X-ray Scattering Factors of Ions in Crystals

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The atomic scattering factors for X-Rays are given for the ions $Li^{\oplus}$, $Be^{2\oplus}$, $B^{3\oplus}$, $C^{4\oplus}$, $N^{5\oplus}$, $N^{3\ominus}$, $O^{2\ominus}$, $F^{\ominus}$, $Na^{\oplus}$, $Mg^{2\oplus}$, $Al^{3\oplus}$, $S^{2\ominus}$, $Cl^{\ominus}$, $K^{\oplus}$, $Ca^{2\oplus}$, $Sc^{3\oplus}$, $Ti^{4\oplus}$, $V^{5\oplus}$, Ni, $Cu^{\oplus}$, $Zn^{2\oplus}$, $Ga^{3\oplus}$, $Se^{2\ominus}$, $Br^{\ominus}$, $Rb^{\oplus}$, $Sr^{2\oplus}$, $Y^{3\oplus}$, Pd, $Ag^{\oplus}$, $Cd^{2\oplus}$, $I^{\ominus}$, $Cs^{\oplus}$, and $Ba^{2\oplus}$ in the crystal. The crystal potential is simulated by a hollow charged sphere (Watson sphere model). The Hartree-Fock-Roothaan-method was used for the calculation. The crystal field affects most strongly the atomic form factors of the negative ions, especially the twofold and threefold ionized negative ions, which are unstable in the gaseous phase.

Introduction

In todays crystal structure determinations the point positions of the atoms in the unit cell and their thermal vibrations are optimized on the basis of the reliability factor R. Whatever approach one choses, R is minimized and thereby the method relates to the given "theoretical" atomic scattering factors. The atomic scattering factors f_{theor} are gained from the spherical charge distribution of the atoms determined by quantum mechanical calculations. Any nonspherical charge distribution is neglected in f_{theor}. For solids in which covalent bonds between the atoms are present, this problem was recognized since a long time. McWeeny [1, 2, 3] first pointed out, that the free atom approach to f_{theor} has to be improved by more elaborate models, which take the chemical bond into account. Effective scattering factors were introduced by him to describe the x-ray scattering of "bonded" atoms. Further improvement of the theory of x-ray scattering on bonded atoms was made since, see e.g. the discussions given by Coppens [4].

A different situation arises in coherent x-ray scattering of ionic crystals. Dawson [5] has introduced the expansion of the atomic charge distribution in cubic harmonics around the nuclei. Further progress along this line is due to Kurki-Suonio and Ruuskanen [6, 7, 8]. Several approaches have been made, to take the deformation of the electronic distribution of ions in crystals into account. An important step was done by Löwdin [9, 10] in introducing the overlap model, Yamashita and Kojima [11] account for the crystal field by considering overlap and Madelung potential. A very simple model for ions in crystals was introduced by Watson [12].

The most famous example for the influence of the crystal field on ions is the ion $O^{2\ominus}$. Elaborate Hartree-Fock calculations show, that the free ion is unstable [13]. Either by the approach of Yamashita [14, 15] or by the use of the Watson sphere model [12, 16] this ion becomes stable by incorporation into the solid. The use of the Watson sphere potential for ions in crystals has shown up to be very useful in calculating physical properties which depend strongly on the charge distribution around the nucleus, such as the diamagnetic suszeptibility [16, 17], the dipole polarizabilities [16, 18] and the Sternheimer antishielding factors [16, 19]. We therefore propose the application of this model to calculate the f_{theor} for ions in crystals. Thereby a set of f_{theor}-values is available, which in general should lead to a better starting point in judging the reliability and accuracy of crystal structure data by minimizing $R \sim |f_{\text{theor}} - f_{\text{exp}}|$.

Theory

The atomic scattering factor is calculated from the spherical charge distribution of atoms and ions by

$$f(\boldsymbol{k}) = \int \varrho(\boldsymbol{r}) \exp\{i\,\boldsymbol{k}\,\boldsymbol{r}\}\,\mathrm{d}\tau\,, \qquad (1)$$

where $\varrho(\boldsymbol{r})$ is the electron density of the isolated atom (ion) and $k = 4\pi \sin\vartheta/\lambda$ is the magnitude of the vector $\boldsymbol{k}$ in the reciprocal space. Since we assume

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the electronic charge density to be spherical symmetric, $\varrho(\boldsymbol{r}) = U(r)$, (1) reduces to

$$f(k) = \int_0^\infty U(r) \frac{\sin k\,r}{k\,r}\,\mathrm{d}r \tag{2}$$

$U(r)$ is taken from self consistent field treatments of the atoms (ions). By changing the free ion approach by application of the Watson-sphere model [12] we put around the spherical ion a charged hollow sphere of radius R_0. For compensation the charge qe of the sphere has opposite sign but equal magnitude to the charge of the ion. The system: (ion + sphere) is now neutral. In Fig. 1 the model is shown. The model crystal potential is given by the form [16]

$$V_w(r) = \begin{cases} q/R_0 & \text{for} \quad r \leqq R_0\,, \\ q/r & \text{for} \quad r > R_0\,, \end{cases} \tag{3}$$

and $q_{\text{sphere}} = -\,q_{\text{ion}}$.

The resulting Hamiltonian of the ion in the crystal is then

$$\mathscr{H} = -\sum_{i=1}^{N}\left[\frac{1}{2}\Delta_i + \frac{Z}{r_i} + V_w(r_i) + \sum_{j>i}^{N}\frac{1}{r_{ij}}\right] \tag{4}$$

(N is the number of electrons, Ze the nuclear charge).

In the frame of the SCF-HF-Roothaan theory the one electron wave functions are given by

$$\begin{aligned} \varphi_{nlm} &= \sum_{\mathrm{p}} c_{nlp}\, R_{lp}(r)\, Y_{lm}(\vartheta, \varphi)\,; \\ R_{lp}(r) &= N_{lp}\, r^{n_{lp}-1} \exp\{-\zeta_{lp}\, r\}\,; \\ N_{lp} &= [(2n_{lp})!]^{1/2}\,(2\zeta_{lp})^{n_{lp}+1/2}\,. \end{aligned} \tag{5}$$

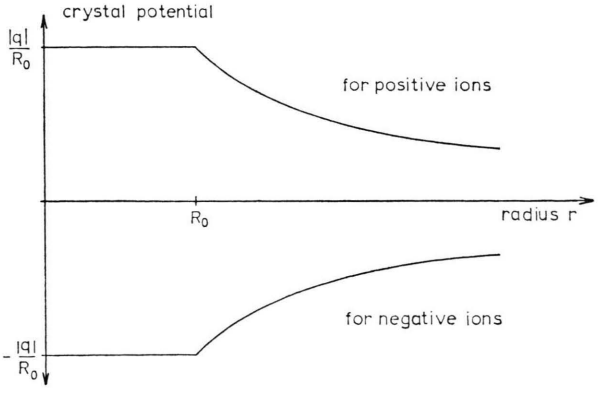

Fig. 1. Crystal potential for negative and positive ions within the Watson sphere model. R_0 is the Watson sphere radius and q is the charge of the Watson sphere.

The radial electron distribution functions of the ions in the crystal is easily found. The radial electron density for closed shell ions is

$$P^2(r) = \sum_{nl} 2(2l+1) \cdot \sum_{pp'} c_{nlp}\, c_{nlp'}\, r^2\, R_{lp}(r)\, R_{lp'}(r)\,. \tag{6}$$

From (6) and (2) for $k \neq 0$ the atomic scattering factors are given by the expression

$$\begin{aligned} f(k) = \frac{1}{k} \sum_{nl} 2(2l+1) \\ \cdot \sum_{pp'} c_{nlp}\, c_{nlp'}\, N_{lp} N_{lp'} (\zeta_{lp} + \zeta_{lp'})^{-(n_{lp}+n_{lp'})} \\ \cdot S_{n_{lp}+n_{lp'}-1}\left(\frac{k}{\zeta_{lp}+\zeta_{lp'}}\right) \end{aligned} \tag{7}$$

where the integral

$$S_m(x) = \int_0^\infty t^m \sin(x\,t) \exp\{-t\}\,\mathrm{d}t \tag{8}$$

is not calculated numerically but by a simple recurrence formula.

Results

The electron distribution, respectively the radial distribution functions of ions, changes considerably through the influence of the spherical potential. In general cations expand, anions shrink [16]. The radial density distribution depends on the radius of the charged sphere. We have choosen the ionic radii of Pauling, but $P^2(r)$ was also calculated for $R_0 \lessgtr r_{\text{Pauling}}$. There is no doubt, that the arbitrariness in selecting R_0 is a major disadvantage of the model. Nevertheless the R_0-dependence at $R_0 \approx r_{\text{Pauling}}$ is small compared with the total effect of the charged sphere on $P^2(r)$. In Fig. 2 the radial distribution function $P^2(r)$ is shown for $F^{\ominus}$. The difference in the radial charge density for the ion in the Watson sphere for different radii R_0, $(P^2(r))_{R_0}$, can not be resolved within the plot of Figure 2. In Fig. 3 the differences

$$P^2(r) = (P^2(r))_{R_0=\infty} - (P^2(r))_{R_0}$$

are listed for $F^{\ominus}$, $Br^{\ominus}$ and $Rb^{\oplus}$.

In Table 1 the f_{theor} are given for 33 ions. For comparison the data calculated from HF^- radial distribution functions for free ions as used in todays crystal structure determination are listed too. No approval has been made to include f_{theor} based on

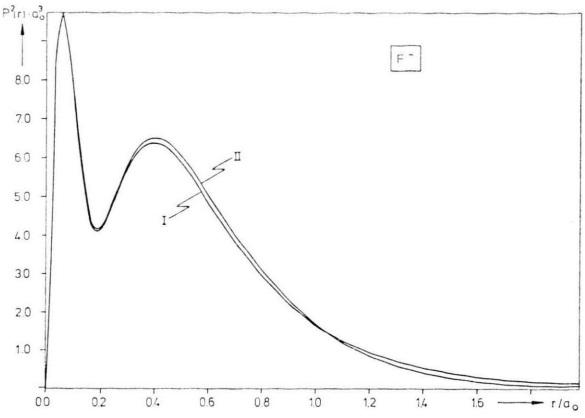

Fig. 2 Total radial charge density $P^2(r)$ in units of a_0^{-3} ($a_0 = 0.529$Å) for $F^{\ominus}$. Curve I shows $P^2(r)$ for the free ion whereas curve II gives $P^2(r)$ for the ion in the Watson sphere.

Table 1. Atomic scattering factors f for free ions and ions in the crystal potential based on Hartree-Fock-Rothaan wave functions. The first line of the table gives the chemical symbol and the charge q_{ion} of the ion. The first column gives the value of $X = \sin\vartheta/\lambda$ in Å^{-1}. In the further columns the f values for each ion are given for three different radii R_0 of the Watson sphere. The first column for one ion is calculated with $R_0 = \infty$ (free ion). The second and third column for the same ion are calculated for two different radii, which are given in Å in the second line of the table. Besides Pd^0 and Ni^0 the charge of the Watson sphere q_w is equal to $-q_{ion}$.

For Pd^0 and Ni^0 there are five columns. The first column gives the free atom result, the second and third column the crystalatom result for two values R_0 with $q_w = -1$, and the last two columns the f-values for two values R_0 and for $q_w = +1$.

X	$Li^{\oplus}$	$Li^{\oplus}$	$Li^{\oplus}$	$Be^{2\oplus}$	$Be^{2\oplus}$	$Be^{2\oplus}$	$B^{3\oplus}$	$B^{3\oplus}$	$B^{3\oplus}$	$C^{4\oplus}$	$C^{4\oplus}$	$C^{4\oplus}$	$N^{5\oplus}$	$N^{5\oplus}$	$N^{5\oplus}$
		0.66	0.60		0.34	0.31		0.22	0.20		0.18	0.15		0.13	0.11
0.0	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0.02	1.997	1.997	1.997	1.999	1.998	1.998	1.999	1.999	1.999	1.999	1.999	1.999	2.000	1.999	1.999
0.04	1.990	1.989	1.989	1.995	1.993	1.993	1.997	1.995	1.994	1.998	1.996	1.995	1.998	1.996	1.995
0.05	1.984	1.983	1.983	1.991	1.990	1.989	1.995	1.992	1.991	1.996	1.994	1.992	1.997	1.994	1.992
0.06	1.977	1.976	1.975	1.988	1.985	1.984	1.993	1.988	1.987	1.995	1.991	1.988	1.996	1.992	1.988
0.08	1.959	1.957	1.957	1.978	1.974	1.972	1.987	1.979	1.976	1.991	1.985	1.979	1.994	1.985	1.979
0.10	1.936	1.934	1.933	1.966	1.959	1.957	1.979	1.968	1.963	1.986	1.976	1.967	1.990	1.977	1.968
0.12	1.909	1.906	1.905	1.952	1.942	1.939	1.970	1.954	1.948	1.980	1.966	1.953	1.985	1.966	1.954
0.14	1.878	1.874	1.872	1.935	1.922	1.917	1.960	1.938	1.930	1.973	1.954	1.937	1.980	1.955	1.938
0.15	1.861	1.857	1.855	1.925	1.911	1.906	1.954	1.929	1.920	1.969	1.947	1.928	1.977	1.948	1.929
0.16	1.843	1.838	1.836	1.915	1.899	1.893	1.948	1.920	1.909	1.964	1.940	1.919	1.974	1.941	1.919
0.18	1.804	1.799	1.796	1.894	1.874	1.867	1.934	1.899	1.886	1.955	1.925	1.898	1.968	1.926	1.899
0.20	1.762	1.757	1.753	1.870	1.846	1.838	1.919	1.877	1.862	1.945	1.908	1.876	1.960	1.909	1.876
0.25	1.648	1.640	1.636	1.803	1.769	1.757	1.876	1.815	1.792	1.915	1.860	1.813	1.938	1.862	1.812
0.30	1.523	1.514	1.509	1.726	1.682	1.667	1.825	1.744	1.714	1.879	1.805	1.742	1.912	1.807	1.739
0.35	1.394	1.385	1.379	1.641	1.589	1.571	1.767	1.668	1.631	1.838	1.745	1.665	1.881	1.746	1.659
0.40	1.266	1.256	1.251	1.551	1.492	1.472	1.704	1.587	1.544	1.792	1.680	1.584	1.847	1.681	1.575
0.45	1.141	1.132	1.127	1.458	1.394	1.372	1.637	1.504	1.456	1.743	1.612	1.503	1.810	1.613	1.489
0.50	1.024	1.015	1.010	1.364	1.297	1.274	1.567	1.421	1.369	1.690	1.543	1.421	1.769	1.543	1.402
0.60	0.815	0.808	0.803	1.179	1.112	1.088	1.420	1.259	1.201	1.576	1.403	1.262	1.680	1.402	1.234
0.70	0.643	0.638	0.634	1.007	0.944	0.921	1.273	1.106	1.047	1.457	1.266	1.115	1.583	1.267	1.080
0.80	0.506	0.503	0.500	0.852	0.797	0.776	1.131	0.967	0.909	1.335	1.137	0.983	1.482	1.140	0.944
0.90	0.400	0.397	0.395	0.718	0.670	0.651	0.997	0.842	0.787	1.215	1.017	0.865	1.379	1.024	0.826
1.00	0.317	0.314	0.313	0.603	0.562	0.546	0.875	0.732	0.682	1.100	0.907	0.762	1.276	0.919	0.726
1.10	0.252	0.251	0.249	0.505	0.472	0.458	0.764	0.636	0.590	0.991	0.807	0.671	1.176	0.826	0.640
1.20	0.202	0.201	0.200	0.424	0.396	0.385	0.666	0.552	0.511	0.889	0.718	0.592	1.079	0.742	0.567
1.30	0.163	0.162	0.161	0.357	0.334	0.324	0.580	0.479	0.443	0.796	0.638	0.523	0.987	0.667	0.504
1.40	0.133	0.132	0.131	0.301	0.282	0.274	0.505	0.417	0.385	0.711	0.567	0.463	0.900	0.600	0.450
1.50	0.109	0.108	0.108	0.254	0.238	0.232	0.439	0.363	0.335	0.635	0.505	0.410	0.819	0.540	0.402
1.60	0.090	0.089	0.089	0.216	0.203	0.197	0.383	0.316	0.292	0.566	0.449	0.363	0.745	0.487	0.361
1.70	0.074	0.074	0.074	0.184	0.173	0.168	0.334	0.276	0.255	0.504	0.400	0.323	0.676	0.439	0.324
1.80	0.062	0.062	0.061	0.157	0.148	0.144	0.292	0.242	0.223	0.450	0.356	0.287	0.613	0.397	0.292
1.90	0.052	0.052	0.052	0.135	0.127	0.123	0.256	0.212	0.196	0.401	0.318	0.256	0.556	0.359	0.263
2.00	0.044	0.044	0.044	0.116	0.109	0.106	0.224	0.186	0.172	0.358	0.284	0.229	0.504	0.324	0.238

Table 1 (continued)

X	$N^{3\ominus}$	$N^{3\ominus}$	$N^{3\ominus}$	$O^{2\ominus}$	$O^{2\ominus}$	$O^{2\ominus}$	$F^{\ominus}$	$F^{\ominus}$	$F^{\ominus}$	$Na^{\oplus}$	$Na^{\oplus}$	$Na^{\oplus}$	$Mg^{2\oplus}$	$Mg^{2\oplus}$	$Mg^{2\oplus}$
		1.59	1.24		1.40	1.32		1.36	1.33		1.05	0.95		0.72	0.65
0.0	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000	10.000
0.02	9.133	9.917	9.921	9.826	9.942	9.944	9.953	9.960	9.960	9.981	9.981	9.981	9.986	9.986	9.986
0.04	7.279	9.673	9.707	9.396	9.771	9.780	9.816	9.840	9.841	9.925	9.924	9.924	9.945	9.943	9.943
0.05	6.373	9.497	9.559	9.140	9.647	9.660	9.716	9.752	9.754	9.883	9.882	9.882	9.914	9.912	9.911
0.06	5.603	9.288	9.388	8.878	9.499	9.517	9.597	9.647	9.649	9.832	9.832	9.831	9.876	9.873	9.872
0.08	4.532	8.789	8.978	8.372	9.141	9.170	9.309	9.388	9.391	9.705	9.704	9.703	9.781	9.777	9.773
0.10	3.950	8.206	8.488	7.895	8.715	8.754	8.968	9.073	9.078	9.546	9.544	9.542	9.662	9.655	9.649
0.12	3.653	7.576	7.939	7.436	8.241	8.290	8.587	8.714	8.720	9.356	9.354	9.352	9.519	9.509	9.502
0.14	3.497	6.928	7.353	6.985	7.739	7.795	8.181	8.322	8.330	9.141	9.138	9.135	9.354	9.341	9.332
0.15	3.445	6.606	7.055	6.763	7.483	7.542	7.973	8.118	8.126	9.024	9.021	9.018	9.264	9.249	9.239
0.16	3.402	6.290	6.756	6.543	7.226	7.287	7.762	7.910	7.918	8.903	8.899	8.896	9.169	9.153	9.141
0.18	3.326	5.685	6.167	6.113	6.717	6.780	7.341	7.487	7.496	8.645	8.641	8.637	8.967	8.948	8.934
0.20	3.249	5.125	5.603	5.702	6.224	6.286	6.924	7.062	7.072	8.372	8.367	8.362	8.750	8.727	8.711
0.25	3.016	3.972	4.369	4.777	5.105	5.159	5.937	6.042	6.051	7.644	7.637	7.632	8.153	8.124	8.102
0.30	2.746	3.162	3.441	4.014	4.194	4.235	5.067	5.136	5.143	6.891	6.885	6.879	7.510	7.475	7.449
0.35	2.481	2.625	2.796	3.407	3.488	3.517	4.330	4.370	4.375	6.156	6.149	6.144	6.851	6.814	6.786
0.40	2.247	2.274	2.368	2.935	2.959	2.977	3.723	3.744	3.748	5.466	5.460	5.455	6.204	6.167	6.139
0.45	2.054	2.043	2.087	2.572	2.567	2.578	3.233	3.243	3.245	4.840	4.835	4.831	5.589	5.553	5.527
0.50	1.899	1.884	1.899	2.296	2.278	2.284	2.841	2.846	2.847	4.285	4.282	4.278	5.018	4.987	4.962
0.60	1.684	1.685	1.676	1.926	1.907	1.908	2.288	2.289	2.289	3.390	3.389	3.387	4.039	4.017	4.000
0.70	1.547	1.556	1.542	1.706	1.695	1.693	1.945	1.946	1.945	2.748	2.748	2.748	3.281	3.269	3.258
0.80	1.448	1.452	1.440	1.566	1.560	1.558	1.729	1.729	1.729	2.301	2.302	2.302	2.718	2.713	2.707
0.90	1.363	1.356	1.348	1.463	1.460	1.459	1.585	1.585	1.585	1.994	1.994	1.995	2.310	2.310	2.308
1.00	1.279	1.263	1.257	1.377	1.376	1.374	1.481	1.481	1.481	1.781	1.782	1.783	2.019	2.021	2.021
1.10	1.195	1.171	1.168	1.297	1.296	1.295	1.397	1.396	1.396	1.631	1.632	1.632	1.810	1.813	1.814
1.20	1.110	1.080	1.079	1.220	1.218	1.218	1.322	1.322	1.322	1.521	1.522	1.522	1.658	1.661	1.663
1.30	1.026	0.993	0.993	1.144	1.141	1.141	1.252	1.252	1.252	1.436	1.436	1.436	1.545	1.548	1.549
1.40	0.943	0.910	0.910	1.068	1.065	1.065	1.184	1.183	1.183	1.364	1.364	1.365	1.457	1.459	1.460
1.50	0.864	0.831	0.831	0.994	0.991	0.991	1.117	1.116	1.116	1.302	1.302	1.302	1.385	1.387	1.388
1.60	0.789	0.758	0.758	0.923	0.919	0.919	1.051	1.050	1.050	1.244	1.244	1.244	1.323	1.324	1.325
1.70	0.719	0.690	0.690	0.854	0.851	0.850	0.987	0.986	0.986	1.188	1.188	1.188	1.267	1.268	1.268
1.80	0.654	0.627	0.627	0.789	0.785	0.785	0.924	0.923	0.923	1.134	1.134	1.134	1.215	1.215	1.216
1.90	0.594	0.569	0.569	0.728	0.724	0.724	0.864	0.863	0.863	1.082	1.082	1.081	1.165	1.165	1.165
2.00	0.539	0.517	0.517	0.671	0.667	0.667	0.806	0.805	0.805	1.030	1.030	1.030	1.116	1.116	1.116

X	$Al^{3\oplus}$	$Al^{3\oplus}$	$Al^{3\oplus}$	$S^{2\ominus}$	$S^{2\ominus}$	$S^{2\ominus}$	$Cl^{\ominus}$	$Cl^{\ominus}$	$Cl^{\ominus}$	$K^{\oplus}$	$K^{\oplus}$	$K^{\oplus}$	$Ca^{2\oplus}$	$Ca^{2\oplus}$	$Ca^{2\oplus}$
		0.55	0.50		1.83	1.66		1.81	1.63		1.33	1.30		1.06	0.99
0.0	10.000	10.000	10.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000
0.02	9.989	9.989	9.988	17.798	17.870	17.879	17.888	17.899	17.903	17.943	17.942	17.942	17.955	17.953	17.952
0.04	9.957	9.955	9.953	17.239	17.496	17.529	17.564	17.605	17.618	17.773	17.769	17.769	17.820	17.813	17.810
0.05	9.933	9.930	9.927	16.861	17.229	17.278	17.332	17.393	17.411	17.647	17.642	17.642	17.720	17.709	17.705
0.06	9.904	9.899	9.896	16.439	16.917	16.982	17.059	17.141	17.167	17.497	17.490	17.489	17.600	17.585	17.578
0.08	9.831	9.821	9.816	15.531	16.185	16.281	16.416	16.541	16.579	17.126	17.115	17.113	17.300	17.276	17.265
0.10	9.737	9.723	9.715	14.615	15.358	15.478	15.684	15.842	15.893	16.673	16.657	16.655	16.931	16.895	16.879
0.12	9.625	9.605	9.594	13.747	14.486	14.620	14.908	15.085	15.145	16.154	16.135	16.132	16.500	16.454	16.434
0.14	9.495	9.469	9.453	12.950	13.613	13.751	14.125	14.306	14.369	15.586	15.564	15.560	16.021	15.964	15.939
0.15	9.424	9.394	9.377	12.580	13.187	13.324	13.740	13.917	13.981	15.289	15.265	15.262	15.766	15.705	15.678
0.16	9.349	9.315	9.296	12.229	12.773	12.907	13.364	13.533	13.597	14.986	14.961	14.958	15.503	15.438	15.410
0.18	9.187	9.146	9.122	11.581	11.991	12.114	12.644	12.792	12.852	14.368	14.343	14.340	14.959	14.889	14.858
0.20	9.011	8.963	8.934	11.002	11.282	11.389	11.977	12.097	12.150	13.748	13.724	13.720	14.401	14.327	14.294
0.25	8.520	8.454	8.415	9.826	9.859	9.921	10.569	10.615	10.647	12.261	12.243	12.240	13.001	12.931	12.899
0.30	7.975	7.893	7.844	8.970	8.888	8.912	9.512	9.507	9.520	10.957	10.947	10.945	11.695	11.641	11.615
0.35	7.399	7.305	7.250	8.337	8.236	8.235	8.734	8.708	8.708	9.885	9.882	9.881	10.555	10.522	10.504
0.40	6.813	6.713	6.653	7.838	7.763	7.752	8.150	8.122	8.117	9.038	9.040	9.040	9.608	9.594	9.584
0.45	6.236	6.135	6.074	7.411	7.373	7.359	7.688	7.668	7.661	8.381	8.385	8.385	8.846	8.846	8.842
0.50	5.682	5.584	5.524	7.016	7.007	6.996	7.295	7.284	7.278	7.868	7.872	7.873	8.242	8.249	8.250

Table 1 (continued)

X	$Al^{3\oplus}$	$Al^{3\oplus}$	$Al^{3\oplus}$	$S^{2\ominus}$	$S^{2\ominus}$	$S^{2\ominus}$	$Cl^{\ominus}$	$Cl^{\ominus}$	$Cl^{\ominus}$	$K^{\oplus}$	$K^{\oplus}$	$K^{\oplus}$	$Ca^{2\oplus}$	$Ca^{2\oplus}$	$Ca^{2\oplus}$
0.60	4.681	4.598	4.547	6.252	6.269	6.266	6.589	6.591	6.590	7.108	7.110	7.111	7.370	7.380	7.383
0.70	3.850	3.790	3.752	5.497	5.516	5.518	5.907	5.913	5.914	6.508	6.508	6.508	6.746	6.751	6.754
0.80	3.195	3.157	3.130	4.777	4.790	4.795	5.234	5.239	5.241	5.947	5.946	5.946	6.213	6.213	6.214
0.90	2.693	2.673	2.657	4.122	4.131	4.136	4.592	4.596	4.598	5.389	5.388	5.387	5.700	5.697	5.697
1.00	2.319	2.311	2.303	3.554	3.560	3.565	4.006	4.009	4.011	4.839	4.838	4.838	5.189	5.185	5.184
1.10	2.041	2.042	2.039	3.076	3.082	3.085	3.492	3.494	3.496	4.315	4.314	4.314	4.686	4.683	4.681
1.20	1.837	1.842	1.842	2.685	2.690	2.692	3.054	3.056	3.057	3.832	3.831	3.831	4.207	4.204	4.202
1.30	1.685	1.692	1.694	2.371	2.375	2.377	2.689	2.691	2.692	3.400	3.400	3.400	3.764	3.761	3.760
1.40	1.569	1.576	1.579	2.121	2.125	2.126	2.391	2.392	2.393	3.023	3.023	3.023	3.364	3.362	3.361
1.50	1.479	1.486	1.488	1.925	1.928	1.928	2.149	2.151	2.151	2.701	2.701	2.701	3.013	3.011	3.010
1.60	1.406	1.411	1.414	1.770	1.772	1.773	1.956	1.957	1.957	2.430	2.429	2.429	2.708	2.707	2.706
1.70	1.344	1.348	1.350	1.647	1.649	1.649	1.801	1.801	1.802	2.203	2.203	2.203	2.448	2.447	2.447
1.80	1.289	1.292	1.294	1.550	1.551	1.551	1.676	1.677	1.677	2.016	2.016	2.016	2.229	2.228	2.228
1.90	1.239	1.241	1.242	1.470	1.471	1.471	1.576	1.577	1.577	1.862	1.862	1.862	2.046	2.045	2.044
2.00	1.192	1.193	1.194	1.404	1.405	1.405	1.494	1.494	1.495	1.735	1.735	1.735	1.892	1.892	1.891

X	$Sc^{3\oplus}$	$Sc^{3\oplus}$	$Sc^{3\oplus}$	$Ti^{4\oplus}$	$Ti^{4\oplus}$	$Ti^{4\oplus}$	$V^{5\oplus}$	$V^{5\oplus}$	$V^{5\oplus}$	Ni	Ni	Ni	Ni	Ni
		0.91	0.81		0.68	0.58		0.65	0.49		1.37	1.24	1.37	1.24
0.0	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	18.000	28.000	28.000	28.000	28.000	28.000
0.02	17.963	17.961	17.959	17.969	17.962	17.955	17.974	17.946	17.950	27.925	27.923	27.922	27.932	27.933
0.04	17.853	17.844	17.836	17.877	17.848	17.822	17.895	17.788	17.804	27.704	27.696	27.691	27.729	27.735
0.05	17.771	17.757	17.745	17.808	17.764	17.724	17.837	17.670	17.695	27.543	27.530	27.523	27.579	27.589
0.06	17.672	17.652	17.636	17.725	17.663	17.607	17.766	17.529	17.564	27.349	27.331	27.322	27.400	27.413
0.08	17.425	17.392	17.364	17.516	17.411	17.317	17.587	17.179	17.241	26.877	26.848	26.833	26.958	26.980
0.10	17.117	17.068	17.027	17.255	17.101	16.963	17.363	16.751	16.844	26.308	26.268	26.247	26.419	26.451
0.12	16.755	16.690	16.636	16.945	16.740	16.558	17.095	16.257	16.387	25.663	25.613	25.588	25.801	25.841
0.14	16.346	16.266	16.198	16.593	16.338	16.112	16.789	15.714	15.883	24.962	24.906	24.877	25.121	25.167
0.15	16.127	16.039	15.965	16.403	16.125	15.878	16.623	15.429	15.618	24.596	24.538	24.507	24.762	24.810
0.16	15.899	15.805	15.725	16.204	15.904	15.638	16.448	15.137	15.347	24.223	24.163	24.132	24.393	24.444
0.18	15.422	15.316	15.226	15.785	15.445	15.146	16.078	14.543	14.794	23.460	23.400	23.368	23.634	23.687
0.20	14.924	14.809	14.712	15.341	14.971	14.645	15.683	13.947	14.238	22.685	22.627	22.597	22.855	22.908
0.25	13.637	13.516	13.411	14.169	13.763	13.405	14.620	12.538	12.914	20.750	20.706	20.682	20.885	20.932
0.30	12.376	12.269	12.172	12.978	12.590	12.244	13.509	11.363	11.790	18.884	18.858	18.843	18.969	19.004
0.35	11.219	11.139	11.062	11.843	11.511	11.208	12.417	10.490	10.926	17.137	17.126	17.119	17.178	17.200
0.40	10.212	10.162	10.103	10.814	10.557	10.312	11.393	9.898	10.301	15.539	15.539	15.537	15.547	15.559
0.45	9.367	9.344	9.312	9.917	9.738	9.556	10.469	9.512	9.848	14.104	14.109	14.111	14.093	14.097
0.50	8.677	8.673	8.659	9.158	9.050	8.927	9.662	9.238	9.486	12.837	12.844	12.847	12.818	12.817
0.60	7.667	7.683	7.689	8.012	8.003	7.969	8.396	8.718	8.783	10.784	10.790	10.793	10.767	10.763
0.70	6.980	6.994	7.005	7.234	7.266	7.280	7.515	8.025	7.963	9.291	9.293	9.294	9.283	9.279
0.80	6.445	6.451	6.458	6.664	6.699	6.728	6.888	7.225	7.121	8.227	8.227	8.227	8.227	8.225
0.90	5.962	5.961	5.963	6.188	6.210	6.233	6.398	6.485	6.402	7.467	7.465	7.465	7.471	7.470
1.00	5.489	5.484	5.482	5.744	5.748	5.758	5.968	5.887	5.851	6.904	6.902	6.901	6.909	6.909
1.10	5.018	5.011	5.006	5.305	5.295	5.291	5.556	5.415	5.425	6.459	6.457	6.457	6.463	6.463
1.20	4.556	4.549	4.543	4.869	4.849	4.834	5.147	5.015	5.055	6.080	6.079	6.079	6.082	6.082
1.30	4.115	4.109	4.103	4.442	4.418	4.397	4.741	4.642	4.692	5.734	5.734	5.734	5.734	5.734
1.40	3.706	3.701	3.695	4.035	4.010	3.985	4.344	4.274	4.324	5.403	5.403	5.404	5.402	5.401
1.50	3.335	3.330	3.325	3.655	3.631	3.606	3.965	3.911	3.954	5.079	5.080	5.080	5.077	5.076
1.60	3.004	3.001	2.996	3.309	3.286	3.264	3.610	3.563	3.597	4.761	4.762	4.762	4.757	4.756
1.70	2.716	2.713	2.709	2.998	2.979	2.959	3.284	3.239	3.265	4.449	4.450	4.450	4.445	4.444
1.80	2.467	2.464	2.461	2.724	2.708	2.690	2.991	2.946	2.967	4.146	4.147	4.148	4.142	4.141
1.90	2.254	2.252	2.249	2.485	2.471	2.457	2.729	2.687	2.705	3.856	3.857	3.858	3.852	3.851
2.00	2.074	2.072	2.070	2.278	2.268	2.257	2.500	2.462	2.477	3.581	3.582	3.583	3.578	3.577

Table 1 (continued)

X	$Cu^{\oplus}$	$Cu^{\oplus}$	$Cu^{\oplus}$	$Zn^{2\oplus}$	$Zn^{2\oplus}$	$Zn^{2\oplus}$	$Ga^{3\oplus}$	$Ga^{3\oplus}$	$Ga^{3\oplus}$	$Se^{2\ominus}$	$Se^{2\ominus}$	$Se^{2\ominus}$	$Br^{\ominus}$	$Br^{\ominus}$	$Br^{\ominus}$
		1.05	0.96		0.89	0.74		0.68	0.62		1.98	1.78		1.95	1.75
0.0	28.000	28.000	28.000	28.000	28.000	28.000	28.000	28.000	28.000	36.000	36.000	36.000	36.000	36.000	36.000
0.02	27.945	27.944	27.944	27.957	27.954	27.951	27.964	27.960	27.958	35.740	35.834	35.843	35.844	35.860	35.864
0.04	27.783	27.778	27.776	27.828	27.818	27.807	27.856	27.840	27.832	35.026	35.352	35.386	35.394	35.452	35.467
0.05	27.664	27.655	27.651	27.732	27.717	27.700	27.776	27.750	27.739	34.549	35.006	35.055	35.072	35.156	35.179
0.06	27.519	27.507	27.501	27.615	27.595	27.571	27.678	27.642	27.625	34.021	34.599	34.665	34.695	34.806	34.837
0.08	27.159	27.139	27.130	27.324	27.289	27.249	27.433	27.371	27.343	32.891	33.637	33.736	33.809	33.969	34.016
0.10	26.713	26.685	26.671	26.959	26.908	26.850	27.123	27.032	26.989	31.749	32.536	32.661	32.803	32.994	33.056
0.12	26.192	26.156	26.137	26.526	26.459	26.382	26.754	26.630	26.572	30.646	31.364	31.506	31.738	31.738	32.008
0.14	25.609	25.564	25.542	26.033	25.950	25.856	26.330	26.173	26.099	29.598	30.179	30.326	30.662	30.848	30.922
0.15	25.297	25.249	25.226	25.767	25.677	25.574	26.099	25.926	25.844	29.097	29.597	29.742	30.131	30.304	30.377
0.16	24.974	24.923	24.898	25.489	25.392	25.281	25.856	25.668	25.578	28.609	29.028	29.168	29.610	29.767	29.837
0.18	24.299	24.244	24.217	24.899	24.791	24.667	25.339	25.121	25.017	27.679	27.942	28.066	28.602	28.722	28.785
0.20	23.595	23.538	23.509	24.274	24.158	24.024	24.784	24.541	24.425	26.808	26.937	27.040	27.652	27.733	27.785
0.25	21.766	21.711	21.683	22.601	22.480	22.338	23.271	22.988	22.851	24.870	24.797	24.837	25.540	25.548	25.566
0.30	19.929	19.885	19.861	20.857	20.750	20.618	21.649	21.363	21.220	23.202	23.084	23.076	23.760	23.738	23.732
0.35	18.162	18.132	18.115	19.127	19.044	18.936	19.997	19.738	19.605	21.703	21.616	21.585	22.217	22.193	22.176
0.40	16.514	16.498	16.487	17.474	17.418	17.336	18.378	18.165	18.050	20.299	20.256	20.223	20.823	20.807	20.789
0.45	15.012	15.006	15.001	15.936	15.904	15.848	16.839	16.678	16.586	18.953	18.941	18.917	19.517	19.509	19.496
0.50	13.667	13.669	13.668	14.536	14.523	14.488	15.408	15.299	15.229	17.653	17.656	17.644	18.268	18.264	18.258
0.60	11.451	11.457	11.459	12.176	12.182	12.175	12.936	12.903	12.870	15.219	15.227	15.229	15.906	15.907	15.909
0.70	9.802	9.807	9.809	10.374	10.384	10.388	10.994	10.999	10.989	13.076	13.081	13.086	13.768	13.770	13.773
0.80	8.609	8.611	8.612	9.042	9.048	9.055	9.527	9.542	9.543	11.283	11.286	11.290	11.919	11.921	11.923
0.90	7.751	7.750	7.750	8.073	8.074	8.079	8.441	8.454	8.459	9.845	9.848	9.850	10.392	10.394	10.394
1.00	7.121	7.120	7.119	7.363	7.362	7.365	7.642	7.649	7.654	8.729	8.730	8.731	9.174	9.176	9.176
1.10	6.638	6.636	6.636	6.829	6.826	6.827	7.045	7.046	7.051	7.876	7.876	7.876	8.227	8.228	8.228
1.20	6.242	6.240	6.240	6.405	6.402	6.403	6.582	6.580	6.584	7.226	7.226	7.226	7.500	7.500	7.500
1.30	5.893	5.892	5.892	6.046	6.044	6.045	6.202	6.200	6.203	6.725	6.725	6.724	6.939	6.939	6.939
1.40	5.568	5.568	5.568	5.723	5.722	5.723	5.872	5.871	5.873	6.327	6.326	6.325	6.500	6.499	6.499
1.50	5.255	5.256	5.256	5.417	5.418	5.419	5.569	5.570	5.572	5.995	5.994	5.994	6.143	6.142	6.143
1.60	4.948	4.949	4.949	5.121	5.123	5.125	5.280	5.283	5.285	5.705	5.705	5.705	5.840	5.840	5.840
1.70	4.646	4.647	4.648	4.830	4.832	4.835	4.998	5.003	5.005	5.439	5.440	5.440	5.571	5.571	5.571
1.80	4.351	4.352	4.353	4.543	4.546	4.549	4.722	4.728	4.730	5.187	5.188	5.188	5.322	5.322	5.322
1.90	4.065	4.066	4.067	4.264	4.267	4.270	4.450	4.458	4.460	4.943	4.944	4.944	5.083	5.083	5.083
2.00	3.791	3.793	3.793	3.993	3.996	3.999	4.185	4.193	4.196	4.702	4.703	4.704	4.850	4.850	4.850

X	$Rb^{\oplus}$	$Rb^{\oplus}$	$Rb^{\oplus}$	$Sr^{2\oplus}$	$Sr^{2\oplus}$	$Sr^{2\oplus}$	$Y^{3\oplus}$	$Y^{3\oplus}$	$Y^{3\oplus}$	Pd	Pd	Pd	Pd	Pd
		1.48	1.43		1.24	1.13		0.97	0.93		1.51	1.37	1.51	1.37
0.0	36.000	36.000	36.000	36.000	36.000	36.000	36.000	36.000	36.000	46.000	46.000	46.000	46.000	46.000
0.02	35.907	35.905	35.904	35.922	35.919	35.917	35.933	35.926	35.925	45.876	45.875	45.874	45.879	45.880
0.04	35.631	35.625	35.622	35.689	35.679	35.672	35.732	35.707	35.702	45.509	45.507	45.504	45.521	45.528
0.05	35.428	35.420	35.414	35.518	35.502	35.492	35.584	35.546	35.538	45.241	45.237	45.233	45.259	45.268
0.06	35.185	35.174	35.166	35.311	35.290	35.276	35.405	35.352	35.340	44.919	44.913	44.909	44.945	44.958
0.08	34.588	34.571	34.558	34.801	34.766	34.743	34.960	34.872	34.852	44.132	44.123	44.116	44.175	44.197
0.10	33.867	33.844	33.826	34.175	34.126	34.093	34.410	34.283	34.255	43.184	43.171	43.161	43.244	43.275
0.12	33.047	33.019	32.997	33.453	33.391	33.350	33.768	33.604	33.568	42.111	42.094	42.081	42.187	42.227
0.14	32.158	32.127	32.102	32.656	32.584	32.536	33.052	32.856	32.811	40.949	40.930	40.915	41.040	41.087
0.15	31.696	31.664	31.639	32.236	32.161	32.110	32.671	32.461	32.413	40.346	40.325	40.309	40.442	40.492
0.16	31.226	31.195	31.169	31.806	31.728	31.675	32.278	32.056	32.005	39.733	39.712	39.695	39.834	39.886
0.18	30.277	30.247	30.222	30.923	30.843	30.787	31.462	31.224	31.169	38.491	38.468	38.451	38.597	38.653
0.20	29.331	29.305	29.281	30.026	29.948	29.893	30.621	30.377	30.320	37.246	37.223	37.205	37.353	37.409
0.25	27.077	27.063	27.049	27.816	27.759	27.715	28.495	28.279	28.227	34.227	34.208	34.193	34.319	34.368
0.30	25.079	25.076	25.071	25.781	25.753	25.728	26.467	26.320	26.281	31.457	31.444	31.434	31.518	31.551
0.35	23.356	23.361	23.363	23.986	23.984	23.976	24.630	24.561	24.539	28.995	28.990	28.985	29.024	29.041
0.40	21.866	21.872	21.877	22.427	22.439	22.443	23.011	23.004	22.997	26.856	26.856	26.855	26.858	26.861

Table 1 (continued)

X	$Rb^{\oplus}$	$Rb^{\oplus}$	$Rb^{\oplus}$	$Sr^{2\oplus}$	$Sr^{2\oplus}$	$Sr^{2\oplus}$	$Y^{3\oplus}$	$Y^{3\oplus}$	$Y^{3\oplus}$	Pd	Pd	Pd	Pd	Pd
0.45	20.544	20.549	20.553	21.059	21.075	21.084	21.592	21.621	21.625	25.025	25.028	25.030	25.010	25.004
0.50	19.334	19.336	19.340	19.832	19.845	19.855	20.332	20.375	20.383	23.472	23.477	23.480	23.450	23.439
0.60	17.107	17.106	17.107	17.634	17.637	17.643	18.130	18.160	18.170	21.028	21.032	21.035	21.008	20.997
0.70	15.053	15.052	15.052	15.631	15.629	15.629	16.166	16.174	16.179	19.161	19.163	19.164	19.153	19.148
0.80	13.184	13.183	13.183	13.785	13.782	13.781	14.353	14.349	14.349	17.586	17.586	17.585	17.588	17.589
0.90	11.546	11.546	11.545	12.128	12.126	12.124	12.697	12.689	12.686	16.139	16.138	16.137	16.146	16.149
1.00	10.167	10.167	10.167	10.695	10.694	10.692	11.231	11.222	11.219	14.755	14.754	14.753	14.762	14.766
1.10	9.045	9.044	9.044	9.499	9.498	9.496	9.976	9.969	9.966	13.428	13.427	13.426	13.434	13.436
1.20	8.152	8.152	8.152	8.529	8.528	8.527	8.935	8.930	8.928	12.178	12.177	12.177	12.181	12.183
1.30	7.453	7.453	7.453	7.757	7.756	7.756	8.092	8.089	8.088	11.029	11.028	11.028	11.030	11.030
1.40	6.907	6.907	6.907	7.149	7.149	7.149	7.419	7.418	7.418	9.998	9.998	9.998	9.999	9.999
1.50	6.475	6.475	6.475	6.669	6.669	6.669	6.886	6.886	6.886	9.097	9.097	9.097	9.097	9.097
1.60	6.124	6.124	6.124	6.285	6.285	6.285	6.460	6.461	6.461	8.323	8.323	8.323	8.323	8.323
1.70	5.829	5.830	5.830	5.967	5.968	5.968	6.114	6.115	6.115	7.670	7.670	7.670	7.670	7.670
1.80	5.571	5.571	5.571	5.696	5.697	5.697	5.825	5.826	5.826	7.125	7.125	7.125	7.125	7.125
1.90	5.335	5.335	5.335	5.455	5.455	5.455	5.574	5.574	5.575	6.673	6.673	6.673	6.673	6.673
2.00	5.112	5.112	5.112	5.232	5.232	5.232	5.347	5.348	5.348	6.297	6.297	6.297	6.298	6.298

X	$Ag^{\oplus}$	$Ag^{\oplus}$	$Ag^{\oplus}$	$Cd^{2\oplus}$	$Cd^{2\oplus}$	$Cd^{2\oplus}$	$I^{\ominus}$	$I^{\ominus}$	$I^{\ominus}$	$Cs^{\oplus}$	$Cs^{\oplus}$	$Cs^{\oplus}$	$Ba^{2\oplus}$	$Ba^{2\oplus}$	$Ba^{2\oplus}$
		1.26	1.13		1.07	0.97		2.38	2.16		1.69	1.52		1.46	1.35
0.0	46.000	46.000	46.000	46.000	46.000	46.000	54.000	54.000	54.000	54.000	54.000	54.000	54.000	54.000	54.000
0.02	45.899	45.898	45.897	45.914	45.912	45.910	53.768	53.783	53.788	53.846	53.843	53.842	53.867	53.863	53.860
0.04	45.599	45.596	45.593	45.658	45.649	45.644	53.098	53.155	53.173	53.392	53.383	53.376	53.473	53.458	53.448
0.05	45.377	45.372	45.368	45.469	45.455	45.446	52.622	52.704	52.730	53.061	53.047	53.037	53.183	53.162	53.147
0.06	45.111	45.104	45.097	45.240	45.221	45.208	52.068	52.175	52.209	52.665	52.646	52.634	52.836	52.808	52.787
0.08	44.451	44.439	44.429	44.671	44.638	44.617	50.778	50.926	50.974	51.704	51.676	51.656	51.986	51.943	51.912
0.10	43.642	43.624	43.610	43.964	43.916	43.886	49.333	49.500	49.557	50.556	50.521	50.496	50.955	50.901	50.861
0.12	42.707	42.683	42.666	43.138	43.075	43.034	47.821	47.983	48.041	49.274	49.234	49.207	49.785	49.723	49.677
0.14	41.671	41.643	41.622	42.209	42.133	42.084	46.308	46.444	46.497	47.907	47.868	47.840	48.516	48.451	48.402
0.15	41.124	41.094	41.071	41.713	41.631	41.578	45.565	45.684	45.732	47.207	47.169	47.141	47.857	47.792	47.743
0.16	40.561	40.530	40.505	41.199	41.111	41.055	44.837	44.936	44.979	46.502	46.466	46.440	47.187	47.124	47.074
0.18	39.400	39.366	39.340	40.126	40.030	39.968	43.434	43.493	43.524	45.096	45.066	45.043	45.832	45.774	45.727
0.20	38.211	38.176	38.148	39.010	38.908	38.843	42.109	42.132	42.151	43.719	43.696	43.678	44.481	44.431	44.389
0.25	35.227	35.195	35.170	36.136	36.038	35.974	39.130	39.100	39.096	40.517	40.512	40.506	41.258	41.233	41.209
0.30	32.390	32.367	32.349	33.314	33.238	33.187	36.529	36.492	36.480	37.725	37.731	37.733	38.380	38.379	38.372
0.35	29.822	29.810	29.799	30.693	30.647	30.614	34.169	34.146	34.136	35.289	35.297	35.303	35.866	35.877	35.883
0.40	27.570	27.568	27.565	28.354	28.336	28.320	31.968	31.961	31.955	33.105	33.111	33.116	33.644	33.659	33.670
0.45	25.639	25.643	25.646	26.321	26.326	26.324	29.903	29.905	29.904	31.094	31.097	31.100	31.635	31.647	31.658
0.50	24.002	24.010	24.015	24.585	24.603	24.610	27.983	27.988	27.989	29.218	29.218	29.220	29.779	29.786	29.794
0.60	21.437	21.445	21.450	21.863	21.885	21.897	24.638	24.641	24.643	25.852	25.850	25.849	26.439	26.437	26.437
0.70	19.511	19.515	19.517	19.851	19.863	19.871	21.988	21.989	21.990	23.044	23.043	23.041	23.591	23.587	23.583
0.80	17.928	17.928	17.928	18.247	18.248	18.250	19.952	19.952	19.953	20.802	20.801	20.801	21.263	21.260	21.256
0.90	16.505	16.503	16.502	16.846	16.841	16.838	18.371	18.370	18.370	19.047	19.046	19.046	19.417	19.416	19.414
1.00	15.158	15.156	15.154	15.538	15.531	15.527	17.076	17.075	17.075	17.649	17.649	17.649	17.952	17.952	17.952
1.10	13.864	13.862	13.860	14.279	14.274	14.270	15.937	15.936	15.936	16.480	16.480	16.480	16.749	16.750	16.750
1.20	12.630	12.629	12.628	13.068	13.065	13.062	14.873	14.873	14.872	15.438	15.438	15.438	15.702	15.703	15.703
1.30	11.478	11.478	11.477	11.920	11.919	11.917	13.845	13.845	13.844	14.457	14.458	14.458	14.736	14.736	14.737
1.40	10.428	10.428	10.428	10.857	10.856	10.855	12.842	12.842	12.842	13.507	13.507	13.507	13.808	13.809	13.809
1.50	9.493	9.493	9.493	9.894	9.894	9.894	11.873	11.873	11.873	12.578	12.578	12.578	12.903	12.903	12.902
1.60	8.677	8.677	8.677	9.042	9.042	9.042	10.951	10.952	10.952	11.677	11.677	11.677	12.018	12.018	12.018
1.70	7.979	7.979	7.979	8.303	8.302	8.302	10.092	10.092	10.092	10.816	10.815	10.815	11.164	11.164	11.164
1.80	7.389	7.389	7.389	7.671	7.670	7.670	9.306	9.306	9.306	10.007	10.007	10.007	10.353	10.353	10.353
1.90	6.896	6.896	6.896	7.137	7.137	7.136	8.600	8.601	8.601	9.262	9.262	9.262	9.597	9.597	9.596
2.00	6.485	6.485	6.485	6.690	6.689	6.689	7.977	7.977	7.977	8.587	8.587	8.587	8.903	8.903	8.903

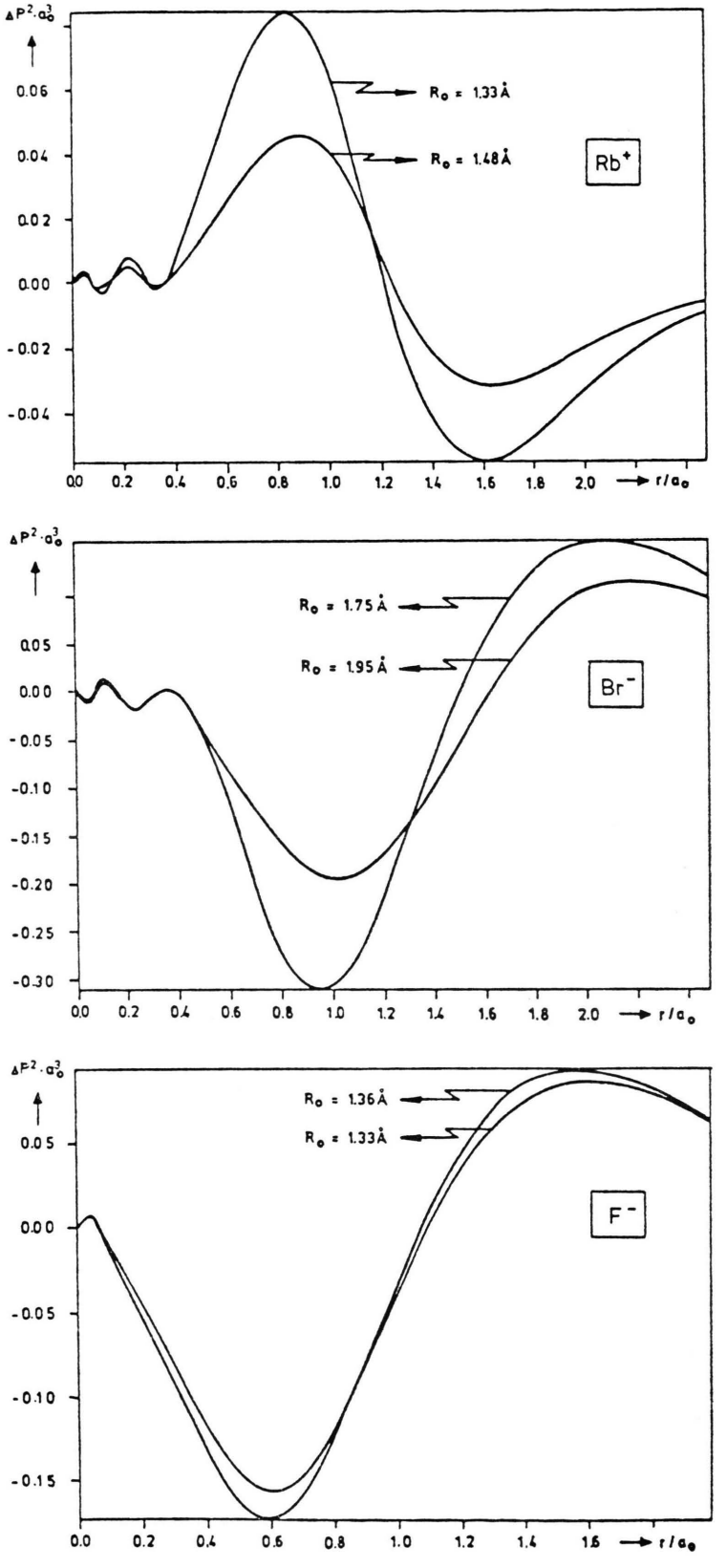

Fig. 3. Difference in the total radial charge density
$P^2(r) = (P^2(r))_{\text{free}} - (P^2(r))_{\text{Watson sphere}}$
for $F^{\ominus}$, $Br^{\ominus}$ and $Rb^{\oplus}$ for two different Watson sphere radii R_0.

more sophisticated quantum mechanical calculation which take configuration interaction into account [20] nor were relativistic effects considered [21]. In good approximation the corrections for anomalious dispersion can be applied to $f_{\text{theor, crystal}}$ in the usual way [22].

Discussion

Comparison of the charge density $P^2(r)$ for the free ions and the ions within the hollow charge sphere shows that the model crystal potential causes an expansion of the electron cloud in the cations and a shrinkage of it in the anions (see Figs. 2 and 3). The influence of the crystal potential on the electron distribution is larger for anions than for cations, an effect which is due to the more loosely bonded valence shell electrons of the anions in comparison with the cations.

The shrinkage of the anion electron cloud within the crystal potential induces an increase of the atomic scattering factor f for small $\sin\vartheta/\lambda$. This is shown in Fig. 4 for $F^{\ominus}$.

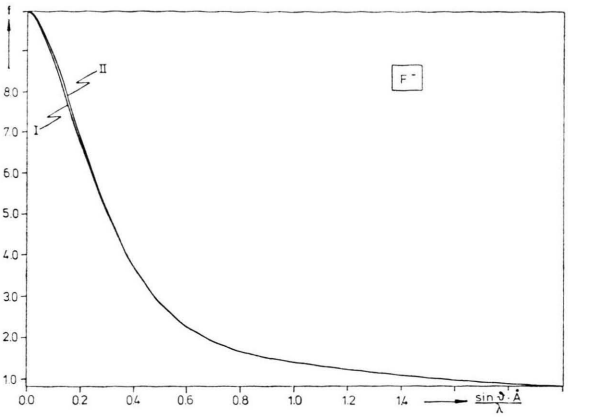

Fig. 4. Atomic scattering factor f for $F^{\ominus}$. Curve I shows f for the free ion whereas curve II gives f for the ion in the Watson sphere.

In contrast, the atomic scattering factors f_{cation} are lowered by the Watson-sphere potential (see Table 1 and Figure 5). Analogously with the density function $P^2(r)$ the effect of the crystal potential on the atomic scattering factor is larger for anions than for cations. Considering for example the ion $F^{\ominus}$ the maximum of the relative deviation

$$\frac{\Delta f}{f} = \frac{(f_{\text{theor, free}} - f_{\text{theor, crystal}})}{f_{\text{theor, free}}} \qquad (9)$$

is found at $\sin\vartheta/\lambda = 0.16$ Å^{-1} and is equal to -2%, whereas for $Na^{\oplus}$ $(\Delta f/f)_{\max}$ at $\sin\vartheta/\lambda = 0.40$ Å^{-1} is 0.1 to 0.2%, depending on the choosen Watson sphere radius (see Table 1).

Table 2 gives $(\Delta f)_{\max}$ and $(\Delta f/f)_{\max}$ for some ions. It shows that for equally charged ions $(\Delta f)_{\max}$ increases with increasing atomic number. For single charged negative ions $(\Delta f/f)_{\max}$ is decreasing with increasing atomic number Z because $f(\sin\vartheta/\lambda = 0) = Z + 1$ increases linearly with Z, whereas the spherical crystal potential influences mainly the valence shell electrons, which are constant in number within this series. Therefore f is increasing faster with Z than Δf.

For single charged positive ions the (small) change of f_{crystal} compared to f_{free} is sensitive to the chosen Watson sphere radius, and no general trend for $(\Delta f/f)_{\max}$ for these ions is found. Twofold (and three fold) positive ions show larger $(\Delta f/f)_{\max}$ than singly ionized iones because of the stronger crystal potential (see Figure 3). The large changes Δf for the multiple charged ions is somewhat surprising. One reason for this effect may be that the Watson sphere model overestimates the true crystal potential for these ions. This assumption is supported by the fact that for the multiple charged ions considerable electron density (between 1.5 to 3 electrons) is found outside the hollow charged sphere.

The strongest effect of the crystal potential on the atomic scattering factors is experienced by the twofold and threefold negative ions. The free ion atomic scattering factor for these ions, given in Table 1, has no physical meaning because they are unstable in the gaseous phase. A comparison of the f_{free} and f_{crystal} for multiple charged negative ions is therefore of no use. The two- and threefold negative ions have extremely weakly bonded electrons in the outermost shell, where from a distinct difference up to 10% in the atomic scattering factors for the same ion within different crystal potentials (different Watson sphere radii in our model) results.

It will be of interest to apply $f_{\text{theor, crystal}}$ to experimentally well investigated ionic crystals, such as the alkali halides and oxides and other halides with simple crystal structures.

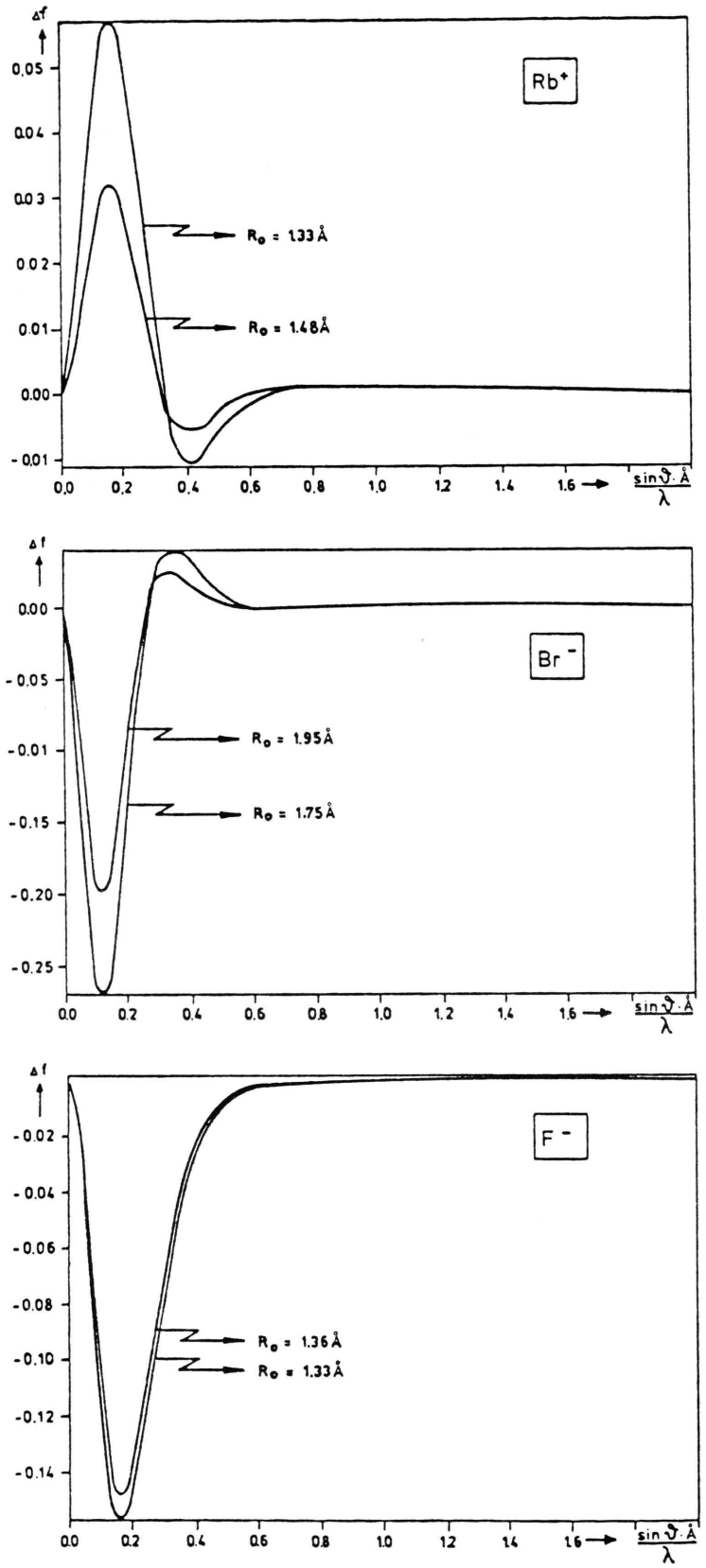

Fig. 5. Difference in the atomic scattering factor $\Delta f = f_{\text{free}} - f_{\text{Watson sphere}}$ for $F^{\ominus}$, $Br^{\ominus}$ and $Rb^{\oplus}$ for two different Watson sphere radii R_0.

Table 2. Differences ($f_{\text{free ion}} - f_{\text{ion crystal}}$) $= \Delta f$ at the point $(\sin \vartheta/\lambda)_{\max}$ where the relative deviation $\Delta f/f_{\text{free}}$ is a maximum; λ in Å.

Ion	$(\sin \vartheta/\lambda)_{\max}$	$\Delta f \cdot 10^2$	$\Delta f/f$
F^-	0.15	− 0.148	− 1.91
Cl^-	0.15	− 0.177	− 1.29
Br^-	0.12	− 0.250	− 0.63
Na^+	0.35	0.007	0.11
K^+	0.20	0.028	0.17
Rb^+	0.15	0.032	0.10
Mg^{2+}	0.45	0.062	0.64
Ca^{2+}	0.25	0.070	0.78
Sr^{2+}	0.18	0.080	0.26
Al^{3+}	0.45	0.101	1.62
Sc^{3+}	0.25	0.121	0.89
Y^{3+}	0.20	0.244	0.80

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