

## BOHR MODEL FOR ISOELECTRONIC IONS

Exact energies of atomic ions were taken from E. R. Davidson's table available on-line at <http://php.indiana.edu/~davidson/atom/tub.4>.

For a given number of electrons  $N$ , and nuclear charge  $Z$ , the functional of energy is defined as

$$W = W_1 + W_2, \quad (1)$$

where

$$W_1 = \sum_{n=1}^N \left( \frac{Q(n)^2}{2R_n^2} - \frac{Z}{R_n} \right), \quad (2)$$

$$W_2 = \sum_{m=1}^{N-1} \sum_{n=m+1}^N \frac{1}{R_{mn}}, \quad (3)$$

$$R_n = \sqrt{x_n^2 + y_n^2 + z_n^2}, \quad (4)$$

$$R_{mn} = \sqrt{(x_m - x_n)^2 + (y_m - y_n)^2 + (z_m - z_n)^2}, \quad (5)$$

and

$$y_1 = z_1 = z_2 = 0. \quad (6)$$

In (2),  $Q(n)$  for  $n = 1, 2, 3, \dots, N$  is a principal quantum number of  $n$ th electron (as an example for Li,  $Q(1) = Q(2) = 1$ ,  $Q(3) = 2$ ). The energy  $W$  is expressed by means of equations (1) - (6) through Cartesian coordinates  $x_1, x_2, y_2, x_3, y_3, z_3, x_4, y_4, z_4, \dots, x_N, y_N, z_N$ , in total 1 coordinate if  $N = 1$ , 3 coordinates if  $N = 2$ , or  $3N - 3$  coordinates if  $N \geq 3$ . Then, the energy is minimized in respect to these coordinates.

Calculations were done by the following *Mathematica* program, that accepts two arguments,  $N$  and  $Z$ , and returns the energy and distances with tallies.

```
(* Bohr model for any atom or ion *)
<< Miscellaneous'ChemicalElements';
bohr[npart_Integer, zz_Integer] := Module[
{name, shortname, config, conf, title, mshells, n, mels, qnumber, x, y, z, r, en1, en2, w, vars, enz, sol,
rs, rads, mrads, radms, time},
If[!ValueQ[prec], prec = 128]; (* working precision *)
If[!ValueQ[maxit], maxit = 333]; (* maximal number of iterations *)
name = Elements[npart];
shortname = Abbreviation[name];
config = ElectronConfigurationFormat[name] // TeXForm // ToString;
conf = Plus @@ # & /@ ElectronConfiguration[name];
title = ToString[name] <> " isoelectronic series - " <> ToString[npart] <> " electrons: ";
mshells = Length[conf];
n = 0;
Do[
  mels = conf[[nshell]];
  Do[
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n++;
qnumber[n] = nshell, {mels}, {nshell, mshells}];
y[1] = z[1] = z[2] = 0;
en1 =
Sum[
r[n] = Sqrt[x[n]^2 + y[n]^2 + z[n]^2];
-zz/r[n] + qnumber[n]^2/2/r[n]^2, {n, npart}];
en2 =
Sum[Sum[
r[n, m] = Sqrt[(x[n] - x[m])^2 + (y[n] - y[m])^2 + (z[n] - z[m])^2];
1/r[n, m], {m, n + 1, npart}], {n, npart}];
w = en1 + en2;
vars = Table[{x[n], y[n], z[n]}, {n, npart}] // Flatten;
vars = Cases[vars, _[.]];
time = Timing[
{enz, sol} = NMinimize[{w}, vars,
WorkingPrecision -> prec,
MaxIterations -> maxit];
][[1]];
enz = N[enz];
rs = N[Table[r[n], {n, npart}] /. sol] // Sort;
rads = rs // Union;
mrads = Length[rads];
radms = Table[Length[Select[rs, # == rads[[nrad]] &]], {nrad, mrads}];
Print[title, " Z = ", zz, " R = ", {rads, radms} // TableForm, " E = ",
enz, " ", time];
{enz, rads, radms}]

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Results are printed in tables given below. Third column of each table lists the distances between electrons and the nucleus  $R_1, R_2, R_3, \dots, R_N$ . If several distances are equal, they are listed as one number with the multiplicity shown in parenthesis. The fourth column gives result of the energy minimization  $E_{\text{Bohr}}$ , and the fifth column exact energy  $E_{\text{exact}}$ . The sixth (last) column shows an error as a percentage  $100(E_{\text{Bohr}} - E_{\text{exact}})/E_{\text{exact}}$ .

TABLE I: Helium isoelectronic series. Configuration  $1s^2$ . 2 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
1	H <sup>-</sup>	1.333(2)	-0.5625	-0.5278	6.58
2	He	0.571(2)	-3.0625	-2.9037	5.47
3	Li <sup>+</sup>	0.364(2)	-7.5625	-7.2799	3.88
4	Be <sup>2+</sup>	0.267(2)	-14.0625	-13.6556	2.98
5	B <sup>3+</sup>	0.211(2)	-22.5625	-22.031	2.41
6	C <sup>4+</sup>	0.174(2)	-33.0625	-32.4062	2.03
7	N <sup>5+</sup>	0.148(2)	-45.5625	-44.7814	1.74
8	O <sup>6+</sup>	0.129(2)	-60.0625	-59.1566	1.53
9	F <sup>7+</sup>	0.114(2)	-76.5625	-75.5317	1.36
10	Ne <sup>8+</sup>	0.103(2)	-95.0625	-93.9068	1.23
11	Na <sup>9+</sup>	0.093(2)	-115.5625	-114.2819	1.12
12	Mg <sup>10+</sup>	0.085(2)	-138.0625	-136.6569	1.03
13	Al <sup>11+</sup>	0.078(2)	-162.5625	-161.032	0.95
14	Si <sup>12+</sup>	0.073(2)	-189.0625	-187.4071	0.88
15	P <sup>13+</sup>	0.068(2)	-217.5625	-215.7821	0.83
16	S <sup>14+</sup>	0.063(2)	-248.0625	-246.1571	0.77
17	Cl <sup>15+</sup>	0.06(2)	-280.5625	-278.5322	0.73
18	Ar <sup>16+</sup>	0.056(2)	-315.0625	-312.9072	0.69
19	K <sup>17+</sup>	0.053(2)	-351.5625	-349.2822	0.65
20	Ca <sup>18+</sup>	0.051(2)	-390.0625	-387.6572	0.62
21	Sc <sup>19+</sup>	0.048(2)	-430.5625	-428.0323	0.59
22	Ti <sup>20+</sup>	0.046(2)	-473.0625	-470.4073	0.56
23	V <sup>21+</sup>	0.044(2)	-517.5625	-514.7823	0.54
24	Cr <sup>22+</sup>	0.042(2)	-564.0625	-561.1573	0.52
25	Mn <sup>23+</sup>	0.04(2)	-612.5625	-609.5323	0.5
26	Fe <sup>24+</sup>	0.039(2)	-663.0625	-659.9073	0.48
27	Co <sup>25+</sup>	0.037(2)	-715.5625	-712.2823	0.46
28	Ni <sup>26+</sup>	0.036(2)	-770.0625	-766.6574	0.44

TABLE II: Lithium isoelectronic series. Configuration  $1s^2 2s^1$ . 3 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
3	Li	0.364(2), 3.849	-7.6905	-7.4781	2.84
4	Be <sup>+</sup>	0.267(2), 1.909	-14.5767	-14.3248	1.76
5	B <sup>2+</sup>	0.211(2), 1.275	-23.7185	-23.4246	1.25
6	C <sup>3+</sup>	0.174(2), 0.96	-35.1134	-34.7755	0.97
7	N <sup>4+</sup>	0.148(2), 0.771	-48.7602	-48.3769	0.79
8	O <sup>5+</sup>	0.129(2), 0.644	-64.6581	-64.2285	0.67
9	F <sup>6+</sup>	0.114(2), 0.554	-82.8067	-82.3303	0.58
10	Ne <sup>7+</sup>	0.103(2), 0.486	-103.2058	-102.6822	0.51
11	Na <sup>8+</sup>	0.093(2), 0.433	-125.8553	-125.2842	0.46
12	Mg <sup>9+</sup>	0.085(2), 0.39	-150.755	-150.1362	0.41
13	Al <sup>10+</sup>	0.079(2), 0.356	-177.9049	-177.2382	0.38
14	Si <sup>11+</sup>	0.073(2), 0.326	-207.305	-206.5903	0.35
15	P <sup>12+</sup>	0.068(2), 0.302	-238.9553	-238.1924	0.32
16	S <sup>13+</sup>	0.064(2), 0.28	-272.8556	-272.0445	0.3
17	Cl <sup>14+</sup>	0.06(2), 0.262	-309.006	-308.1466	0.28
18	Ar <sup>15+</sup>	0.056(2), 0.246	-347.4064	-346.4987	0.26
19	K <sup>16+</sup>	0.053(2), 0.232	-388.057	-387.1008	0.25
20	Ca <sup>17+</sup>	0.051(2), 0.219	-430.9575	-429.953	0.23
21	Sc <sup>18+</sup>	0.048(2), 0.207	-476.1081	-475.0551	0.22
22	Ti <sup>19+</sup>	0.046(2), 0.197	-523.5088	-522.4073	0.21
23	V <sup>20+</sup>	0.044(2), 0.188	-573.1595	-572.0094	0.2
24	Cr <sup>21+</sup>	0.042(2), 0.18	-625.0602	-623.8616	0.19
25	Mn <sup>22+</sup>	0.04(2), 0.172	-679.2109	-677.9638	0.18
26	Fe <sup>23+</sup>	0.039(2), 0.165	-735.6116	-734.3159	0.18
27	Co <sup>24+</sup>	0.037(2), 0.158	-794.2624	-792.9181	0.17
28	Ni <sup>25+</sup>	0.036(2), 0.152	-855.1632	-853.7702	0.16

TABLE III: Beryllium isoelectronic series. Configuration  $1s^2 2s^2$ . 4 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
3	Li <sup>-</sup>	0.364(2), 5.233(2)	-7.7049	-7.5008	2.72
4	Be	0.267(2), 2.232(2)	-14.8403	-14.6674	1.18
5	B <sup>+</sup>	0.211(2), 1.421(2)	-24.4825	-24.3489	0.55
6	C <sup>2+</sup>	0.174(2), 1.044(2)	-36.6286	-36.5349	0.26
7	N <sup>3+</sup>	0.148(2), 0.826(2)	-51.2772	-51.2229	0.11
8	O <sup>4+</sup>	0.129(2), 0.683(2)	-68.4273	-68.4118	0.02
9	F <sup>5+</sup>	0.114(2), 0.583(2)	-88.0784	-88.1012	-0.03
10	Ne <sup>6+</sup>	0.103(2), 0.508(2)	-110.2303	-110.291	-0.06
11	Na <sup>7+</sup>	0.093(2), 0.451(2)	-134.8827	-134.981	-0.07
12	Mg <sup>8+</sup>	0.085(2), 0.405(2)	-162.0355	-162.1711	-0.08
13	Al <sup>9+</sup>	0.079(2), 0.368(2)	-191.6887	-191.8614	-0.09
14	Si <sup>10+</sup>	0.073(2), 0.337(2)	-223.8421	-224.0517	-0.09
15	P <sup>11+</sup>	0.068(2), 0.31(2)	-258.4956	-258.7421	-0.1
16	S <sup>12+</sup>	0.064(2), 0.288(2)	-295.6494	-295.9325	-0.1
17	Cl <sup>13+</sup>	0.06(2), 0.269(2)	-335.3033	-335.623	-0.1
18	Ar <sup>14+</sup>	0.056(2), 0.252(2)	-377.4573	-377.8135	-0.09
19	K <sup>15+</sup>	0.053(2), 0.237(2)	-422.1113	-422.5041	-0.09
20	Ca <sup>16+</sup>	0.051(2), 0.224(2)	-469.2655	-469.6946	-0.09
21	Sc <sup>17+</sup>	0.048(2), 0.212(2)	-518.9197	-519.3852	-0.09
22	Ti <sup>18+</sup>	0.046(2), 0.201(2)	-571.074	-571.5758	-0.09
23	V <sup>19+</sup>	0.044(2), 0.191(2)	-625.7283	-626.2664	-0.09
24	Cr <sup>20+</sup>	0.042(2), 0.183(2)	-682.8827	-683.457	-0.08
25	Mn <sup>21+</sup>	0.04(2), 0.175(2)	-742.5371	-743.1477	-0.08
26	Fe <sup>22+</sup>	0.039(2), 0.167(2)	-804.6916	-805.3383	-0.08
27	Co <sup>23+</sup>	0.037(2), 0.161(2)	-869.3461	-870.0289	-0.08
28	Ni <sup>24+</sup>	0.036(2), 0.154(2)	-936.5006	-937.2196	-0.08

TABLE IV: Boron isoelectronic series. Configuration  $1s^2 2s^2 2p^1$ . 5 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
4	Be <sup>-</sup>	0.267(2), 2.758(3)	-14.8313	-14.6674	1.12
5	B	0.211(2), 1.618(3)	-24.7936	-24.6539	0.57
6	C <sup>+</sup>	0.174(2), 1.146(3)	-37.5131	-37.431	0.22
7	N <sup>2+</sup>	0.148(2), 0.888(3)	-52.9872	-52.9664	0.04
8	O <sup>3+</sup>	0.129(2), 0.725(3)	-71.2144	-71.2556	-0.06
9	F <sup>4+</sup>	0.115(2), 0.613(3)	-92.1936	-92.2972	-0.11
10	Ne <sup>5+</sup>	0.103(2), 0.531(3)	-115.9243	-116.0902	-0.14
11	Na <sup>6+</sup>	0.093(2), 0.469(3)	-142.4061	-142.6342	-0.16
12	Mg <sup>7+</sup>	0.085(2), 0.419(3)	-171.6388	-171.929	-0.17
13	Al <sup>8+</sup>	0.079(2), 0.379(3)	-203.622	-203.9742	-0.17
14	Si <sup>9+</sup>	0.073(2), 0.346(3)	-238.3558	-238.7698	-0.17
15	P <sup>10+</sup>	0.068(2), 0.319(3)	-275.8399	-276.3157	-0.17
16	S <sup>11+</sup>	0.064(2), 0.295(3)	-316.0744	-316.6119	-0.17
17	Cl <sup>12+</sup>	0.06(2), 0.275(3)	-359.0592	-359.6582	-0.17
18	Ar <sup>13+</sup>	0.056(2), 0.257(3)	-404.7942	-405.4547	-0.16
19	K <sup>14+</sup>	0.053(2), 0.242(3)	-453.2793	-454.0012	-0.16
20	Ca <sup>15+</sup>	0.051(2), 0.228(3)	-504.5147	-505.2979	-0.16
21	Sc <sup>16+</sup>	0.048(2), 0.215(3)	-558.5002	-559.3447	-0.15
22	Ti <sup>17+</sup>	0.046(2), 0.204(3)	-615.2357	-616.1415	-0.15
23	V <sup>18+</sup>	0.044(2), 0.194(3)	-674.7214	-675.6884	-0.14
24	Cr <sup>19+</sup>	0.042(2), 0.185(3)	-736.9572	-737.9853	-0.14
25	Mn <sup>20+</sup>	0.04(2), 0.177(3)	-801.9431	-803.0323	-0.14
26	Fe <sup>21+</sup>	0.039(2), 0.17(3)	-869.679	-870.8293	-0.13
27	Co <sup>22+</sup>	0.037(2), 0.163(3)	-940.165	-941.3764	-0.13
28	Ni <sup>23+</sup>	0.036(2), 0.156(3)	-1013.401	-1014.673	-0.13

TABLE V: Carbon isoelectronic series. Configuration  $1s^2 2s^2 2p^2$ . 6 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
6	C	0.174(2), 1.294(4)	-37.8156	-37.8168	-0.03
7	N <sup>+</sup>	0.148(2), 0.976(4)	-53.9059	-54.0546	-0.28
8	O <sup>2+</sup>	0.129(2), 0.783(4)	-72.9976	-73.275	-0.38
9	F <sup>3+</sup>	0.114(2), 0.654(4)	-95.0916	-95.5014	-0.43
10	Ne <sup>4+</sup>	0.103(2), 0.562(4)	-120.1873	-120.7315	-0.45
11	Na <sup>5+</sup>	0.093(2), 0.492(4)	-148.2845	-148.964	-0.46
12	Mg <sup>6+</sup>	0.085(2), 0.438(4)	-179.3828	-180.1983	-0.45
13	Al <sup>7+</sup>	0.079(2), 0.395(4)	-213.4821	-214.4338	-0.44
14	Si <sup>8+</sup>	0.073(2), 0.359(4)	-250.5822	-251.6703	-0.43
15	P <sup>9+</sup>	0.068(2), 0.33(4)	-290.683	-291.9075	-0.42
16	S <sup>10+</sup>	0.064(2), 0.304(4)	-333.7843	-335.1453	-0.41
17	Cl <sup>11+</sup>	0.06(2), 0.283(4)	-379.8861	-381.3835	-0.39
18	Ar <sup>12+</sup>	0.056(2), 0.264(4)	-428.9882	-430.6221	-0.38
19	K <sup>13+</sup>	0.053(2), 0.248(4)	-481.0907	-482.861	-0.37
20	Ca <sup>14+</sup>	0.051(2), 0.233(4)	-536.1935	-538.1002	-0.35
21	Sc <sup>15+</sup>	0.048(2), 0.22(4)	-594.2966	-596.3395	-0.34
22	Ti <sup>16+</sup>	0.046(2), 0.209(4)	-655.3998	-657.5791	-0.33
23	V <sup>17+</sup>	0.044(2), 0.198(4)	-719.5033	-721.8188	-0.32
24	Cr <sup>18+</sup>	0.042(2), 0.189(4)	-786.607	-789.0586	-0.31
25	Mn <sup>19+</sup>	0.04(2), 0.181(4)	-856.7107	-859.2985	-0.3
26	Fe <sup>20+</sup>	0.039(2), 0.173(4)	-929.8147	-932.5385	-0.29
27	Co <sup>21+</sup>	0.037(2), 0.166(4)	-1005.919	-1008.779	-0.28
28	Ni <sup>22+</sup>	0.036(2), 0.159(4)	-1085.023	-1088.019	-0.28

TABLE VI: Nitrogen isoelectronic series. Configuration  $1s^2 2s^2 2p^3$ . 7 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
7	N	0.148, 0.148, 1.052(2), 1.061(2), 1.159	-54.161	-54.5893	-0.78
8	O <sup>+</sup>	0.129, 0.129, 0.835(2), 0.836(2), 0.895	-73.928	-74.5669	-0.86
9	F <sup>2+</sup>	0.114, 0.114, 0.691(4), 0.732	-96.947	-97.808	-0.88
10	Ne <sup>3+</sup>	0.103, 0.103, 0.588(4), 0.62	-123.2169	-124.307	-0.88
11	Na <sup>4+</sup>	0.093, 0.093, 0.513(4), 0.537	-152.7374	-154.0612	-0.86
12	Mg <sup>5+</sup>	0.085, 0.085, 0.454(4), 0.474	-185.5084	-187.0689	-0.83
13	Al <sup>6+</sup>	0.079(2), 0.408(2), 0.408, 0.415(2)	-221.5306	-223.3292	-0.81
14	Si <sup>7+</sup>	0.073(2), 0.37(2), 0.37, 0.376(2)	-260.8048	-262.8414	-0.77
15	P <sup>8+</sup>	0.068(2), 0.338(2), 0.339, 0.344(2)	-303.3297	-305.605	-0.74
16	S <sup>9+</sup>	0.064(2), 0.312(2), 0.312, 0.316(2)	-349.1051	-351.6199	-0.72
17	Cl <sup>10+</sup>	0.06(2), 0.289(2), 0.29, 0.293(2)	-398.131	-400.8856	-0.69
18	Ar <sup>11+</sup>	0.056(2), 0.27(2), 0.27, 0.273(2)	-450.4073	-453.402	-0.66
19	K <sup>12+</sup>	0.053(2), 0.253(2), 0.253, 0.256(2)	-505.934	-509.1691	-0.64
20	Ca <sup>13+</sup>	0.051(2), 0.238(2), 0.238, 0.24(2)	-564.711	-568.1866	-0.61
21	Sc <sup>14+</sup>	0.048(2), 0.224(2), 0.225, 0.227(2)	-626.7383	-630.4546	-0.59
22	Ti <sup>15+</sup>	0.046(2), 0.212(2), 0.213, 0.214(2)	-692.0158	-695.973	-0.57
23	V <sup>16+</sup>	0.044(2), 0.202(2), 0.202, 0.203(2)	-760.5436	-764.7416	-0.55
24	Cr <sup>17+</sup>	0.042(2), 0.192(2), 0.192, 0.194(2)	-832.3215	-836.7605	-0.53
25	Mn <sup>18+</sup>	0.04(2), 0.183(2), 0.183, 0.185(2)	-907.3496	-912.0296	-0.51
26	Fe <sup>19+</sup>	0.039(2), 0.175(2), 0.175, 0.177(2)	-985.6278	-990.5489	-0.5
27	Co <sup>20+</sup>	0.037(2), 0.168(2), 0.168, 0.169(2)	-1067.156	-1072.318	-0.48
28	Ni <sup>21+</sup>	0.036(2), 0.161(2), 0.161, 0.162(2)	-1151.935	-1157.338	-0.47

TABLE VII: Oxygen isoelectronic series. Configuration  $1s^2 2s^2 2p^4$ . 8 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
8	O	0.129(2), 0.878(4), 1.027(2)	-74.178	-75.0674	-1.18
9	F <sup>+</sup>	0.114(2), 0.726(4), 0.8(2)	-97.9282	-99.093	-1.18
10	Ne <sup>2+</sup>	0.103(2), 0.63(6)	-125.1863	-126.6373	-1.15
11	Na <sup>3+</sup>	0.093(2), 0.544(6)	-155.9469	-157.6923	-1.11
12	Mg <sup>4+</sup>	0.085(2), 0.479(6)	-190.2084	-192.2543	-1.06
13	Al <sup>5+</sup>	0.078(2), 0.428(6)	-227.9705	-230.3214	-1.02
14	Si <sup>6+</sup>	0.073(2), 0.386(6)	-269.2334	-271.8921	-0.98
15	P <sup>7+</sup>	0.068(2), 0.352(6)	-313.9967	-316.9657	-0.94
16	S <sup>8+</sup>	0.064(2), 0.324(6)	-362.2605	-365.5414	-0.9
17	Cl <sup>9+</sup>	0.06(2), 0.3(6)	-414.0247	-417.6188	-0.86
18	Ar <sup>10+</sup>	0.056(2), 0.279(6)	-469.2893	-473.1976	-0.83
19	K <sup>11+</sup>	0.053(2), 0.26(6)	-528.0541	-532.2776	-0.79
20	Ca <sup>12+</sup>	0.051(2), 0.245(6)	-590.3193	-594.8585	-0.76
21	Sc <sup>13+</sup>	0.048(2), 0.23(6)	-656.0846	-660.9402	-0.73
22	Ti <sup>14+</sup>	0.046(2), 0.218(6)	-725.3502	-730.5225	-0.71
23	V <sup>15+</sup>	0.044(2), 0.207(6)	-798.1159	-803.6054	-0.68
24	Cr <sup>16+</sup>	0.042(2), 0.196(6)	-874.3818	-880.1888	-0.66
25	Mn <sup>17+</sup>	0.04(2), 0.187(6)	-954.1478	-960.2726	-0.64
26	Fe <sup>18+</sup>	0.039(2), 0.179(6)	-1037.414	-1043.857	-0.62
27	Co <sup>19+</sup>	0.037(2), 0.171(6)	-1124.18	-1130.941	-0.6
28	Ni <sup>20+</sup>	0.036(2), 0.164(6)	-1214.447	-1221.526	-0.58

TABLE VIII: Fluorine isoelectronic series. Configuration  $1s^2 2s^2 2p^5$ . 9 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
9	F	0.114,0.114,0.716(2),0.735(2),0.802,0.805,3.656	-98.059	-99.7341	-1.68
10	Ne <sup>+</sup>	0.103(2),0.661(5),0.704(2)	-125.9247	-128.1437	-1.73
11	Na <sup>2+</sup>	0.093(2),0.567(5),0.598(2)	-157.6955	-160.3258	-1.64
12	Mg <sup>3+</sup>	0.085(2),0.497(5),0.52(2)	-193.2168	-196.2715	-1.56
13	Al <sup>4+</sup>	0.078(2),0.442(5),0.46(2)	-232.4881	-235.9763	-1.48
14	Si <sup>5+</sup>	0.073(2),0.398(2),0.398(2),0.399,0.412,0.412	-275.5098	-279.4376	-1.41
15	P <sup>6+</sup>	0.068(2),0.362,0.362(2),0.363(2),0.372(2)	-322.2825	-326.6538	-1.34
16	S <sup>7+</sup>	0.064(2),0.332,0.332(2),0.333(2),0.34(2)	-372.8059	-377.6237	-1.28
17	Cl <sup>8+</sup>	0.06(2),0.306,0.307(2),0.308(2),0.313(2)	-427.0799	-432.3465	-1.22
18	Ar <sup>9+</sup>	0.056(2),0.285(2),0.285,0.286(2),0.29(2)	-485.1044	-490.8217	-1.16
19	K <sup>10+</sup>	0.053(2),0.266,0.266(2),0.267(2),0.27(2)	-546.8792	-553.0488	-1.12
20	Ca <sup>11+</sup>	0.051(2),0.249,0.25(2),0.25(2),0.253(2)	-612.4044	-619.0275	-1.07
21	Sc <sup>12+</sup>	0.048(2),0.234,0.235(2),0.236(2),0.238(2)	-681.6798	-688.7576	-1.03
22	Ti <sup>13+</sup>	0.046(2),0.221,0.222(2),0.222(2),0.225(2)	-754.7055	-762.2387	-0.99
23	V <sup>14+</sup>	0.044(2),0.21,0.21(2),0.211(2),0.213(2)	-831.4815	-839.4708	-0.95
24	Cr <sup>15+</sup>	0.042(2),0.199,0.2(2),0.2(2),0.202(2)	-912.0076	-920.4537	-0.92
25	Mn <sup>16+</sup>	0.04(2),0.19,0.19(2),0.191(2),0.192(2)	-996.2839	-1005.187	-0.89
26	Fe <sup>17+</sup>	0.039(2),0.181,0.182(2),0.182(2),0.183(2)	-1084.31	-1093.672	-0.86
27	Co <sup>18+</sup>	0.037(2),0.173,0.174(2),0.174(2),0.175(2)	-1176.087	-1185.906	-0.83
28	Ni <sup>19+</sup>	0.036(2),0.166,0.166(2),0.167(2),0.168(2)	-1271.614	-1281.892	-0.8

TABLE IX: Neon isoelectronic series. Configuration  $1s^2 2s^2 2p^6$ . 10 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
9	F <sup>-</sup>	0.114(2),0.725(4),0.803(2),5.216(2)	-98.0708	-99.859	-1.79
10	Ne	0.103,0.103,0.656(2),0.664(2),0.667,0.693,0.713,3.781	-126.0531	-128.9383	-2.24
11	Na <sup>+</sup>	0.093(2),0.611(8)	-158.3715	-162.0667	-2.28
12	Mg <sup>2+</sup>	0.085(2),0.53(8)	-194.9627	-199.2214	-2.14
13	Al <sup>3+</sup>	0.078(2),0.468(8)	-235.555	-240.3925	-2.01
14	Si <sup>4+</sup>	0.073(2),0.419(8)	-280.1483	-285.5747	-1.9
15	P <sup>5+</sup>	0.068(2),0.379(8)	-328.7423	-334.7651	-1.8
16	S <sup>6+</sup>	0.064(2),0.346(8)	-381.337	-387.9615	-1.71
17	Cl <sup>7+</sup>	0.06(2),0.319(8)	-437.9322	-445.1628	-1.62
18	Ar <sup>8+</sup>	0.056(2),0.295(8)	-498.528	-506.3678	-1.55
19	K <sup>9+</sup>	0.053(2),0.275(8)	-563.1243	-571.5758	-1.48
20	Ca <sup>10+</sup>	0.051(2),0.257(8)	-631.721	-640.7864	-1.41
21	Sc <sup>11+</sup>	0.048(2),0.242(8)	-704.318	-713.9991	-1.36
22	Ti <sup>12+</sup>	0.046(2),0.228(8)	-780.9153	-791.2135	-1.3
23	V <sup>13+</sup>	0.044(2),0.215(8)	-861.5129	-872.4294	-1.25
24	Cr <sup>14+</sup>	0.042(2),0.204(8)	-946.1108	-957.6465	-1.2
25	Mn <sup>15+</sup>	0.04(2),0.195(8)	-1034.709	-1046.865	-1.16
26	Fe <sup>16+</sup>	0.039(2),0.185(8)	-1127.307	-1140.084	-1.12
27	Co <sup>17+</sup>	0.037(2),0.177(8)	-1223.906	-1237.304	-1.08
28	Ni <sup>18+</sup>	0.036(2),0.17(8)	-1324.504	-1338.525	-1.05

TABLE X: Sodium isoelectronic series. Configuration  $1s^2 2s^2 2p^6 3s^1$ . 11 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
11	Na	0.093,0.093,0.61(4),0.612(4),8.927	-158.4273	-162.2554	-2.36
12	Mg <sup>+</sup>	0.085,0.085,0.528(4),0.532(4),4.43	-195.187	-199.7732	-2.3
13	Al <sup>2+</sup>	0.078,0.078,0.466(4),0.47(4),2.936	-236.0611	-241.4362	-2.23
14	Si <sup>3+</sup>	0.073,0.073,0.417(4),0.421(4),2.192	-281.0498	-287.2305	-2.15
15	P <sup>4+</sup>	0.068,0.068,0.377(4),0.381(4),1.748	-330.1532	-337.1494	-2.08
16	S <sup>5+</sup>	0.064,0.064,0.344(4),0.348(4),1.453	-383.3708	-391.1892	-2.
17	Cl <sup>6+</sup>	0.06,0.06,0.317(4),0.321(4),1.243	-440.7025	-449.3474	-1.92
18	Ar <sup>7+</sup>	0.056,0.056,0.293(4),0.297(4),1.087	-502.1479	-511.6223	-1.85
19	K <sup>8+</sup>	0.053,0.053,0.273(4),0.276(4),0.965	-567.7067	-578.0129	-1.78
20	Ca <sup>9+</sup>	0.051,0.051,0.256(4),0.259(4),0.869	-637.3786	-648.5182	-1.72
21	Sc <sup>10+</sup>	0.048,0.048,0.24(4),0.243(4),0.79	-711.1633	-723.1376	-1.66
22	Ti <sup>11+</sup>	0.046,0.046,0.227(4),0.229(4),0.724	-789.0608	-801.8706	-1.6
23	V <sup>12+</sup>	0.044,0.044,0.215(4),0.217(4),0.669	-871.0707	-884.7169	-1.54
24	Cr <sup>13+</sup>	0.042,0.042,0.204(4),0.206(4),0.621	-957.1929	-971.676	-1.49
25	Mn <sup>14+</sup>	0.04,0.04,0.194(4),0.196(4),0.58	-1047.427	-1062.748	-1.44
26	Fe <sup>15+</sup>	0.039,0.039,0.185(4),0.186(4),0.544	-1141.774	-1157.932	-1.4
27	Co <sup>16+</sup>	0.037,0.037,0.177(4),0.178(4),0.512	-1240.232	-1257.228	-1.35
28	Ni <sup>17+</sup>	0.036,0.036,0.169(2),0.169,0.17(2),0.17(2),0.171,0.493	-1342.596	-1360.637	-1.33

 TABLE XI: Magnesium isoelectronic series. Configuration  $1s^2 2s^2 2p^6 3s^2$ . 12 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
11	Na <sup>-</sup>	0.093(2),0.611(8),11.95(2)	-158.4341	-162.275	-2.37
12	Mg	0.085(2),0.53(8),5.101(2)	-195.3048	-200.054	-2.37
13	Al <sup>+</sup>	0.078(2),0.468(8),3.234(2)	-236.4013	-242.127	-2.36
14	Si <sup>2+</sup>	0.073(2),0.419(8),2.365(2)	-281.7242	-288.459	-2.33
15	P <sup>3+</sup>	0.068(2),0.379(8),1.862(2)	-331.2736	-339.036	-2.29
16	S <sup>4+</sup>	0.064(2),0.346(8),1.535(2)	-385.0495	-393.851	-2.23
17	Cl <sup>5+</sup>	0.06(2),0.319(8),1.306(2)	-443.0515	-452.899	-2.17
18	Ar <sup>6+</sup>	0.056,0.056,0.294(2),0.295(4),0.296(2),1.159(2)	-505.1943	-516.178	-2.13
19	K <sup>7+</sup>	0.053(2),0.274(4),0.275(4),1.025(2)	-571.6248	-583.685	-2.07
20	Ca <sup>8+</sup>	0.051(2),0.257(8),0.902(2)	-642.4119	-655.42	-1.98
21	Sc <sup>9+</sup>	0.048(2),0.241(4),0.242(4),0.833(2)	-717.1569	-731.382	-1.94
22	Ti <sup>10+</sup>	0.046(2),0.228(8),0.748(2)	-796.4441	-811.569	-1.86
23	V <sup>11+</sup>	0.044(2),0.215(4),0.216(4),0.701(2)	-879.5837	-895.981	-1.83
24	Cr <sup>12+</sup>	0.042(2),0.205(8),0.639(2)	-967.3737	-984.618	-1.75
25	Mn <sup>13+</sup>	0.04(2),0.195(8),0.596(2)	-1059.175	-1077.48	-1.7
26	Fe <sup>14+</sup>	0.039(2),0.186(8),0.558(2)	-1155.199	-1174.565	-1.65
27	Co <sup>15+</sup>	0.037(2),0.177(8),0.525(2)	-1255.447	-1275.874	-1.6
28	Ni <sup>16+</sup>	0.036(2),0.17(8),0.496(2)	-1359.919	-1381.407	-1.56

TABLE XII: Aluminium isoelectronic series. Configuration  $1s^2 2s^2 2p^6 3s^2 3p^1$ . 13 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
13	Al	0.078,0.078,0.467(2),0.468(4),0.468(2),3.655,3.731(2)	-236.5348	-242.347	-2.4
14	Si <sup>+</sup>	0.073,0.073,0.418(2),0.419(4),0.419(2),2.584,2.639(2)	-282.1046	-289.06	-2.41
15	P <sup>2+</sup>	0.068,0.068,0.378,0.379,0.379(2),0.379(2),0.38(2),2.002,2.03,2.046	-332.01	-340.145	-2.39
16	S <sup>3+</sup>	0.064,0.064,0.346,0.346,0.346(2),0.346(2),0.347(2),1.633,1.652,1.667	-386.2511	-395.589	-2.36
17	Cl <sup>4+</sup>	0.06,0.06,0.318,0.318,0.318(2),0.319(2),0.319(2),1.379,1.392,1.407	-444.8281	-455.384	-2.32
18	Ar <sup>5+</sup>	0.056,0.056,0.294,0.295,0.295(2),0.295(2),0.296(2),1.193,1.203,1.216	-507.7409	-519.525	-2.27
19	K <sup>6+</sup>	0.053,0.053,0.274,0.275,0.275(2),0.275(2),0.276(2),1.051,1.058,1.071	-574.9896	-588.01	-2.21
20	Ca <sup>7+</sup>	0.051,0.051,0.256,0.257,0.257(2),0.257(2),0.258(2),0.939,0.945,0.956	-646.5742	-660.836	-2.16
21	Sc <sup>8+</sup>	0.048,0.048,0.241,0.241,0.242(2),0.242(2),0.242(2),0.849,0.853,0.864	-722.4945	-738.001	-2.1
22	Ti <sup>9+</sup>	0.046,0.046,0.227,0.228(2),0.228,0.228(2),0.228(2),0.774,0.778,0.788	-802.7505	-819.504	-2.04
23	V <sup>10+</sup>	0.044,0.044,0.215,0.215(2),0.216,0.216(2),0.216(2),0.712,0.715,0.724	-887.342	-905.346	-1.99
24	Cr <sup>11+</sup>	0.042,0.042,0.204,0.204(2),0.205,0.205(2),0.205(2),0.659,0.661,0.67	-976.2688	-995.524	-1.93
25	Mn <sup>12+</sup>	0.04,0.04,0.194,0.195(2),0.195,0.195(2),0.195(2),0.613,0.615,0.623	-1069.531	-1090.038	-1.88
26	Fe <sup>13+</sup>	0.039,0.039,0.185,0.185(2),0.186,0.186(2),0.186(2),0.573,0.575,0.582	-1167.128	-1188.888	-1.83
27	Co <sup>14+</sup>	0.037,0.037,0.177,0.177(2),0.177(2),0.177,0.178(2),0.539,0.54,0.547	-1269.06	-1292.074	-1.78
28	Ni <sup>15+</sup>	0.036,0.036,0.169,0.17(2),0.17(2),0.17,0.17(2),0.508,0.509,0.515	-1375.327	-1399.594	-1.73

 TABLE XIII: Silicon isoelectronic series. Configuration  $1s^2 2s^2 2p^6 3s^2 3p^2$ . 14 electrons.

$Z$	Ion	Distances	$E_{\text{Bohr}}$	$E_{\text{exact}}$	Error, %
13	Al <sup>-</sup>	0.078(2),0.468(8),4.185,4.369,4.372(2)	-236.518	-242.364	-2.41
14	Si	0.073(2),0.418(8),2.857,2.938,2.941(2)	-282.2589	-289.36	-2.45
15	P <sup>+</sup>	0.068(2),0.379(8),2.16,2.217,2.22(2)	-332.4456	-340.872	-2.47
16	S <sup>2+</sup>	0.064,0.064,0.346,0.346(2),0.346(2),0.346,0.347(2),1.734,1.779(2),1.783	-387.0779	-396.87	-2.47
17	Cl <sup>3+</sup>	0.06,0.06,0.318,0.318(2),0.318(2),0.319,0.319(2),1.449,1.486(2),1.49	-446.156	-457.339	-2.45
18	Ar <sup>4+</sup>	0.056(2),0.295(2),0.295(2),0.295(2),0.295(2),1.26(2),1.276(2)	-509.6792	-522.272	-2.41
19	K <sup>5+</sup>	0.053(2),0.274(2),0.275(2),0.275(2),0.275(2),1.104(2),1.118(2)	-577.6495	-591.664	-2.37
20	Ca <sup>6+</sup>	0.051(2),0.257(2),0.257(2),0.257(2),0.257(2),0.982(2),0.994(2)	-650.066	-665.512	-2.32
21	Sc <sup>7+</sup>	0.048(2),0.241(2),0.242(2),0.242(2),0.242(2),0.884(2),0.895(2)	-726.9289	-743.812	-2.27
22	Ti <sup>8+</sup>	0.046(2),0.228(2),0.228(2),0.228(2),0.228(2),0.804(2),0.814(2)	-808.2383	-826.565	-2.22
23	V <sup>9+</sup>	0.044(2),0.215(2),0.216(2),0.216(2),0.216(2),0.737(2),0.746(2)	-893.994	-913.767	-2.16
24	Cr <sup>10+</sup>	0.042(2),0.204(2),0.205(2),0.205(2),0.205(2),0.68(2),0.688(2)	-984.1961	-1005.419	-2.11
25	Mn <sup>11+</sup>	0.04(2),0.194(2),0.195(2),0.195(2),0.195(2),0.632(2),0.639(2)	-1078.844	-1101.52	-2.06
26	Fe <sup>12+</sup>	0.039(2),0.185(2),0.186(2),0.186(2),0.186(2),0.59(2),0.597(2)	-1177.939	-1202.068	-2.01
27	Co <sup>13+</sup>	0.037(2),0.177(2),0.177(2),0.177(2),0.178(2),0.553(2),0.559(2)	-1281.48	-1307.064	-1.96
28	Ni <sup>14+</sup>	0.036(2),0.17(2),0.17(2),0.17(2),0.17(2),0.52(2),0.526(2)	-1389.466	-1416.507	-1.91