Solvent-density expansions for $\mathcal{B}_2$, $\mathcal{B}_3$, and $\mathcal{B}_4$

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This file contains solvent reservoir-density expansions for $\mathcal{B}_2$, $\mathcal{B}_3$, and $\mathcal{B}_4$. B_{ij} is the gas-phase virial coefficient for i solvent molecules and j solute molecules.

The B_{ij} and the solvent reservoir-density ρ_1 should be given in a mutually consistent set of units, which together determine the units of the calculated $\mathcal{B}_N$. For example, with B_{ij} given in units of $(liter/mol)^{(i+j-1)}$, and ρ_1 in units of $(mol/liter)$, $\mathcal{B}_N$ will be in units of $(liter/mol)^{(N-1)}$.

Second osmotic virial coefficient

$$\mathcal{B}_2 \;=\; B_{02} + A\rho_1 + B\rho_1^2 + C\rho_1^3 + D\rho_1^4 + E\rho_1^5 + F\rho_1^6 \tag{1a}$$

where $A, B, \ldots, F$ are defined as follows:

$$A \;=\; -2B_{11}^2 + (3B_{12})/2 \tag{1b}$$

$$B \;=\; 2(2B_{20}B_{11}^2 - 3B_{11}B_{21} + B_{22}) \tag{1c}$$

$$C \;=\; (-16B_{20}^2B_{11}^2 + 12B_{30}B_{11}^2 + 24B_{20}B_{11}B_{21} - 9B_{21}^2 - 16B_{11}B_{31} + 5B_{32})/2 \tag{1d}$$

$$
\begin{aligned}
D \;=\; & (-12B_{21}B_{31} - 10B_{11}B_{41} - (-8B_{20}^3 + 12B_{20}B_{30} - 4B_{40})(2B_{11}^2 - (3B_{12})/2) \\
& + 6B_{40}B_{12} - (4B_{20}^2 - 3B_{30})(6B_{11}B_{21} - 3B_{20}B_{12} - 2B_{22}) + 6B_{30}B_{22} \\
& + B_{20}(9B_{21}^2 + 16B_{11}B_{31} - 9B_{30}B_{12} - 8B_{20}B_{22} - 5B_{32}) + 5B_{20}B_{32} + 3B_{42})
\end{aligned}
\tag{1e}
$$

$$
\begin{aligned}
E \;=\; & ((-16B_{20}^4 + 36B_{20}^2B_{30} - 9B_{30}^2 - 16B_{20}B_{40} + 5B_{50})(2B_{11}^2 - (3B_{12})/2) - (-8B_{20}^3 \\
& + 12B_{20}B_{30} - 4B_{40})(6B_{11}B_{21} - 3B_{20}B_{12} - 2B_{22}) - ((4B_{20}^2 - 3B_{30})(9B_{21}^2 + 16B_{11}B_{31} \\
& - 9B_{30}B_{12} - 8B_{20}B_{22} - 5B_{32}))/2 + 2B_{20}(12B_{21}B_{31} + 10B_{11}B_{41} - 6B_{40}B_{12} \\
& - 6B_{30}B_{22} - 5B_{20}B_{32} - 3B_{42}) + (-16B_{31}^2 - 30B_{21}B_{41} - 24B_{11}B_{51} + 15B_{50}B_{12} \\
& + 16B_{40}B_{22} + 15B_{30}B_{32} + 12B_{20}B_{42} + 7B_{52})/2)
\end{aligned}
\tag{1f}
$$

$$F = (-20B_{31}B_{41} - 18B_{21}B_{51} - 14B_{11}B_{61} - (-32B_{20}^5 + 96B_{20}^3B_{30} - 54B_{20}B_{30}^2 - 48B_{20}^2B_{40}$$
$$+ 24B_{30}B_{40} + 20B_{20}B_{50} - 6B_{60})(2B_{11}^2 - (3B_{12})/2) + 9B_{60}B_{12} - (16B_{20}^4 - 36B_{20}^2B_{30}$$
$$+ 9B_{30}^2 + 16B_{20}B_{40} - 5B_{50})(6B_{11}B_{21} - 3B_{20}B_{12} - 2B_{22}) + 10B_{50}B_{22} - ((-8B_{20}^3$$
$$+ 12B_{20}B_{30} - 4B_{40})(9B_{21}^2 + 16B_{11}B_{31} - 9B_{30}B_{12} - 8B_{20}B_{22} - 5B_{32}))/2 + 10B_{40}B_{32}$$
$$- (4B_{20}^2 - 3B_{30})(12B_{21}B_{31} + 10B_{11}B_{41} - 6B_{40}B_{12} - 6B_{30}B_{22} - 5B_{20}B_{32} - 3B_{42})$$
$$+ 9B_{30}B_{42} + B_{20}(16B_{31}^2 + 30B_{21}B_{41} + 24B_{11}B_{51} - 15B_{50}B_{12} - 16B_{40}B_{22} - 15B_{30}B_{32}$$
$$- 12B_{20}B_{42} - 7B_{52}) + 7B_{20}B_{52} + 4B_{62}) \tag{1g}$$

Third osmotic virial coefficient

$$\mathcal{B}_3 = B_{03} + A\rho_1 + B\rho_1^2 + C\rho_1^3 + D\rho_1^4 + E\rho_1^5 \tag{2a}$$

where $A, B, \ldots, E$ are defined as follows:

$$A = 2(4B_{11}^3 - 9B_{11}B_{12} + 4B_{13})/3 \tag{2b}$$

$$B = (-16B_{20}B_{11}^3 + 24B_{11}^2B_{21} + 12B_{20}B_{11}B_{12} - 9B_{21}B_{12} - 16B_{11}B_{22} + 5B_{23}) \tag{2c}$$

$$C = 2(32B_{20}^2B_{11}^3 - 16B_{30}B_{11}^3 - 60B_{20}B_{11}^2B_{21} + 27B_{11}B_{21}^2 + 24B_{11}^2B_{31} - 12B_{20}^2B_{11}B_{12}$$
$$+ 9B_{30}B_{11}B_{12} + 9B_{20}B_{21}B_{12} - 6B_{31}B_{12} + 16B_{20}B_{11}B_{22} - 12B_{21}B_{22} - 15B_{11}B_{32}$$
$$+ 4B_{33}) \tag{2d}$$

$$D = (-640B_{20}^3B_{11}^3 + 720B_{20}B_{30}B_{11}^3 - 160B_{40}B_{11}^3 + 1296B_{20}^2B_{11}^2B_{21} - 648B_{30}B_{11}^2B_{21}$$
$$- 756B_{20}B_{11}B_{21}^2 + 108B_{21}^3 - 672B_{20}B_{11}^2B_{31} + 576B_{11}B_{21}B_{31} + 240B_{11}^2B_{41}$$
$$+ 144B_{20}^3B_{11}B_{12} - 216B_{20}B_{30}B_{11}B_{12} + 72B_{40}B_{11}B_{12} - 108B_{20}^2B_{21}B_{12}$$
$$+ 81B_{30}B_{21}B_{12} + 72B_{20}B_{31}B_{12} - 45B_{41}B_{12} - 192B_{20}^2B_{11}B_{22} + 144B_{30}B_{11}B_{22}$$
$$+ 144B_{20}B_{21}B_{22} - 96B_{31}B_{22} + 180B_{20}B_{11}B_{32} - 135B_{21}B_{32} - 144B_{11}B_{42} + 35B_{43})/3 \tag{2e}$$

$$E = 2(320B_{20}^4 B_{11}^3 - 576B_{20}^2 B_{30} B_{11}^3 + 108B_{30}^2 B_{11}^3 + 192B_{20} B_{40} B_{11}^3 - 40B_{50} B_{11}^3$$
$$- 672B_{20}^3 B_{11}^2 B_{21} + 756B_{20} B_{30} B_{11}^2 B_{21} - 168B_{40} B_{11}^2 B_{21} + 432B_{20}^2 B_{11} B_{21}^2$$
$$- 216B_{30} B_{11} B_{21}^2 - 81B_{20} B_{21}^3 + 384B_{20}^2 B_{11}^2 B_{31} - 192B_{30} B_{11}^2 B_{31}$$
$$- 432B_{20} B_{11} B_{21} B_{31} + 90B_{21}^2 B_{31} + 80B_{11} B_{31}^2 - 180B_{20} B_{11}^2 B_{41} + 150B_{11} B_{21} B_{41}$$
$$+ 60B_{11}^2 B_{51} - 48B_{20}^4 B_{11} B_{12} + 108B_{20}^2 B_{30} B_{11} B_{12} - 27B_{30}^2 B_{11} B_{12} - 48B_{20} B_{40} B_{11} B_{12}$$
$$+ 15B_{50} B_{11} B_{12} + 36B_{20}^3 B_{21} B_{12} - 54B_{20} B_{30} B_{21} B_{12} + 18B_{40} B_{21} B_{12} - 24B_{20}^2 B_{31} B_{12}$$
$$+ 18B_{30} B_{31} B_{12} + 15B_{20} B_{41} B_{12} - 9B_{51} B_{12} + 64B_{20}^3 B_{11} B_{22} - 96B_{20} B_{30} B_{11} B_{22}$$
$$+ 32B_{40} B_{11} B_{22} - 48B_{20}^2 B_{21} B_{22} + 36B_{30} B_{21} B_{22} + 32B_{20} B_{31} B_{22} - 20B_{41} B_{22}$$
$$- 60B_{20}^2 B_{11} B_{32} + 45B_{30} B_{11} B_{32} + 45B_{20} B_{21} B_{32} - 30B_{31} B_{32} + 48B_{20} B_{11} B_{42}$$
$$- 36B_{21} B_{42} - 35B_{11} B_{52} + 8B_{53}) \tag{2f}$$

Fourth osmotic virial coefficient

$$\mathcal{B}_4 = B_{04} + A\rho_1 + B\rho_1^2 + C\rho_1^3 + D\rho_1^4 \tag{3a}$$

where $A, \ldots, D$ are defined as follows:

$$A = -2B_{11}^4 + 9B_{11}^2 B_{12} - 8B_{11} B_{13} - \frac{27}{8} B_{12}^2 + \frac{15}{4} B_{14} \tag{3b}$$

$$B = (56B_{20} B_{11}^4 - 108B_{20} B_{11}^2 B_{12} + 32B_{20} B_{11} B_{13} + \frac{27}{2} B_{20} B_{12}^2 - 96B_{11}^3 B_{21}$$
$$+ 96B_{11}^2 B_{22} + 108B_{11} B_{21} B_{12} - 60B_{11} B_{23} - 24B_{21} B_{13} - 36B_{12} B_{22} + 18B_{24})/2 \tag{3c}$$

$$C = (-1200B_{20}^2 B_{11}^4 + 1296B_{20}^2 B_{11}^2 B_{12} - 192B_{20}^2 B_{11} B_{13} - 81B_{20}^2 B_{12}^2 + 2736B_{20} B_{11}^3 B_{21}$$
$$- 1440B_{20} B_{11}^2 B_{22} - 1620B_{20} B_{11} B_{21} B_{12} + 360B_{20} B_{11} B_{23} + 144B_{20} B_{21} B_{13}$$
$$+ 216B_{20} B_{12} B_{22} + 468B_{30} B_{11}^4 - 648B_{30} B_{11}^2 B_{12} + 144B_{30} B_{11} B_{13} + \frac{243}{4} B_{30} B_{12}^2$$
$$- 864B_{11}^3 B_{31} - 1458B_{11}^2 B_{21}^2 + 810B_{11}^2 B_{32} + 1296B_{11} B_{21} B_{22} + 648B_{11} B_{31} B_{12}$$
$$- 432B_{11} B_{33} + \frac{729}{2} B_{21}^2 B_{12} - 270B_{21} B_{23} - 96B_{31} B_{13} - \frac{405}{2} B_{12} B_{32} - 144B_{22}^2$$
$$+ 105B_{34})/6 \tag{3d}$$

$$
\begin{aligned}
D &= (24960B_{20}^3B_{11}^4 - 14400B_{20}^3B_{11}^2B_{12} + 768B_{20}^3B_{11}B_{13} + 432B_{20}^3B_{12}^2 - 60480B_{20}^2B_{11}^3B_{21} \\
&\quad + 18432B_{20}^2B_{11}^2B_{22} + 16200B_{20}^2B_{11}B_{21}B_{12} - 1440B_{20}^2B_{11}B_{23} - 576B_{20}^2B_{21}B_{13} \\
&\quad - 1152B_{20}^2B_{12}B_{22} - 23040B_{20}B_{30}B_{11}^4 + 16200B_{20}B_{30}B_{11}^2B_{12} - 1152B_{20}B_{30}B_{11}B_{13} \\
&\quad - 648B_{20}B_{30}B_{12}^2 + 26880B_{20}B_{11}^3B_{31} + 44064B_{20}B_{11}^2B_{21}^2 - 14040B_{20}B_{11}^2B_{32} \\
&\quad - 19008B_{20}B_{11}B_{21}B_{22} - 7200B_{20}B_{11}B_{31}B_{12} + 1728B_{20}B_{11}B_{33} - 4050B_{20}B_{21}^2B_{12} \\
&\quad + 1080B_{20}B_{21}B_{23} + 384B_{20}B_{31}B_{13} + 1080B_{20}B_{12}B_{32} + 768B_{20}B_{22}^2 + 23112B_{30}B_{11}^3B_{21} \\
&\quad - 9216B_{30}B_{11}^2B_{22} - 8100B_{30}B_{11}B_{21}B_{12} + 1080B_{30}B_{11}B_{23} + 432B_{30}B_{21}B_{13} \\
&\quad + 864B_{30}B_{12}B_{22} + 4032B_{40}B_{11}^4 - 3600B_{40}B_{11}^2B_{12} + 384B_{40}B_{11}B_{13} + 216B_{40}B_{12}^2 \\
&\quad - 7320B_{11}^3B_{41} - 25200B_{11}^2B_{21}B_{31} + 6624B_{11}^2B_{42} - 9234B_{11}B_{21}^3 + 11610B_{11}B_{21}B_{32} \\
&\quad - 36B_{11}B_{21}(16B_{20}^2B_{11}^2 - 24B_{20}B_{11}B_{21} - 12B_{30}B_{11}^2 + 16B_{11}B_{31} + 9B_{21}^2 - 5B_{32}) \\
&\quad + 6B_{11}B_{21}(12B_{20}^2B_{12} + 32B_{20}B_{22} + 12B_{30}B_{11}^2 + 18B_{30}B_{12} - 24B_{11}(B_{20}B_{21} + 2B_{31}) \\
&\quad - 27B_{21}^2 + 15B_{32}) + 6528B_{11}B_{31}B_{22} + 2250B_{11}B_{41}B_{12} - 3360B_{11}B_{43} + 3240B_{21}^2B_{22} \\
&\quad + 2700B_{21}B_{31}B_{12} - 648B_{21}B_{33} - 720B_{31}B_{23} - 240B_{41}B_{13} - 864B_{12}B_{42} \\
&\quad - 6B_{12}(-108B_{20}B_{21}^2 + 144B_{21}B_{31}) + 18B_{12}(2B_{11}(-32B_{20}B_{31} + B_{21}(36B_{20}^2 - 18B_{30}) \\
&\quad + 15B_{41}) + 12B_{21}B_{31} + 3B_{21}(-12B_{20}B_{21} + 8B_{31})) + 12B_{12}(3B_{11}(-32B_{20}B_{31} \\
&\quad + B_{21}(36B_{20}^2 - 18B_{30}) + 15B_{41}) + 54B_{21}B_{31} + 9B_{21}(-12B_{20}B_{21} + 8B_{31})) \\
&\quad - 3B_{12}(32B_{20}^2B_{22} + 4B_{20}(9B_{30}B_{12} - 9B_{21}^2 + 15B_{32}) + 48B_{30}B_{22} + 32B_{40}B_{11}^2 \\
&\quad + 24B_{40}B_{12} - 8B_{11}(8B_{20}B_{31} + 10B_{41}) - 96B_{21}B_{31} + 24B_{42}) - 48B_{12}(16B_{20}^3B_{11}^2 \\
&\quad - 24B_{20}^2B_{11}B_{21} - 24B_{20}B_{30}B_{11}^2 + 16B_{20}B_{11}B_{31} + 9B_{20}B_{21}^2 + 18B_{30}B_{11}B_{21} + 8B_{40}B_{11}^2 \\
&\quad - 10B_{11}B_{41} - 12B_{21}B_{31} + 3B_{42}) - 1440B_{22}B_{32} + 6B_{22}(8B_{11}(-12B_{20}B_{21} + 8B_{31}) + 36B_{21}^2) \\
&\quad + 12B_{22}(8B_{11}(-12B_{20}B_{21} + 8B_{31}) + 72B_{21}^2) + 6B_{13}(-64B_{20}B_{31} + 4B_{21}(12B_{20}^2 - 9B_{30}) \\
&\quad + 60B_{41}) - 12B_{13}(-48B_{20}B_{31} + 4B_{11}(-8B_{20}^3 + 12B_{20}B_{30} - 4B_{40}) + 4B_{21}(12B_{20}^2 - 9B_{30}) \\
&\quad + 40B_{41}) - 24B_{13}(-8B_{20}B_{31} + B_{11}(-16B_{20}^3 + 24B_{20}B_{30} - 8B_{40}) + B_{21}(12B_{20}^2 - 9B_{30}) \\
&\quad + 5B_{41}) + 6B_{23}(-90B_{20}B_{21} + 120B_{31}) - 12B_{23}(-90B_{20}B_{21} + 15B_{11}(4B_{20}^2 - 3B_{30}) \\
&\quad + 90B_{31}) - 18B_{23}(-30B_{20}B_{21} + 5B_{11}(8B_{20}^2 - 6B_{30}) + 20B_{31}) + 6B_{33}(-96B_{20}B_{11} \\
&\quad + 72B_{21}) - 12B_{33}(-72B_{20}B_{11} + 108B_{21}) - 24B_{33}(-60B_{20}B_{11} + 45B_{21}) + 720B_{44} \\
&\quad + (-4B_{11}^2 + 3B_{12})(2B_{11}(-64B_{20}B_{31} + B_{21}(120B_{20}^2 - 36B_{30}) + 15B_{41}) + 12B_{21}B_{31} \\
&\quad + 3B_{21}(-24B_{20}B_{21} + 8B_{31})) + 2(-4B_{11}^2 + 3B_{12})(2B_{11}(-32B_{20}B_{31} + B_{21}(36B_{20}^2 - 18B_{30}) \\
&\quad + 15B_{41}) + 12B_{21}B_{31} + 3B_{21}(-12B_{20}B_{21} + 8B_{31})) - 1(-4B_{11}^2 + 3B_{12})(-90B_{20}B_{32} \\
&\quad + B_{12}(-240B_{20}^3 + 216B_{20}B_{30} - 36B_{40}) + B_{22}(192B_{20}^2 - 72B_{30}) + 24B_{42}) - 2(-4B_{11}^2 \\
&\quad + 3B_{12})(-30B_{20}B_{32} + B_{12}(-24B_{20}^3 + 36B_{20}B_{30} - 12B_{40}) + B_{22}(32B_{20}^2 - 24B_{30}) + 24B_{42}) \\
&\quad - 1(-18B_{20}B_{12} + 8B_{22})(12B_{20}^2B_{12} + 32B_{20}B_{22} + 12B_{30}B_{11}^2 + 18B_{30}B_{12} - 24B_{11}(B_{20}B_{21} \\
&\quad + 2B_{31}) - 27B_{21}^2 + 15B_{32}) - 2(18B_{20}B_{12} - 24B_{22})(16B_{20}^2B_{11}^2 - 24B_{20}B_{11}B_{21} - 12B_{30}B_{11}^2 \\
&\quad + 16B_{11}B_{31} + 9B_{21}^2 - 5B_{32}) - 1(8B_{11}(-24B_{20}B_{21} + 8B_{31}) + 36B_{21}^2)(-3B_{20}B_{12} + 6B_{11}B_{21} \\
&\quad - 2B_{22}) + 2(16B_{11}(-12B_{20}B_{21} + 8B_{31}) + 72B_{21}^2)(2B_{20}B_{11}^2 - 3B_{11}B_{21} + B_{22}) - 2(16B_{20}B_{11}^2 - 24B_{11}B_{21} \\
&\quad + 8B_{22})(-16B_{20}B_{22} + B_{12}(12B_{20}^2 - 9B_{30}) + 15B_{32}) + (-12B_{20}B_{12} + 24B_{11}B_{21} - 8B_{22})(-48B_{20}B_{22} \\
&\quad + B_{12}(72B_{20}^2 - 27B_{30}) + 15B_{32}))/24 \qquad \text{S4}
\end{aligned}
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(3e)