Form factor of truncated octahedron along one axis

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July 2021

1 Notations and axes

1.1 Dimensions

We start from a general octahedron with dimensions a, b, c from center to vertices along the x, y and z axes. A truncature of the two vertices on the z axis is added. The truncature parameter is $0 < t < 1$ (see Figure 3).
$t = 1$ corresponds to the general octahedron shape.

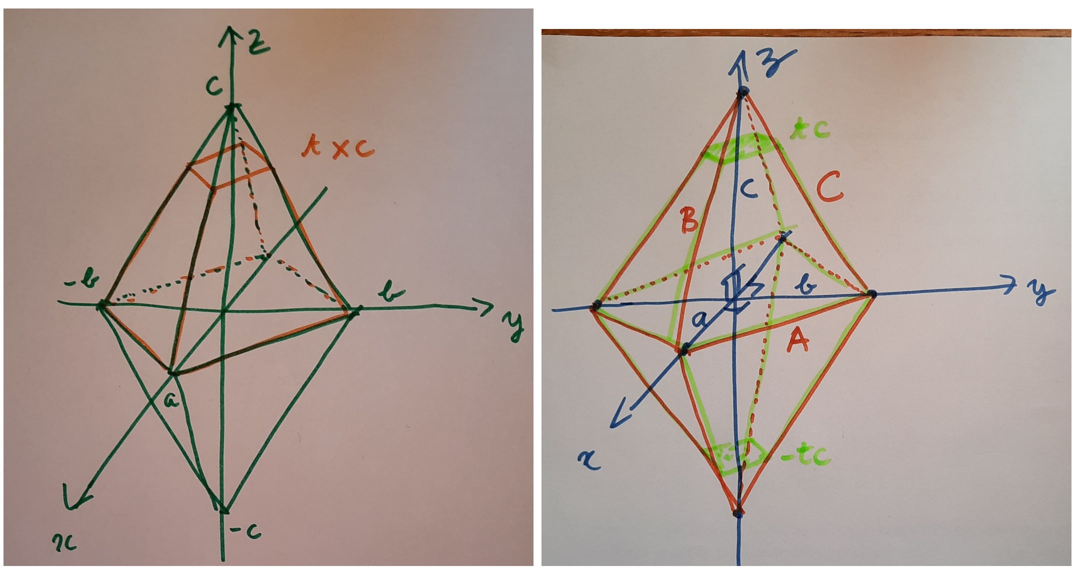

Figure 1: General octahedron with truncature along z axis

1.2 List of vertices

$$
\begin{aligned}
&(a, 0, 0) \\
&(-a, 0, 0) \\
&(0, b, 0) \\
&(0, -b, 0) \\
&((1-t)a, 0, tc) \\
&(-(1-t)a, 0, tc) \\
&(0, (1-t)b, tc) \\
&(0, -(1-t)b, tc) \\
&((1-t)a, 0, -tc) \\
&(-(1-t)a, 0, -tc) \\
&(0, (1-t)b, -tc) \\
&(0, -(1-t)b, -tc)
\end{aligned}
$$

For $t = 1$, one obtains the general octahedron with 6 vertices :

$$
\begin{aligned}
&(a, 0, 0) \\
&(-a, 0, 0) \\
&(0, b, 0) \\
&(0, -b, 0) \\
&(0, 0, c) \\
&(0, 0, -c)
\end{aligned}
$$

1.3 Parameters list in SASView

Four parameters are used in the corresponding model in SASView a, $b2a_{ratio}$, $c2a_{ratio}$ and t :

$$
\begin{aligned}
&a \\
&b2a_{ratio} = b/a \\
&c2a_{ratio} = c/a \\
&0 < t < 1
\end{aligned}
$$

2 Rescaling along the x,y,z directions

The shape is streched along the x, y and z axes into a regular octahedron truncated along the z axis (see Figure 4. After rescaling, the base is a square in the plane perpendicular to z'z.

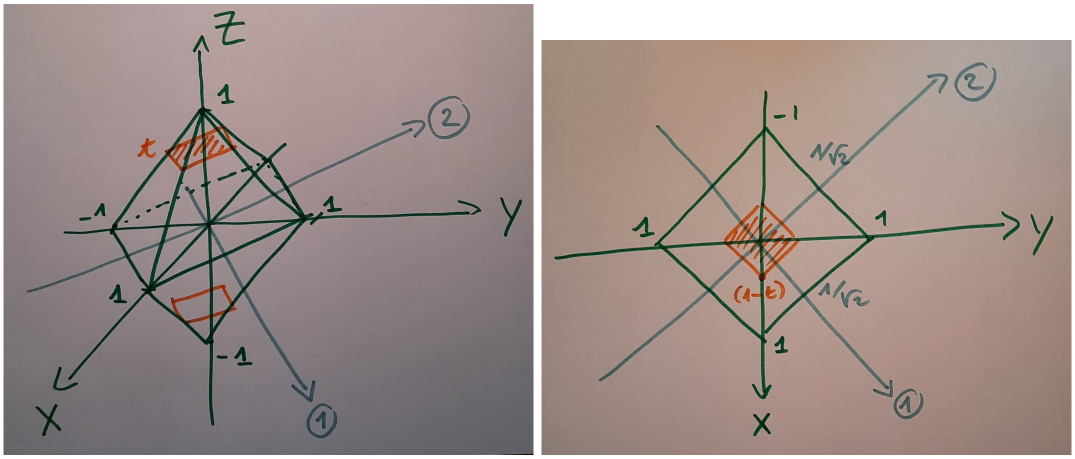

Figure 2: After rescaling: Regular octahedron with truncature along one direction or square based bi frustum.

2.1 Rescaling in real space

$$
\begin{aligned}
X &= x/a \\
Y &= y/b \\
Z &= z/c
\end{aligned}
$$

2.2 Coordinates of the vertices after rescaling

$$
\begin{aligned}
&(1, 0, 0) \\
&(-1, 0, 0) \\
&(0, 1, 0) \\
&(0, -1, 0) \\
&((1-t), 0, t) \\
&(-(1-t), 0, t) \\
&(0, (1-t), t) \\
&(0, -(1-t), t) \\
&((1-t), 0, -t) \\
&(-(1-t), 0, -t) \\
&(0, (1-t), -t) \\
&(0, -(1-t), -t)
\end{aligned}
$$

2.3 Rescaling in reciprocal space

$$
\begin{aligned}
Q_x &= aq_x \\
Q_y &= bq_y \\
Q_z &= cq_z
\end{aligned}
$$

3 Integration of the form factor

3.1 Definition of the form factor

$$A(\vec{q}) = \int\int\int_V \rho_D(\vec{r})\, e^{-i\vec{q}\cdot\vec{r}} d^3\vec{r} \quad \text{with} \qquad \rho_D(\vec{r}) = \begin{cases} 1 & \text{if } \vec{r} \text{ inside } V \\ 0 & \text{if } \vec{r} \text{ outside } V \end{cases}$$

with $\vec{r} = (x, y, z)$ and $\vec{q} = (q_x, q_y, q_z)$

3.2 Integral after rescaling

$$A\left(\vec{Q}\right) = abc \int\int\int_{V_{res}} \rho_D\left(\vec{R}\right) e^{-i\vec{Q}\cdot\vec{R}} d^3\vec{R}$$

with $\vec{R} = (X = x/a, Y = y/b, Z = z/c)$ and $\vec{Q} = (Q_x = aq_x, Q_y = bq_y, Q_z = cq_z)$
And V_{res} is the volume of the rescaled shape (see figure 4).

3.3 Ancillary axes in the square base plane

It is easier to perform the integral by introducing two ancillary axes X_1 and X_2 in the base plane (see figure 4). They are turned by $\pi/4$ with respect to the X and Y axes.

$$\begin{aligned}
\vec{e_1} &= \frac{1}{\sqrt{2}}(\vec{e_X} + \vec{e_Y}) \\
\vec{e_2} &= \frac{1}{\sqrt{2}}(-\vec{e_X} + \vec{e_Y}) \\
\vec{R} &= X\vec{e_X} + Y\vec{e_Y} + Z\vec{e_Z} = X_1\vec{e_1} + X_2\vec{e_2} + Z\vec{e_Z} \\
X_1 &= \frac{X+Y}{\sqrt{2}} \\
X_2 &= \frac{-X+Y}{\sqrt{2}}
\end{aligned}$$

3.4 Integration limits for the square based pyramid

Integration over the entire volume is decomposed in the sum of two integrals over each pyramids.
Limits for integration for the upper pyramid ($Z > 0$) are :

$$\begin{gathered}
-\frac{1}{\sqrt{2}}(1-Z) < X_1 < \frac{1}{\sqrt{2}}(1-Z) \\
-\frac{1}{\sqrt{2}}(1-Z) < X_2 < \frac{1}{\sqrt{2}}(1-Z) \\
0 < Z < t
\end{gathered}$$

One can define the function $L(Z)$ for the limit with $L(Z) = \frac{1}{\sqrt{2}}(1-Z)$ and the form factor for one pyramid reads:

$$
\begin{aligned}
A_{py}\left(\vec{Q}\right) &= abc\int_0^t dZ\int_{-L(Z)}^{L(Z)} dX_1\int_{-L(Z)}^{L(Z)} dX_2 e^{-i(Q_1X_1+Q_2X_2+Q_zZ)}\\
Q_1 &= \frac{Q_x+Q_y}{\sqrt{2}}\\
Q_2 &= \frac{-Q_x+Q_y}{\sqrt{2}}
\end{aligned}
$$

3.5 Integration for the truncated pyramid

First, integration in the base plane is done over X_1 and X_2. And after, the Q_x and Q_y coordinates are introduced instead of the Q_1 and Q_2.
The last integration to do is over the Z coordinate with a sum of four exponential terms.

$$
\begin{aligned}
A_{py}\left(\vec{Q}\right) &= \frac{abc}{Q_1Q_2}\int_0^t dZ e^{-iQ_zZ}(e^{i(Q_1-Q_2)(1-Z)/\sqrt{2}} + e^{-i(Q_1-Q_2)(1-Z)/\sqrt{2}} - e^{i(Q_1+Q_2)(1-Z)/\sqrt{2}} - e^{-i(Q_1+Q_2)(1-Z)/\sqrt{2}})\\
Q_x &= \frac{Q_1-Q_2}{\sqrt{2}}\\
Q_y &= \frac{Q_1+Q_2}{\sqrt{2}}\\
A_{py}\left(\vec{Q}\right) &= \frac{2abc}{Q_y^2-Q_x^2}\int_0^t dZ e^{-iQ_zZ}(e^{iQ_x(1-Z)} + e^{-iQ_x(1-Z)} - e^{iQ_y(1-Z)} - e^{-iQ_y(1-Z)})
\end{aligned}
$$

3.6 Integration for the truncated octahedron

We perform the last integration over Z directly only for the octahedron, by combining the two integrals. The whole function is real, contrary to the case of a single pyramid.

$$
A_{Otz}(Q_x,Q_y,Q_z) = A_{py}(Q_x,Q_y,Q_z) + A_{py}(Q_x,Q_y,-Q_z)
$$

The whole calculation is long, but, after a few pages, we obtain the final expression !!!

$$
\begin{aligned}
A_{Otz}(\vec{Q}) &= \frac{8abc}{Q_x^2-Q_y^2}(AA+BB)\\
AA &= \frac{1}{Q_x^2-Q_z^2}[-Q_x\sin Q_x + \frac{1}{2}[(Q_x-Q_z)\sin\left(Q_x(1-t)-Q_zt\right) + (Q_x+Q_z)\sin\left(Q_x(1-t)+Q_zt\right)]]\\
BB &= \frac{1}{Q_y^2-Q_z^2}[Q_y\sin Q_y - \frac{1}{2}[(Q_y-Q_z)\sin\left(Q_y(1-t)-Q_zt\right) + (Q_y+Q_z)\sin\left(Q_y(1-t)+Q_zt\right)]]
\end{aligned}
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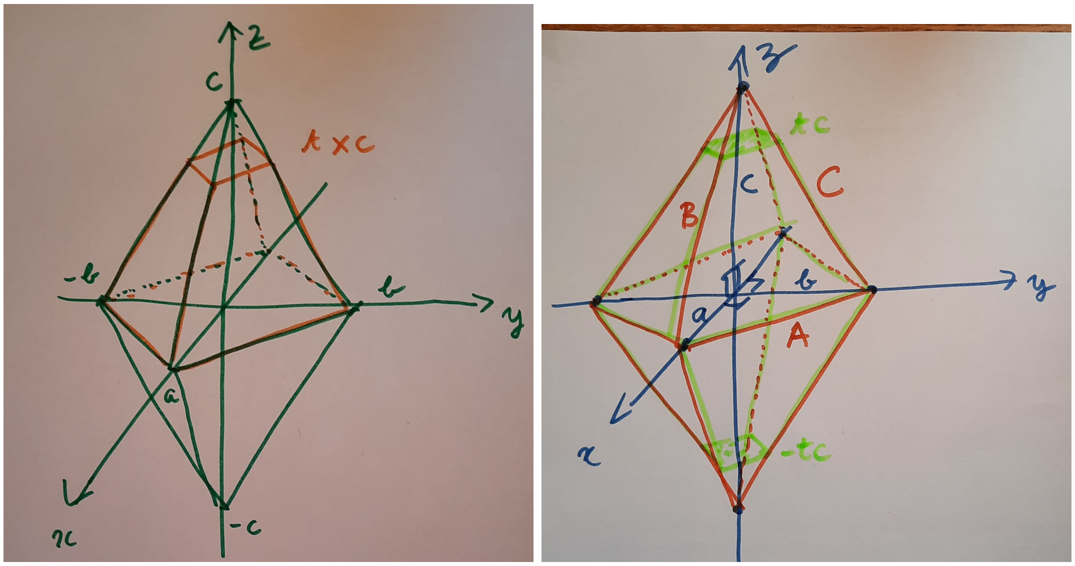

Figure 3: General octahedron with truncature along z axis

3.7 List of vertices

$$(a, 0, 0)$$
$$(-a, 0, 0)$$
$$(0, b, 0)$$
$$(0, -b, 0)$$
$$((1-t)a, 0, tc)$$
$$(-(1-t)a, 0, tc)$$
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For $t = 1$, one obtains the general octahedron with 6 vertices :

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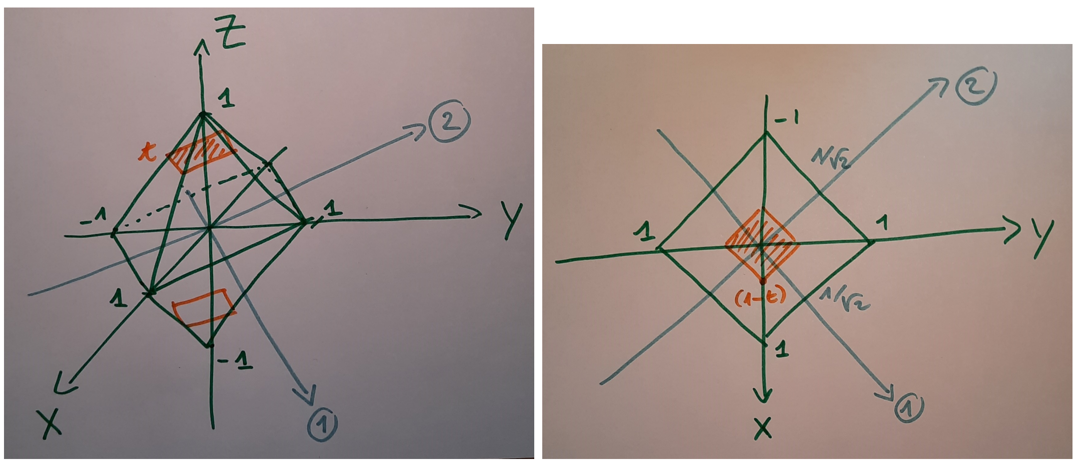

Figure 4: After rescaling: Regular octahedron with truncature along one direction or square based bi frustum.

4.1 Rescaling in real space

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Z &= z/c
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&(0,-1,0)\\
&((1-t),0,t)\\
&(-(1-t),0,t)\\
&(0,(1-t),t)\\
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\end{aligned}
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\begin{aligned}
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5 Integration of the form factor

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$$

with $\vec{r} = (x, y, z)$ and $\vec{q} = (q_x, q_y, q_z)$

5.2 Integral after rescaling

$$
A\left(\vec{Q}\right) = abc \int\int\int_{V_{res}} \rho_D\left(\vec{R}\right) e^{-i\vec{Q}\cdot\vec{R}} d^3\vec{R}
$$

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It is easier to perform the integral by introducing two ancillary axes X_1 and X_2 in the base plane (see figure 4). They are turned by $\pi/4$ with respect to the X and Y axes.

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\vec{e_2} &= \frac{1}{\sqrt{2}}(-\vec{e_X} + \vec{e_Y}) \\
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X_1 &= \frac{X+Y}{\sqrt{2}} \\
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Integration over the entire volume is decomposed in the sum of two integrals over each pyramids.
Limits for integration for the upper pyramid ($Z > 0$) are :

$$
\begin{aligned}
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One can define the function $L(Z)$ for the limit with $L(Z) = \frac{1}{\sqrt{2}}(1-Z)$ and the form factor for one pyramid reads:

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$$Q_x = \frac{Q_1 - Q_2}{\sqrt{2}}$$

$$Q_y = \frac{Q_1 + Q_2}{\sqrt{2}}$$

$$A_{py}\left(\vec{Q}\right) = \frac{2abc}{Q_y^2 - Q_x^2}\int_0^t dZ e^{-iQ_z Z}(e^{iQ_x(1-Z)} + e^{-iQ_x(1-Z)} - e^{iQ_y(1-Z)} - e^{-iQ_y(1-Z)})$$

5.6 Integration for the truncated octahedron

We perform the last integration over Z directly only for the octahedron, by combining the two integrals. The whole function is real, contrary to the case of a single pyramid.

$$A_{Otz}(Q_x, Q_y, Q_z) = A_{py}(Q_x, Q_y, Q_z) + A_{py}(Q_x, Q_y, -Q_z)$$

The whole calculation is long, but, after a few pages, we obtain the final expression !!!

$$A_{Otz}(\vec{Q}) = \frac{8abc}{Q_x^2 - Q_y^2}(AA + BB)$$

$$AA = \frac{1}{Q_x^2 - Q_z^2}[-Q_x \sin Q_x + \frac{1}{2}[(Q_x - Q_z)\sin(Q_x(1-t) - Q_z t) + (Q_x + Q_z)\sin(Q_x(1-t) + Q_z t)]]$$

$$BB = \frac{1}{Q_y^2 - Q_z^2}[Q_y \sin Q_y - \frac{1}{2}[(Q_y - Q_z)\sin(Q_y(1-t) - Q_z t) + (Q_y + Q_z)\sin(Q_y(1-t) + Q_z t)]]$$

5.7 Expression for the general octahedron

It is when $t = 1$.

$$A_O(\vec{Q}) = \frac{8abc}{Q_x^2 - Q_y^2}(\frac{1}{Q_x^2 - Q_z^2}(-Q_x \sin Q_x + Q_z \sin Q_z) + \frac{1}{Q_y^2 - Q_z^2}(Q_y \sin Q_y - Q_z \sin Q_z))$$

This can be rewritten in the sum of three terms :

$$A_O(\vec{Q}) = -8abc\left(\frac{Q_x \sin Q_x}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)} + \frac{Q_y \sin Q_y}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)} + \frac{Q_z \sin Q_z}{(Q_z^2 - Q_x^2)(Q_z^2 - Q_y^2)}\right)$$

In this form, the invariance by permutation of the three axes is evidenced. The three terms of the sum can be derived from each other by circular permutation: $(Qx, Qy, Qz) \to (Qy, Qz, Qx) \to (Qz, Qx, Qy)$.

6 Building models in SASView

6.1 General octahedron

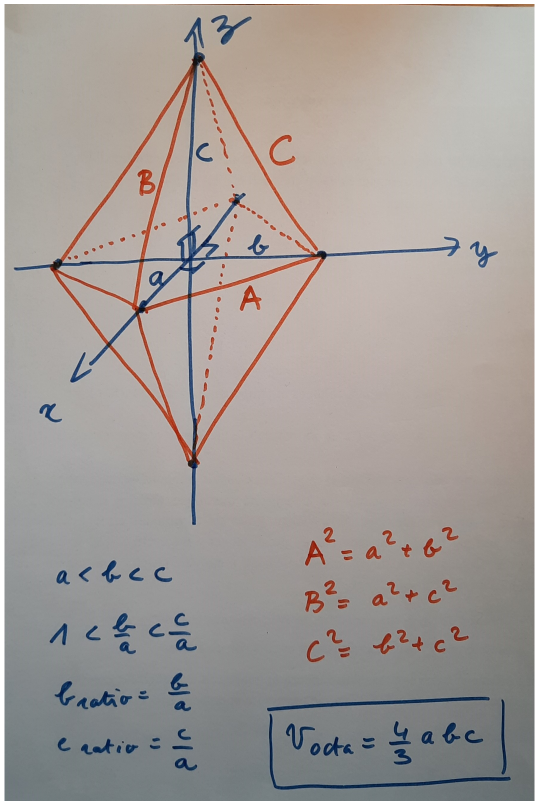

Figure 5: General octahedron

The volume of the octahedron is:

$$V = \frac{4}{3}abc = \frac{4}{3}a^3 \cdot b2a_{ratio} \cdot c2a_{ratio}$$

The lengths of the edges are equal to:

$$A^2 = a^2 + b^2$$
$$B^2 = a^2 + c^2$$
$$C^2 = b^2 + c^2$$

For a regular octahedron, this simplifies to:

$$b2a_{ratio} = c2a_{ratio} = 1$$
$$A = B = C = a \cdot \sqrt{2}$$
$$a = b = c = \frac{A}{\sqrt{2}}$$
$$V = \frac{4}{3} \cdot a^3 = \frac{\sqrt{2}}{3} \cdot A^3$$

The Amplitude of the form factor AP is calculated with a scaled scattering vector (Qx, Qy, Qz) and it is normalised by the volume of the shape:

$$AP = A_O(\vec{Q})/V$$

$$\begin{aligned}
AP &= \frac{6}{Qx^2 - Qy^2}(AA + BB) \\
AA &= \frac{Qy \cdot \sin Qy - Qz \cdot \sin Qz}{Qy^2 - Qz^2} \\
BB &= \frac{Qz \cdot \sin Qz - Qx \cdot \sin Qx}{Qx^2 - Qz^2}
\end{aligned}$$

and:

$$\begin{aligned}
q_x &= q \cdot \sin\theta \cdot \cos\phi \\
q_y &= q \cdot \sin\theta \cdot \sin\phi \\
q_z &= q \cdot \cos\theta \\
Q_x &= q_x \cdot a \\
Q_y &= q_y \cdot b \\
Q_z &= q_z \cdot c
\end{aligned}$$

θ is the angle between the z axis and the c axis of the octahedron ($length_c$), and ϕ is the angle between the scattering vector (lying in the xy plane) and the y axis. The normalized form factor in 1D is obtained averaging over all possible orientations. This is the same code as already used in the rectangular prism model.
The code is given in the http://marketplace.sasview.org/models/134/SasView Marketplace and as well as in Appendix B.
July 2021 : A version with the more symmetric expression with three terms is made :

$$AP = A_O(\vec{Q})/V$$

$$\begin{aligned}
AP &= -6(AA + BB + CC) \\
AA &= \frac{Q_x \sin Q_x}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)} \\
BB &= \frac{Q_y \sin Q_y}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)} \\
CC &= \frac{Q_z \sin Q_z}{(Q_z^2 - Q_x^2)(Q_z^2 - Q_y^2)}
\end{aligned}$$

6.2 Truncated octahedron along the z direction

The volume of the truncated octahedron along one axis is obtained by subtracting the volume of the two small pyramids that are truncated:

$$V_{tz} = \frac{4}{3}abc(1 - (1-t)^3)$$

The amplitude of the form factor is :

$$AP = A_{Otz}(\vec{Q})/V_{tz}$$
$$AP = \frac{6}{Q_x^2 - Q_y^2}\frac{1}{(1-(1-t)^3)}(AA+BB)$$
$$AA = \frac{1}{Q_x^2 - Q_z^2}[-Q_x \sin Q_x + \frac{1}{2}[(Q_x - Q_z)\sin(Q_x(1-t) - Q_z t) + (Q_x + Q_z)\sin(Q_x(1-t) + Q_z t)]]$$
$$BB = \frac{1}{Q_y^2 - Q_z^2}[Q_y \sin Q_y - \frac{1}{2}[(Q_y - Q_z)\sin(Q_y(1-t) - Q_z t) + (Q_y + Q_z)\sin(Q_y(1-t) + Q_z t)]]$$

The expression can be rewritten with the sum of three terms :

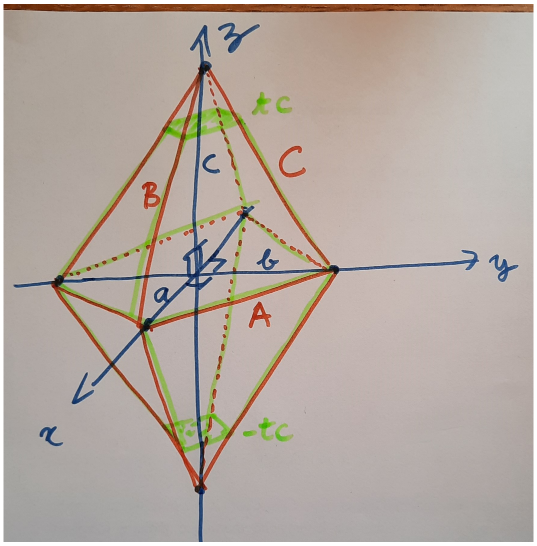

Figure 6: Truncated octahedron along one axis

$$AP = A_O(\vec{Q})/V$$

$$AP = -\frac{6}{1-(1-t)^3}(AA+BB+CC)$$
$$AA = \frac{Q_x \sin Q_x}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)}$$
$$BB = \frac{Q_y \sin Q_y}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)}$$
$$CC = -\frac{1}{2}\frac{1}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)}[(Q_x - Q_z)\sin(Q_x(1-t) - Q_z t) + (Q_x + Q_z)\sin(Q_x(1-t) + Q_z t)] +$$
$$-\frac{1}{2}\frac{1}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)}[(Q_y - Q_z)\sin(Q_y(1-t) - Q_z t) + (Q_y + Q_z)\sin(Q_y(1-t) + Q_z t)]$$

For $t = 1$, without truncature, CC term is :

$$CC = \frac{Q_z \sin Q_z}{(Q_z^2 - Q_x^2)(Q_z^2 - Q_y^2)}$$

6.3 Truncated octahedron along the three directions

Truncature parameter is $1/2 < t < 1$.
$t = 1/2$ corresponds to a general cuboctahedron shape.
The volume of the truncated octahedron is obtained by subtracting the volume of the six small pyramids that are truncated:

$$V_t = \frac{4}{3}abc(1 - 3(1-t)^3)$$

Calculation on the form factor can be done using a general formula from Bernard Croset or Joachim Wuttke. But it is possible to 'guess' an analytical expression based on the one with the truncature along z only. By symmetry, on gets the following expression :

$$AP = A_O(\vec{Q})/V_t$$

$$AP = \frac{6}{1-3(1-t)^3}(AA + BB + CC)$$

$$\begin{aligned}
AA &= \frac{1}{2}\frac{1}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)}[(Q_y - Q_x)\sin(Q_y(1-t) - Q_x t) + (Q_y + Q_x)\sin(Q_y(1-t) + Q_x t)] + \\
&+ \frac{1}{2}\frac{1}{(Q_z^2 - Q_x^2)(Q_z^2 - Q_y^2)}[(Q_z - Q_x)\sin(Q_z(1-t) - Q_x t) + (Q_z + Q_x)\sin(Q_z(1-t) + Q_x t)] \\
BB &= \frac{1}{2}\frac{1}{(Q_z^2 - Q_x^2)(Q_z^2 - Q_y^2)}[(Q_z - Q_y)\sin(Q_z(1-t) - Q_y t) + (Q_z + Q_y)\sin(Q_z(1-t) + Q_y t)] + \\
&+ \frac{1}{2}\frac{1}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)}[(Q_x - Q_y)\sin(Q_x(1-t) - Q_y t) + (Q_x + Q_y)\sin(Q_x(1-t) + Q_y t)] \\
CC &= \frac{1}{2}\frac{1}{(Q_x^2 - Q_y^2)(Q_x^2 - Q_z^2)}[(Q_x - Q_z)\sin(Q_x(1-t) - Q_z t) + (Q_x + Q_z)\sin(Q_x(1-t) + Q_z t)] + \\
&+ \frac{1}{2}\frac{1}{(Q_y^2 - Q_z^2)(Q_y^2 - Q_x^2)}[(Q_y - Q_z)\sin(Q_y(1-t) - Q_z t) + (Q_y + Q_z)\sin(Q_y(1-t) + Q_z t)]
\end{aligned}$$

For $t = 1$, the expression for the octahedron is recovered. The cuboctahedron corresponds to $t = 1/2$.

6.4 Truncated octahedron along the three directions with three different truncatures

Finally, a different truncature can be applied along the three axes and the expressions are modified as follows:

$$V_{t_x t_y t_z} = \frac{4}{3}abc(1 - (1-t_x)^3 - (1-t_y)^3 - (1-t_z)^3)$$

$$AP = A_O(\vec{Q})/V_{t_x t_y t_z}$$

$$AP = \frac{6}{1-(1-t_x)^3-(1-t_y)^3-(1-t_z)^3}(AA+BB+CC)$$

$$\begin{aligned}
AA = &\frac{1}{2}\frac{1}{(Q_y^2-Q_z^2)(Q_y^2-Q_x^2)}[(Q_y-Q_x)\sin(Q_y(1-t_x)-Q_x t_x)+(Q_y+Q_x)\sin(Q_y(1-t_x)+Q_x t_x)]+\\
&+\frac{1}{2}\frac{1}{(Q_z^2-Q_x^2)(Q_z^2-Q_y^2)}[(Q_z-Q_x)\sin(Q_z(1-t_x)-Q_x t_x)+(Q_z+Q_x)\sin(Q_z(1-t_x)+Q_x t_x)]\\
BB = &\frac{1}{2}\frac{1}{(Q_z^2-Q_x^2)(Q_z^2-Q_y^2)}[(Q_z-Q_y)\sin(Q_z(1-t_y)-Q_y t_y)+(Q_z+Q_y)\sin(Q_z(1-t_y)+Q_y t_y)]+\\
&+\frac{1}{2}\frac{1}{(Q_x^2-Q_y^2)(Q_x^2-Q_z^2)}[(Q_x-Q_y)\sin(Q_x(1-t_y)-Q_y t_y)+(Q_x+Q_y)\sin(Q_x(1-t_y)+Q_y t_y)]\\
CC = &\frac{1}{2}\frac{1}{(Q_x^2-Q_y^2)(Q_x^2-Q_z^2)}[(Q_x-Q_z)\sin(Q_x(1-t_z)-Q_z t_z)+(Q_x+Q_z)\sin(Q_x(1-t_z)+Q_z t_z)]+\\
&+\frac{1}{2}\frac{1}{(Q_y^2-Q_z^2)(Q_y^2-Q_x^2)}[(Q_y-Q_z)\sin(Q_y(1-t_z)-Q_z t_z)+(Q_y+Q_z)\sin(Q_y(1-t_z)+Q_z t_z)]
\end{aligned}$$