P-izoelektronės sekos energijos spektro ir radiacinių šuolių teorinis tyrimas

Theoretical study of energy spectra and radiative transitions of P-like ions

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Accurate atomic data for (highly) ionized atoms are needed in astrophysics and plasma physics. Iron group elements are important in the study of astrophysical plasmas, as many of their emission lines are frequently observed from different ionization stages. These observations provide a wealth of data about the plasma characteristics, such as temperature, density, and chemical composition. Atomic data, including energy levels and transition data, are required for many ions.

In this work energy spectrum calculations were performed for 147 even states of the $3s3p^4$, $3s^23p^23d$, $3p^43d$, $3s3p^23d^2$ configurations and for 124 odd states of the $3s^23p^3$, $3p^5$, $3s3p^43d$, $3s^23p3d^2$ configurations in Co XIII - Zn XVI ions. The calculations are in progress and some other ions of P-isoelectronic sequence will be studied. In the abstract the part of energy spectra of P-like Co ion is presented. Energy levels are compared with data from NIST and other theoretical computations when it is available. All calculations were performed using the general relativistic atomic structure package GRASP2K [1].

The calculation was done using multiconfiguration Dirac-Hartree-Fock (MCDHF) approximation [2]. As a final step, a relativistic configuration interaction (RCI) calculation was performed to include the transverse-photon (Breit) interaction describing the transversely polarized photon contribution to the electron-electron interactions in the Coulomb gauge, the vacuum polarization (VP), and the self-energy (SE) corrections.

In the present work, the atomic state functions (ASFs) were obtained as expansions over jj-coupled CSFs. To provide the LSJ labeling system the ASFs were transformed from a jj-coupled CSF basis into an LSJ-coupled CSF basis using the method provided by Gaigalas *et al.* [3].

In the Table 1 energy levels of this work are compared with data from NIST, theoretical computations performed by Vilkas and Ishikawa [4] who used relativistic multireference Moller-Plesset (MR-MP) perturbation theory and Fritzsche *et al.* [5] who used multiconfiguration Dirac-Fock approach. In the NIST database for P-like Co ion just 31 energy levels are given. Vilkas and Ishikawa [4] calculated the energy levels of $3s^23p^3$, $3s3p^4$, $3s^23p^23d$ and $3s3p^33d$ configurations, whereas Fritzsche *et al.* [5] have studied $3s^23p^3$, $3s3p^4$, $3s^23p^23d$ configurations.

As it seen from the Table 1 there is good agreement between present work, MR-MP calculations and NIST. The mean energy differences for presented energy levels in Table 1 comparing with NIST are 0.11% for this work, 0.03% for [4], and 1.32% for [5]. There are some disagreements in the identifications of the levels comparing with this work: level $3s^2\,3p^2(^3_2P)\;^3P\,3d\;^2P_{1/2}$ in NIST and in Vilkas paper [4] was identified as $3s3p^4\;^2P_{1/2}$. And level $3s^2\,3p^2(^1_2D)\;^1D\,3d\;^2F_{7/2}$ in Vilkas column have $^4D_{7/2}$ identification.

Table 1. Energy levels in cm^{-1} from RCI calculations for P-like Co ion. Energies are compared with NIST, and theoretical results from Vilkas *et al.* [4] and from Fritzsche *et al.* [5].

State	RCI	NIST	[4]	[5]
$3s^2\,3p^3(^4_3S)\;^4S^o_{3/2}$	0	0	0	0
$3s^2\,3p^3(^2_3D)\;^2D^o_{3/2}$	43742	43650	43630	45284
$3s^2\,3p^3(^2_3D)\;^2D^o_{5/2}$	49725	49690	49657	51225
$3s^2\,3p^3(^2_1P)\;^2P^o_{1/2}$	79706	79460	79507	81491
$3s^2\,3p^3(^2_1P)\;^2P^o_{3/2}$	88215	88170	88192	89980
$3s\;^2S\,3p^4(^3_2P)\;^4P_{5/2}$	295145	295160	295037	295717
$3s\;^2S\,3p^4(^3_2P)\;^4P_{3/2}$	307093	307030	306917	307475
$3s\;^2S\,3p^4(^3_2P)\;^4P_{1/2}$	312376	312110	312000	312564
$3s\;^2S\,3p^4(^1_2D)\;^2D_{3/2}$	365933	365530	365493	367592
$3s\;^2S\,3p^4(^1_2D)\;^2D_{5/2}$	368496	368250	368161	370221
$3s\;^2S\,3p^4(^3_2P)\;^2P_{3/2}$	419100	418480	418519	421348
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^2P_{1/2}$	423852	423290	423250	426855
$3s\;^2S\,3p^4(^1_0S)\;^2S_{1/2}$	443092		442206	446179
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^4F_{3/2}$	457680		456371	458742
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^4F_{5/2}$	462393		461086	463389
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^4F_{7/2}$	469198		468017	470240
$3s^2\,3p^2(^1_2D)\;^1D\,3d\;^2F_{5/2}$	475172		474008	476754
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^4F_{9/2}$	477485		476358	
$3s^2\,3p^2(^1_2D)\;^1D\,3d\;^2F_{7/2}$	480425		479395	481939
$3s^2\,3p^2(^3_2P)\;^3P\,3d\;^4D_{1/2}$	480678		479765	482164

Keywords: energy spectra, transition data, multiconfiguration Dirac-Hartree-Fock method, relativistic configuration interaction method.

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