbitals for the EAL calculation, also included the configurations $2s2p^6 3s$ (2 levels), $2s2p^6 3p$ (4 levels), $2s2p^6 3d$ (4 levels) and $2s^2 2p^6$ (the ground level). Perturbative corrections were included to account for the finite size of the nucleus and the Breit interaction, as well as vacuum polarization, electron self-energy, and other quantum electrodynamic effects. Electric dipole transition probabilities were computed using both Coulomb and Babushkin gauge, and the Coulomb gauge results were selected for presentation. Table I reports calculations of selected transition wavelengths, lifetimes, and branching ratios among the $2s^2 2p^5 nl$ levels (the transition probabilities can be obtained as the quotient of the branching ratio and the lifetime). The selection criteria for inclusion in this table were that transition probabilities for the Ni^{+18} ion be greater than $3.5 \times 10^9 s^{-1}$ for the $3s$–$3p$ transitions, and greater than $10 \times 10^9 s^{-1}$ for the $3p$–$3d$ transitions. The wavelength estimates are in close agreement with MCDF energy level calculations reported by Cogordan and Lunell [15].

The MCDF lifetime estimates are generally somewhat shorter than earlier nonrelativistic calculations by Loulergue and Nussbaumer [20] and similar calculations with Breit–Pauli corrections by Bureeva and Safronova [21]. Agreement is satisfactory with the calculations of Bhatia *et al.* [25] in which relativistic effects were included as perturbations.

4. Results

Figure 1 shows a partial spectrum, obtained using 49 MeV ions. The strongest lines in our spectra are transitions in Ni XVIII and Ni XVII, whereas several of the less intense transitions can be ascribed to $3s$–$3p$ and $3p$–$3d$ transitions in Ni XIX.

In classifying these Ni XIX transitions we took advantage of the previous experimental work [9–14], the present calculations (Table I) and those of Cogordan and Lunell [15]. The latter, also performed using the MCDF code of Grant and coworkers [24], have been shown to give transition wave-

Table II. *Experimental and theoretical wavelengths in Ni XIX. Wavelength (Å)*

Transition	Theory[a]	Theory[b]	Extrapolation[b]	Experiment[b]	Solar flare spectrum[c]
$3p(1/2, 1/2)_1$–$3d(1/2, 3/2)_2$	234.55	234.54	235.36	235.4	
$3p(3/2, 3/2)_2$–$3d(3/2, 5/2)_3$	249.42	249.42	250.21	250.3	
$3p(1/2, 3/2)_1$–$3d(1/2, 5/2)_2$	250.92	250.87	251.33	251.5	
$3p(3/2, 1/2)_2$–$3d(3/2, 3/2)_3$	236.88	236.88	237.60	237.6	237.61
$3p(3/2, 3/2)_3$–$3d(3/2, 5/2)_4$	253.63	253.66	254.19	254.3	254.53
$3p(1/2, 3/2)_2$–$3d(1/2, 5/2)_3$	249.71	249.69	250.52	250.3	
$3s(1/2, 1/2)_1$–$3p(1/2, 3/2)_2$	303.81	302.95	303.99	303.9	303.63
$3s(3/2, 1/2)_2$–$3p(3/2, 3/2)_3$	305.30	305.17	306.39	306.2	306.29
$3s(3/2, 1/2)_1$–$3p(3/2, 1/2)_2$	348.00	346.95	347.95	348.0	

[a] Cogordan and Lunell [15].
[b] This work.
[c] Jupén [6], Dere [26].

Table III. *Predicted wavelengths (Å) of some 3s–3p and 3p–3d transitions in Ne-like Co XVIII, Cu XX and Zn XXI*

Transition	Co XVIII	Cu XX	Zn XXI
$3s(1/2,\ 1/2)_1-3p(1/2,\ 3/2)_2$	324.87	284.97	267.55
$3s(3/2,\ 1/2)_2-3p(3/2,\ 3/2)_3$	327.39	287.23	269.68
$3s(3/2,\ 1/2)_1-3p(3/2,\ 1/2)_2$	367.43	330.43	314.35
$3s(3/2,\ 1/2)_2-3p(3/2,\ 1/2)_1$	384.07	340.71	322.26
$3p(1/2,\ 1/2)_1-3d(1/2,\ 3/2)_2$	250.28	221.76	209.28
$3p(3/2,\ 1/2)_2-3d(3/2,\ 3/2)_3$	252.73	223.78	211.13
$3p(3/2,\ 3/2)_2-3d(3/2,\ 5/2)_3$	264.37	237.40	225.75
$3p(1/2,\ 3/2)_2-3d(1/2,\ 5/2)_3$	264.58	237.79	226.18
$3p(1/2,\ 3/2)_1-3d(1/2,\ 5/2)_2$	265.44	238.54	226.89
$3p(3/2,\ 3/2)_3-3d(3/2,\ 5/2)_4$	268.32	241.38	229.71

lengths that are very close to the experimental results. By forming the expression $(\sigma_{th} - \sigma_{exp})/\xi$ where σ_{th} and σ_{exp} are the theoretical and experimental wavenumbers for a given transition and ξ the net charge of the core (spectrum number) we can compete the wavelengths for the $3s$–$3p$ and $3p$–$3d$ lines in Ni XIX to a high accuracy (estimated to ± 0.05 Å) using the available experimental data for Ca XI–Fe XVII, quoted above.

Some plots are shown in Fig. 2. In the work of Jupén [6] four Ni XIX transitions were tentatively identified in the spectrum of solar flares published by Dere [26]. These assignments are confirmed in the present work. Table II gives the wavelengths of the Ni XIX lines classified in the present work, together with the results obtained from extrapolation of the difference discussed above. We also include the theoretical wavelengths obtained by Cogordan and Lunell [15], as well as the results from our new calculations (see also Table I). The agreement between theoretical and experimental wavelengths is within 1 Å.

In the course of the isoelectronic analysis of differences between theoretical and experimental wavenumbers it became evident that the classification of the $3p(1/2,\ 3/2)_2$–$3d(1/2,\ 5/2)_3$ line in Fe XVII ($3p\ ^3P_2$–$3d\ ^3D_3$ in *LS* notation) has to be revised. The wavelength of this transition has been given as 279.21 Å [6, 7, 14]. However, a linear fit of the difference between theoretical and experimental wavenumbers predicts a wavelength of 280.20 Å for this transition in Fe XVII, i.e., the line would practically coincide with the Fe XVII $3p(3/2,\ 3/2)_2$–$3d(3/2,\ 5/2)_3$ combination ($3p\ ^1D_2$–$3d\ ^1F_3$) at 280.14 Å [6]. The 279.21 Å line, present in the spectra of flares [26] is probably due to a transition in F-like Fe XVIII [27].

Thanks to the high quality of the previous experimental material and the accuracy of the MCDF calculations, it is also possible to provide wavelengths for several $3s$–$3p$ and $3p$–$3d$ transitions in Co XVIII, Cu XX and Zn XXI for which no experimental data have been reported. This material which also is based on linear fits of the difference between theoretical and experimental transition energies, divided by the spectrum number, is given in Table III, Here, also, the accuracies are estimated to be ± 0.05 Å.

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