Supporting Information for "Polarizable Atomic Multipole Solutes in a Generalized Kirkwood Continuum" by Schnieders and Ponder:

Appendix A. Intermediate Terms in the Derivation of the Solvent Field Approximation

Table A-1. Multipole moment conversions.

$Q_0^{(0)} = q$
$Q_1^{(0)} = \mu_z$
$Q_1^{(1)} = \mu_x$
$Q_1^{(-1)} = \mu_y$
$Q_2^{(0)} = \Theta_{zz}$
$Q_2^{(1)} = \frac{2}{\sqrt{3}}\Theta_{xz}$
$Q_2^{(-1)} = \frac{2}{\sqrt{3}}\Theta_{yz}$
$Q_2^{(2)} = \frac{1}{\sqrt{3}}\left(\Theta_{xx} - \Theta_{yy}\right)$
$Q_2^{(-2)} = \frac{2}{\sqrt{3}}\Theta_{xy}$

Table A-2. Unit vacuum potentials.

l	m	$\Phi_l^{(m)}(r,\theta,\phi)$
0	0	$\frac{1}{r}$
1	0	$\frac{\cos\theta}{r^2}$
	1	$\frac{\sin\theta\cos\phi}{r^2}$
	-1	$\frac{\sin\theta\sin\phi}{r^2}$
2	0	$\frac{1}{2}\frac{3\cos^2\theta-1}{r^3}$
	1	$\frac{\sqrt{3}\cos\theta\sin\theta\cos\phi}{r^3}$
	-1	$\frac{\sqrt{3}\cos\theta\sin\theta\sin\phi}{r^3}$
	2	$-\frac{\sqrt{3}}{2}\frac{\left(\sin^2\theta+2\cos^2\theta\cos^2\phi-2\cos^2\phi\right)}{r^3}$
	-2	$\frac{\sqrt{3}\sin^2\theta\sin\phi\cos\phi}{r^3}$

Table A-3. Unit vacuum fields.

l	m	$\mathbf{E}_l^{(m)}$
0	0	$\frac{1}{r^2}\hat{\mathbf{r}}$
1	0	$\frac{2\cos\theta}{r^3}\hat{\mathbf{r}}+\frac{\sin\theta}{r^3}\hat{\boldsymbol{\theta}}$
	1	$\frac{2\sin\theta\cos\phi}{r^3}\hat{\mathbf{r}}-\frac{\cos\theta\cos\phi}{r^3}\hat{\boldsymbol{\theta}}+\frac{\sin\phi}{r^3}\hat{\boldsymbol{\phi}}$
	-1	$\frac{2\sin\theta\sin\phi}{r^3}\hat{\mathbf{r}}-\frac{\cos\theta\sin\phi}{r^3}\hat{\boldsymbol{\theta}}-\frac{\cos\phi}{r^3}\hat{\boldsymbol{\phi}}$
2	0	$\frac{3}{2}\frac{\left(3\cos^2\theta-1\right)}{r^4}\hat{\mathbf{r}}+\frac{3\cos\theta\sin\theta}{r^4}\hat{\boldsymbol{\theta}}$
	1	$\frac{3\sqrt{3}\cos\theta\sin\theta\cos\phi}{r^4}\hat{\mathbf{r}}-\frac{\sqrt{3}\left(2\cos^2\theta-1\right)\cos\phi}{r^4}\hat{\boldsymbol{\theta}}+\frac{\sqrt{3}\cos\theta\sin\phi}{r^4}\hat{\boldsymbol{\phi}}$
	-1	$\frac{3\sqrt{3}\cos\theta\sin\theta\sin\phi}{r^4}\hat{\mathbf{r}}-\frac{\sqrt{3}\left(2\cos^2\theta-1\right)\sin\phi}{r^4}\hat{\boldsymbol{\theta}}-\frac{\sqrt{3}\cos\theta\cos\phi}{r^4}\hat{\boldsymbol{\phi}}$
	2	$\frac{3\sqrt{3}}{2}\frac{\sin^2\theta\cos 2\phi}{r^4}\hat{\mathbf{r}}-\frac{\sqrt{3}\sin\theta\cos\theta\cos 2\phi}{r^4}\hat{\boldsymbol{\theta}}+\frac{\sqrt{3}\sin\theta\sin 2\phi}{r^4}\hat{\boldsymbol{\phi}}$
	-2	$\frac{3\sqrt{3}}{2}\frac{\sin^2\theta\sin 2\phi}{r^4}\hat{\mathbf{r}}-\frac{\sqrt{3}\sin\theta\cos\theta\sin 2\phi}{r^4}\hat{\boldsymbol{\theta}}-\frac{\sqrt{3}\sin\theta\cos 2\phi}{r^4}\hat{\boldsymbol{\phi}}$

Table A-4. Selected scalar products of unit magnitude vacuum spherical harmonic fields.

$(l,m)_1$	$(l,m)_2$	$\mathbf{E}_{l_1}^{(m_1)} \cdot \mathbf{E}_{l_2}^{(m_2)}$
(0, 0)	(0, 0)	$\frac{1}{r^4}$
	(1, 0)	$\frac{2\cos\theta}{r^5}$
	(2, 0)	$\frac{3}{2}\frac{\left(3\cos^2\theta-1\right)}{r^6}$
(1, 0)	(1, 0)	$\frac{3\cos^2\theta+1}{r^6}$
	(2, 0)	$\frac{6\cos^3\theta}{r^7}$
(1, 1)	(1, 1)	$\frac{\left(4\sin^2\theta+\cos^2\theta\right)\cos^2\phi+\sin^2\phi}{r^6}$
	(2, 1)	$\frac{\sqrt{3}\cos\theta\left(6\cos^2\phi\sin^2\theta-\cos^2\phi+2\cos^2\theta\cos^2\phi+\sin^2\phi\right)}{r^7}$
(1,-1)	(1,-1)	$\frac{\left(4\sin^2\theta+\cos^2\theta\right)\sin^2\phi+\cos^2\phi}{r^6}$
	(2,-1)	$\frac{\sqrt{3}\cos\theta\left(6\sin^2\phi\sin^2\theta-\sin^2\phi+2\sin^2\phi\cos^2\theta+\cos^2\phi\right)}{r^7}$
(2, 0)	(2, 0)	$\frac{1}{4}\frac{9+81\cos^4\theta+\left(36\sin^2\theta-54\right)\cos^2\theta}{r^8}$
(2, 1)	(2, 1)	$\frac{12\cos^2\phi\cos^4\theta+\left(\left(27\sin^2\theta-12\right)\cos^2\phi+3\sin^2\phi\right)\cos^2\theta+3\cos^2\phi}{r^8}$
(2,-1)	(2,-1)	$\frac{12\sin^2\phi\cos^4\theta+\left(\left(27\sin^2\theta-12\right)\sin^2\phi+3\cos^2\phi\right)\cos^2\theta+3\sin^2\phi}{r^8}$
(2, 2)	(2, 2)	$\frac{1}{4}\frac{\left(27\cos^4\theta+27+\left(12\sin^2\theta-54\right)\cos^2\theta\right)\cos^2 2\phi+12\sin^2 2\phi\sin^2\theta}{r^8}$
(2,-2)	(2,-2)	$\frac{3}{4}\frac{\sin^2\theta\left(9\sin^2 2\phi\sin^2\theta+4\sin^2 2\phi\cos^2\theta+4\cos^2 2\phi\right)}{r^8}$

Appendix B. Factoring of Generalized Kirkwood Tensors

Cartesian multipole interaction tensors can be computed via recurrence relationships, which can greatly improve the efficiency of their use for high degree expansions.[70,71] Unfortunately, we have not found an analogous approach for generalized Kirkwood tensors. In this appendix we present a practical factoring of the associated algebra that mirrors our implementation of GK, but it is conceivable superior alternatives exist.

The GK auxiliary potential tensor $\mathbf{A}^{(n)}$ of rank n has 3^n elements, but because it is totally symmetric only $(n+1)(n+2)/2$ elements are distinct. For example, the dipole auxiliary potential tensor $\mathbf{A}^{(1)}$ has 3 elements $\left(-c_1 \frac{x}{f^3}, -c_1 \frac{y}{f^3}, -c_1 \frac{z}{f^3}\right)$, where the generalizing function f was defined in Eq. (6) and c_l was defined in Eq. (19). In compressed tensor notation[72,73], elements are denoted as $\mathrm{A}^{(n)}_{\{n_1,n_2,n_3\}}$, where n_1, n_2, and n_3 are called degree indices that satisfy the constraint $n_1 + n_2 + n_3 = n$. All components of the GK auxiliary potential tensor of any degree can be decomposed as $\mathrm{A}^{(n)}_{\{n_1,n_2,n_3\}} = x^{n_1} y^{n_2} z^{n_3} t_{(n,0)}$ where $t_{(n,0)}$ is an entry in the first column of a matrix $\boldsymbol{t}$ that we construct purely for convenience, and detail below. Using this notation, one element of the auxiliary dipole potential is $\mathrm{A}^{(1)}_{\{1,0,0\}} = x t_{(1,0)}$, where $t_{(1,0)}$ is $-c_1 \frac{1}{f^3}$.

Generation of Cartesian derivatives for any element $\mathrm{A}^{(n)}_{\{n_1,n_2,n_3\}}$ will now be described. Unlike tensors built from derivatives of $1/r$, GK auxiliary potential tensors do not, in general, obey the relationship

$$\frac{\partial \mathrm{A}_{\{n_1,n_2,n_3\}}^{(n)}}{\partial x} \neq \mathrm{A}_{\{n_1+1,n_2,n_3\}}^{(n+1)} . \tag{B1}$$

However, we present a factoring scheme that facilitates generation of the mth order auxiliary potential gradient for any GK auxiliary potential tensor, which we denote as

$$\mathrm{A}_{\{n_1,n_2,n_3\},\{m_1,m_2,m_3\}}^{(n)} = \frac{\partial^m}{\partial x^{m_1} \partial y^{m_2} \partial z^{m_3}} \mathrm{A}_{\{n_1,n_2,n_3\}}^{(n)} \tag{B2}$$

where $m_1 + m_2 + m_3 = m$. All potential gradients are composed of sums of terms that have the form $p_1 x^{p_2} y^{p_3} z^{p_4} t_{(i,j)}$, where p_1, p_2, p_3, and p_4 are constants. These are enumerated in Table B-1 through Table B-10 for moments through the quadrupole. For example, Table B-2 contains the auxiliary reaction potential $\mathrm{A}_{\{1,0,0\}}^{(1)}$ and its gradients for the x-component of a dipole.

The effective radii chain rule terms are denoted $\frac{\partial}{\partial a_1} \mathrm{A}_{\{n_1,n_2,n_3\},\{m_1,m_2,m_3\}}^{(n)}$, where a_1 denotes the derivative is with respect to the effective radii of site 1. They are composed of sums of terms that have the form $a_2 p_1 x^{p_2} y^{p_3} z^{p_4} b_{(i,j)}$ where $b_{(i,j)} = \frac{\partial t_{(i,j)}}{\partial a_1} \frac{1}{a_2} = \frac{\partial t_{(i,j)}}{\partial a_2} \frac{1}{a_1}$ is an element from a second matrix **b**, again defined for convenience. This matrix contains the derivatives of the **t** matrix elements with respect to an effective radius, normalized by the effective radius of the other site in the pairwise interaction. The chain rule term with respect to an effective radius for any entry in Table B-1 through Table B-10 is given by substituting the **t** matrix elements with corresponding elements from the **b** matrix and multiplying by the opposite effective radius. For example, the chain rule term for the first entry in Table B-2 with respect to effective radius 1 is $\frac{\partial}{\partial a_1}\mathrm{A}^{(1)}_{\{1,0,0\},\{0,0,0\}} = a_2 x b_{(1,0)}$ and that for the 2nd entry is $\frac{\partial}{\partial a_1}\mathrm{A}^{(1)}_{\{1,0,0\},\{1,0,0\}} = a_2\left(b_{(1,0)} + x^2 b_{(1,1)}\right)$.

All that remains is to describe an efficient mechanism to generate all elements of the **t** and **b** matrices. The matrix **t** is of size $n \times m$, whose rows and columns are indexed from $0..n-1$ and $0..m-1$, respectively. The first column contains the GK auxiliary reaction potential tensors given in Eq. (35) without factors of x, y or z in the numerator. All other columns contain derivatives with respect to r_α of the previous column, where α represents x, y or z. The results are normalized by r_α such that the terms are independent of which derivative was taken.

$$\mathbf{t} = \begin{bmatrix} c_0 \frac{1}{f} & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(0,0)} & \cdots & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(0,m-2)} \\ -c_1 \frac{1}{f^3} & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(1,0)} & \cdots & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(1,m-2)} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{(n-1)} c_{n-1} \frac{(2(n-1)-1)!!}{f^{2(n-1)+1}} & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(n-1,0)} & \cdots & \frac{1}{r_\alpha}\frac{\partial}{\partial r_\alpha} t_{(n-1,m-2)} \end{bmatrix} \quad \text{(B3)}$$

We note that all the elements of the 2nd column $t_{(i,1)}$ are related to elements of the first column by a constant factor f_1,

$$f_1 = \left(\frac{\partial t_{(i,0)}}{\partial r_\alpha}\right)\frac{1}{r_\alpha t_{(i+1,0)}} = 1 - \frac{e^{-r_{ij}^2 / c_f a_1 a_2}}{c_f} \quad \text{(B4)}$$

such that all $t_{(i,1)}$ can be found as

$$t_{(i,1)} = f_1 t_{(i+1,0)} \quad \text{(B5)}$$

By the chain rule, all components in the 3rd column of **t** are related to those in the first two columns as

$$t_{(i,2)} = f_1 t_{(i+1,1)} + f_2 t_{(i+1,0)} \tag{B6}$$

where f_2 is the derivative of f_1 normalized by r_α

$$f_2 = \left(\frac{\partial f_1}{\partial r_\alpha}\right)\frac{1}{r_\alpha} = \frac{2}{c_f^2 a_1 a_2} e^{-r_{ij}^2 / c_f a_1 a_2} \tag{B7}$$

All higher order (normalized) derivatives f_i can be determined as

$$f_i = f_r^{i-2} f_2, \quad i \geq 2 \tag{B8}$$

where,

$$f_r = -\frac{2}{c_f a_1 a_2}. \tag{B9}$$

For example, f_3 is the last such term needed for the GK quadrupole-quadrupole energy gradient

$$f_3 = \left(\frac{\partial f_2}{\partial r_\alpha}\right)\frac{1}{r_\alpha} = f_r f_2 \tag{B10}$$

and the final column needed for **t** is

$$t_{(i,3)} = f_1 t_{(i+1,2)} + 2 f_2 t_{(i+1,1)} + f_3 t_{(i+1,0)}. \tag{B11}$$

However, for arbitrary order tensors, any entry can be determined from entries in previous columns as a sum

$$t_{(i,j)} = \left(\frac{\partial t_{(i,j-1)}}{\partial r_\alpha} \right) \frac{1}{r_\alpha} = \sum_{k=1}^{j} \omega_{j,k} f_k t_{(i+1,j-k)} \tag{B12}$$

where each row of the coefficient matrix $\boldsymbol{\omega}$ can be determined from the previous row

$$\omega = \begin{bmatrix} 0 & & & & & & \\ 1 & 0 & & & & & \\ 1 & 1 & 0 & & & & \\ 1 & 2 & 1 & 0 & & & \\ 1 & 3 & 3 & 1 & 0 & & \\ 1 & 4 & 6 & 4 & 1 & 0 & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \tag{B13}$$

Note that row j of the coefficient matrix is used for all elements in column j of the matrix **t**.

The matrix of effective radius chain rule terms **b** is of size $n \times m - 1$. It has one fewer columns than **t** because the last column in **t** is itself only needed for energy gradients and not the energy. Therefore effective radius chain rule terms are not needed for this column. We note that any term in the first column $b_{(i,0)}$ is related to an element in the first column of **t** by a factor we label g

$$g = \left(\frac{\partial t_{(i,0)}}{\partial a_1} \right) \frac{1}{a_2 t_{(i+1,0)}} = \frac{1}{2} e^{-r_{ij}^2 / c_f a_1 a_2} \left(1 + \frac{r_{ij}^2}{c_f a_1 a_2} \right) \tag{B14}$$

such that

$$b_{(i,0)} = g t_{(i+1,0)} . \tag{B15}$$

Elements in the 2nd column of **b** can be found from elements in the first columns of **t** and **b** via the chain rule as

$$b_{(i,1)} = \left(\frac{\partial t_{(i,1)}}{\partial a_1} \right) \frac{1}{a_2} = g_1 t_{(i+1,0)} + f_1 b_{(i+1,0)} \tag{B16}$$

where g_1 is defined as

$$g_1 = \left(\frac{\partial f_1}{\partial a_1} \right) \frac{1}{a_2} = -\frac{r_{ij}^2 e^{-r_{ij}^2 / c_f a_1 a_2}}{c_f^2 a_1^2 a_2^2} . \tag{B17}$$

Similarly, the 3rd column is

$$b_{(i,2)} = \left(\frac{\partial t_{(i,2)}}{\partial a_1} \right) \frac{1}{a_2} = g_1 t_{(i+1,1)} + g_2 t_{(i+1,0)} + f_1 b_{(i+1,1)} + f_2 b_{(i+1,0)} \tag{B18}$$

where

$$g_2 = \left(\frac{\partial f_2}{\partial a_1} \right) \frac{1}{a_2} = \frac{2e^{-r_{ij}^2 / c_f a_1 a_2}}{\left(c_f a_1 a_2 \right)^2} \left(\frac{r_{ij}^2}{c a_1 a_2} - 1 \right) . \tag{B19}$$

All further terms g_i are determined from f_i as

$$g_i = \left(\frac{\partial f_i}{\partial a_1} \right) \frac{1}{a_2} = \left(i - 2 \right) f_r^{i-3} g_r f_2 + f_r^{i-2} g_2, \quad i \geq 2 \tag{B20}$$

where

$$g_r = \frac{2}{c_f \left(a_1 a_2 \right)^2} . \tag{B21}$$

For example,

$$g_3 = g_r f_2 + f_r g_2 . \tag{B22}$$

It is now possible to define all elements of the matrix **b**,

$$b_{(i,j)} = \left(\frac{\partial t_{(i,j)}}{\partial a_1} \right) \frac{1}{a_2} = \sum_{k=1}^{j} \omega_{j,k} \left(g_k t_{(i+1,j-k)} + f_k b_{(i+1,j-k)} \right) \qquad \text{(B23)}$$

to facilitate determination of energy gradients for any order multipole interaction.

Table B-1. Gradients of $A^{(0)}_{\{0,0,0\}}$.

m	$\{m\}$	$A^{(0)}_{\{0,0,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$t_{(0,0)}$
1	1,0,0	$xt_{(0,1)}$
	0,1,0	$yt_{(0,1)}$
	0,0,1	$zt_{(0,1)}$
2	2,0,0	$t_{(0,1)} + x^2 t_{(0,2)}$
	1,1,0	$xyt_{(0,2)}$
	1,0,1	$xzt_{(0,2)}$
	0,2,0	$t_{(0,1)} + y^2 t_{(0,2)}$
	0,1,1	$yzt_{(0,2)}$
	0,0,2	$t_{(0,1)} + z^2 t_{(0,2)}$
3	3,0,0	$3xt_{(0,2)} + x^3 t_{(0,3)}$
	2,1,0	$yt_{(0,2)} + x^2 yt_{(0,3)}$
	2,0,1	$zt_{(0,2)} + x^2 zt_{(0,3)}$
	1,2,0	$xt_{(0,2)} + xy^2 t_{(0,3)}$
	1,1,1	$xyzt_{(0,3)}$
	1,0,2	$xt_{(0,2)} + xz^2 t_{(0,3)}$
	0,3,0	$3yt_{(0,2)} + y^3 t_{(0,3)}$
	0,2,1	$zt_{(0,2)} + y^2 zt_{(0,3)}$
	0,1,2	$yt_{(0,2)} + yz^2 t_{(0,3)}$
	0,0,3	$3zt_{(0,2)} + z^3 t_{(0,3)}$

Table B-2. Gradients of $A^{(1)}_{1,0,0}$.

m	$\{m\}$	$A^{(1)}_{\{1,0,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$xt_{(1,0)}$
1	1,0,0	$t_{(1,0)} + x^2t_{(1,1)}$
	0,1,0	$xyt_{(1,1)}$
	0,0,1	$xzt_{(1,1)}$
2	2,0,0	$3xt_{(1,1)} + x^3t_{(1,2)}$
	1,1,0	$yt_{(1,1)} + x^2yt_{(1,2)}$
	1,0,1	$zt_{(1,1)} + x^2zt_{(1,2)}$
	0,2,0	$xt_{(1,1)} + xy^2t_{(1,2)}$
	0,1,1	$xyzt_{(1,2)}$
	0,0,2	$xt_{(1,1)} + xz^2t_{(1,2)}$
3	3,0,0	$3t_{(1,1)} + 6x^2t_{(1,2)} + x^4t_{(1,3)}$
	2,1,0	$3xyt_{(1,2)} + x^3yt_{(1,3)}$
	2,0,1	$3xzt_{(1,2)} + x^3zt_{(1,3)}$
	1,2,0	$t_{(1,1)} + x^2t_{(1,2)} + y^2t_{(1,2)} + x^2y^2t_{(1,3)}$
	1,1,1	$yzt_{(1,2)} + x^2yzt_{(1,3)}$
	1,0,2	$t_{(1,1)} + x^2t_{(1,2)} + z^2t_{(1,2)} + x^2z^2t_{(1,3)}$
	0,3,0	$3xyt_{(1,2)} + xy^3t_{(1,3)}$
	0,2,1	$xzt_{(1,2)} + xy^2zt_{(1,3)}$
	0,1,2	$xyt_{(1,2)} + xyz^2t_{(1,3)}$
	0,0,3	$3xzt_{(1,2)} + xz^3t_{(1,3)}$

Table B-3. Gradients of $A^{(1)}_{\{0,1,0\}}$.

m	$\{m\}$	$A^{(1)}_{\{0,1,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$yt_{(1,0)}$
1	1,0,0	$xyt_{(1,1)}$
	0,1,0	$t_{(1,0)} + y^2t_{(1,1)}$
	0,0,1	$yzt_{(1,1)}$
2	2,0,0	$yt_{(1,1)} + x^2yt_{(1,2)}$
	1,1,0	$xt_{(1,1)} + xy^2t_{(1,2)}$
	1,0,1	$xyzt_{(1,2)}$
	0,2,0	$3yt_{(1,1)} + y^3t_{(1,2)}$
	0,1,1	$zt_{(1,1)} + y^2zt_{(1,2)}$
	0,0,2	$yt_{(1,1)} + yz^2t_{(1,2)}$
3	3,0,0	$3xyt_{(1,2)} + x^3yt_{(1,3)}$
	2,1,0	$t_{(1,1)} + x^2t_{(1,2)} + y^2t_{(1,2)} + x^2y^2t_{(1,3)}$
	2,0,1	$yzt_{(1,2)} + x^2yzt_{(1,3)}$
	1,2,0	$3xyt_{(1,2)} + xy^3t_{(1,3)}$
	1,1,1	$xzt_{(1,2)} + xy^2zt_{(1,3)}$
	1,0,2	$xyt_{(1,2)} + xyz^2t_{(1,3)}$
	0,3,0	$3t_{(1,1)} + 6y^2t_{(1,2)} + y^4t_{(1,3)}$
	0,2,1	$3yzt_{(1,2)} + y^3zt_{(1,3)}$
	0,1,2	$t_{(1,1)} + y^2t_{(1,2)} + z^2t_{(1,2)} + y^2z^2t_{(1,3)}$
	0,0,3	$3yzt_{(1,2)} + yz^3t_{(1,3)}$

Table B-4. Gradients of $A^{(1)}_{\{0,0,1\}}$.

m	$\{m\}$	$A^{(1)}_{\{0,0,1\},\{m_1,m_2,m_3\}}$
0	0,0,0	$zt_{(1,0)}$
1	1,0,0	$xzt_{(1,1)}$
	0,1,0	$yzt_{(1,1)}$
	0,0,1	$t_{(1,0)} + z^2t_{(1,1)}$
2	2,0,0	$zt_{(1,1)} + x^2zt_{(1,2)}$
	1,1,0	$xyzt_{(1,2)}$
	1,0,1	$xt_{(1,1)} + xz^2t_{(1,2)}$
	0,2,0	$zt_{(1,1)} + y^2zt_{(1,2)}$
	0,1,1	$yt_{(1,1)} + yz^2t_{(1,2)}$
	0,0,2	$3zt_{(1,1)} + z^3t_{(1,2)}$
3	3,0,0	$3xzt_{(1,2)} + x^3zt_{(1,3)}$
	2,1,0	$yzt_{(1,2)} + x^2yzt_{(1,3)}$
	2,0,1	$t_{(1,1)} + x^2t_{(1,2)} + z^2t_{(1,2)} + x^2z^2t_{(1,3)}$
	1,2,0	$xzt_{(1,2)} + xy^2zt_{(1,3)}$
	1,1,1	$xyt_{(1,2)} + xyz^2t_{(1,3)}$
	1,0,2	$3xzt_{(1,2)} + xz^3t_{(1,3)}$
	0,3,0	$3yzt_{(1,2)} + y^3zt_{(1,3)}$
	0,2,1	$t_{(1,1)} + y^2t_{(1,2)} + z^2t_{(1,2)} + y^2z^2t_{(1,3)}$
	0,1,2	$3yzt_{(1,2)} + yz^3t_{(1,3)}$
	0,0,3	$3t_{(1,1)} + 6z^2t_{(1,2)} + z^4t_{(1,3)}$

Table B-5. Gradients of $A^{(2)}_{\{2,0,0\}}$.

m	$\{m\}$	$A^{(2)}_{\{2,0,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$x^2 t_{(2,0)}$
1	1,0,0	$2xt_{(2,0)} + x^3 t_{(2,1)}$
	0,1,0	$x^2 y t_{(2,1)}$
	0,0,1	$x^2 z t_{(2,1)}$
2	2,0,0	$2t_{(2,0)} + 5x^2 t_{(2,1)} + x^4 t_{(2,2)}$
	1,1,0	$2xyt_{(2,1)} + x^3 y t_{(2,2)}$
	1,0,1	$2xzt_{(2,1)} + x^3 z t_{(2,2)}$
	0,2,0	$x^2 t_{(2,1)} + x^2 y^2 t_{(2,2)}$
	0,1,1	$x^2 yz t_{(2,2)}$
	0,0,2	$x^2 t_{(2,1)} + x^2 z^2 t_{(2,2)}$
3	3,0,0	$12xt_{(2,1)} + 9x^3 t_{(2,2)} + x^5 t_{(2,3)}$
	2,1,0	$2yt_{(2,1)} + 5x^2 yt_{(2,2)} + x^4 yt_{(2,3)}$
	2,0,1	$2zt_{(2,1)} + 5x^2 zt_{(2,2)} + x^4 zt_{(2,3)}$
	1,2,0	$2xt_{(2,1)} + x^3 t_{(2,2)} + 2xy^2 t_{(2,2)} + x^3 y^2 t_{(2,3)}$
	1,1,1	$2xyzt_{(2,2)} + x^3 yzt_{(2,3)}$
	1,0,2	$2xt_{(2,1)} + x^3 t_{(2,2)} + 2xz^2 t_{(2,2)} + x^3 z^2 t_{(2,3)}$
	0,3,0	$3x^2 yt_{(2,2)} + x^2 y^3 t_{(2,3)}$
	0,2,1	$x^2 zt_{(2,2)} + x^2 y^2 zt_{(2,3)}$
	0,1,2	$yx^2 t_{(2,2)} + x^2 yz^2 t_{(2,3)}$
	0,0,3	$3x^2 zt_{(2,2)} + x^2 z^3 t_{(2,3)}$

Table B-6. Gradients of $A^{(2)}_{\{1,1,0\}}$.

m	$\{m\}$	$A^{(2)}_{\{1,1,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$xyt_{(2,0)}$
1	1,0,0	$yt_{(2,0)} + x^2yt_{(2,1)}$
	0,1,0	$xt_{(2,0)} + xy^2t_{(2,1)}$
	0,0,1	$xyzt_{(2,1)}$
2	2,0,0	$3xyt_{(2,1)} + x^3yt_{(2,2)}$
	1,1,0	$t_{(2,0)} + x^2t_{(2,1)} + y^2t_{(2,1)} + x^2y^2t_{(2,2)}$
	1,0,1	$yzt_{(2,1)} + x^2yzt_{(2,2)}$
	0,2,0	$3xyt_{(2,1)} + xy^3t_{(2,2)}$
	0,1,1	$xzt_{(2,1)} + xy^2zt_{(2,2)}$
	0,0,2	$xyt_{(2,1)} + xyz^2t_{(2,2)}$
3	3,0,0	$3yt_{(2,1)} + 6x^2yt_{(2,2)} + x^4yt_{(2,3)}$
	2,1,0	$3xt_{(2,1)} + 3xy^2t_{(2,2)} + x^3t_{(2,2)} + x^3y^2t_{(2,3)}$
	2,0,1	$3xyzt_{(2,2)} + x^3yzt_{(2,3)}$
	1,2,0	$3yt_{(2,1)} + 3x^2yt_{(2,2)} + y^3t_{(2,2)} + x^2y^3t_{(2,3)}$
	1,1,1	$zt_{(2,1)} + x^2zt_{(2,2)} + y^2zt_{(2,2)} + x^2y^2zt_{(2,3)}$
	1,0,2	$yt_{(2,1)} + x^2yt_{(2,2)} + yz^2t_{(2,2)} + x^2yz^2t_{(2,3)}$
	0,3,0	$3xt_{(2,1)} + 6xy^2t_{(2,2)} + xy^4t_{(2,3)}$
	0,2,1	$3xyzt_{(2,2)} + xy^3zt_{(2,3)}$
	0,1,2	$xt_{(2,1)} + xy^2t_{(2,2)} + xz^2t_{(2,2)} + xy^2z^2t_{(2,3)}$
	0,0,3	$3xyzt_{(2,2)} + xyz^3t_{(2,3)}$

Table B-7. Gradients of $A^{(2)}_{\{1,0,1\}}$.

m	$\{m\}$	$A^{(2)}_{\{1,0,1\},\{m_1,m_2,m_3\}}$
0	0,0,0	$xzt_{(2,0)}$
1	1,0,0	$zt_{(2,0)} + x^2zt_{(2,1)}$
	0,1,0	$xyzt_{(2,1)}$
	0,0,1	$xt_{(2,0)} + xz^2t_{(2,1)}$
2	2,0,0	$3xzt_{(2,1)} + x^3zt_{(2,2)}$
	1,1,0	$yzt_{(2,1)} + x^2yzt_{(2,2)}$
	1,0,1	$t_{(2,0)} + x^2t_{(2,1)} + z^2t_{(2,1)} + x^2z^2t_{(2,2)}$
	0,2,0	$xzt_{(2,1)} + xy^2zt_{(2,2)}$
	0,1,1	$xyt_{(2,1)} + xyz^2t_{(2,2)}$
	0,0,2	$3xzt_{(2,1)} + xz^3t_{(2,2)}$
3	3,0,0	$3zt_{(2,1)} + 6x^2zt_{(2,2)} + x^4zt_{(2,3)}$
	2,1,0	$3xyzt_{(2,2)} + x^3yzt_{(2,3)}$
	2,0,1	$3xt_{(2,1)} + 3xz^2t_{(2,2)} + x^3t_{(2,2)} + x^3z^2t_{(2,3)}$
	1,2,0	$zt_{(2,1)} + x^2zt_{(2,2)} + y^2zt_{(2,2)} + x^2y^2zt_{(2,3)}$
	1,1,1	$yt_{(2,1)} + x^2yt_{(2,2)} + yz^2t_{(2,2)} + x^2yz^2t_{(2,3)}$
	1,0,2	$3zt_{(2,1)} + 3x^2zt_{(2,2)} + z^3t_{(2,2)} + x^2z^3t_{(2,3)}$
	0,3,0	$3xyzt_{(2,2)} + xy^3zt_{(2,3)}$
	0,2,1	$xt_{(2,1)} + xy^2t_{(2,2)} + xz^2t_{(2,2)} + xy^2z^2t_{(2,3)}$
	0,1,2	$3xyzt_{(2,2)} + xyz^3t_{(2,3)}$
	0,0,3	$3xt_{(2,1)} + 6xz^2t_{(2,2)} + xz^4t_{(2,3)}$

Table B-8. Gradients of $A^{(2)}_{\{0,2,0\}}$.

m	$\{m\}$	$A^{(2)}_{\{0,2,0\},\{m_1,m_2,m_3\}}$
0	0,0,0	$y^2 t_{(2,0)}$
1	1,0,0	$xy^2 t_{(2,1)}$
	0,1,0	$2yt_{(2,0)} + y^3 t_{(2,1)}$
	0,0,1	$y^2 zt_{(2,1)}$
2	2,0,0	$y^2 t_{(2,1)} + x^2 y^2 t_{(2,2)}$
	1,1,0	$2xyt_{(2,1)} + xy^3 t_{(2,2)}$
	1,0,1	$xy^2 zt_{(2,2)}$
	0,2,0	$2t_{(2,0)} + 5y^2 t_{(2,1)} + y^4 t_{(2,2)}$
	0,1,1	$2yzt_{(2,1)} + y^3 zt_{(2,2)}$
	0,0,2	$y^2 t_{(2,1)} + y^2 z^2 t_{(2,2)}$
3	3,0,0	$3xy^2 t_{(2,2)} + x^3 y^2 t_{(2,3)}$
	2,1,0	$2yt_{(2,1)} + y^3 t_{(2,2)} + 2x^2 yt_{(2,2)} + x^2 y^3 t_{(2,3)}$
	2,0,1	$y^2 zt_{(2,2)} + x^2 y^2 zt_{(2,3)}$
	1,2,0	$2xt_{(2,1)} + 5xy^2 t_{(2,2)} + xy^4 t_{(2,3)}$
	1,1,1	$2xyzt_{(2,2)} + xy^3 zt_{(2,3)}$
	1,0,2	$xy^2 t_{(2,2)} + xy^2 z^2 t_{(2,3)}$
	0,3,0	$12yt_{(2,1)} + 9y^3 t_{(2,2)} + y^5 t_{(2,3)}$
	0,2,1	$2zt_{(2,1)} + 5y^2 zt_{(2,2)} + y^4 zt_{(2,3)}$
	0,1,2	$2yt_{(2,1)} + y^3 t_{(2,2)} + 2yz^2 t_{(2,2)} + y^3 z^2 t_{(2,3)}$
	0,0,3	$3y^2 zt_{(2,2)} + y^2 z^3 t_{(2,3)}$

Table B-9. Gradients of $A^{(2)}_{\{0,1,1\}}$.

m	$\{m\}$	$A^{(2)}_{\{0,1,1\},\{m_1,m_2,m_3\}}$
0	0,0,0	$yzt_{(2,0)}$
1	1,0,0	$xyzt_{(2,1)}$
	0,1,0	$zt_{(2,0)} + y^2zt_{(2,1)}$
	0,0,1	$yt_{(2,0)} + yz^2t_{(2,1)}$
2	2,0,0	$yzt_{(2,1)} + x^2yzt_{(2,2)}$
	1,1,0	$xzt_{(2,1)} + xy^2zt_{(2,2)}$
	1,0,1	$xyt_{(2,1)} + xyz^2t_{(2,2)}$
	0,2,0	$3yzt_{(2,1)} + y^3zt_{(2,2)}$
	0,1,1	$t_{(2,0)} + z^2t_{(2,1)} + y^2t_{(2,1)} + y^2z^2t_{(2,2)}$
	0,0,2	$3yzt_{(2,1)} + yz^3t_{(2,2)}$
3	3,0,0	$3xyzt_{(2,2)} + x^3yzt_{(2,3)}$
	2,1,0	$zt_{(2,1)} + y^2zt_{(2,2)} + x^2zt_{(2,2)} + x^2y^2zt_{(2,3)}$
	2,0,1	$yt_{(2,1)} + x^2yt_{(2,2)} + yz^2t_{(2,2)} + x^2yz^2t_{(2,3)}$
	1,2,0	$3xyzt_{(2,2)} + xy^3zt_{(2,3)}$
	1,1,1	$xt_{(2,1)} + xy^2t_{(2,2)} + xz^2t_{(2,2)} + xy^2z^2t_{(2,3)}$
	1,0,2	$3xyzt_{(2,2)} + xyz^3t_{(2,3)}$
	0,3,0	$3zt_{(2,1)} + 6y^2zt_{(2,2)} + y^4zt_{(2,3)}$
	0,2,1	$3yt_{(2,1)} + 3yz^2t_{(2,2)} + y^3t_{(2,2)} + y^3z^2t_{(2,3)}$
	0,1,2	$3zt_{(2,1)} + 3y^2zt_{(2,2)} + z^3t_{(2,2)} + y^2z^3t_{(2,3)}$
	0,0,3	$3yt_{(2,1)} + 6yz^2t_{(2,2)} + yz^4t_{(2,3)}$

Table B-10. Gradients of $A^{(2)}_{\{0,0,2\}}$.

m	$\{m\}$	$A^{(2)}_{\{0,0,2\},\{m_1,m_2,m_3\}}$
0	0,0,0	$z^2t_{(2,0)}$
1	1,0,0	$xz^2t_{(2,1)}$
	0,1,0	$yz^2t_{(2,1)}$
	0,0,1	$2zt_{(2,0)} + z^3t_{(2,1)}$
2	2,0,0	$z^2t_{(2,1)} + x^2z^2t_{(2,2)}$
	1,1,0	$xyz^2t_{(2,2)}$
	1,0,1	$2xzt_{(2,1)} + xz^3t_{(2,2)}$
	0,2,0	$z^2t_{(2,1)} + y^2z^2t_{(2,2)}$
	0,1,1	$2yzt_{(2,1)} + yz^3t_{(2,2)}$
	0,0,2	$2t_{(2,0)} + 5z^2t_{(2,1)} + z^4t_{(2,2)}$
3	3,0,0	$3xz^2t_{(2,2)} + x^3z^2t_{(2,3)}$
	2,1,0	$yz^2t_{(2,2)} + x^2yz^2t_{(2,3)}$
	2,0,1	$2zt_{(2,1)} + z^3t_{(2,2)} + 2x^2zt_{(2,2)} + x^2z^3t_{(2,3)}$
	1,2,0	$xz^2t_{(2,2)} + xy^2z^2t_{(2,3)}$
	1,1,1	$2xyzt_{(2,2)} + xyz^3t_{(2,3)}$
	1,0,2	$2xt_{(2,1)} + 5xz^2t_{(2,2)} + xz^4t_{(2,3)}$
	0,3,0	$3yz^2t_{(2,2)} + y^3z^2t_{(2,3)}$
	0,2,1	$2zt_{(2,1)} + z^3t_{(2,2)} + 2y^2zt_{(2,2)} + y^2z^3t_{(2,3)}$
	0,1,2	$2yt_{(2,1)} + 5yz^2t_{(2,2)} + yz^4t_{(2,3)}$
	0,0,3	$12zt_{(2,1)} + 9z^3t_{(2,2)} + z^5t_{(2,3)}$