

Direct parameterization of the volume on pressure dependence by using  
an inverted approximative Vinet equation of state

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Supplementary material

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# 1 Inversions of the third order Vinet EoS approximation

In the following all 4 different solutions of the inversion of the third order Vinet EoS approximation can be found. Some plus and minus signs are colored in red to mark the differences.

## 1.1 Solution 1

With the specified range of positive parameters in the publication this gives an wrong physical behavior, with increasing volume with increasing pressure.

$$\begin{aligned}
f(P) = & \frac{4uv^3 + 3uv^2}{4uv^3} + \frac{1}{2} \left[ \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} \right. \\
& - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& - 512uv^6P^3) \left. \right)^{\frac{1}{2}} uv^2 \left. \right)^{\frac{1}{3}} + \left( 2(-(u^2v^2) - 6uv^2P \right. \\
& + 2P^2 - 4uv^3P - 4uvP) \left. \right) \Bigg/ \left( uv^3 (36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& - 512uv^6P^3) \left. \right)^{\frac{1}{2}} uv^2 \left. \right)^{\frac{1}{3}} \Bigg) - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \Bigg]^{\frac{1}{2}} \\
& + \frac{1}{2} \left[ \frac{1}{2} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& - \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v} (-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& - 512uv^6P^3) \left. \right)^{\frac{1}{2}} uv^2 \left. \right)^{\frac{1}{3}} - \left( 2(-(u^2v^2) - 6uv^2P + 2P^2 \right. \\
& - 4uv^3P - 4uvP) \left. \right) \Bigg/ \left( uv^3 \cdot (36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P
\end{aligned}$$

$$\begin{aligned}
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& + \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \\
& + \left( \frac{(9uv^2 - 6P + 6uv^3 + 6uv)(-4uv^3 - 3uv^2)}{u^2v^6} \right. \\
& \left. - \frac{2(-4uv^3 - 9uv^2 - 12uv - 6u)}{uv^3} - \frac{(-4uv^3 - 3uv^2)^3}{4u^3v^9} \right) \Big/ \\
& \left( \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} + \left( 2(-u^2v^2) - 6uv^2P + 2P^2 \right. \\
& \left. - 4uv^3P - 4uvP \right) \Big/ \left( uv^3(36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P \\
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& \left. - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \right)^{\frac{1}{2}} \Bigg]^{\frac{1}{2}} \quad (1)
\end{aligned}$$

## 1.2 Solution 2

This is the solution given in the publication with the specified range of positive values.

$$\begin{aligned}
f(P) = & \frac{4uv^3 + 3uv^2}{4uv^3} + \frac{1}{2} \left[ \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} \right. \\
& - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) \Big/ \left( uv^3 \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \Big]^{1/2} \\
& - \frac{1}{2} \left[ \frac{1}{2} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& - \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v} (-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) - \left( 2 \left( -(u^2v^2) - 6uv^2P + 2P^2 \right. \right. \\
& \left. \left. - 4uv^3P - 4uvP \right) \right) \Big) \Big/ \left( uv^3 \cdot \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P
\end{aligned}$$

$$\begin{aligned}
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& + \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \\
& + \left( \frac{(9uv^2 - 6P + 6uv^3 + 6uv)(-4uv^3 - 3uv^2)}{u^2v^6} \right. \\
& \left. - \frac{2(-4uv^3 - 9uv^2 - 12uv - 6u)}{uv^3} - \frac{(-4uv^3 - 3uv^2)^3}{4u^3v^9} \right) \Big/ \\
& \left( \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} + \left( 2(-u^2v^2) - 6uv^2P + 2P^2 \right. \\
& \left. - 4uv^3P - 4uvP \right) \Big/ \left( uv^3(36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P \\
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& \left. - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \right)^{\frac{1}{2}} \Bigg]^{\frac{1}{2}} \quad (2)
\end{aligned}$$

### 1.3 Solution 3

This solution is needed in the case of a negative  $B'_0$ . For example in chapter 4. For positive values of  $B'_0$  this equation can lead to complex solutions.

$$\begin{aligned}
f(P) = & \frac{4uv^3 + 3uv^2}{4uv^3} - \frac{1}{2} \left[ \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} \right. \\
& - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right] \frac{1}{2} uv^2 \Big) \Big) \Big/ \left( uv^3 \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right) \frac{1}{2} uv^2 \Big) \Big) \Big/ \left( uv^3 \left( -3uv^2 + 2P - 2uv^3 - 2uv \right) \right)^{\frac{1}{2}} \\
& + \frac{1}{2} \left[ \frac{1}{2} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& \left. - \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v} (-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right] \frac{1}{2} uv^2 \Big) \Big) \Big/ \left( uv^3 \cdot \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P
\end{aligned}$$

$$\begin{aligned}
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& + \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \\
& - \left( \frac{(9uv^2 - 6P + 6uv^3 + 6uv)(-4uv^3 - 3uv^2)}{u^2v^6} \right. \\
& \left. - \frac{2(-4uv^3 - 9uv^2 - 12uv - 6u)}{uv^3} - \frac{(-4uv^3 - 3uv^2)^3}{4u^3v^9} \right) \Bigg) \Bigg/ \\
& \left( \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} + \left( 2(-u^2v^2) - 6uv^2P + 2P^2 \right. \\
& \left. - 4uv^3P - 4uvP \right) \Big) \Big/ \left( uv^3(36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P \\
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& \left. - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \right)^{\frac{1}{2}} \Bigg] \Bigg)^{\frac{1}{2}} \tag{3}
\end{aligned}$$

## 1.4 Solution 4

Similar to solution 1, but only reliable for negative  $B'_0$ .

$$\begin{aligned}
f(P) = & \frac{4uv^3 + 3uv^2}{4uv^3} - \frac{1}{2} \left[ \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} \right. \\
& - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) \Big/ \left( uv^3 \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 \\
& + \left( -\frac{1}{v} (-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P \right. \\
& - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 \\
& - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \Big]^{1/2} \\
& - \frac{1}{2} \left[ \frac{1}{2} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& - \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v} (-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. \left. - 512uv^6P^3) \right) \right]^{1/2} uv^2 \Big) \Big) \Big/ \left( uv^3 \cdot \left( 36u^2v^3P + 21u^2v^4P \right. \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P
\end{aligned}$$

$$\begin{aligned}
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& + \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \\
& - \left( \frac{(9uv^2 - 6P + 6uv^3 + 6uv)(-4uv^3 - 3uv^2)}{u^2v^6} \right. \\
& \left. - \frac{2(-4uv^3 - 9uv^2 - 12uv - 6u)}{uv^3} - \frac{(-4uv^3 - 3uv^2)^3}{4u^3v^9} \right) \Big/ \\
& \left( \frac{1}{4} \frac{(-4uv^3 - 3uv^2)^2}{u^2v^6} - \frac{9uv^2 - 6P + 6uv^3 + 6uv}{uv^3} \right. \\
& + \frac{1}{uv^3} \left( 36u^2v^3P + 21u^2v^4P + 8u^3v^3 - 8P^3 + 24uv^3P^2 \right. \\
& + 24uvP^2 - 6u^2v^2P + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 \right. \\
& - 720u^3v^3P - 756u^2vP^2 - 432u^3v^4P - 3060u^2v^3P^2 \\
& - 3024P^3uv - 2664u^2v^4P^2 - 1296u^2v^2P^2 - 7920uv^2P^3 \\
& + 288P^3u - 825u^2v^5P^2 - 9576P^3uv^3 + 1152vP^4 \\
& - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 - 2304uv^5P^3 + 192P^4v^3 \\
& \left. - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} + \left( 2(-u^2v^2) - 6uv^2P + 2P^2 \right. \\
& \left. - 4uv^3P - 4uvP \right) \Big/ \left( uv^3(36u^2v^3P + 21u^2v^4P \right. \\
& + 8u^3v^3 - 8P^3 + 24uv^3P^2 + 24uvP^2 - 6u^2v^2P \\
& + 36uv^2P^2 + \left( -\frac{1}{v}(-72u^4v^3 - 720u^3v^3P - 756u^2vP^2 \right. \\
& - 432u^3v^4P - 3060u^2v^3P^2 - 3024P^3uv - 2664u^2v^4P^2 \\
& - 1296u^2v^2P^2 - 7920uv^2P^3 + 288P^3u - 825u^2v^5P^2 \\
& - 9576P^3uv^3 + 1152vP^4 - 6000uv^4P^3 + 576v^2P^4 + 1152P^4 \\
& \left. - 2304uv^5P^3 + 192P^4v^3 - 512uv^6P^3) \right)^{\frac{1}{2}}uv^2 \Big)^{\frac{1}{3}} \Big) \\
& \left. - \frac{-3uv^2 + 2P - 2uv^3 - 2uv}{uv^3} \right)^{\frac{1}{2}} \Bigg]^{\frac{1}{2}} \quad (4)
\end{aligned}$$

## 2 Validity of the third order Vinet EoS approximation for transition metals, diamond and osmium

Table 1: Pressure difference between the Vinet EoS and the third order Vinet EoS approximation at a volume compression ratio of 20%. Bulk modulus and pressure derivative values for the transitions metals are obtained from Raju et al. (1997), whereas diamond osmium values are obtained from Cynn et al. (2002).

Element	$B_0$ (GPa)	$B'_0$	Vinet EoS (GPa)	third order Vinet EoS approximation (GPa)	Difference (GPa)
Sc	60	2	16.672	16.672	0
Ti	105	4.37	37.644	37.624	0.02
V	160	4.26	56.688	56.661	0.027
Cr	180	4.89	68.244	68.181	0.063
Mn	131	5	50.257	50.206	0.051
Fe	170	5.29	67.285	67.197	0.088
Co	192	4.26	68.026	67.993	0.0323
Ni	183	5.26	72.197	72.105	0.092
Cu	137	5.48	55.343	55.258	0.085
Y	40	2	11.115	11.115	0
Zr	89	4.11	31.028	31.016	0.012
Nb	170	4.06	58.950	58.927	0.023
Mo	267	4.5	97.071	97.011	0.06
Tc	281	0	62.972	62.972	0
Ru	310	6.61	141.407	140.923	0.484
Rh	269	4.5	97.798	97.738	0.06
Pd	184	5.42	73.851	73.743	0.108
Ag	101	6.12	43.707	43.599	0.108
La	22.6	3.2	7.145	7.144	0.001
Hf	109	3.95	37.353	37.340	0.013
Ta	200	3.79	67.368	67.350	0.018
W	317	4.33	113.162	113.103	0.059
Re	368	5.41	147.544	147.330	0.214
Os	410	3.4	132.433	132.413	0.02
Ir	364	4.83	137.116	136.998	0.118
Pt	280	5.18	109.519	109.389	0.13
Au	173	6.29	76.245	76.033	0.212
C	444	4	152.972	152.919	0.053
Os	462	2.4	134.016	134.014	0.002

### 3 Input files and macros for TOPAS

Listing 1: Input files and macros for TOPAS

```
,  
,
```

---

```
', Information  
,
```

---

```
', This examples shows how to determine the bulk modulus, the pressure derivative  
' and the volume and/or lattice parameters at zero pressure with the inverted  
' third order Vinet EoS approximation.  
,
```

---

```
', By default this example determines the linearized values. Please check the  
' additional comments in the code, in order to change this example to the  
' determination of the bulk values.  
,
```

---

```
', Questions and suggestions can be submitted to:  
,
```

---

```
', Prof Dr. Robert E. Dinnebier (r.dinnebier@fkf.mpg)  
,
```

---

```
', and / or  
,
```

---

```
', Martin Etter (m.etter@fkf.mpg.de)  
,
```

---

```
,
```

---

```
,
```

---

```
', Global definitions  
,
```

---

```
r_exp 2.665616807 r_exp_dash 6.368603465 r_wp 1.702419589 r_wp_dash 4.067364546  
    r_p 1.047127023 r_p_dash 4.65611926 weighted_Durbin_Watson 0.8127132928 gof  
    0.6386587842  
iters 100000  
do_errors  
conserve_memory  
,
```

---

```
', Global parametric parameters  
,
```

---

```
', Parameter for bulk inverted third order Vinet EoS approximation  
prm V0      242.875   min =100; max=400;  
prm VK0     200.0      min =0; max=400;  
prm VKp0    5.0        min =0; max=100;  
  
prm uuu = 3 * VK0;    :0  
prm vvv = 3/2*(VKp0 - 1); :0
```

---

```
' Parameter for linearized and inverted third order Vinet EoS  
approximation
```

```
prm A0_Ma 5.55904 min =5; max=6;  
prm A0_Mb 5.56612 min =5; max=6;  
prm A0_Mc 7.85481 min =6; max=9;  
  
prm AK0_Ma 206.88492 min =0; max=400;  
prm AK0_Mb 141.71096 min =0; max=400;  
prm AK0_Mc 174.72222 min =0; max=400;  
  
prm AKp0_Ma 9.23128 min =-100; max=100;  
prm AKp0_Mb 4.31478 min =-100; max=100;  
prm AKp0_Mc 1.79863 min =-100; max=100;  
  
prm uuu_Ma = 3 * AK0_Ma; :0  
prm uuu_Mb = 3 * AK0_Mb; :0  
prm uuu_Mc = 3 * AK0_Mc; :0  
prm vvv_Ma = 3/2*(AKp0_Ma - 1); :0  
prm vvv_Mb = 3/2*(AKp0_Mb - 1); :0  
prm vvv_Mc = 3/2*(AKp0_Mc - 1); :0
```

---

```
' Macro for Header information
```

---

```
macro Header_info {
```

```
    r_exp 2.665616807 r_exp_dash 6.368603465 r_wp 1.702419589 r_wp_dash  
    4.067364546 r_p 1.047127023 r_p_dash 4.65611926 weighted_Durbin_Watson  
    0.8127132928 gof 0.6386587842  
    start_X 5  
    finish_X 20.8  
    LP_Factor( 90)  
    Zero_Error(, -0.00003)  
    convolution_step 5  
    Rp 217.5  
    Rs 217.5  
    lam  
        ymin_on_ymax 0.0001  
        la 1 lo 0.45587 lh 1e-005  
    x_calculation_step 0.014
```

```
}
```

---

```
' Macro for EoS + Structure parameter
```

---

```
macro Structure {
```

```
    str  
    local prss = pressure_loc; :0
```

---

```
,
```

```

local vinetvolume = -(1/4)*(-4*uuu*vvv^3-3*uuu*vvv^2)/(uuu*
vvv^3)+(1/2)*((1/4)*(-4*uuu*vvv^3-3*uuu*vvv^2)^2/(uuu^2*
vvv^6)-(9*uuu*vvv^2-6*prss+6*uuu*vvv^3+6*uuu*vvv)/(uuu*
vvv^3)+(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*uuu^3*vvv^3-8*
prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv^2*prss^2-6*uuu^2*vvv^2*
prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*uuu^3*vvv^3-
prss-756*uuu^2*vvv*prss^2-432*uuu^3*vvv^4*prss-3060*uuu^2*vvv^3*
prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*prss^2-1296*uuu^2*vvv^2*
vvv^2*prss^2-7920*uuu^2*vvv^3+288*uuu*prss^3-825*uuu^2*vvv^5*prss^2-
9576*prss^3*uuu*vvv^3+1152*vvv*prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+
192*prss^4*vvv^3-512*uuu*vvv^6*prss^3)/vvv)^(1/2)*uuu*vvv^2*(uuu*vvv^3)+2*(-(uuu^2*vvv^2)-6*uuu*vvv^2*prss+2*prss^2-4*uuu*vvv^3*prss-4*uuu*vvv*prss)/(uuu*vvv^3*(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*uuu^3*vvv^3-8*prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv*prss^2-6*uuu^2*vvv^2*prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*uuu^3*vvv^3*prss-756*uuu^2*vvv^2*vvv^2*prss^2-432*uuu^3*vvv^4*prss-3060*uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu^2*vvv^3+288*uuu*prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^2*prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3))-(-3*uuu*vvv^2+2*prss-2*uuu*vvv^3-2*uuu*vvv^2)/((uuu*vvv^3)^(1/2)-(1/2)*((1/2)*(-4*uuu*vvv^3-3*uuu*vvv^2)^2/(uuu^2*vvv^6)-(9*uuu*vvv^2-6*prss+6*uuu*vvv^3+6*uuu*vvv)/(uuu*vvv^3)-(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*uuu^3*vvv^3-8*prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv*prss^2-6*uuu^2*vvv^2*prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*uuu^3*vvv^3*prss-756*uuu^2*vvv^2*vvv^2*prss^2-432*uuu^3*vvv^4*prss-3060*uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu^2*vvv^3+288*uuu*prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^2*prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3))/((uuu*vvv^3)-2*(-(uuu^2*vvv^2)-6*uuu*vvv^2*prss+2*prss^2-4*uuu*vvv^3*prss-4*uuu*vvv*prss)/(uuu*vvv^3*(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*uuu^3*vvv^3-8*prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv*prss^2-6*uuu^2*vvv^2*prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*uuu^3*vvv^3*prss-756*uuu^2*vvv^2*vvv^2*prss^2-432*uuu^3*vvv^4*prss-3060*uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu^2*vvv^3+288*uuu*prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^2*prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3))+(-3*uuu*vvv^2+2*prss-2*uuu*vvv^3-2*uuu*vvv^2)/((uuu*vvv^3)+((9*uuu*vvv^2-6*prss+6*uuu*vvv^3+6*uuu*vvv)*(-4*uuu*vvv^3-3*uuu*vvv^2)/(uuu^2*vvv^6)-2*(-4*uuu*vvv^3-9*uuu*vvv^2-12*uuu*vvv^6*uuu)/(uuu*vvv^3)-(1/4)*(-4*uuu*vvv^3-3*uuu*vvv^2)^3/(uuu^3*vvv^9))/((1/4)*(-4*uuu*vvv^3-3*uuu*vvv^2)^2/(uuu^2*vvv^6)-(9*uuu*vvv^2-6*prss+6*uuu*vvv^3+6*uuu*vvv)/(uuu*vvv^3)+(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*uuu^3*vvv^3-8*prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv*prss^2-6*uuu^2*vvv^2*prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*uuu^3*vvv^3*prss-756*uuu^2*vvv^2*vvv^2*prss^2-432*uuu^3*vvv^4*prss-3060*uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu^2*vvv^3+288*uuu*prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^2*prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3))

```

```

uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*
prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu*vvv^2*prss^3+288*uuu*
prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^
prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*
uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*
prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3)/(uuu*vvv^3)+2*(-(uuu^2*
vvv^2)-6*uuu*vvv^2*prss+2*prss^2-4*uuu*vvv^3*prss-4*uuu*vvv^
prss)/(uuu*vvv^3*(36*uuu^2*vvv^3*prss+21*uuu^2*vvv^4*prss+8*
uuu^3*vvv^3-8*prss^3+24*uuu*vvv^3*prss^2+24*uuu*vvv^prss^2-6*
uuu^2*vvv^2*prss+36*uuu*vvv^2*prss^2+(-(-72*uuu^4*vvv^3-720*
uuu^3*vvv^3*prss-756*uuu^2*vvv^prss^2-432*uuu^3*vvv^4*prss-3060*
uuu^2*vvv^3*prss^2-3024*prss^3*uuu*vvv-2664*uuu^2*vvv^4*
prss^2-1296*uuu^2*vvv^2*prss^2-7920*uuu*vvv^2*prss^3+288*uuu*
prss^3-825*uuu^2*vvv^5*prss^2-9576*prss^3*uuu*vvv^3+1152*vvv^
prss^4-6000*uuu*vvv^4*prss^3+576*vvv^2*prss^4+1152*prss^4-2304*
uuu*vvv^5*prss^3+192*prss^4*vvv^3-512*uuu*vvv^6*
prss^3)/vvv)^(1/2)*uuu*vvv^2)^(1/3))-(-3*uuu*vvv^2+2*prss-2*uuu*
vvv^3-2*uuu*vvv)/(uuu*vvv^3))^(1/2))^(1/2); :0

```

```

local volume_loc = vinetvolume^3*V0;
local multparam = (lp_a_predet*lp_b_predet*
lp_c_predet)/(volume_loc);

```

---

, \_\_\_\_\_  
' linearized and inverted third order Vinet EoS approximation  
, \_\_\_\_\_

---

```

local vinetflatticea = -(1/4)*(-4*uuu_Ma*vvv_Ma^3-3*uuu_Ma*
vvv_Ma^2)/(uuu_Ma*vvv_Ma^3)+(1/2)*((1/4)*(-4*uuu_Ma*vvv_Ma^3-3*
uuu_Ma*vvv_Ma^2)^2/(uuu_Ma^2*vvv_Ma^6)-(9*uuu_Ma*vvv_Ma^2-6*
prss+6*uuu_Ma*vvv_Ma^3+6*uuu_Ma*vvv_Ma)/(uuu_Ma*vvv_Ma^3)+(36*
uuu_Ma^2*vvv_Ma^3*prss+21*uuu_Ma^2*vvv_Ma^4*prss+8*uuu_Ma^3*
vvv_Ma^3-8*prss^3+24*uuu_Ma*vvv_Ma^3*prss^2+24*uuu_Ma*vvv_Ma*
prss^2-6*uuu_Ma^2*vvv_Ma^2*prss+36*uuu_Ma*vvv_Ma^2*
prss^2+(-(-72*uuu_Ma^4*vvv_Ma^3-720*uuu_Ma^3*vvv_Ma^3*prss-756*
uuu_Ma^2*vvv_Ma*prss^2-432*uuu_Ma^3*vvv_Ma^4*prss-3060*uuu_Ma^2*
vvv_Ma^3*prss^2-3024*prss^3*uuu_Ma*vvv_Ma-2664*uuu_Ma^2*
vvv_Ma^4*prss^2-1296*uuu_Ma^2*vvv_Ma^2*prss^2-7920*uuu_Ma*
vvv_Ma^2*prss^3+288*uuu_Ma*prss^3-825*uuu_Ma^2*vvv_Ma^5*
prss^2-9576*prss^3*uuu_Ma*vvv_Ma^3+1152*vvv_Ma*prss^4-6000*
uuu_Ma*vvv_Ma^4*prss^3+576*vvv_Ma^2*prss^4+1152*prss^4-2304*
uuu_Ma*vvv_Ma^5*prss^3+192*prss^4*vvv_Ma^3-512*uuu_Ma*vvv_Ma^6*
prss^3)/vvv_Ma)^(1/2)*uuu_Ma*vvv_Ma^2)^(1/3)/(uuu_Ma*
vvv_Ma^3)+2*(-(uuu_Ma^2*vvv_Ma^2)-6*uuu_Ma*vvv_Ma^2*prss+2*
prss^2-4*uuu_Ma*vvv_Ma^3*prss-4*uuu_Ma*vvv_Ma*prss)/(uuu_Ma*
vvv_Ma^3*(36*uuu_Ma^2*vvv_Ma^3*prss+21*uuu_Ma^2*vvv_Ma^4*prss+8*
uuu_Ma^3*vvv_Ma^3-8*prss^3+24*uuu_Ma*vvv_Ma^3*prss^2+24*uuu_Ma*
vvv_Ma*prss^2-6*uuu_Ma^2*vvv_Ma^2*prss+36*uuu_Ma*vvv_Ma^2*
prss^2+(-(-72*uuu_Ma^4*vvv_Ma^3-720*uuu_Ma^3*vvv_Ma^3*prss-756*
uuu_Ma^2*vvv_Ma*prss^2-432*uuu_Ma^3*vvv_Ma^4*prss-3060*uuu_Ma^2*
vvv_Ma^3*prss^2-3024*prss^3*uuu_Ma*vvv_Ma-2664*uuu_Ma^2*
vvv_Ma^4*prss^2-1296*uuu_Ma^2*vvv_Ma^2*prss^2-7920*uuu_Ma*
vvv_Ma^2*prss^3+288*uuu_Ma*prss^3-825*uuu_Ma^2*vvv_Ma^5*
prss^2-9576*prss^3*uuu_Ma*vvv_Ma^3+1152*vvv_Ma*prss^4-6000*
uuu_Ma*vvv_Ma^4*prss^3+576*vvv_Ma^2*prss^4+1152*prss^4-2304*
```

$$\begin{aligned}
& \text{uuu\_Ma}^* \text{vvv\_Ma}^5 \text{prss}^3 + 192 \text{prss}^4 \text{vvv\_Ma}^3 - 512 \text{uuu\_Ma}^* \text{vvv\_Ma}^6 \\
& (\text{prss}^3) / \text{vvv\_Ma}^{(1/2)} \text{uuu\_Ma}^* \text{vvv\_Ma}^2 \text{)^{(1/3)}} - (-3 \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2 + 2 \text{prss} - 2 \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 2 \text{uuu\_Ma}^* \text{vvv\_Ma}) / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3) \text{)^{(1/2)}} - (1/2) * ((1/2) * (-4 \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 3 \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2) \text{)^2} / (\text{uuu\_Ma}^2 \text{vvv\_Ma}^6) - (9 \text{uuu\_Ma}^* \text{vvv\_Ma}^2 - 6 \text{prss} + 6 \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 6 \text{uuu\_Ma}^* \text{vvv\_Ma}) / (\text{uuu\_Ma}^* \text{vvv\_Ma}^3) - (36 \text{uuu\_Ma}^2 \\
& \text{vvv\_Ma}^3 * \text{prss} + 21 \text{uuu\_Ma}^2 \text{vvv\_Ma}^4 * \text{prss} + 8 \text{uuu\_Ma}^3 \text{vvv\_Ma}^3 - 8 \\
& \text{prss}^3 + 24 \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss}^2 + 24 \text{uuu\_Ma}^* \text{vvv\_Ma}^* \text{prss}^2 - 6 \\
& \text{uuu\_Ma}^2 \text{vvv\_Ma}^2 * \text{prss} + 36 \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \text{prss}^2 + (-72 \\
& \text{uuu\_Ma}^4 \text{vvv\_Ma}^3 - 720 \text{uuu\_Ma}^3 \text{vvv\_Ma}^3 * \text{prss} - 756 \text{uuu\_Ma}^2 \\
& \text{vvv\_Ma}^* \text{prss}^2 - 432 \text{uuu\_Ma}^3 \text{vvv\_Ma}^4 * \text{prss} - 3060 \text{uuu\_Ma}^2 \text{vvv\_Ma}^3 * \\
& \text{prss}^2 - 3024 \text{uuu\_Ma}^3 \text{vvv\_Ma}^* \text{prss} - 2664 \text{uuu\_Ma}^2 \text{vvv\_Ma}^4 * \\
& \text{prss}^2 - 1296 \text{uuu\_Ma}^2 \text{vvv\_Ma}^2 * \text{prss}^2 - 7920 \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \\
& \text{prss}^3 + 288 \text{uuu\_Ma}^* \text{prss}^3 - 825 \text{uuu\_Ma}^2 \text{vvv\_Ma}^5 * \text{prss}^2 - 9576 * \\
& \text{prss}^3 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 1152 \text{vvv\_Ma}^* \text{prss}^4 - 6000 \text{uuu\_Ma}^* \text{vvv\_Ma}^4 * \\
& \text{prss}^3 + 576 \text{vvv\_Ma}^2 * \text{prss}^4 + 1152 \text{prss}^4 - 2304 \text{uuu\_Ma}^* \text{vvv\_Ma}^5 * \\
& \text{prss}^3 + 192 \text{prss}^4 \text{vvv\_Ma}^3 - 512 \text{uuu\_Ma}^* \text{vvv\_Ma}^6 * \\
& \text{prss}^3) / \text{vvv\_Ma}^{(1/2)} \text{uuu\_Ma}^* \text{vvv\_Ma}^2 \text{)^{(1/3)}} / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3) - 2 * ((\text{uuu\_Ma}^2 \text{vvv\_Ma}^2) - 6 \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \text{prss} + 2 * \\
& \text{prss}^2 - 4 \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss} - 4 \text{uuu\_Ma}^* \text{vvv\_Ma}^* \text{prss}) / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3 * (36 \text{uuu\_Ma}^2 \text{vvv\_Ma}^3 * \text{prss} + 21 \text{uuu\_Ma}^2 \text{vvv\_Ma}^4 * \text{prss} + 8 * \\
& \text{uuu\_Ma}^3 \text{vvv\_Ma}^3 - 8 * \text{prss}^3 + 24 \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss}^2 + 24 \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^* \text{prss}^2 - 6 \text{uuu\_Ma}^2 \text{vvv\_Ma}^2 * \text{prss} + 36 \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \\
& \text{prss}^2 + (-72 \text{uuu\_Ma}^4 \text{vvv\_Ma}^3 - 720 \text{uuu\_Ma}^3 \text{vvv\_Ma}^3 * \text{prss} - 756 * \\
& \text{uuu\_Ma}^2 \text{vvv\_Ma}^* \text{prss}^2 - 432 \text{uuu\_Ma}^3 \text{vvv\_Ma}^4 * \text{prss} - 3060 \text{uuu\_Ma}^2 * \\
& \text{vvv\_Ma}^3 * \text{prss}^2 - 3024 \text{uuu\_Ma}^3 \text{vvv\_Ma}^* \text{prss} - 2664 \text{uuu\_Ma}^2 * \\
& \text{vvv\_Ma}^4 * \text{prss}^2 - 1296 \text{uuu\_Ma}^2 \text{vvv\_Ma}^2 * \text{prss}^2 - 7920 \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2 * \text{prss}^3 + 288 \text{uuu\_Ma}^* \text{prss}^3 - 825 \text{uuu\_Ma}^2 \text{vvv\_Ma}^5 * \\
& \text{prss}^2 - 9576 * \text{prss}^3 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 1152 \text{vvv\_Ma}^* \text{prss}^4 - 6000 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^4 * \text{prss}^3 + 576 \text{vvv\_Ma}^2 * \text{prss}^4 + 1152 * \text{prss}^4 - 2304 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^5 * \text{prss}^3 + 192 * \text{prss}^4 * \text{vvv\_Ma}^3 - 512 * \text{uuu\_Ma}^* \text{vvv\_Ma}^6 * \\
& \text{prss}^3) / \text{vvv\_Ma}^{(1/2)} \text{uuu\_Ma}^* \text{vvv\_Ma}^2 \text{)^{(1/3)}} + (-3 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2 + 2 * \text{prss} - 2 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 2 * \text{uuu\_Ma}^* \text{vvv\_Ma}) / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3) + ((9 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2 - 6 * \text{prss} + 6 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 6 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}) * (-4 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 3 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2) / (\text{uuu\_Ma}^2 * \\
& \text{vvv\_Ma}^6) - 2 * ((-4 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 9 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2 - 12 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma} - 6 * \text{uuu\_Ma}) / (\text{uuu\_Ma}^* \text{vvv\_Ma}^3) - (1/4) * (-4 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 - 3 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^2) ^3 / (\text{uuu\_Ma}^3 * \text{vvv\_Ma}^9)) / ((1/4) * (-4 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3 - 3 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2) ^2 / (\text{uuu\_Ma}^2 * \text{vvv\_Ma}^6) - (9 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2 - 6 * \text{prss} + 6 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 6 * \text{uuu\_Ma}^* \text{vvv\_Ma}) / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3) + (36 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^3 * \text{prss} + 21 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^4 * \\
& \text{prss} + 8 * \text{uuu\_Ma}^3 * \text{vvv\_Ma}^3 - 8 * \text{prss}^3 + 24 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss}^2 + 24 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^* \text{prss}^2 - 6 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^2 * \text{prss} + 36 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^2 * \text{prss}^2 + (-72 * \text{uuu\_Ma}^4 * \text{vvv\_Ma}^3 - 720 * \text{uuu\_Ma}^3 * \text{vvv\_Ma}^3 * \\
& \text{prss} - 756 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^* \text{prss}^2 - 432 * \text{uuu\_Ma}^3 * \text{vvv\_Ma}^4 * \text{prss} - 3060 * \\
& \text{uuu\_Ma}^2 * \text{vvv\_Ma}^3 * \text{prss}^2 - 3024 * \text{prss}^3 * \text{uuu\_Ma}^* \text{vvv\_Ma} - 2664 * \\
& \text{uuu\_Ma}^2 * \text{vvv\_Ma}^4 * \text{prss}^2 - 1296 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^2 * \text{prss}^2 - 7920 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \text{prss}^3 + 288 * \text{uuu\_Ma}^* \text{prss}^3 - 825 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^5 * \\
& \text{prss}^2 - 9576 * \text{prss}^3 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 + 1152 * \text{vvv\_Ma}^* \text{prss}^4 - 6000 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^4 * \text{prss}^3 + 576 * \text{vvv\_Ma}^2 * \text{prss}^4 + 1152 * \text{prss}^4 - 2304 * \\
& \text{uuu\_Ma}^* \text{vvv\_Ma}^5 * \text{prss}^3 + 192 * \text{prss}^4 * \text{vvv\_Ma}^3 - 512 * \text{uuu\_Ma}^* \text{vvv\_Ma}^6 * \\
& \text{prss}^3) / \text{vvv\_Ma}^{(1/2)} \text{uuu\_Ma}^* \text{vvv\_Ma}^2 \text{)^{(1/3)}} / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3) + 2 * ((-4 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^2) - 6 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \text{prss} + 2 * \\
& \text{prss}^2 - 4 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss} - 4 * \text{uuu\_Ma}^* \text{vvv\_Ma}^* \text{prss}) / (\text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^3 * (36 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^3 * \text{prss} + 21 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^4 * \text{prss} + 8 * \\
& \text{uuu\_Ma}^3 * \text{vvv\_Ma}^3 - 8 * \text{prss}^3 + 24 * \text{uuu\_Ma}^* \text{vvv\_Ma}^3 * \text{prss}^2 + 24 * \text{uuu\_Ma}^* \\
& \text{vvv\_Ma}^* \text{prss}^2 - 6 * \text{uuu\_Ma}^2 * \text{vvv\_Ma}^2 * \text{prss} + 36 * \text{uuu\_Ma}^* \text{vvv\_Ma}^2 * \\
& \text{prss}^2 + (-72 * \text{uuu\_Ma}^4 * \text{vvv\_Ma}^3 - 720 * \text{uuu\_Ma}^3 * \text{vvv\_Ma}^3 * \text{prss} - 756 *
\end{aligned}$$

```

uuu_Ma^2*vvv_Ma*prss^2-432*uuu_Ma^3*vvv_Ma^4*prss-3060*uuu_Ma^2*
vvv_Ma^3*prss^2-3024*prss^3*uuu_Ma*vvv_Ma-2664*uuu_Ma^2*
vvv_Ma^4*prss^2-1296*uuu_Ma^2*vvv_Ma^2*prss^2-7920*uuu_Ma^2*
vvv_Ma^2*prss^3+288*uuu_Ma*prss^3-825*uuu_Ma^2*vvv_Ma^5*
prss^2-9576*prss^3*uuu_Ma*vvv_Ma^3+1152*vvv_Ma*prss^4-6000*
uuu_Ma*vvv_Ma^4*prss^3+576*vvv_Ma^2*prss^4+1152*prss^4-2304*
uuu_Ma*vvv_Ma^5*prss^3+192*prss^4*vvv_Ma^3-512*uuu_Ma*vvv_Ma^6*
prss^3)/vvv_Ma^(1/2)*uuu_Ma*vvv_Ma^2)^(1/3))-(-3*uuu_Ma*
vvv_Ma^2+2*prss-2*uuu_Ma*vvv_Ma^3-2*uuu_Ma*vvv_Ma)/(uuu_Ma*
vvv_Ma^3))^(1/2))^(1/2); :0

```

```
local lp_a = vinetlatticea*A0_Ma;
```

```

local vinetlatticeb = -(1/4)*(-4*uuu_Mb*vvv_Mb^3-3*uuu_Mb*
vvv_Mb^2)/(uuu_Mb*vvv_Mb^3)+(1/2)*((1/4)*(-4*uuu_Mb*vvv_Mb^3-3*
uuu_Mb*vvv_Mb^2)^2/(uuu_Mb^2*vvv_Mb^6)-(9*uuu_Mb*vvv_Mb^2-6*
prss+6*uuu_Mb*vvv_Mb^3+6*uuu_Mb*vvv_Mb)/(uuu_Mb*vvv_Mb^3)+(36*
uuu_Mb^2*vvv_Mb^3*prss+21*uuu_Mb^2*vvv_Mb^4*prss+8*uuu_Mb^3*
vvv_Mb^3-8*prss^3+24*uuu_Mb*vvv_Mb^3*prss^2+24*uuu_Mb*vvv_Mb*
prss^2-6*uuu_Mb^2*vvv_Mb^2*prss+36*uuu_Mb*vvv_Mb^2*
prss^2+(-(-72*uuu_Mb^4*vvv_Mb^3-720*uuu_Mb^3*vvv_Mb^3*prss-756*
uuu_Mb^2*vvv_Mb*prss^2-432*uuu_Mb^3*vvv_Mb^4*prss-3060*uuu_Mb^2*
vvv_Mb^3*prss^2-3024*prss^3*uuu_Mb*vvv_Mb-2664*uuu_Mb^2*
vvv_Mb^4*prss^2-1296*uuu_Mb^2*vvv_Mb^2*prss^2-7920*uuu_Mb^2*
vvv_Mb^2*prss^3+288*uuu_Mb*prss^3-825*uuu_Mb^2*vvv_Mb^5*
prss^2-9576*prss^3*uuu_Mb*vvv_Mb^3+1152*vvv_Mb*prss^4-6000*
uuu_Mb*vvv_Mb^4*prss^3+576*vvv_Mb^2*prss^4+1152*prss^4-2304*
uuu_Mb*vvv_Mb^5*prss^3+192*prss^4*vvv_Mb^3-512*uuu_Mb*vvv_Mb^6*
prss^3)/vvv_Mb^(1/2)*uuu_Mb*vvv_Mb^2)^(1/3)/(uuu_Mb*
vvv_Mb^3)+2*(-(uuu_Mb^2*vvv_Mb^2)-6*uuu_Mb*vvv_Mb^2*prss+2*
prss^2-4*uuu_Mb*vvv_Mb^3*prss-4*uuu_Mb*vvv_Mb*prss)/(uuu_Mb*
vvv_Mb^3*(36*uuu_Mb^2*vvv_Mb^3*prss+21*uuu_Mb^2*vvv_Mb^4*prss+8*
uuu_Mb^3*vvv_Mb^3-8*prss^3+24*uuu_Mb*vvv_Mb^3*prss^2+24*uuu_Mb*
vvv_Mb*prss^2-6*uuu_Mb^2*vvv_Mb^2*prss+36*uuu_Mb*vvv_Mb^2*
prss^2+(-(-72*uuu_Mb^4*vvv_Mb^3-720*uuu_Mb^3*vvv_Mb^3*prss-756*
uuu_Mb^2*vvv_Mb*prss^2-432*uuu_Mb^3*vvv_Mb^4*prss-3060*uuu_Mb^2*
vvv_Mb^3*prss^2-3024*prss^3*uuu_Mb*vvv_Mb-2664*uuu_Mb^2*
vvv_Mb^4*prss^2-1296*uuu_Mb^2*vvv_Mb^2*prss^2-7920*uuu_Mb^2*
vvv_Mb^2*prss^3+288*uuu_Mb*prss^3-825*uuu_Mb^2*vvv_Mb^5*
prss^2-9576*prss^3*uuu_Mb*vvv_Mb^3+1152*vvv_Mb*prss^4-6000*
uuu_Mb*vvv_Mb^4*prss^3+576*vvv_Mb^2*prss^4+1152*prss^4-2304*
uuu_Mb*vvv_Mb^5*prss^3+192*prss^4*vvv_Mb^3-512*uuu_Mb*vvv_Mb^6*
prss^3)/vvv_Mb^(1/2)*uuu_Mb*vvv_Mb^2)^(1/3))-(-3*uuu_Mb*
vvv_Mb^2+2*prss-2*uuu_Mb*vvv_Mb^3-2*uuu_Mb*vvv_Mb)/(uuu_Mb*vvv_Mb^3)-(36*uuu_Mb^2*
vvv_Mb^3*prss+21*uuu_Mb^2*vvv_Mb^4*prss+8*uuu_Mb^3*vvv_Mb^3-8*prss^3+24*uuu_Mb*vvv_Mb^3*prss^2+24*uuu_Mb*vvv_Mb^2*prss^2+(-72*
uuu_Mb^2*vvv_Mb^2*prss+36*uuu_Mb*vvv_Mb^2*prss^2+(-72*
uuu_Mb^4*vvv_Mb^3-720*uuu_Mb^3*vvv_Mb^3*prss-756*uuu_Mb^2*
vvv_Mb*prss^2-432*uuu_Mb^3*vvv_Mb^4*prss-3060*uuu_Mb^2*vvv_Mb^3*prss^2-3024*prss^3*uuu_Mb*vvv_Mb-2664*uuu_Mb^2*vvv_Mb^4*prss^2-1296*uuu_Mb^2*vvv_Mb^2*prss^2-7920*uuu_Mb*vvv_Mb^2*prss^3+288*uuu_Mb*prss^3-825*uuu_Mb^2*vvv_Mb^5*prss^2-9576*prss^3*uuu_Mb*vvv_Mb^3+1152*vvv_Mb*prss^4-6000*uuu_Mb*vvv_Mb^4*prss^3+576*vvv_Mb^2*prss^4+1152*prss^4-2304*uuu_Mb*vvv_Mb^5*prss^3+192*prss^4*vvv_Mb^3-512*uuu_Mb*vvv_Mb^6*
```

```

local lp_b = vinetlatticeb*A0 Mb;
local vinetlatticec = -(1/4)*(-4*uuu_Mc*vvv_Mc^3-3*uuu_Mc*
vvv_Mc^2)/(uuu_Mc*vvv_Mc^3)+(1/2)*((1/4)*(-4*uuu_Mc*vvv_Mc^3-3*
uuu_Mc*vvv_Mc^2)^2/(uuu_Mc^2*vvv_Mc^6)-(9*uuu_Mc*vvv_Mc^2-6*
prss+6*uuu_Mc*vvv_Mc^3+6*uuu_Mc*vvv_Mc)/(uuu_Mc*vvv_Mc^3)+(36*

```



$$\begin{aligned}
& vvv\_Mc) * (-4*uuu\_Mc*vvv\_Mc^3 - 3*uuu\_Mc*vvv\_Mc^2) / (uuu\_Mc^2 * \\
& vvv\_Mc^6) - 2*(-4*uuu\_Mc*vvv\_Mc^3 - 9*uuu\_Mc*vvv\_Mc^2 - 12*uuu\_Mc* \\
& vvv\_Mc - 6*uuu\_Mc) / (uuu\_Mc*vvv\_Mc^3) - (1/4)*(-4*uuu\_Mc*vvv\_Mc^3 - 3* \\
& uuu\_Mc*vvv\_Mc^2)^3 / (uuu\_Mc^3*vvv\_Mc^9)) / ((1/4)*(-4*uuu\_Mc* \\
& vvv\_Mc^3 - 3*uuu\_Mc*vvv\_Mc^2)^2 / (uuu\_Mc^2*vvv\_Mc^6) - (9*uuu\_Mc* \\
& vvv\_Mc^2 - 6*prss + 6*uuu\_Mc*vvv\_Mc^3 + 6*uuu\_Mc*vvv\_Mc) / (uuu\_Mc* \\
& vvv\_Mc^3) + (36*uuu\_Mc^2*vvv\_Mc^3*prss + 21*uuu\_Mc^2*vvv\_Mc^4* \\
& prss + 8*uuu\_Mc^3*vvv\_Mc^3 - 8*prss^3 + 24*uuu\_Mc*vvv\_Mc^3*prss^2 + 24* \\
& uuu\_Mc*vvv\_Mc*prss^2 - 6*uuu\_Mc^2*vvv\_Mc^2*prss + 36*uuu\_Mc* \\
& vvv\_Mc^2*prss^2 + (-(-72*uuu\_Mc^4*vvv\_Mc^3 - 720*uuu\_Mc^3*vvv\_Mc^3* \\
& prss - 756*uuu\_Mc^2*vvv\_Mc*prss^2 - 432*uuu\_Mc^3*vvv\_Mc^4*prss - 3060* \\
& uuu\_Mc^2*vvv\_Mc^3*prss^2 - 3024*prss^3*uuu\_Mc*vvv\_Mc - 2664* \\
& uuu\_Mc^2*vvv\_Mc^4*prss^2 - 1296*uuu\_Mc^2*vvv\_Mc^2*prss^2 - 7920* \\
& uuu\_Mc*vvv\_Mc^2*prss^3 + 288*uuu\_Mc*prss^3 - 825*uuu\_Mc^2*vvv\_Mc^5* \\
& prss^2 - 9576*prss^3*uuu\_Mc*vvv\_Mc^3 + 1152*vvv\_Mc*prss^4 - 6000* \\
& uuu\_Mc*vvv\_Mc^4*prss^3 + 576*vvv\_Mc^2*prss^4 + 1152*prss^4 - 2304* \\
& uuu\_Mc*vvv\_Mc^5*prss^3 + 192*prss^4*vvv\_Mc^3 - 512*uuu\_Mc*vvv\_Mc^6* \\
& prss^3) / vvv\_Mc)^(1/2)*uuu\_Mc*vvv\_Mc^2)^(1/3) / (uuu\_Mc* \\
& vvv\_Mc^3) + 2*(-(uuu\_Mc^2*vvv\_Mc^2) - 6*uuu\_Mc*vvv\_Mc^2*prss + 2* \\
& prss^2 - 4*uuu\_Mc*vvv\_Mc^3*prss - 4*uuu\_Mc*vvv\_Mc*prss) / (uuu\_Mc* \\
& vvv\_Mc^3*(36*uuu\_Mc^2*vvv\_Mc^3*prss + 21*uuu\_Mc^2*vvv\_Mc^4*prss + 8* \\
& uuu\_Mc^3*vvv\_Mc^3 - 8*prss^3 + 24*uuu\_Mc*vvv\_Mc^3*prss^2 + 24*uuu\_Mc* \\
& vvv\_Mc*prss^2 - 6*uuu\_Mc^2*vvv\_Mc^2*prss + 36*uuu\_Mc*vvv\_Mc^2* \\
& prss^2 + (-(-72*uuu\_Mc^4*vvv\_Mc^3 - 720*uuu\_Mc^3*vvv\_Mc^3*prss - 756* \\
& uuu\_Mc^2*vvv\_Mc*prss^2 - 432*uuu\_Mc^3*vvv\_Mc^4*prss - 3060*uuu\_Mc^2* \\
& vvv\_Mc^3*prss^2 - 3024*prss^3*uuu\_Mc*vvv\_Mc - 2664*uuu\_Mc^2* \\
& vvv\_Mc^4*prss^2 - 1296*uuu\_Mc^2*vvv\_Mc^2*prss^2 - 7920*uuu\_Mc* \\
& vvv\_Mc^2*prss^3 + 288*uuu\_Mc*prss^3 - 825*uuu\_Mc^2*vvv\_Mc^5* \\
& prss^2 - 9576*prss^3*uuu\_Mc*vvv\_Mc^3 + 1152*vvv\_Mc*prss^4 - 6000* \\
& uuu\_Mc*vvv\_Mc^4*prss^3 + 576*vvv\_Mc^2*prss^4 + 1152*prss^4 - 2304* \\
& uuu\_Mc*vvv\_Mc^5*prss^3 + 192*prss^4*vvv\_Mc^3 - 512*uuu\_Mc*vvv\_Mc^6* \\
& prss^3) / vvv\_Mc)^(1/2)*uuu\_Mc*vvv\_Mc^2)^(1/3)) - (-3*uuu\_Mc* \\
& vvv\_Mc^2 + 2*prss - 2*uuu\_Mc*vvv\_Mc^3 - 2*uuu\_Mc*vvv\_Mc) / (uuu\_Mc* \\
& vvv\_Mc^3))^(1/2); :0
\end{aligned}$$

```
local lp_c = vinetlatticec*A0_Mc;
```

---

' Structure

---

```
r_bragg 0.8278468831
MW( 971.0024577, 241.9655836, 100)
scale @ 1.99061161e-005
space_group Pbnm
Phase_LAC_1_on_cm( 82.73346431)
Phase_Density_g_on_cm3( 6.663710563)

' If you want to determine the bulk inverted third order Vinet
' EoS approximation,
' please change the lattice parameters to the equations which are
' commented behind
' the particular line!
```

```
a = lp_a;           ' a =lp_a_bulk;
```

```

b = lp_b;           ' b =lp_b_bulk ;
c = lp_c;           ' c =lp_c_bulk ;

site La1 num_posns 4 x =La1_x; y =La1_y; z =La1_z; occ La+3
=La1_occ; beq =La1_beq;
site Fe1 num_posns 4 x =Fe1_x; y =Fe1_y; z =Fe1_z; occ Fe+3
=Fe1_occ; beq =Fe1_beq;
site O1 num_posns 4 x =O1_x; y =O1_y; z =O1_z; occ O-2
=O1_occ; beq =O1_beq;
site O2 num_posns 8 x =O2_x; y =O2_y; z =O2_z; occ O-2
=O2_occ; beq =O2_beq;

}

,

```

---

```

' list of all data files with corresponding individual parameters

```

---

```
xdd "r596042.xy"
```

```

local !pressure_loc 0.0 ' local pressure value (in GPa) for that
measurement
Header_info
bkg @ 1551.74228`_0.441933891 337.752184`_0.723691278
-154.465511`_0.69367704 -1.61793378`_0.66210448
7.96843609`_0.648085549 1.64117618`_0.620984183
-10.8823511`_0.61474511 0.333632182`_0.582640942
10.224038`_0.587608764 -11.777764`_0.535611434
2.30890721`_0.523207601
Structure
local csl 579.10727`_22.13431 min =0.3; max =10000;
local csg 68.78826`_0.19359 min =0.3; max =10000;
local stl 0.03869`_0.00147 min =0.0001; max =5;
CS_L( csl)
CS_G( csg)
Strain_G( stl)
Strain_L( stl)
local lp_a_predet 5.55696`_0.00007
local lp_b_predet 5.56405`_0.00009
local lp_c_predet 7.85508`_0.00011
local lp_a_bulk = multparam * lp_a_predet;
local lp_b_bulk = multparam * lp_b_predet;
local lp_c_bulk = multparam * lp_c_predet;

local La1_x 0.00602`_0.00026
local La1_y 0.02917
local !La1_z 0.25

local !Fe1_x 0
local !Fe1_y 0.5
local !Fe1_z 0

local O1_x 0.07608`_0.00192
local O1_y 0.48650`_0.00076
local !O1_z 0.25

```

```

local O2_x -0.27783‘_0.00134
local O2_y 0.28344‘_0.00125
local O2_z 0.03850‘_0.00076

' Occ parameters

local !La1_occ 1
local !Fe1_occ 1
local !O1_occ 1
local !O2_occ 1

' Temperature / Displacement Factors

local La1_beq 0.3 min =0; max =10;
local Fe1_beq =La1_beq; min =0; max =10;
local O1_beq =La1_beq; min =0; max =10;
local O2_beq =La1_beq; min =0; max =10;

phase_name "r596042"

xdd "Z:\Data\LaFeO3_High-Pressure\Datens (XY)\r596043.xy"
...

```

## 4 As<sub>2</sub>O<sub>5</sub> as an example for high $B'_0$ values

The arsenic pentoxide (space group  $P2_12_12_1$  at ambient conditions) builds a framework of corner-sharing distorted AsO<sub>6</sub>-octahedra and AsO<sub>4</sub>-tetrahedra (Jansen 1977, Locherer et al. 2010). As the empty channels of As<sub>2</sub>O<sub>5</sub> provide much additional space for the framework structure to deform under pressure, it is a good candidate to investigate channel framework structures which tend to have much smaller bulk moduli in contrast to perovskites which are normally described as three-dimensional frameworks with higher moduli (Hazen & Finger 1979). Because nitrogen as the used pressure medium has a very low hydrostatic limit (3.0 GPa according to Angel et al. (2007)), the parameterized data of Locherer et al. (2010) were taken in the non-hydrostatic regime and therefore in a range of  $2.74 \text{ GPa} \leq P \leq 19.5 \text{ GPa}$ .

Following the same procedure as for LaFeO<sub>3</sub>, parametric refinements were carried out determining the lattice parameters in a first run with the Le Bail method (LeBail et al. 1988) and fixing them in a second run to fit equation 2. The determination of the linear modulus etc. were performed as described above. Fitted curves obtained by the parametric refinement as well as the data points of the sequential refinement can be seen in figure 1. In table 2 the obtained values of the inverted approximative Vinet EoS can be found compared to the values of the pure Vinet EoS determined by (Locherer et al. 2010) with the program EOSFIT 5.2 (Angel 2000).

Figure 1: Volume and lattice parameters (a) and the corresponding f-F plot (b) for As<sub>2</sub>O<sub>5</sub> (space group  $P2_12_12_1$ ) obtained by sequential Rietveld refinement (points) and by parametric Rietveld refinement with an inverted third order Vinet EoS approximation. The dotted line for the lattice parameter  $a$  is fitted by another solution of the inverted third order Vinet EoS approximation as one has to respect the negative value of  $B'_0$ .

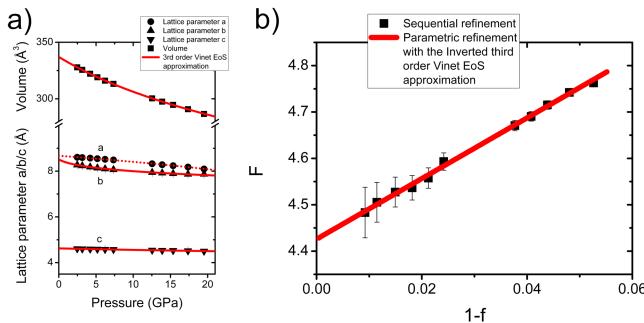


Table 2: Bulk modulus, its pressure derivative and the volume at ambient conditions of As<sub>2</sub>O<sub>5</sub> determined by the inverted third order Vinet EoS approximation as well as the linearized versions in the non-hydrostatic regime of nitrogen which is used as pressure medium ( $2.74 \text{ GPa} \leq P \leq 19.5 \text{ GPa}$ ). Due to reasons of comparison the values obtained by Locherer et al. (2010) with a usual Vinet EoS are also listed. The values for the lattice direction  $a$  are obtained by another solution of the inverted third order Vinet EoS approximation as one has to respect the negative value of  $B'_0$ .

	inv. approx. Vinet (3rd ord.)	Vinet (Locherer et al. 2010)
$V_0$	337.038(1)	337.93(5)
$B_0$	83.6(1)	78.1(24)
$B'_0$	4.7(1)	5.29(45)
$a_0$	8.674(1)	8.65(1)
$B_{0a}$	117.0(1)	125.06(167592)
$B'_{0a}$	-2.1(1)	-2.28(21060)
$b_0$	8.513(1)	8.45(30)
$B_{0b}$	15.5(2)	23.60(6749)
$B'_{0b}$	14.0(1)	11.95(3684)
$c_0$	4.624(1)	4.626(2)
$B_{0c}$	207.1(13)	186.88(183733)
$B'_{0c}$	5.3(2)	8.36(400.53)

In table 2, the values for the direction of the lattice parameter  $a$  cannot be directly obtained by the given linearized inverted third order Vinet EoS approximation displayed in equation 2. This is due to one of the seldom

cases, where the pressure derivative becomes negative and this leads to a complex solution of equation 2. To overcome this issue, it is possible to use another solution of the inverse function of the third order Vinet EoS approximation (chapter 1, equation 3) where a negative pressure derivative does not result in a complex solution. In general this will lead to the correct results for the linear modulus, its pressure derivative and the lattice parameter at ambient conditions.

Comparing the values of the linear moduli and the pressure derivatives it seems that the magnitude of the determined values is the same within three estimated standard deviations for both equations, bearing in mind that the same values are not completely reached. This can be attributed to the large pressure derivatives of  $B'_{0b} = 11.95$  and  $B'_{0c} = 8.36$  and the total volume compression of 15% in the investigated pressure range, which is slightly beyond the validity of the third order Vinet EoS approximation.

## 5 Graphical overview of $P(V)$ and $V(P)$

### 5.1 Graphical overview of $P(V)$

The following graphics are obtained by an analytical investigation of the Vinet EoS and the third order Vinet EoS approximation.

Figure 2: Selected fixed volume contractions and selected values of the bulk modulus showing the pressure differences between the Vinet EoS and the third order Vinet EoS approximation for the positive parameter space of the pressure derivative of the bulk modulus  $B'_0$ .

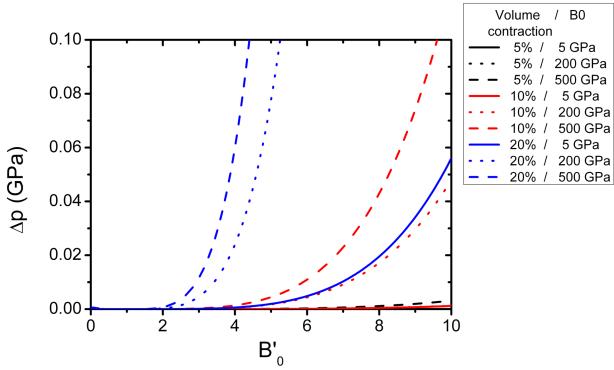


Figure 3: 3D map showing the differences of the calculated pressure values between Vinet EoS and third order Vinet EoS approximation at a fixed volume contraction of 5% for the positive parameter space of the bulk modulus  $B_0$  and its derivative  $B'_0$ .

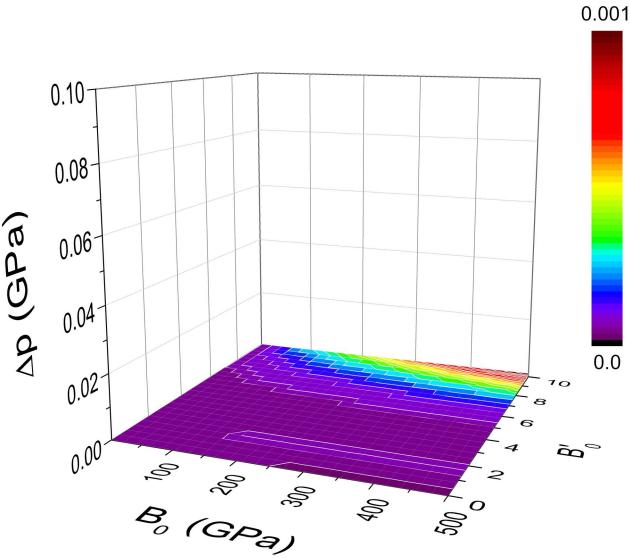


Figure 4: 3D map showing the differences of the calculated pressure values between Vinet EoS and third order Vinet EoS approximation at a fixed volume contraction of 10% for the positive parameter space of the bulk modulus  $B_0$  and its derivative  $B'_0$ .

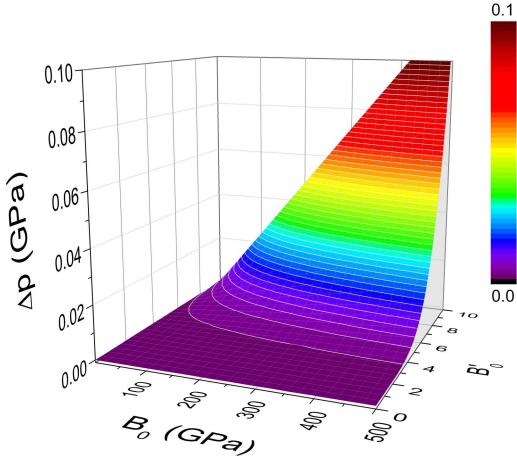
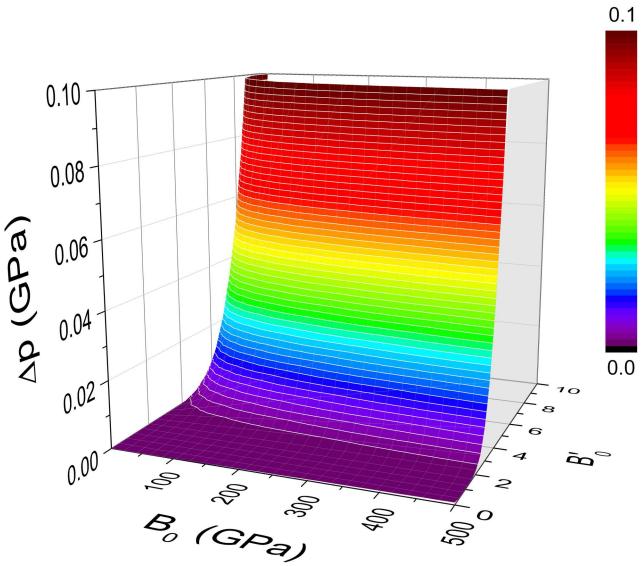


Figure 5: 3D map showing the differences of the calculated pressure values between Vinet EoS and third order Vinet EoS approximation at a fixed volume contraction of 20% for the positive parameter space of the bulk modulus  $B_0$  and its derivative  $B'_0$ .



## 5.2 Graphical overview of V(P)

The following graphics are obtained by an investigation of the numerically inverted Vinet EoS and the inverted third order Vinet EoS approximation.

Figure 6: Selected fixed pressures and selected values of the bulk modulus showing the volume differences between the numerical inverted Vinet EoS and the inverted third order Vinet EoS approximation for the positive parameter space of the pressure derivative of the bulk modulus  $B'_0$ .

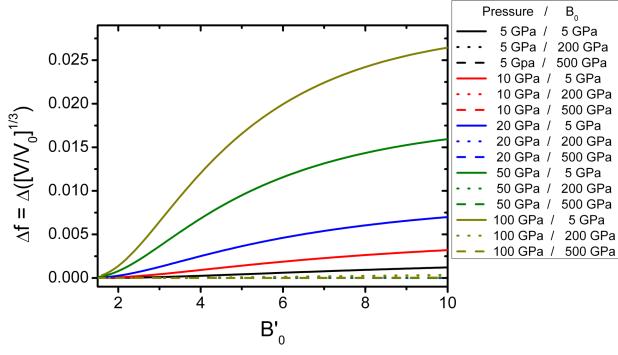
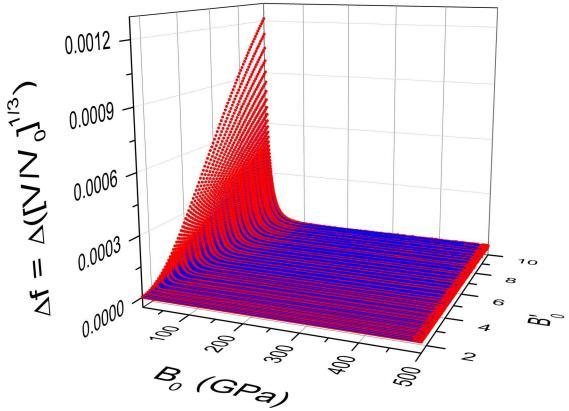


Figure 7: 3D map showing the volume differences of the calculated volume values between numerical inverted Vinet EoS and inverted third order Vinet EoS approximation at a fixed pressure of 10 GPa for the positive parameter space of the bulk modulus  $B_0$  and its derivative  $B'_0$ .



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