ОРДЕНА ЛЕНИНА
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РАН

IONIZATION ENERGIES OF MULTICHARGED IONS OF PALLADIUM GROUP ELEMENTS

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Content

- Available data sources
- Semiclassical method
- Features of the multicharged ions
- Isoelectronic serries
- Ionization potentials of the element
- Conclusion

Available data on ion ionization potentials (energies, eV)

[1] NIST Atomic Spectra Database Ionization Energies Data

1. Experiment
2. Interpolation or extrapolation of known experimental values or semiempirical calculation […]
3. Dirac – Fock approach in “Systematic calculation of total atomic energies of ground state configurations” by G.C.Rodrigues et al. (…)

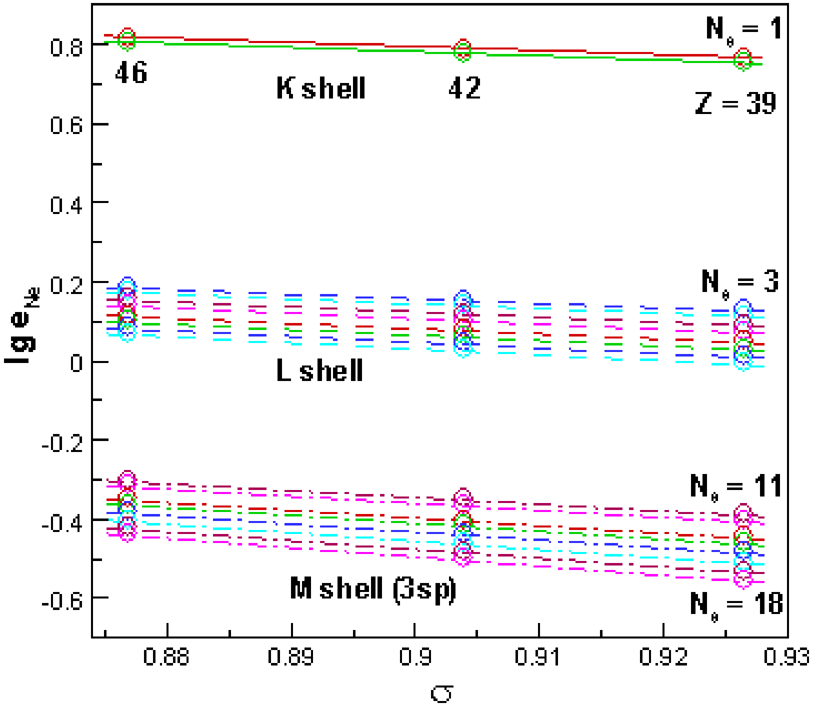
Semiclassical method for representing ionization energies $I_{Ne}(Z)$ eV from [1]

$$e_{Ne}(\sigma) = (I_{Ne}^{(Z)} / E_h) Z^{-4/3},$$

$$\sigma = \pi Z^{-1/3},$$

$$E_h = 27.211386\ eV.$$

Functions $e(\sigma)$, reconstructed from the available data for ions with N_e = 1 - 18 of elements Z = 39, 42, 46



$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$

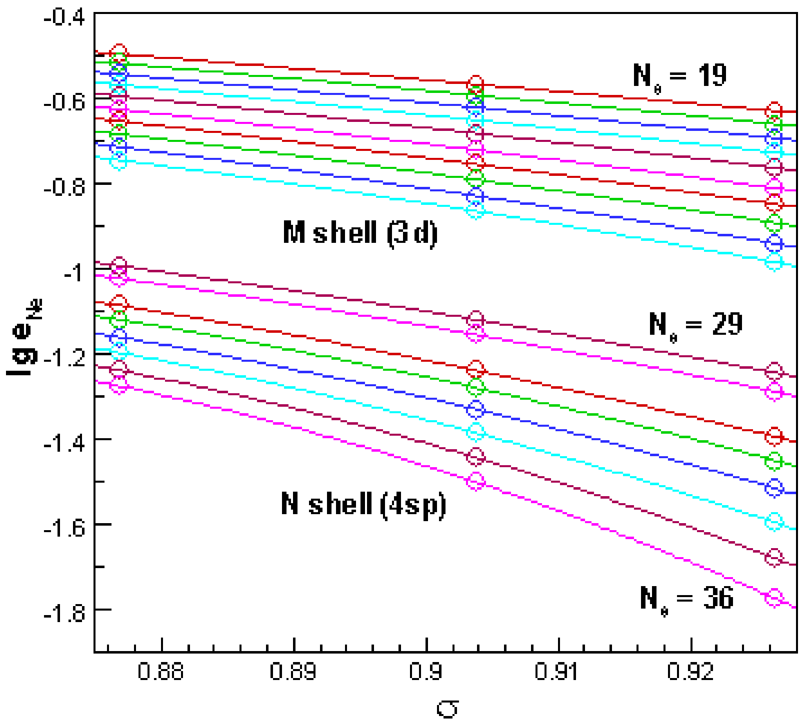
Polynomial approximation of the ionization energies for isoelectronic series with N_e = 1 - 18

$$\lg e_{Ne} = \sum_{i=0}^{i_{\max}} a_i(N_e)\sigma^i,$$

$$\sigma = \pi Z^{-1/3},\ i_{\max} = 1,$$

$$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$$

Functions *e(σ)*, reconstructed from the available data for ions with N_e = 19 - 36 of elements Z = 39, 42, 46



$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$

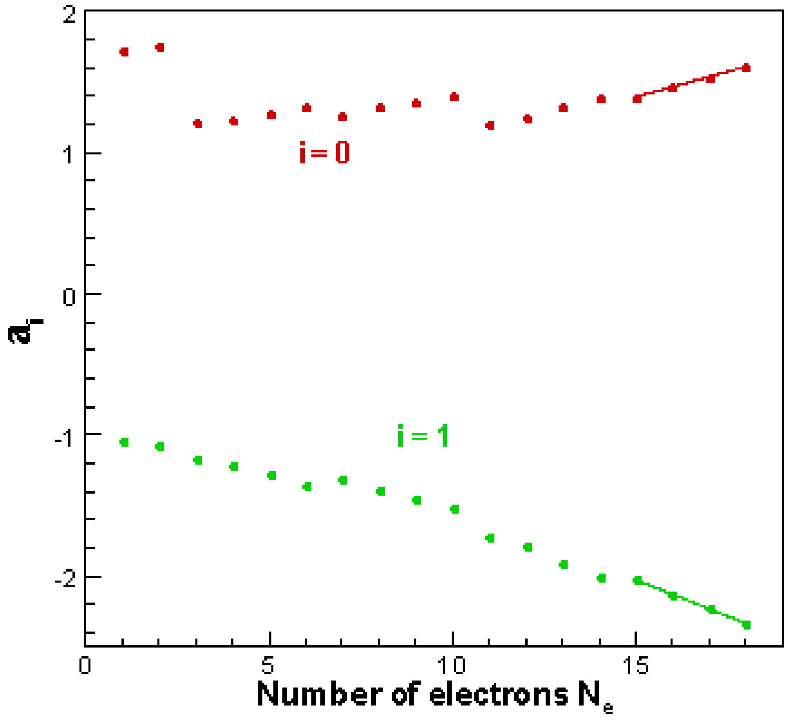
Polynomial approximation of the ionization energies for isoelectronic series with N_e = 19 - 36

$$\lg e_{Ne} = \sum_{i=0}^{i_{\max}} a_i (N_e) \sigma^i ,$$

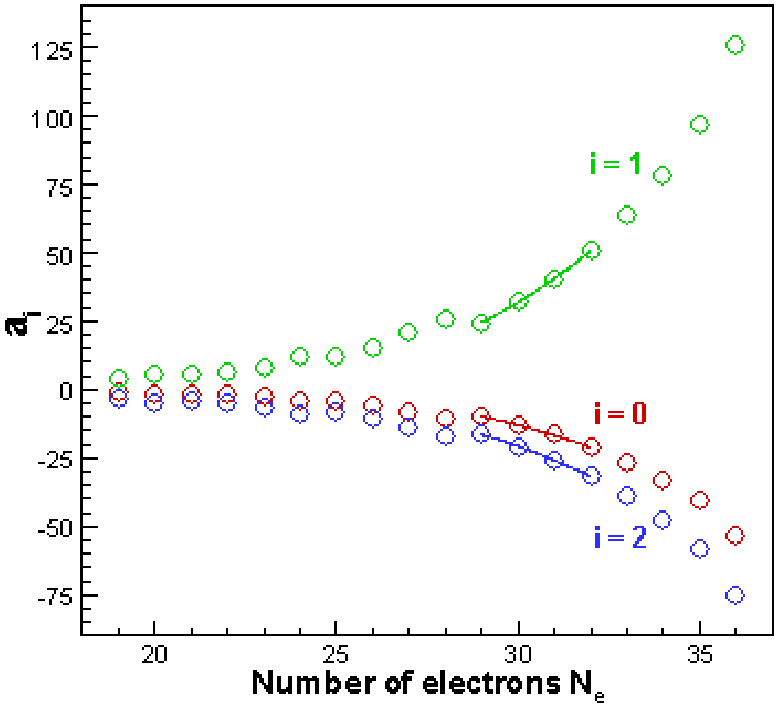
$$\sigma = \pi Z^{-1/3}, \quad i_{\max} = 2,$$

$$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$$

Coefficients $a_i(N_e)$ for ions with N_e = 1 - 18 of elements Z = 39, 42, 46



Coefficients $a_i(N_e)$ for ions with N_e = 19 - 36 of elements Z = 39, 42, 46



$I_{Ne}^{(Z)} = Z^{4/3}10^{\lg e_{Ne}(\sigma)} E_h$

Ionization potentials of one element depending on the number of electrons N_e

$$a_i = \sum_{k=0}^{k_{\max}} b_{ik} Ne^k, \quad N_m < Ne < N_{m+1}$$

$$\lg e_{Ne} = \sum_{i=0}^{i_{\max}} \sum_{k=0}^{k_{\max}} b_{ik} Ne^k \sigma^i$$

$$I_{Ne}^{(Z)} = Z^{4/3} 10^{\lg e_{Ne}(\sigma)} E_h$$

$N_e = 1 – 18$, coefficients b_{ik}

N_e	1, 2		3 – 6		7 - 10	
i\k	**0**	**1**	**0**	**1**	**0**	**1**
0	1.705942	0.023449	1.085078	0.040560	0.956438	0.045162
1	-0.996401	-0.041093	-0.965807	-0.064175	-0.832332	-0.069227

N_e	11 - 14		15 – 18	
i\k	**0**	**1**	**0**	**1**
0	0.492862	0.064189	0.323159	0.714368
1	-0.636596	-0.097331	-0.486187	-0.102609

$N_e = 19 – 36$, coefficients b_{ik}

N_e	19 – 24			25 – 28		
i\k	**0**	**1**	**2**	**0**	**1**	**2**
0	-60.296321	6.271472	-0.159450	-73.280436	7.088374	-0.172949
1	144.94636	-14.370625	0.367337	159.15625	-15.496224	0.383620
2	-83.983541	8.252046	-0.212791	-86.147062	8.420669	-0.212691

N_e	29 – 32			33 – 36		
i\k	**0**	**1**	**2**	**0**	**1**	**2**
0	-186.65381	14.985556	-0.306609	-1690.9062	104.87552	-1.649896
1	437.37352	-35.008116	0.716368	3804.6552	-236.28106	3.724736
2	-256.60262	20.439315	-0.419222	-2139.9722	133.03252	-2.102266

Comparison estimation with [1]. $N_e = Z - q$

Ion	[1]	anal	Ion	[1]	anal	Ion	[1]	anal
Y^{37+}	20 416	20 408	Y^{3+}	60.607	60.647	Y^{17+}	677±3	677.49
Zr^{33+}	4 300±30	4 302	Zr^{4+}	80.348	79.483	Zr^{16+}	622±3	624.25
Nb^{29+}	1 626±2	1 600	Nb^{9+}	180±2.2	178.13	Nb^{15+}	581±3	580.41
Mo^{24+}	1 263±4	1 257	Mo^{14+}	544±0.5	543.71	Mo^{14+}	544±0.5	543.71
Tc^{22+}	1 032±4	1 035	Tc^{15+}	604±3	606.59	Tc^{13+}	311±3	305.08
Ru^{20+}	905±5	908	Ru^{18+}	905±4	907.68	Ru^{12+}	271±3	270.7
Rh^{17+}	739±3	740	Rh^{25+}	1 274±4	1 274.8	Rh^{11+}	252±2.5	253.29
Pd^{14+}	342±3	340	Pd^{36+}	5 284±3	5 284.9	Pd^{10+}	238.57	238.29

Conclusion

- Certain **regularities** in the dependence of the ionization potentials of ions from filled shells **on the atomic number and the number of electrons** are shown for the palladium group elements
- The **polynomial approximation** of these patterns makes it possible to **analytically estimate** the ionization potentials of multicharged ions with an **error** of the order of and **less than one percent**.