integrity basis of polynomial invariants and of the linear bases of polynomial covariants.

(3) *Twinning group*: This option works for the first group of the set of conjugate subgroups only. It displays a table that contains consecutive normalizers of the set of conjugate subgroups, left, right and double coset resolutions of the parent group G with respect to the subgroup F_1, and the twinning groups assigned to double cosets. This is the basic information concerning pairs of domain states.

Lattices of equitranslational subgroups of the space groups. The importance of these lattices was realized by Ascher (1968), who prepared the first tables. However, his tables do not contain full information about subgroups; neither the parent group nor the subgroups are completely specified. The current version gives the full information about subgroups including their settings and origins. The pull-down menu *Groups* contains two options: *Point* and *Space*. The choice of the second option brings to the screen another panel, in the right-hand part of which are listed space groups of the geometric class G through Hermann–Mauguin symbols corresponding to all settings and cell choices where applicable. The number of the space-group type, the Schoenflies symbol, the setting and the cell choice are shown in the left-hand part of the panel when you click on one of these Hermann–Mauguin symbols. At the same time, the symbols of the point groups in the lattice change to Schoenflies symbols of oriented space-group types. As you click on any of these subgroups, the Hermann–Mauguin symbol that specifies the subgroup completely appears in the lower bar of the panel, reserved for this information. Though the embellished lattice symbols used in this presentation are self-explanatory, consultation of the manual is recommended.

The option *Point* returns the lattice to its original form of the lattice of point groups.

The following is a list of tabular appendices contained in the manual:

Appendix A: correlation of various notations and Jones' faithful representation symbols;

Appendix B: Schoenflies and Hermann–Mauguin symbols of groups in standard orientations and of their subgroups;

Appendix C: isomorphisms used for defining irreducible representations;

Appendix D: standard polynomials;

Appendix E: labelling of covariants and conversion equations;

Appendix F: list of symmetry descents;

Appendix G: nonstandard lattice letters.

Our symbols for point-symmetry operations are compared with other sources in Appendix A. Symbols of all groups used in the software are given in Appendix B and isomorphisms in Appendix C. Standard polynomials in Appendix D are abbreviated symbols for more complicated polynomials that appear in the main tables. Appendix E is of primary importance for consideration of the relationship between tensor parameters and their contribution to Cartesian tensor components as already indicated in the text explaining Table 3.1.3.1. In Appendix F are listed and classified all symmetry descents considered in the main table. Consultation of Appendix G is strongly recommended to all users who want to use the lattices of equitranslational subgroups of the space groups.

3.1.7. Glossary

(*a*) Groups

G	point-group symmetry of the parent (prototype, high-symmetry) phase
$\mathcal{G}$	space-group symmetry of the parent (prototype, high-symmetry) phase
F	point-group symmetry of the ferroic (low-symmetry) phase (domain state not specified)
$\mathcal{F}$	space-group symmetry of the ferroic (low-symmetry) phase (domain state not specified)
F_1	point-group symmetry of the first ferroic single domain state
$\mathcal{F}_1$	space-group symmetry of the first ferroic single domain state
$G \Downarrow F$	point-group symmetry descent from G to F
$\mathcal{G} \Downarrow \mathcal{F}$	space-group symmetry descent from $\mathcal{G}$ to $\mathcal{F}$
$\mathcal{G} \Downarrow^t \mathcal{F}$	equitranslational symmetry descent from $\mathcal{G}$ to $\mathcal{F}$
Γ_η	representation of $\mathcal{G}$ (or of G) according to which η transforms
$D^{(\eta)}$	irreducible matrix representation of the order parameter η
χ_η	character of the matrix representation $D^{(\eta)}$
R-irep	physically irreducible representation
n_F	number of subgroups conjugate under G to subgroup F_1
n_f	number of ferroic single domain states
n_a	number of ferroelastic single domain states
n_e	number of ferroelectric single domain states

(*b*) Physical quantities

c	specific heat
$d_{i\mu}$	piezoelectric tensor
F, G	free energy
g_μ	optical activity
P_i	dielectric polarization
S	entropy
s_{ij}	elastic compliance
T_c	Curie temperature
u_{ij}, u_μ	strain tensor
V	cell volume
χ	dielectric susceptibility
ε	enantiomorphism, chirality
ε_{ij}	dielectric permittivity
η	order parameter (primary)
λ	order parameter (secondary)
$\omega_{\rm LO}$	longitudinal optic mode frequency
$\omega_{\rm TO}$	transverse optic mode frequency
$\pi_{\mu\nu}$	piezo-optic tensor

References

Aizu, K. (1969). *Possible species of ferroelastic crystals and of simultaneously ferroelectric and ferroelastic crystals. J. Phys. Soc. Jpn*, **27**, 387–396.

Aizu, K. (1970). *Possible species of ferromagnetic, ferroelectric, and ferroelastic crystals. Phys. Rev. B*, **2**, 754–772.

Aizu, K. (1973). *Second order ferroic states. J. Phys. Soc. Jpn*, **34**, 121–128.

Altmann, S. L. & Herzig, P. (1994). *Point-group theory tables.* Oxford: Clarendon Press.

Aroyo, M. I. & Perez-Mato, J. M. (1998). *Symmetry mode analysis of displacive phase transitions using International Tables for Crystallography. Acta Cryst.* A**54**, 19–30.

Ascher, E. (1968). *Lattices of equi-translation subgroups of the space groups.* Geneva: Battelle.

Ascher, E. & Kobayashi, J. (1977). *Symmetry and phase transitions: the inverse Landau problem. J. Phys. C: Solid State Phys.* **10**, 1349–1363.

Balkanski, M., Teng, M. K. & Nusimovici, M. (1969). *Lattice dynamics in KNO_3. Phases I, II and III*. In *Light scattering spectra of solids*, edited by G. B. Wright, pp. 731–746. Paris: Flammarion.

Blinc, R. (1960). *On the isotopic effects in the ferroelectric behaviour of crystals with short hydrogen bonds. J. Phys. Chem. Solids*, **13**, 204–211.

Blinc, R., Jamsek-Vilfan, M., Lahajnar, G. & Hajdukovic, G. (1970). *Nuclear magnetic resonance study of the ferroelectric transition in diglycine nitrate and tris-sarcosine calcium chloride. J. Chem. Phys.* **52**, 6407–6411.

Bradley, C. J. & Cracknell, A. P. (1972). *The mathematical theory of symmetry in solids. Representation theory for point groups and space groups.* Oxford: Clarendon Press.

Chan, L. Y. Y. & Geller, S. (1977). *Crystal structure and conductivity of 26-silver 18-iodine tetratungstate. J. Solid State Chem.* **21**, 331–347.

Cochran, W. (1960). *Crystal stability and the theory of ferroelectricity; Part I. Adv. Phys.* **9**, 387–402.

Cochran, W. (1961). *Crystal stability and the theory of ferroelectricity; Part II. Piezoelectric crystals. Adv. Phys.* **10**, 401–420.

Cowley, R. A. (1962). *Temperature dependence of a transverse optic mode in strontium titanate. Phys. Rev. Lett.* **9**, 159–161.

Cowley, R. A. (1964). *Lattice dynamics and phase transitions mode in strontium titanate. Phys. Rev. A*, **134**, 981–997.

Cowley, R. A. (1970). *On the dielectric properties of an anharmonic crystal. J. Phys. Soc. Jpn*, **28**, Suppl., 205–209.

Devonshire, A. F. (1954). *Theory of ferroelectrics. Adv. Phys.* **3**, 85.

Dvořák, V. (1974). *Improper ferroelectrics. Ferroelectrics*, **7**, 1–9.

Errandonea, G., Tolédano, J.-C., Litzler, A., Schneck, J., Savary, H. & Aubrée, J. (1984). *Kinetic characteristics of the thermal hysteresis in an incommensurate system. J. Phys. Lett.* **45**, L329–L334.

Fleury, P. A., Scott, J. F. & Worlock, J. M. (1968). *Soft phonon modes and the 110 K phase transition in strontium titanate. Phys. Rev. Lett.* **21**, 16–19.

Fox, D. L., Scott, J. F. & Bridenbaugh, P. M. (1976). *Soft modes in ferroelastic LaP_5O_{14} and NdP_5O_{14}. Solid State Commun.* **18**, 111–113.

Geller, S. & Bala, V. B. (1956). *Crystallographic studies of perovskite-like compounds. II. Rare earth alluminates. Acta Cryst.* **9**, 1019–1024.

Geller, S., Wilber, S. A., Ruse, G. F., Akridge, J. R. & Turkovic, A. (1980). *Anisotropic electrical conductivity and low-temperature phase transitions of the solid electrolyte $Ag_{26}I_{18}W_4O_{16}$. Phys. Rev. B*, **21**, 2506–2512.

Greer, A. L., Habbal, F., Scott, J. F. & Takahashi, T. (1980). *Specific heat anomalies and phase transitions in the solid electrolyte $Ag_{26}I_{18}W_4O_{16}$. J. Chem. Phys.* **73**, 5833–5867.

Habbal, F., Zvirgzds, J. A. & Scott, J. F. (1978). *Raman spectra of structural phase transitions in $Ag_{26}I_{18}W_4O_{16}$. J. Chem. Phys.* **69**, 4984–4989.

Habbal, F., Zvirgzds, J. A. & Scott, J. F. (1980). *Ferroelectric phase transition in the superionic conductor $Ag_{26}I_{18}W_4O_{16}$. J. Chem. Phys.* **72**, 2760–2763.

Huang, C. Y., Dries, L. T., Hor, P. H., Meng, R. I., Chu, C. W. & Frankel, R. B. (1987). *Observation of possible superconductivity at 230 K. Nature (London)*, **238**, 403–404.

Hulm, J. K. (1950). *The dielectric properties of some alkaline earth titanates at low temperatures. Proc. Phys. Soc. London Ser. A*, **63**, 1184–1185.

Hulm, J. K. (1953). *Low-temperature properties of cadmium and lead niobates. Phys. Rev.* **92**, 504.

IEEE Standard on Piezoelectricity STD 176–1987. (1987). New York: The Institute of Electrical and Electronics Engineers, Inc. This IEEE Std 176–1987 is reproduced in *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control.* (1996). **43**, No. 5.

Indenbom, V. L. (1960). *Phase transitions without change in the number of atoms in the unit cell of the crystal. Sov. Phys. Crystallogr.* **5**, 105–115.

International Tables for Crystallography (2004). Vol. A1. *Symmetry relations between space groups*, edited by H. Wondratschek & U. Müller. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2005). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Heidelberg: Springer.

Izyumov, Yu. A. & Syromiatnikov, V. N. (1990). *Phase transitions and crystal symmetry.* Dordrecht: Kluwer Academic Publishers.

Janovec, V., Dvořák, V. & Petzelt, J. (1975). *Symmetry classification and properties of equi-translation structural phase transitions. Czech. J. Phys.* **B25**, 1362–1396.

Jansen, L. & Boon, M. (1967). *Theory of finite groups. Applications in physics. Symmetry groups of quantum mechanical systems.* Amsterdam: North-Holland.

Kociński, J. (1983). *Theory of symmetry changes at continuous phase transitions*. Warsaw: PWN – Polish Scientific Publishers; Amsterdam: Elsevier.

Kociński, J. (1990). *Commensurate and incommensurate phase transitions*. Warsaw: PWN – Polish Scientific Publishers; Amsterdam: Elsevier.

Kopský, V. (1976*a*). *The use of the Clebsch–Gordan reduction of the Kronecker square of the typical representation in symmetry problems of crystal physics. I. Theoretical foundations. J. Phys. C: Solid State Phys.* **9**, 3391–3405.

Kopský, V. (1976*b*). *The use of the Clebsch–Gordan reduction of the Kronecker square of the typical representation in symmetry problems of crystal physics. II. Tabulation of Clebsch–Gordan products for classical and magnetic crystal point groups. J. Phys. C: Solid State Phys.* **9**, 3405–3420.

Kopský, V. (1979*a*). *Tensorial covariants of the 32 crystal point groups. Acta Cryst.* A**35**, 83–95.

Kopský, V. (1979*b*). *A simplified calculation and tabulation of tensorial covariants for magnetic point groups belonging to the same Laue class. Acta Cryst.* A**35**, 95–101.

Kopský, V. (1979*c*). *Extended integrity bases of irreducible matrix groups. The crystal point groups. J. Phys. A: Math. Gen.* **12**, 943–957.

Kopský, V. (1979*d*). *Representation generating theorem and interaction of improper quantities with order parameter. J. Phys. A. Math. Gen.* **12**, L291–L294.

Kopský, V. (1982). *Group lattices, subduction of bases and fine domain structures for magnetic crystal point groups.* Prague: Academia.

Kopský, V. (2000). *The change of tensor properties at ferroic phase transitions. Ferroelectrics*, **237**, 127–134.

Kopský, V. (2001). *Tensor parameters of ferroic phase transitions. I. Theory and tables. Phase Transit.* **73**, No. 1–2, 1–422.

Koster, G. F., Dimmock, J. O., Wheeler, R. E. & Statz, H. (1963). *Properties of the 32 groups.* Cambridge: MIT Press.

Kozlov, G. V.., Volkov, A. A., Scott, J. F. & Petzelt, J. (1983). *Millimeter wavelength spectroscopy of the ferroelectric phase transition in tris-sarcosine calcium chloride. Phys. Rev. B*, **28**, 255–261.

Laegreid, T., Fossheim, K., Sandvold, E. & Juisrud, S. (1987). *Specific heat anomaly at 220 K connected with superconductivity at 90 K in ceramic $YBa_2Cu_3O_{7-x}$. Nature (London)*, **330**, 637–638.

Landau, L. D. (1937). *Theory of phase transitions. I. Phys. Z. Sowjun.* **11**, 26–47; *II. Phys. Z. Sowjun.* **11**, 545–555.

Landau, L. D. & Lifshitz, E. M. (1969). *Course in theoretical physics*, Vol. 5, *Statistical physics*, 2nd ed. Oxford: Pergamon Press.

Levanyuk, A. P. & Sannikov, D. G. (1974). *Improper seignetoelectrics. Uspekhi Fiz. Nauk.* **112**, 561–589. (In Russian.)

Lines, M. E. & Glass, A. M. (1977). *Principles and applications of ferroelectrics and related materials.* Oxford University Press.

Lytle, F. W. (1964). *X-ray diffractometry of low-temperature phase transformations in strontium titanate. J. Appl. Phys.* **35**, 2212–2214.

Lyubarskii, G. Ya. (1960). *The application of group theory in physics*. Oxford: Pergamon Press.

MacFarlane, R. M., Rosen, H. & Seki, H. (1987). *Temperature dependence of the Raman spectra of the high-T_c superconductor $YBa_2Cu_3O_{7-x}$. Solid State Commun.* **63**, 831–834.

Nimmo, J. K. & Lucas, D. W. (1973). *The crystal structures of γ- and β-KNO_3 and the $\alpha \leftarrow \gamma \leftarrow \beta$ phase transformations. Acta Cryst.* B**32**, 1968–1971.

Nowick, A. S. (1995). *Crystal properties via group theory.* Cambridge University Press.

Nye, J. F. (1985). *Physical properties of crystals.* Oxford: Clarendon Press.

Oliver, W. F. (1990). PhD thesis, University of Colorado.

Patera, J., Sharp, R. T. & Winternitz, P. (1978). *Polynomial irreducible tensors for point groups. J. Math. Phys.* **19**, 2362–2376.

Peercy, P. S. (1975*a*). *Soft mode and coupled modes in the ferroelectric phase of KH_2PO_4. Solid State Commun.* **16**, 439–442.

Peercy, P. S. (1975*b*). *Measurement of the soft mode and coupled modes in the paraelectric and ferroelectric phases of KH_2PO_4. Phys. Rev. B*, **12**, 2741–2746.

Pick, R. (1969). Private communication.

Prokhorova, S. D., Smolensky, G. A., Siny, I. G., Kuzminov, E. G., Mikvabia, V. D. & Arndt, H. (1980). *Light scattering study of the phase transition in tris-sarcosine calcium chloride. Ferroelectrics*, **25**, 629–632.

Rebane, L., Fimberg, T. A., Fefer, E. M., Blumberg, G. E. & Joon, E. R. (1988). *Raman scattering study of lattice instability in $YBa_2Cu_3O_{7-x}$ at 200–240 K. Solid State Commun.* **65**, 1535–1537.

Rousseau, D. L., Bauman, R. P. & Porto, S. P. S. (1981). *Normal mode determination in crystals. J. Raman Spectrosc.* **10**, 253–290.

Schneck, J. (1982). Thèse de Doctorat d'Etat ès Sciences Physiques, Université Pierre et Marie Curie (Paris).

Schneck, J., Primot, J., Von der Muhl, R. & Ravez, J. (1977). *New phase transition with increasing symmetry on cooling in barium sodium niobate. Solid State Commun.* **21**, 57–60.

Scott, J. F. (1969). *Raman study of trigonal–cubic phase transitions in rare-earth aluminates. Phys. Rev.* **183**, 823–825.

Scott, J. F. (1999). *A comparison of Ag- and proton-conducting ferroelectrics. Solid State Ionics*, **125**, 141–146.

Scott, J. F. & Pouligny, B. (1988). *Raman spectroscopic study of submicron KNO_3 films. J. Appl. Phys.* **64**, 1547–1551.

Scott, J. F. & Remeika, J. P. (1970). *High-temperature Raman study of $SmAlO_3$. Phys. Rev. B*, **1**, 4182–4185.

Shannon, R. D. & Prewitt, C. T. (1969). *Effective ionic radii in oxides and fluorides. Acta Cryst.* B**25**, 925–945.

Shapiro, S. M., Cowley, R. A., Cox, D. E., Eibschutz, M. & Guggenheim, H. J. (1976). *Neutron scattering study of incommensurate $BaMnF_4$.* In *Proc. Natl Conf. Neutron Scat.* edited by R. M. Moon, pp. 399–406. Springfield, VA: Nat. Tech. lnfo. Serv.

Shawabkeh, A. & Scott, J. F. (1989). *Raman spectra of low-temperature phase transitions in $RbAg_4I_5$. J. Raman Spectrosc.* **20**, 277–281.

Shawabkeh, A. & Scott, J. F. (1991). *Raman spectroscopy of incommensurate $Ba_2NaNb_5O_{15}$. Phys. Rev. B*, **43**, 10999–11004.

Shinnaka, Y. (1962). *X-ray study on the disordered structure above the ferroelectric Curie point in KNO_3. J. Phys. Soc. Jpn*, **17**, 820–828.

Shuvalov, L. A. (1988). Editor. *Modern crystallography IV. Physical properties of crystals.* Berlin: Springer-Verlag.

Sirotin, Yu. I. & Shaskolskaya, M. P. (1982). *Fundamentals of crystal physics.* Moscow: Mir Publishers.

Spencer, E. G., Guggenheim, H. J. & Kominiak, G. J. (1970). *$BaMnF_4$, a new crystal for microwave ultrasonics. Appl. Phys. Lett.* **17**, 300–301.

Stokes, H. T. & Hatch, D. M. (1988). *Isotropy groups of the 230 crystallographic space groups.* Singapore: World Scientific.

Strukov, B. A. & Levanyuk, A. P. (1998). *Ferroelectric phenomena in crystals.* Berlin: Springer.

Tahvonen, P. E. (1947). *X-ray structure of potassium nitrate. Ann. Acad. Sci. Fenn. Ser. A*, 44–51.

Tokunaga, M. (1987). *Two different mechanisms of the Curie–Weiss dielectric susceptibility in displacive-type ferroelectrics. J. Phys. Soc. Jpn*, **56**, 1653–1656.

Tolédano, J.-C., Schneck, J. & Errandonea, G. (1986). *Incommensurate phase of barium sodium niobate.* In *Incommensurate phases in dielectric materials*, edited by R. Blinc & A. P. Levanyuk, pp. 233–252. Amsterdam: North-Holland.

Tolédano, J.-C. & Tolédano, P. (1980). *Order parameter symmetries and free-energy expansions for purely ferroelastic transitions. Phys. Rev. B*, **21**, 1139–1172.

Tolédano, J.-C. & Tolédano, P. (1987). *The Landau theory of phase transitions.* Singapore: World Scientific.

Tolédano, P. & Dmitriev, V. (1996). *Reconstructive phase transitions.* Singapore: World Scientific.

Tolédano, P. & Tolédano, J.-C. (1976). *Order parameter symmetries for ferroelectric nonferroelastic transitions. Phys. Rev. B*, **14**, 3097–3109.

Tolédano, P. & Tolédano, J.-C. (1977). *Order parameter symmetries for the phase transitions of nonmagnetic secondary and higher order ferroics. Phys. Rev. B*, **16**, 386–407.

Tolédano, P. & Tolédano, J.-C. (1982). *Non-ferroic phase transitions. Phys. Rev. B*, **25**, 1946–1964.

Unoki, H. & Sakudo, T. (1967). *Electron spin resonance of Fe^{+3} in strontium titanate with specific reference to the 110 K phase transition. J. Phys. Soc. Jpn*, **23**, 546–552.

Van der Waals, J. D. (1873). PhD thesis, University of Leiden.

Volkov, A. A., Kozlov, G. V., Mirzoyants, G. I. & Petzelt, J. (1985). *Submicron dielectric spectroscopy of superionic conductors. Jpn. J. Appl. Phys.* **24**, Suppl. 24–2, 531–533.

Wadhawan, V. K. (2000) *Introduction to ferroic materials.* Australia: Gordon and Breach Science Publishers.

Wang, Y., Shen, H., Zhu, J., Xu, Z., Gu, M., Niu, Z. & Zhang, Z. (1987). *Ultrasonic anomaly in $YBa_2Cu_3O_{7-x}$ at 235 K. J. Phys. Condens. Mat.* **20**, L665.

Weiss, P. (1907). *L'hypothèse du champ moléculaire et la propriété ferromagnétique. J. Phys. Radium*, **6**, 661–690.

Weitzenböck, R. (1923). *Invariantentheorie.* Groningen: Noordhof.

Western, A. B., Baker, A. G., Bacon, C. R. & Schmidt, V. H. (1978). *Pressure-induced critical point in the ferroelectric phase transition in KH_2PO_4. Phys. Rev. B*, **17**, 4461–4473.

Weyl, H. (1946). *The classical groups.* Princeton: UP.

Windsch, W. & Volkel, G. (1980). *EPR investigation of the dynamics of ferroelectric tris-sarcosine calcium chloride. Ferroelectrics*, **24**, 195–202.

Wondre, F. R. (1977). Unpublished. Cited in Scott, J. F. (1978). *Spectroscopy of magnetoelectric $BaMnF_4$ and ferroelastic NdP_5O_{14}. Ferroelectrics*, **20**, 69–74.

Worlock, J. M. (1971). *Light scattering studies of structural phase transitions*. In *Structural phase transitions and soft modes*, edited by E. Samuelsen, E. Andersen & Z. Feder, pp. 329–370. Oslo: Universitetsforlaget.

Zhang, M.-S., Chen, Q., Sun, D., Ji, R.-F., Qin, Z.-K., Yu, Z. & Scott, J. F. (1988). *Raman studies of phonon anomalies at 235 K in $YBa_2Cu_3O_{7-x}$. Solid State Commun.* **65**, 487–490; see also Huang *et al.* (1987).