International Tables for Crystallography (2006). Vol. B, Table 1.2.7.3, pp. 16–17.

Table 1.2.7.3. *'Kubic Harmonic' functions*

(*a*) Coefficients in the expression $K_{lj} = \sum_{mp} k^l_{mpj} y_{lmp}$ with normalization $\int_0^\pi \int_0^{2\pi} |K_{lj}|^2 \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\varphi = 1$ (Kara & Kurki-Suonio, 1981).

Even l		mp					
l	j	0+	2+	4+	6+	8+	10+
0	1	1					
4	1	$\frac{1}{2}\left(\frac{7}{3}\right)^{1/2}$ 0.76376		$\frac{1}{2}\left(\frac{5}{3}\right)^{1/2}$ 0.64550			
6	1	$\frac{1}{2}\left(\frac{1}{2}\right)^{1/2}$ 0.35355		$-\frac{1}{2}\left(\frac{7}{2}\right)^{1/2}$ −0.93541			
6	2		$\frac{1}{4}11^{1/2}$ 0.82916		$-\frac{1}{4}5^{1/2}$ −0.55902		
8	1	$\frac{1}{8}33^{1/2}$ 0.71807		$\frac{1}{4}\left(\frac{7}{3}\right)^{1/2}$ 0.38188		$\frac{1}{8}\left(\frac{65}{3}\right)^{1/2}$ 0.58184	
10	1	$\frac{1}{8}\left(\frac{65}{6}\right)^{1/2}$ 0.41143		$-\frac{1}{4}\left(\frac{11}{2}\right)^{1/2}$ −0.58630		$-\frac{1}{8}\left(\frac{187}{6}\right)^{1/2}$ −0.69784	
10	2		$\frac{1}{8}\left(\frac{247}{6}\right)^{1/2}$ 0.80202		$\frac{1}{16}\left(\frac{19}{3}\right)^{1/2}$ 0.15729		$\frac{1}{16}85^{1/2}$ 0.57622
l	j		2−	4−	6−	8−	
3	1		1				
7	1		$\frac{1}{2}\left(\frac{13}{6}\right)^{1/2}$ 0.73598		$\frac{1}{2}\left(\frac{11}{16}\right)^{1/2}$ 0.41458		
9	1		$\frac{1}{4}3^{1/2}$ 0.43301		$-\frac{1}{4}13^{1/2}$ −0.90139		
9	2		$\frac{1}{2}\left(\frac{17}{6}\right)^{1/2}$ 0.84163		$-\frac{1}{2}\left(\frac{7}{6}\right)^{1/2}$ −0.54006		

(*b*) Coefficients k^l_{mpj} and density normalization factors N_{lj} in the expression $K_{lj} = N_{lj} \sum_{mp} k^l_{mpj} u_{lmp}$ where $u_{lm\pm} = P^m_l(\cos\theta)^{\cos m\varphi}_{\sin m\varphi}$ (Su & Coppens, 1994).

Even l		N_{lj}	mp					
l	j		0+	2+	4+	6+	8+	10+
0	1	$1/4\pi = 0.079577$	1					
4	1	0.43454	1		$+1/168$			
6	1	0.25220	1		$-1/360$			
6	2	0.020833		1		$-1/792$		

Table 1.2.7.3. *'Kubic Harmonic' functions* (*cont.*)

Even l		N_{lj}	mp					
8	1	0.56292	1		1/5940		$\frac{1}{672} \times \frac{1}{5940}$	
10	1	0.36490	1		1/5460		$\frac{1}{4320} \times \frac{1}{5460}$	
10	2	0.0095165	1			$1/43680$		$-\frac{1}{456} \times \frac{1}{43680}$
l	j			2−	4−	6−	8−	
3	1	0.066667		1				
7	1	0.014612		1		$1/1560$		
9	1	0.0059569		1		$1/2520$		
9	2	0.00014800			1		$-1/4080$	

(*c*) Density-normalized Kubic harmonics as linear combinations of density-normalized spherical harmonic functions. Coefficients in the expression $K_{lj} = \sum_{mp} k''^{l}_{mpj} d_{lmp}$. Density-type normalization is defined as $\int_0^{\pi}\int_0^{2\pi} |K_{lj}| \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\varphi = 2 - \delta_{l0}$.

Even l		mp					
l	j	0+	2+	4+	6+	8+	10+
0	1	1					
4	1	0.78245		0.57939			
6	1	0.37790		−0.91682			
6	2		0.83848		−0.50000		
l	j	2−	4−	6−	8−		
3	1	1					
7	1	0.73145		0.63290			

(*d*) Index rules for cubic symmetries (Kurki-Suonio, 1977; Kara & Kurki-Suonio, 1981).

l	j	23 T	$m\bar{3}$ T_h	432 O	$\bar{4}3m$ T_d	$m\bar{3}m$ O_h
0	1	×	×	×	×	×
3	1	×			×	
4	1	×	×	×	×	×
6	1	×	×	×	×	×
6	2	×	×			
7	1	×			×	
8	1	×	×	×	×	×
9	1	×			×	
9	2	×		×		
10	1	×	×	×	×	×
10	2	×	×			

1.2.8. Fourier transform of orbital products

If the wavefunction is written as a sum over normalized Slater determinants, each representing an antisymmetrized combination of occupied molecular orbitals χ_i expressed as linear combinations of atomic orbitals φ_ν, *i.e.* $\chi_i = \sum_\nu c_{i\nu}\varphi_\nu$, the electron density is given by (Stewart, 1969*a*)

$$\rho(\mathbf{r}) = \sum_i n_i \chi_i^2 = \sum_\mu \sum_\nu P_{\mu\nu}\varphi_\mu(\mathbf{r})\varphi_\nu(\mathbf{r}), \qquad (1.2.8.1)$$

with $n_i = 1$ or 2. The coefficients $P_{\mu\nu}$ are the populations of the

references