Let $\mathbf{x}$ be a vector, whose matrix representation is

$$\mathbf{x} \longleftrightarrow \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{1}$$

Let

$$\mathbf{x}^{\otimes l} \equiv \mathbf{x} \otimes \mathbf{x} \otimes \cdots \otimes \mathbf{x} \tag{2}$$

be the tensor product of l copies of vector $\mathbf{x}$. The matrix representation of $\mathbf{x}^{\otimes l}$ is a column vector of dimension 3^l:

$$\mathbf{x}^{\otimes l} \longleftrightarrow \begin{bmatrix} xx\cdots xx \\ xx\cdots xy \\ xx\cdots xz \\ xx\cdots yx \\ \cdots \\ zz\cdots zz \end{bmatrix} \tag{3}$$

If we define

$$\mathbf{M}^l = \int \rho(\mathbf{x})\mathbf{x}^{\otimes l} d^3x \tag{4}$$

we see that the Cartesian multipole moment $M^{(l)}_{\alpha\beta\gamma}$ is just a component of the tensor $\mathbf{M}^l$ after full symmetrization. So the $SO(3)$ reducibility theory will apply.

Now the number of unique symmetrizations of rank-l tensor is the same as the number of unique ways to arrange ordered triple (α,β,γ) such that $\alpha+\beta+\gamma=l$. It's straightforward to verify that this is exactly

$$M(l) = \frac{(l+1)(l+2)}{2} \tag{5}$$

For an arbitrary (α,β,γ) with $\alpha+\beta+\gamma=l$, consider the inner product (which indicates close relationship to the definition of q_{lm})

$$\int Y^*_{l'm}(\theta,\phi)\frac{x^\alpha y^\beta z^\gamma}{r^l}d^3x \tag{6}$$

On the surface, it seems reasonable to expect this inner product to vanish unless $l=l'$ since $x^\alpha y^\beta z^\gamma/r^l$ is a linear combination of order-l spherical harmonics. But the "trace" operation can yield lower order spherical harmonics. For example, with $l=3$

$$\frac{x^2z+y^2z+z^3}{r^3} = \frac{z}{r} \tag{7}$$

therefore

$$\int Y^*_{l'm}(\theta,\phi)\left(\frac{x^2z+y^2z+z^3}{r^3}\right)d^3x = \int Y^*_{l'm}(\theta,\phi)\frac{z}{r}d^3x \tag{8}$$

actually vanishes except for $l'=1$, as opposed to $l'=3$.

In fact, let's count among the total $M(l)=(l+1)(l+2)/2$ components $x^\alpha y^\beta z^\gamma/r^l$, how many can participate in the "trace" operation.

This is easy to do, since for any (α',β',γ') satisfying $\alpha'+\beta'+\gamma'=l-2$ will produce a trace

$$\frac{x^{\alpha'+2}y^{\beta'}z^{\gamma'} + x^{\alpha'}y^{\beta'+2}z^{\gamma'} + x^{\alpha'}y^{\beta'}z^{\gamma'+2}}{r^l} = \frac{x^{\alpha'}y^{\beta'}z^{\gamma'}}{r^{l-2}} \tag{9}$$

which means out of the $M(l)=(l+1)(l+2)/2$ components, $M(l-2)$ of them can participate in the trace operation, leaving

$$q(l) = M(l) - M(l-2) = \frac{(l+1)(l+2)-l(l-1)}{2} = 2l+1 \tag{10}$$

"traceless" components. These components can produce non-zero inner product with $Y_{l'm}(\theta,\phi)$ only when $l'=l$, hence belong to the $(2l+1)$-dimensional irreducible subspace of $SO(3)$. Per form (6), they are linear combinations of q_{lm}.

This operation doesn't end at one round. Among the $M(l-2)$ components participating the first round of trace, $M(l-4)$ of them can participate one more round. Thus those which cannot participate this second round of trace are in number

$$q\,(l-2) = M\,(l-2) - M\,(l-4) = 2l-3 \tag{11}$$

which belong to the $(2l-3)$-dimensional irreducible subspace of $SO(3)$ and are linear combinations of $q_{l-2,m}$, so on and so forth.

In general, we can decompose $M(l)$ as the sum

$$\begin{aligned} M\,(l) &= q(l) + M\,(l-2) \\ &= q(l) + q(l-2) + M\,(l-4) \\ &= q\,(l) + q\,(l-2) + q\,(l-4) + \cdots \end{aligned} \tag{12}$$

which is easy to prove. We have also listed the first few orders in the table below:

l	$q(l)=2l+1$	$M(l)=(l+1)(l+2)/2$
0	1	1
1	3	3
2	5	6
3	7	10
4	9	15
5	11	21
6	13	28

Let's briefly comment on the irreducibility of spherical multipole moments q_{lm}:

$$q_{lm} = \int Y^*_{lm}\,(\theta,\phi)\,r^l\rho\,(\mathbf{x})\,d^3x \tag{13}$$

Under rotation, any Y_{lm}s will transform into linear combinations of $Y_{lm'}$s with the same l only. We are not going to give the rigorous proof here, but instead, we draw analogy from the theory of angular momentum in quantum mechanics.

Since the total angular momentum operator $\mathbf{L}^2$ commutes with rotation operator R, then for $|lm\rangle$ a simultaneous eigenstate of $\mathbf{L}^2$ and L_z, the rotation will leave its total angular momentum invariant:

$$\mathbf{L}^2\,(R|lm\rangle) = R\left(\mathbf{L}^2|lm\rangle\right) = l(l+1)\hbar^2\,(R\,|lm\rangle) \tag{14}$$

This means the rotated state $R\,|lm\rangle$ is necessarily a linear combination of $|lm'\rangle$s. In other words, the states $\{|lm\rangle\}$ form a complete orthonormal basis of the $(2l+1)$-dimensional irreducible subspace of $SO(3)$.

Recall $Y_{lm}\,(\theta,\phi)$ is just the position representation of $|lm\rangle$, the "invariant eigenvalue" relation (14) in this representation is given by the correspondence

$$\mathbf{L}^2 \longleftrightarrow -\hbar^2\boldsymbol{\nabla}^2 \tag{15}$$

and the Laplace equation

$$\boldsymbol{\nabla}^2 Y_{lm}\,(\theta,\phi) = -l(l+1)Y_{lm}\,(\theta,\phi) \tag{16}$$