

other than $3d^n$ for which the calculations were carried out.

Comparison with experiment

There have been very few experimental determinations of the incoherent scattering intensities (for C, Al, KCl, CaF₂ and NaCl) but these have not included any of the atoms considered in this paper. While the agreement between theory and experiment has been very good for these cases, it would be valuable to have accurate measurements for the transition elements, both for their own inherent interest and to compare with theory in order to test its validity. While the experiments are not easy to perform we hope that they will soon be undertaken.

APPENDIX A

We give in Table 3 a listing of the atoms and ions for which accurate incoherent scattering functions are now known in order to provide a convenient summary of the data available to date. The results of the present work are not included.

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Some Calculations using the Ewald Transformation

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The calculation of the energy, dispersion relations of the normal modes, and elastic constants of a crystal requires a knowledge of the long-range Coulomb interactions between the atoms. The summations involved can be expressed in dimensionless form and converted to a rapidly convergent form by using the Ewald transformation. Machine programs have been written to calculate the Madelung coefficients, Coulomb coefficients, and the expansions of the Coulomb coefficients, (which are required to calculate the elastic constants), for crystals which have at least orthorhombic symmetry. Both the Madelung coefficients, and the Coulomb coefficients for wave-vectors parallel to the ferro-electric axis, have been calculated for barium titanate, using the atomic positions both of the paraelectric phase and of the ferroelectric phase at 20 °C.

The total energy of a non-metallic crystal is usually divided into two parts—one from the Coulomb interaction of point charges, dipoles and higher multipole moments representing the long-range interactions between the atoms in the crystal, and the other from

the short-range or repulsive forces. Although the potential for the interaction of point charges and multipoles is readily obtained from classical electrostatics, the short-range interaction is essentially of a quantum-mechanical nature, and cannot usually be

calculated explicitly. If however the short-range interaction between different pairs of atoms within the crystal is either known or assumed to have some particular form, then the contributions from the short-range interactions to both the energy of the crystal and the forces on an atom are obtained by summing these interactions over comparatively few atoms. On the other hand the potential for the Coulomb interaction is easily obtained but the long-range nature of the force makes the summation much more difficult. The summations involved can however be made more rapidly convergent by using the Ewald transformation, (Ewald, 1920; Born & Huang, 1954), which is based on the identity

$$1/|\mathbf{x}(l) - \mathbf{x}| = 2/\sqrt{\pi} \int_0^\infty \exp -|\mathbf{x}(l) - \mathbf{x}|^2 \varrho^2 d\varrho. \quad (1)$$

The contribution to the energy of the crystal from the interaction of an atom at $\mathbf{x}(k)$ carrying charge z_k with atoms at $\mathbf{x}(k')$ having charge $z_{k'}$ is given by

$$z_k z_{k'} \alpha_{kk'}/r = z_k z_{k'} \frac{1}{2} \sum_{l'} 1/|\mathbf{x}(k') - \mathbf{x}(l)|.$$

The prime over the summation sign indicates the omission of the term $(k) = (k')$, and r is any convenient characteristic dimension of the lattice.

The total electrostatic or Madelung energy is then given by

$$\sum_{kk'} z_k z_{k'} \alpha_{kk'}/r.$$

The coefficients $\alpha_{kk'}$ are dimensionless and can be written as two rapidly convergent sums, one in real space and the other in reciprocal space, (Born & Huang, 1954), giving

$$\alpha_{kk'} = \frac{1}{2} c \sum_{l'} H(c|\mathbf{x}(k') - \mathbf{x}(l)|/r) - \delta_{kk'} c/\sqrt{\pi} + \pi/2c^2 s \sum_h G(\pi^2 |\mathbf{b}(h)|^2 r^2/c^2) \exp [2\pi i \mathbf{b}(h) \cdot \mathbf{x}(k')], \quad (2)$$

where

$$H(x) = (2/\sqrt{\pi}) (1/x) \int_x^\infty \exp(-\varrho^2) d\varrho,$$

$$G(x) = (1/x) \exp(-x),$$

and

$$\mathbf{x}(k') = \mathbf{x}(k) - \mathbf{x}(l);$$

the volume of a unit cell is $v = sr^3$, $\mathbf{b}(h)$ is a reciprocal-lattice vector and c is a number which is chosen so that the convergence is obtained as rapidly as possible.

The forces between the effective dipoles created at the atomic sites during the lattice vibrations can be calculated in a similar way. If the total dipole associated with the atomic site (k') is

$$\mathbf{p}(k') = \mathbf{p}(k') \exp [2\pi i \mathbf{y} \cdot \mathbf{x}(k')]$$

then the α component of the electric field at $\mathbf{x}(k)$ due to these dipoles is given by

$$E_\alpha \exp [2\pi i \mathbf{y} \cdot \mathbf{x}(k)] = \sum_\beta p_\beta(k') \frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} \sum_{l'} \frac{\exp [2\pi i \mathbf{y} \cdot \mathbf{x}(k')]}{|\mathbf{x}(k') - \mathbf{x}(l)|}.$$

The forces can then be expressed in terms of dimensionless Coulomb coefficients $C_{\alpha\beta}^{(y)}(kk')$ defined by

$$C_{\alpha\beta}^{(y)}(kk') = -v \left[\frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} \sum_{l'} \frac{\exp [2\pi i \mathbf{y} \cdot \mathbf{x}(k')]}{|\mathbf{x}(k') - \mathbf{x}(l)|} \right] \times \exp 2\pi i \mathbf{y} \cdot \mathbf{x}(k').$$

The part of this expression which is enclosed in the brackets is periodic in \mathbf{y} and all the distinct values are obtained if we restrict \mathbf{y} to one reciprocal lattice cell. The exponential term outside depends on the phase factors which are chosen to describe the electric field and the dipoles or, for the lattice vibrations, on the phase factors of the displacements. Although the phases will in general vary as \mathbf{y} changes by a reciprocal-lattice vector, the frequencies of the lattice vibrations will not. It is therefore necessary to tabulate these Coulomb coefficients only within one reciprocal-lattice cell.

The Coulomb coefficients can be transformed by using the transformation (1) to give (Born & Huang, 1954),

$$C_{\alpha\beta}^{(y)}(kk') = -c^3 s \sum_{l'} H_{\alpha\beta}(c|\mathbf{x}(k') - \mathbf{x}(l)|/r) \exp [2\pi i \mathbf{y} \cdot \mathbf{x}(k')] + (4\pi^2 r^2/c^2) \sum_h (b_\alpha(h) + y_\alpha)(b_\beta(h) + y_\beta) G(\pi^2 |\mathbf{b}(h) + \mathbf{y}|^2 r^2/c^2) \times \exp [2\pi i \mathbf{b}(h) \cdot \mathbf{x}(k')], \quad (3)$$

where

$$H_{\alpha\beta}(|\mathbf{x}|) = \frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} H(|\mathbf{x}|).$$

The term corresponding to the dipole at (k) must be eliminated in calculating the forces or effective field at (k) and this is done by replacing $H(|\mathbf{x}|)$ by $H^0(|\mathbf{x}|)$, when $l=0$ and $k'=k$, such that

$$H^0(|\mathbf{x}|) = -\frac{2}{\sqrt{\pi} x} \int_0^x \exp(-\varrho^2) d\varrho.$$

It is also well known that the value of the term involving $h=0$ in the second summation is ambiguous when $y=0$ and can be associated with the macroscopic field (Born & Huang, 1954). This term may however be calculated by taking the limit as $\mathbf{y} \rightarrow 0$ in a particular specified direction.

The elastic constants are obtained from the expansions of the Coulomb coefficients near wave number zero, (Born & Huang, 1954). The coefficients may be expanded in dimensionless form as:

$$C_{\alpha\beta}^{(\varepsilon y)}(kk') = C_{\alpha\beta}^{(0)}(kk') + i\varepsilon \sum_\gamma C_{\alpha\beta,\gamma}^{(1)}(kk') y_\gamma a_\gamma + \frac{1}{2} \varepsilon^2 \sum_{\gamma\lambda} C_{\alpha\beta,\gamma\lambda}^{(2)}(kk') y_\gamma y_\lambda a_\gamma a_\lambda + \dots$$

a_γ is the repeat distance along the γ axis. It then follows that

$$\begin{aligned}
C_{\alpha\beta,\gamma}^{(1)}(kk') = & -2\pi c^3 s \sum_{\nu} H_{\alpha\beta} \left(\frac{c|\mathbf{x}(k' \frac{0}{k})|}{r} \right) \frac{x_{\nu}(k' \frac{0}{k})}{a_{\nu}} \\
& - \frac{4\pi^3 r^2 i}{c^2 a_{\gamma}} \sum_h \left[(b_{\alpha}(h) \delta_{\beta\gamma} + b_{\beta}(h) \delta_{\alpha\gamma}) G \left(\frac{\pi^2 |\mathbf{b}(h)|^2 r^2}{c^2} \right) \right. \\
& \left. + \frac{2\pi^2 r^2}{c^2} b_{\alpha}(h) b_{\beta}(h) b_{\gamma}(h) G' \left(\frac{\pi^2 |\mathbf{b}(h)|^2 r^2}{c^2} \right) \right] \\
& \times \exp [2\pi i \mathbf{b}(h) \cdot \mathbf{x}(k' \frac{0}{k})], \quad (4)
\end{aligned}$$

while the second-order coefficient is

$$\begin{aligned}
C_{\alpha\beta,\gamma\lambda}^{(2)}(kk') = & -\frac{4\pi^3 r^2}{c^2} (\delta_{\alpha\gamma} \delta_{\beta\lambda} + \delta_{\alpha\lambda} \delta_{\beta\gamma}) \\
& + 4\pi^2 c^3 s \sum_{\nu} H_{\alpha\beta} \left(\frac{c|\mathbf{x}(k' \frac{0}{k})|}{r} \right) \frac{x_{\nu}(k' \frac{0}{k}) x_{\lambda}(k' \frac{0}{k})}{a_{\nu} a_{\lambda}} \\
& + \frac{4\pi^3 r^2}{c^2 a_{\gamma} a_{\lambda}} \sum_h \left[(\delta_{\beta\gamma} \delta_{\alpha\lambda} + \delta_{\beta\lambda} \delta_{\alpha\gamma}) G \left(\frac{\pi^2 |\mathbf{b}(h)|^2 r^2}{c^2} \right) \right. \\
& \left. + \frac{4\pi^4 r^4}{c^4} b_{\alpha}(h) b_{\beta}(h) b_{\gamma}(h) b_{\lambda}(h) G'' \left(\frac{\pi^2 |\mathbf{b}(h)|^2 r^2}{c^2} \right) \right. \\
& \left. + \frac{2\pi^2 r^2}{c^2} (b_{\alpha}(h) b_{\beta}(h) \delta_{\gamma\lambda} + b_{\alpha}(h) b_{\gamma}(h) \delta_{\beta\lambda} + b_{\alpha}(h) b_{\lambda}(h) \delta_{\beta\gamma} \right. \\
& \left. + b_{\beta}(h) b_{\gamma}(h) \delta_{\alpha\lambda} + b_{\beta}(h) b_{\lambda}(h) \delta_{\alpha\gamma}) G' \left(\frac{\pi^2 |\mathbf{b}(h)|^2 r^2}{c^2} \right) \right] \\
& \times \exp [2\pi i \mathbf{b}(h) \cdot \mathbf{x}(k' \frac{0}{k})]. \quad (5)
\end{aligned}$$

This expression differs from that of Born & Huang (1954) who include a term

$$\delta_{\alpha\beta} b_{\gamma}(h) b_{\lambda}(h)$$

in the last part of the expression; we can find no justification for this.

Machine programs have been written for the Edsac II which calculate the expressions (2), (3), (4) and (5) for structures for which orthogonal axes can be chosen; the summation is then performed over all the points on a simple orthorhombic lattice. The lattice is specified by the two axial ratios, a_1/a_3 and a_2/a_3 , while the lattice parameter r is chosen to be a_3 . The adjustable number c is fixed at π , for which value the time taken for the calculations was found usually to be a minimum. The summation is performed on successively larger and larger rectangular volumes in both real and reciprocal space and is stopped when the partial sum over all the points lying outside one of the volumes but inside the next is less in magnitude than some predetermined value.

The coefficients can be calculated for any point k' in the unit cell and by combining several coefficients, it is possible to obtain the coefficients for all structures with orthorhombic or higher symmetry. Provision is included within the programs for calculating the coefficients of face-centred and body-centred structures, and also for the printing of either the real or both the real and imaginary parts of the Coulomb coefficients.

The Coulomb coefficients and the partial Madelung coefficients have been calculated for the Perovskite structure; the Coulomb coefficients have been calculated for a series of wave-numbers parallel to the

ferro-electric axis of barium titanate, $\langle 001 \rangle$. They have been calculated both for the atomic positions in the undistorted paraelectric phase and for the tetragonal ferro-electric phase, using the axial ratio obtained by Rhodes (1951), and the atomic positions measured by Frazer, Danner & Pepinsky (1955).

The axial ratio of the tetragonal ferroelectric phase at 20 °C. $a_1/a_3 = 0.9892$.

The atomic positions		
Atom	Paraelectric phase	Ferroelectric phase
Ti	(0 0 0)	(0 0 0)
Ba	(0.5 0.5 0.5)	(0.5 0.5 0.486)
O _I	(0 0 0.5)	(0 0 0.463)
O _{II}	(0.5 0 0)	(0.5 0 -0.028)
O _{III}	(0 0.5 0)	(0 0.5 -0.028)

Four different sets of coefficients are needed to describe the Madelung electrostatic interactions in the paraelectric phase while eight are needed in the ferroelectric one.

Partial Madelung coefficients

Interaction	Paraelectric phase	Ferroelectric phase
Ti-Ti(Ba-Ba)(O-O)	1.25950	1.26625
Ti-Ba	0.24181	0.24107
Ti-O _I	-0.11119	-0.11503
Ti-O _{II} (Ti-O _{III})	-0.11119	-0.11776
Ba-O _I	0.13210	0.12617
Ba-O _{II} (Ba-O _{III})	0.13210	0.13290
O _I -O _{II} (O _I -O _{III})	0.13210	0.13316
O _{II} -O _{III}	0.13210	0.12554

Coulomb coefficients

The Coulomb coefficients have been calculated for a wave-vector parallel to the ferro-electric axis $\langle 0, 0, 1 \rangle$ and are described by $q = ya_3$. A reasonable survey of the coefficients is obtained if we divide the range of q , within one zone, $-0.5 < q \leq 0.5$, into tenths. The frequencies of the lattice vibrations will then be the same for q and $-q$ and the coefficients are tabulated in the range $0 \leq q \leq 0.5$. Moreover each atom is situated on a centre of symmetry in the paraelectric phase and so there is no imaginary part to the Coulomb coefficients in that phase.

Paraelectric phase

Ti-Ti interaction			
Wave-vector	$C_{\alpha\beta}(kk') = C_{11}(\text{Ti-Ti})$	$C_{22}(\text{Ti-Ti})$	$C_{33}(\text{Ti-Ti})$
q	11	22	33
0.5	-4.844	-4.844	9.687
0.4	-4.782	-4.782	9.563
0.3	-4.618	-4.618	9.236
0.2	-4.416	-4.416	8.832
0.1	-4.252	-4.252	8.503
0	-4.189	-4.189	8.378
Ti-Ba interaction			
q	11	22	33
0.5	0	0	0
0.4	-1.281	-1.281	2.561
0.3	-2.443	-2.443	4.886
0.2	-3.375	-3.375	6.750
0.1	-3.979	-3.979	7.958
0	-4.189	-4.189	8.378

Ti-O _I interaction			
<i>q</i>	11	22	33
0.5	0	0	0
0.4	3.339	3.339	-6.678
0.3	6.359	6.359	-12.717
0.2	8.765	8.765	-17.530
0.1	10.316	10.316	-20.632
0	10.852	10.852	-21.704

Ti-O _{II} interaction			
<i>q</i>	11	22	33
0.5	-33.622	10.323	23.299
0.4	-33.684	10.373	23.311
0.3	-33.845	10.505	23.341
0.2	-34.046	10.668	23.377
0.1	-34.208	10.801	23.407
0	-34.271	10.852	23.419

Ba-O _I interaction			
<i>q</i>	11	22	33
0.5	-7.996	-7.996	15.992
0.4	-8.046	-8.046	16.091
0.3	-8.177	-8.177	16.354
0.2	-8.340	-8.340	16.679
0.1	-8.472	-8.472	16.944
0	-8.523	-8.523	17.045

Ba-O _{II} interaction			
<i>q</i>	11	22	33
0.5	0	0	0
0.4	1.370	-2.619	1.249
0.3	2.614	-4.989	2.376
0.2	3.610	-6.880	3.271
0.1	4.255	-8.101	3.846
0	4.479	-8.523	4.044

Ferroelectric phase

Ti-Ti interaction								
<i>q</i>	11		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-4.874	0	-4.874	0	9.748	0	9.748	0
0.4	-4.815	0	-4.815	0	9.630	0	9.630	0
0.3	-4.662	0	-4.662	0	9.323	0	9.323	0
0.2	-4.471	0	-4.471	0	8.942	0	8.942	0
0.1	-4.317	0	-4.317	0	8.633	0	8.633	0
0	-4.258	0	-4.258	0	8.515	0	8.515	0

Ti-Ba interaction								
<i>q</i>	11		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-0.012	-0.278	-0.012	-0.278	0.024	0.555	0.024	0.555
0.4	-1.273	-0.220	-1.273	-0.220	2.546	0.440	2.546	0.440
0.3	-2.416	-0.162	-2.416	-0.162	4.833	0.324	4.833	0.324
0.2	-3.332	-0.106	-3.332	-0.106	6.665	0.212	6.665	0.212
0.1	-3.926	-0.052	-3.926	-0.052	7.853	0.105	7.853	0.105
0	-4.132	0	-4.132	0	8.264	0	8.264	0

Ti-O _I interaction								
<i>q</i>	11		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	0.366	3.131	0.366	3.131	-0.731	-6.262	-0.731	-6.262
0.4	3.656	2.671	3.656	2.671	-7.312	-5.342	-7.312	-5.342
0.3	6.622	2.097	6.622	2.097	-13.244	-4.194	-13.244	-4.194
0.2	8.980	1.441	8.980	1.441	-17.961	-2.853	-17.961	-2.853
0.1	10.499	0.733	10.499	0.733	-20.997	-1.467	-20.997	-1.467
0	11.023	0	11.023	0	-22.046	0	-22.046	0

Ti-O _{II} interaction										
<i>q</i>	11		22		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-33.565	2.960	10.340	-0.912	23.225	-2.048	23.225	-2.048	23.225	-2.048
0.4	-33.673	2.340	10.404	-0.708	23.268	-1.632	23.268	-1.632	23.268	-1.632
0.3	-33.864	1.735	10.542	-0.516	23.322	-1.219	23.322	-1.219	23.322	-1.219
0.2	-34.081	1.146	10.707	-0.336	23.375	-0.810	23.375	-0.810	23.375	-0.810
0.1	-34.252	0.569	10.839	-0.165	23.413	-0.404	23.413	-0.404	23.413	-0.404
0	-34.316	0	10.889	0	23.428	0	23.428	0	23.428	0

Ba-O _I interaction										
<i>q</i>	11		22		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-8.047	0.582	-8.047	0.582	16.095	-1.165	16.095	-1.165	16.095	-1.165
0.4	-8.104	0.448	-8.104	0.448	16.208	-0.897	16.208	-0.897	16.208	-0.897
0.3	-8.235	0.324	-8.235	0.324	16.470	-0.648	16.470	-0.648	16.470	-0.648
0.2	-8.395	0.210	-8.395	0.210	16.789	-0.419	16.789	-0.419	16.789	-0.419
0.1	-8.523	0.103	-8.523	0.103	17.046	-0.205	17.046	-0.205	17.046	-0.205
0	-8.572	0	-8.572	0	17.144	0	17.144	0	17.144	0

Ba-O _{II} interaction										
<i>q</i>	11		22		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	0.014	0.315	-0.033	-0.748	0.019	0.433	0.019	0.433	0.019	0.433
0.4	1.361	0.252	-2.591	-0.622	1.230	0.369	1.230	0.369	1.230	0.369
0.3	2.582	0.188	-4.905	-0.478	2.323	0.290	2.323	0.290	2.323	0.290
0.2	3.560	0.124	-6.750	-0.323	3.190	0.199	3.190	0.199	3.190	0.199
0.1	4.194	0.061	-7.941	-0.163	3.747	0.101	3.747	0.101	3.747	0.101
0	4.413	0	-8.352	0	3.939	0	3.939	0	3.939	0

O _I -O _{II} interaction										
<i>q</i>	11		22		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-0.013	0.481	0.006	-0.202	0.008	-0.278	0.008	-0.278	0.008	-0.278
0.4	-2.572	0.400	1.353	-0.162	1.218	-0.237	1.218	-0.237	1.218	-0.237
0.3	-4.886	0.307	2.575	-0.121	2.311	-0.186	2.311	-0.186	2.311	-0.186
0.2	-6.732	0.208	3.554	-0.080	3.178	-0.128	3.178	-0.128	3.178	-0.128
0.1	-7.922	0.105	4.188	-0.040	3.735	-0.065	3.735	-0.065	3.735	-0.065
0	-8.334	0	4.407	0	3.926	0	3.926	0	3.926	0

O _{II} -O _{III} interaction										
<i>q</i>	11		22		22		33		33	
	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0.5	-8.100	0	-8.100	0	16.200	0	16.200	0	16.200	0
0.4	-8.147	0	-8.147	0	16.294	0	16.294	0	16.294	0
0.3	-8.271	0	-8.271	0	16.543	0	16.543	0	16.543	0
0.2	-8.425	0	-8.425	0	16.851	0	16.851	0	16.851	0
0.1	-8.551	0	-8.551	0	17.102	0	17.102	0	17.102	0
0	-8.599	0	-8.599	0	17.198	0	17.198	0	17.198	0

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