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LETTER TO THE EDITOR

On the isotropic averaging of fifth-order Cartesian tensors

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Abstract. We demonstrate the equivalence of two published formulae for the isotropic averaging of fifth-order Cartesian tensors.

General formulae for the isotropic averaging of three-dimensional Cartesian tensors of order not exceeding six have been published recently (Power and Thirunamachandran 1974, Healy 1974). These obviate the necessity of expressing physical quantities in terms of spherical tensors in order to carry through the averaging process and are of wide applicability, eg to multipole moments of molecules randomly oriented in solution. Some years ago Kielich (1961, 1968) presented results which, except for the case of fifth-order tensors, are evidently equivalent to those in the papers cited above. Our aim in this note is to demonstrate the equivalence of the fifth-order formulae given by equations (4) and (5) below and which are due to Kielich (1968) and to Power and Thirunamachandran (1974) respectively.

The problem of isotropically averaging an nth-order tensor reduces to the determination of the quantities

$$I^{(n)}_{i_1 i_2 \ldots i_n;\lambda_1\lambda_2\ldots\lambda_n} \equiv \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} R_{i_1\lambda_1}R_{i_2\lambda_2}\ldots R_{i_n\lambda_n}\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta\,\mathrm{d}\psi. \qquad (1)$$

$(R_{i\lambda}(\phi,\theta,\psi))$ is the 3×3 orthogonal matrix of direction cosines specifying the relative orientation of the laboratory and body-fixed frames and is parameterized by the Euler angles ϕ, θ, ψ. $I^{(n)}$ is expressible (Power and Thirunamachandran 1974, Healy 1975) in a bilinear form,

$$I^{(n)}_{i_1 i_2\ldots i_n;\lambda_1\lambda_2\ldots\lambda_n} = \sum_r\sum_s T^r_{i_1 i_2\ldots i_n}A_{rs}T^s_{\lambda_1\lambda_2\ldots\lambda_n} \qquad (2)$$

where the A_{rs} are numerical coefficients and $\{T^r\}$ is a maximal linearly independent set of nth-order isotropic tensors. (By an m-dimensional isotropic tensor is meant here a tensor invariant under the proper orthogonal group R_m and not necessarily invariant under the full orthogonal group O_m.) In three dimensions the nth-order isotropic tensors (Jeffreys 1973) are sums of products of $\frac{1}{2}n$ Kronecker deltas (n even) or of $\frac{1}{2}(n-3)$ Kronecker deltas and one Levi-Civita alternating tensor ($n\geqslant3$ and odd).

Smith (1968) has given a procedure to determine a maximal independent set for any particular m and n. For $m=3$ and $n=5$ this procedure yields

$$\{T^r_{i_1i_2i_3i_4i_5}\} = \{\epsilon_{i_1i_2i_3}\delta_{i_4i_5}, \epsilon_{i_1i_2i_4}\delta_{i_3i_5}, \epsilon_{i_1i_2i_5}\delta_{i_3i_4}, \epsilon_{i_1i_3i_4}\delta_{i_2i_5}, \epsilon_{i_1i_3i_5}\delta_{i_2i_4}, \epsilon_{i_1i_4i_5}\delta_{i_2i_3}\}. \qquad (3)$$

The orthogonality properties of the matrix $(R_{i\lambda})$ may now be used on the right-hand sides of equations (1) and (2) to deduce the values of the A_{rs}. The result is Kielich's formula, which may be written

$$I^{(5)}_{i_1i_2i_3i_4i_5;\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5}$$
$$= \frac{1}{30}\begin{pmatrix} \epsilon_{i_1i_2i_3}\,\delta_{i_4i_5} \\ \epsilon_{i_1i_2i_4}\,\delta_{i_3i_5} \\ \epsilon_{i_1i_2i_5}\,\delta_{i_3i_4} \\ \epsilon_{i_1i_3i_4}\,\delta_{i_2i_5} \\ \epsilon_{i_1i_3i_5}\,\delta_{i_2i_4} \\ \epsilon_{i_1i_4i_5}\,\delta_{i_2i_3} \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 3 & -1 & -1 & 1 & 1 & 0 \\ -1 & 3 & -1 & -1 & 0 & 1 \\ -1 & -1 & 3 & 0 & -1 & -1 \\ 1 & -1 & 0 & 3 & -1 & 1 \\ 1 & 0 & -1 & -1 & 3 & -1 \\ 0 & 1 & -1 & 1 & -1 & 3 \end{pmatrix} \begin{pmatrix} \epsilon_{\lambda_1\lambda_2\lambda_3}\,\delta_{\lambda_4\lambda_5} \\ \epsilon_{\lambda_1\lambda_2\lambda_4}\,\delta_{\lambda_3\lambda_5} \\ \epsilon_{\lambda_1\lambda_2\lambda_5}\,\delta_{\lambda_3\lambda_4} \\ \epsilon_{\lambda_1\lambda_3\lambda_4}\,\delta_{\lambda_2\lambda_5} \\ \epsilon_{\lambda_1\lambda_3\lambda_5}\,\delta_{\lambda_2\lambda_4} \\ \epsilon_{\lambda_1\lambda_4\lambda_5}\,\delta_{\lambda_2\lambda_3} \end{pmatrix}. \tag{4}$$

T denotes the transposed matrix and we have assumed that both frames have the same handedness, so that $\det(R_{i\lambda})$ is unity.

There are in all ten distinct isomers (Smith 1968) of $\epsilon_{i_1i_2i_3}\,\delta_{i_4i_5}$. The remaining four—$\epsilon_{i_2i_3i_4}\,\delta_{i_1i_5}$, $\epsilon_{i_2i_3i_5}\,\delta_{i_1i_4}$, $\epsilon_{i_2i_4i_5}\,\delta_{i_1i_3}$ and $\epsilon_{i_3i_4i_5}\,\delta_{i_1i_2}$—must therefore be linearly dependent on the six isomers appearing in equation (3). Smith's procedure does not give the explicit linear combinations; we have derived them by elementary means.

We denote the complete set of ten isomers by $\{S^r\}$ and the zero fifth-order tensor by O, and suppose

$$\sum_{r=1}^{10} a_r S^r_{i_1i_2i_3i_4i_5} \equiv O.$$

Assigning all possible values to the tensorial suffixes we obtain for the a_r a system of 3^5 homogeneous equations of which only ten are non-trivial and distinct. The 10×10 matrix of coefficients of the a_r in these equations has rank six, and the four independent solutions imply the following relations:

$$\begin{aligned}
\epsilon_{i_2i_3i_4}\,\delta_{i_1i_5} &= \epsilon_{i_1i_2i_3}\,\delta_{i_4i_5} - \epsilon_{i_1i_2i_4}\,\delta_{i_3i_5} + \epsilon_{i_1i_3i_4}\,\delta_{i_2i_5} \\
\epsilon_{i_2i_3i_5}\,\delta_{i_1i_4} &= \epsilon_{i_1i_2i_3}\,\delta_{i_4i_5} - \epsilon_{i_1i_2i_5}\,\delta_{i_3i_4} + \epsilon_{i_1i_3i_5}\,\delta_{i_2i_4} \\
\epsilon_{i_2i_4i_5}\,\delta_{i_1i_3} &= \epsilon_{i_1i_2i_4}\,\delta_{i_3i_5} - \epsilon_{i_1i_2i_5}\,\delta_{i_3i_4} + \epsilon_{i_1i_4i_5}\,\delta_{i_2i_3} \\
\epsilon_{i_3i_4i_5}\,\delta_{i_1i_2} &= \epsilon_{i_1i_3i_4}\,\delta_{i_2i_5} - \epsilon_{i_1i_3i_5}\,\delta_{i_2i_4} + \epsilon_{i_1i_4i_5}\,\delta_{i_2i_3}.
\end{aligned}$$

If these are used in conjunction with the formula of Power and Thirunamachandran, namely

$$\begin{aligned}
I^{(5)}_{i_1i_2i_3i_4i_5;\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5}
&= \tfrac{1}{30}(\epsilon_{i_1i_2i_3}\,\delta_{i_4i_5}\,\epsilon_{\lambda_1\lambda_2\lambda_3}\,\delta_{\lambda_4\lambda_5} + \epsilon_{i_1i_2i_4}\,\delta_{i_3i_5}\,\epsilon_{\lambda_1\lambda_2\lambda_4}\,\delta_{\lambda_3\lambda_5} + \epsilon_{i_1i_2i_5}\,\delta_{i_3i_4}\,\epsilon_{\lambda_1\lambda_2\lambda_5}\,\delta_{\lambda_3\lambda_4} \\
&\quad + \epsilon_{i_1i_3i_4}\,\delta_{i_2i_5}\,\epsilon_{\lambda_1\lambda_3\lambda_4}\,\delta_{\lambda_2\lambda_5} + \epsilon_{i_1i_3i_5}\,\delta_{i_2i_4}\,\epsilon_{\lambda_1\lambda_3\lambda_5}\,\delta_{\lambda_2\lambda_4} \\
&\quad + \epsilon_{i_1i_4i_5}\,\delta_{i_2i_3}\,\epsilon_{\lambda_1\lambda_4\lambda_5}\,\delta_{\lambda_2\lambda_3} + \epsilon_{i_2i_3i_4}\,\delta_{i_1i_5}\,\epsilon_{\lambda_2\lambda_3\lambda_4}\,\delta_{\lambda_1\lambda_5} + \epsilon_{i_2i_3i_5}\,\delta_{i_1i_4}\,\epsilon_{\lambda_2\lambda_3\lambda_5}\,\delta_{\lambda_1\lambda_4} \\
&\quad + \epsilon_{i_2i_4i_5}\,\delta_{i_1i_3}\,\epsilon_{\lambda_2\lambda_4\lambda_5}\,\delta_{\lambda_1\lambda_3} + \epsilon_{i_3i_4i_5}\,\delta_{i_1i_2}\,\epsilon_{\lambda_3\lambda_4\lambda_5}\,\delta_{\lambda_1\lambda_2}),
\end{aligned} \tag{5}$$

then equation (4) is immediately recovered.

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