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DODATAK APPENDIX

Addendum to:

Irreducible Tensors of the Point Groups with Fivefold Rotational Axes

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(on the following referred to as »**BC**«)

The basic formula for the calculation of the components of the irreducible tensors (»Tensorial Covariants«[a]) deduced from an extension of the Neumann's principle, as quoted in the publication **BC** (p. 268) in eq. (4) and (5), is not correct. For the components of a polar tensor results[b]

$$^{j}d_{p,\rho\sigma\tau}\cdots^{(\gamma)} = \Delta ij^{(\gamma)}\,(R^{-1})\; R_{a\rho}\; R_{b\sigma}\; R_{c\tau} \cdots {}^{i}d_{p,abc} \cdots {}^{(\gamma)}. \qquad (4')$$

In analogy follows for the components of an axial tensor

$$^{j}d_{ax,\rho\sigma\tau}\cdots^{(\gamma)} = \det R^{-1}\; \Delta ij^{(\gamma)}\,(R^{-1})\; R_{a\rho}\; R_{b\sigma}\; R_{c\tau} \cdots {}^{i}d_{ax,abc} \cdots {}^{(\gamma)}. \qquad (5')$$

According to De Groot and Mazur[4] the two relations (1′) and (2′) can be summarized to

$$^{j}d_{p,\rho\sigma\tau}\cdots^{(\gamma)} = (\det R^{-1})\varepsilon\; \Delta ij^{(\gamma)}\,(R^{-1})\; R_{a\rho}\; R_{b\sigma}\; R_{c\tau} \cdots {}^{i}d_{abc} \cdots {}^{(\gamma)}. \qquad (5a')$$

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[a] Kopský[1] named the property tensors »Tensorial Covariants« explicitely following Weitzenböck[2] and Weyl.[3] Kopský gave these tensorial covariants for same special intrinsic symmetries for tensors up to the fourth rank for the 32 classical crystallographic point groups. In addition the general tensors are given as well in this paper as for metacrystallographic point groups.

[b] One of us (J.B.) is grateful to Prof. Dr. Rainer Dirl, Technical University Vienna, for help.

with ε = 0 for polar and ε = 1 for axial tensors. Eq. (5a′) has been justified Brandmüller and Winter.[5] With this new basic formula (5a′) the calculations of the tensorial covariants were again made for the degenerated irreducible representations of point groups. There is no change for the one-dimensional irreducible representations. The Raman and hyper Raman tensors are special cases.

We have to correct the forms given by **BC**:

1) For the 5 pentagonal point groups 5, $\overline{5}$, 52, 5m, $\overline{5}$ and for the decagonal point groups $\overline{10}$ and $\overline{10}$m2 all components of the second part tensors in the twofold degenerate irreducible representation have to be multiplied with the factor (–1).

2) For the 2 icosahedral point groups 235 and $\frac{2}{\mathrm{m}}\overline{3}\,\overline{5}$ a factor (–1) has to be added in the following cases: α) the second and third part tensors for the threefold degenerate irreducible representations; β) the third and fourth part tensors for the fourfold degenerate irreducible representation, and γ) the second and third part tensors for the fivefold degenerate irreducible representation.

The problem was generalized mathematically. The forms of polar and axial tensors without intrinsic symmetries were calculated up to the 4$^{\mathrm{th}}$ rank for the 32 crystallographic point groups., for the 5 pentagonal point groups, the 2 icosaedric, the 7 decagonal (10, $\overline{10}$, 10/m, 1022, 10mm, $\overline{10}$m2, and 10/mmm) and finally for the 5 continuous one-parametric (Curie) point groups (∞, ∞/m, ∞2, ∞m, and ∞/mm), always for all irreducible representations. These results are available on a Macintosh discette which can read with the programs Microsoft Word 3.02, Word 4.00, and Mac Write II. A Version for MS-DOS PC with Windows and Word for Windows is coming. The printout consists of 25 pages of text and 165 pages of tables. Copies thereof can be obtained upon request by Fachinformationszentrum Energie-Physik-Mathematik, W–7514 Eggenstein-Leopoldshafen 2, F.R.G. Code: CSD 51 318.

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