The Platinum Group Ion Project

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1 Introduction

Elements of the 5d-sequence show complex spectra and large relativistic effects, reflected in a strong mixing of levels and high values of the spin orbit interactions. Over the last decade many investigations focusing on the resonance transitions of 5d-elements were published [1]. One reason for these investigations is the increase of interest in 5d-elements in astrophysics after the observation of spectral lines of 5d-elements in chemically peculiar stars, such as χ Lupi and κ Cancri [2]. Another reason is the development of sophisticated computational methods, such as the orthogonal operator approach [3], [4], [5] and the Multi Configuration Dirac Fock code [6]. These new computational methods allow the successful investigation of the complex systems of the 5d-sequence, thanks to far better values for initial estimates of the energy level values and transition probabilities. A third reason for exploring the 5d-elements is interest in relativistic effects that appear to be strong for these heavy elements. The orthogonal operator approach provides the tools to investigate these small, thus far neglected higher order correlation and relativistic effects quantitatively, as was recently showed for the 3d-elements [7]. To study these effects properly, however, many data from different elements in the 5d-sequence and from different stages of ionization are necessary.

Efforts of our team have resulted in many investigations of elements in the platinum group. The state of these analyses is shown in table 1. These analyses have resulted in experimental wavelengths and energy level values, as well as calculated transition probabilities. In most of the spectra indicated in table 1 about 400 lines have been identified. The high dispersive 10m normal incidence vacuum spectrograph in Meudon was used to obtain the spectrograms. This spectrograph is equipped with a 3600 l/mm grating, resulting in a plate factor of 0.26 Å/mm. Other observational instruments are the 6.6 m normal incidence vacuum spectrograph at the Institute for Spectroscopy in Troitsk and the 3 m normal incidence spectrograph of the St. Francis Xavier University in Antigonish. Spectrograms have been measured with semi-automatic and fully-automatic comparators in Antigonish and Troitsk, respectively. The analyses were supported by the "package IDEN" [8], [9] developed in Troitsk.

2 Present Investigations

The main objective of the project presented here is the extension of the analyses, focussed in the past on spectra of doubly ionized elements of the platinum group. These lower stages of ionization are more interesting from the astrophysical point of view, but they are also a challenge due to the complexity of these systems. The lower stages of ionization are dominated by strong correlation effects. For this reason the energy matrix has to be extended to ($5d^N$ + $5d^{N-1}6s$ + $5d^{N-2}6s^2$) for the even system and to ($5d^{N-1}6p$ + $5d^{N-2}6s6p$ + $5d^{N-3}6s^26p$) for the odd system. This extension of the basis will result in complicated calculations of energy level values and transition probabilities using orthogonal operators along the lines presented in [5]. The transition probabilities, in combination with the wavelengths calculated from the experimental energy level values, provide a large amount of valuable data.

Another result from these efforts is the possibility to quantize higher order magnetic and electrostatic effects as was done in the 3d-elements [7]. To undertake these studies a large amount of data is necessary together with a good knowledge of interacting configurations. For the higher stages of ionization the latter is not that relevant. We show an example of the consistency of small, thus far neglected 3-particle electrostatic higher order effects, observed in Os V and Au V [10] (see table 2). Here we have chosen a comparison between two iso-ionic spectra. Iso-ionic comparisons are far more relevant since they are less sensitive to the reproduction of errors, as is the case for iso-electronic comparisons. The example given for four times ionized platinum group elements shows the stability of our computational method in providing reliable estimates for starting the analyses of unknown systems of doubly ionized 5d-elements. For the strong 2-particle electrostatic interactions and the 1-particle magnetic interactions this stability was already known for years, but the stability of the small higher order effects in the orthogonal operator approach offers the possibility to extrapolate even these small effects to unknown spectra and to obtain good predictions, necessary to investigate the complex systems successfully.

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Table 1: State of knowledge of platinum group ion spectra.

	W 74	**Re** 5	**Os** 76	**Ir** 77	**Pt** 78	**Au** 79
I	$\mathbf{5d}^6$	$\mathbf{5d}^7$	$\mathbf{5d}^8$	$\mathbf{5d}^9$	$\mathbf{5d}^{10}$	
II	$\mathbf{5d}^5$	$\mathbf{5d}^6$	$\mathbf{5d}^7$	$\mathbf{5d}^8$	$\mathbf{5d}^9$	$\mathbf{5d}^{10}$
III	$\mathbf{5d}^4$	$5d^5$	$5d^6$	$5d^7$	$\mathbf{5d}^8$	$\mathbf{5d}^9$
IV	$\mathbf{5d}^3$	$5d^4$	$\mathbf{5d}^5$	$5d^6$	$5d^7$	$\mathbf{5d}^8$
V	$5d^2$	$\mathbf{5d}^3$	$\mathbf{5d}^4$	$5d^5$	$5d^6$	$\mathbf{5d}^7$
VI	$\mathbf{5d}^1$	$\mathbf{5d}^2$	$\mathbf{5d}^3$	$5d^4$	$5d^5$	$5d^6$
VII		$\mathbf{5d}^1$	$\mathbf{5d}^2$	$\mathbf{5d}^3$	$5d^4$	$5d^5$
VIII			$\mathbf{5d}^1$	$\mathbf{5d}^2$	$5d^3$	$5d^4$
IX				$\mathbf{5d}^1$	$\mathbf{5d}^2$	$5d^3$
X					$\mathbf{5d}^1$	$5d^2$

$5d^N$: unknown
$\mathbf{5d}^N$: known in past and from others
$5d^N$: in progress in our team
$\mathbf{5d}^N$: finished in our team

Table 2: Comparison between the 3-particle electrostatic ddp-type parameters in Os V and Au V

Parameter	Os V	Au V
T_{16}	-25.4	-25.2
T_{17}	14.5	10.5
T_{18}	-18.2	-16.1
T_{19}	-15.6	-10.0
T_{20}	-38.2	-47.1
T_{21}	-11.5	-19.4
T_{22}	-48.9	-15.1
T_{23}	-12.7	-3.2
T_{24}	-15.1	-17.7
T_{25}	7.9	5.1
T_{26}	-41.6	-33.5
T_{27}	14.2	1.7
T_{28}	59.0	44.6
T_{29}	-30.1	-20.5
T_{30}	8.0	29.6
T_{31}	-5.9	-17.7
T_{32}	-11.0	2.6
T_{33}	14.5	7.2
T_{34}	-40.8	-46.1
T_{35}	-64.0	-65.5