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The third spectrum of rhenium (Re III): Analysis of the $(5d^5 + 5d^46s)-(5d^46p + 5d^36s6p)$ transition array

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ABSTRACT

The spectrum of rhenium was observed in the (1017–2074) Å wavelength region. The $(5d^5 + 5d^46s)-(5d^46p + 5d^36s6p)$ transition array of two times ionized rhenium, Re III, has been investigated and 1305 spectral lines have been classified in the region. The analysis has led to the determination of the $5d^5$, $5d^46s$, $5d^46p$ and $5d^36s6p$ configurations. Seventy levels of the $5d^5$ and $5d^46s$ configurations in the even system and 161 levels of the $5d^46p$ and $5d^36s6p$ configurations in the odd system have been established. The orthogonal operators technique was used to calculate the level structure and transition probabilities. The energy parameters have been determined by the least squares fit to the observed levels. Calculated transition probability and energy values, as well as *LS*-compositions obtained from the fitted parameters are presented.

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1. Introduction and experiment

Re III is the last unknown rhenium spectrum with an open 5d shell. It was never studied before. The first, second, fourth, fifth, sixth and seventh spectra of rhenium have been successfully studied [1–6]. The ion Re^{2+} is astrophysically more interesting than other rhenium ions with higher ionization. The interest came up from the observation of heavy elements in the spectra of the chemically peculiar stars κ Cancri and χ Lupi. Observations by the Goddard High Resolution Spectrograph on board of the Hubble Space Telescope proved presence of Re, Os, Pt, Au and Hg [7–9] in these objects. It concerns especially the lower stages of ionization.

The Re III spectrum is one of the most complicated and difficult to study spectra. First, it is because of the number of levels that have to be established. The total number of levels in the three lowest configurations $5d^5$, $5d^46s$ and $5d^46p$ is 280. In order to determine these configurations reliably, the minimal number of spectral lines that have to be classified is about 900. Secondly, the Re III spectrum exhibits overlapping of the lowest configurations in both parities, significant level mixing and strong configuration interaction. The spectrum, in addition to the three lowest configurations of the type $5d^N$, $5d^{N-1}6s$ and $5d^{N-1}6p$ commonly studied in the 5d spectra, has closely lying disturbing configurations $5d^{N-2}6s^2$, $5d^{N-2}6s6p$ and $5d^{N-3}6s^26p$. These configurations strongly affect levels of the investigated configurations, but it is very difficult to establish them experimentally. Parameters of these disturbing configurations and corresponding configuration interaction integrals are unknown in the isoelectronic spectra with higher ionization, therefore these parameters cannot be isoelectronically extrapolated, and transition probabilities cannot be reliably calculated. For laboratory light sources, levels of the $5d^{N-2}6s6p$ and $5d^{N-3}6s^26p$ configurations are usually much less populated than those of the $5d^{N-1}6p$ configuration.

In addition, if the investigated spectrum is III or lower, it is more difficult to extrapolate parameters of the investigated configurations ($5d^N$, $5d^{N-1}6s$ and $5d^{N-1}6p$) from isoelectronic spectra with higher ionization [10–13]. When the ionization lowers, the trends of parameters, or their scaling factors (ratios of fitted and *ab initio* Hartree–Fock values of parameters), along isoelectronic sequences become more irregular. For instance, the scaling factors for electrostatic parameters fall down sharply when we approach the third and second spectra [10–13]. It is worth quoting an opinion of leaders in the theoretical and experimental atomic spectroscopy (Wyart et al. [11]), which described a situation on analyses of 5d spectra in 1993: “Although the second and third spectra have a larger astronomical interest than the spectra of higher charge ions, a straight attempt to analyze Re III, Os III or Ir III looks hopeless to us”. Research on the Re III spectrum is also of interest to fundamental physics for better understanding of complex atomic

spectra and for improvement of theoretical methods of treatment of multi-electron heavy atoms.

The purpose of the present work is to study the spectrum of two times ionized rhenium, Re III. The study is essentially based on theoretical calculations utilizing the orthogonal operators approach [10,14–16] and the program suite IDEN [17,18].

The spectrograms for the current analysis have been photographed in the wavelength region of (1017–2074) Å at the Institute of Spectroscopy, Troitsk, Moscow, Russian Federation. Rhenium spectra of different ionization stages were obtained on a 6.65 m normal incidence spectrograph with a plate factor of 1.25 Å/mm. The sources used were vacuum triggered and sliding sparks with operating voltage of (4.0–4.5) kV. The sparks were fed from a low-inductance 10 μF capacitor. The photographic plates were measured on an automatic comparator controlled by the system for automatic processing of photo-spectrograms [19]. Conversion of line positions to wavelengths included: (i) conversion of line positions to wavelengths using theoretical curve of the spectrograph and (ii) construction of a correction (calibration) curve by spline interpolation of positions of available reference lines. For a particular spectrograph, the approximate form of the correction curve is usually known. It reflects imperfection of the plate holder. For well developed symmetrical spectral lines, the statistical uncertainty, $\text{Unc}_{\text{stat}}(\lambda)$, of our wavelength measurements is less than 2 mÅ. It resulted from the statistical uncertainty of measurements of positions of lines. Conversion of line positions to wavelengths using reference lines resulted in addition of a systematic component, $\text{Unc}_{\text{sys}}(\lambda)$, to wavelength uncertainties. For each of three parts of our linelist corresponding to three photographic plates (see below), the added value $\text{Unc}_{\text{sys}}(\lambda)$ gradually varies along the linelist. These values reflect smooth adjustment possibly needed for the interpolated correction curve of the spectrograph. In calculations of wavelength distances between spectral lines, if two lines are close enough, the systematic component $\text{Unc}_{\text{sys}}(\lambda)$ in the wavelength uncertainties of the two lines can be neglected. Another example of possibility of more accurate calculations of the distances by neglecting $\text{Unc}_{\text{sys}}(\lambda)$ is the case when, for some region, lines of the same element, ionization stage and accuracy are used as reference lines for wavelengths calculation. To take into account a possible shift of all reference lines used in the region, we may add a component $\text{Unc}_{\text{sys}}(\lambda) = \text{const}$, which will not affect uncertainty of the calculated wavelength differences for the region. In general, to correctly account for the $\text{Unc}_{\text{sys}}(\lambda)$ component in the wavelength differences calculations, it is necessary to specify the complete covariance matrix of all wavelength measurements. In Ref. [18] (see Sec. 3.1) we introduced a simplified method in which, for each linelist part, we specify the covariance component of any two wavelength measurements as a formula depending on two parameters: the maximal covariance of the measurements and the

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