

IPPJ-AM-63

**PARTIAL ELECTRONIC STOPPING CROSS SECTIONS
OF ATOMS FOR PROTONS**

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February 1989

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Abstract

Based on a newly developed wave packet theory, the partial electronic stopping cross sections for protons in collisions with atoms with atomic number Z_2 ranging from 2(He) to 54(Xe) are calculated shell by shell.

The electronic stopping power of matter for energetic ions has attracted our attention theoretically[1-11] as well as experimentally because it is one of the basic problems in the studies of both the plasma-wall interaction in a fusion reactor and the atomic collision phenomena in solids. So far, the theoretical estimates have been performed of the stoppings for both a free electron gas[1-4] and atomic electrons based either on Born approximation[5,6] or on the momentum exchange between electron clouds of a projectile and of a target atom[7]. In addition, the density functional calculations [8], the binary-encounter theory[9] with the aid of Bethe stopping model, and the calculations on the basis of the local electron density models (LEDM's)[10,11] were also presented. Recently, some effort has been made to estimate shellwise partial stoppings on the basis of binary-encounter model[12]. Quite recently, the wave packet theory of the stopping of weakly bound electrons(WBE's) was newly presented[13]. The main thrust of the wave packet theory is the use of momentum space representation to describe bound electrons, where the localized nature is held in the momentum distribution function. Then the system can be regarded as an interacting electron gas. Hereby, one can study the dielectric response and discuss many-body effect, which have ever been neither considered nor evaluated in the existing theoretical approaches to the stopping of bound electrons. This theory has been shown to be useful for the evaluation of the partial electronic stoppings of atoms and solids shell by shell on the independent shell model. The aim of this report is to present series of tables of theoretical values of the partial as well as total electronic stopping cross

sections for protons in collisions with neutral target atoms. Hereafter, m , e , v_0 , a_0 , and \hbar denote the electron rest mass, the elementary charge, the Bohr velocity, the Bohr radius and the Planck constant divided by 2π , respectively.

In general, the atomic state is degenerate with respect to magnetic quantum number without external magnetic field. The wave function of an atomic electron is represented by a linear combination of plane waves in the momentum space. In this case the absolute square of expansion coefficients is closely related to the occupation probability of momenta. Then, we can introduce the momentum-occupation probability $w(\vec{q})$ for momentum $\hbar\vec{q}$ into the system of the wave packet, which is classified by the principal and angular momentum quantum numbers, i.e., (n,l) . According to the basic principle of the statistical physics[14], a gaussian distribution : $w(\vec{q})=\exp(-q^2/\bar{q}^2)$ is assumed from a simple discussion[15]. Here \bar{q} denotes the characteristic momentum for a shell(n,l). When a shell(n,l) contains N electrons per atom and $M(>>1)$ atoms are assumed to be confined in a normalization volume V , one find that the following relation holds:

$$2 V/(2\pi)^3 \int d^3q w(\vec{q}) = N \times M , \quad (1)$$

by connecting the volume occupied in the phase space with the electron number contained. Then \bar{q} is determined by $\bar{q}=(\pi)^{1/2} \times (4N \cdot M/V)^{1/3}$ or $\bar{q} = N^{1/3} q_1$, where $q_1 = (4M/V)^{1/3}$ denoting the value of \bar{q} in the case of $N=1$. It is required that the momentum-occupation probability, $w_1(\vec{q})$ (for $N=1$) = $\exp(-q^2/q_1^2)$, should be proportional to the momentum distribution of one electron in the shell (n,l).

Fortunately, the Hartree-Fock(HF) momentum distribution function [16,17], $f_{HF}(\vec{q})$, obtained from the normalized wavefunction $\phi_{HF}(\vec{r})$ through $f_{HF}(\vec{q}) = (2\pi)^{-3} |\int d^3r \exp(i\vec{q}\cdot\vec{r}) \phi_{HF}(\vec{r})|^2$, can be well approximated by a gaussian form:

$$f_{HF}(\vec{q}) = (\pi Q^2)^{-3/2} \exp(-q^2/Q^2). \quad (2)$$

If the parameter Q is determined from $f_{HF}(0)$ value such as $Q = [\{f_{HF}(0)\}^{-2/3}/\pi]^{1/2}$, this Q is equivalent to q_1 . The wave packet system is treated as an interacting electron gas with the gaussian momentum occupation probability.

According to the wave packet theory[13,15], the RPA (Random Phase Approximation)[18,19] dielectric function of the electronic shell considered can be expressed by the reduced variables $z=k/2\bar{q}$ and $u=m\omega/k\hbar\bar{q}$ instead of usual variables k and ω as follows:

$$\epsilon(z, u) = 1 + \chi^2/z^2 [f_1(z, u) + i f_2(z, u)] , \quad (3)$$

$$f_1(z, u) = (\pi)^{1/2}/(4z) [G(u+z) - G(u-z)] , \quad (4)$$

$$f_2(z, u) = \pi/(8z) [\exp(-(u-z)^2) - \exp(-(u+z)^2)] , \quad (5)$$

$$G(y) = y \exp(-y^2) \Phi(1/2, 3/2, y^2) , \quad (6)$$

in the framework of the linear response theory. In the above equations, $\chi^2 = mv_0/(\pi\hbar q)$ and $\Phi(1/2, 3/2, y^2)$ denotes a degenerate hypergeometric function[20]. Note that our dielectric function $\epsilon(\vec{k}, \omega)$ satisfies the sum rules:

$$\int_0^\infty d\omega \omega \operatorname{Im}\{\epsilon(\vec{k}, \omega)\} = \pi \omega_p^2 / 2 , \quad (7)$$

$$\int_0^\infty d\omega \omega \operatorname{Im}\{\epsilon^{-1}(\vec{k}, \omega)\} = -\pi \omega_p^2 / 2 , \quad (8)$$

in which $\omega_p = (4\pi \rho e^2/m)^{1/2}$ denotes the plasma frequency for a shell considered and $\rho = NM/V$. According to the dielectric function method, the stopping power S of the one-shell for an ion with charge $Z_1 e$ moving at velocity \vec{v} on a straight-line trajectory is calculated as

$$S = 4\pi (Z_1 e^2)^2 / mv^2 \cdot \rho \cdot L , \quad (9)$$

$$L = 8 / (\pi^{3/2} \chi^2) \int_0^\infty dz z \int_0^{v/\bar{v}} du u \operatorname{Im}\{\epsilon^{-1}(z, u) - 1\} , \quad (10)$$

where $\bar{v} = \hbar \bar{q} / m$.

First, we mention general features derived from our dielectric function. It is remarked that in the momentum space there isn't any characteristic surface like the Fermi surface (see Figure 1). Therefore the collective excitation has a finite life time except for that in the region of small z and large u in $z-u$ space. Figure 2 shows comparison between the real and imaginary parts of our dielectric function and of Lindhard's. In our case, the collective excitation has the dispersion relation in the region of $k \ll \bar{q}$:

$$\omega^2 = \omega_p^2 + \langle v^2 \rangle k^2 + (\hbar k^2 / 2m)^2 , \quad (11)$$

with $\langle v^2 \rangle = 3\bar{v}^2/2$.

At low velocities, the stopping power S is of the form

$$S \sim \frac{4Z_1^2}{3\pi} \frac{mv_0^2}{a_0} \frac{v}{v_0} \int_0^\infty dz \frac{z^3 \exp(-z^2)}{[z^2 + \frac{\pi^{1/2}}{2} x^2 \exp(-z^2) \Phi(\frac{1}{2}, \frac{3}{2}, z^2)]^2} \quad (12)$$

which is proportional to the ion velocity v . On the other hand, at high velocities the stopping number L has the following form of Bethe-Bloch type :

$$L \sim \ln(2mv^2/\hbar\omega_p) - \langle v^2 \rangle / v^2 - (1/2) \langle v^2 \rangle^2 / v^4 + \dots , \quad (13)$$

where $\hbar\omega_p$ corresponds to the mean excitation energy. It is worth while comparing the electronic stopping powers calculated using the present dielectric function $\epsilon(z, u)$ with those by Lindhard-Winther (LW) theory at the same electron densities. We found that the steep increases around the stopping maximum predicted by LW theory are suppressed and the peak of the stopping curves shifts a bit to the higher energy side.

Figure 3 shows partial and total stopping cross section of Ar for a proton at energies ranging from 1 keV/amu to 10^4 keV/amu. The states are classified independently by sets of principal and angular-momentum quantum numbers. The calculated total stopping cross section agrees well with the data [21-28] over the specific energy range considered. At lower velocities, the calculated total stopping curve deviates from the data. In general, the stopping data for low-energy protons tend to deviate from each other, whether they are obtained for solid or gaseous targets. Therefore, further data compilation is necessary to discuss a quantitative agreement with the data. It should be added that

the wave packet theory can also predict the Z_e (target atomic number) oscillations of the electronic stopping cross sections for protons[15]. At high energies, the stopping curves obtained by this theory are not so different from those by the atomic and solid LEDM's [11]. At low energies, on the other hand, this theory provides a velocity-proportionality, while the atomic LEDM with the use of LW theory predicts the unreasonable energy dependences[10,11].

In conclusion, the wave packet treatment was newly presented for studying the dielectric response of an ensemble of bound electrons by using the momentum space representation. Here a new type of the RPA dielectric function was obtained, and it was applied to estimate the electronic stoppings on the independent shell model. In the framework of linear response, the formalism presented could be straightforwardly extended to the evaluation of electronic stoppings and straggling for heavier ions.

The author would like to thank Mr. K. Iwashinaka, K. Makino, Y. Nagata, and H. Yamada for preparing tables of data, and Mr. Y. Imanaka, M. Tokuhiro, S. Watanabe for making the tables. He expresses sincere thanks to Dr. H. Tawara of IPP, Nagoya University for useful comments. This work was supported in part by the Special Project Research on Ion Beam Interactions with Solids from Ministry of Education, Science, and Culture, Japan.

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FIGURE CAPTIONS

Figure 1:

The momentum distribution used in comparison with the Fermi-Dirac distribution function for $r_s=1$, where $q = 1.745$ and $q_f = 1.919$ in atomic units. $\theta(x)$ is the step function.

Figure 2:

Real and imaginary parts, $f_1(z,u)$ and $f_2(z,u)$, of the present dielectric function with respect to u at $z=0.2$. For comparison, the corresponding parts, $f_1^L(z,u)$ and $f_2^L(z,u)$, of Lindhard dielectric function[4] ($z=k'/2k$, and $u=\omega/kv$, in this case) are drawn in the same coordinate system.

Figure 3:

Calculated total and partial stopping cross sections of Ar for protons together with the results of the kinetic theory: X-[12], and with the data: C-[21], Δ -[22], \odot -[23], \triangle -[24], ∇ -[25], ∇ -[26], \square -[27], \wedge -[28].

FIGURE 1

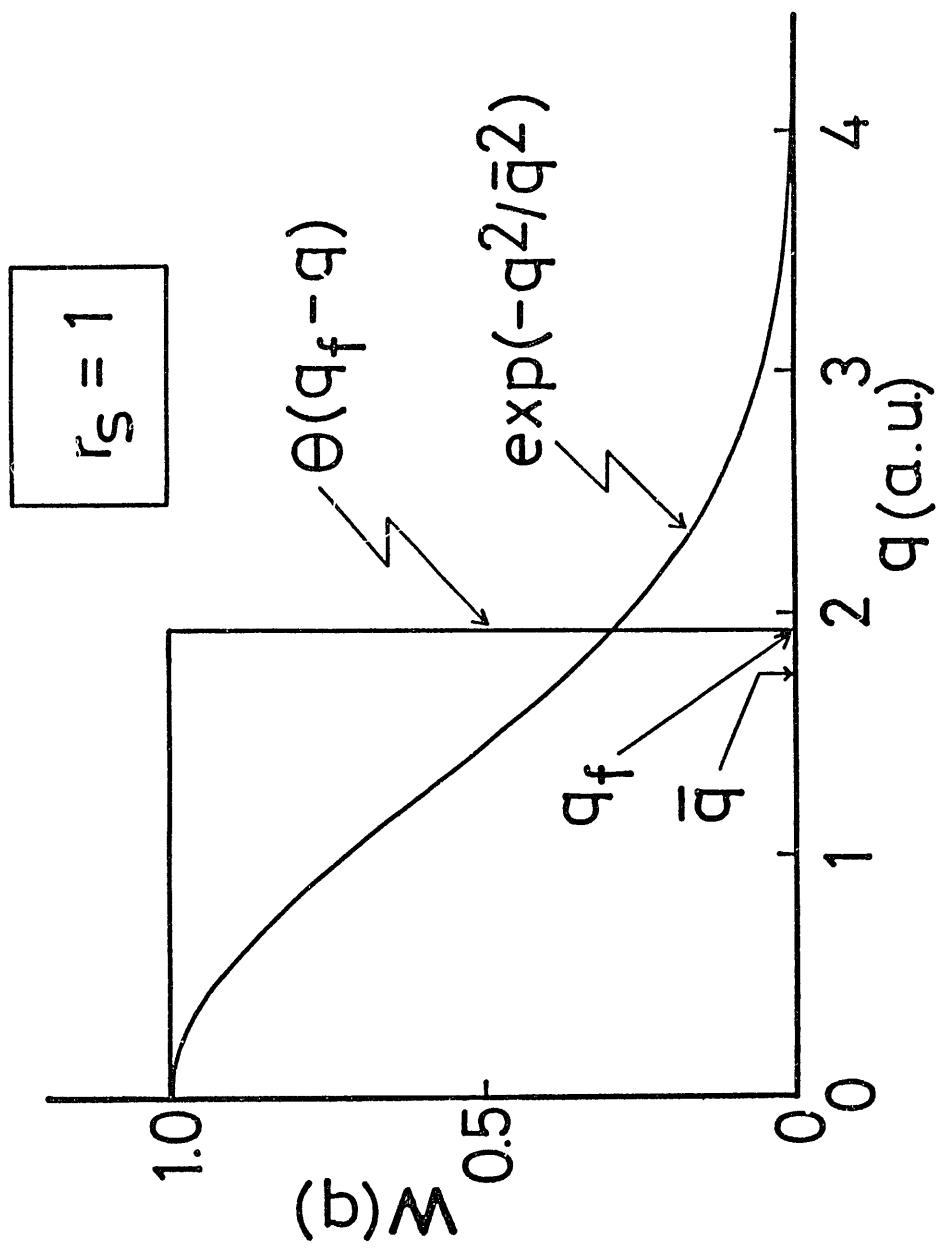
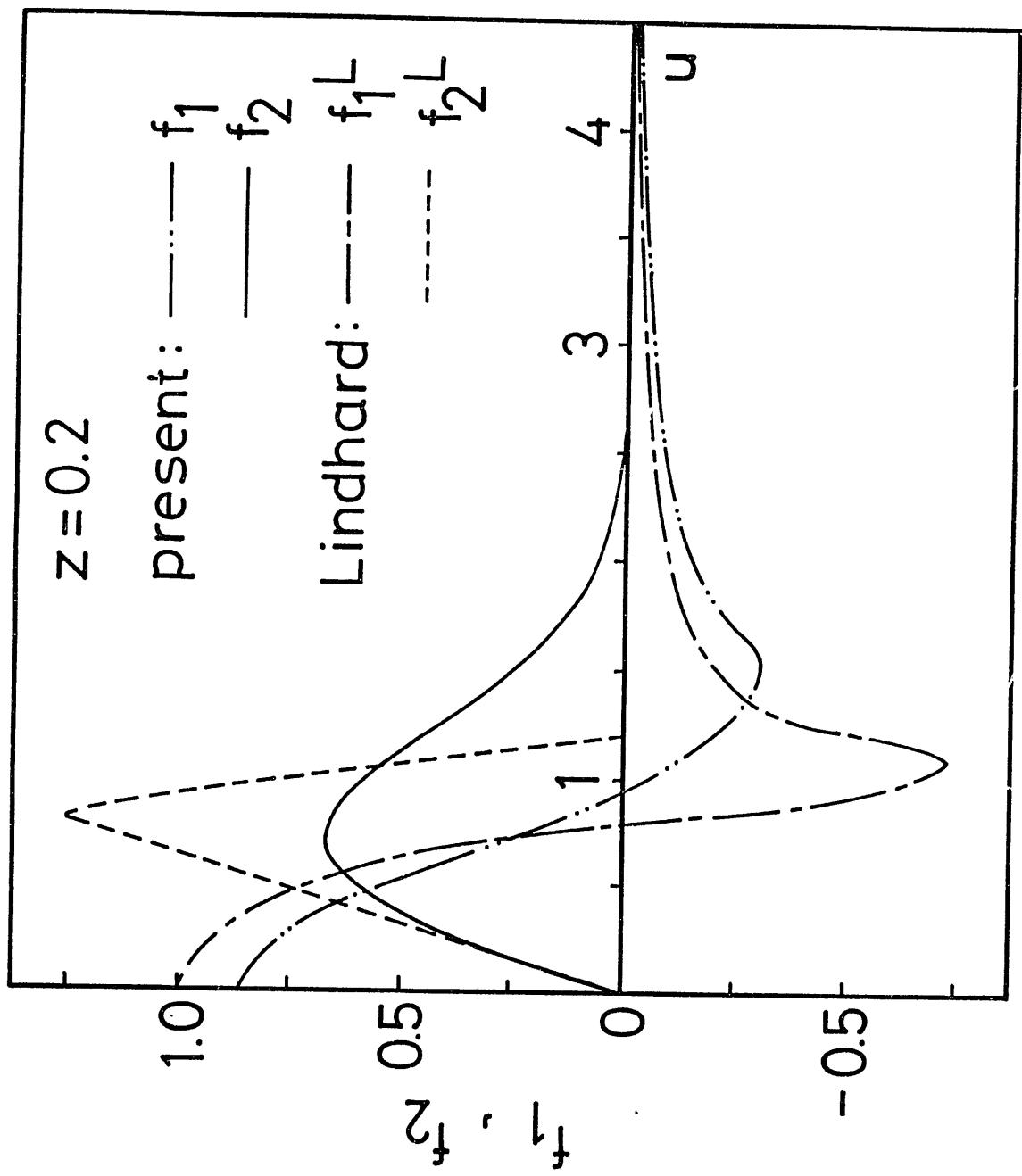


FIGURE 2



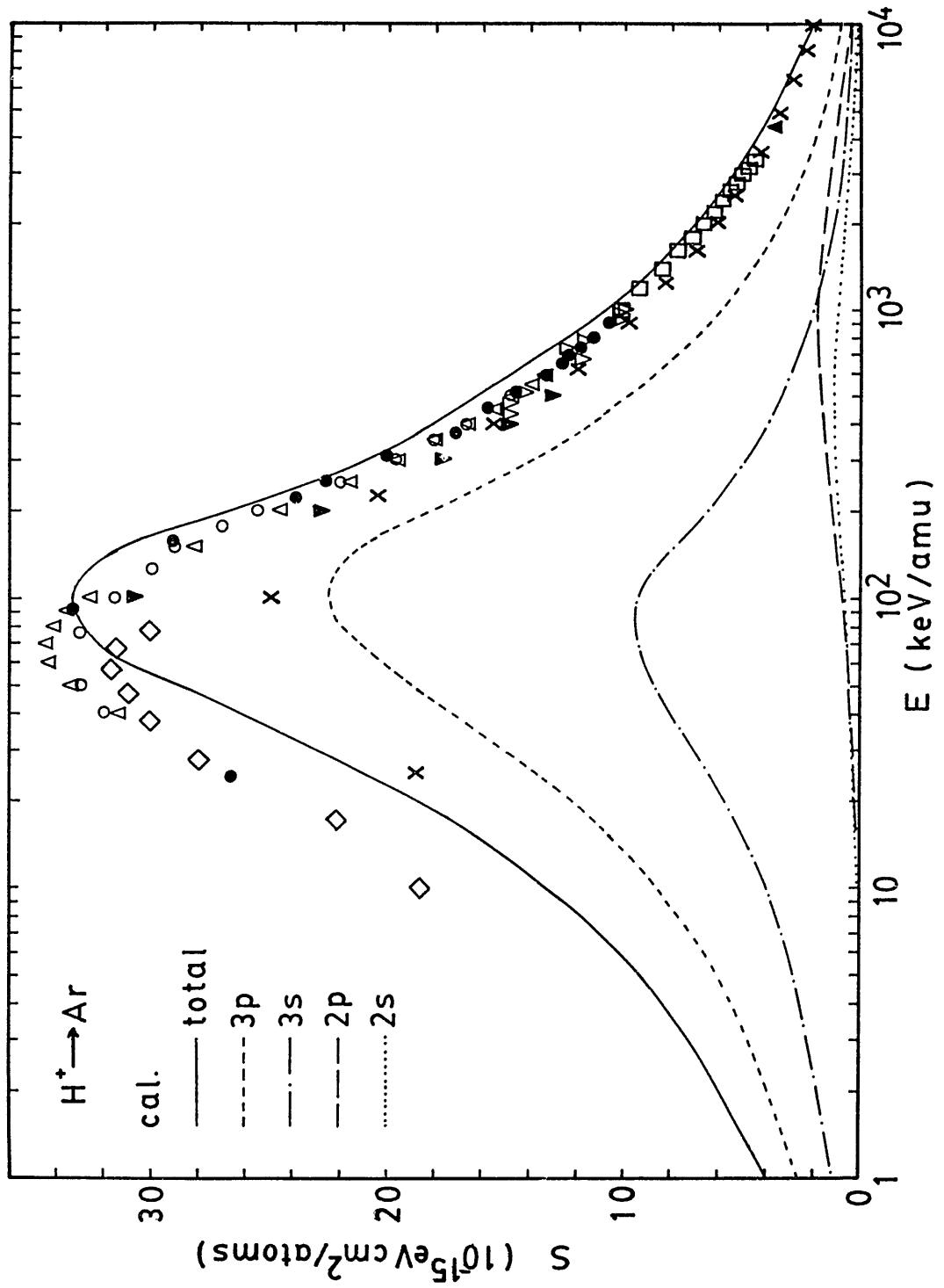


FIGURE 3

EXPLANATION OF TABLES

(1) Symbol of a target element.

(2) Electron state and the number N of electrons in the state.

(3) Parameter of the one-electron momentum distribution q_1 .

(4) Proton velocity v in atomic units (v_J).
 $v = 1$ (a.u.) corresponds to the kinetic energy $E = 25$ kev/amu.

(5) Stopping cross sections in $10^{-15} \text{ eV cm}^2 / \text{amu}$.

$\Rightarrow A1 \quad 1s(2)2s(2)2p(6)3s(2)3p(1)$

$\rightarrow q_1 \quad ---- \quad 7.276 \quad 1.713 \quad 1.625 \quad 0.4228 \quad 0.3202$

$\rightarrow v \quad \text{total} \quad 1s(2) \quad 2s(2) \quad 2p(6) \quad 3s(2) \quad 3p(1)$

0.2 12.72 0.00405 0.164 0.225 4.689 7.635

0.4 27.46 0.00812 0.328 0.450 9.709 16.96

0.6 42.63 0.0122 0.492 0.675 15.10 26.35

0.8 50.05 0.0162 0.655 0.898 20.29 28.19

1.0 48.97 0.0203 0.817 1.120 23.81 23.20

1.2 45.40 0.0243 0.977 1.340 24.30 18.76

1.4 40.56 0.0284 1.133 1.557 22.48 15.36

1.6 35.40 0.0324 1.287 1.771 19.50 12.81

1.8 31.10 0.0364 1.435 1.981 16.82 10.83

2.0 27.76 0.0404 1.576 2.186 14.68 9.280

2.2 25.17 0.0443 1.710 2.386 12.96 8.068

2.4 23.01 0.0483 1.831 2.578 11.49 7.059

2.6 21.26 0.0522 1.941 2.763 10.25 6.252

2.8 19.81 0.0561 2.037 2.938 9.211 5.563

3.0 18.60 0.0599 2.117 3.102 8.323 4.999

3.2 17.56 0.0638 2.179 3.255 7.560 4.498

3.4 17.00 0.0676 2.222 3.394 6.909 4.046

3.6 15.83 0.0713 2.247 3.519 6.331 3.659

3.8 15.11 0.0751 2.254 3.628 5.831 3.318

4.0 14.46 0.0788 2.244 3.721 5.391 3.029

5 11.84 0.0966 2.015 3.924 3.788 2.021

6 9.735 0.113 1.660 3.739 2.768 1.455

7 9.072 0.128 1.321 3.336 2.091 1.098

8 6.516 0.142 1.098 2.776 1.642 0.858

9 5.408 0.153 0.927 2.305 1.322 0.701

10 4.562 0.162 0.793 1.940 1.092 0.575

12 3.521 0.173 0.602 1.550 0.784 0.412

14 2.773 0.174 0.472 1.226 0.593 0.308

16 2.249 0.166 0.381 1.001 0.461 0.240

18 1.840 0.152 0.315 0.838 0.371 0.195

20 1.574 0.135 0.266 0.706 0.305 0.162

He 1s(2)						Li 1s(2)2s(1)						Be 1s(2)2s(2)					
q ₁	total	1s(2)	v	total	1s(1)	1s(2)	2s(1)	2s(2)	v	total	1s(2)	v	total	1s(2)	2s(1)	2s(2)	
0.2	0.704	0.704	0.2	1.590	0.206	1.384	0.6754	0.2	5.737	0.0967	5.640						
0.4	1.426	1.426	0.4	3.160	0.414	2.746	0.4	11.95	0.194	11.76							
0.6	2.150	2.150	0.6	4.830	0.621	4.209	0.6	18.68	0.291	18.39							
0.8	2.873	2.873	0.8	6.511	0.827	5.684	0.8	24.90	0.387	24.51							
1.0	3.588	3.588	1.0	8.043	1.032	7.011	1.0	28.29	0.482	27.81							
1.2	4.279	4.279	1.2	9.158	1.233	7.925	1.2	27.65	0.577	27.07							
1.4	4.921	4.921	1.4	9.632	1.431	8.201	1.4	24.98	0.670	24.31							
1.6	5.480	5.480	1.6	9.516	1.623	7.893	1.6	21.39	0.762	20.63							
1.8	5.918	5.918	1.8	9.060	1.806	7.254	1.8	18.65	0.852	17.80							
2.0	6.202	6.202	2.0	8.447	1.979	6.468	2.0	16.36	0.939	15.42							
2.2	6.313	6.313	2.2	7.840	2.139	5.701	2.2	14.60	1.023	13.58							
2.4	6.255	6.255	2.4	7.408	2.282	5.126	2.4	13.12	1.103	12.02							
2.6	6.052	6.052	2.6	6.993	2.404	4.589	2.6	11.91	1.179	10.73							
2.8	5.696	5.696	2.8	6.663	2.504	4.159	2.8	10.86	1.250	9.606							
3.0	5.232	5.232	3.0	6.302	2.579	3.723	3.0	9.977	1.315	8.662							
3.2	4.783	4.783	3.2	6.068	2.628	3.440	3.2	9.238	1.374	7.864							
3.4	4.376	4.376	3.4	5.796	2.651	3.145	3.4	8.608	1.426	7.182							
3.6	4.012	4.012	3.6	5.540	2.649	2.891	3.6	8.043	1.469	6.574							
3.8	3.750	3.750	3.8	5.301	2.624	2.677	3.8	7.552	1.505	6.047							
4.0	3.526	3.526	4.0	5.047	2.579	2.468	4.0	7.106	1.532	5.574							
5	2.618	2.618	5	3.951	2.186	1.762	5	5.434	1.544	3.890							
6	2.022	2.022	6	3.024	1.727	1.315	6	4.206	1.402	2.804							
7	1.610	1.610	7	2.423	1.402	1.021	7	3.317	1.188	2.129							
8	1.311	1.311	8	1.965	1.161	0.804	8	2.641	0.966	1.675							
9	1.093	1.093	9	1.619	0.972	0.647	9	2.151	0.797	1.354							
10	0.928	0.928	10	1.364	0.830	0.534	10	1.827	0.710	1.117							
12	0.689	0.689	12	1.011	0.628	0.383	12	1.335	0.544	0.791							
14	0.523	0.523	14	0.783	0.492	0.291	14	1.034	0.429	0.605							
16	0.410	0.410	16	0.621	0.395	0.226	16	0.813	0.350	0.463							
18	0.332	0.332	18	0.509	0.326	0.183	18	0.662	0.290	0.372							
20	0.274	0.274	20	0.423	0.273	0.150	20	0.565	0.245	0.320							

B 1s(2)2s(2)2p(1)

C 1s(2)2s(2)2p(2)						N 1s(2)2s(2)2p(3)											
q ₁	total	1s(2)	2s(2)	2p(1)	v	q ₁	total	1s(2)	2s(2)	2p(2)	v	q ₁	total	1s(2)	2s(2)	2p(3)	
0.2	6.424	0.0528	2.915	3.459	0.2	4.070	0.0324	1.745	2.293	0.2	2.936	0.0209	1.153	1.762			
0.4	16.15	0.105	5.951	7.285	0.4	8.308	0.0645	3.559	4.684	0.4	5.911	0.0417	2.321	3.548			
0.6	20.75	0.158	9.138	11.45	0.6	12.66	0.0962	5.412	7.156	0.6	8.934	0.0626	3.507	5.364			
0.8	27.57	0.211	12.34	15.02	0.8	17.07	0.127	7.285	9.656	0.8	11.98	0.0835	4.704	7.195			
1.0	31.63	0.263	15.17	16.20	1.0	21.22	0.160	9.084	11.98	1.0	14.98	0.104	5.880	8.992			
1.2	32.25	0.315	16.97	14.96	1.2	24.59	0.192	10.63	13.77	1.2	17.76	0.125	6.976	10.66			
1.4	30.28	0.366	17.31	12.60	1.4	26.54	0.223	11.69	14.63	1.4	20.13	0.145	7.905	12.08			
1.6	27.57	0.417	16.43	10.72	1.6	26.81	0.254	12.09	14.47	1.6	21.81	0.166	8.569	13.07			
1.8	24.77	0.467	15.07	9.232	1.8	25.71	0.285	11.83	13.59	1.8	22.61	0.186	8.892	13.53			
2.0	21.58	0.515	13.06	8.000	2.0	23.76	0.315	11.12	12.32	2.0	22.53	0.206	8.868	13.46			
2.2	19.18	0.563	11.61	7.010	2.2	21.12	0.344	10.08	10.70	2.2	21.77	0.225	8.566	12.98			
2.4	17.19	0.610	10.39	6.193	2.4	18.86	0.373	8.872	9.613	2.4	20.55	0.245	8.087	12.22			
2.6	15.50	0.655	9.342	5.500	2.6	17.08	0.401	7.995	8.680	2.6	19.12	0.264	7.523	11.35			
2.8	14.05	0.699	8.426	4.924	2.8	15.62	0.428	7.268	7.921	2.8	17.94	0.283	7.042	10.61			
3.0	12.81	0.740	7.630	4.444	3.0	14.30	0.454	6.647	7.196	3.0	16.25	0.301	6.344	9.603			
3.2	11.78	0.780	6.976	4.025	3.2	13.26	0.480	6.127	6.655	3.2	15.01	0.319	5.846	8.846			
3.4	10.85	0.817	6.369	3.662	3.4	12.19	0.504	5.650	6.034	3.4	13.90	0.337	5.414	8.147			
3.6	10.09	0.852	5.866	3.354	3.6	11.32	0.528	5.245	5.543	3.6	12.90	0.354	5.010	7.537			
3.8	9.373	0.884	5.406	3.083	3.8	10.51	0.550	4.812	5.151	3.8	12.00	0.370	4.633	7.002			
4.0	8.770	0.914	5.004	2.852	4.0	10.19	0.571	4.465	4.774	4.0	11.21	0.386	4.322	6.502			
5	6.525	1.010	3.553	1.962	5	7.299	0.653	3.252	3.394	5	8.263	0.456	3.118	4.689			
6	5.088	1.020	2.659	1.409	6	5.688	0.689	2.449	2.550	6	6.421	0.507	2.363	3.551			
7	4.068	0.960	2.048	1.060	7	4.600	0.675	1.924	2.001	7	5.190	0.535	1.856	2.799			
8	3.303	0.856	1.609	0.838	8	3.732	0.621	1.531	1.580	8	4.307	0.540	1.504	2.263			
9	2.696	0.726	1.299	0.671	9	3.102	0.551	1.265	1.286	9	2.638	0.525	1.242	1.871			
10	2.243	0.616	1.074	0.553	10	2.591	0.483	1.052	1.056	10	3.096	0.492	1.040	1.564			
12	1.643	0.476	0.768	0.399	12	1.855	0.370	0.740	0.754	12	2.268	0.395	0.749	1.124			
14	1.257	0.381	0.578	0.298	14	1.449	0.302	0.571	0.576	14	1.726	0.313	0.564	0.849			
16	0.999	0.313	0.454	0.232	16	1.135	0.252	0.437	0.446	16	1.364	0.259	0.442	0.663			
18	0.818	0.262	0.367	0.189	18	0.936	0.214	0.361	0.361	18	1.116	0.220	0.359	0.537			
20	0.681	0.223	0.303	0.155	20	0.773	0.184	0.291	0.298	20	0.928	0.188	0.297	0.443			

Ne 1s(2)2s(2)2p(6)									
0	1s(2)2s(2)2p(4)	q ₁	0.8894	0.7787	q ₁	-----	4.995	1.014	0.8776
v	total	1s(2)	2s(2)	2p(4)	v	total	1s(2)	2s(2)	2p(5)
0.2	2.107	0.0149	0.811	1.281	0.2	1.591	0.0109	0.585	0.995
0.4	4.232	0.0297	1.630	2.572	0.4	3.193	0.0217	1.181	1.990
0.6	6.369	0.0445	2.456	3.868	0.6	4.813	0.0325	1.779	3.001
0.8	8.509	0.0594	3.284	5.166	0.8	6.421	0.0432	2.376	4.001
1.0	10.63	0.0742	4.104	6.453	1.0	8.010	0.0538	2.965	4.991
1.2	12.68	0.0890	4.892	7.702	1.2	9.563	0.0642	3.539	5.960
1.4	14.59	0.104	5.611	8.875	1.4	11.05	0.0749	4.081	6.896
1.6	16.25	0.118	6.216	9.917	1.6	12.43	0.0856	4.570	7.776
1.8	17.56	0.133	6.658	10.77	1.8	13.65	0.0962	4.981	8.575
2.0	18.43	0.147	6.902	11.38	2.0	14.66	0.107	5.288	9.265
2.2	18.80	0.161	6.940	11.70	2.2	15.40	0.117	5.471	9.816
2.4	18.72	0.175	6.800	11.74	2.4	15.85	0.127	5.522	10.20
2.6	18.25	0.189	6.528	11.53	2.6	15.99	0.137	5.447	10.41
2.8	17.52	0.202	6.186	11.13	2.8	15.84	0.147	5.261	10.43
3.0	16.67	0.216	5.841	10.61	3.0	15.36	0.157	4.945	10.26
3.2	15.68	0.229	5.372	10.08	3.2	14.66	0.166	4.568	9.921
3.4	14.57	0.242	4.946	9.379	3.4	13.78	0.176	4.203	9.398
3.6	13.81	0.254	4.572	8.980	3.6	12.85	0.185	3.868	8.796
3.8	12.81	0.267	4.278	8.266	3.8	11.97	0.194	3.567	8.195
4.0	12.01	0.279	3.991	7.744	4.0	11.16	0.203	3.329	7.629
5	8.922	0.334	2.910	5.678	5	8.350	0.243	2.493	5.614
6	6.955	0.378	2.229	4.348	6	6.621	0.276	1.943	4.402
7	5.609	0.409	1.756	3.444	7	5.412	0.301	1.552	3.559
8	4.651	0.425	1.424	2.802	8	4.510	0.315	1.266	2.929
9	3.935	0.427	1.179	2.329	9	3.832	0.320	1.057	2.455
10	3.379	0.416	1.000	1.963	10	3.309	0.314	0.899	2.096
12	2.552	0.362	0.733	1.457	12	2.533	0.282	0.671	1.580
14	1.957	0.295	0.553	1.109	14	1.986	0.239	0.516	1.231
16	1.543	0.240	0.433	0.870	16	1.588	0.200	0.406	0.982
18	1.249	0.199	0.351	0.699	18	1.290	0.168	0.327	0.795
20	1.041	0.176	0.288	0.577	20	1.073	0.146	0.270	0.657

Na	1s(2)2s(2)2p(6)3s(1)	q ₁	-----	6.121	1.312	0.2617	1.205	q ₁	-----	6.689	1.518	1.420	0.3347
v	total	1s(2)	2s(2)	2p(6)	3s(1)	v	total	1s(2)	2s(2)	2s(2)	2p(6)	3s(2)	
0.2	13.04	0.00638	0.316	0.473	12.24	0.2	11.70	0.00505	0.221	0.315	8.062		
0.4	29.97	0.0128	0.634	0.950	28.37	0.4	18.20	0.0101	0.443	0.631	17.12		
0.6	42.41	0.0191	0.950	1.424	40.02	0.6	28.62	0.0152	0.664	0.946	26.99		
0.8	37.93	0.0255	1.266	1.896	34.74	0.8	36.88	0.0202	0.885	1.259	34.72		
1.0	30.68	0.0319	1.579	2.354	26.72	1.0	38.47	0.0253	1.103	1.570	35.77		
1.2	25.85	0.0382	1.888	2.826	21.10	1.2	35.37	0.0303	1.318	1.878	32.14		
1.4	22.60	0.0446	2.187	3.281	17.09	1.4	30.25	0.0354	1.529	2.182	26.50		
1.6	20.33	0.0509	2.474	3.725	14.08	1.6	26.71	0.0404	1.734	2.480	22.46		
1.8	18.80	0.0571	2.742	4.154	11.85	1.8	23.93	0.0453	1.929	2.771	19.18		
2.0	17.70	0.0634	2.982	4.565	10.09	2.0	21.82	0.0503	2.112	3.053	16.60		
2.2	16.94	0.0696	3.190	4.952	8.731	2.2	20.18	0.0552	2.279	3.324	14.52		
2.4	16.36	0.0757	3.357	5.310	7.616	2.4	18.84	0.0601	2.428	3.583	12.77		
2.6	15.89	0.0818	3.477	5.634	6.693	2.6	17.78	0.0650	2.553	3.826	11.34		
2.8	15.46	0.0878	3.549	5.917	5.903	2.8	16.91	0.0698	2.652	4.052	10.14		
3.0	15.03	0.0938	3.571	6.155	5.210	3.0	16.18	0.0746	2.723	4.257	9.130		
3.2	14.64	0.0997	3.548	6.344	4.646	3.2	15.56	0.0793	2.766	4.439	8.280		
3.4	14.23	0.1056	3.486	6.480	4.160	3.4	14.99	0.0840	2.779	4.596	7.535		
3.6	13.84	0.1111	3.393	6.564	3.768	3.6	14.47	0.0887	2.766	4.727	6.891		
3.8	13.39	0.1117	3.279	6.596	3.402	3.8	14.06	0.0933	2.730	4.829	6.407		
4.0	12.95	0.1223	3.146	6.578	3.101	4.0	13.50	0.0978	2.674	4.902	5.831		
5	10.67	0.150	2.493	5.953	2.076	5	11.16	0.120	2.231	4.859	3.951		
6	8.548	0.174	1.938	4.944	1.492	6	9.085	0.140	1.763	4.342	2.840		
7	6.805	0.195	1.553	3.940	1.117	7	7.362	0.157	1.425	3.622	2.158		
8	5.626	0.212	1.270	3.257	0.887	8	5.969	0.173	1.177	2.932	1.687		
9	4.754	0.226	1.064	2.753	0.711	9	4.939	0.185	0.986	2.416	1.352		
10	4.077	0.234	0.900	2.354	0.589	10	4.324	0.195	0.840	2.169	1.120		
12	3.119	0.238	0.676	1.789	0.416	12	3.295	0.203	0.632	1.657	0.803		
14	2.471	0.226	0.527	1.404	0.314	14	2.618	0.199	0.497	1.307	0.615		
16	2.005	0.201	0.421	1.138	0.245	16	2.125	0.184	0.400	1.063	0.478		
18	1.656	0.173	0.344	0.942	0.197	18	1.753	0.163	0.330	0.882	0.378		
20	3.102	0.149	0.283	0.852	0.162	20	1.481	0.142	0.275	0.747	0.317		

A1 1s(2)2s(2)2p(6)3s(2)3p(1)

Si 1s(2)2s(2)2p(6)3s(2)3p(2)

<u>q₁</u>	<u>--</u>	<u>7.276</u>	<u>1.713</u>	<u>1.625</u>	<u>0.4228</u>	<u>0.3202</u>	<u>q₁</u>	<u>-----</u>	<u>7.988</u>	<u>1.890</u>	<u>1.797</u>	<u>0.5014</u>	<u>0.3833</u>
<u>v</u>	<u>total</u>	<u>1s(2)</u>	<u>2s(2)</u>	<u>2p(6)</u>	<u>3s(2)</u>	<u>3p(1)</u>	<u>v</u>	<u>total</u>	<u>1s(2)</u>	<u>2s(2)</u>	<u>2p(6)</u>	<u>3s(2)</u>	<u>3p(2)</u>
0.2	12.72	0.00405	0.164	0.225	4.689	7.635	0.2	9.345	0.00317	0.128	0.174	3.152	5.883
0.4	27.46	0.00812	0.328	0.450	0.675	15.10	0.4	19.37	0.00635	0.257	0.349	6.446	12.31
0.6	42.63	0.0122	0.492	0.655	0.898	20.29	0.6	30.09	0.00952	0.385	0.523	9.917	19.26
0.8	50.05	0.0162	0.817	1.120	23.81	23.20	0.8	40.23	0.0127	0.513	0.697	13.40	25.61
1.0	48.97	0.0203	0.817	1.120	24.30	18.76	1.0	46.69	0.0158	0.640	0.870	16.39	28.77
1.2	45.40	0.0243	0.977	1.340	22.48	15.36	1.2	47.64	0.0190	0.765	1.040	18.13	27.69
1.4	40.56	0.0284	1.133	1.557	19.50	12.81	1.4	45.20	0.0222	0.888	1.210	18.20	24.88
1.6	35.40	0.0324	1.287	1.771	11.49	7.059	1.6	40.36	0.0253	1.009	1.376	17.03	20.92
1.8	31.10	0.0364	1.435	1.981	16.82	10.83	1.8	36.27	0.0285	1.126	1.541	15.49	18.08
2.0	27.76	0.0404	1.576	2.186	14.68	9.280	2.0	32.09	0.0316	1.240	1.702	13.40	15.72
2.2	25.17	0.0443	1.710	2.386	12.96	8.068	2.2	28.88	0.0347	1.348	1.859	11.86	13.78
2.4	23.01	0.0483	1.831	2.578	11.49	7.059	2.4	26.27	0.0378	1.449	2.012	10.60	12.17
2.6	21.26	0.0522	1.941	2.763	10.25	6.252	2.6	24.11	0.0409	1.544	2.160	9.521	10.84
2.8	19.31	0.0561	2.037	2.938	9.21	5.563	2.8	22.26	0.0439	1.629	2.301	8.585	9.693
3.0	13.50	0.0599	2.117	3.102	8.32	4.999	3.0	20.75	0.0470	1.704	2.437	7.796	8.765
3.2	17.56	0.0638	2.179	3.255	7.560	4.198	3.2	19.11	0.0500	1.768	2.565	7.097	7.932
3.4	16.64	0.0676	2.222	3.394	6.909	4.046	3.4	18.28	0.0530	1.820	2.685	6.477	7.242
3.6	15.83	0.0713	2.247	3.519	6.331	3.659	3.6	17.30	0.0560	1.859	2.795	5.962	6.629
3.8	15.11	0.0751	2.254	3.628	5.831	3.318	3.8	16.43	0.0583	1.886	2.896	5.494	6.098
4.0	14.16	0.0788	2.244	3.721	5.391	3.029	4.0	15.65	0.0619	1.899	2.987	5.084	5.619
5	11.84	0.0966	2.015	3.924	3.788	2.021	5	12.64	0.0760	1.803	3.265	3.597	3.902
6	9.735	0.113	1.660	3.739	2.768	1.155	6	10.41	0.0894	1.565	3.249	2.687	2.822
7	9.072	0.128	1.321	3.336	2.091	1.028	7	8.550	0.102	1.250	3.011	2.063	2.124
8	6.516	0.142	1.098	2.776	1.642	0.858	8	7.068	0.113	1.034	2.634	1.62	1.657
9	5.408	0.153	0.927	2.205	1.32	0.701	9	5.875	0.123	0.875	2.214	1.311	1.551
10	4.562	0.162	0.793	1.940	1.092	0.575	10	4.961	0.131	0.756	1.881	1.082	1.111
12	3.521	0.173	0.602	1.550	0.784	0.412	12	3.749	0.143	0.573	1.457	0.775	0.201
14	2.773	0.174	0.472	1.226	0.593	0.308	14	2.960	0.147	0.453	1.174	0.587	0.549
16	2.249	0.166	0.381	1.001	0.461	0.240	16	2.573	0.145	0.366	1.061	0.497	0.504
18	1.840	0.152	0.315	0.838	0.371	0.196	18	1.979	0.137	0.303	0.800	0.367	0.372
20	1.574	0.135	0.266	0.706	0.305	0.162	20	1.679	0.125	0.257	0.680	0.301	0.316

C1 1s(2)2s(2)3s(2)2P(6)3P(5)
Ar 1s(2)2s(2)3s(2)2P(6)3p(6)

q ₁	-----	9.665	2.443	0.720	2.440	0.576	q ₁	-----	10.37	2.610	0.7869	2.635	0.6231
v	total	1s(2)	2s(2)	3s(2)	2P(6)	3P(5)	v	total	1s(2)	2s(2)	3s(2)	2p(6)	3p(6)
0.2	4.184	0.00193	0.0676	1.326	0.0804	2.708	0.2	3.586	0.00158	0.0571	1.088	0.0658	2.374
0.4	8.546	0.00386	0.134	2.707	0.160	5.541	0.4	7.208	0.00318	0.114	2.189	0.132	4.770
0.6	12.92	0.00578	0.199	4.101	0.239	8.376	0.6	10.86	0.00477	0.171	3.306	0.197	7.183
0.8	17.33	0.00770	0.267	5.506	0.317	11.23	0.8	14.54	0.00636	0.228	4.432	0.263	9.606
1.0	21.65	0.00961	0.334	6.880	0.396	14.03	1.0	18.16	0.00794	0.285	5.540	0.329	12.00
1.2	25.68	0.0115	0.400	8.134	0.476	16.66	1.2	21.63	0.00952	0.341	6.580	0.394	14.31
1.4	29.10	0.0134	0.465	9.143	0.554	18.92	1.4	24.76	0.0111	0.396	7.476	0.458	16.42
1.6	31.54	0.0153	0.529	9.775	0.631	20.59	1.6	27.34	0.0127	0.451	8.141	0.522	18.21
1.8	32.74	0.0172	0.591	9.953	0.708	21.47	1.8	29.15	0.0143	0.505	8.501	0.586	19.54
2.0	32.68	0.0190	0.652	9.714	0.782	21.51	2.0	30.06	0.0159	0.557	8.539	0.648	20.30
2.2	31.61	0.0209	0.711	9.191	0.856	20.83	2.2	30.11	0.0174	0.609	8.305	0.710	20.47
2.4	29.70	0.0227	0.768	8.346	0.928	19.64	2.4	29.44	0.0190	0.659	7.892	0.771	20.10
2.6	27.07	0.0246	0.823	7.441	0.999	17.78	2.6	28.30	0.0206	0.708	7.392	0.831	19.35
2.8	24.62	0.0265	0.875	6.670	1.068	15.98	2.8	26.98	0.0221	0.754	6.934	0.890	18.38
3.0	22.61	0.0283	0.923	6.128	1.135	14.40	3.0	25.39	0.0237	0.799	6.259	0.948	17.36
3.2	21.16	0.0302	0.969	5.657	1.200	13.30	3.2	23.65	0.0252	0.841	5.758	1.004	16.02
3.4	19.82	0.0320	1.011	5.219	1.262	12.30	3.4	22.20	0.0267	0.880	5.308	1.059	14.93
3.6	18.73	0.0338	1.048	4.837	1.323	11.49	3.6	20.76	0.0282	0.917	4.915	1.113	13.79
3.8	17.66	0.0356	1.081	4.500	1.380	10.66	3.8	19.52	0.0298	0.950	4.570	1.164	12.81
4.0	16.74	0.0374	1.110	4.184	1.435	9.970	4.0	18.48	0.0313	0.980	4.245	1.214	12.01
5	13.17	0.0461	1.166	3.032	1.662	7.261	5	14.41	0.0386	1.074	3.081	1.432	8.789
6	10.76	0.0543	1.080	2.304	1.789	5.535	6	11.76	0.0457	1.072	2.336	1.586	6.724
7	8.982	0.0619	0.923	1.813	1.802	4.382	7	9.841	0.0525	0.996	1.836	1.667	5.289
8	7.575	0.0689	0.772	1.473	1.708	3.553	6	8.366	0.0589	0.874	1.489	1.674	4.270
9	6.441	0.0752	0.649	1.213	1.553	2.951	9	7.203	0.0648	0.736	1.231	1.616	3.555
10	5.513	0.0808	0.5645	1.0091	1.381	2.477	10	6.259	0.0702	0.626	1.031	1.504	3.028
12	4.122	0.0895	0.4423	0.7260	1.076	1.788	12	4.744	0.3794	0.485	0.746	1.198	2.236
14	3.215	0.0947	0.3569	0.5478	0.864	1.351	14	3.664	0.3862	0.388	0.565	0.945	1.680
16	2.603	0.0964	0.2942	0.4299	0.723	1.060	16	2.942	0.3902	0.318	0.441	0.781	1.312
18	2.158	0.0949	0.2462	0.3459	0.617	0.854	18	2.423	0.3916	0.266	0.354	0.663	1.048
20	1.821	0.0909	0.2099	0.2858	0.530	0.704	20	2.062	0.3903	0.226	0.292	0.568	0.886

<u>K</u>	Ca 1s(2)2s(2)3s(2)2p(6)3p(6)4s(1)						Ca 1s(2)2s(2)3s(2)2p(6)3p(6)4s(2)								
q ₁	-----	10.75	2.813	0.8905	2.8678	0.7610	0.2185	q ₁	-----	11.35	2.997	0.9972	0.2707	3.071	0.8695
v	total	1s(2)	2s(2)	3s(2)	2p(6)	3p(6)	4s(1)	v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)
0.2	21.19	0.00144	0.0472	0.809	0.0529	1.465	18.81	0.2	14.95	0.00125	0.0402	0.616	13.19	0.0444	1.058
0.4	49.84	0.00289	0.0944	1.625	0.106	2.939	45.07	0.4	32.48	0.00250	0.0803	1.236	28.95	0.0887	2.123
0.6	59.41	0.00434	0.142	2.448	0.159	4.414	52.24	0.6	50.74	0.00376	0.121	1.859	45.44	0.133	3.186
0.8	48.50	0.00589	0.189	3.274	0.212	5.888	38.93	0.8	58.56	0.00501	0.161	2.482	51.49	0.177	4.245
1.0	41.52	0.00723	0.234	4.092	0.264	7.350	29.57	1.0	54.78	0.00625	0.201	3.100	45.95	0.222	5.296
1.2	37.26	0.00867	0.282	4.887	0.317	8.780	22.99	1.2	47.32	0.00750	0.240	3.701	36.78	0.266	6.329
1.4	34.97	0.0101	0.328	5.595	0.369	10.15	18.52	1.4	42.43	0.00874	0.280	4.267	30.23	0.309	7.331
1.6	33.55	0.0116	0.373	6.199	0.420	11.41	15.14	1.6	38.99	0.00999	0.318	4.773	25.25	0.353	8.282
1.8	32.74	0.0130	0.418	6.641	0.472	12.53	12.67	1.8	36.48	0.0112	0.357	5.193	21.36	0.396	9.160
2.0	32.12	0.0144	0.462	6.886	0.522	13.43	10.81	2.0	34.58	0.0125	0.394	5.500	18.30	0.438	9.937
2.2	31.36	0.0159	0.505	6.924	0.572	14.09	9.253	2.2	33.09	0.0137	0.431	5.674	15.90	0.481	10.59
2.4	30.38	0.0173	0.547	6.787	0.622	14.46	7.951	2.4	31.77	0.0150	0.467	5.713	13.96	0.522	11.09
2.6	29.29	0.0187	0.588	6.519	0.671	14.55	6.924	2.6	30.48	0.0162	0.503	5.631	12.36	0.563	11.41
2.8	27.94	0.0201	0.628	6.179	0.719	14.38	6.012	2.8	29.21	0.0174	0.537	5.455	11.03	0.604	11.57
3.0	26.61	0.0215	0.666	5.835	0.766	14.00	5.320	3.0	27.92	0.0186	0.570	5.220	9.915	0.644	11.55
3.2	25.10	0.0229	0.702	5.368	0.812	13.48	4.713	3.2	26.59	0.0199	0.602	4.960	8.944	0.683	11.38
3.4	23.70	0.0243	0.736	4.940	0.857	12.89	4.255	3.4	25.20	0.0211	0.632	4.636	8.088	0.722	11.10
3.6	22.29	0.0257	0.769	4.567	0.901	12.17	3.857	3.6	23.97	0.0223	0.661	4.445	7.349	0.760	10.73
3.8	21.19	0.0271	0.799	4.140	0.944	11.80	3.483	3.8	22.58	0.0235	0.689	4.092	6.671	0.796	10.31
4.0	19.82	0.0285	0.827	3.987	0.986	10.85	3.146	4.0	21.30	0.0247	0.714	3.824	6.065	0.832	9.837
5	14.79	0.0352	0.925	2.908	1.173	7.612	2.133	5	16.38	0.0305	0.811	2.807	4.049	0.996	7.682
6	11.61	0.0417	0.950	2.227	1.317	5.579	1.497	6	13.06	0.0362	0.850	2.152	2.934	1.128	5.960
7	10.13	0.0479	0.909	1.755	1.408	4.880	1.130	7	10.75	0.0416	0.833	1.705	2.188	1.221	4.765
8	8.620	0.0538	0.826	1.422	1.444	3.982	0.892	8	9.110	0.0468	0.775	1.387	1.726	1.270	3.905
9	7.406	0.0593	0.710	1.178	1.428	3.316	0.715	9	7.821	0.0517	0.685	1.154	1.406	1.277	3.247
10	6.460	0.0644	0.605	0.999	1.366	2.814	0.612	10	6.773	0.0562	0.588	0.974	1.145	1.246	2.764
12	4.928	0.0731	0.465	0.733	1.141	2.096	0.420	12	5.189	0.0641	0.447	0.725	0.808	1.085	2.060
14	3.861	0.0796	0.373	0.552	0.913	1.625	0.318	14	4.093	0.0704	0.360	0.554	0.620	0.885	1.604
16	3.092	0.0839	0.306	0.433	0.739	1.279	0.251	16	3.293	0.0747	0.298	0.434	0.477	0.721	1.288
18	2.560	0.0857	0.258	0.633	1.033	0.200	18	2.724	0.0771	0.250	0.352	0.401	0.606	1.038	2.056
20	2.151	0.0852	0.219	0.852	0.543	0.164	20	2.288	0.0776	0.213	0.290	0.324	0.527	0.856	0.

Sc 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)3d(1)

Ti 1s(2)2s(2)3s(2)2p(6)3p(6)3d(2)4s(2)

q ₁	----	11.96	3.181	1.071	0.2859	3.273	0.9463	0.6286	q ₁	----	12.54	3.364	1.140	0.2973	3.473	1.010	0.718
v	total	1s (2)	2s (2)	3s (2)	4s (2)	2p (6)	3p (6)	3d (1)	v	total	1s (2)	2s (2)	3s (2)	4s (2)	2p (6)	3p (6)	3d (2)
0.2	14.67	0.00108	0.0346	0.518	11.62	0.0376	0.866	1.594	0.2	13.20	0.000954	0.0300	0.445	10.61	0.0323	0.732	1.355
0.4	31.43	0.00218	0.0690	1.040	25.26	0.0753	1.725	3.261	0.4	28.14	0.00192	0.0598	0.893	22.92	0.0645	1.470	2.732
0.6	49.22	0.00327	0.104	1.562	39.83	0.113	2.588	5.019	0.6	44.07	0.00288	0.0899	1.341	36.20	0.0966	2.204	4.136
0.8	59.71	0.00436	0.138	2.084	47.11	0.150	3.447	6.780	0.8	54.49	0.00384	0.120	1.788	43.96	0.129	2.935	5.555
1.0	58.58	0.00544	0.173	2.602	43.03	0.188	4.299	8.287	1.0	54.60	0.00480	0.150	2.232	41.45	0.161	3.661	6.941
1.2	52.95	0.00652	0.207	3.108	35.13	0.225	5.138	9.152	1.2	49.66	0.00575	0.179	2.667	34.04	0.193	4.376	8.203
1.4	48.23	0.00760	0.240	3.590	29.01	0.262	5.956	9.167	1.4	45.99	0.00671	0.208	3.084	28.18	0.225	5.075	9.213
1.6	44.22	0.00869	0.274	4.033	24.31	0.299	6.742	8.561	1.6	43.33	0.00766	0.237	3.474	23.77	0.257	5.750	9.839
1.8	40.98	0.00977	0.307	4.417	20.66	0.336	7.480	7.772	1.8	40.99	0.00862	0.266	3.823	20.21	0.288	6.391	10.01
2.0	38.08	0.0109	0.339	4.724	17.76	0.372	8.155	6.716	2.0	38.89	0.00957	0.294	4.116	17.40	0.319	6.987	9.774
2.2	35.88	0.0119	0.371	4.936	15.44	0.408	8.748	5.968	2.2	36.97	0.0105	0.322	4.339	15.15	0.350	7.526	9.272
2.4	34.01	0.0130	0.402	5.043	13.56	0.444	9.241	5.311	2.4	35.24	0.0115	0.350	4.483	13.35	0.381	7.992	8.669
- 2.6	32.38	0.0141	0.433	5.049	12.02	0.479	9.619	4.768	2.6	33.55	0.0124	0.377	4.543	11.79	0.411	8.375	8.038
2.8	30.86	0.0152	0.463	4.965	10.73	0.514	9.871	4.300	2.8	31.90	0.0134	0.403	4.524	10.56	0.441	8.664	7.295
3.0	29.42	0.0162	0.492	4.812	9.649	0.548	9.995	3.905	3.0	30.36	0.0143	0.428	4.439	9.478	0.471	8.852	6.678
3.2	27.99	0.0173	0.520	4.612	8.711	0.581	9.995	3.555	3.2	28.95	0.0152	0.453	4.302	8.600	0.500	8.940	6.139
3.4	26.63	0.0183	0.547	4.400	7.911	0.615	9.884	3.255	3.4	27.52	0.0162	0.477	4.128	7.798	0.529	8.931	5.644
3.6	25.24	0.0194	0.573	4.136	7.201	0.647	9.680	2.985	3.6	26.18	0.0171	0.500	3.940	7.123	0.557	8.835	5.211
3.8	23.97	0.0204	0.598	3.950	6.565	0.679	9.404	2.751	3.8	24.89	0.0180	0.522	3.749	6.505	0.585	8.667	4.842
4.0	22.64	0.0215	0.621	3.656	6.001	0.710	9.084	2.547	4.0	23.61	0.0190	0.543	3.547	5.959	0.612	8.441	4.491
5	17.44	0.0266	0.713	2.694	4.007	0.854	7.346	1.805	5	18.20	0.0235	0.630	2.595	3.988	0.739	7.004	3.225
6	13.72	0.0136	0.760	2.073	2.893	0.973	5.656	1.349	6	14.30	0.0279	0.681	2.003	2.856	0.847	5.447	2.439
7	11.27	0.0364	0.761	1.646	2.184	1.063	4.543	1.032	7	11.72	0.0322	0.694	1.602	2.162	0.932	4.388	1.913
8	9.479	0.0409	0.723	1.342	1.702	1.120	3.740	0.811	8	9.861	0.0363	0.672	1.309	1.700	0.991	3.601	1.552
9	8.105	0.0453	0.656	1.118	1.368	1.142	3.121	0.655	9	8.448	0.0401	0.623	1.091	1.375	1.022	3.027	1.270
10	7.027	0.0493	0.571	0.948	1.131	1.131	2.656	0.541	10	7.312	0.0438	0.553	0.922	1.132	1.026	2.577	1.058
12	5.422	0.0565	0.431	0.705	0.825	1.024	1.991	0.389	12	5.621	0.0504	0.422	0.690	0.804	0.959	1.937	0.759
14	4.268	0.0624	0.350	0.545	0.608	0.854	1.555	0.294	14	4.453	0.0558	0.337	0.536	0.612	0.822	1.514	0.576
16	3.443	0.0667	0.288	0.429	0.479	0.702	1.249	0.229	16	3.589	0.0600	0.278	0.424	0.481	0.683	1.218	0.445
18	2.830	0.0694	0.243	0.345	0.381	0.586	1.022	0.184	18	2.959	0.0629	0.236	0.341	0.383	0.570	1.003	0.363
20	2.379	0.0705	0.207	0.285	0.316	0.505	0.844	0.151	20	2.485	0.0644	0.201	0.282	0.315	0.490	0.831	0.302

V 1s(2)2s(2)3s(2)2p(6)3p(6)3d(3)4s(2)

q, v	---	13.15	3.546	1.207	0.3078	3.673	1.075	0.7885
	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(3)
0.2	12.03	0.000840	0.0262	0.387	9.789	0.0279	0.627	1.175
0.4	25.54	0.00169	0.0523	0.777	21.04	0.0558	1.260	2.360
0.6	40.00	0.00254	0.0786	1.166	33.23	0.0836	1.890	3.554
0.8	50.22	0.00338	0.105	1.554	41.18	0.112	2.516	4.752
1.0	51.11	0.00423	0.131	1.940	39.82	0.139	3.137	5.938
1.2	47.08	0.00507	0.157	2.318	33.61	0.167	3.750	7.079
1.4	43.56	0.00591	0.182	2.683	28.02	0.195	4.351	8.127
1.6	40.88	0.00675	0.208	3.028	23.47	0.222	4.934	9.017
1.8	39.20	0.00759	0.233	3.343	20.20	0.249	5.492	9.682
2.0	37.56	0.00843	0.258	3.617	17.32	0.277	6.018	10.07
2.2	36.09	0.00927	0.282	3.839	15.00	0.303	6.501	10.16
2.4	34.87	0.0101	0.306	4.000	13.30	0.330	6.933	9.991
2.6	33.41	0.0110	0.330	4.094	11.69	0.356	7.303	9.626
2.8	32.09	0.0118	0.353	4.121	10.47	0.382	7.602	9.150
3.0	30.84	0.0126	0.376	4.087	9.494	0.408	7.825	8.640
3.2	29.34	0.0134	0.398	4.001	8.540	0.434	7.968	7.989
3.4	28.13	0.0143	0.419	3.877	7.813	0.459	8.031	7.515
3.6	26.67	0.0151	0.440	3.729	7.082	0.483	8.018	6.904
3.8	25.42	0.0159	0.460	3.554	6.540	0.508	7.936	6.407
4.0	22.91	0.0167	0.479	3.412	4.706	0.531	7.796	5.971
5	18.68	0.0207	0.560	2.527	3.975	0.644	6.584	4.369
6	14.80	0.0247	0.612	1.961	2.903	0.741	5.210	3.343
7	12.04	0.0284	0.632	1.563	2.154	0.820	4.216	2.623
8	10.12	0.0321	0.622	1.277	1.688	0.879	3.489	2.128
9	8.668	0.0356	0.588	1.072	1.365	0.916	2.920	1.771
10	7.524	0.0389	0.533	0.906	1.121	0.929	2.491	1.505
12	5.856	0.0448	0.413	0.678	0.833	0.893	1.885	1.109
14	4.615	0.0499	0.325	0.530	0.610	0.787	1.476	0.837
16	3.729	0.0539	0.271	0.422	0.475	0.664	1.189	0.654
18	3.071	0.0569	0.230	0.342	0.380	0.557	0.981	0.524
20	2.587	0.0587	0.197	0.281	0.314	0.472	0.823	0.441

Cr 1s(2)2s(2)3s(2)2p(6)3p(6)3d(4)4s(2)

q ₁	-----	13.77	3.728	1.273	0.3175	3.872	1.139	0.8529
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(4)
0.2	11.07	0.000742	0.0230	0.340	9.110	0.0243	0.544	1.028
0.4	23.42	0.00149	0.0460	0.682	19.49	0.0487	1.092	2.062
0.6	36.67	0.00224	0.0691	1.024	30.77	0.0729	1.638	3.099
0.8	46.60	0.00299	0.0921	1.364	38.73	0.0972	2.181	4.134
1.0	48.17	0.00374	0.115	1.701	38.35	0.122	2.719	5.161
1.2	45.26	0.00448	0.138	2.033	33.53	0.146	3.250	6.165
1.4	41.29	0.00522	0.160	2.355	27.71	0.170	3.772	7.122
1.6	38.63	0.00596	0.183	2.662	23.31	0.194	4.280	8.002
1.8	36.78	0.00670	0.205	2.946	19.87	0.218	4.769	8.757
2.0	35.41	0.00745	0.227	3.199	17.13	0.241	5.234	9.379
2.2	34.33	0.00819	0.249	3.413	14.93	0.265	5.667	9.805
2.4	33.39	0.00894	0.270	3.580	13.16	0.288	6.062	10.03
2.6	32.42	0.00968	0.291	3.694	11.67	0.311	6.411	10.04
2.8	31.44	0.0104	0.311	3.752	10.44	0.334	6.707	9.884
3.0	30.37	0.0112	0.331	3.757	9.383	0.356	6.944	9.586
3.2	29.24	0.0119	0.351	3.713	8.474	0.379	7.117	9.193
3.4	28.15	0.0126	0.370	3.630	7.737	0.401	7.226	8.773
3.6	26.91	0.0133	0.389	3.516	7.045	0.423	7.270	8.249
3.8	25.87	0.0141	0.407	3.386	6.479	0.444	7.253	7.884
4.0	24.56	0.0148	0.424	3.232	5.942	0.465	7.181	7.303
5	19.30	0.0184	0.499	2.545	3.998	0.565	6.295	5.382
6	15.29	0.0218	0.551	1.979	2.871	0.652	5.073	4.140
7	12.45	0.0252	0.576	1.577	2.180	0.726	4.078	3.288
8	10.46	0.0285	0.576	1.288	1.721	0.783	3.382	2.662
9	8.929	0.0316	0.553	1.078	1.376	0.822	2.836	2.232
10	7.751	0.0345	0.511	0.914	1.133	0.842	2.422	1.894
12	6.009	0.0400	0.403	0.681	0.811	0.828	1.836	1.410
14	4.771	0.0447	0.317	0.531	0.600	0.750	1.439	1.089
16	3.605	0.0485	0.265	0.425	0.469	0.644	1.166	0.587
18	3.205	0.0514	0.224	0.346	0.391	0.544	0.960	0.689
20	2.682	0.0534	0.192	0.286	0.312	0.463	0.808	0.568

Mn 1s(2) 2s(2) 3s(2) 4s(2) 2p(6) 3p(6) 3d(5)

q_1	---	14.38	3.908	1.339	0.326	4.070	1.201	0.918
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(5)
0.2	12.17	0.000659	0.0204	0.301	8.551	0.0213	0.477	0.897
0.4	25.56	0.00133	0.0408	0.603	18.22	0.0427	0.958	1.799
0.6	29.88	0.00199	0.0612	0.905	28.75	0.0640	1.436	2.700
0.8	51.63	0.00266	0.0816	1.205	36.62	0.0853	1.912	3.597
1.0	55.96	0.00332	0.102	1.503	37.03	0.107	2.384	4.488
1.2	56.26	0.00399	0.122	1.797	32.93	0.128	2.850	5.364
1.4	53.40	0.00465	0.142	2.082	27.04	0.149	3.309	6.212
1.6	49.81	0.00531	0.162	2.356	22.87	0.170	3.756	7.017
1.8	44.46	0.00596	0.182	2.612	19.50	0.191	4.189	7.758
2.0	44.26	0.00663	0.201	2.845	16.87	0.212	4.603	8.413
2.2	42.22	0.00729	0.220	3.048	14.70	0.233	4.993	8.957
2.4	40.53	0.00795	0.239	3.214	12.96	0.253	5.353	9.371
2.6	39.02	0.00861	0.258	3.338	11.51	0.273	5.678	9.638
2.8	37.58	0.00926	0.276	3.416	10.28	0.294	5.962	9.755
3.0	36.21	0.00992	0.294	3.449	9.253	0.313	6.201	9.730
3.2	34.83	0.0106	0.312	3.438	8.384	0.333	6.389	9.580
3.4	33.46	0.0112	0.329	3.389	7.635	0.353	6.524	9.331
3.6	32.07	0.0119	0.346	3.309	6.976	0.372	6.606	9.008
3.8	30.68	0.0125	0.362	3.206	6.388	0.391	6.635	8.647
4.0	29.33	0.0132	0.378	3.087	5.881	0.410	6.615	8.255
5	23.15	0.0163	0.447	2.471	3.982	0.498	5.975	6.394
6	18.31	0.0195	0.497	1.909	2.862	0.578	4.953	4.963
7	14.77	0.0225	0.526	1.534	2.149	0.646	3.947	3.967
8	12.32	0.0254	0.532	1.254	1.686	0.700	3.282	3.249
9	10.49	0.0282	0.518	1.052	1.370	0.740	2.756	2.711
10	9.066	0.0309	0.487	0.895	1.123	0.764	2.370	2.299
12	6.985	0.0358	0.394	0.671	0.798	0.766	1.790	1.725
14	5.565	0.0402	0.312	0.523	0.607	0.711	1.405	1.347
16	4.526	0.0438	0.255	0.420	0.473	0.622	1.142	1.076
18	3.724	0.0466	0.217	0.341	0.389	0.531	0.943	0.859
20	3.116	0.0487	0.188	0.280	0.316	0.454	0.792	0.705

Fe 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)3d(6)

q_1	---	14.97	4.089	1.406	0.337	4.269	1.266	0.963
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(6)
0.2	9.509	0.000592	0.0182	0.266	7.963	0.0188	0.419	0.823
0.4	20.00	0.00119	0.0363	0.535	16.90	0.0377	0.841	1.653
0.6	31.29	0.00179	0.0545	0.802	26.64	0.0565	1.261	2.479
0.8	40.52	0.00239	0.0727	1.068	34.32	0.0753	1.678	3.302
1.0	43.23	0.00298	0.0907	1.332	35.50	0.0942	2.093	4.118
1.2	41.10	0.00358	0.0109	1.593	31.94	0.113	2.502	4.922
1.4	37.05	0.00417	0.127	1.846	26.33	0.132	2.905	5.706
1.6	34.47	0.00477	0.144	2.091	22.32	0.150	3.299	6.460
1.8	32.64	0.00536	0.162	2.322	19.13	0.169	3.682	7.172
2.0	31.35	0.00595	0.179	2.535	16.57	0.187	4.050	7.825
2.2	30.38	0.00654	0.196	2.725	14.44	0.206	4.399	8.404
2.4	29.70	0.00714	0.213	2.886	12.75	0.224	4.725	8.891
2.6	29.11	0.00773	0.230	3.013	11.32	0.242	5.026	9.273
2.8	28.57	0.00832	0.247	3.104	10.12	0.260	5.294	9.538
3.0	28.03	0.00891	0.263	3.156	9.118	0.277	5.526	9.682
3.2	27.45	0.00949	0.279	3.171	8.265	0.295	5.719	9.709
3.4	26.79	0.0101	0.294	3.151	7.521	0.312	5.870	9.628
3.6	26.06	0.0107	0.309	3.100	6.877	0.329	5.977	9.455
3.8	25.27	0.0112	0.324	3.025	6.319	0.346	6.039	9.210
4.0	24.43	0.0118	0.338	2.933	5.811	0.363	6.059	8.916
5	21.15	0.0147	0.402	2.407	4.968	0.442	5.637	7.275
6	16.10	0.0175	0.450	1.853	2.836	0.514	4.814	5.618
7	13.05	0.0202	0.481	1.490	2.150	0.577	3.814	4.515
8	10.94	0.0229	0.492	1.229	1.687	0.628	3.182	3.699
9	9.339	0.0254	0.485	1.026	1.353	0.668	2.693	3.089
10	8.115	0.0279	0.462	0.873	1.123	0.694	2.306	2.629
12	6.302	0.0324	0.383	0.655	0.807	0.708	1.745	1.972
14	5.056	0.0364	0.306	0.511	0.612	0.671	1.378	1.542
16	4.135	0.0398	0.248	0.412	0.480	0.599	1.113	1.243
18	3.424	0.0426	0.212	0.338	0.377	0.517	0.922	1.015
20	2.891	0.0446	0.184	0.279	0.318	0.444	0.779	0.842

Co 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)3d(7)

q_1	---	15.58	4.269	1.472	0.346	4.467	1.629	1.014
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(7)
0.2	8.868	0.000531	0.0163	0.238	7.480	0.0167	0.371	0.745
0.4	18.58	0.00107	0.0325	0.478	15.82	0.0335	0.745	1.467
0.6	29.09	0.00161	0.0487	0.716	24.91	0.0502	1.117	2.245
0.8	37.93	0.00214	0.0650	0.954	32.37	0.0668	1.486	2.989
1.0	41.07	0.00268	0.0812	1.189	34.13	0.0836	1.853	3.727
1.2	39.19	0.00322	0.0973	1.422	30.90	0.100	2.216	4.456
1.4	35.43	0.00375	0.113	1.649	25.80	0.117	2.574	5.169
1.6	32.84	0.00428	0.129	1.868	21.92	0.134	2.924	5.861
1.8	30.97	0.00481	0.145	2.077	18.81	0.150	3.265	6.523
2.0	29.64	0.00534	0.161	2.272	16.30	0.166	3.594	7.146
2.2	28.66	0.00588	0.176	2.448	14.22	0.183	3.909	7.717
2.4	27.98	0.00641	0.191	2.602	12.55	0.200	4.205	8.226
2.6	27.46	0.00694	0.206	2.729	11.16	0.215	4.481	8.660
2.8	27.10	0.00748	0.221	2.827	9.981	0.231	4.732	9.009
3.0	26.60	0.00800	0.236	2.892	8.998	0.247	4.954	9.266
3.2	26.18	0.00853	0.250	2.925	8.164	0.262	5.145	9.426
3.4	25.70	0.00906	0.264	2.926	7.426	0.278	5.303	9.491
3.6	25.17	0.00958	0.278	2.900	6.795	0.293	5.424	9.466
3.8	24.57	0.0101	0.291	2.849	6.245	0.308	5.508	9.360
4.0	23.92	0.0106	0.304	2.778	5.762	0.323	5.556	9.185
5	20.04	0.0132	0.363	2.304	3.927	0.395	5.315	7.724
6	16.23	0.0157	0.409	1.796	2.821	0.460	4.635	6.096
7	13.21	0.0182	0.440	1.449	2.131	0.517	3.728	4.931
8	12.08	0.0206	0.454	1.196	1.674	0.566	3.084	4.081
9	9.488	0.0229	0.453	1.000	1.357	0.605	2.616	3.434
10	6.997	0.0251	0.437	0.853	1.114	0.632	2.244	2.929
12	6.420	0.0393	0.372	0.641	0.800	0.654	1.711	2.204
14	5.139	0.0330	0.300	0.504	0.599	0.632	1.346	1.725
16	5.024	0.0362	0.244	0.405	0.472	0.574	1.094	1.389
18	3.512	0.0388	0.207	0.333	0.376	0.503	0.907	1.147
20	2.972	0.0409	0.178	0.278	0.314	0.435	0.766	0.960

Ni 1s(2) 2s(2) 3s(2) 4s(2) 2p(6) 3p(6) 3d(8)

q_1	---	16.18	4.449	1.538	0.3546	4.664	1.392	1.065
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(8)
0.2	8.300	0.000480	0.0146	0.213	7.053	0.0149	0.331	0.676
0.4	17.4	0.000967	0.0292	0.429	14.87	0.0299	0.663	1.375
0.6	27.14	0.00145	0.0438	0.643	23.38	0.0449	0.995	2.034
0.8	35.61	0.00194	0.0585	0.856	30.60	0.0597	1.324	2.708
1.0	39.07	0.00242	0.0730	1.068	32.82	0.0747	1.651	3.376
1.2	37.62	0.00291	0.0875	1.276	30.15	0.0896	1.975	4.037
1.4	33.98	0.00339	0.102	1.480	25.32	0.105	2.294	4.685
1.6	31.42	0.00387	0.116	1.679	21.58	0.119	2.607	5.318
1.8	29.53	0.00435	0.130	1.868	18.56	0.134	2.912	5.928
2.0	28.14	0.00483	0.145	2.046	16.08	0.149	3.208	6.511
2.2	27.12	0.00531	0.158	2.210	14.04	0.163	3.492	7.057
2.4	26.43	0.00580	0.172	2.355	12.40	0.178	3.762	7.558
2.6	25.92	0.00628	0.186	2.480	11.04	0.192	4.015	8.007
2.8	25.51	0.00676	0.199	2.579	9.887	0.206	4.248	8.394
3.0	25.17	0.00724	0.212	2.653	8.915	0.221	4.459	8.712
3.2	24.84	0.00771	0.225	2.698	8.078	0.235	4.644	8.956
3.4	24.49	0.00819	0.238	2.716	7.367	0.248	4.802	9.122
3.6	24.11	0.00866	0.250	2.709	6.748	0.262	4.931	9.210
3.8	23.66	0.00914	0.263	2.678	6.186	0.276	5.029	9.223
4.0	23.15	0.00961	0.275	2.628	5.699	0.289	5.096	9.166
5	19.98	0.0120	0.329	2.208	3.908	0.354	4.998	8.170
6	16.46	0.0142	0.372	1.743	2.817	0.413	4.426	6.679
7	13.43	0.0165	0.403	1.410	2.131	0.466	3.655	5.346
8	11.21	0.0187	0.420	1.166	1.668	0.511	2.989	4.440
9	9.587	0.0208	0.423	0.981	1.346	0.549	2.541	3.725
10	8.324	0.0228	0.413	0.837	1.109	0.577	2.182	3.184
12	6.495	0.0266	0.361	0.630	6.789	0.604	1.668	2.416
14	5.222	0.0301	0.294	0.493	0.594	0.593	1.322	1.896
16	4.297	0.0330	0.240	0.397	0.466	0.549	1.075	1.537
18	3.591	0.0356	0.202	0.328	0.376	0.487	0.891	1.271
20	3.037	0.0376	0.173	0.275	0.310	0.425	0.750	1.066

Cu 1s(2)2s(2)3s(2)4s(1)2p(6)3p(6)3d(10)

q_1	---	16.77	4.625	1.584	0.313	4.856	1.436	1.035
v	total	1s(2)	2s(2)	3s(2)	4s(1)	2p(6)	3p(6)	3d(10)
0.2	9.365	0.000435	0.0132	0.198	8.080	0.0134	0.306	0.754
0.4	20.62	0.000877	0.0264	0.398	18.04	0.0269	0.613	1.513
0.6	31.72	0.00132	0.0396	0.597	27.85	0.0404	0.920	2.269
0.8	34.26	0.00176	0.0529	0.795	29.11	0.0537	1.225	3.020
1.0	30.12	0.00220	0.0660	0.991	23.70	0.0672	1.527	3.766
1.2	26.75	0.00264	0.0792	1.185	19.07	0.0806	1.826	4.503
1.4	24.53	0.00308	0.0922	1.375	15.62	0.0940	2.121	5.227
1.6	23.01	0.00351	0.0105	1.560	12.98	0.107	2.411	5.935
1.8	22.26	0.00395	0.118	1.737	10.96	0.121	2.695	6.621
2.0	21.81	0.00439	0.131	1.904	9.393	0.134	2.970	7.278
2.2	21.64	0.00482	0.143	2.059	8.154	0.147	3.234	7.899
2.4	21.63	0.00526	0.156	2.198	7.144	0.160	3.487	8.477
2.6	21.70	0.00570	0.168	2.319	6.312	0.173	3.725	9.001
2.8	21.83	0.00614	0.180	2.419	5.626	0.186	3.946	9.465
3.0	22.00	0.00657	0.192	2.496	5.039	0.199	4.148	9.859
3.2	22.00	0.00700	0.204	2.548	4.525	0.211	4.328	10.18
3.4	22.00	0.00744	0.216	2.575	4.075	0.224	4.485	10.42
3.6	21.91	0.00787	0.227	2.579	3.675	0.236	4.615	10.57
3.8	21.76	0.00830	0.238	2.560	3.331	0.249	4.719	10.65
4.0	21.52	0.00873	0.249	2.523	3.042	0.261	4.796	10.64
5	19.33	0.0109	0.299	2.160	2.030	0.319	4.781	9.727
6	16.36	0.0129	0.340	1.716	1.455	0.373	4.296	8.165
7	14.10	0.0150	0.371	1.386	1.824	0.422	3.603	6.479
8	11.22	0.0170	0.389	1.148	0.873	0.465	2.932	5.394
9	9.630	0.0189	0.395	0.968	0.691	0.500	2.496	4.561
10	8.383	0.0208	0.389	0.825	0.571	0.528	2.146	3.903
12	6.553	0.0243	0.348	0.621	0.410	0.559	1.642	2.949
14	5.301	0.0275	0.288	0.487	0.309	0.557	1.303	2.329
16	4.390	0.0303	0.236	0.394	0.266	0.524	1.061	1.880
18	3.657	0.0327	0.197	0.325	0.194	0.472	0.880	1.556
20	3.110	0.0346	0.171	0.272	0.160	0.415	0.743	1.314

Zn 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)3d(10)

q_1	---	17.37	4.803	1.668	0.384	5.055	1.520	1.170
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	3d(10)
0.2	6.896	0.000396	0.0120	0.175	5.874	0.0121	0.266	0.557
0.4	14.32	0.000798	0.0240	0.350	12.27	0.0242	0.532	1.116
0.6	22.28	0.001200	0.0359	0.526	19.21	0.0363	0.799	1.673
0.8	29.63	0.001600	0.0479	0.700	25.54	0.0484	1.063	2.227
1.0	33.82	0.002000	0.0599	0.872	28.72	0.0604	1.326	2.777
1.2	33.76	0.002400	0.0718	1.043	27.66	0.0725	1.586	3.321
1.4	31.93	0.002800	0.0840	1.210	24.85	0.0846	1.842	3.857
1.6	28.95	0.003200	0.0954	1.373	20.90	0.0966	2.095	4.384
1.8	27.02	0.00359	0.107	1.531	18.03	0.109	2.342	4.897
2.0	25.61	0.00399	0.119	1.681	15.71	0.120	2.583	5.394
2.2	24.54	0.00439	0.130	1.821	13.77	0.132	2.815	5.871
2.4	23.77	0.00478	0.141	1.949	12.17	0.144	3.039	6.324
2.6	23.21	0.00518	0.153	2.063	10.83	0.156	3.251	6.749
2.8	22.78	0.00558	0.164	2.161	9.694	0.167	3.451	7.140
3.0	22.46	0.00598	0.175	2.240	8.736	0.179	3.636	7.493
3.2	22.22	0.00637	0.185	2.300	7.928	0.190	3.804	7.803
3.4	22.00	0.00677	0.196	2.339	7.240	0.202	3.954	8.066
3.6	21.79	0.00716	0.206	2.358	6.636	0.213	4.085	8.280
3.8	21.54	0.00755	0.217	2.357	6.096	0.224	4.194	8.444
4.0	21.20	0.00794	0.227	2.339	5.559	0.235	4.282	8.551
5	19.30	0.00988	0.273	2.070	3.903	0.288	4.386	8.372
6	16.62	0.0118	0.311	1.680	2.820	0.338	4.052	7.403
7	13.80	0.0137	0.341	1.343	2.125	0.382	3.497	6.102
8	11.42	0.0155	0.360	1.115	1.667	0.422	2.857	4.988
9	9.785	0.0172	0.369	0.941	1.352	0.456	2.410	4.240
10	8.542	0.0190	0.367	0.804	1.111	0.483	2.092	3.666
12	6.684	0.0222	0.335	0.606	0.800	0.517	1.604	2.800
14	5.377	0.0251	0.282	0.478	0.599	0.521	1.272	2.200
16	4.436	0.0278	0.232	0.385	0.467	0.498	1.033	1.793
18	3.713	0.0301	0.193	0.319	0.372	0.455	0.858	1.486
20	3.169	0.0320	0.167	0.267	0.315	0.404	0.726	1.258

Ga 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)4p(1)3d(10)

q_1	---	17.97	4.982	1.755	0.443	5.292	1.594	0.322	1.302
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(1)	3d(10)
0.2	12.61	0.000361	0.0109	0.154	4.207	0.0107	0.236	7.563	0.426
0.4	27.15	0.000728	0.0218	0.309	8.677	0.0215	0.472	16.79	0.853
0.6	42.07	0.00109	0.0327	0.464	13.45	0.0322	0.708	26.10	1.28
0.8	49.51	0.00146	0.0436	0.617	18.12	0.0429	0.942	28.04	1.705
1.0	48.95	0.00183	0.0545	0.770	21.59	0.0536	1.175	23.18	2.126
1.2	46.31	0.00219	0.0653	0.920	22.61	0.0643	1.406	18.70	2.543
1.4	42.49	0.00255	0.0761	1.068	21.35	0.0750	1.633	15.33	2.954
1.6	38.43	0.00292	0.0868	1.213	19.03	0.0856	1.858	12.79	3.359
1.8	34.85	0.00328	0.0974	1.353	16.66	0.0963	2.077	10.81	3.756
2.0	31.83	0.00364	0.108	1.487	14.47	0.107	2.292	9.289	4.143
2.2	29.63	0.00400	0.118	1.613	12.72	0.117	2.501	8.035	4.518
2.4	28.02	0.00437	0.129	1.731	11.38	0.128	2.701	7.065	4.878
2.6	26.70	0.00473	0.139	1.837	10.22	0.138	2.893	6.247	5.226
2.8	25.61	0.00509	0.149	1.931	9.198	0.149	3.075	5.557	5.545
3.0	24.71	0.00546	0.159	2.010	8.292	0.159	3.245	4.993	5.844
3.2	23.94	0.00582	0.169	2.073	7.513	0.169	3.403	4.492	6.119
3.4	23.31	0.00618	0.179	2.120	6.872	0.179	3.545	4.044	6.365
3.6	22.78	0.00654	0.188	2.149	6.335	0.189	3.672	3.658	6.581
3.8	22.25	0.00690	0.198	2.162	5.813	0.199	3.782	3.328	6.765
4.0	21.71	0.00725	0.207	2.159	5.310	0.209	3.874	3.030	6.913
5	19.46	0.00903	0.249	1.964	3.760	0.256	4.054	2.032	7.132
6	16.92	0.0108	0.286	1.640	2.764	0.301	3.829	1.453	6.636
7	14.33	0.0125	0.314	1.299	2.103	0.342	3.387	1.096	5.774
8	11.83	0.0142	0.334	1.081	1.633	0.378	2.800	0.855	4.732
9	10.09	0.0158	0.344	0.915	1.329	0.410	2.421	0.700	3.964
10	8.721	0.0174	0.345	0.783	1.089	0.436	2.028	0.581	3.442
12	6.812	0.0203	0.322	0.595	0.789	0.471	1.560	0.412	2.643
14	5.485	0.0231	0.275	0.467	0.589	0.481	1.241	0.308	2.101
16	4.528	0.0256	0.228	0.379	0.462	0.467	1.013	0.240	1.713
18	3.802	0.0277	0.190	0.313	0.376	0.434	0.842	0.196	1.423
20	3.237	0.0295	0.164	0.263	0.308	0.391	0.714	0.162	1.205

Ge 1s(2) 2s(2) 3s(2) 4s(2) 2p(6) 3p(6) 4p(2) 3d(10)

q_1	---	18.60	5.163	1.843	0.503	5.491	1.686	0.385	1.427
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(2)	3d(10)
0.2	9.733	0.000329	0.00994	0.136	3.122	0.00972	0.205	5.825	0.338
0.4	19.94	0.000997	0.0199	0.274	6.384	0.0195	0.410	12.17	0.677
0.6	30.96	0.000997	0.0298	0.411	9.821	0.0292	0.615	19.04	1.016
0.8	41.40	0.00133	0.0397	0.546	13.27	0.0389	0.819	25.33	1.352
1.0	48.26	0.00166	0.0497	0.681	16.24	0.0486	1.022	28.53	1.687
1.2	49.70	0.00200	0.0596	0.815	17.99	0.0584	1.222	27.54	2.018
1.4	47.70	0.00233	0.0694	0.946	18.10	0.0681	1.421	24.75	2.345
1.6	43.35	0.00266	0.0792	1.074	16.96	0.0778	1.616	20.87	2.668
1.8	39.60	0.00300	0.0888	1.199	15.45	0.0874	1.808	17.98	2.985
2.0	35.75	0.00332	0.0985	1.319	13.32	0.0970	1.996	15.62	3.296
2.2	32.97	0.00365	0.108	1.433	11.84	0.107	2.179	13.70	3.598
2.4	30.72	0.00398	0.118	1.540	10.59	0.116	2.356	12.11	3.890
2.6	28.91	0.00431	0.127	1.638	9.505	0.126	2.526	10.81	4.172
2.8	27.38	0.00464	0.136	1.727	8.571	0.135	2.689	9.676	4.441
3.0	26.12	0.00497	0.145	1.804	7.756	0.144	2.843	8.731	4.695
3.2	25.09	0.00530	0.154	1.868	7.065	0.154	2.986	7.927	4.932
3.4	24.20	0.00563	0.163	1.919	6.470	0.163	3.119	7.210	5.152
3.6	23.48	0.00596	0.172	1.956	5.955	0.172	3.239	6.624	5.352
3.8	22.79	0.00629	0.181	1.978	5.486	0.181	3.346	6.077	5.530
4.0	22.18	0.00661	0.189	1.987	5.077	0.190	3.440	5.637	5.685
5	19.59	0.00823	0.229	1.858	3.592	0.233	3.678	3.903	6.088
6	17.11	0.00982	0.263	1.595	2.684	0.274	3.562	2.815	5.907
7	14.59	0.0114	0.290	1.262	2.014	0.312	3.223	2.126	5.351
8	12.27	0.0129	0.310	1.050	1.618	0.346	2.728	1.669	4.539
9	10.32	0.0144	0.321	0.889	1.311	0.376	2.273	1.352	3.784
10	9.058	0.0159	0.324	0.762	1.081	0.401	1.958	1.114	3.259
12	6.940	0.0186	0.308	0.580	0.774	0.436	1.511	0.797	2.515
14	5.600	0.0212	0.268	0.458	0.586	0.450	1.205	0.601	2.011
16	4.616	0.0235	0.224	0.378	0.459	0.442	0.985	0.465	1.639
18	3.863	0.0255	0.188	0.307	0.365	0.416	0.824	0.372	1.365
20	3.296	0.0272	0.160	0.259	0.301	0.379	0.695	0.317	1.158

As 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)4p(3)3d(10)

q_1	-----	19.20	5.342	1.932	0.558	5.961	1.784	0.442	1.548
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(3)	3d(10)
0.2	7.680	0.0000302	0.00909	0.121	2.450	0.00884	0.178	4.638	0.275
0.4	15.65	0.0000609	0.0182	0.243	4.983	0.0177	0.355	9.481	0.550
0.6	23.98	0.0000916	0.0273	0.365	7.622	0.0266	0.533	14.58	0.827
0.8	32.36	0.001122	0.0364	0.486	10.29	0.0354	0.710	19.70	1.101
1.0	39.82	0.00153	0.0455	0.606	12.74	0.0442	0.885	24.12	1.373
1.2	44.86	0.00183	0.0545	0.725	14.55	0.0531	1.059	26.77	1.643
1.4	46.39	0.00214	0.0635	0.841	15.30	0.0619	1.232	26.98	1.910
1.6	44.99	0.00244	0.0725	0.956	14.98	0.0707	1.401	25.33	2.174
1.8	42.30	0.00275	0.0814	1.068	13.97	0.0795	1.569	23.10	2.434
2.0	38.34	0.00305	0.0902	1.175	12.63	0.0882	1.732	19.93	2.689
2.2	36.21	0.00335	0.0989	1.278	12.17	0.0969	1.892	17.73	2.938
2.4	32.90	0.00366	0.107	1.376	10.23	0.106	2.048	15.85	3.180
2.6	30.70	0.00396	0.116	1.466	9.208	0.114	2.198	14.18	3.415
2.8	28.91	0.00426	0.125	1.549	8.323	0.123	2.342	12.80	3.641
3.0	27.41	0.00457	0.133	1.622	7.562	0.131	2.479	11.62	3.857
3.2	26.10	0.00487	0.141	1.686	6.877	0.140	2.609	10.58	4.061
3.4	25.03	0.00517	0.150	1.738	6.319	0.148	2.730	9.689	4.254
3.6	24.08	0.00547	0.158	1.779	5.813	0.156	2.842	8.890	4.433
3.8	23.27	0.00578	0.166	1.808	5.360	0.165	2.944	8.221	4.597
4.0	21.64	0.00608	0.173	1.826	4.970	0.173	3.035	6.446	4.745
5	19.62	0.00756	0.210	1.754	3.523	0.213	3.310	5.379	5.221
6	17.22	0.00903	0.242	1.533	2.642	0.250	3.284	4.024	5.240
7	14.88	0.0105	0.268	1.239	2.049	0.285	3.035	3.093	4.899
8	12.67	0.0119	0.288	1.018	1.630	0.317	2.646	2.426	4.331
9	10.67	0.0133	0.300	0.869	1.305	0.345	2.221	1.960	3.656
10	9.121	0.0146	0.305	0.746	1.083	0.369	1.886	1.620	3.097
12	7.111	0.0172	0.294	0.569	0.783	0.404	1.472	1.160	2.412
14	5.720	0.0195	0.261	0.448	0.589	0.420	1.177	0.875	1.930
16	4.699	0.0217	0.220	0.364	0.452	0.417	0.963	0.689	1.572
18	3.942	0.0236	0.185	0.302	0.363	0.398	0.802	0.551	1.317
20	3.356	0.0253	0.157	0.254	0.300	0.366	0.681	0.454	1.119

Se 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)4p(4)3d(10)

q ₁	---	19.81	5.525	2.020	0.6111	5.893	1.870	0.4809	1.671
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(4)	3d(10)
0.2	6.526	0.000277	0.00833	0.109	1.981	0.00806	0.158	4.043	0.227
0.4	13.23	0.000559	0.0167	0.218	4.013	0.0162	0.315	8.193	0.454
0.6	20.12	0.000841	0.0250	0.326	6.113	0.0243	0.473	12.48	0.682
0.8	27.11	0.00112	0.0333	0.434	8.239	0.0323	0.630	16.83	0.908
1.0	33.73	0.00140	0.0417	0.542	10.25	0.0404	0.786	20.94	1.133
1.2	39.26	0.00168	0.0499	0.648	11.92	0.0484	0.941	24.30	1.356
1.4	42.76	0.00196	0.0582	0.752	12.93	0.0565	1.094	26.29	1.576
1.6	43.75	0.00224	0.0664	0.855	13.12	0.0645	1.245	26.60	1.795
1.8	42.64	0.00252	0.0746	0.955	12.62	0.0726	1.394	25.51	2.010
2.0	40.49	0.00280	0.0827	1.052	11.77	0.0805	1.540	23.74	2.222
2.2	38.03	0.00308	0.0907	1.146	10.82	0.0885	1.683	21.77	2.429
2.4	34.65	0.00336	0.0987	1.234	9.567	0.0964	1.822	19.20	2.632
2.6	32.30	0.00364	0.107	1.318	8.640	0.104	1.957	17.35	2.829
2.8	30.32	0.00392	0.114	1.395	7.822	0.112	2.087	15.77	3.020
3.0	28.62	0.00420	0.122	1.464	7.129	0.120	2.212	14.37	3.204
3.2	27.14	0.00447	0.130	1.526	6.535	0.128	2.330	13.11	3.380
3.4	25.87	0.00475	0.137	1.578	5.998	0.135	2.442	12.03	3.547
3.6	24.77	0.00503	0.145	1.622	5.512	0.143	2.546	11.10	3.705
3.8	23.80	0.00531	0.152	1.655	5.106	0.150	2.643	10.24	3.853
4.0	22.98	0.00558	0.159	1.678	4.732	0.158	2.730	9.524	3.989
5	19.67	0.00695	0.193	1.651	3.376	0.195	3.020	6.791	4.481
6	17.25	0.00830	0.223	1.466	2.544	0.229	3.053	5.102	4.624
7	15.04	0.00963	0.248	1.215	1.991	0.261	2.875	3.989	4.454
8	12.97	0.0109	0.267	0.994	1.589	0.291	2.565	3.185	4.073
9	11.01	0.0122	0.280	0.845	1.286	0.317	2.175	2.575	3.521
10	9.404	0.0134	0.287	0.726	1.064	0.340	1.845	2.124	3.005
12	7.177	0.0158	0.280	0.554	0.762	0.375	1.427	1.524	2.239
14	5.697	0.0180	0.253	0.439	0.572	0.393	1.143	1.148	1.731
16	4.650	0.0200	0.216	0.357	0.450	0.394	0.937	0.896	1.380
18	3.882	0.0219	0.182	0.297	0.363	0.380	0.787	0.723	1.128
20	3.426	0.0235	0.155	0.250	0.297	0.353	0.668	0.596	1.083

Br 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)4p(5)3d(10)

q_1	----	20.41	5.704	2.110	0.663	6.366	1.962	0.524	1.783
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(5)	3d(10)
0.2	5.545	0.0000256	0.00767	0.0974	1.637	0.00657	0.140	3.464	0.192
0.4	11.18	0.0000516	0.0154	0.195	3.307	0.0132	0.279	6.987	0.384
0.6	16.93	0.0000776	0.0230	0.293	5.021	0.0198	0.419	10.58	0.577
0.8	22.70	0.00104	0.0306	0.340	6.755	0.0264	0.558	14.22	0.769
1.0	28.40	0.00130	0.0383	0.485	8.429	0.0329	0.696	17.76	0.960
1.2	33.53	0.00155	0.0465	0.581	9.896	0.0395	0.833	20.98	1.149
1.4	39.97	0.00181	0.0536	0.675	10.960	0.0461	0.969	23.93	1.337
1.6	40.01	0.00207	0.0611	0.767	11.440	0.0526	1.103	25.06	1.522
1.8	40.68	0.00233	0.0686	0.858	11.330	0.0592	1.235	25.42	1.705
2.0	39.88	0.00259	0.0761	0.945	10.790	0.0657	1.365	24.75	1.886
2.2	38.16	0.00284	0.0835	1.030	10.000	0.0722	1.493	23.42	2.063
2.4	36.13	0.00310	0.0909	1.111	9.148	0.0787	1.617	21.85	2.236
2.6	34.07	0.00336	0.0981	1.187	8.172	0.0851	1.738	20.38	2.406
2.8	31.74	0.00362	0.105	1.258	7.423	0.0915	1.855	18.43	2.570
3.0	29.83	0.00387	0.113	1.324	6.778	0.0979	1.968	16.82	2.730
3.2	28.26	0.00413	0.120	1.383	6.228	0.104	2.075	15.46	2.884
3.4	26.85	0.00439	0.127	1.434	5.724	0.111	2.178	14.24	3.031
3.6	24.69	0.00464	0.133	1.478	5.287	0.117	2.274	12.23	3.171
3.8	24.45	0.00490	0.140	1.514	4.885	0.123	2.364	12.12	3.304
4.0	23.53	0.00515	0.147	1.540	4.553	0.129	2.447	11.28	3.428
5	19.91	0.00642	0.179	1.550	3.255	0.159	2.742	8.109	3.908
6	17.35	0.00767	0.207	1.406	2.461	0.188	2.820	6.142	4.116
7	15.14	0.00890	0.230	1.190	1.928	0.215	2.706	4.801	4.060
8	13.16	0.0101	0.249	0.967	1.555	0.240	2.466	3.873	3.800
9	11.09	0.0112	0.262	0.820	1.268	0.263	2.123	3.193	3.384
10	9.692	0.0124	0.270	0.711	1.048	0.283	1.810	2.641	2.918
12	7.394	0.0146	0.267	0.544	0.751	0.316	1.393	1.908	2.200
14	5.950	0.0167	0.245	0.432	0.568	0.336	1.118	1.444	1.790
16	4.876	0.0186	0.212	0.350	0.446	0.343	0.917	1.116	1.473
18	4.103	0.0203	0.180	0.291	0.360	0.339	0.771	0.902	1.240
20	3.742	0.0219	0.153	0.245	0.540	0.323	0.655	0.747	1.057

Kr 1s(2)2s(2)3s(2)4s(2)2p(6)3p(6)4p(6)3d(10)

q_1	-----	21.00	5.888	2.199	0.7115	6.281	2.078	0.5679	1.898
v	total	1s(2)	2s(2)	3s(2)	4s(2)	2p(6)	3p(6)	4p(6)	3d(10)
0.2	4.734	0.000236	0.00706	0.0378	1.382	0.00681	0.121	2.965	0.164
0.4	9.526	0.000478	0.0141	0.176	2.788	0.0137	0.241	5.965	0.328
0.6	14.38	0.000718	0.0212	0.264	4.223	0.0205	0.362	9.000	0.493
0.8	19.27	0.000958	0.0282	0.351	5.672	0.0273	0.482	12.05	0.657
1.0	24.07	0.00120	0.0353	0.438	7.087	0.0341	0.602	15.07	0.820
1.2	28.61	0.00144	0.0423	0.524	8.371	0.0409	0.720	17.92	0.982
1.4	32.60	0.00168	0.0493	0.689	9.389	0.0477	0.838	20.44	1.142
1.6	35.46	0.00192	0.0563	0.692	10.00	0.0545	0.954	22.40	1.301
1.8	37.20	0.00216	0.0632	0.774	10.15	0.0613	1.069	23.62	1.458
2.0	37.21	0.00239	0.0701	0.853	9.886	0.0681	1.181	23.99	1.162
2.2	37.09	0.00263	0.0769	0.930	9.359	0.0748	1.292	23.59	1.765
2.4	35.86	0.00287	0.0837	1.004	8.733	0.0815	1.401	22.64	1.914
2.6	34.36	0.00311	0.0904	1.074	8.140	0.0882	1.506	21.40	2.060
2.8	32.52	0.00334	0.0971	1.140	7.365	0.0948	1.609	20.01	2.203
3.0	28.92	0.00358	0.104	1.202	6.724	0.101	1.709	18.44	2.342
3.2	28.66	0.00382	0.110	1.258	6.177	0.108	1.804	16.72	2.476
3.4	27.20	0.00406	0.117	1.307	5.690	0.114	1.896	15.49	2.606
3.6	25.95	0.00430	0.123	1.351	5.250	0.121	1.983	14.39	2.730
3.8	24.81	0.00453	0.129	1.387	4.844	0.127	2.065	13.39	2.849
4.0	23.63	0.00477	0.136	1.417	4.525	0.134	2.141	12.45	2.961
5	19.93	0.00594	0.165	1.454	3.241	0.165	2.432	9.051	3.415
6	16.84	0.00710	0.191	1.312	2.339	0.200	2.551	6.554	3.681
7	15.14	0.00824	0.214	1.163	1.919	0.222	2.498	5.428	3.684
8	13.23	0.00936	0.232	0.951	1.549	0.248	2.325	4.392	3.523
9	11.52	0.0105	0.245	0.802	1.273	0.272	2.054	3.642	3.224
10	9.960	0.0115	0.253	0.691	1.057	0.292	1.765	3.065	2.825
12	7.588	0.0136	0.254	0.534	0.762	0.325	1.340	2.219	2.140
14	6.027	0.0155	0.236	0.372	0.578	0.345	1.079	1.578	1.723
16	4.997	0.0173	0.207	0.344	0.446	0.352	0.895	1.316	1.420
18	4.196	0.0189	0.177	0.286	0.361	0.346	0.748	1.060	1.199
20	3.575	0.0204	0.151	0.241	0.299	0.328	0.637	0.876	1.023

Rb 1s(2) 2s(2) 3s(2) 4s(2) 5s(1) 2p(6) 3p(6) 4p(6) 3d(10)

q_1	---	21.44	6.084	2.294	0.786	0.208	6.483	2.175	0.655	2.013
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(1)	2p(6)	3p(6)	4p(6)	3d(10)
0.2	25.22	0.000224	0.00648	0.0790	1.092	21.68	0.00626	0.108	2.103	0.141
0.4	57.86	0.000452	0.0130	0.158	2.197	50.76	0.0126	0.215	4.223	0.282
0.6	66.11	0.000679	0.0194	0.237	3.319	55.41	0.0189	0.323	6.355	0.424
0.8	54.31	0.000907	0.0259	0.316	4.449	40.01	0.0251	0.430	8.492	0.565
1.0	47.97	0.00113	0.0324	0.394	5.561	30.10	0.0314	0.536	10.61	0.705
1.2	44.73	0.00136	0.0389	0.471	6.604	23.43	0.0376	0.642	12.66	0.845
1.4	43.17	0.00159	0.0453	0.548	7.502	18.74	0.0439	0.747	14.56	0.983
1.6	42.42	0.00181	0.0517	0.623	8.167	15.33	0.0501	0.851	16.23	1.120
1.8	41.92	0.00204	0.0580	0.697	8.525	12.83	0.0564	0.953	17.54	1.255
2.0	41.19	0.00227	0.0644	0.769	8.559	10.88	0.0626	1.054	18.41	1.389
2.2	40.03	0.00249	0.0707	0.839	8.322	9.273	0.0688	1.153	18.78	1.520
2.4	38.59	0.00272	0.0769	0.906	7.905	7.946	0.0750	1.251	18.78	1.650
2.6	36.74	0.00294	0.0831	0.970	7.401	6.898	0.0811	1.346	18.18	1.777
2.8	34.94	0.00317	0.0892	1.031	6.941	6.026	0.0872	1.438	17.42	1.901
3.0	32.89	0.00339	0.0953	1.088	6.263	5.320	0.0933	1.528	16.48	2.022
3.2	31.13	0.00362	0.101	1.141	5.761	4.733	0.0993	1.615	15.54	2.140
3.4	29.59	0.00384	0.107	1.188	5.311	4.255	0.105	1.699	14.67	2.254
3.6	28.07	0.00407	0.113	1.231	4.918	3.834	0.111	1.778	13.72	2.364
3.8	26.61	0.00429	0.119	1.267	4.573	3.469	0.117	1.854	12.74	2.470
4.0	25.40	0.00451	0.125	1.298	4.247	3.177	0.123	1.925	11.93	2.571
5	20.79	0.00562	0.152	1.357	3.082	2.120	0.152	2.207	8.724	2.993
6	18.12	0.00672	0.177	1.280	2.337	1.891	0.179	2.343	6.658	3.253
7	15.47	0.00780	0.198	1.131	1.837	1.151	0.205	2.333	5.271	3.333
8	13.50	0.00886	0.215	0.934	1.490	0.903	0.229	2.206	4.265	3.250
9	11.79	0.00990	0.229	0.777	1.231	0.716	0.251	1.990	3.541	3.041
10	10.27	0.0109	0.237	0.676	1.031	0.602	0.271	1.726	2.993	2.723
12	7.861	0.0129	0.241	0.521	0.746	0.432	0.303	1.306	2.209	2.090
14	5.245	0.0147	0.227	0.414	0.565	0.317	0.323	1.055	1.672	1.657
16	5.821	0.0164	0.202	0.333	0.441	0.248	0.332	0.869	1.309	2.066
18	4.318	0.0180	0.174	0.281	0.355	0.199	0.329	0.733	1.059	1.170
20	3.690	0.0194	0.149	0.239	0.292	0.170	0.315	0.625	0.883	0.998

Sr 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10)

q_1	---	22.09	6.267	2.392	0.864	0.255	6.681	2.276	0.733	2.127
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)
0.2	17.99	0.000206	0.00599	0.0711	0.870	15.21	0.00578	0.0958	1.605	0.123
0.4	39.35	0.000416	0.0120	0.142	1.749	33.78	0.0116	0.191	3.220	0.245
0.6	60.86	0.000626	0.0180	0.214	2.635	52.48	0.0174	0.287	4.838	0.368
0.8	67.44	0.000836	0.0240	0.284	3.527	56.25	0.0232	0.383	6.457	0.491
1.0	60.32	0.00105	0.0300	0.355	4.408	46.34	0.0290	0.478	8.061	0.613
1.2	54.20	0.00125	0.0360	0.424	5.250	37.52	0.0347	0.572	9.628	0.734
1.4	49.92	0.00146	0.0419	0.493	6.011	30.69	0.0405	0.666	11.12	0.854
1.6	47.11	0.00167	0.0478	0.561	6.637	25.60	0.0463	0.758	12.48	0.974
1.8	45.05	0.00188	0.0537	0.628	7.073	21.64	0.0521	0.850	13.66	1.091
2.0	43.37	0.00209	0.0596	0.693	7.283	18.55	0.0578	0.940	14.58	1.208
2.2	41.84	0.00230	0.0654	0.756	7.268	16.13	0.0635	1.029	15.20	1.323
2.4	40.21	0.00250	0.0712	0.817	7.068	14.14	0.0692	1.116	15.49	1.436
2.6	38.46	0.00271	0.0769	0.876	6.741	12.47	0.0749	1.202	15.47	1.548
2.8	36.67	0.00292	0.0826	0.932	6.341	11.12	0.0806	1.285	15.17	1.657
3.0	34.92	0.00313	0.0883	0.985	5.965	9.993	0.0862	1.366	14.67	1.763
3.2	33.00	0.00333	0.0939	1.034	5.451	8.991	0.0918	1.445	14.02	1.867
3.4	31.20	0.00354	0.0994	1.079	4.996	8.089	0.0973	1.520	13.35	1.968
3.6	29.52	0.00375	0.105	1.120	4.639	7.317	0.103	1.593	12.57	2.066
3.8	28.10	0.00396	0.110	1.156	4.324	6.634	0.108	1.663	11.94	2.161
4.0	26.51	0.00416	0.116	1.187	4.019	6.059	0.114	1.729	11.03	2.252
5	21.29	0.00519	0.141	1.262	2.937	4.044	0.141	1.998	8.120	2.642
6	18.03	0.00620	0.164	1.214	2.242	2.910	0.166	2.147	6.274	2.903
7	15.60	0.00720	0.184	1.091	1.765	2.194	0.190	2.169	4.979	3.019
8	13.63	0.00818	0.201	0.917	1.436	1.713	0.213	2.083	4.060	2.994
9	11.96	0.00914	0.214	0.763	1.192	1.400	0.233	1.915	3.378	2.851
10	10.45	0.0101	0.223	0.662	1.004	1.152	0.252	1.684	2.853	2.611
12	8.038	0.0119	0.229	0.510	0.733	0.823	0.283	1.279	2.129	2.040
14	6.390	0.0136	0.219	0.406	0.554	0.616	0.303	1.030	1.638	1.610
16	5.240	0.0152	0.197	0.332	0.434	0.480	0.313	0.850	1.285	1.334
18	4.407	0.0167	0.171	0.276	0.350	0.393	0.313	0.718	1.038	1.131
20	3.750	0.0180	0.147	0.235	0.289	0.324	0.303	0.612	0.856	0.966

χ 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(1)

q ₁	----	22.77	6.446	2.478	0.920	0.269	6.878	2.375	0.791	2.198	0.498
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)	4d(1)
0.2	17.80	0.000190	0.00557	0.0651	0.748	13.36	0.00535	0.0859	1.332	0.113	2.086
0.4	39.79	0.000383	0.0112	0.130	1.502	29.36	0.0107	0.171	2.672	0.225	5.712
0.6	62.06	0.000577	0.0167	0.195	2.260	46.04	0.0161	0.258	4.012	0.338	8.922
0.8	73.31	0.000770	0.0223	0.260	3.022	51.93	0.0215	0.343	5.350	0.451	11.91
1.0	71.66	0.000963	0.0278	0.325	3.776	46.24	0.0268	0.429	6.678	0.563	13.59
1.2	64.33	0.00116	0.0334	0.388	4.503	36.88	0.0322	0.513	7.978	0.675	13.33
1.4	58.57	0.00135	0.0389	0.451	5.174	30.30	0.0375	0.597	9.228	0.785	11.96
1.6	53.84	0.00154	0.0445	0.514	5.752	25.30	0.0429	0.680	10.39	0.895	10.22
1.8	50.34	0.00173	0.0499	0.575	6.194	21.45	0.0482	0.763	11.44	1.003	8.820
2.0	47.56	0.00192	0.0554	0.634	6.467	18.40	0.0535	0.844	12.32	1.111	7.672
2.2	45.25	0.00212	0.0608	0.693	6.557	15.99	0.0588	0.924	12.99	1.217	6.759
2.4	43.08	0.00231	0.0662	0.749	6.478	14.00	0.0641	1.002	13.42	1.321	5.979
2.6	41.03	0.00250	0.0715	0.804	6.269	12.39	0.0694	1.079	13.60	1.424	5.323
2.8	39.02	0.00269	0.0768	0.856	5.980	11.03	0.0746	1.155	13.55	1.525	4.766
3.0	37.08	0.00288	0.0821	0.905	5.640	9.906	0.0798	1.228	13.30	1.623	4.312
3.2	35.14	0.00307	0.0873	0.951	5.266	8.935	0.0850	1.300	12.89	1.720	3.906
3.4	33.44	0.00326	0.0924	0.994	5.058	8.080	0.0902	1.369	12.37	1.814	3.568
3.6	31.62	0.00345	0.0975	1.033	4.632	7.337	0.0953	1.436	11.81	1.905	3.266
3.8	29.99	0.00364	0.103	1.069	4.316	6.675	0.100	1.500	11.23	1.993	3.005
4.0	28.47	0.00383	0.108	1.100	4.034	6.078	0.106	1.561	10.63	2.078	2.775
5	22.43	0.00478	0.131	1.184	2.942	4.061	0.130	1.816	7.783	2.448	1.933
6	18.73	0.00571	0.153	1.156	2.239	2.934	0.154	1.971	6.007	2.707	1.404
7	16.13	0.00663	0.172	1.052	1.772	2.202	0.177	2.017	4.833	2.837	1.059
8	14.02	0.00754	0.188	0.901	1.436	1.729	0.198	1.964	3.928	2.840	0.831
9	12.28	0.00843	0.201	0.752	1.193	1.405	0.217	1.834	3.270	2.733	0.669
10	10.74	0.00931	0.211	0.642	1.005	1.143	0.235	1.639	2.765	2.534	0.555
12	8.277	0.0110	0.218	0.500	0.746	0.809	0.264	1.257	2.069	2.008	0.395
14	6.590	0.0126	0.210	0.400	0.566	0.626	0.285	0.995	1.608	1.582	0.301
16	5.399	0.0141	0.191	0.327	0.445	0.479	0.296	0.831	1.279	1.306	0.231
18	4.532	0.0155	0.168	0.272	0.354	0.402	0.298	0.703	1.024	1.108	0.187
20	3.853	0.0167	0.145	0.231	0.287	0.322	0.290	0.600	0.847	0.957	0.157

Zr 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(2)

q ₁	---	23.32	6.633	2.570	0.972	0.283	7.079	2.473	0.844	2.326	0.540
v	total	1s (2)	2s (2)	3s (2)	4s (2)	5s (2)	2p (6)	3p (6)	4p (6)	3d (10)	4d (2)
0.2	16.62	0.000178	0.00517	0.0594	0.655	11.93	0.00495	0.0774	1.140	0.0976	2.649
0.4	35.49	0.000359	0.0104	0.119	1.316	26.00	0.00995	0.155	2.287	0.195	5.397
0.6	55.38	0.000541	0.0155	0.178	1.979	40.97	0.0149	0.232	3.432	0.292	8.269
0.8	67.41	0.000721	0.0207	0.237	2.643	48.05	0.0199	0.309	4.574	0.390	11.17
1.0	67.54	0.000902	0.0258	0.296	3.302	43.53	0.0248	0.386	5.707	0.487	13.78
1.2	63.29	0.00108	0.0310	0.354	3.941	35.46	0.0298	0.463	6.820	0.584	15.61
1.4	59.60	0.00126	0.0361	0.412	4.539	29.26	0.0348	0.539	7.896	0.679	16.20
1.6	56.06	0.00144	0.0413	0.469	5.069	24.50	0.0397	0.614	8.913	0.774	15.64
1.8	52.72	0.00162	0.0463	0.525	5.499	20.80	0.0447	0.688	9.844	0.869	14.40
2.0	49.73	0.00180	0.0514	0.579	5.799	17.88	0.0496	0.761	10.66	0.962	12.99
2.2	46.86	0.00198	0.0564	0.633	5.952	15.54	0.0545	0.834	11.32	1.054	11.41
2.4	44.50	0.00216	0.0614	0.685	5.958	13.64	0.0594	0.905	11.81	1.145	10.23
2.6	42.29	0.00234	0.0664	0.735	5.838	12.09	0.0643	0.975	12.10	1.234	9.189
2.8	40.21	0.00252	0.0713	0.783	5.625	10.80	0.0692	1.044	12.20	1.322	8.294
3.0	38.18	0.00270	0.0762	0.829	5.353	9.704	0.0740	1.111	12.11	1.408	7.515
3.2	36.28	0.00288	0.0811	0.87?	5.078	8.761	0.0788	1.176	11.88	1.493	6.862
3.4	34.40	0.00306	0.0859	0.91:	4.724	7.943	0.0856	1.239	11.52	1.575	6.308
3.6	32.71	0.00324	0.0906	0.950	4.511	7.236	0.0883	1.300	11.09	1.656	5.786
3.8	30.93	0.00342	0.0953	0.984	4.152	6.595	0.0931	1.359	10.59	1.734	5.329
4.0	29.44	0.00359	0.0999	1.015	3.887	6.007	0.0978	1.416	10.16	1.810	4.941
5	23.11	0.00448	0.122	1.106	2.848	4.018	0.121	1.657	7.580	2.145	3.509
6	19.15	0.00536	0.143	1.097	2.181	2.886	0.143	1.814	5.852	2.394	2.637
7	16.41	0.00622	0.161	1.013	1.727	2.192	0.164	1.877	4.698	2.540	2.031
8	14.25	0.00708	0.176	0.883	1.405	1.720	0.184	1.851	3.839	2.581	1.601
9	12.47	0.00791	0.189	0.741	1.167	1.375	0.202	1.752	3.213	2.525	1.303
10	10.96	0.00874	0.198	0.629	0.986	1.142	0.219	1.591	2.730	2.387	1.066
12	8.502	0.0103	0.207	0.491	0.731	0.821	0.247	1.235	2.041	1.948	0.771
14	6.722	0.0118	0.202	0.392	0.556	0.608	0.268	0.972	1.585	1.547	0.580
16	5.060	0.0132	0.186	0.321	0.437	0.479	0.280	0.813	1.262	1.269	0.452
18	4.251	0.0146	0.164	0.268	0.351	0.383	0.283	0.688	1.020	1.079	0.368
20	3.628	0.0158	0.143	0.227	0.289	0.320	0.278	0.588	0.842	0.925	0.299

Nb 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(3)											
q ₁	----	23.96	6.813	2.661	1.022	0.2934	7.318	2.572	0.8935	2.440	0.5890
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)	4d(3)
0.2	15.72	0.000165	0.00482	0.0544	0.580	10.94	0.00454	0.700	0.990	0.0863	2.356
0.4	32.04	0.000334	0.00965	0.109	1.165	23.69	0.00911	0.140	1.986	0.172	4.758
0.6	50.00	0.000502	0.0145	0.163	1.751	37.39	0.0137	0.210	2.980	0.258	7.219
0.8	61.92	0.000670	0.0193	0.217	2.337	45.02	0.0182	0.280	3.970	0.345	9.708
1.0	63.09	0.000838	0.0241	0.271	2.919	42.00	0.0228	0.350	4.953	0.431	12.12
1.2	59.28	0.00101	0.0289	0.325	3.485	34.31	0.0273	0.419	5.919	0.516	14.25
1.4	56.76	0.00117	0.0337	0.377	4.021	28.52	0.0318	0.487	6.858	0.601	15.83
1.6	54.55	0.00134	0.0385	0.429	4.505	23.93	0.0364	0.555	7.753	0.685	16.62
1.8	52.39	0.00151	0.0432	0.481	4.914	20.36	0.0409	0.623	8.584	0.769	16.57
2.0	50.10	0.00168	0.0479	0.531	5.223	17.52	0.0454	0.689	9.329	0.851	15.86
2.2	47.77	0.00184	0.0526	0.580	5.414	15.24	0.0499	0.755	9.964	0.933	14.78
2.4	45.50	0.00201	0.0573	0.628	5.480	13.41	0.0544	0.820	10.46	1.013	13.58
2.6	43.03	0.00218	0.0619	0.675	5.432	11.86	0.0589	0.883	10.82	1.093	12.14
2.8	40.91	0.00234	0.0665	0.719	5.289	10.59	0.0633	0.946	11.01	1.171	11.05
3.0	38.90	0.00251	0.0711	0.762	5.083	9.531	0.0678	1.007	11.04	1.248	10.09
3.2	37.03	0.00267	0.0756	0.803	4.834	8.636	0.0722	1.066	10.94	1.224	9.280
3.4	35.18	0.00284	0.0801	0.841	4.561	7.846	0.0766	1.124	10.71	1.398	8.538
3.6	33.46	0.00301	0.0846	0.876	4.363	7.134	0.0809	1.181	10.40	1.470	7.865
3.8	31.73	0.00317	0.0889	0.909	4.046	6.520	0.0853	1.235	10.03	1.540	7.272
4.0	30.10	0.00334	0.0933	0.939	3.740	5.966	0.0896	1.287	9.590	1.608	6.786
5	23.87	0.00416	0.114	1.034	2.769	3.986	0.111	1.514	7.565	1.915	4.857
6	19.67	0.00498	0.133	1.040	2.125	2.863	0.131	1.670	5.883	2.152	3.665
7	16.77	0.00579	0.151	0.374	1.684	2.165	0.151	1.745	4.715	2.305	2.872
8	14.56	0.00658	0.165	0.863	1.372	1.701	0.169	1.741	3.853	2.369	2.325
9	12.76	0.00736	0.178	0.730	1.142	1.379	0.186	1.668	3.213	2.348	1.904
10	11.19	0.00813	0.187	0.618	0.964	1.123	0.202	1.539	2.726	2.252	1.571
12	8.722	0.00961	0.197	0.481	0.718	0.811	0.229	1.213	2.042	1.891	1.130
14	6.913	0.0110	0.194	0.386	0.550	0.609	0.249	0.954	1.594	1.516	0.850
16	5.654	0.0124	0.180	0.316	0.430	0.480	0.261	0.795	1.278	1.234	0.668
18	4.726	0.0136	0.161	0.263	0.347	0.382	0.266	0.674	1.032	1.051	0.536
20	4.013	0.0147	0.141	0.223	0.286	0.313	0.263	0.576	0.853	0.902	0.441

Mo 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(4)

q_1	----	24.50	6.997	2.752	1.070	0.303	7.477	2.670	0.942	2.552	0.636
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)	4d(4)
0.2	13.81	0.000155	0.00449	0.0499	0.519	10.14	0.00428	0.0636	0.870	0.0768	2.086
0.4	29.22	0.000314	0.00900	0.0998	1.042	21.83	0.00860	0.127	1.747	0.154	4.198
0.6	45.61	0.000473	0.0135	0.150	1.566	34.49	0.0129	0.191	2.620	0.230	6.337
0.8	57.25	0.000631	0.0180	0.200	2.089	42.38	0.0172	0.254	3.490	0.307	8.492
1.0	59.12	0.000789	0.0224	0.249	2.608	40.55	0.0215	0.318	4.352	0.384	10.61
1.2	55.72	0.000947	0.0269	0.298	3.115	33.59	0.0258	0.380	5.202	0.460	12.62
1.4	53.34	0.00111	0.0314	0.347	3.598	27.96	0.0300	0.443	6.030	0.535	14.56
1.6	51.43	0.00126	0.0359	0.395	4.042	23.50	0.0343	0.505	6.824	0.611	15.48
1.8	50.31	0.00142	0.0403	0.442	4.427	20.09	0.0386	0.566	7.570	0.685	16.45
2.0	48.84	0.00158	0.0447	0.488	4.734	17.29	0.0429	0.627	8.251	0.759	16.60
2.2	47.24	0.00173	0.0491	0.534	4.945	15.07	0.0472	0.687	8.848	0.832	16.23
2.4	45.43	0.00189	0.0535	0.578	5.052	13.21	0.0514	0.746	9.343	0.904	15.49
2.6	43.60	0.00205	0.0578	0.621	5.057	11.73	0.0556	0.804	9.719	0.975	14.58
2.8	42.36	0.00220	0.0621	0.662	4.972	10.49	0.0598	0.861	9.967	1.045	13.68
3.0	39.65	0.00236	0.0664	0.702	4.818	9.471	0.0640	0.917	10.08	1.114	12.42
3.2	37.64	0.00252	0.0706	0.740	4.616	8.534	0.0682	0.971	10.08	1.182	11.38
3.4	35.82	0.00267	0.0748	0.776	4.404	7.769	0.0724	1.025	9.956	1.249	10.49
3.6	34.03	0.00283	0.0789	0.810	4.140	7.072	0.0765	1.076	9.744	1.314	9.717
3.8	32.45	0.00299	0.0830	0.841	3.952	6.490	0.0806	1.127	9.459	1.377	9.039
4.0	30.80	0.00314	0.0871	0.870	3.658	5.950	0.0847	1.175	9.131	1.439	8.399
5	24.46	0.00392	0.107	0.967	2.695	4.004	0.105	1.388	7.364	1.721	6.101
6	19.99	0.00469	0.125	0.985	2.073	2.860	0.124	1.541	5.701	1.944	4.631
7	17.00	0.00545	0.141	0.935	1.646	2.174	0.143	1.625	4.576	2.099	3.654
8	14.73	0.00620	0.155	0.842	1.343	1.703	0.160	1.637	3.746	2.178	2.955
9	12.91	0.00694	0.167	0.718	1.118	1.380	0.176	1.587	3.126	2.183	2.448
10	11.39	0.00766	0.176	0.610	0.948	1.134	0.191	1.484	2.659	2.120	2.056
12	8.892	0.00906	0.187	0.472	0.705	0.800	0.217	1.190	1.994	1.830	1.488
14	7.080	0.0104	0.186	0.379	0.546	0.619	0.237	0.940	1.558	1.485	1.120
16	5.771	0.0117	0.175	0.310	0.429	0.482	0.250	0.779	1.249	1.208	0.877
18	4.828	0.0128	0.157	0.259	0.345	0.381	0.256	0.660	1.024	1.026	0.707
20	4.097	0.0139	0.138	0.220	0.285	0.316	0.254	0.565	0.842	0.881	0.582

Tc_1s(2)2s(2)3s(2)4s(2)5s(2)2p(6)3p(6)4p(6)3d(10)4d(5)

q_1	---	25.76	7.178	2.843	1.117	0.311	7.676	2.766	0.983	2.667	0.680
v	total	1s (2)	2s (2)	3s (2)	4s (2)	5s (2)	2p (6)	3p (6)	4p (6)	3d (10)	4d (5)
0.2	12.82	0.000135	0.00420	0.0460	0.468	9.529	0.00399	0.0581	0.782	0.0686	1.8558
0.4	27.04	0.000274	0.00841	0.0919	0.939	20.44	0.00802	0.116	1.570	0.137	3.731
0.6	42.21	0.000412	0.0126	0.138	1.410	32.29	0.0120	0.174	2.355	0.205	5.617
0.8	53.51	0.000551	0.0168	0.184	1.880	40.26	0.0161	0.232	3.136	0.274	7.509
1.0	55.81	0.000689	0.0210	0.229	2.347	39.27	0.0201	0.290	3.911	0.343	9.382
1.2	53.45	0.000827	0.0252	0.275	2.804	33.70	0.0240	0.348	4.675	0.411	11.19
1.4	50.79	0.000964	0.0294	0.319	3.242	28.01	0.0280	0.405	5.420	0.478	12.86
1.6	49.08	0.00110	0.0335	0.364	3.649	23.56	0.0320	0.461	6.139	0.545	14.30
1.8	47.91	0.00124	0.0377	0.407	4.009	20.07	0.0360	0.517	6.819	0.612	15.40
2.0	46.94	0.00138	0.0418	0.450	4.308	17.31	0.0400	0.573	7.447	0.678	16.09
2.2	45.92	0.00151	0.0459	0.492	4.529	15.11	0.0440	0.628	8.009	0.743	16.32
2.4	44.67	0.00165	0.0500	0.533	4.663	13.26	0.0479	0.682	8.488	0.808	16.14
2.6	43.29	0.00179	0.0541	0.573	4.708	11.79	0.0519	0.735	8.872	0.872	15.63
2.8	41.67	0.00193	0.0581	0.612	4.669	10.49	0.0588	0.788	9.149	0.935	14.91
3.0	40.01	0.00206	0.0621	0.649	4.563	9.467	0.0597	0.839	9.315	0.997	14.06
3.2	38.26	0.00220	0.0660	0.684	4.407	8.575	0.0636	0.889	9.370	1.058	13.15
3.4	36.86	0.00234	0.0700	0.718	4.218	7.797	0.0675	0.939	9.322	1.118	12.61
3.6	34.92	0.00247	0.0739	0.750	4.004	7.124	0.0714	0.987	9.185	1.177	11.55
3.8	33.23	0.00261	0.0777	0.780	3.834	6.460	0.0752	1.033	8.974	1.234	10.76
4.0	31.63	0.00275	0.0815	0.807	3.585	5.935	0.0790	1.078	8.710	1.290	10.06
5	25.11	0.00342	0.100	0.906	2.627	4.033	0.0978	1.278	7.180	1.548	7.337
6	20.42	0.00410	0.117	0.933	2.025	2.875	0.116	1.427	5.538	1.758	5.623
7	17.28	0.00476	0.133	0.897	1.618	2.190	0.133	1.516	4.456	1.911	4.421
8	14.90	0.00542	0.146	0.818	1.321	1.686	0.150	1.541	3.654	2.000	3.583
9	13.07	0.00607	0.158	0.708	1.101	1.361	0.165	1.509	3.068	2.025	2.970
10	11.57	0.00670	0.167	0.602	0.930	1.154	0.179	1.428	2.612	1.989	2.507
12	9.128	0.00794	0.178	0.464	0.696	0.823	0.204	1.167	1.960	1.764	1.864
14	7.250	0.00912	0.178	0.372	0.538	0.604	0.224	0.927	1.532	1.452	1.414
16	5.908	0.0103	0.169	0.304	0.425	0.472	0.237	0.761	1.232	1.187	1.111
18	5.414	0.0113	0.154	0.255	0.843	0.381	0.243	0.647	1.011	0.989	0.880
20	4.174	0.0123	0.136	0.217	0.282	0.312	0.243	0.555	0.838	0.861	0.718

Ru 1s(2)2s(2)3s(2)4s(2)5s(1)2p(6)3p(6)4p(6)3d(10)4d(7)

q ₁	----	25.86	7.379	2.906	1.161	0.303	7.887	2.858	1.020	2.778	0.666
v	total	1s (2)	2s (2)	3s (2)	4s (2)	5s (1)	2p (6)	3p (6)	4p (6)	3d (10)	4d (7)
0.2	12.09	0.000134	0.00390	0.0435	0.426	8.703	0.00371	0.0534	0.714	0.0617	2.083
0.4	26.36	0.000271	0.00783	0.0869	0.855	19.56	0.00746	0.107	1.435	0.123	4.180
0.6	40.12	0.000408	0.0117	0.131	1.284	29.90	0.0112	0.160	2.152	0.185	6.285
0.8	43.89	0.000545	0.0156	0.174	1.712	30.26	0.0149	0.214	2.865	0.247	8.391
1.0	44.96	0.000682	0.0195	0.217	2.136	24.37	0.0187	0.267	3.572	0.308	10.48
1.2	39.85	0.000818	0.0234	0.260	2.552	19.52	0.0224	0.320	4.270	0.369	12.51
1.4	39.44	0.000954	0.0273	0.302	2.953	15.95	0.0261	0.372	4.953	0.430	14.43
1.6	39.66	0.00109	0.0312	0.344	3.329	13.24	0.0298	0.424	5.613	0.491	16.16
1.8	40.17	0.00123	0.0351	0.385	3.667	11.17	0.0335	0.476	6.240	0.551	17.61
2.0	40.66	0.00136	0.0389	0.426	3.954	9.563	0.0372	0.527	6.825	0.610	18.68
2.2	40.94	0.00150	0.0427	0.466	4.178	8.275	0.0409	0.577	7.355	0.669	19.33
2.4	40.86	0.00163	0.0465	0.505	4.328	7.244	0.0446	0.627	7.816	0.728	19.52
2.6	40.43	0.00177	0.0503	0.543	4.401	6.412	0.0483	0.676	8.198	0.785	19.31
2.8	39.62	0.00191	0.0541	0.579	4.398	5.699	0.0519	0.725	8.490	0.842	18.76
3.0	38.51	0.00204	0.0578	0.615	4.330	5.097	0.0556	0.772	8.685	0.898	18.00
3.2	37.20	0.00218	0.0615	0.649	4.209	4.566	0.0592	0.819	8.783	0.954	17.10
3.4	35.70	0.00231	0.0652	0.681	4.051	4.104	0.0628	0.865	8.787	1.008	16.07
3.6	34.51	0.00245	0.0688	0.712	3.879	3.702	0.0664	0.909	8.706	1.061	15.40
3.8	32.77	0.00258	0.0724	0.741	3.677	3.355	0.0700	0.952	8.552	1.114	14.23
4.0	31.25	0.00272	0.0760	0.767	3.551	3.054	0.0736	0.994	8.340	1.165	13.23
5	24.94	0.00339	0.0932	0.865	2.567	2.041	0.0912	1.183	6.917	1.401	9.774
6	20.40	0.00406	0.109	0.898	1.995	1.472	0.108	1.327	5.391	1.598	7.495
7	17.27	0.00471	0.124	0.870	1.587	1.107	0.124	1.418	4.348	1.748	5.941
8	14.95	0.00536	0.137	0.801	1.298	0.862	0.140	1.453	3.590	1.843	4.817
9	13.26	0.00600	0.148	0.698	1.081	0.697	0.154	1.436	3.002	1.881	4.005
10	11.61	0.00664	0.157	0.597	0.919	0.571	0.168	1.372	2.557	1.866	3.395
12	9.199	0.00786	0.168	0.456	0.685	0.408	0.191	1.143	1.922	1.696	2.522
14	7.370	0.00903	0.170	0.366	0.534	0.307	0.210	0.915	1.510	1.418	1.931
16	6.005	0.0102	0.163	0.301	0.422	0.243	0.223	0.744	1.215	1.167	1.517
18	5.003	0.0112	0.150	0.254	0.342	0.194	0.230	0.633	1.000	0.969	1.220
20	4.254	0.0122	0.134	0.215	0.281	0.159	0.232	0.545	0.832	0.840	1.004

Rh 1s(2) 2s(2) 3s(2) 4s(2) 5s(1) 2p(6) 3p(6) 4p(6) 3d(10) 4d(8)

q_1	----	26.37	7.555	3.000	1.202	0.304	8.089	2.953	1.065	2.884	0.709
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(1)	2p(6)	3p(6)	4p(6)	3d(10)	4d(8)
0.2	11.64	0.000127	0.00367	0.0401	0.391	8.617	0.00347	0.0491	0.642	0.0560	1.837
0.4	26.30	0.000257	0.00735	0.0801	0.785	19.35	0.00697	0.981	1.290	0.112	3.685
0.6	38.72	0.000387	0.0110	0.120	1.178	29.62	0.0105	0.147	1.934	0.168	5.533
0.8	42.26	0.000516	0.0147	0.160	1.570	30.11	0.0140	0.196	2.575	0.224	7.379
1.0	39.24	0.000646	0.0183	0.200	1.959	24.31	0.0174	0.245	3.211	0.280	9.210
1.2	37.57	0.000775	0.0220	0.240	2.341	19.48	0.0209	0.294	3.838	0.335	11.00
1.4	36.82	0.000905	0.0257	0.279	2.710	15.87	0.0244	0.342	4.453	0.391	12.72
1.6	36.83	0.00103	0.0293	0.317	3.059	13.18	0.0278	0.390	5.049	0.446	14.33
1.8	37.25	0.00116	0.0330	0.356	3.376	11.15	0.0313	0.437	5.619	0.500	15.75
2.0	37.80	0.00129	0.0366	0.393	3.651	9.530	0.0348	0.485	6.155	0.554	16.96
2.2	38.25	0.00142	0.0402	0.430	3.874	8.260	0.0383	0.531	6.646	0.608	17.82
2.4	38.52	0.00155	0.0438	0.466	4.034	7.235	0.0417	0.577	7.083	0.661	18.38
2.6	38.49	0.00168	0.0473	0.501	4.126	6.392	0.0451	0.622	7.456	0.714	18.58
2.8	38.13	0.00181	0.0508	0.535	4.150	5.692	0.0486	0.667	7.755	0.765	18.46
3.0	37.45	0.00193	0.0543	0.569	4.113	5.096	0.0520	0.711	7.975	0.817	18.06
3.2	36.50	0.00206	0.0578	0.600	4.024	4.561	0.0554	0.754	8.111	0.867	17.47
3.4	35.36	0.00219	0.0613	0.631	3.896	4.102	0.0588	0.797	8.164	0.917	16.73
3.6	34.09	0.00232	0.0647	0.660	3.745	3.693	0.0621	0.838	8.140	0.966	15.92
3.8	32.89	0.00245	0.0681	0.687	3.567	3.355	0.0655	0.878	8.046	1.014	15.21
4.0	31.49	0.00258	0.0715	0.713	3.425	3.053	0.0688	0.917	7.894	1.061	14.28
5	24.98	0.00321	0.0877	0.809	2.522	2.042	0.0852	1.094	6.630	1.279	10.43
6	20.50	0.00384	0.103	0.848	1.966	1.474	0.101	1.233	5.230	1.464	8.082
7	17.37	0.00447	0.117	0.832	1.575	1.106	0.116	1.326	4.257	1.608	6.430
8	15.02	0.00509	0.129	0.774	1.286	0.864	0.131	1.369	3.500	1.706	5.252
9	13.18	0.00570	0.140	0.684	1.074	0.697	0.145	1.363	2.945	1.755	4.373
10	11.34	0.00629	0.149	0.588	0.908	0.572	0.158	1.315	2.511	1.755	3.377
12	9.295	0.00746	0.160	0.446	0.679	0.409	0.180	1.118	1.890	1.628	2.778
14	6.583	0.00858	0.163	0.360	0.531	0.307	0.198	0.901	1.479	1.385	2.151
16	5.959	0.00964	0.158	0.298	0.423	0.244	0.211	0.731	1.197	1.148	1.697
18	5.018	0.0106	0.146	0.250	0.343	0.194	0.219	0.620	0.907	0.956	1.372
20	4.330	0.0116	0.131	0.213	0.282	0.159	0.222	0.538	0.823	0.820	1.130

Pd 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(8)

q_1	----	26.89	7.731	3.096	1.255	0.336	8.288	3.051	1.125	2.980	0.794
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)	4d(8)
0.2	10.44	0.000120	0.00345	0.0370	0.352	7.996	0.00325	0.0451	0.561	0.0514	1.393
0.4	21.88	0.000244	0.00692	0.0739	0.706	16.97	0.00654	0.0902	1.126	0.103	2.796
0.6	34.11	0.000367	0.0104	0.111	1.060	26.75	0.00981	0.135	1.689	0.154	4.195
0.8	44.26	0.000490	0.0138	0.148	1.412	34.45	0.0131	0.180	2.248	0.206	5.590
1.0	47.83	0.000612	0.0173	0.185	1.762	35.59	0.0164	0.225	2.803	0.257	6.974
1.2	46.64	0.000735	0.0207	0.221	2.106	32.01	0.0196	0.270	3.351	0.308	8.335
1.4	43.41	0.000858	0.0242	0.257	2.439	26.45	0.0228	0.314	3.889	0.359	9.654
1.6	41.61	0.000980	0.0276	0.293	2.756	22.42	0.0261	0.359	4.412	0.409	10.91
1.8	40.44	0.00110	0.0310	0.328	3.048	19.15	0.0294	0.402	4.916	0.460	12.07
2.0	39.76	0.00123	0.0344	0.363	3.307	16.57	0.0326	0.446	5.393	0.509	13.10
2.2	39.29	0.00135	0.0378	0.397	3.523	14.45	0.0359	0.489	5.837	0.559	13.96
2.4	38.96	0.00147	0.0412	0.431	3.689	12.76	0.0391	0.531	6.240	0.608	14.62
2.6	38.57	0.00159	0.0445	0.463	3.799	11.33	0.0423	0.573	6.593	0.656	15.07
2.8	38.06	0.00171	0.0479	0.495	3.850	10.13	0.0455	0.614	6.891	0.704	15.28
3.0	37.40	0.00183	0.0512	0.526	3.845	9.124	0.0487	0.655	7.126	0.751	15.27
3.2	36.58	0.00196	0.0545	0.556	3.791	8.270	0.0519	0.695	7.295	0.798	15.07
3.4	35.61	0.00208	0.0577	0.584	3.697	7.527	0.0551	0.734	7.395	0.844	14.71
3.6	34.50	0.00220	0.0610	0.612	3.573	6.883	0.0583	0.772	7.428	0.889	14.22
3.8	33.34	0.00232	0.0642	0.638	3.434	6.322	0.0614	0.810	7.399	0.933	13.68
4.0	32.07	0.00244	0.0673	0.662	3.277	5.814	0.0645	0.846	7.314	0.977	13.05
5	26.22	0.00305	0.0827	0.757	2.559	3.943	0.0800	0.102	6.361	1.180	10.24
6	21.37	0.00365	0.0971	0.801	1.985	2.836	0.0949	0.145	5.099	1.355	7.950
7	17.95	0.00424	0.110	0.794	1.587	2.151	0.109	0.238	4.096	1.494	6.362
8	15.45	0.00483	0.122	0.747	1.301	1.690	0.123	0.286	3.397	1.592	5.184
9	13.50	0.00540	0.133	0.670	1.082	1.352	0.136	0.292	2.864	1.648	4.313
10	11.95	0.00597	0.141	0.579	0.920	1.121	0.148	0.257	2.445	1.660	3.669
12	9.513	0.00708	0.153	0.438	0.687	0.806	0.170	0.091	1.843	1.565	2.753
14	7.671	0.00815	0.157	0.353	0.534	0.613	0.187	0.087	1.444	1.353	2.135
16	6.295	0.00916	0.153	0.296	0.429	0.479	0.200	0.722	1.170	1.129	1.708
18	5.236	0.0101	0.143	0.245	0.346	0.378	0.209	0.608	0.966	0.944	1.387
20	5.147	0.0110	0.129	0.209	0.911	0.285	0.318	0.528	0.802	0.810	1.144

Ag 1s(2) 2s(2) 3s(2) 4s(2) 5s(1) 2p(6) 3p(6) 4p(6) 3d(10) 4d(10)

q_1	----	28.25	7.886	3.180	1.278	0.3045	8.456	3.126	1.138	3.634	0.7370
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(1)	2p(6)	3p(6)	4p(6)	3d(10)	4d(10)
0.2	11.33	0.000105	0.00328	0.0346	0.337	8.574	0.00308	0.0424	0.545	0.0491	1.742
0.4	24.80	0.000213	0.00657	0.0690	0.676	19.27	0.00620	0.0847	1.095	0.0982	3.496
0.6	37.82	0.000321	0.00985	0.104	1.014	29.52	0.00930	0.127	1.641	0.147	5.246
0.8	41.10	0.000428	0.0131	0.138	1.351	30.05	0.0124	0.169	2.185	0.196	6.990
1.0	38.00	0.000535	0.0164	0.173	1.685	24.21	0.0155	0.212	2.725	0.245	8.720
1.2	35.95	0.000643	0.0197	0.207	2.014	19.47	0.0186	0.254	3.257	0.294	10.42
1.4	34.97	0.000750	0.0229	0.240	2.333	15.86	0.0217	0.295	3.780	0.343	12.07
1.6	34.79	0.000857	0.0262	0.274	2.637	13.17	0.0247	0.337	4.289	0.391	13.64
1.8	35.09	0.000964	0.0295	0.307	2.919	11.12	0.0278	0.378	4.779	0.439	15.09
2.0	35.62	0.00107	0.0327	0.339	3.170	9.525	0.0309	0.419	5.245	0.486	16.37
2.2	36.21	0.00118	0.0359	0.371	3.384	8.259	0.0340	0.459	5.679	0.533	17.45
2.4	36.70	0.00129	0.0391	0.403	3.550	7.232	0.0371	0.499	6.075	0.580	18.28
2.6	37.00	0.00139	0.0423	0.433	3.665	6.388	0.0401	0.538	6.424	0.626	18.84
2.8	37.04	0.00150	0.0455	0.463	3.725	5.688	0.0432	0.577	6.725	0.672	19.10
3.0	36.79	0.00160	0.0486	0.492	3.732	5.086	0.0462	0.616	6.956	0.717	19.09
3.2	36.26	0.00171	0.0517	0.521	3.692	4.558	0.0492	0.653	7.130	0.762	18.84
3.4	35.49	0.00182	0.0548	0.548	3.611	4.100	0.0522	0.690	7.238	0.806	18.39
3.6	34.52	0.00192	0.0579	0.573	3.500	3.694	0.0552	0.726	7.281	0.849	17.78
3.8	33.47	0.00203	0.0609	0.598	3.373	3.356	0.0582	0.762	7.263	0.892	17.10
4.0	32.26	0.00214	0.0640	0.621	3.221	3.053	0.0612	0.796	7.191	0.934	16.32
5	26.63	0.00267	0.0786	0.714	2.528	2.044	0.0758	0.954	6.300	1.129	12.80
6	21.78	0.00319	0.0923	0.761	1.968	1.473	0.0900	1.083	5.075	1.298	9.938
7	18.30	0.00371	0.105	0.761	1.577	1.107	0.104	1.175	4.079	1.434	7.952
8	15.73	0.00423	0.116	0.723	1.287	0.864	0.117	1.227	3.384	1.533	6.480
9	13.75	0.00473	0.126	0.656	1.077	0.696	0.129	1.239	2.837	1.591	5.391
10	12.17	0.00523	0.135	0.571	0.910	0.572	0.141	1.214	2.423	1.608	4.587
12	9.718	0.00621	0.147	0.431	0.683	0.410	0.162	1.069	1.837	1.530	3.443
14	7.347	0.00715	0.151	0.350	0.533	0.307	0.179	0.875	1.440	1.335	2.669
16	6.443	0.00805	0.148	0.289	0.424	0.244	0.192	0.716	1.167	1.119	2.136
18	5.366	0.00891	0.139	0.243	0.347	0.194	0.200	0.662	0.960	0.937	1.735
20	4.522	0.00971	0.127	0.207	0.286	0.160	0.204	0.452	0.808	0.797	1.431

Cd 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 3d(10) 4d(10)

q_1	----	28.11	8.103	3.298	1.344	0.349	8.694	3.241	1.213	3.209	0.874
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	3d(10)	4d(10)
0.2	9.334	0.000106	0.00305	0.0315	0.298	7.308	0.00286	0.0386	0.466	0.0424	1.144
0.4	19.50	0.000216	0.00612	0.0629	0.598	15.43	0.00575	0.0772	0.934	0.0849	2.298
0.6	32.04	0.000325	0.00917	0.0946	0.896	24.29	0.00864	0.116	1.865	0.170	4.590
0.8	39.78	0.000434	0.0122	0.126	1.194	31.66	0.0115	0.154	1.865	0.170	4.590
1.0	43.74	0.000543	0.0153	0.157	1.489	33.61	0.0144	0.193	2.325	0.212	5.723
1.2	42.70	0.000651	0.0183	0.188	1.780	30.59	0.0173	0.231	2.780	0.254	6.841
1.4	39.62	0.000760	0.0214	0.219	2.063	25.57	0.0201	0.269	3.228	0.296	7.935
1.6	37.69	0.000868	0.0244	0.250	2.335	21.75	0.0230	0.307	3.664	0.338	8.994
1.8	36.41	0.000977	0.0274	0.280	2.589	18.68	0.0258	0.344	4.087	0.379	10.00
2.0	35.64	0.00109	0.0304	0.310	2.820	16.20	0.0287	0.382	4.492	0.421	10.95
2.2	35.12	0.00119	0.0334	0.339	3.022	14.13	0.0316	0.419	4.874	0.462	11.81
2.4	34.85	0.00130	0.0364	0.368	3.188	12.48	0.0344	0.455	5.228	0.502	12.56
2.6	34.66	0.00141	0.0394	0.396	3.312	11.10	0.0373	0.491	5.548	0.542	13.19
2.8	34.48	0.00152	0.0423	0.423	3.392	9.957	0.0401	0.527	5.829	0.582	13.69
3.0	34.22	0.00163	0.0453	0.450	3.426	8.974	0.0429	0.562	6.067	0.621	14.03
3.2	33.84	0.00173	0.0482	0.476	3.417	8.114	0.0457	0.596	6.257	0.660	14.22
3.4	33.35	0.00184	0.0511	0.501	3.371	7.392	0.0485	0.630	6.396	0.699	14.26
3.6	32.74	0.00195	0.0539	0.525	3.293	6.773	0.0513	0.663	6.483	0.736	14.16
3.8	32.00	0.00206	0.0568	0.548	3.192	6.218	0.0541	0.696	6.520	0.774	13.94
4.0	31.17	0.00216	0.0596	0.570	3.076	5.733	0.0569	0.728	6.508	0.810	13.63
5	26.27	0.00270	0.0733	0.659	2.467	3.918	0.0705	0.875	5.910	0.983	11.31
6	21.54	0.00323	0.0862	0.709	1.909	2.818	0.0837	0.996	4.928	1.134	8.868
7	18.03	0.00376	0.0981	0.717	1.531	2.132	0.0965	1.086	3.903	1.261	7.206
8	15.50	0.00428	0.109	0.690	1.253	1.670	0.109	1.142	3.250	1.357	5.918
9	13.59	0.00480	0.119	0.635	1.051	1.350	0.120	1.162	2.747	1.421	4.977
10	12.02	0.00530	0.127	0.560	0.890	1.111	0.131	1.149	2.350	1.451	4.242
12	9.611	0.00629	0.138	0.425	0.670	0.796	0.151	1.034	1.786	1.416	3.189
14	7.807	0.00725	0.144	0.343	0.521	0.596	0.168	0.859	1.402	1.272	2.495
16	6.435	0.00816	0.142	0.283	0.419	0.468	0.180	0.705	1.137	1.084	2.009
18	5.390	0.00902	0.135	0.239	0.341	0.376	0.189	0.589	0.941	0.915	1.656
20	4.572	0.00983	0.124	0.204	0.282	0.311	0.193	0.507	0.788	0.776	1.377

In 1s(2)2s(2)3s(2)4s(2)5s(2)2p(6)3p(6)4p(6)5p(1)3d(10)4d(10)

q ₁	---	28.77	8.289	3.378	1.403	0.405	8.905	3.344	1.264	0.3020	3.317	0.9545
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	5p(1)	3d(10)	4d(10)
0.2	15.64	0.997(-4)	0.00287	0.0297	0.268	5.170	0.00268	0.0356	0.420	8.751	0.0389	0.921
0.4	33.86	0.000203	0.00576	0.0592	0.537	10.74	0.00539	0.0712	0.844	19.67	0.0779	1.850
0.6	52.00	0.000305	0.00864	0.0890	0.806	16.76	0.00810	0.107	1.265	30.06	0.117	2.774
0.8	59.66	0.000407	0.0115	0.119	1.073	22.43	0.0108	0.142	1.684	30.34	0.156	3.693
1.0	58.89	0.000509	0.0144	0.148	1.339	25.90	0.0135	0.178	2.099	24.40	0.194	4.604
1.2	55.61	0.000611	0.0172	0.177	1.600	25.79	0.0162	0.213	2.510	19.55	0.233	5.504
1.4	51.21	0.000713	0.0201	0.206	1.855	23.33	0.0189	0.248	2.914	15.96	0.272	6.387
1.6	46.78	0.000815	0.0230	0.235	2.101	20.00	0.0215	0.283	3.310	13.25	0.310	7.247
1.8	43.57	0.000917	0.0258	0.263	2.333	17.31	0.0242	0.318	3.693	11.18	0.348	8.075
2.0	41.26	0.00102	0.0287	0.291	2.547	15.13	0.0269	0.352	4.062	9.573	0.386	8.860
2.2	39.53	0.00112	0.0315	0.319	2.737	13.30	0.0296	0.386	4.413	8.301	0.424	9.592
2.4	38.21	0.00122	0.0343	0.346	2.898	11.77	0.0323	0.419	4.740	7.252	0.461	10.26
2.6	37.20	0.00132	0.0371	0.372	3.026	10.49	0.0350	0.453	5.040	6.412	0.498	10.84
2.8	36.40	0.00143	0.0399	0.399	3.116	9.423	0.0376	0.486	5.309	5.710	0.535	11.34
3.0	35.64	0.00153	0.0427	0.424	3.168	8.502	0.0403	0.519	5.542	5.099	0.571	11.73
3.2	34.92	0.00163	0.0454	0.449	3.181	7.722	0.0429	0.551	5.735	4.566	0.607	12.02
3.4	34.17	0.00173	0.0481	0.472	3.160	7.038	0.0455	0.582	5.885	4.106	0.642	12.19
3.6	33.38	0.00183	0.0508	0.495	3.108	6.444	0.0482	0.613	5.991	3.706	0.677	12.25
3.8	32.56	0.00193	0.0535	0.517	3.032	5.930	0.0508	0.643	6.053	3.355	0.711	12.21
4.0	31.70	0.00203	0.0562	0.538	2.939	5.477	0.0534	0.673	6.072	3.062	0.745	12.08
5	26.97	0.00254	0.0691	0.625	2.410	3.841	0.0662	0.810	5.546	2.041	0.905	10.55
6	22.22	0.00304	0.0814	0.676	1.854	2.782	0.0786	0.926	4.818	1.472	1.047	8.478
7	18.39	0.00353	0.0927	0.689	1.491	2.111	0.0907	1.014	3.316	1.107	1.167	6.812
8	15.79	0.00402	0.103	0.668	1.229	1.652	0.102	1.072	3.183	0.864	1.261	5.650
9	13.79	0.00450	0.112	0.621	1.026	1.334	0.113	1.098	2.694	0.698	1.327	4.763
10	12.17	0.00498	0.120	0.551	0.874	1.096	0.124	1.093	2.307	0.572	1.363	4.067
12	9.727	0.00592	0.132	0.421	0.655	0.791	0.143	1.001	1.755	0.409	1.348	3.056
14	7.906	0.00681	0.137	0.336	0.512	0.592	0.158	0.843	1.379	0.307	1.221	2.404
16	6.534	0.00768	0.137	0.278	0.412	0.467	0.171	0.696	1.113	0.243	1.062	1.947
18	5.476	0.00850	0.131	0.236	0.338	0.378	0.179	0.578	0.923	0.194	0.901	1.609
20	4.654	0.00927	0.121	0.201	0.279	0.306	0.184	0.502	0.779	0.159	0.766	1.348

Sn 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 5p(2) 3d(10) 4d(10)

q_1	---	29.38	8.482	3.480	1.460	0.451	9.103	3.442	1.326	0.354	3.415	1.035
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	5p(2)	3d(10)	4d(10)
0.2	12.58	0.941(-4)	0.00270	0.0275	0.243	4.033	0.00253	0.0330	0.373	7.077	0.0360	0.755
0.4	26.19	0.000191	0.00542	0.0549	0.487	8.307	0.00509	0.0661	0.749	14.93	0.0722	1.515
0.6	40.75	0.000288	0.00813	0.0824	0.731	12.86	0.00764	0.089	1.123	23.47	0.108	2.272
0.8	53.96	0.000385	0.0108	0.110	0.973	17.34	0.0102	0.132	1.494	30.72	0.144	3.024
1.0	61.05	0.000481	0.0135	0.137	1.213	20.77	0.0127	0.165	1.863	32.93	0.180	3.770
1.2	60.97	0.000577	0.0162	0.164	1.450	21.95	0.0153	0.198	2.228	30.22	0.216	4.508
1.4	56.18	0.000674	0.0189	0.191	1.682	20.91	0.0178	0.230	2.587	25.36	0.252	5.233
1.6	52.00	0.000770	0.0216	0.218	1.906	18.79	0.0203	0.263	2.939	21.61	0.287	5.942
1.8	48.07	0.000866	0.0243	0.244	2.119	16.58	0.0229	0.295	3.282	18.55	0.323	6.629
2.0	44.84	0.000962	0.0270	0.270	2.317	14.51	0.0254	0.327	3.613	16.10	0.358	7.287
2.2	42.32	0.00106	0.0297	0.296	2.495	12.78	0.0279	0.359	3.929	14.10	0.393	7.909
2.4	40.33	0.00115	0.0323	0.321	2.650	11.36	0.0304	0.390	4.227	12.41	0.427	8.486
2.6	38.79	0.00125	0.0349	0.346	2.778	10.17	0.0330	0.421	4.503	11.93	0.462	9.011
2.8	37.54	0.00135	0.0376	0.370	2.874	9.150	0.0355	0.452	4.755	9.896	0.496	9.475
3.0	36.46	0.00144	0.0402	0.394	2.938	8.262	0.0380	0.482	4.978	8.924	0.529	9.870
3.2	35.50	0.00154	0.0428	0.417	2.968	7.509	0.0405	0.512	5.169	8.086	0.563	10.19
3.4	34.63	0.00163	0.0453	0.439	2.966	6.869	0.0429	0.541	5.326	7.374	0.596	10.43
3.6	33.73	0.00173	0.0479	0.460	2.935	6.277	0.0454	0.570	5.447	6.736	0.628	10.58
3.8	32.88	0.00182	0.0504	0.481	2.880	5.775	0.0479	0.598	5.531	6.206	0.660	10.65
4.0	32.01	0.00192	0.0529	0.501	2.806	5.347	0.0503	0.626	5.577	5.703	0.692	10.65
5	27.38	0.00240	0.0652	0.584	2.328	3.765	0.0624	0.755	5.329	3.911	0.842	9.732
6	22.86	0.00287	0.0767	0.636	1.814	2.787	0.0742	0.865	4.644	2.818	0.975	8.167
7	18.78	0.00334	0.0875	0.654	1.462	2.106	0.0856	0.951	3.732	2.133	1.090	6.480
8	16.03	0.00380	0.0974	0.640	1.200	1.650	0.0966	1.009	3.086	1.668	1.181	5.396
9	13.98	0.00426	0.106	0.601	1.008	1.336	0.107	1.040	2.618	1.348	1.247	4.562
10	12.33	0.00471	0.114	0.540	0.855	1.111	0.117	1.041	2.245	1.110	1.287	3.903
12	9.816	0.00559	0.125	0.416	0.645	0.779	0.135	0.969	1.712	0.790	1.288	2.951
14	7.998	0.00645	0.131	0.330	0.505	0.586	0.150	0.827	1.346	0.595	1.193	2.329
16	6.613	0.00727	0.132	0.276	0.405	0.462	0.162	0.686	1.095	0.467	1.040	1.880
18	5.544	0.00805	0.127	0.231	0.334	0.374	0.171	0.572	0.907	0.376	0.888	1.556
20	4.720	0.00878	0.118	0.198	0.278	0.303	0.176	0.491	0.766	0.310	0.757	1.314

St. 1s(2)2s(2)3s(2)4s(2)5s(2)2p(6)3p(6)4p(6)5p(3)3d(10)4d(10)

q_1	---	30.03	8.664	3.572	1.520	0.4933	9.302	3.539	1.391	0.4000	3.520	1.111
v	total	1s (2)	2s (2)	3s (2)	4s (2)	5s (2)	2p (6)	3p (6)	4p (6)	5p (3)	3d (10)	4d (10)
0.2	16.39	0.886(-4)	0.00255	0.0257	0.219	3.274	0.30239	0.0307	0.331	5.836	0.0333	0.632
0.4	21.37	0.020180	0.00512	0.0513	0.441	6.702	0.00480	0.0615	0.664	12.02	0.0667	1.268
0.6	32.75	0.000271	0.00769	0.0771	0.662	10.32	0.00721	0.0920	0.996	18.59	0.1000	1.902
0.8	44.14	0.000362	0.0102	0.103	0.881	13.94	0.00961	0.123	1.326	25.08	0.133	2.532
1.0	53.54	0.000453	0.0128	0.128	1.098	17.01	0.0120	0.154	1.653	30.15	0.167	3.157
1.2	58.46	0.000544	0.0153	0.154	1.313	18.71	0.0144	0.184	1.977	32.12	0.200	3.775
1.4	58.34	0.000635	0.0180	0.179	1.523	18.63	0.0168	0.214	2.297	30.84	0.233	4.384
1.6	55.30	0.000726	0.0205	0.204	1.727	17.33	0.0192	0.245	2.610	27.90	0.266	4.980
1.8	51.50	0.000816	0.0220	0.290	1.921	15.66	0.0216	0.275	2.916	24.63	0.298	5.560
2.0	47.46	0.000907	0.0255	0.253	2.104	13.56	0.0240	0.304	3.212	21.53	0.331	6.120
2.2	44.51	0.000997	0.0280	0.277	2.271	12.04	0.0264	0.354	3.496	19.02	0.363	6.654
2.4	42.07	0.00109	0.0305	0.301	2.418	10.71	0.0287	0.363	3.766	16.90	0.395	7.158
2.6	40.14	0.00118	0.0330	0.324	2.544	9.615	0.0311	0.392	4.020	15.13	0.427	7.624
2.8	38.50	0.00127	0.0355	0.347	2.643	8.667	0.0335	0.421	4.253	13.59	0.459	8.047
3.0	37.13	0.00136	0.0380	0.369	2.715	7.866	0.0358	0.449	4.464	12.28	0.490	8.422
3.2	35.95	0.00145	0.0404	0.391	2.757	7.161	0.0382	0.477	4.649	11.17	0.521	8.742
3.4	34.89	0.00154	0.0429	0.412	2.771	6.535	0.0405	0.504	4.808	10.22	0.551	9.002
3.6	32.91	0.00163	0.0453	0.432	2.759	6.013	0.0429	0.531	4.936	9.369	0.581	9.201
3.8	32.99	0.00172	0.0477	0.452	2.723	5.540	0.0452	0.558	5.034	8.642	0.611	9.336
4.0	32.07	0.00181	0.0501	0.470	2.668	5.126	0.0475	0.584	5.101	7.969	0.641	9.408
4.2	27.57	0.00226	0.0617	0.551	2.228	3.621	0.0590	0.705	5.002	5.606	0.780	8.956
4.4	23.30	0.00270	0.0757	0.603	1.762	2.704	0.0701	0.810	4.428	4.151	0.906	7.788
4.6	19.23	0.00314	0.0830	0.624	1.424	2.069	0.0803	0.893	3.656	3.144	1.014	6.236
4.8	16.27	0.00353	0.0924	0.646	1.177	1.622	0.0913	0.952	2.929	2.466	1.103	5.157
5.0	14.16	0.00491	0.101	0.713	0.986	1.308	0.101	0.985	2.541	2.009	1.169	4.373
5.2	12.47	0.0044	0.102	0.720	0.810	1.080	0.111	0.993	2.197	1.645	1.212	3.719
5.4	11.12	0.37523	0.110	0.714	0.632	0.780	0.126	0.937	1.668	1.177	1.226	2.758
5.6	10.24	0.00693	0.119	0.724	0.557	0.581	0.143	0.311	1.494	0.893	1.151	2.260
5.8	9.79	0.00686	0.127	0.710	0.400	0.456	0.155	0.677	1.075	0.698	1.017	1.827
6.0	9.52	0.00750	0.123	0.729	0.320	0.370	0.163	0.566	0.891	0.556	0.873	1.514
6.2	9.78	0.00736	0.115	0.716	0.275	0.304	0.181	0.750	0.452	0.748	1.230	

T_e 1s(2)2s(2)3s(2)4s(2)5s(2)2p(6)3p(6)4p(6)5p(4)3d(10)4d(10)

q ₁	---	30.54	8.844	3.664	1.578	0.534	9.498	3.637	1.449	0.430	3.624	1.185
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	5p(4)	3d(10)	4d(10)
0.2	9.121	0.846(-4)	0.00242	0.0241	0.200	2.722	0.00226	0.0286	0.299	5.273	0.0309	0.539
0.4	18.55	0.000172	0.00485	0.0481	0.402	5.548	0.00545	0.0573	0.600	10.74	0.0618.	1.079
0.6	28.34	0.000259	0.00728	0.0722	0.603	8.506	0.00682	0.0857	0.899	16.45	0.0927	1.619
0.8	38.22	0.000346	0.00970	0.0963	0.802	11.49	0.00909	0.114	1.197	22.22	0.123	2.155
1.0	47.21	0.000433	0.0121	0.120	1.000	14.16	0.0114	0.143	1.493	27.43	0.154	2.687
1.2	53.79	0.000520	0.0145	0.144	1.196	15.99	0.0136	0.171	1.786	31.08	0.185	3.214
1.4	56.63	0.000606	0.0170	0.168	1.388	16.52	0.0159	0.200	2.074	32.30	0.216	3.733
1.6	55.95	0.000693	0.0194	0.191	1.574	15.87	0.0181	0.228	2.358	31.20	0.246	4.242
1.8	53.24	0.000780	0.0218	0.214	1.752	14.57	0.0204	0.256	2.635	28.75	0.277	4.740
2.0	49.81	0.000866	0.0242	0.237	1.921	12.98	0.0227	0.284	2.904	25.91	0.307	5.222
2.2	46.09	0.000952	0.0266	0.260	2.077	11.44	0.0249	0.311	3.164	22.76	0.337	5.685
2.4	43.46	0.00104	0.0289	0.282	2.217	10.24	0.0272	0.338	3.411	20.42	0.367	6.126
2.6	41.19	0.00113	0.0313	0.304	2.338	9.203	0.0294	0.365	3.645	18.34	0.396	6.540
2.8	39.30	0.00121	0.0337	0.325	2.438	8.305	0.0317	0.392	3.863	16.56	0.425	6.923
3.0	37.83	0.00130	0.0360	0.346	2.515	7.560	0.0339	0.418	4.062	15.13	0.454	7.269
3.2	36.35	0.00138	0.0383	0.367	2.566	6.897	0.0361	0.445	4.241	13.70	0.483	7.577
3.4	35.18	0.00147	0.0406	0.386	2.592	6.303	0.0384	0.470	4.396	12.60	0.512	7.839
3.6	34.02	0.00156	0.0429	0.406	2.595	5.794	0.0406	0.495	4.527	11.52	0.540	8.055
3.8	33.11	0.00164	0.0452	0.424	2.575	5.337	0.0428	0.520	4.633	10.74	0.567	8.222
4.0	32.08	0.00173	0.0475	0.442	2.536	4.945	0.0450	0.545	4.711	9.871	0.595	8.338
5	27.62	0.00216	0.0585	0.519	2.166	3.510	0.0558	0.659	4.718	6.990	0.725	8.220
6	23.50	0.00258	0.0690	0.571	1.719	2.632	0.0664	0.758	4.258	5.267	0.844	7.310
7	19.74	0.00300	0.0788	0.595	1.388	2.043	0.0766	0.839	3.587	4.112	0.947	6.066
8	16.53	0.00342	0.0878	0.592	1.149	1.609	0.0865	0.898	2.922	3.203	1.032	4.945
9	14.36	0.00384	0.0960	0.565	0.968	1.295	0.0960	0.934	2.489	2.597	1.098	4.220
10	12.62	0.00424	0.103	0.519	0.826	1.072	0.105	0.946	2.139	2.133	1.142	3.626
12	10.06	0.00504	0.114	0.407	0.622	0.765	0.122	0.905	1.638	1.540	1.167	2.771
14	8.210	0.00582	0.121	0.321	0.487	0.583	0.136	0.794	1.299	1.157	1.110	2.196
16	6.789	0.00656	0.123	0.266	0.394	0.452	0.147	0.668	1.057	0.905	0.992	1.778
18	5.712	0.00728	0.120	0.226	0.365	0.560	0.156	0.877	0.735	0.859	1.481	1.250
20	4.850	0.00795	0.113	0.193	0.272	0.301	0.162	0.476	0.739	0.598	0.738	1.250

1 1s(2)2s(2)3s(2)4s(2)5s(2)2p(6)3p(6)4p(6)5p(5)3d(10)4d(10)

q_1	---	31.27	9.026	3.760	1.637	0.572	9.709	3.732	1.506	0.463	3.729	1.259
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	5p(5)	3d(10)	4d(10)
0.2	7.939	0.792(-4)	0.00229	0.0225	0.183	2.312	0.00213	0.0268	0.272	4.630	0.0286	0.463
0.4	16.07	0.000161	0.00460	0.0450	0.367	4.696	0.00428	0.0535	0.544	9.372	0.0574	0.928
0.6	24.44	0.000243	0.00690	0.0676	0.550	7.174	0.00643	0.0802	0.816	14.26	0.0860	1.392
0.8	32.88	0.000324	0.00919	0.0901	0.733	9.680	0.00857	0.107	1.087	19.20	0.114	1.853
1.0	40.93	0.000406	0.0115	0.113	0.913	12.01	0.0107	0.134	1.355	23.93	0.143	2.310
1.2	47.48	0.000487	0.0138	0.135	1.092	13.79	0.0129	0.160	1.621	27.92	0.172	2.763
1.4	52.11	0.000568	0.0161	0.157	1.267	14.64	0.0150	0.187	1.883	30.53	0.200	3.210
1.6	53.68	0.000650	0.0184	0.179	1.438	14.48	0.0171	0.213	2.141	31.31	0.229	3.649
1.8	52.87	0.000731	0.0206	0.200	1.602	13.62	0.0192	0.239	2.393	30.44	0.257	4.079
2.0	50.65	0.000812	0.0229	0.222	1.758	12.40	0.0214	0.265	2.639	28.54	0.285	4.498
2.2	48.26	0.000893	0.0252	0.243	1.903	11.23	0.0235	0.291	2.876	26.45	0.313	4.902
2.4	44.90	0.000974	0.0274	0.264	2.036	10.06	0.0256	0.317	3.104	23.44	0.340	5.289
2.6	42.38	0.00106	0.0297	0.284	2.152	9.050	0.0277	0.342	3.320	21.15	0.368	5.656
2.8	40.36	0.00114	0.0319	0.305	2.251	8.206	0.0299	0.367	3.523	19.25	0.395	6.000
3.0	38.55	0.00122	0.0341	0.324	2.330	7.435	0.0320	0.392	3.711	17.55	0.422	6.317
3.2	37.00	0.00130	0.0363	0.344	2.388	6.811	0.0341	0.416	3.881	16.03	0.449	6.605
3.4	35.64	0.00138	0.0385	0.362	2.423	6.242	0.0362	0.440	4.033	14.73	0.475	6.859
3.6	34.42	0.00146	0.0407	0.381	2.437	5.729	0.0383	0.464	4.163	13.59	0.501	7.077
3.8	33.31	0.00154	0.0429	0.398	2.430	5.302	0.0403	0.487	4.272	12.55	0.527	7.258
4.0	32.27	0.00162	0.0450	0.415	2.405	4.908	0.0424	0.510	4.359	11.63	0.553	7.399
5	27.79	0.00202	0.0555	0.489	2.104	3.488	0.0526	0.619	4.447	8.337	0.675	7.517
6	23.73	0.00242	0.0655	0.541	1.693	2.617	0.0626	0.713	4.091	6.271	0.786	6.885
7	20.11	0.00282	0.0748	0.567	1.361	2.044	0.0723	0.791	3.514	4.911	0.883	5.887
8	16.89	0.00321	0.0835	0.568	1.128	1.612	0.0817	0.849	2.867	3.936	0.966	4.796
9	15.42	0.00360	0.0913	0.546	0.946	1.306	0.0967	0.887	2.418	3.201	1.030	4.074
10	12.82	0.00398	0.0983	0.507	0.808	1.079	0.0992	0.903	2.097	2.643	1.076	3.507
12	10.18	0.00474	0.109	0.402	0.613	0.768	0.1115	0.873	1.609	1.893	1.109	2.687
14	8.316	0.00546	0.116	0.316	0.480	0.579	0.129	0.777	1.277	1.434	1.068	2.135
16	6.889	0.00617	0.118	0.259	0.389	0.456	0.140	0.658	1.035	1.122	0.967	1.739
18	5.796	0.00684	0.116	0.222	0.321	0.373	0.149	0.554	0.864	0.903	0.843	1.444
20	4.817	0.00748	0.110	0.192	0.270	0.302	0.155	0.469	0.728	0.744	0.728	1.222

Xe 1s(2) 2s(2) 3s(2) 4s(2) 5s(2) 2p(6) 3p(6) 4p(6) 5p(6) 3d(10) 4d(10)

q_1	---	31.82	9.215	3.844	1.691	0.608	9.916	3.824	1.577	0.497	3.836	1.328
v	total	1s(2)	2s(2)	3s(2)	4s(2)	5s(2)	2p(6)	3p(6)	4p(6)	5p(6)	3d(10)	4d(10)
0.2	6.966	0.755(-4)	0.00217	0.0213	0.169	2.006	0.00201	0.0251	0.242	4.067	0.0266	0.405
0.4	14.06	0.000154	0.00435	0.0426	0.339	4.066	0.00404	0.0503	0.485	8.201	0.0533	0.812
0.6	21.30	0.000232	0.00653	0.0639	0.508	6.195	0.00607	0.0753	0.728	12.42	0.0799	1.218
0.8	28.61	0.000309	0.00870	0.0852	0.677	8.350	0.00810	0.100	0.969	16.68	0.106	1.621
1.0	35.69	0.000387	0.0109	0.106	0.844	10.39	0.0101	0.126	1.208	20.84	0.133	2.022
1.2	42.03	0.000464	0.0130	0.127	1.009	12.06	0.0121	0.151	1.446	24.63	0.160	2.418
1.4	46.93	0.000542	0.0152	0.148	1.171	13.07	0.0142	0.175	1.680	27.66	0.186	2.810
1.6	50.19	0.000619	0.0174	0.169	1.329	13.23	0.0162	0.200	1.910	29.53	0.212	3.574
1.8	50.63	0.000697	0.0195	0.190	1.482	12.71	0.0182	0.225	2.136	30.04	0.239	3.574
2.0	49.87	0.000774	0.0217	0.210	1.627	11.84	0.0202	0.249	2.357	29.34	0.265	3.943
2.2	48.15	0.000851	0.0238	0.230	1.763	10.86	0.0222	0.273	2.571	27.82	0.291	4.300
2.4	45.83	0.000929	0.0260	0.250	1.889	9.590	0.0242	0.297	2.777	26.01	0.316	4.645
2.6	43.72	0.00101	0.0281	0.269	2.001	8.660	0.0262	0.321	2.973	24.13	0.342	4.973
2.8	41.37	0.00108	0.0302	0.288	2.098	7.874	0.0282	0.345	3.159	21.89	0.367	5.287
3.0	39.43	0.00116	0.0323	0.307	2.177	7.175	0.0302	0.368	3.333	20.04	0.392	5.574
3.2	37.75	0.00124	0.0344	0.325	2.238	6.549	0.0322	0.391	3.493	18.43	0.417	5.841
3.4	36.21	0.00131	0.0365	0.343	2.280	6.009	0.0342	0.414	3.637	16.93	0.442	6.083
3.6	34.88	0.00139	0.0385	0.360	2.302	5.543	0.0362	0.436	3.765	15.64	0.466	6.296
3.8	33.71	0.00147	0.0406	0.377	2.305	5.116	0.0381	0.458	3.875	14.53	0.490	6.480
4.0	32.59	0.00154	0.0426	0.394	2.291	4.740	0.0461	0.480	3.967	13.48	0.514	6.631
5	27.88	0.00193	0.0526	0.465	2.042	3.391	0.0498	0.582	4.131	9.676	0.628	6.863
6	23.95	0.00231	0.0621	0.516	1.670	2.548	0.0593	0.673	3.882	7.320	0.733	6.481
7	20.44	0.00269	0.0710	0.543	1.337	1.994	0.0684	0.748	3.415	5.741	0.825	5.698
8	17.28	0.00366	0.0793	0.547	1.110	1.592	0.0773	0.805	2.814	4.654	0.904	4.693
9	14.84	0.00343	0.0868	0.530	0.932	1.286	0.0859	0.844	2.360	3.809	0.968	3.935
10	13.03	0.00380	0.0936	0.496	0.796	1.062	0.0940	0.863	2.035	3.174	1.014	3.394
12	10.36	0.00452	0.104	0.397	0.604	0.761	0.109	0.844	1.575	2.278	1.054	2.627
14	8.394	0.00522	0.111	0.314	0.474	0.574	0.122	0.760	1.245	1.687	1.026	2.076
16	6.981	0.00589	0.114	0.259	0.384	0.449	0.133	0.649	1.016	1.337	0.940	1.694
18	5.877	0.00653	0.112	0.221	0.318	0.362	0.142	0.548	0.844	1.088	0.827	1.408
20	5.012	0.00715	0.107	0.189	0.267	0.297	0.148	0.465	0.716	0.905	0.718	1.193

LIST OF IPPJ-AM REPORTS

- IPPJ-AM-1* "Cross Sections for Charge Transfer of Hydrogen Beams in Gases and Vapors in the Energy Range 10 eV–10 keV"
H. Tawara (1977) [Published in Atomic Data and Nuclear Data Tables 22, 491 (1978)]
- IPPJ-AM-2* "Ionization and Excitation of Ions by Electron Impact –Review of Empirical Formulae–"
T. Kato (1977)
- IPPJ-AM-3 "Grotrian Diagrams of Highly Ionized Iron FeVIII-FeXXVI"
K. Mori, M. Otsuka and T. Kato (1977) [Published in Atomic Data and Nuclear Data Tables 23, 196 (1979)]
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