International Tables for Crystallography (2006). Vol. B, Table 1.2.11.1, p. 21.

Table 1.2.8.3. *Products of two real spherical harmonic functions y_{lmp} in terms of the density functions d_{lmp} defined by equation (1.2.7.3b)*

$$
\begin{aligned}
y_{00}\, y_{00} &= 1.0000d_{00}\\
y_{10}\, y_{00} &= 0.43301d_{10}\\
y_{10}\, y_{10} &= 0.38490d_{20} + 1.0d_{00}\\
y_{11\pm}\, y_{00} &= 0.43302d_{11\pm}\\
y_{11\pm}\, y_{10} &= 0.31831d_{21\pm}\\
y_{11\pm}\, y_{11\pm} &= 0.31831d_{22+} - 0.19425d_{20} + 1.0d_{00}\\
y_{11+}\, y_{11-} &= 0.31831d_{22-}\\
y_{20}\, y_{00} &= 0.43033d_{20}\\
y_{20}\, y_{10} &= 0.37762d_{30} + 0.38730d_{10}\\
y_{20}\, y_{11\pm} &= 0.28864d_{31\pm} - 0.19365d_{11\pm}\\
y_{20}\, y_{20} &= 0.36848d_{40} + 0.27493d_{20} + 1.0d_{00}\\
y_{21\pm}\, y_{00} &= 0.41094d_{21\pm}\\
y_{21\pm}\, y_{10} &= 0.33329d_{31\pm} + 0.33541d_{11\pm}\\
y_{21\pm}\, y_{11\pm} &= \pm 0.26691d_{32+} - 0.21802d_{30} + 0.33541d_{10}\\
y_{21\pm}\, y_{11\mp} &= -0.26691d_{32-}\\
y_{21\pm}\, y_{20} &= 0.31155d_{41\pm} + 0.13127d_{21\pm}\\
y_{21\pm}\, y_{21\pm} &= \pm 0.25791d_{42+} \pm 0.22736d_{22+} - 0.24565d_{40} + 0.13747d_{20}\\
&\quad + 1.0d_{00}\\
y_{21+}\, y_{21-} &= 0.25790d_{42-} + 0.22736d_{22-}\\
y_{22\pm}\, y_{00} &= 0.41094d_{22\pm}\\
y_{22\pm}\, y_{10} &= 0.26691d_{32\pm}\\
y_{22\pm}\, y_{11\pm} &= \pm\, 0.31445d_{33+} - 0.083323d_{31+} + 0.33541d_{11+}\\
y_{22\pm}\, y_{11\mp} &= 0.31445d_{33-} \pm 0.083323d_{31-} \mp 0.33541d_{11-}\\
y_{22\pm}\, y_{20} &= 0.22335d_{42\pm} - 0.26254d_{22\pm}\\
y_{22\pm}\, y_{21\pm} &= \pm\, 0.23873d_{43+} - 0.089938d_{41+} + 0.22736d_{21+}\\
y_{22\pm}\, y_{21\mp} &= 0.23873d_{43-} \pm 0.089938d_{41-} \mp 0.22736d_{21-}\\
y_{22\pm}\, y_{22\pm} &= \pm\, 0.31831d_{44+} + 0.061413d_{40} - 0.27493d_{20} + 1.0d_{00}\\
y_{22+}\, y_{22-} &= 0.31831d_{44-}
\end{aligned}
$$

Table 1.2.11.1. *The arrays G_{ijkl} and H_{ijkl} to be used in the observational equations $U_{ij} = G_{ijkl}L_{kl} + H_{ijkl}S_{kl} + T_{ij}$ [equation (1.2.11.9)]*

G_{ijkl}

	kl					
ij	11	22	33	23	31	12
11	0	z^2	y^2	$-2yz$	0	0
22	z^2	0	x^2	0	$-2xz$	0
33	y^2	x^2	0	0	0	$-2xy$
23	$-yz$	0	0	$-x^2$	xy	xz
31	0	$-xz$	0	xy	$-y^2$	yz
12	0	0	$-xy$	xz	yz	$-z^2$

H_{ijkl}

	kl								
ij	11	22	33	23	31	12	32	13	21
11	0	0	0	0	$-2y$	0	0	0	$2z$
22	0	0	0	0	0	$-2z$	$2x$	0	0
33	0	0	0	$-2x$	0	0	0	$2y$	0
23	0	$-x$	x	0	0	y	0	$-z$	0
31	y	0	$-y$	z	0	0	0	0	$-x$
12	$-z$	z	0	0	x	0	$-y$	0	0

the same vibration tensor. When the observational equations for these two atoms are added, the terms involving elements of **S** disappear since they are linear in the components of **r**. The other terms, involving elements of the **T** and **L** tensors, are simply doubled, like the $\mathbf{U}^n$ components.

The physical meaning of the **T** and **L** tensor elements is as follows. $T_{ij}l_il_j$ is the mean-square amplitude of translational vibration in the direction of the unit vector l with components l_1, l_2, l_3 along the Cartesian axes and $L_{ij}l_il_j$ is the mean-square amplitude of libration about an axis in this direction. The quantity $S_{ij}l_il_j$ represents the mean correlation between libration about the axis l and translation parallel to this axis. This quantity, like $T_{ij}l_il_j$, depends on the choice of origin, although the sum of the two quantities is independent of the origin.

The non-symmetrical tensor **S** can be written as the sum of a symmetric tensor with elements $S^S_{ij} = (S_{ij} + S_{ji})/2$ and a skew-symmetric tensor with elements $S^A_{ij} = (S_{ij} - S_{ji})/2$. Expressed in terms of principal axes, $\mathbf{S}^S$ consists of three principal screw correlations $\langle \lambda_I t_I \rangle$. Positive and negative screw correlations correspond to opposite senses of helicity. Since an arbitrary constant may be added to all three correlation terms, only the differences between them can be determined from the data.

The skew-symmetric part $\mathbf{S}^A$ is equivalent to a vector $(\boldsymbol{\lambda} \times \mathbf{t})/2$ with components $(\boldsymbol{\lambda} \times \mathbf{t})_i/2 = (\lambda_j t_k - \lambda_k t_j)/2$, involving correlations between a libration and a perpendicular translation. The components of $\mathbf{S}^A$ can be reduced to zero, and **S** made symmetric, by a change of origin. It can be shown that the origin shift that symmetrizes **S** also minimizes the trace of **T**. In terms of the coordinate system based on the principal axes of **L**, the required origin shifts $\widehat{\rho}_i$ are

$$\widehat{\rho}_1 = \frac{\widehat{S}_{23} - \widehat{S}_{32}}{\widehat{L}_{22} + \widehat{L}_{33}} \quad \widehat{\rho}_2 = \frac{\widehat{S}_{31} - \widehat{S}_{13}}{\widehat{L}_{11} + \widehat{L}_{33}} \quad \widehat{\rho}_3 = \frac{\widehat{S}_{12} - \widehat{S}_{21}}{\widehat{L}_{11} + \widehat{L}_{22}}, \quad (1.2.11.10)$$

in which the carets indicate quantities referred to the principal axis system.

The description of the averaged motion can be simplified further by shifting to three generally non-intersecting libration axes, one each for each principal axis of **L**. Shifts of the $\mathbf{L}_1$ axis in the $\mathbf{L}_2$ and $\mathbf{L}_3$ directions by

$${}^1\widehat{\rho}_2 = -\widehat{S}_{13}/\widehat{L}_{11} \text{ and } {}^1\widehat{\rho}_3 = \widehat{S}_{12}/\widehat{L}_{11}, \quad (1.2.11.11)$$

respectively, annihilate the S_{12} and S_{13} terms of the symmetrized **S** tensor and simultaneously effect a further reduction in Tr(**T**) (the presuperscript denotes the axis that is shifted, the subscript the direction of the shift component). Analogous equations for displacements of the $\mathbf{L}_2$ and $\mathbf{L}_3$ axes are obtained by permutation of the indices. If all three axes are appropriately displaced, only the diagonal terms of **S** remain. Referred to the principal axes of **L**, they represent screw correlations along these axes and are independent of origin shifts.

The elements of the reduced **T** are

$$
\begin{aligned}
{}^rT_{II} &= \widehat{T}_{II} - \sum_{K \neq I} (\widehat{S}_{KI})^2/\widehat{L}_{KK}\\
{}^rT_{IJ} &= \widehat{T}_{IJ} - \sum_{K} \widehat{S}_{KI}\widehat{S}_{KJ}/\widehat{L}_{KK}, \quad J \neq I. \qquad (1.2.11.12)
\end{aligned}
$$

The resulting description of the average rigid-body motion is in terms of six independently distributed instantaneous motions – three screw librations about non-intersecting axes (with screw pitches given by $\widehat{S}_{11}/\widehat{L}_{11}$ *etc.*) and three translations. The parameter set consists of three libration and three translation amplitudes, six

references