Int. J. Solids Structures, Vol. 18, No. 2, pp. 107–119, 1982
Printed in Great Britain.

0020-7683/82/020107-13$03.00/0
Pergamon Press Ltd.

CONSTITUTIVE EQUATIONS FOR KDP BY GROUP THEORETIC METHODS†

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(*Received* 3 *November* 1980)

Abstract—Methods of group representation theory and Schur's lemma are employed to impose restrictions on the constitutive equations for elastic dielectrics which remain invariant under a group of symmetry transformations. The method is discussed in detail and used to derive constitutive equations for Potassium Dyhydrogen Phosphate (KDP), a dielectric which has only one phase transition point at 123°K. The constitutive equations are constructed both in the paraelectric phase ($T > 123$°K), where the crystal has tetragonal symmetry ($\bar{4}2m$, (D_{2d})) and also in the ferroelectric phase ($T < 123$°K) where the symmetry is of orthorhombic type ($mm2(C_{2v})$). The number of independent material constants is found to reduce from 171 to 30 and 54 for the two (phases) symmetry groups, respectively.

1. INTRODUCTION

Next to establishing balance laws, incorporation of symmetry restrictions in constitutive theory are the major aspects of the linear and non-linear theories of continuous media. Recent years have witnessed increased interest and activity in these areas resulting in explicit constitutive equations for several classes of materials which remain invariant under a group of symmetry transformations. The most frequently employed symmetry groups are the 32 crystallographic groups and the 90 magnetic groups. To simplify the non-linear constitutive equations which incorporate symmetry restrictions, it was customary to follow the method of Voigt[1] in which polynomial expansions are employed and the coefficients in such expansions simplified, using material restrictions. This method becomes cumbersome and increasingly complex as the number of terms in the equations increases. Finite groups and various other procedures for simplifying constitutive equations have been developed by a number of authors[2–5]. An extensive survey on the use of continuous groups to construct integrity bases for isotropic materials is given by Spencer[6]. The book by Lomont[7] further enhances the use of finite symmetry groups to problems of mechanics and constitutive theory.

Smith and Kiral[8, 9] have recently developed a more direct method of group representation theory to simplify constitutive equations. The present authors used their method to construct constitutive equations for alpha quartz[10].

In this paper, we use the method of group representation theory and Schur's lemma to derive constitutive equations for the elastic dielectric, Potassium Dyhydrogen Phosphate (KDP). Amongst all the ferro-electrics, KDP has the simplest macroscopic behaviour with only one phase transition point at 123°K. Above this "Currie point", the crystal is in a paraelectric phase, with tetragonal symmetry ($\bar{4}2m$) while below this temperature it is in a ferroelectric phase, with orthorhombic symmetry ($mm2$). Elements of the symmetry groups $\bar{4}2m$ and $mm2$, together with corresponding irreducible representations are listed. Constitutive equations are constructed in both phases using the methods of group representation theory.

In the natural state, with no symmetry, the number of constants for an elastic dielectric equals 171. It is observed that as the temperature increases through the Curie point, the symmetry changes from $mm2$ to $\bar{4}2m$ and the number of elastic and dielectric constants decreases from 54 to 30.

2. FUNDAMENTAL EQUATIONS

The general quadratic expression for the strain energy density function of deformation and polarization of a homogeneous linear elastic dielectric is given by

$$W^L(S_{ij}, P_i, P_{i,j}) = \tfrac{1}{2} c_{klij}S_{ij}S_{kl} + \tfrac{1}{2} a_{ij}P_iP_j + \tfrac{1}{2} b_{ijkl}\Pi_{ij}\Pi_{kl} + f_{ijk}S_{jk}P_i + j_{ijk}P_i\Pi_{jk} + d_{ijkl}\Pi_{ij}S_{kl} \quad (2.1)$$

†The results presented here were obtained in the course of research sponsored by the Natural Sciences and Engineering Research Council of Canada, Grant No. A-2736.

where S_{ij} are the components of the symmetric strain tensor, P_i are components of the polarization vector, and $\Pi_{ij} = P_{i,j}$ are the components of the polarization gradient tensor. The coefficient tensors c_{ijkl}, a_{ij}, b_{ijkl}, f_{ijk}, j_{ijk} and d_{ijkl} are the constant elastic and dielectric tensors.

The constitutive equations for the components of stress tensor σ_{ij}, the local electric vector ${}_LE_i$ and the electric tensor ϵ_{ij} are given by

$$\sigma_{ij} = \frac{\partial W^L}{\partial S_{ij}} = c_{ijkl}S_{kl} + f_{kij}P_k + d_{klij}\Pi_{kl} \tag{2.2}$$

$$-{}_LE_i = \frac{\partial W^L}{\partial P_i} = f_{ikl}S_{kl} + a_{ik}P_k + j_{ikl}\Pi_{kl} \tag{2.3}$$

$$\epsilon_{ij} = \frac{\partial W^L}{\partial \Pi_{ij}} = d_{ijkl}S_{kl} + j_{kij}P_k + b_{ijkl}\Pi_{kl}. \tag{2.4}$$

We introduce the following abbreviated matrix notation

$$\begin{gathered} \sigma^t = [\sigma_{11},\sigma_{22},\sigma_{33},\sigma_{23},\sigma_{31},\sigma_{12}],\quad S^t = [S_{11},S_{22},S_{33},S_{23},S_{31},S_{12}] \\ L^{\bar{E}^t} = [{}_LE_1,{}_LE_2,{}_LE_3],\quad \bar{P}^t = [P_1,P_2,P_3] \\ \bar{\epsilon}^t = [\epsilon_{11},\epsilon_{22},\epsilon_{33},\epsilon_{23},\epsilon_{32},\epsilon_{31},\epsilon_{13},\epsilon_{12},\epsilon_{21}] \\ \bar{\Pi}^t = [\Pi_{11},\Pi_{22},\Pi_{33},\Pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21}] \end{gathered} \tag{2.5}$$

where the superscript t denotes the transpose of the column vector. The scheme for indexing the various tensors is indicated in [10].

The strain energy density function of deformation and polarization and the constitutive equations can now be written in matrix form as

$$W^L(\bar{S},\bar{P},\bar{\Pi}) = \tfrac{1}{2}[\bar{S},\bar{P},\bar{\Pi}]\bar{\bar{M}}[\bar{S},\bar{P},\bar{\Pi}]^t \tag{2.6}$$

$$[\bar{\sigma},-{}_L\bar{E},\bar{\epsilon}]^t = \left[\frac{\partial}{\partial\bar{S}},\frac{\partial}{\partial\bar{P}},\frac{\partial}{\partial\bar{\Pi}}\right]^t W^L = \bar{\bar{M}}[\bar{S},\bar{P},\bar{\Pi}]^t \tag{2.7}$$

where

$$\bar{\bar{M}} = \begin{bmatrix} \bar{\bar{c}} & \bar{\bar{f}}^t & \bar{\bar{d}}^t \\ (6\times 6) & (6\times 3) & (6\times 9) \\ \bar{\bar{f}} & \bar{\bar{a}} & \bar{\bar{j}} \\ (3\times 6) & (3\times 3) & (3\times 9) \\ \bar{\bar{d}} & \bar{\bar{f}}^t & \bar{\bar{b}} \\ (9\times 6) & (9\times 3) & (9\times 9) \end{bmatrix} \tag{2.8}$$

and the numbers in parentheses below the matrix indicate the order of the matrix. For an elastic dielectric with arbitrary symmetry, the total number of independent material constants is 171.

Let the crystallographic group $\{\bar{A}\} = \bar{I},\bar{A}_2,\bar{A}_3,\ldots,\bar{A}_N$ of N 3×3 matrices define the symmetry transformations of the crystal. The matrix $\bar{A}_K$ is orthogonal and the rectangular Cartesian coordinate system $\bar{A}_k\bar{x}$ is said to be equivalent to the reference frame $\bar{x}$.

The independent components of vectors $\bar{S}$, $\bar{P}$ and $\bar{\Pi}$ in the reference frames $\bar{x}$ and $\bar{A}_k\bar{x}$ are related by

$$\bar{\bar{S}}(A_k) = \bar{A}_k\bar{\bar{S}}(\bar{x})\bar{A}_k^t,\ \bar{P}(A_k) = \bar{A}_k\bar{P},\ \bar{\bar{\Pi}}(\bar{A}_k) = \bar{A}_k\bar{\bar{\Pi}}(x)\bar{A}_k^t \tag{2.9}$$

which lead to

$$\underset{(6\times 1)}{\bar{S}(A_k)} = \underset{(6\times 6)(6\times 1)}{\bar{T}_S(\bar{A}_k)\bar{S}(\bar{x})},\ \underset{(3\times 1)}{\bar{P}(A_k)} = \underset{(3\times 3)(3\times 1)}{\bar{T}_{(P)}(\bar{A}_k)\bar{P}}, \tag{2.9a}$$

$$\underset{(9\times 1)}{\bar{\Pi}(A_k)} = \underset{(9\times 9)(9\times 1)}{\bar{T}_{(\Pi)}(\bar{A}_k)\bar{\Pi}}. \tag{2.10}$$

The group of each of N transformation matrices $\bar{T}_{(S)}(A_k)$, $\bar{T}_{(P)}(\bar{A}_k)$ and $\bar{T}_{(\Pi)}(A_k)$ of order 6×6, 3×3 and 9×9, respectively, which describe the transformation properties of the strain vector, $\bar{S}$, polarization vector $\bar{P}$ and the polarization gradient vector $\bar{\Pi}$ under the symmetry group $\{A\}$ are said to form its matrix representation $\{\bar{\Gamma}_{(S)}\}$, $\{\bar{\Gamma}_{(P)}\}$, $\{\bar{\Gamma}_{(\Pi)}\}$ of degree 6, 3 and 9, respectively. The strain vector $\bar{S}(S_{11},S_{22},S_{33},S_{23},S_{31},S_{12})$, the polarization vector $\bar{P}(P_1,P_2,P_3)$ and the polarization gradient vector $\bar{\Pi}(\Pi_{11},\Pi_{22},\Pi_{33},\Pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21})$ are said to form the carrier spaces of the representations. There are n inequivalent irreducible representations $D_r(A_k)(r = 1,\ldots,n)$ associated with each of N elements of the symmetry group.

The representations

$$\{\Gamma_{(S)}\} = \{\bar{T}_{(S)}(\bar{A}_1),\ \bar{T}_{(S)}(\bar{A}_2),\ \bar{T}_{(S)}(\bar{A}_3)\ldots,\ \bar{T}_{(S)}(\bar{A}_N)\} \tag{2.11a}$$

$$\{\Gamma_{(P)}\} = \{\bar{T}_{(P)}(\bar{A}_1),\ \bar{T}_{(P)}(\bar{A}_2),\ \bar{T}_{(P)}(\bar{A}_3)\ldots,\ \bar{T}_{(P)}(\bar{A}_N)\} \tag{2.11b}$$

$$\{\Gamma_{(\Pi)}\} = \{\bar{T}_{(\Pi)}(\bar{A}_1),\ \bar{T}_{(\Pi)}(\bar{A}_2),\ \bar{T}_{(\Pi)}(\bar{A}_3)\ldots,\ \bar{T}_{(\Pi)}(\bar{A}_N)\} \tag{2.11c}$$

can be decomposed into a direct sum of the irreducible representations $D_1,D_2,\ldots D_n$ of $\{A\}$ by constructing matrices $\bar{Q}_{(S)}(6\times 6)$, $\bar{Q}_{(P)}(3\times 3)$ $\bar{Q}_{(\Pi)}(9\times 9)$, associated with this group, from the basic quantities. The number of times $\alpha_r^{(\Gamma_R)D_j}(R = S,P,\Pi)$, the irreducible representation $D_j(A_k)$ appears in the decomposition of $\{\Gamma_R\} = \{\bar{T}_{(R)}(\bar{A}_k),\ k = 1-N\}$ is given by[9]

$$\alpha_r^{(\Gamma_R)D_j} = \frac{1}{N}\sum_{k=1}^{N} \operatorname{tr} \bar{T}_{(\bar{R})}(\bar{A}_k) \operatorname{tr} D_j(\bar{A}_k) \tag{2.12}$$

where the suffix tr before the matrix stands for its trace.

The components $U_1^S,U_2^S,U_3^S\ldots$; $U_1^P,U_2^P,U_3^P\ldots$; $U_1^\Pi,U_2^\Pi,U_3^\Pi\ldots$; which from the carrier spaces of the irreducible representations $D_j(A_k)$ of the group $\{A\} = \{A_1,A_2\ldots A_N\}$ are linear combinations of components of $\bar{S} = \{S_{11},S_{22},S_{33},S_{23},S_{31},S_{12}\}$, $P = \{P_1,P_2,P_3\}$ and $\Pi = \{\Pi_{11},\Pi_{22},\Pi_{33},\pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21}\}$, respectively, and are determined from the formula[9]

$$\bar{U}_p^{(j)} = \sum_{k=1}^{N} D_j(\bar{\bar{A}}_k)\bar{\bar{T}}_{pq}(\bar{\bar{A}}_k)\bar{R}_q \tag{2.13}$$

which may be written as

$$\bar{U}_{(R)} = \bar{Q}_{(R)}\bar{R}(\bar{R} = \bar{S},\bar{P}\bar{\Pi}) \tag{2.14}$$

The matrices $\bar{Q}_{(S)}$, $\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$ can be explicitly constructed for the group $\{A\}$ from the basic quantities generated in (2.13).

The correctness of matrices $\bar{Q}_{(R)}$, $(\bar{R} = \bar{S},\bar{P},\bar{\Pi})$ can be verified by observing that $\bar{Q}_{(R)}\bar{T}_{(R)}(A_k)\bar{Q}_{(\bar{R})}^{-1}$, $(\bar{R} = \bar{S},\bar{P},\bar{\Pi})$ reduces to the direct sum of the irreducible representation of every symmetry operator $\bar{A}_k$ of the group $\{A\}$, the number of times of its occurrence being given by (2.12). The matrices $\bar{Q}_{\bar{R}}(\bar{R} = \bar{S},\bar{P},\bar{\Pi})$, together with Schur's lemma are used to simplify the constitutive equations.

3. BASIC QUANTITIES FOR PARAELECTRIC PHASE—$\bar{4}2m(T > 123°K)$

Of all the elastic dielectrics, Potassium Dyhydrogen Phosphate has the simplest macroscopic behaviour and has only one phase transition point at 123°K. Here we construct the constitutive equations in the paraelectric phase ($T > 123°K$) where the crystal has tetragonal symmetry $\bar{4}2m(D_{2d})$.

The matrices comprising the symmetry group $\{\bar{A}\}$ of this crystal class are given by

$$\bar{A}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \bar{A}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \bar{A}_3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\bar{A}_4 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \bar{A}_5 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \bar{A}_6 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\bar{A}_7 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \bar{A}_8 = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{3.1}$$

There are five inequivalent irreducible representations[7] $D_1(\bar{A}_k), D_2(\bar{A}_k), D_3(\bar{A}_k), D_4(\bar{A}_k)$ and $D_5(\bar{A}_k)$, $k = 1-8$ as ociated with the group $\{\bar{A}\} = \{\bar{A}_1, \bar{A}_2, \ldots, \bar{A}_8\}$ which are of degree one and two and are listed below.

The matrices $\bar{T}_{(R)}(\bar{A}_k)$ $[\bar{R} = \bar{S}, \bar{P}, \bar{\Pi}, k = 1-8]$ which describe the transformation properties of the vectors $\bar{S}, \bar{P}$ and $\bar{\Pi}$ can be determined from eqs. (2.9) and (2.10). The values of $\alpha^{(\Gamma_R)D_j}$ found from (2.12) are given by

$$\alpha^{(\Gamma_S)D_1} = 2,\ \alpha^{(\Gamma_S)D_2} = 0,\ \alpha^{(\Gamma_S)D_3} = \alpha^{(\Gamma_S)D_4} = \alpha^{(\Gamma_S)D_5} = 1$$

$$\alpha^{(\Gamma_P)D_1} = \alpha^{(\Gamma_P)D_2} = \alpha^{(\Gamma_P)D_4} = 0,\ \alpha^{(\Gamma_P)D_3} = \alpha^{(\Gamma_P)D_5} = 1$$

$$\alpha^{(\Gamma_\Pi)D_1} = \alpha^{(\Gamma_\Pi)D_5} = 2,\ \alpha^{(\Gamma_\Pi)D_2} = \alpha^{(\Gamma_\Pi)D_3} = \alpha^{(\Gamma_\Pi)D_4} = 1 \tag{3.3}$$

The six independent components of $\bar{S}(S_{11}, S_{22}, S_{33}, S_{23}, S_{31}, S_{12})$, the three independent components of $\bar{P}(P_1, P_2, P_3)$ and the nine independent components of $\bar{\Pi}(\Pi_{11}, \Pi_{22}, \Pi_{33}, \Pi_{23}, \Pi_{32}, \Pi_{31}, \Pi_{13}, \Pi_{12}, \Pi_{21})$ can be split into basic quantities using eqn (2.13). The basic quantities associated with the appropriate irreducible representation are found to be

$$\begin{aligned}
&(1)\ S_{33}^{(1)}, (S_{11} + S_{22})^{(1)}; \text{——}; \Pi_{33}^{(1)}, (\Pi_{11} + \Pi_{22})^{(1)} \\
&(2)\ \text{——}; \text{——}; (\Pi_{21} - \Pi_{12})^{(2)} \\
&(3)\ S_{12}^{(3)}; P_3^{(3)}; (\Pi_{21} + \Pi_{12})^{(3)} \\
&(4)\ (S_{11} - S_{22})^{(4)}; \text{——}; (\Pi_{11} - \Pi_{22})^{(4)} \\
&(5)\ (S_{23}, S_{13})^{(5)}; (P_1, P_2)^{(5)}: (\Pi_{23}, \Pi_{13})^{(5)}; (\Pi_{32}, \Pi_{31})^{(5)}.
\end{aligned} \tag{3.4}$$

Table 1. Irreducible Representations of $\bar{4}2m$ (D_{2d})

	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
D_1	1	1	1	1	1	1	1	1
D_2	1	-1	-1	1	-1	1	1	-1
D_3	1	-1	-1	1	1	-1	-1	1
D_4	1	1	1	1	-1	-1	-1	-1
D_5	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

The matrices $\bar{Q}_{(S)},\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$ are generated from the above basic quantities using the following set of equations

$$(S_{33}^{(1)},(S_{11}+S_{22})^{(1)},S_{12}^{(3)},(S_{11}-S_{22})^{(4)},(S_{23},S_{13})^{(5)})^t$$
$$=\bar{Q}_{(S)}(S_{11},S_{22},S_{33},S_{23},S_{31},S_{12})^t \quad (3.5)$$

$$(P_3^{(3)},(P_1,P_2)^{(5)})^t=\bar{Q}_{(P)}(P_1,P_2,P_3)^t \quad (3.6)$$

$$(\Pi_{33},(\Pi_{11}+\Pi_{22})^{(1)},(\Pi_{21}-\Pi_{12})^{(2)},(\Pi_{21}+\Pi_{12})^{(3)},(\Pi_{11}-\Pi_{22})^{(4)},$$
$$(\Pi_{23},\Pi_{13})^{(5)},(\Pi_{32},\Pi_{31})^{(5)})=\bar{Q}_{(\Pi)}(\Pi_{11},\Pi_{22},\Pi_{33},\Pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21}). \quad (3.7)$$

The matrices $\bar{Q}_{(S)}$, $\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$ and their inverses are listed in Appendix A.

4. BASIC QUANTITIES FOR FERROELECTRIC PHASE—$mm2(T<123°K)$

The group comprising the symmetry operators of this crystal class is given by

$$A_1=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\quad A_2=\begin{bmatrix}1&0&0\\0&-1&0\\0&0&-1\end{bmatrix}\quad A_3=\begin{bmatrix}1&0&0\\0&1&0\\0&0&-1\end{bmatrix}$$

$$A_4=\begin{bmatrix}1&0&0\\0&-1&0\\0&0&1\end{bmatrix} \quad (4.1)$$

There are four inequivalent irreducible representations $D_i(\bar{A}_k)(i=1–4,k=1–4)$, associated with the group $\{A\}$, which are all of degree 1 and are given in Table 2.

The matrices $\bar{T}_{(\bar{R})}(\bar{A}_k)[\bar{R}=\bar{S},\bar{P},\bar{\Pi},\ k=1–4]$ which describe the transformation properties of vectors $\bar{S},\bar{P},\bar{\Pi}$ can be determined from eqns (2)–(9). The values of α found from the formula (2.12) are given by

$$\alpha^{(\Gamma_S)D_1}=3,\ \alpha^{(\Gamma_S)D_2}=\alpha^{(\Gamma_S)D_2}=\alpha^{(\Gamma_S)D_4}=1$$

$$\alpha^{(\Gamma_P)D_2}=0,\ \alpha^{(\Gamma_P)D_1}=\alpha^{(\Gamma_P)D_3}=\alpha^{(\Gamma_P)D_4}=1$$

$$\alpha^{(\Gamma_\Pi)D_1}=3,\ \alpha^{(\Gamma_\Pi)D_2}=\alpha^{(\Gamma_\Pi)D_3}=\alpha^{(\Gamma_\Pi)D_3}=\alpha^{(\Gamma_\Pi)D_4}=2. \quad (4.3)$$

The six independent components of $\bar{S}(S_{11},S_{22},S_{33},S_{23},S_{13},S_{12})$, the three independent components of $\bar{P}(P_1,P_2,P3)$ and the nine independent components of $\bar{\Pi}(\Pi_{11},\Pi_{22},\Pi_{33},\Pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21})$ can be split into basic quantities using the formula (2.13). The basic quantities are found to be

Table 2. Irreducible representations of $mm2$

	A_1	A_2	A_3	A_4
D_1	1	1	1	1
D_2	1	1	-1	-1
D_3	1	-1	1	-1
D_4	1	-1	-1	1

$$(1)\ S_{11}^{(1)},S_{22}^{(1)},S_{33}^{(1)};P_1^{(1)};\Pi_{11}^{(1)},\Pi_{22}^{(1)},\Pi_{33}^{(1)}$$

$$(2)\ S_{23}^{(1)};\text{——};\Pi_{23}^{(2)},\Pi_{32}^{(2)}$$

$$(3)\ S_{12}^{(3)};P_2^{(3)};\Pi_{21}^{(3)},\Pi_{12}^{(3)}$$

$$(4)\ S_{13}^{(4)};P_3^{(4)};\Pi_{13}^{(4)};\Pi_{31}^{(4)}. \tag{4.4}$$

The matrices $\bar{Q}_{(S)}$, $\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$ are generated from the basic quantities constructed above and are given by the following system of equations

$$[S_{11}^{(1)},S_{22}^{(1)},S_{33}^{(1)},S_{23}^{(2)},S_{12}^{(3)},S_{13}^{(4)}]^t$$

$$= \bar{Q}_{(S)}[S_{11},S_{22},S_{33},S_{23},S_{31},S_{12}]^t \tag{4.5}$$

$$[P_1^{(1)},P_2^{(3)},P_3^{(4)}]^t = \bar{Q}_{(P)}[P_1,P_2,P_3] \tag{4.6}$$

$$[\Pi_{11}^{(1)},\Pi_{22}^{(1)},\Pi_{33}^{(1)},\Pi_{23}^{(2)},\Pi_{32}^{(2)},\Pi_{21}^{(3)},\Pi_{12}^{(3)},\Pi_{13}^{(4)},\Pi_{31}^{(4)}]$$

$$= \bar{Q}_{(\Pi)}[\Pi_{11},\Pi_{22},\Pi_{33},\Pi_{23},\Pi_{32},\Pi_{31},\Pi_{13},\Pi_{12},\Pi_{21}\}. \tag{4.7}$$

The transformation matrices $\bar{Q}_{(\bar{R})}[\bar{R} = \bar{S},\bar{P},\bar{\Pi}]$ and their inverses are listed in Appendix B.

5. REDUCTION OF CONSTITUTIVE COEFFICIENTS BY SCHUR'S LEMMA

The system of constitutive equations (2.7), with rows multiplied by the matrices $\bar{Q}_{(S)}$, $\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$, may be written in the form

$$\begin{bmatrix} \bar{\sigma}^* \\ -{}_L\bar{E}^* \\ \bar{\epsilon}^* \end{bmatrix} = \begin{bmatrix} \bar{c}^* & \bar{f}^{*t} & d^{*t} \\ \bar{f}^* & \bar{a}^* & \bar{j}^* \\ \bar{d}^* & \bar{j}^{*t} & \bar{b}^* \end{bmatrix} \begin{bmatrix} \bar{S}^* \\ \bar{P}^* \\ \bar{\Pi}^* \end{bmatrix} \tag{5.1}$$

where

$$(\bar{\sigma}^*, \bar{S}^*) = \bar{Q}_{(S)}(\bar{\sigma}, \bar{S}),({}_LE^*, P^*) = \bar{Q}_{(P)}({}_L\bar{E},\bar{P}),(\bar{\epsilon}^*,\bar{\Pi}^*) = \bar{Q}_{(\Pi)}(\bar{\epsilon},\bar{\Pi})$$

and the coefficient matrices are given by

$$\begin{bmatrix} \bar{c}^* & \bar{f}^{*t} & \bar{d}^{*t} \\ \bar{f}^* & \bar{a}^* & \bar{j}^* \\ \bar{d}^* & \bar{j}^{*t} & \bar{b}^* \end{bmatrix} = \begin{bmatrix} Q_{(S)} & \cdot & \cdot \\ \cdot & Q_{(P)} & \cdot \\ \cdot & \cdot & Q_{(\Pi)} \end{bmatrix} \begin{bmatrix} \bar{c} & \bar{f}^t & \bar{d}^t \\ \bar{f} & \bar{a} & \bar{j} \\ \bar{d} & \bar{j}^t & \bar{b} \end{bmatrix} \times \begin{bmatrix} Q_{(S)}^{-1} & \cdot & \cdot \\ \cdot & Q_{(P)}^{-1} & \cdot \\ \cdot & \cdot & Q_{(\Pi)}^{-1} \end{bmatrix}. \tag{5.2}$$

Making use of the matrices $\bar{Q}_{(S)}$, $\bar{Q}_{(P)}$ and $\bar{Q}_{(\Pi)}$ for the para-electric phase $-\bar{4}2m$ ($T > 123°K$) and the ferroelectric phase $-mm2$ ($T < 123°K$) constructed in Sections 3 and 4, and using Schur's lemma, the star coefficient matrices assume the forms as shown in Appendices A and B, respectively.

(a) *Paraelectric phase*: $-\bar{4}2m$, $T > 123°K$)

A direct comparison of corresponding elements of matrices and their irreducible forms from Appendix A leads to the following non-zero elastic and dielectric constants.

$$c_{12},c_{33},c_{66},c_{11} = c_{22},c_{13} = c_{23},c_{44} = c_{55}$$

$$f_{36},f_{14} = f_{25};a_{33},a_{11} = a_{22};$$

$$j_{15} = f_{26},j_{14} = j_{27},j_{38} = j_{39}$$

$$d_{33}; d_{11} = d_{22}, d_{12} = d_{21}, d_{13} = d_{23}, d_{31} = d_{32},$$

$$d_{54} = d_{65}, d_{44} = d_{75}, d_{86} = d_{96}$$

$$b_{33}, b_{31} = b_{32}, b_{11} = b_{22}, b_{44} = b_{77}, b_{45} = b_{76},$$

$$b_{54} = b_{67}, b_{12}, b_{89}, b_{88} = b_{99}$$

and all other elements in matrices $\bar{c}, \bar{a}, \bar{f}, \bar{j}, \bar{d}, \bar{b} = 0$.

Keeping in mind the above values of the material ciefficients, the explicit constitutive equations for KDP in the paraelectric phase $\bar{4}2m$ ($T > 123°K$) are given in Table 3.

(b) *Ferroelectric phase*: ($mm2$, $T < 123°K$)

A comparison of the corresponding elements of matrices and their irreducible forms from Appendix B leads to the following set of non-zero elastic and dielectric constants

$$c_{ij}(i = 1-3, j = 1-3), c_{44}, c_{55}, c_{66}$$

$$f_{11}, f_{12}, f_{13}, f_{26}, f_{35}$$

$$a_{11}, a_{22}, a_{33}; j_{11}, j_{12}, j_{13}, j_{28}, j_{29}, j_{36}, j_{37}$$

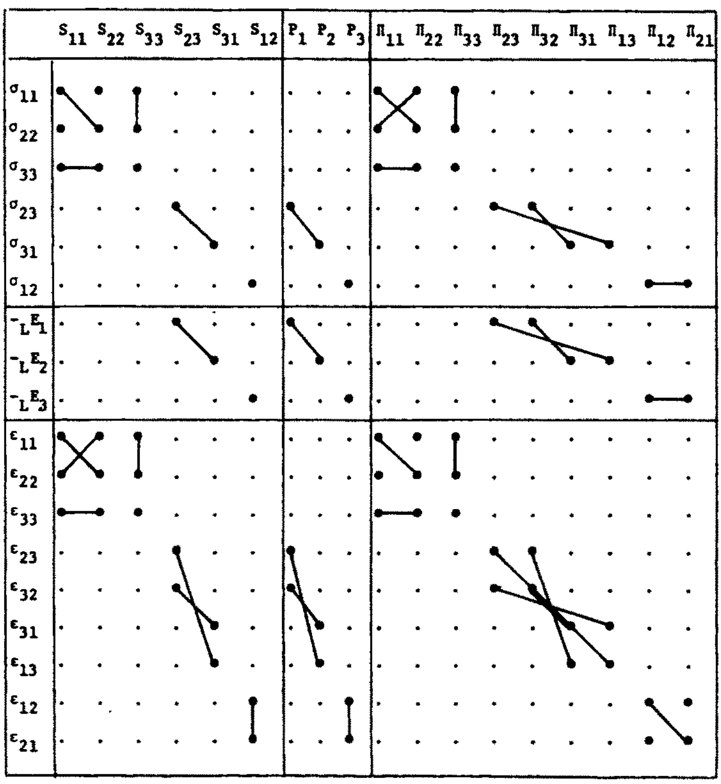
$$d_{ij}(i = 1-3, j = 1-3), d_{44}, d_{54}, d_{65}, d_{75}, d_{86}, d_{96}$$

$$b_{ij}(i = 1\text{-}3, j = 1\text{-}3), b_{44}, b_{45}, b_{54}, b_{55}, b_{68}, b_{69}$$

$$b_{78}, b_{79}, b_{86}, b_{87}, b_{96}, b_{97}$$

all other constants in matrices $\bar{a}, \bar{b}, \bar{c}, \bar{d}, \bar{f}, \bar{j}$ being zero.

Table 3. Constitutive equations for KDP in Paraelectric Phase $\bar{4}2m$)



zero element, ● non-zero element, ●—● non-zero equal element

Table 4. Constitutive equations for KDP in Ferroelectric Phase (*mm*2)

	s_{11}	s_{22}	s_{33}	s_{23}	s_{31}	s_{12}	P_1	P_2	P_3	Π_{11}	Π_{22}	Π_{33}	Π_{23}	Π_{32}	Π_{31}	Π_{13}	Π_{12}	Π_{21}
σ_{11}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
σ_{22}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
σ_{33}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
σ_{23}	·	·	·	●	·	·	·	·	·	·	·	·	●	●	·	·	·	·
σ_{31}	·	·	·	·	●	·	·	·	●	·	·	·	·	·	●	●	●	●
σ_{12}	·	·	·	·	·	●	·	●	·	·	·	·	·	·	·	·	●	●
$-{}_LE_1$	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
$-{}_LE_2$	·	·	·	·	·	●	·	●	·	·	·	·	·	·	·	·	●	●
$-{}_LE_3$	·	·	·	·	●	·	·	·	●	·	·	·	·	·	●	●	·	·
ϵ_{11}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
ϵ_{22}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
ϵ_{33}	●	●	●	·	·	·	●	·	·	●	●	●	·	·	·	·	·	·
ϵ_{23}	·	·	·	●	·	·	·	·	·	·	·	·	●	●	·	·	·	·
ϵ_{32}	·	·	·	●	·	·	·	·	·	·	·	·	●	●	·	·	·	·
ϵ_{31}	·	·	·	·	●	·	·	·	●	·	·	·	·	·	·	·	●	●
ϵ_{13}	·	·	·	·	●	·	·	·	●	·	·	·	·	·	·	·	●	●
ϵ_{12}	·	·	·	·	·	●	·	●	·	·	·	·	·	·	●	●	·	·
ϵ_{21}	·	·	·	·	·	●	·	●	·	·	·	·	·	·	●	●	·	·

· zero element, ● non-zero element

Table 5. Number of independent constants in coefficient matrices

Matrix	No. Symmetry	mm2-Symmetry Ferroelectric Phase	$\bar{4}2m$-Symmetry Paraelectric Phase
$\bar{c}$	21	9	6
$\bar{f}$	18	5	2
$\bar{a}$	6	3	2
$\bar{d}$	54	15	8
$\bar{b}$	45	15	9
$\bar{j}$	27	7	3
Total	171	54	30

The explicit constitutive equations for the KDP in ferroelectric phase ($mm2$, $T < 123°K$) are now written in the form of Table 4.

Results obtained in the constitutive tables generated above lead to distinct non-zero independent elastic and dielectric constants and their number in the matrices $\bar{c}, \bar{f}, \bar{a}, \bar{d}, \bar{b}, \bar{j}$, are presented in Table 5.

We observe that in the natural state of an elastic dielectric when there is no symmetry, the number of material constants equals 171. As the temperature of KDP increases through the Currie point, its symmetry changes from $mm2$ to $\bar{4}2m$ and the total number of constants decreases from 54 to 30.

Acknowledgements—The financial assistance provided by the Natural Sciences and Engineering Research Council of Canada in the form of a research grant to the second author, N.S.E.R.C. grant N9. A-2736 is gratefully acknowledged.

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APPENDIX A

Paraelectric phase ($\bar{4}2m$ (D_{2d}), $T > 123°$K)

The matrices $\mathring{Q}_{(S)}, \mathring{Q}_{(S)}^{-1}; \mathring{Q}_{(P)}, \mathring{Q}_{(P)}^{-1}; \mathring{Q}_{\Pi}$ and $\mathring{Q}_{\Pi}^{-1}$ which describe the transformation properties of $\bar{S}$, $\bar{P}$ and $\bar{\Pi}$ respectively, are listed as:

$$\mathring{Q}_{(S)} = \begin{bmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & -1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{bmatrix}$$

$$\mathring{Q}_{(S)}^{-1} = \begin{bmatrix} \cdot & \frac{1}{2} & \cdot & \frac{1}{2} & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & -\frac{1}{2} & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{bmatrix} \qquad \mathring{Q}_{(P)} = \begin{bmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{bmatrix}$$

$$\mathring{Q}_{(P)}^{-1} = \begin{bmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{bmatrix}$$

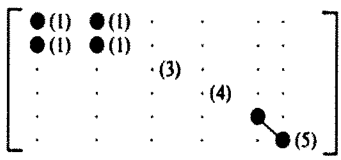
$$\mathring{Q}_{(\Pi)} = \begin{bmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & 1 \\ 1 & -1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{bmatrix}$$

$$\mathring{Q}_{(\Pi)}^{-1} = \begin{bmatrix} \cdot & \frac{1}{2} & \cdot & \cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot & \cdot & -\frac{1}{2} & \cdot & \cdot & \cdot & \cdot \\ 1 & & & & & & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & -\frac{1}{2} & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{1}{2} & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

The matrices $\mathring{c}^*, \mathring{f}^*, \mathring{a}^*, \mathring{f}^*, \mathring{d}^*$ and $\mathring{b}^*$ listed in eqn (5.1) are evaluated using eqns (5.2) and the matrices $\mathring{Q}_{(S)}, \mathring{Q}_{(S)}^{-1}, \mathring{Q}_{(P)}, \mathring{Q}_{(P)}^{-1}, \mathring{Q}_{(\Pi)} \mathring{Q}_{(\pi)}^{-1}$ listed above. The corresponding forms are obtained by multiplying the irreducible representations.

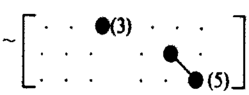
(1) The matrix $\bar{c}^*$ (symmetric):

$$c^* = \mathring{Q}_{(S)}\bar{c}\mathring{Q}^{-1}_{(S)} = \begin{bmatrix} c_{33} & \frac{c_{31}+c_{32}}{2} & c_{36} & \frac{c_{31}-c_{32}}{2} & c_{34} & c_{35} \\ c_{13}+c_{23} & \frac{c_{11}+c_{22}}{2} & c_{16}+c_{26} & \frac{c_{11}-c_{22}}{2} & c_{14}+c_{24} & c_{15}+c_{25} \\ c_{63} & \frac{c_{61}+c_{62}}{2} & c_{66} & \frac{c_{61}-c_{62}}{2} & c_{64} & c_{65} \\ c_{13}-c_{23} & \frac{c_{11}-c_{22}}{2} & c_{16}-c_{26} & \frac{c_{11}+c_{22}}{2} & c_{14}-c_{24} & c_{15}-c_{25} \\ c_{43} & \frac{c_{41}+c_{42}}{2} & c_{46} & \frac{c_{41}-c_{42}}{2} & c_{44} & c_{45} \\ c_{53} & \frac{c_{51}+c_{52}}{2} & c_{56} & \frac{c_{51}-c_{52}}{2} & c_{54} & c_{55} \end{bmatrix}$$



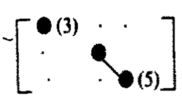
(2) The matrix $\bar{f}^*$:

$$\bar{f}^* = \mathring{Q}_{(P)}\bar{f}\mathring{Q}^{-1}_{(S)} = \begin{bmatrix} f_{33} & \frac{f_{31}+f_{32}}{2} & f_{36} & \frac{f_{31}-f_{32}}{2} & f_{34} & f_{35} \\ f_{13} & \frac{f_{11}+f_{12}}{2} & f_{16} & \frac{f_{11}-f_{12}}{2} & f_{14} & f_{15} \\ f_{23} & \frac{f_{21}+f_{22}}{2} & f_{26} & \frac{f_{21}-f_{22}}{2} & f_{24} & f_{25} \end{bmatrix} \sim$$

$\sim$ 

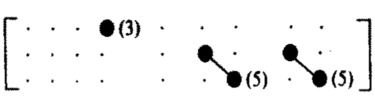
(3) The matrix $\bar{a}^*$ (symmetric):

$$\bar{a}^* = \mathring{Q}_{(P)}\bar{a}\mathring{Q}^{-1}_{(P)} = \begin{bmatrix} a_{33} & a_{31} & a_{32} \\ a_{13} & a_{11} & a_{12} \\ a_{23} & a_{21} & a_{22} \end{bmatrix} \sim$$



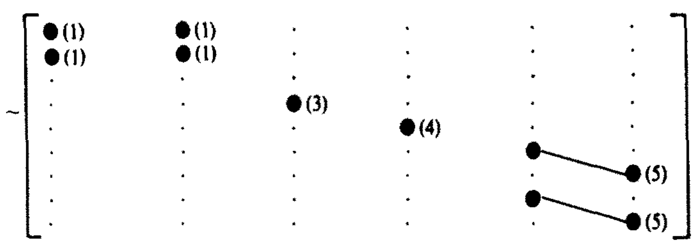
(4) The matrix $\bar{j}^*$:

$$\bar{j}^* = \mathring{Q}_{(P)}\bar{j}\mathring{Q}^{-1}_{(\Pi)} = \begin{bmatrix} j_{33} & \frac{j_{31}+j_{32}}{2} & \frac{-j_{38}+j_{39}}{2} & \frac{j_{38}+j_{39}}{2} & \frac{j_{31}-j_{32}}{2} & j_{34} & j_{37} & j_{35} & j_{36} \\ j_{13} & \frac{j_{11}+j_{12}}{2} & \frac{-j_{18}+j_{19}}{2} & \frac{j_{18}+j_{19}}{2} & \frac{j_{11}-j_{12}}{2} & j_{14} & j_{17} & j_{15} & j_{16} \\ j_{23} & \frac{j_{21}+j_{22}}{2} & \frac{-j_{28}+j_{29}}{2} & \frac{j_{28}+j_{29}}{2} & \frac{j_{21}-j_{22}}{2} & j_{24} & j_{27} & j_{25} & j_{26} \end{bmatrix}$$



(5) The matrix $\tilde{d}^*$:

$$\tilde{d}^* = \tilde{Q}_{(\Pi)}\tilde{d}\tilde{Q}^{-1}_{(S)} = \begin{bmatrix} d_{33} & \frac{d_{31}+d_{32}}{2} & d_{36} & \frac{d_{31}-d_{32}}{2} & d_{34} & d_{35} \\ d_{13}+d_{23} & \frac{\begin{pmatrix} d_{11}+d_{12} \\ +d_{21}+d_{22}\end{pmatrix}}{2} & d_{16}+d_{26} & \frac{\begin{pmatrix} d_{11}+d_{21} \\ -d_{12}-d_{22}\end{pmatrix}}{2} & d_{14}+d_{24} & d_{15}+d_{25} \\ -d_{83}+d_{93} & \frac{\begin{pmatrix} -d_{81}+d_{91} \\ -d_{82}+d_{92}\end{pmatrix}}{2} & -d_{86}+d_{96} & \frac{\begin{pmatrix} -d_{81}+d_{91} \\ +d_{82}-d_{92}\end{pmatrix}}{2} & -d_{84}+d_{94} & -d_{85}+d_{95} \\ d_{83}+d_{93} & \frac{\begin{pmatrix} d_{81}+d_{91} \\ d_{82}+d_{92}\end{pmatrix}}{2} & d_{86}+d_{96} & \frac{\begin{pmatrix} d_{81}+d_{91} \\ -d_{81}-d_{91}\end{pmatrix}}{2} & d_{84}+d_{94} & d_{85}+d_{95} \\ d_{13}-d_{23} & \frac{\begin{pmatrix} d_{11}-d_{21} \\ d_{12}-d_{22}\end{pmatrix}}{2} & d_{16}-d_{26} & \frac{\begin{pmatrix} d_{11}-d_{21} \\ -d_{12}+d_{22}\end{pmatrix}}{2} & d_{14}-d_{24} & d_{15}-d_{25} \\ d_{43} & \frac{d_{41}+d_{42}}{2} & d_{46} & \frac{d_{41}-d_{42}}{2} & d_{44} & d_{45} \\ d_{73} & \frac{d_{71}+d_{72}}{2} & d_{76} & \frac{d_{71}-d_{72}}{2} & d_{74} & d_{75} \\ d_{53} & \frac{d_{51}+d_{52}}{2} & d_{56} & \frac{d_{51}-d_{52}}{2} & d_{54} & d_{55} \\ d_{63} & \frac{d_{61}+d_{62}}{2} & d_{66} & \frac{d_{61}-d_{62}}{2} & d_{64} & d_{65} \end{bmatrix}$$



(6) The matrix $\tilde{b}^*$ (symmetric):

$\tilde{b}^* = \tilde{Q}_{(\Pi)}\tilde{b}\tilde{Q}^{-1}_{(\Pi)} =$

$$\begin{bmatrix} b_{33} & \frac{b_{31}+b_{32}}{2} & \frac{-b_{38}+b_{39}}{2} & \frac{b_{38}+b_{39}}{2} & \frac{b_{31}-b_{32}}{2} & b_{34} & b_{37} & b_{35} & b_{36} \\ b_{13}+b_{23} & \frac{b_{11}+b_{22}}{2}+b_{12} & \frac{\begin{pmatrix} -b_{18}-b_{28} \\ b_{19}+b_{29}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{18}+b_{28} \\ b_{19}+b_{29}\end{pmatrix}}{2} & \frac{b_{11}-b_{22}}{2} & b_{14}+b_{24} & b_{17}+b_{27} & b_{15}+b_{25} & b_{16}+b_{36} \\ -b_{83}+b_{93} & \frac{\begin{pmatrix} -b_{81}+b_{91} \\ -b_{82}+b_{92}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{88}-b_{98} \\ +b_{89}+b_{99}\end{pmatrix}}{2} & \frac{\begin{pmatrix} -b_{88}+b_{98} \\ +b_{89}+b_{99}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{81}+b_{91} \\ -b_{82}-b_{92}\end{pmatrix}}{2} & -b_{84}+b_{94} & -b_{87}+b_{97} & -b_{85}+b_{95} & -b_{86}+b_{96} \\ b_{83}+b_{93} & \frac{\begin{pmatrix} b_{81}+b_{91} \\ b_{82}+b_{92}\end{pmatrix}}{2} & \frac{\begin{pmatrix} -b_{88}-b_{98} \\ +b_{89}+b_{99}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{88}+b_{98} \\ b_{89}+b_{99}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{81}+b_{91} \\ -b_{82}-b_{92}\end{pmatrix}}{2} & b_{84}+b_{94} & b_{87}+b_{97} & b_{85}+b_{95} & b_{86}+b_{96} \\ b_{13}-b_{23} & \frac{b_{11}-b_{22}}{2} & \frac{\begin{pmatrix} -b_{18}+b_{28} \\ +b_{19}-b_{29}\end{pmatrix}}{2} & \frac{\begin{pmatrix} b_{18}-b_{28} \\ b_{19}-b_{29}\end{pmatrix}}{2} & \frac{b_{11}+b_{22}}{2}-b_{12} & b_{14}-b_{24} & b_{17}-b_{27} & b_{15}-b_{25} & b_{16}-b_{26} \\ b_{43} & \frac{b_{41}+b_{42}}{2} & \frac{-b_{48}+b_{49}}{2} & \frac{b_{48}+b_{49}}{2} & \frac{b_{41}-b_{42}}{2} & b_{44} & b_{47} & b_{45} & b_{46} \\ b_{73} & \frac{d_{71}+d_{72}}{2} & \frac{-b_{78}+b_{79}}{2} & \frac{b_{78}+b_{79}}{2} & \frac{b_{71}-b_{72}}{2} & b_{74} & b_{77} & b_{75} & b_{76} \\ b_{53} & \frac{b_{51}+b_{52}}{2} & \frac{-b_{58}+b_{59}}{2} & \frac{b_{58}+b_{59}}{2} & \frac{b_{51}-b_{52}}{2} & b_{54} & b_{57} & b_{55} & b_{56} \\ b_{63} & \frac{b_{61}+b_{62}}{2} & \frac{-b_{68}+b_{69}}{2} & \frac{b_{68}+b_{69}}{2} & \frac{b_{61}-b_{62}}{2} & b_{64} & b_{67} & b_{65} & b_{66} \end{bmatrix} \sim$$

$$
\begin{bmatrix}
\bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \bullet(2) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \bullet(3) & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \bullet(4) & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \bullet & \cdot & \bullet & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(5) & \cdot & \bullet(5) \\
\cdot & \cdot & \cdot & \cdot & \cdot & \bullet & \cdot & \bullet & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(5) & \cdot & \bullet(5)
\end{bmatrix}
$$

APPENDIX B

Ferro-electric phase [$mm2\ (C_{2v})$, $T < 123°K$

The matrices $\bar{Q}_{(S)}, \bar{Q}^{-1}_{(S)}, \bar{Q}_{(P)}, \bar{Q}^{-1}_{(P)}, \bar{Q}_{(\Pi)}, \bar{Q}^{-1}_{(\Pi)}$ which describe the transformation properties of $\bar{S}$, $\bar{P}$ and $\bar{\Pi}$ are listed below:

$$
\bar{Q}_{(S)} = \bar{Q}^{-1}_{(S)} = \begin{bmatrix}
1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot
\end{bmatrix}
$$

$$
\bar{Q}_{(\Pi)} = \bar{Q}^{-1}_{(\Pi)} = \begin{bmatrix}
1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot
\end{bmatrix}
$$

$$
\bar{Q}_{(P)} = \bar{Q}^{-1}_{(P)} = \begin{bmatrix}
1 & \cdot & \cdot \\
\cdot & 1 & \cdot \\
\cdot & \cdot & 1
\end{bmatrix}.
$$

The matrices $\bar{c}^*$, $\bar{f}^*$, $\bar{a}^*$, $\bar{j}^*$, $\bar{d}^*$ and $\bar{b}^*$ are evaluated by eqns (5.1) and (5.2) and are compared to the corresponding forms obtained by multiplication of the irreducible representations.

(1) The matrix $\bar{c}^*$ (symmetric):

$$
\bar{c}^* = \bar{Q}_{(S)} \bar{c} \bar{Q}^{-1}_{(S)} = \begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{16} & c_{15} \\
c_{21} & c_{22} & c_{23} & c_{24} & c_{26} & c_{25} \\
c_{31} & c_{32} & c_{33} & c_{34} & c_{36} & c_{35} \\
c_{41} & c_{42} & c_{43} & c_{44} & c_{46} & c_{45} \\
c_{61} & c_{62} & c_{63} & c_{64} & c_{66} & c_{65} \\
c_{51} & c_{52} & c_{53} & c_{54} & c_{56} & c_{55}
\end{bmatrix} \sim
$$

$$
\sim \begin{bmatrix}
\bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\
\bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\
\bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \bullet(2) & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \bullet(3) & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4)
\end{bmatrix}
$$

(2) The matrix $\bar{f}^*$:

$$
\bar{f}^* = \bar{Q}_{(P)} \bar{f} \bar{Q}^{-1}_{(S)} = \begin{bmatrix}
f_{11} & f_{12} & f_{13} & f_{14} & f_{16} & f_{15} \\
f_{21} & f_{22} & f_{23} & f_{24} & f_{26} & f_{25} \\
f_{31} & f_{32} & f_{33} & f_{34} & f_{36} & f_{35}
\end{bmatrix} \sim
$$

$$
\begin{bmatrix}
\bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \bullet(3) & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4)
\end{bmatrix}
$$

(3) The matrix $\check{a}^*$ (symmetric):

$$\check{a}^* = \check{Q}_{(P)}\check{a}\check{Q}^{-1}_{(P)} = \check{a} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \sim \begin{bmatrix} \bullet(1) & \cdot & \cdot \\ \cdot & \bullet(3) & \cdot \\ \cdot & \cdot & \bullet(4) \end{bmatrix}.$$

(4) The matrix $\check{j}$:

$$\check{j} = \check{Q}_{(P)}\check{j}\check{Q}^{-1}_{(\Pi)} = \begin{bmatrix} j_{11} & j_{12} & j_{13} & j_{14} & j_{15} & j_{19} & j_{18} & j_{17} & j_{16} \\ j_{21} & j_{22} & j_{23} & j_{24} & j_{25} & h_{29} & j_{28} & j_{27} & j_{26} \\ j_{31} & j_{32} & j_{33} & j_{34} & j_{35} & j_{39} & j_{38} & j_{37} & j_{36} \end{bmatrix}$$

$$\begin{bmatrix} \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(3) & \bullet(3) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4) & \bullet(4) \end{bmatrix}$$

(5) The matrix d^*:

$$\check{d}^* = \check{Q}_{(\Pi)}\check{d}\check{Q}^{-1}_{(S)} = \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{16} & d_{15} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{26} & d_{25} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{36} & d_{35} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{46} & d_{45} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{56} & d_{55} \\ d_{91} & d_{92} & d_{93} & d_{94} & d_{96} & d_{95} \\ d_{81} & d_{82} & d_{83} & d_{84} & d_{86} & d_{85} \\ d_{71} & d_{72} & d_{73} & d_{74} & d_{76} & d_{75} \\ d_{61} & d_{62} & d_{63} & d_{64} & d_{66} & d_{65} \end{bmatrix}$$

$$\begin{bmatrix} \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\ \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\ \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bullet(2) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bullet(2) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \bullet(3) & \cdot \\ \cdot & \cdot & \cdot & \cdot & \bullet(3) & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4) \\ \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4) \end{bmatrix}$$

(6) The matrix $\check{b}^*$:

$$\check{b}^* = \check{Q}_{(\Pi)}\check{b}\check{Q}^{-1}_{(\Pi)} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{19} & b_{18} & b_{17} & b_{16} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{29} & b_{28} & b_{27} & b_{26} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{39} & b_{38} & b_{37} & b_{36} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{49} & b_{48} & b_{47} & b_{46} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{59} & b_{58} & b_{57} & b_{56} \\ b_{61} & b_{62} & b_{63} & b_{64} & b_{65} & b_{69} & b_{68} & b_{67} & b_{66} \\ b_{71} & b_{72} & b_{73} & b_{74} & b_{75} & b_{79} & b_{78} & b_{77} & b_{76} \\ b_{81} & b_{82} & b_{83} & b_{84} & b_{85} & b_{89} & b_{88} & b_{87} & b_{86} \\ b_{91} & b_{92} & b_{93} & b_{94} & b_{95} & b_{99} & b_{98} & b_{97} & b_{96} \end{bmatrix}$$

$$\begin{bmatrix} \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \bullet(1) & \bullet(1) & \bullet(1) & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bullet(2) & \bullet(2) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \bullet(2) & \bullet(2) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(3) & \bullet(3) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(3) & \bullet(3) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4) & \bullet(4) \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \bullet(4) & \bullet(4) \end{bmatrix}$$