Nuclear Instruments and Methods in Physics Research B31 (1988) 280–283
North-Holland, Amsterdam

MULTICONFIGURATION DIRAC–FOCK CALCULATIONS OF ENERGY LEVELS AND TRANSITION PROBABILITIES IN Ne-LIKE S VII, Cl VIII AND Ar IX

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A multiconfiguration Dirac–Fock (MCDF) calculation using the program of Grant and collaborators has been performed for the Ne-like systems S VII, Cl VIII and Ar IX. Excitation energies and transition probabilities have been calculated for all 3s, 3p and 3d levels in these spectra. The theoretical results are in excellent agreement with recent experimental data.

1. Introduction

The structure of Ne-like ions has been vigorously investigated in recent years. In addition to the basic relevance to atomic physics there are interesting applications in astrophysics, e.g. in interpreting spectra of solar flares, as well as in plasma physics where Ne-like ions of Cr, Fe and Ni are observed in tokamaks. The demonstration of laser action in the far UV and X-ray regions in Ne-like ions [1] has provided additional strong motivation for experimental and theoretical studies of these systems.

Experimental investigations of the transitions between the 3s–3p and 3p–3d levels in Ne-like ions have been carried out using sparks, laser-produced plasmas and foil-excited ions. The available material is extensive up to Cu XX [2]. On the theoretical side a number of methods have been applied, including nonrelativistic as well as relativistic calculations. For example, Fawcett [3] has employed the Hartree–Fock method of Cowan [4], which involves a semiempirical optimization of Slater integrals, whereas Cogordan et al. [5] have performed relativistic ab initio calculations, by means of the multiconfiguration Dirac–Fock code of Grant et al. [6], for a number of ions up to $Z = 54$. In both cases excellent agreement with experimental results has been obtained.

While there thus exist experimental data for wavelengths and excitation energies for the transitions involving the 3s, 3p and 3d levels, much less is known concerning transition probabilities and lifetimes. Furthermore, here also the theoretical results seem to differ from each other. For example, this holds for Ni XIX where the lifetimes from MCDF calculations [7] differ from those based on $1/Z$ perturbation calculations with Breit–Pauli corrections included [8]. Similar differences can also be noted for lower ionization stages. Thus, for Cl VIII and Ar IX the calculations of Fawcett [3] and Loginov [9], both of which use semiempirical parametrization, give similar results, whereas they seem to disagree with ab initio results of Bureeva and Safronova [8].

To study such problems we have undertaken new ab initio calculations using the MCDF approach [6]. The ions S VII, Cl VIII and Ar IX were selected. In these systems there exist some experimental lifetime data, as discussed below. Furthermore, since these spectra have been recently analyzed, cf. refs [10,11] (S VII), [12] (Cl VIII) and [3,13–15] (Ar IX), there also exist reliable experimental wavelengths for comparison with theoretical data.

2. Calculations

The calculations were carried out by network using the CRAY X-MP E machine at the National MFE Computer Center in Livermore, California. The code used was an improved version of the program MCDF developed by Grant and coworkers [6]. Computations were made using the MCDF-EAL option of the code, and included the desired configurations $2s^2 2p^5 3s$, $2s^2 2p^5 3p$, $2s^2 2p^5 3d$ and, to provide a balanced set of orbitals for the EAL calculation, also included the configurations $2s2p^6 3s$, $2s2p^6 3p$ and $2s2p^6 3d$. To optimize the calculation of the 3s–3p and 3p–3d transition wavelengths, the ground state $2s^2 2p^6$ was treated separately in some of the computations. 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 gauges, but the Coulomb gauge results were selected for presentation.

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0168-583X/88/$03.50

3. Results

The calculations yielded the wavelengths and spontaneous transition probabilities of all possible electric dipole (E1) transitions between the $2p^6\ ^1S_0$ ground level and the $2p^5 3s$ (4 levels), $2p^5 3p$ (10 levels) and $2p^5 3d$ (12 levels) excited configurations for the three spectra S VII, Cl VIII and Ar IX.

The complete set of data, together with similar results for neighboring ions will be published later. In the present brief report only a selected number of results will be given. Thus, in table 1 we give the calculated wavelengths of a number of 3s–3p and 3p–3d transitions in S VII–Ar IX. Only the most intense decay of each 3p and 3d level has been included. Note also that the mixing of the 3p $^1D_2$ and 3p $^3P_2$ levels is very pronounced and here the *LS* notations are only nominal. (The level denoted by us as 3p $^3P_2$ is lower in energy whereas the opposite labeling is used in experimental and some previous theoretical work. Our choice is based on fact that the contributions of the $^3P_2$ and $^1D_2$ squared-amplitudes are about 60% and 40% for the lower and 30% and 40% for the higher of these states in the three ions considered here.)

Table 1 also includes the most recent experimental wavelengths [11,12,15] for these three ions. It can be noted that the wavelength agreement between theory and experiment is quite satisfactory. For two of the strongest lines we show (in fig. 1) the variation of the

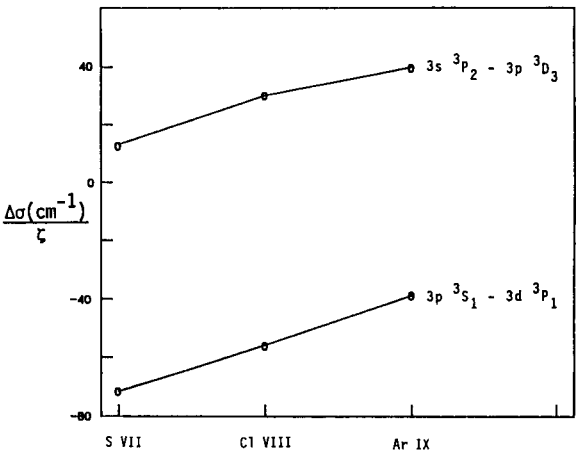

Fig. 1. Isoelectronic study of the difference between theoretical and experimental wavenumbers (divided by the core charge ζ) for two transitions in S VII–Ar IX.

Table 1
Wavelengths (Å) of some 3s–3p and 3p–3d transitions in S VII, Cl VIII and Ar IX.

Transition	S VII		Cl VIII		Ar IX	
	MCDF [a]	Expt. [b]	MCDF [a]	Expt. [c]	MCDF [a]	Expt. [d]
3s $^3P_2$–3p $^3S_1$	1048.55	1051.57	916.26	919.04	812.08	814.60
$^3P_2$– $^3D_3$	897.10	897.82	784.19	785.68	695.67	697.42
$^3P_1$– $^3D_2$	923.76	924.06	811.95	813.00	724.56	725.86
$^3P_1$– $^3D_1$	893.74	894.35	781.98	783.43	694.74	696.49
$^3P_2$– $^3P_2$	827.65	828.43 [e]	722.72	724.32 [e]	640.75	642.54 [e]
$^1P_1$– $^1P_1$	930.90	930.20	816.14	816.65	726.63	727.73
$^3P_1$– $^3P_0$	816.52	816.81	710.68	711.74	627.20	629.36
$^1P_1$– $^1D_2$	905.67	903.13 [e]	789.07	788.00 [e]	698.04	697.83 [e]
$^1P_1$– $^3P_1$	895.03	893.24	781.16	780.95	692.52	693.70
3p $^3S_1$–3d $^3P_0$	640.52	638.00	561.40	559.86	500.65	499.80
$^3S_1$– $^3P_1$	635.66	633.35	556.48	555.10	495.64	494.79
$^3S_1$– $^3P_2$	625.66	623.49	546.46	545.32	485.53	484.92
$^3D_3$– $^3F_4$	680.21	680.65	594.39	595.20	528.67	529.62
$^3D_2$– $^3F_3$	676.54	677.69	589.46	590.90	522.54	524.05
$^3D_1$– $^3F_2$	678.13	678.80	591.29	592.32	524.58	525.77
$^3P_2$– $^1F_3$	684.70	687.67 [e]	595.80	598.62 [e]	528.07	530.65 [e]
$^3P_0$– $^3D_1$	683.17	685.07	594.91		527.81	
$^1P_1$– $^1D_2$	670.94	671.93	583.22	584.44	516.34	517.69
$^1D_2$– $^3D_3$	679.16	680.95 [e]	591.67	593.73 [e]	525.01	527.15 [e]
$^3P_1$– $^3D_2$	682.55	683.59	594.54	595.80	527.53	528.89

[a] This work.
[b] Kononov et al [11] (laser plasma).
[c] Jupén [12] (beam-foil spectroscopy).
[d] Engström and Berry [15] (beam-foil spectroscopy).
[e] The levels 3p $^3P_2$ and 3p $^1D_2$ are strongly mixed and the labels differ in this work and the experimental analysis.

Table 2
Lifetimes of the 3s, 3p and 3d levels in Ar IX

Level		Lifetime (ps)				
		This work (MCDF)	Other theory [a]	Other theory [b]	Other theory [c]	Experiment
3s	$^1P_1$	6.89	8.3	13.1		6.5(20) [d]
	$^3P_1$	18.50	20.6	35.7		19(4) [d]
3p	$^3S_1$	779	700	1080	717	
	$^3D_3$	363	411	562	415	340(20) [e]
	$^3D_2$	393	436	629	441	
	$^3D_1$	391	412	671	424	
	$^3P_2$	386	353	410	359	360(20) [e], 590(60) [f,g]
	$^1P_1$	403	424	581	916	
	$^3P_0$	398	322	463	336	
	$^1D_2$	382	388	588	389	
	$^3P_1$	397	350	368	365	
3d	$^3P_0$	170	157	324	197	
	$^3P_1$	88.9	70	96	75	
	$^3P_2$	172	160	260	170	230(20) [f]
	$^3F_4$	145	164	279	165	170(20) [e]
	$^3F_3$	140	158	289	161	
	$^3F_2$	143	155	244	159	
	$^1F_3$	148	160	267	161	
	$^3D_1$	7.02	4.4	5.62	4.5	
	$^1D_2$	145	153	260	155	
	$^3D_3$	148	158	265	161	
	$^3D_2$	154	154	228	162	

[a] Loginov [9] (semiempirical calculation).
[b] Bureeva and Safronova [8] ($1/Z$ expansion).
[c] Fawcett [3] (Hartree–Fock method of Cowan [4]).
[d] Berry et al. [19] (beam–foil spectroscopy).
[e] Buchet-Poulizac and Buchet [13] (beam–foil spectroscopy).
[f] Knystautas et al [20] (beam–foil spectroscopy).
[g] The levels 3p $^3P_2$ and 3p $^1D_2$ are strongly mixed and the labels differ in this work and the experimental analysis.

difference between theory and experiment as a function of ζ, the net charge of the core. The small remaining difference between theory and experiment is probably due to correlations from the $n = 4$ and higher shells, not included in the theoretical calculations.

A comparison of our data with other theoretical results [3,8,16–18] also shows good agreement. The MCDF wavelengths are, in several cases, closer to the experimental data than the results of previous ab initio calculations.

It should be noted that we do not include results for transitions involving the levels 3p $^1S_0$ and 3d $^1P_1$, because here the MCDF code gives results which deviate strongly from the experimental data. As shown by Cogordan et al. [5] a separate optimization would be necessary to obtain better agreement with the experimental material.

Of all the calculated lifetimes we here present the theoretical results for Ar IX only. Three other sets of theoretical results, by Bureeva and Safronova [8], by Loginov [9] and by Fawcett [3], are included for comparison. It is clear that the MCDF results are in much better agreement with the semiempirical calculations [9], which incidentally also are in accord with other similar results [16,18], not included in table 2.

Experimental data from beam–foil measurements are available for several of the $n = 3$ levels in Ar IX. Berry et al. [19] thus measured the lifetimes of the 3s $^1P_1$ and 3s $^3P_1$ levels which combine with the $2p^6$ $^1S_0$ ground state and therefore have very high transition probabilities. Our results are in excellent agreement with the experimental values as well as previous relativistic calculations of the two resonance lines (for references to such work see [19]). For the 3p $^1D_2$, 3p $^3D_3$ and 3d $^3F_4$ levels there also exist experimental results. Here Buchet-Poulizac and Buchet [13] seem to have improved the previous data of Knystautas et al. [20]. The MCDF results are in excellent agreement with the experimental results of ref. [13].

This work has demonstrated that the MCDF method

is capable of giving accurate energy differences and transition probabilities for the Ne-like ions S VII–Ar IX. Agreement with the experimental wavelengths is typically within 1–2 Å. In the case of lifetimes we support previous semiempirical results over ab initio calculations. The present data are thus the first ab initio results which are in satisfactory agreement with beam–foil measured lifetimes.

It is finally interesting to note that there exist experimental lifetime data for most of the 3p and 3d levels in Ne-like Ti XIII [21]. Here, also, agreement is good with the calculations of Fawcett [22]. However, the MCDF calculations here predict somewhat shorter lifetimes than the experimentally determined data. Additional theoretical and experimental studies of transition probabilities in Ne-like ions would clearly be of considerable interest.

One of the authors (I.M.) is grateful for the hospitality extended to him at the Department of Physics and Astronomy, University of Toledo. The work was supported by the US Department of Energy, Division of Chemical Sciences, Office of Basic Energy Sciences under contract number DE-AS05-80ER10676 (L.J.C. and R.R.H.) and by EFN, the Swedish Energy Research Committee (I.M.).

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