KOPSKY, V. (1979a). Acta Cryst. A35, 83–95.
KOPSKY, V. (1979b). Acta Cryst. A35, 95–101.
LITVIN, D. B., JANOVEC, V. & LITVIN, S. Y. (1994). Ferroelectrics. In the press.
LITVIN, S. Y. & LITVIN, D. B. (1991). Acta Cryst. A47, 290–292
NYE, J. F. (1957). Physical Properties of Crystals. Oxford: Clarendon Press.
SANDS, D. E. (1982). Vectors and Tensors in Crystallography. Reading, MA: Addison-Wesley.
SIROTIN, YU. & SHASKOLSKAYA, M. P. (1975). Osnovi Kristallogfiziki. Moscow: Nauka.

Acta Cryst. (1994). **A50**, 408–409

Normalization factors for Kubic harmonic density functions.

By ZHENGWEI SU and PHILIP COPPENS, *Department of Chemistry, State University of New York at Buffalo, Buffalo, New York* 14214-3094, *USA*

(*Received* 19 *August* 1993; *accepted* 22 *November* 1993)

Abstract

Normalization factors N_{lj} for the Kubic harmonics K_{lj} defined by

$$\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} N_{lj}|K_{lj}|\sin\theta\,d\theta\,d\varphi = 2-\delta_{l0}$$

have been evaluated numerically for $l \leq 10$.

Introduction

For cubic site symmetries, the symmetry-adapted functions for describing the angular dependence of the atomic charge density are the Kubic harmonics K_{lj} (Kurki-Suonio, 1977; Dawson, 1967). However, the normalization factors available in the literature, defined by

$$(1/M_{lj}^2)\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} K_{lj}^2 \sin\theta\,d\theta\,d\varphi = 1 \qquad (1)$$

(Von der Lage & Bethe, 1947; Kurki-Suonio, 1977), apply to the normalization of wave functions. For density functions, the normalization

$$N_{lj}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} |K_{lj}|\sin\theta\,d\theta\,d\varphi = 2-\delta_{l0} \qquad (2)$$

is appropriate. With this normalization, a population coefficient $P_{lj}=1$ implies, for $l=0$, a population of one electron and, for $l>0$, that one electron has been transferred from the negative to the positive lobes of the function $R_l(r)N_{lj}K_{lj}$, where $R_l(r)$ is a normalized radial function.

The unnormalized Kubic harmonics K_{lj} have been expressed in different forms (Kurki-Suonio, 1977; Dawson, 1967; Von der Lage & Bethe, 1947). We adopt the expressions given by Kurki-Suonio (1977).

The calculation

Table 1 lists the definitions of K_{lj} up to $l=10$, together with the N_{lj} values. Except for K_0 ($N_0 = 1/4\pi$) and K_3 ($N_3 = 1/15$), the values have been calculated by numerical integration using the Gaussian quadrature (Press, Flannery, Teukolsky & Vetterling, 1986). Satisfactory results have been obtained by dividing the intervals of integration for θ and φ into about 200 parts, evaluating the integral in each small solid angle by the 10-point Gaussian formula and subsequently summing the integrals. Finer divisions did not change the values to seven significant figures. For example, the numerical result for N_3 is 0.9999999997/15 for both a 200-by-200 and a 300-by-300 division of $\theta\varphi$ space.

Table 1. *Normalization factors for Kubic harmonics*

$u_{lm\pm}$ is given here as $P_l^m(\cos\theta)\,{}^{\cos(m\varphi)}_{\sin(m\varphi)}$.

Unnormalized $K_{lj}(0, 0)$	Normalization factor N_{lj}
$K_0 = u_{00+} = 1$	$1/4\pi = 0.07957747$
$K_3 = u_{32-}$	$2/30 = 1/15 = 0.06666667$
$K_4 = u_{40+} + (1/168)u_{44+}$	$2/4.602568 = 0.4345400$
$K_{6,1} = u_{60+} - (1/360)u_{64+}$	$2/7.930299 = 0.2521973$
$K_{6,2} = u_{62+} - (1/792)u_{66+}$	$2/96.00000 = 0.02083333$
$K_7 = u_{72-} + (1/1560)u_{76-}$	$2/136.8711 = 0.01461229$
$K_8 = u_{80+} + (1/5940)[u_{84+} + (1/672)u_{88+}]$	$2/3.552877 = 0.5629241$
$K_{9,1} = u_{92-} - (1/2520)u_{96-}$	$2/335.7424 = 0.005956948$
$K_{9,2} = u_{94-} - (1/4080)u_{98-}$	$2/13513.50 = 0.0001480001$
$K_{10,1} = u_{10,0+} - (1/5460)[u_{10,4+} + (1/4320)u_{10,8+}]$	$2/5.480931 = 0.3649015$
$K_{10,2} = u_{10,2+} + (1/43680)[u_{10,6+} - (1/456)u_{10,10+}]$	$2/210.1611 = 0.009516509$

Table 2. *Some high-order* $y_{lm\pm}$ $[z = \cos(\theta)]$

u_{80+}	$(1/128)(6435z^8 - 12012z^6 + 6930z^4 - 1260z^2 + 35)$
u_{84+}	$(1/8)(10395)(z^2-1)^2(65z^4 - 26z^2 + 1)\cos(4\varphi)$
u_{88+}	$2027025(z^2-1)^4\cos(8\varphi)$
u_{92-}	$(495/16)z(1-z^2)(221z^6 - 273z^4 + 91z^2 - 7)\sin(2\varphi)$
u_{94-}	$(135135/8)z(z^2-1)^2(17z^4 - 10z^2 + 1)\sin(4\varphi)$
u_{96-}	$(675675/2)z(1-z^2)^3(17z^2 - 3)\sin(6\varphi)$
u_{98-}	$34459425z(z^2-1)^4\sin(8\varphi)$
$u_{10,0+}$	$(1/256)(46189z^{10} - 109395z^8 + 90090z^6 - 30030z^4 + 3465z^2 - 63)$
$u_{10,2+}$	$(495/128)(1-z^2)(4199z^8 - 6188z^6 + 2730z^4 - 364z^2 + 7)$
$u_{10,4+}$	$(45045/16)(z^2-1)^2(323z^6 - 255z^4 + 45z^2 - 1)\cos(4\varphi)$
$u_{10,6+}$	$(675675/8)(1-z^2)^3(323z^4 - 102z^2 + 3)\cos(6\varphi)$
$u_{10,8+}$	$(34459425/2)(z^2-1)^4(19z^2 - 1)\cos(8\varphi)$
$u_{10,10+}$	$654729075(1-z^2)^5\cos(10\varphi)$

ISSN 0108-7673 © 1994

The real spherical harmonics (Arfken, 1970)

$$u_{lm\pm} = P_l^m(\cos\theta)\,{}^{\cos(m\varphi)}_{\sin(m\varphi)}, \quad l=0,1,\ldots, \quad m=0,1,\ldots,l \quad (3)$$

[where $P_l^m(x)$ is the associated Legendre function] have been tabulated in the literature for $l \leq 7$ (Paturle & Coppens, 1988; Coppens, 1993). Table 2 lists those $u_{lm\pm}$ ($8 \leq l \leq 10$), with their normalization factors, which appear in the expressions for K_{lj} ($8 \leq l \leq 10$).

Support of this work by the National Science Foundation (CHE9021069) is gratefully acknowledged.

References

ARFKEN, G. (1970). *Mathematical Methods for Physicists*, 2nd ed. New York, London: Academic Press.

DAWSON, B. (1967). *Proc. R. Soc. London Ser. A*, **298**, 255–263, 264–288.

KURKI-SUONIO, K. (1977). *Isr. J. Chem.* **16**, 115–123.

PATURLE, A. & COPPENS, P. (1988). *Acta Cryst.* A**44**, 6–7.

PRESS, W. H., FLANNERY, B. P., TEUKOLSKY, S. A. & VETTERLING, W. T. (1986). *Numerical Recipes: the Art of Scientific Computing*. Cambridge Univ. Press.

VON DER LAGE, F. C. & BETHE, H. A. (1947). *Phys. Rev.* **71**, 612–622.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

Acta Cryst. (1994). A**50**, 409–410

P. P. Ewald and his dynamical theory of X-ray diffraction. (IUCr Monograph on Crystallography No. 2.) Edited by D. W. J. CRUICKSHANK, H. J. JURETSCHKE and N. KATO. Pp. xi + 161. Oxford: International Union of Crystallography/Oxford Univ. Press, 1992. Price £37.50. ISBN 0-19-855379-X.

This is an opportune time to re-examine the dynamical theory of X-ray diffraction by Ewald. The advent of synchrotrons all over the world has given new impetus to diffraction and scattering studies and with them a new demand for the understanding of basic diffraction theory. This new monograph by the IUCr is therefore timely, offering a concise presentation of Ewald's work for the specialist with a thorough grounding in physics and mathematics. With the rapid growth of X-ray and neutron studies of biological systems, it also would be extremely helpful if the major aspects of the dynamical theory could be presented in a manner understandable to scientists who are nonphysicists. We may hope that someone will now attempt that.

Ewald as a great scientist and gentle person comes to life in this book, with the authors presenting some glimpses into his private life and providing a well rounded presentation of his major scientific contributions.

The monograph begins with an introductory chapter by Kato on the significance of Ewald's dynamical theory. This is followed by four contributions constituting Section *B*, 'Ewald as seen by others'. This section is of particular interest and brings the man to life - a different person from the formal, rather Germanic, scientist encountered by the audience of his lectures. Since one of us (JFM) spent many hours with Ewald, both in Australia and elsewhere, we approached this book with a deep respect for his brilliance and deep insight into the physical basis of crystal optics and crystallography. What we had only glimpsed, and what underlies many of the comments and revelations in this book, is the humanity of the man - even humility, yet without any display of false modesty. He knew he was foremost in his field, but had great tolerance of the difficulties experienced by others, even senior scientists in crystallography, in understanding his work. He often came up with appropriate comparisons from other fields, such as the *Pendellösung* fringes described well in this monograph. Reading his history, one marvels at the range of his interests and contributions to science. It is difficult enough today to try to understand subjects like his dynamical theory, or the quantum-mechanical approach to the interaction between matter and radiation; how much more difficult it must have been without the knowledge of crystal structure that we now possess and the myriad of related experiments from so many other fields. A lot of his personal charm and diplomacy was revealed at a NATO conference on direct methods, organized by Michael Woolfson and held in Parma, Italy. Parma was then a stronghold of the Communist movement in Italy, with very vocal representation by the students of the University. Martin Buerger was lecturing when a group of students entered and disrupted the meeting. Buerger was furious and looked like providing provocation for a confrontation, these being only too common at the time. However, Woolfson, who chaired the session, calmed down Buerger and invited a few of the troublemakers to talk things over. He managed to propitiate some of the delegation, but a very pretty and fiery young woman still protested against 'fascists in a NATO-sponsored conference' using their university. At this stage, Professor Nardelli, host of the conference, wanted to call in the police, but Ewald interceded and asked if he might talk to the demonstrators. The organizers could hardly refuse this request from an elder statesman of science. None of the demonstrators spoke English, but some of them understood French, and Ewald explained in fluent French that many of the participants in the meeting were from non-NATO countries, including the Soviet Union, Hungary, Yugoslavia *etc.* The students left quietly and presented no further problems. The conferees continued to use the university dormitories, but moved the