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List of publications

The work presented in this thesis is published as

- Gorrey, R. P., Jindal, V., Sarma, B. N., and Lele, S. (2020). Analytical Solutions for the Correlation Functions of Perfectly Ordered Binary Phases based on BCC, FCC and CPH Structures using Cluster Variation Method. *Calphad*, **71**, 101773. https://doi.org/10.1016/j.calphad.2020.101773

- Gorrey, R. P., Jindal, V., Sarma, B. N., and Lele, S. (2021). Polynomial Functions for Configurational Correlation Functions in Gibbs Energies of Solid Solutions using Cluster Variation Method. *Comp. Mater. Sci.*, **186**, 109746. https://doi.org/10.1016/j.commatsci.2020.109746

- Gorrey, R. P., Jindal, V., Sarma, B. N., and Lele, S. (2021). Modification of Cluster Variation Method Entropy Functional for Binary FCC Phases using Tetrahedron Approximation. *T Indian I Metals*, **74**(1), 129136. https://doi.org/10.1007/s12666-020-02119-z

Appendix A

Thermodynamics of ordered phases in the limit of perfect ordering

A.1 BCC based ordered phases

A.1.1 Thermodynamics of $B32$ phase using tetrahedron approximation

The tetrahedron cluster considered for $B32$ phase is shown in Figure A.1 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.1.

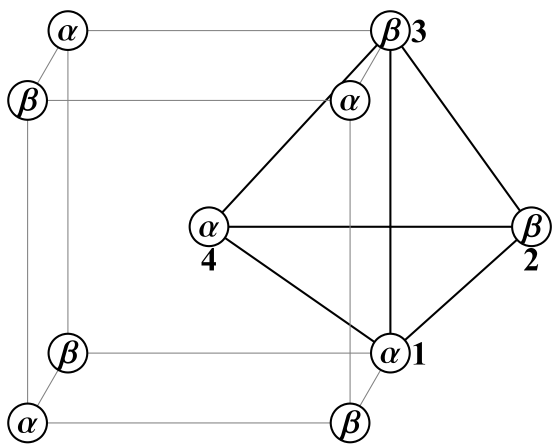

Figure A.1: The irregular tetrahedron basic cluster in $B32$ phase along with the sublattice sites designated α and β.

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2})/2 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Table A.1: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $B32$ phase using tetrahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Irregular tetrahedron	$\alpha\alpha\beta\beta$ (1,4,2,3)	4.1	1	1
Isosceles triangle	$\alpha\beta\beta$ (1,2,3)	3.2	6	-1
	$\alpha\alpha\beta$ (1,4,2)	3.1	6	
II-n pair	$\alpha\beta$ (1,3)	2.1	3	1
I-n pair	$\beta\beta$ (2,3)	1.3	1	1
	$\alpha\beta$ (1,2)	1.2	2	
	$\alpha\alpha$ (1,4)	1.1	1	
point	β (2)	0.2	1/2	-1
	α (1)	0.1	1/2	

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \eta_1\eta_3^3\eta_4^{3/2}; \qquad v^0_{1.2} = \frac{\eta_4^{3/2}}{\eta_1}; \qquad v^0_{1.3} = \frac{\eta_1\eta_4^{3/2}}{\eta_3^3}; \qquad v^0_{2.1} = \frac{\eta_4}{\eta_2}$$

$$v^0_{3.1} = \frac{\eta_3^2\eta_4^3}{\eta_2}; \qquad v^0_{3.2} = \frac{\eta_4^3}{\eta_2\eta_3^2}; \qquad v^0_{4.1} = \frac{\eta_4^5}{\eta_2^2}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = -v^0_{1.1}\left(2 + v^0_{1.1} - 3v^0_{1.2} - 3v^0_{2.1}\right) - 3v^0_{3.1}$$

$$v^0_{(1.2)0} = \frac{3}{2}v^0_{1.2}\left(-v^0_{1.1} + v^0_{1.3}\right) + 3\frac{v^0_{3.1} - v^0_{3.2}}{2}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(2 - 3v^0_{1.2} + v^0_{1.3} - 3v^0_{2.1}\right) + 3v^0_{3.2}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(-v^0_{1.1} + v^0_{1.3}\right) + v^0_{3.1} - v^0_{3.2}$$

$$v^0_{(3.1)0} = \frac{v^0_{3.1}}{2}\left(-3 - 5v^0_{1.1} + 4v^0_{1.2} + 3v^0_{1.3} + 4v^0_{2.1} - 3\frac{v^0_{3.1}}{v^0_{1.1}} + \frac{2v^0_{3.1} - v^0_{3.2}}{v^0_{1.2}} + \frac{v^0_{3.1}}{v^0_{2.1}}\right) - v^0_{4.1}$$

$$v^0_{(3.2)0} = \frac{v^0_{3.2}}{2}\left(3 - 3v^0_{1.1} - 4v^0_{1.2} + 5v^0_{1.3} - 4v^0_{2.1} + \frac{v^0_{3.1} - 2v^0_{3.2}}{v^0_{1.2}} + 3\frac{v^0_{3.2}}{v^0_{1.3}} - \frac{v^0_{3.2}}{v^0_{2.1}}\right) + v^0_{4.1}$$

$$v^0_{(4.1)0} = v^0_{4.1}\left(-3v^0_{1.1} + 3v^0_{1.3} - \frac{v^0_{3.1}}{v^0_{1.1}} + \frac{v^0_{3.1} - v^0_{3.2}}{v^0_{1.2}} + \frac{v^0_{3.2}}{v^0_{1.3}} - \frac{v^0_{4.1}}{v^0_{3.1}} + \frac{v^0_{4.1}}{v^0_{3.2}}\right)$$

and

$$v^0_{(1.1)\xi} = v^0_{1.1}\left(-4 + v^0_{1.1} + 3v^0_{1.2} + 3v^0_{3.1}\right) - 3v^0_{3.1}$$
$$v^0_{(1.2)\xi} = \frac{v^0_{1.2}}{2}\left(-8 + 3v^0_{1.1} + 2v^0_{1.2} + 3v^0_{1.3} + 6v^0_{2.1}\right) - 3\frac{v^0_{3.1} + v^0_{3.2}}{2}$$
$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-4 + 3v^0_{1.2} + v^0_{1.3} + 3v^0_{2.1}\right) - 3v^0_{3.2}$$
$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-3 + v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + v^0_{2.1}\right) - v^0_{3.1} - v^0_{3.2}$$
$$v^0_{(3.1)\xi} = \frac{v^0_{3.1}}{2}\left(-17 + 5v^0_{1.1} + 8v^0_{1.2} + 3v^0_{1.3} + 10v^0_{2.1} - 3\frac{v^0_{3.1}}{v^0_{1.1}} - \frac{2v^0_{3.1} + v^0_{3.2}}{v^0_{1.2}} - \frac{v^0_{3.1}}{v^0_{2.1}}\right) - v^0_{4.1}$$
$$v^0_{(3.2)\xi} = \frac{v^0_{3.2}}{2}\left(-17 + 3v^0_{1.1} + 8v^0_{1.2} + 5v^0_{1.3} + 10v^0_{2.1} - \frac{v^0_{3.1} + 2v^0_{3.2}}{v^0_{1.2}} - 3\frac{v^0_{3.2}}{v^0_{1.3}} - \frac{v^0_{3.2}}{v^0_{2.1}}\right) - v^0_{4.1}$$
$$v^0_{(4.1)\xi} = v^0_{4.1}\left(-14 + 3v^0_{1.1} + 6v^0_{1.2} + 3v^0_{1.3} + 8v^0_{2.1} - \frac{v^0_{3.1}}{v^0_{1.1}} - \frac{v^0_{3.1} + v^0_{3.2}}{v^0_{1.2}} - \frac{v^0_{3.2}}{v^0_{1.3}} - \frac{v^0_{4.1}}{v^0_{3.1}} - \frac{v^0_{4.1}}{v^0_{3.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = 1$; $u^0_{1.2} = -1$; $u^0_{1.3} = 1$; $u^0_{2.1} = -1$
$u^0_{3.1} = 1$; $u^0_{3.2} = -1$; $u^0_{4.1} = 1$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = -2$; $u^0_{(1.2)0} = 0$; $u^0_{(1.3)0} = 2$; $u^0_{(2.1)0} = 0$
$u^0_{(3.1)0} = -1$; $u^0_{(3.2)0} = -1$; $u^0_{(4.1)0} = 0$
$u^0_{(1.1)\xi} = 2$; $u^0_{(1.2)\xi} = -2$; $u^0_{(1.3)\xi} = 2$; $u^0_{(2.1)\xi} = -2$
$u^0_{(3.1)\xi} = 3$; $u^0_{(3.2)\xi} = -3$; $u^0_{(4.1)\xi} = 4$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi 0}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1}$; $u^0_{(1.2)00} = 2v^0_{1.2}$; $u^0_{(1.3)00} = 2v^0_{1.3}$
$u^0_{(2.1)00} = 2v^0_{2.1}$; $u^0_{(3.1)00} = 2v^0_{1.1} - 2v^0_{1.2} - 2v^0_{2.1}$; $u^0_{(3.2)00} = 2v^0_{1.2} - 2v^0_{1.3} + 2v^0_{2.1}$
$u^0_{(4.1)00} = 2v^0_{1.1} - 4v^0_{1.2} + 2v^0_{1.3} - 4v^0_{2.1}$
$u^0_{(1.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(1.2)\xi 0} = 0$; $u^0_{(1.3)\xi 0} = 2v^0_{1.3}$
$u^0_{(2.1)\xi 0} = 0$; $u^0_{(3.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(3.2)\xi 0} = -2v^0_{1.3}$
$u^0_{(4.1)\xi 0} = 2v^0_{1.3} - 2v^0_{1.1}$

and

$u^0_{(1.1)\xi\xi} = 2v^0_{1.1}$; $u^0_{(1.2)\xi\xi} = -2v^0_{1.2}$; $u^0_{(1.3)\xi\xi} = 2v^0_{1.3}$
$u^0_{(2.1)\xi\xi} = -2v^0_{2.1}$; $u^0_{(3.1)\xi\xi} = 2v^0_{1.1} + 2v^0_{1.2} + 2v^0_{2.1}$; $u^0_{(3.2)\xi\xi} = -2v^0_{1.2} - 2v^0_{1.3} - 2v^0_{2.1}$
$u^0_{(4.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 4v^0_{2.1}$

A.1.2 Thermodynamics of $D0_3$ phase using tetrahedron approximation

The tetrahedron cluster considered for $D0_3$ phase is shown in Figure A.2 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.2.

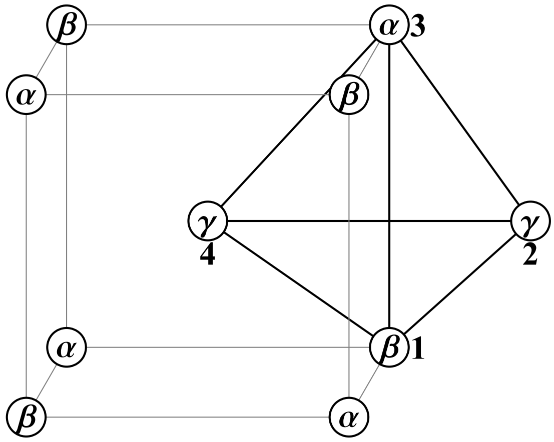

Figure A.2: The irregular tetrahedron basic cluster in $D0_3$ phase along with the sublattice sites designated α, β and γ.

Table A.2: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $D0_3$ phase using tetrahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Irregular tetrahedron	$\alpha\beta\gamma\gamma$ (3,1,2,4)	4.1	6	1
Isosceles triangle	$\beta\gamma\gamma$ (1,2,4)	3.3	3	-1
	$\alpha\gamma\gamma$ (3,2,4)	3.2	3	
	$\alpha\beta\gamma$ (3,1,2)	3.1	6	
II-n pair	$\gamma\gamma$ (2,4)	2.2	3/2	1
	$\alpha\beta$ (3,1)	2.1	3/2	
I-n pair	$\beta\gamma$ (1,2)	1.2	2	1
	$\alpha\gamma$ (3,2)	1.1	2	

cont...

cont...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Point	γ (2)	0.3	1/2	-1
	β (1)	0.2	1/4	
	α (2)	0.1	1/4	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2} + 2u_{0.3})/4, \xi_1 = (2u_{0.3} - u_{0.2} - u_{0.1})/4 \text{ and } \xi_2 = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{1}{\eta_1\eta_3^3\eta_4^{3/2}}; \quad v^0_{1.2} = \frac{\eta_1}{\eta_4^{3/2}}; \quad v^0_{2.1} = \frac{1}{\eta_2\eta_3^2\eta_4}; \quad v^0_{2.2} = \frac{\eta_2}{\eta_4}$$

$$v^0_{3.1} = \frac{1}{\eta_2\eta_3^4\eta_4^3}; \quad v^0_{3.2} = \frac{\eta_2}{\eta_1^2\eta_3^5\eta_4^3}; \quad v^0_{3.3} = \frac{\eta_1^2\eta_2}{\eta_3\eta_4^3}; \quad v^0_{4.1} = \frac{1}{\eta_3^6\eta_4^5}$$

The limiting first derivatives of the transformed CFs with respect to u_0, ξ_1 and ξ_2, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi_k}$, are:

$$v^0_{(1.1)0} = \frac{3}{2}v^0_{1.1}\left(-2 + v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2}\right) - 3\frac{v^0_{3.1} + v^0_{3.2}}{2}$$

$$v^0_{(1.2)0} = \frac{v^0_{1.2}}{2}\left(-2 - 3v^0_{1.1} + 5v^0_{1.2} - 3v^0_{2.1} + 3v^0_{2.2}\right) + 3\frac{v^0_{3.1} - v^0_{3.3}}{2}$$

$$v^0_{(2.1)0} = 2v^0_{2.1}\left(-1 + v^0_{1.1} + v^0_{1.2}\right) - 2v^0_{3.1}$$

$$v^0_{(2.2)0} = v^0_{2.2}\left(-1 - 2v^0_{1.1} + 2v^0_{1.2} + v^0_{2.2}\right) + v^0_{3.2} - v^0_{3.3}$$

$$v^0_{(3.1)0} = \frac{v^0_{3.1}}{2}\left(-9 + 2v^0_{1.1} + 8v^0_{1.2} + 4v^0_{2.2} - \frac{2v^0_{3.1} + v^0_{3.2}}{v^0_{1.1}} + \frac{2v^0_{3.1} - v^0_{3.3}}{v^0_{1.2}} - \frac{v^0_{3.1}}{v^0_{2.1}}\right) - v^0_{4.1}$$

$$v^0_{(3.2)0} = \frac{v^0_{3.2}}{2}\left(-11 + 2v^0_{1.1} + 6v^0_{1.2} + 4v^0_{2.1} + 6v^0_{2.2} - \frac{2v^0_{3.1} + 4v^0_{3.2}}{v^0_{1.1}} + \frac{v^0_{3.2}}{v^0_{2.2}}\right) - v^0_{4.1}$$

$$v^0_{(3.3)0} = v^0_{3.3}\left(-\frac{5}{2} - 3v^0_{1.1} + 5v^0_{1.2} - 2v^0_{2.1} + 3v^0_{2.2} + \frac{v^0_{3.1} - 2v^0_{3.3}}{v^0_{1.2}} - \frac{v^0_{3.3}}{2v^0_{2.2}}\right) + v^0_{4.1}$$

$$v^0_{(4.1)0} = v^0_{4.1}\left(-7 + 6v^0_{1.2} + 4v^0_{2.2} - \frac{v^0_{3.1} + v^0_{3.2}}{v^0_{1.1}} + \frac{v^0_{3.1} - v^0_{3.3}}{v^0_{1.2}} - \frac{v^0_{4.1}}{v^0_{3.1}} - \frac{v^0_{4.1}}{2v^0_{3.2}} + \frac{v^0_{4.1}}{2v^0_{3.3}}\right)$$

$$v^0_{(1.1)\xi_1} = \frac{v^0_{1.1}}{2}\left(-2 + 5v^0_{1.1} - 3v^0_{1.2} - 3v^0_{2.1} + 3v^0_{2.2}\right) + 3\frac{v^0_{3.1} - v^0_{3.2}}{2}$$
$$v^0_{(1.2)\xi_1} = \frac{3}{2}v^0_{1.2}\left(-2 + v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2}\right) - 3\frac{v^0_{3.1} + v^0_{3.3}}{2}$$
$$v^0_{(2.1)\xi_1} = 2v^0_{2.1}\left(-1 + v^0_{1.1} + v^0_{1.2}\right) - 2v^0_{3.1}$$
$$v^0_{(2.2)\xi_1} = v^0_{2.2}\left(-1 + 2v^0_{1.1} - 2v^0_{1.2} + v^0_{2.2}\right) - v^0_{3.2} + v^0_{3.3}$$
$$v^0_{(3.1)\xi_1} = v^0_{3.1}\left(-\frac{9}{2} + 4v^0_{1.1} + v^0_{1.2} + 2v^0_{2.2} + \frac{2v^0_{3.1} - v^0_{3.2}}{2v^0_{1.1}} - \frac{2v^0_{3.1} + v^0_{3.3}}{2v^0_{1.2}} - \frac{v^0_{3.1}}{2v^0_{2.1}}\right) - v^0_{4.1}$$
$$v^0_{(3.2)\xi_1} = v^0_{3.2}\left(-\frac{5}{2} + 5v^0_{1.1} - 3v^0_{1.2} - 2v^0_{2.1} + 3v^0_{2.2} + \frac{v^0_{3.1} - 2v^0_{3.2}}{v^0_{1.1}} - \frac{v^0_{3.2}}{2v^0_{2.2}}\right) + v^0_{4.1}$$
$$v^0_{(3.3)\xi_1} = \frac{v^0_{3.3}}{2}\left(-11 + 6v^0_{1.1} + 2v^0_{1.2} + 4v^0_{2.1} + 6v^0_{2.2} - \frac{2v^0_{3.1} + 4v^0_{3.3}}{v^0_{1.2}} + \frac{v^0_{3.3}}{v^0_{2.2}}\right) - v^0_{4.1}$$
$$v^0_{(4.1)\xi_1} = v^0_{4.1}\left(-7 + 6v^0_{1.1} + 4v^0_{2.2} + \frac{v^0_{3.1} - v^0_{3.2}}{v^0_{1.1}} - \frac{v^0_{3.1} + v^0_{3.3}}{v^0_{1.2}} - \frac{v^0_{4.1}}{v^0_{3.1}} + \frac{v^0_{4.1}}{2v^0_{3.2}} - \frac{v^0_{4.1}}{2v^0_{3.3}}\right)$$

and

$$v^0_{(1.1)\xi_2} = \frac{v^0_{1.1}}{2}\left(-4 + v^0_{1.1} + 3v^0_{1.2} + 3v^0_{2.1}\right) - \frac{3}{2}v^0_{3.1}$$
$$v^0_{(1.2)\xi_2} = \frac{v^0_{1.2}}{2}\left(-4 + 3v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1}\right) - \frac{3}{2}v^0_{3.1}$$
$$v^0_{(2.1)\xi_2} = v^0_{2.1}\left(-1 + v^0_{2.1}\right)$$
$$v^0_{(2.2)\xi_2} = 2v^0_{2.2}\left(-1 + v^0_{1.1} + v^0_{1.2}\right) - v^0_{3.2} - v^0_{3.3}$$
$$v^0_{(3.1)\xi_2} = v^0_{3.1}\left(-4 + \frac{3}{2}v^0_{1.1} + \frac{3}{2}v^0_{1.2} + 3v^0_{2.1} - \frac{v^0_{3.1}}{v^0_{1.1}} - \frac{v^0_{3.1}}{v^0_{1.2}}\right)$$
$$v^0_{(3.2)\xi_2} = v^0_{3.2}\left(-\frac{9}{2} + 2v^0_{1.1} + 3v^0_{1.2} + 2v^0_{2.1} - \frac{v^0_{3.1}}{v^0_{1.1}} - \frac{v^0_{3.2}}{2v^0_{2.2}}\right) - v^0_{4.1}$$
$$v^0_{(3.3)\xi_2} = v^0_{3.3}\left(-\frac{9}{2} + 3v^0_{1.1} + 2v^0_{1.2} + 2v^0_{2.1} - \frac{v^0_{3.1}}{v^0_{1.2}} - \frac{v^0_{3.3}}{2v^0_{2.2}}\right) - v^0_{4.1}$$
$$v^0_{(4.1)\xi_2} = v^0_{4.1}\left(-7 + 3v^0_{1.1} + 3v^0_{1.2} + 4v^0_{2.1} - \frac{v^0_{3.1}}{v^0_{1.1}} - \frac{v^0_{3.1}}{v^0_{1.2}} - \frac{v^0_{4.1}}{2v^0_{3.2}} - \frac{v^0_{4.1}}{2v^0_{3.3}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = -1$; $u^0_{1.2} = 1$; $u^0_{2.1} = -1$; $u^0_{2.2} = 1$
$u^0_{3.1} = -1$; $u^0_{3.2} = -1$; $u^0_{3.3} = 1$; $u^0_{4.1} = -1$

The limiting first derivatives of the CFs with respect to u_0, ξ_1 and ξ_2, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = \ \ 0;$ $u^0_{(1.2)0} = \ \ 2;$ $u^0_{(2.1)0} = \ \ 0;$ $u^0_{(2.2)0} = \ \ 2$

$u^0_{(3.1)0} = -1;$ $u^0_{(3.2)0} = -1;$ $u^0_{(3.3)0} = \ \ 3;$ $u^0_{(4.1)0} = -2$

$u^0_{(1.1)\xi_1} = -2;$ $u^0_{(1.2)\xi_1} = \ \ 0;$ $u^0_{(2.1)\xi_1} = \ \ 0;$ $u^0_{(2.2)\xi_1} = \ \ 2$

$u^0_{(3.1)\xi_1} = -1;$ $u^0_{(3.2)\xi_1} = -3;$ $u^0_{(3.3)\xi_1} = \ \ 1;$ $u^0_{(4.1)\xi_1} = -2$

$u^0_{(1.1)\xi_2} = -1;$ $u^0_{(1.2)\xi_2} = \ \ 1;$ $u^0_{(2.1)\xi_2} = -2;$ $u^0_{(2.2)\xi_2} = \ \ 0$

$u^0_{(3.1)\xi_2} = -2;$ $u^0_{(3.2)\xi_2} = -1;$ $u^0_{(3.3)\xi_2} = \ \ 1;$ $u^0_{(4.1)\xi_2} = -2$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi_1 0}$, $u^0_{(i.j)\xi_2 0}$, $u^0_{(i.j)\xi_1\xi_1}$ and $u^0_{(i.j)\xi_2\xi_2}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1};$ $u^0_{(1.2)00} = 2v^0_{1.2};$ $u^0_{(2.1)00} = 2v^0_{2.1}$

$u^0_{(2.2)00} = 2v^0_{2.2};$ $u^0_{(3.1)00} = 2v^0_{1.1} - 2v^0_{1.2} + 2v^0_{2.1};$ $u^0_{(3.2)00} = 4v^0_{1.1} - 2v^0_{2.2}$

$u^0_{(3.3)00} = 4v^0_{1.2} + 2v^0_{2.2};$ $u^0_{(4.1)00} = 4v^0_{1.1} - 4v^0_{1.2} + 2v^0_{2.1} - 2v^0_{2.2}$

$u^0_{(1.1)\xi_1 0} = 0;$ $u^0_{(1.2)\xi_1 0} = 0;$ $u^0_{(2.1)\xi_1 0} = -\,2v^0_{2.1}$

$u^0_{(2.2)\xi_1 0} = 2v^0_{2.2};$ $u^0_{(3.1)\xi_1 0} = -\,2v^0_{2.1};$ $u^0_{(3.2)\xi_1 0} = -\,2v^0_{2.2}$

$u^0_{(3.3)\xi_1 0} = 2v^0_{2.2};$ $u^0_{(4.1)\xi_1 0} = -\,2v^0_{2.1} - 2v^0_{2.2}$

$u^0_{(1.1)\xi_2 0} = -\,v^0_{1.1};$ $u^0_{(1.2)\xi_2 0} = v^0_{1.2};$ $u^0_{(2.1)\xi_2 0} = 0$

$u^0_{(2.2)\xi_2 0} = 0;$ $u^0_{(3.1)\xi_2 0} = -\,v^0_{1.1} - v^0_{1.2};$ $u^0_{(3.2)\xi_2 0} = -\,2v^0_{1.1}$

$u^0_{(3.3)\xi_2 0} = 2v^0_{1.2};$ $u^0_{(4.1)\xi_2 0} = -\,2v^0_{1.1} - 2v^0_{1.2}$

$u^0_{(1.1)\xi_1\xi_1} = -2v^0_{1.1};$ $u^0_{(1.2)\xi_1\xi_1} = -2v^0_{1.2};$ $u^0_{(2.1)\xi_1\xi_1} = 2v^0_{2.1}$

$u^0_{(2.2)\xi_1\xi_1} = 2v^0_{2.2};$ $u^0_{(3.1)\xi_1\xi_1} = -2v^0_{1.1} + 2v^0_{1.2} + 2v^0_{2.1};$ $u^0_{(3.2)\xi_1\xi_1} = -4v^0_{1.1} - 2v^0_{2.2}$

$u^0_{(3.3)\xi_1\xi_1} = -4v^0_{1.2} + 2v^0_{2.2};$ $u^0_{(4.1)\xi_1\xi_1} = -4v^0_{1.1} + 4v^0_{1.2} + 2v^0_{2.1} - 2v^0_{2.2}$

and

$u^0_{(1.1)\xi_2\xi_2} = 0;$ $u^0_{(1.2)\xi_2\xi_2} = 0;$ $u^0_{(2.1)\xi_2\xi_2} = -2v^0_{2.1};$ $u^0_{(2.2)\xi_2\xi_2} = 0$

$u^0_{(3.1)\xi_2\xi_2} = -2v^0_{2.1};$ $u^0_{(3.2)\xi_2\xi_2} = 0;$ $u^0_{(3.3)\xi_2\xi_2} = 0;$ $u^0_{(4.1)\xi_2\xi_2} = -2v^0_{2.1}$

A.2 FCC based ordered phases

A.2.1 Thermodynamics of $L1_0$ phase using tetrahedron – octahedron approximation

The tetrahedron–octahedron clusters considered for $L1_0$ phase is shown in Figure A.3 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.3.

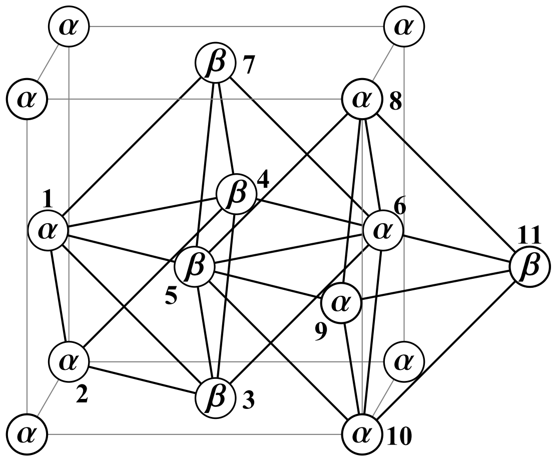

Figure A.3: The tetrahedron–octahedron basic clusters in $L1_0$ phase along with the sublattice sites designated α and β.

Table A.3: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $L1_0$ phase using tetrahedron–octahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Octahedron	$\alpha\alpha\beta\beta\beta\beta$(O2) (1,6,3,4,5,7)	9.2	1/2	1
	$\alpha\alpha\alpha\alpha\beta\beta$(O1) (6,8,9,10,5,11)	9.1	1/2	
Square pyramid	$\alpha\beta\beta\beta\beta$ (1,3,4,5,7)	8.4	1	0
	$\alpha\alpha\beta\beta\beta$ (1,6,3,4,5)	8.3	2	
	$\alpha\alpha\alpha\beta\beta$ (6,8,9,5,11)	8.2	2	
	$\alpha\alpha\alpha\alpha\beta$ (6,8,9,10,5)	8.1	1	

cont ...

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Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Square	$\beta\beta\beta\beta$ (3,4,5,7)	7.4	1/2	0
	$\alpha\alpha\beta\beta$(O2) (1,6,4,5)	7.3	1	
	$\alpha\alpha\beta\beta$(O1) (6,9,5,11)	7.2	1	
	$\alpha\alpha\alpha\alpha$ (6,8,9,10)	7.1	1/2	
Irregular tetrahedron	$\alpha\beta\beta\beta$ (1,3,4,5)	6.4	4	0
	$\alpha\alpha\beta\beta$(O2) (1,6,3,4)	6.3	2	
	$\alpha\alpha\beta\beta$(O1) (6,8,5,11)	6.2	2	
	$\alpha\alpha\alpha\beta$ (6,8,9,5)	6.1	4	
Regular tetrahedron	$\alpha\alpha\beta\beta$ (1,2,3,4)	5.1	2	1
Isosceles triangle	$\beta\beta\beta$ (3,4,5)	4.6	2	0
	$\alpha\beta\beta$(O2) (1,3,7)	4.5	2	
	$\alpha\beta\beta$(O1) (6,5,11)	4.4	2	
	$\alpha\alpha\beta$(O2) (1,6,3)	4.3	2	
	$\alpha\alpha\beta$(O1) (6,9,5)	4.2	2	
	$\alpha\alpha\alpha$ (6,8,9)	4.1	2	
Equilateral triangle	$\alpha\beta\beta$ (1,3,4)	3.2	4	-1
	$\alpha\alpha\beta$ (1,2,3)	3.1	4	
II-n pair	$\beta\beta$(O2) (3,7)	2.4	1	0
	$\beta\beta$(O1) (5,11)	2.3	1/2	
	$\alpha\alpha$(O2) (1,6)	2.2	1/2	
	$\alpha\alpha$(O1) (6,9)	2.1	1	

cont ...

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
I-n pair	$\beta\beta$ (3,4)	1.3	1	1
	$\alpha\beta$ (1,3)	1.2	4	
	$\alpha\alpha$ (1,2)	1.1	1	
Point	β (3)	0.2	1/2	-1
	α (1)	0.1	1/2	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2})/2 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{\eta_1\eta_3^2\eta_9^{1/8}}{\eta_4^2\eta_6^{3/2}}\sqrt{\eta_5\eta_7}; \qquad v^0_{1.2} = \frac{\eta_9^{1/8}}{\eta_1}\sqrt{\frac{\eta_5\eta_7}{\eta_6}}; \qquad v^0_{1.3} = \frac{\eta_1\eta_4^2\eta_9^{1/8}}{\eta_3^2\eta_6^{3/2}}\sqrt{\eta_5\eta_7}$$

$$v^0_{2.1} = \frac{\eta_2\eta_9^{1/16}}{\eta_6}\sqrt{\eta_7}; \qquad v^0_{2.2} = \eta_2\eta_4^2\eta_6\sqrt{\eta_7\eta_8}\eta_9^{1/16}; \qquad v^0_{2.3} = \frac{\eta_2\eta_6\eta_9^{1/16}}{\eta_4^2}\sqrt{\frac{\eta_7}{\eta_8}}$$

$$v^0_{2.4} = \frac{\eta_2\eta_9^{1/16}}{\eta_6}\sqrt{\eta_7}; \qquad v^0_{3.1} = \frac{\eta_3\eta_5\eta_7^{3/2}\eta_8^{1/4}\eta_9^{1/4}}{\eta_1\eta_4^2\eta_6^2}; \qquad v^0_{3.2} = \frac{\eta_4^2\eta_5\eta_7^{3/2}\eta_9^{1/4}}{\eta_1\eta_3\eta_6^2\eta_8^{1/4}}$$

$$v^0_{4.1} = \frac{\eta_1^2\eta_2\eta_3^4\eta_5\eta_7\eta_9^{3/16}}{\eta_4^3\eta_6^3\eta_8^{1/4}}; \qquad v^0_{4.2} = \frac{\eta_2\eta_5\eta_7\eta_8^{1/4}\eta_9^{3/16}}{\eta_1^2\eta_4\eta_6}; \qquad v^0_{4.3} = \frac{\eta_2\eta_4\eta_5\eta_7\eta_9^{3/16}}{\eta_1^2\eta_6\eta_8^{1/4}}$$

$$v^0_{4.4} = \frac{\eta_2\eta_5\eta_7\eta_8^{1/4}\eta_9^{3/16}}{\eta_1^2\eta_4\eta_6}; \qquad v^0_{4.5} = \frac{\eta_2\eta_4\eta_5\eta_7\eta_9^{3/16}}{\eta_1^2\eta_6\eta_8^{1/4}}; \qquad v^0_{4.6} = \frac{\eta_1^2\eta_2\eta_4^3\eta_5\eta_7\eta_8^{1/4}\eta_9^{3/16}}{\eta_3^4\eta_6^3}$$

$$v^0_{5.1} = \frac{\eta_5^2\eta_7^3\eta_9^{1/4}}{\eta_1^2\eta_6^3}; \qquad v^0_{6.1} = \frac{\eta_2\eta_3^2\eta_5^{3/2}\eta_7^2\eta_9^{7/16}}{\eta_1\eta_4^4\eta_6^{7/2}}\sqrt{\eta_8}; \qquad v^0_{6.2} = \frac{\eta_2\eta_5^{3/2}\eta_7^2\eta_9^{7/16}}{\eta_1^3\eta_4^2\eta_6^{5/2}}\sqrt{\eta_8}$$

$$v^0_{6.3} = \frac{\eta_2\eta_4^2\eta_5^{3/2}\eta_7^2\eta_9^{7/16}}{\eta_1^3\eta_6^{5/2}\sqrt{\eta_8}}; \qquad v^0_{6.4} = \frac{\eta_2\eta_4^4\eta_5^{3/2}\eta_7^2\eta_9^{7/16}}{\eta_1\eta_3^2\eta_6^{7/2}\sqrt{\eta_8}}; \qquad v^0_{7.1} = \frac{\eta_1^4\eta_2^2\eta_3^8\eta_5^2\eta_7^2\eta_9^{3/8}}{\eta_4^4\eta_6^4}$$

$$v^0_{7.2} = \frac{\eta_2^2\eta_5^2\eta_7^2\eta_9^{3/8}}{\eta_1^4\eta_4^2\eta_6^2}\sqrt{\eta_8}; \qquad v^0_{7.3} = \frac{\eta_2^2\eta_4^2\eta_5^2\eta_7^2\eta_9^{3/8}}{\eta_1^4\eta_6^2\sqrt{\eta_8}}; \qquad v^0_{7.4} = \frac{\eta_1^4\eta_2^2\eta_4^4\eta_5^2\eta_7^2\eta_9^{3/8}}{\eta_3^8\eta_6^4}$$

$$v^0_{8.1} = \frac{\eta_2^2\eta_3^4\eta_5^2\eta_7^3\eta_9^{5/8}}{\eta_4^6\eta_6^6}\sqrt{\eta_8}; \qquad v^0_{8.2} = \frac{\eta_2^2\eta_5^2\eta_7^3\eta_8\eta_9^{5/8}}{\eta_1^4\eta_4^4\eta_6^4}; \qquad v^0_{8.3} = \frac{\eta_2^2\eta_4^4\eta_5^2\eta_7^3\eta_9^{5/8}}{\eta_1^4\eta_6^4\eta_8}$$

$$v^0_{8.4} = \frac{\eta_2^2\eta_4^6\eta_5^2\eta_7^3\eta_9^{5/8}}{\eta_3^4\eta_6^6\sqrt{\eta_8}}; \qquad v^0_{9.1} = \frac{\eta_2^3\eta_5^2\eta_7^{9/2}\eta_8^{3/2}\eta_9^{15/16}}{\eta_1^4\eta_4^6\eta_6^7}; \qquad v^0_{9.2} = \frac{\eta_2^3\eta_4^6\eta_5^2\eta_7^{9/2}\eta_9^{15/16}}{\eta_1^4\eta_6^7\eta_8^{3/2}}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(1 - 3v^0_{1.1} + 4v^0_{1.2} - 2v^0_{2.1}\right) - 2v^0_{3.1} + 2v^0_{4.1}$$
$$v^0_{(1.2)0} = \frac{v^0_{1.2}}{2}\left(-2v^0_{1.1} + 2v^0_{1.3} - v^0_{2.1} - v^0_{2.2} + v^0_{2.3} + v^0_{2.4}\right) + v^0_{3.1} - v^0_{3.2} + \frac{1}{2}\left(v^0_{4.2} + v^0_{4.3} - v^0_{4.4} - v^0_{4.5}\right)$$
$$v^0_{(1.3)0} = v^0_{1.3}\left(-1 - 4v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.4}\right) + 2v^0_{3.2} - 2v^0_{4.6}$$
$$v^0_{(2.1)0} = v^0_{2.1}\left(1 - 2v^0_{1.1} + 2v^0_{1.2} - v^0_{2.1}\right) + v^0_{4.1} - v^0_{4.2}$$
$$v^0_{(2.2)0} = v^0_{2.2}\left(-1 + 4v^0_{1.2} - v^0_{2.2}\right) - 2v^0_{4.3}$$
$$v^0_{(2.3)0} = v^0_{2.3}\left(1 - 4v^0_{1.2} + v^0_{2.3}\right) + 2v^0_{4.4}$$
$$v^0_{(2.4)0} = v^0_{2.4}\left(-1 - 2v^0_{1.2} + 2v^0_{1.3} + v^0_{2.4}\right) + v^0_{4.5} - v^0_{4.6}$$
$$v^0_{(3.1)0} = \frac{v^0_{3.1}}{2}\left(1 - 6v^0_{1.1} + 6v^0_{1.2} + 3v^0_{1.3} - 4v^0_{2.1} - 2v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} - \frac{v^0_{3.1} - 2v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.2} - v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right) - \frac{v^0_{5.1} + v^0_{6.2}}{2} + v^0_{6.1}$$
$$v^0_{(3.2)0} = \frac{v^0_{3.2}}{2}\left(-1 - 3v^0_{1.1} - 6v^0_{1.2} + 6v^0_{1.3} - 2v^0_{2.1} - v^0_{2.2} + 2v^0_{2.3} + 4v^0_{2.4} + 2\frac{v^0_{3.1} + v^0_{4.2} - v^0_{4.4}}{v^0_{1.2}} + \frac{v^0_{3.2} - 2v^0_{4.6}}{v^0_{1.3}}\right) + \frac{v^0_{5.1} + v^0_{6.3}}{2} - v^0_{6.4}$$
$$v^0_{(4.1)0} = v^0_{4.1}\left(2 - 5v^0_{1.1} + 7v^0_{1.2} - \frac{7}{2}v^0_{2.1} - 2\frac{v^0_{3.1} - v^0_{4.1}}{v^0_{1.1}}\right) - v^0_{6.1} + \frac{v^0_{7.1}}{2}$$
$$v^0_{(4.2)0} = v^0_{4.2}\left(-2v^0_{1.1} + 2v^0_{1.2} + 2v^0_{1.3} - v^0_{2.1} - v^0_{2.2} + \frac{v^0_{2.3}}{2} + v^0_{2.4} - \frac{2v^0_{3.2} - v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right) + v^0_{6.1} - \frac{v^0_{7.2}}{2}$$
$$v^0_{(4.3)0} = v^0_{4.3}\left(-2v^0_{1.1} + v^0_{1.2} + v^0_{1.3} - v^0_{2.1} - v^0_{2.2} + v^0_{2.3} + \frac{v^0_{2.4}}{2} + \frac{2v^0_{3.1} + v^0_{4.2} - v^0_{4.4}}{v^0_{1.2}}\right) - v^0_{6.3} - \frac{v^0_{7.3}}{2}$$
$$v^0_{(4.4)0} = v^0_{4.4}\left(-v^0_{1.1} - v^0_{1.2} + 2v^0_{1.3} - \frac{v^0_{2.1}}{2} - v^0_{2.2} + v^0_{2.3} + v^0_{2.4} - \frac{2v^0_{3.2} - v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right) + v^0_{6.2} + \frac{v^0_{7.2}}{2}$$
$$v^0_{(4.5)0} = v^0_{4.5}\left(-2v^0_{1.1} - 2v^0_{1.2} + 2v^0_{1.3} - v^0_{2.1} - \frac{v^0_{2.2}}{2} + v^0_{2.3} + v^0_{2.4} + \frac{2v^0_{3.1} + v^0_{4.2} - v^0_{4.4}}{v^0_{1.2}}\right) - v^0_{6.4} + \frac{v^0_{7.3}}{2}$$
$$v^0_{(4.6)0} = v^0_{4.6}\left(-2 - 7v^0_{1.2} + 5v^0_{1.3} + \frac{7}{2}v^0_{2.4} + 2\frac{v^0_{3.2} - v^0_{4.6}}{v^0_{1.3}}\right) + v^0_{6.4} - \frac{v^0_{7.4}}{2}$$
$$v^0_{(5.1)0} = v^0_{5.1}\left(-3v^0_{1.1} + 3v^0_{1.3} - 2v^0_{2.1} - v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} + \frac{2v^0_{6.1} - v^0_{6.2}}{v^0_{3.1}} + \frac{v^0_{6.3} - 2v^0_{6.4}}{v^0_{3.2}}\right)$$
$$v^0_{(6.1)0} = \frac{v^0_{6.1}}{2}\left(2 - 10v^0_{1.1} + 12v^0_{1.2} + 4v^0_{1.3} - 7v^0_{2.1} - 3v^0_{2.2} + v^0_{2.3} + 3v^0_{2.4} - \frac{2v^0_{3.1} - 4v^0_{4.1}}{v^0_{1.1}} - \frac{2v^0_{3.2} - 3v^0_{4.3} + 3v^0_{4.5}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) + \frac{v^0_{8.1} - v^0_{8.2}}{2}$$
$$v^0_{(6.2)0} = v^0_{6.2}\left(-3v^0_{1.1} + 2\left(v^0_{1.2} - v^0_{2.1} - v^0_{2.2} + v^0_{2.4}\right) + 3v^0_{1.3} + v^0_{2.3} + \frac{v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.2} - v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right.$$

$$- \frac{v_{5.1}^0}{v_{3.1}^0}\Bigg) + v_{8.2}^0$$

$$v_{(6.3)0}^0 = v_{6.3}^0 \Bigg(-3v_{1.1}^0 - 2\left(v_{1.2}^0 + v_{2.1}^0 - v_{2.3}^0 - v_{2.4}^0\right) + 3v_{1.3}^0 - v_{2.2}^0 + 2\frac{v_{3.1}^0 + v_{4.2}^0 - v_{4.4}^0}{v_{1.2}^0} - \frac{v_{4.6}^0}{v_{1.3}^0}$$

$$+ \frac{v_{5.1}^0}{v_{3.2}^0}\Bigg) - v_{8.3}^0$$

$$v_{(6.4)0}^0 = \frac{v_{6.4}^0}{2} \Bigg(-2 - 4v_{1.1}^0 - 12v_{1.2}^0 + 10v_{1.3}^0 - 3v_{2.1}^0 - v_{2.2}^0 + 3v_{2.3}^0 + 7v_{2.4}^0 + \frac{2v_{3.1}^0 + 3v_{4.2}^0 - 3v_{4.4}^0}{v_{1.2}^0}$$

$$+ \frac{2v_{3.2}^0 - 4v_{4.6}^0}{v_{1.3}^0} + 2\frac{v_{5.1}^0}{v_{3.2}^0}\Bigg) + \frac{v_{8.3}^0 - v_{8.4}^0}{2}$$

$$v_{(7.1)0}^0 = v_{7.1}^0 \left(3 - 8v_{1.1}^0 + 12v_{1.2}^0 - 6v_{2.1}^0 - 4\frac{v_{3.1}^0 - v_{4.1}^0}{v_{1.1}^0} \right) - v_{8.1}^0$$

$$v_{(7.2)0}^0 = v_{7.2}^0 \left(-1 - 2\left(v_{1.1}^0 - v_{1.2}^0 + v_{2.2}^0 - v_{2.4}^0\right) + 4v_{1.3}^0 - v_{2.1}^0 + v_{2.3}^0 - \frac{4v_{3.2}^0 - 2v_{4.3}^0}{v_{1.2}^0} - 2\frac{v_{4.5}^0}{v_{1.2}^0} \right) + v_{8.2}^0$$

$$v_{(7.3)0}^0 = v_{7.3}^0 \left(1 - 4v_{1.1}^0 - 2\left(v_{1.2}^0 - v_{1.3}^0 + v_{2.1}^0 - v_{2.3}^0\right) - v_{2.2}^0 + v_{2.4}^0 + \frac{4v_{3.1}^0 + 2v_{4.2}^0}{v_{1.2}^0} - 2\frac{v_{4.4}^0}{v_{1.2}^0} \right) - v_{8.3}^0$$

$$v_{(7.4)0}^0 = v_{7.4}^0 \left(-3 - 12v_{1.2}^0 + 8v_{1.3}^0 + 6v_{2.4}^0 + 4\frac{v_{3.2}^0 - v_{4.6}^0}{v_{1.3}^0} \right) + v_{8.4}^0$$

$$v_{(8.1)0}^0 = v_{8.1}^0 \Bigg(2\left(1 + v_{1.3}^0 - v_{2.2}^0 + v_{2.4}^0\right) - 8v_{1.1}^0 + 10v_{1.2}^0 - 6v_{2.1}^0 + \frac{v_{2.3}^0}{2} - \frac{2v_{3.1}^0 - 4v_{4.1}^0}{v_{1.1}^0} + 2\frac{v_{4.3}^0 - v_{4.5}^0}{v_{1.2}^0}$$

$$- 2\frac{v_{5.1}^0}{v_{3.1}^0}\Bigg) - \frac{v_{9.1}^0}{2}$$

$$v_{(8.2)0}^0 = v_{8.2}^0 \Bigg(-5v_{1.1}^0 + 5v_{1.2}^0 + 4v_{1.3}^0 - \frac{7}{2}v_{2.1}^0 - 3v_{2.2}^0 + v_{2.3}^0 + 3v_{2.4}^0 + 2\frac{v_{4.1}^0}{v_{1.1}^0} - \frac{2v_{3.2}^0 - 3v_{4.3}^0 + 3v_{4.5}^0}{v_{1.2}^0}$$

$$- 2\frac{v_{5.1}^0}{v_{3.1}^0}\Bigg) + \frac{v_{9.1}^0}{2}$$

$$v_{(8.3)0}^0 = v_{8.3}^0 \Bigg(-4v_{1.1}^0 - 5v_{1.2}^0 + 5v_{1.3}^0 - 3v_{2.1}^0 - v_{2.2}^0 + 3v_{2.3}^0 + \frac{7}{2}v_{2.4}^0 + \frac{2v_{3.1}^0 + 3v_{4.2}^0 - 3v_{4.4}^0}{v_{1.2}^0} - 2\frac{v_{4.6}^0}{v_{1.3}^0}$$

$$+ 2\frac{v_{5.1}^0}{v_{3.2}^0}\Bigg) - \frac{v_{9.2}^0}{2}$$

$$v_{(8.4)0}^0 = 2v_{8.4}^0 \Bigg(-1 - v_{1.1}^0 - 5v_{1.2}^0 + 4v_{1.3}^0 - v_{2.1}^0 - \frac{v_{2.2}^0}{4} + v_{2.3}^0 + 3v_{2.4}^0 + \frac{v_{3.2}^0}{v_{1.3}^0} + \frac{v_{4.2}^0 - v_{4.4}^0}{v_{1.2}^0} - 2\frac{v_{4.6}^0}{v_{1.3}^0}$$

$$+ \frac{v_{5.1}^0}{v_{3.2}^0}\Bigg) + \frac{v_{9.2}^0}{2}$$

$$v_{(9.1)0}^0 = 4v_{9.1}^0 \left(\frac{1}{4} - 2v_{1.1}^0 + 2v_{1.2}^0 + v_{1.3}^0 - \frac{3}{2}v_{2.1}^0 - v_{2.2}^0 + \frac{v_{2.3}^0}{4} + v_{2.4}^0 + \frac{v_{4.1}^0}{v_{1.1}^0} + \frac{v_{4.3}^0 - v_{4.5}^0}{v_{1.2}^0} - \frac{v_{5.1}^0}{v_{3.1}^0} \right)$$

$$v_{(9.2)0}^0 = 4v_{9.2}^0 \left(-\frac{1}{4} - v_{1.1}^0 - 2v_{1.2}^0 + 2v_{1.3}^0 - v_{2.1}^0 - \frac{v_{2.2}^0}{4} + v_{2.3}^0 + \frac{3}{2}v_{2.4}^0 + \frac{v_{4.2}^0 - v_{4.4}^0}{v_{1.2}^0} - \frac{v_{4.6}^0}{v_{1.3}^0} + \frac{v_{5.1}^0}{v_{3.2}^0} \right)$$

and

$$v_{(1.1)\xi}^0 = v_{1.1}^0 \left(-5 + 3v_{1.1}^0 + 4v_{1.2}^0 + 2v_{2.1}^0 \right) - 2v_{3.1}^0 - 2v_{4.1}^0$$

$$v^0_{(1.2)\xi} = \frac{v^0_{1.2}}{2}\left(-10 + 2v^0_{1.1} + 10v^0_{1.2} + 2v^0_{1.3} + v^0_{2.1} + v^0_{2.2} + v^0_{2.3} + v^0_{2.4}\right) - v^0_{3.1} - v^0_{3.2} - \frac{1}{2}\left(v^0_{4.2} + v^0_{4.3} + v^0_{4.4} + v^0_{4.5}\right)$$

$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-5 + 4v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.4}\right) - 2v^0_{3.2} - 2v^0_{4.6}$$

$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-3 + 2v^0_{1.1} + 2v^0_{1.2} + v^0_{2.1}\right) - v^0_{4.1} - v^0_{4.2}$$

$$v^0_{(2.2)\xi} = v^0_{2.2}\left(-3 + 4v^0_{1.2} + v^0_{2.2}\right) - 2v^0_{4.3}$$

$$v^0_{(2.3)\xi} = v^0_{2.3}\left(-3 + 4v^0_{1.2} + v^0_{2.3}\right) - 2v^0_{4.4}$$

$$v^0_{(2.4)\xi} = v^0_{2.4}\left(-3 + 2v^0_{1.2} + 2v^0_{1.3} + v^0_{2.4}\right) - v^0_{4.5} - v^0_{4.6}$$

$$v^0_{(3.1)\xi} = \frac{v^0_{3.1}}{2}\left(-23 + 6v^0_{1.1} + 18v^0_{1.2} + 3v^0_{1.3} + 4v^0_{2.1} + 2v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} - \frac{v^0_{3.1} + 2v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.2} + v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right) - \frac{v^0_{5.1} + v^0_{6.2}}{2} - v^0_{6.1}$$

$$v^0_{(3.2)\xi} = \frac{v^0_{3.1}}{2}\left(-23 + 3v^0_{1.1} + 18v^0_{1.2} + 6v^0_{1.3} + 2v^0_{2.1} + v^0_{2.2} + 2v^0_{2.3} + 4v^0_{2.4} - 2\frac{v^0_{3.1} + v^0_{4.2} + v^0_{4.4}}{v^0_{1.2}} - \frac{v^0_{3.2} + 2v^0_{4.6}}{v^0_{1.3}}\right) - \frac{v^0_{5.1} + v^0_{6.2}}{2} - v^0_{6.1}$$

$$v^0_{(4.1)\xi} = v^0_{4.1}\left(-10 + 5v^0_{1.1} + 7v^0_{1.2} + \frac{7}{2}v^0_{2.1} - 2\frac{v^0_{3.1} + v^0_{4.1}}{v^0_{1.1}}\right) - v^0_{6.1} - \frac{v^0_{7.1}}{2}$$

$$v^0_{(4.2)\xi} = v^0_{4.2}\left(-10 + 2v^0_{1.1} + 8v^0_{1.2} + 2v^0_{1.3} + v^0_{2.1} + v^0_{2.2} + \frac{v^0_{2.3}}{2} + v^0_{2.4} - \frac{2v^0_{3.2} + v^0_{4.3}}{v^0_{1.2}} - \frac{v^0_{4.5}}{v^0_{1.2}}\right) - v^0_{6.1} - \frac{v^0_{7.2}}{2}$$

$$v^0_{(4.3)\xi} = v^0_{4.3}\left(-10 + 2v^0_{1.1} + 9v^0_{1.2} + v^0_{1.3} + v^0_{2.1} + v^0_{2.2} + v^0_{2.3} + \frac{v^0_{2.4}}{2} - \frac{2v^0_{3.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{4.4}}{v^0_{1.2}}\right) - v^0_{6.3} - \frac{v^0_{7.3}}{2}$$

$$v^0_{(4.4)\xi} = v^0_{4.4}\left(-10 + v^0_{1.1} + 9v^0_{1.2} + 2v^0_{1.3} + \frac{v^0_{2.1}}{2} + v^0_{2.2} + v^0_{2.3} + v^0_{2.4} - \frac{2v^0_{3.2} + v^0_{4.3}}{v^0_{1.2}} - \frac{v^0_{4.5}}{v^0_{1.2}}\right) - v^0_{6.2} - \frac{v^0_{7.2}}{2}$$

$$v^0_{(4.5)\xi} = v^0_{4.5}\left(-10 + 2v^0_{1.1} + 8v^0_{1.2} + 2v^0_{1.3} + v^0_{2.1} + \frac{v^0_{2.2}}{2} + v^0_{2.3} + v^0_{2.4} - \frac{2v^0_{3.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{4.4}}{v^0_{1.2}}\right) - v^0_{6.4} - \frac{v^0_{7.3}}{2}$$

$$v^0_{(4.6)\xi} = v^0_{4.6}\left(-10 + 7v^0_{1.2} + 5v^0_{1.3} + \frac{7}{2}v^0_{2.4} - 2\frac{v^0_{3.2} + v^0_{4.6}}{v^0_{1.3}}\right) - v^0_{6.4} - \frac{v^0_{7.4}}{2}$$

$$v^0_{(5.1)\xi} = v^0_{5.1}\left(-18 + 3v^0_{1.1} + 12v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.1} + v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} - \frac{2v^0_{6.1} + v^0_{6.2}}{v^0_{3.1}} - \frac{v^0_{6.3}}{v^0_{3.2}} - 2\frac{v^0_{6.4}}{v^0_{3.2}}\right)$$

$$v^0_{(6.1)\xi} = \frac{v^0_{6.1}}{2}\left(-36 + 10v^0_{1.1} + 26v^0_{1.2} + 4v^0_{1.3} + 7v^0_{2.1} + 3v^0_{2.2} + v^0_{2.3} + 3v^0_{2.4} - \frac{2v^0_{3.1} + 4v^0_{4.1}}{v^0_{1.1}} - \frac{2v^0_{3.2} + 3v^0_{4.3} + 3v^0_{4.5}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{8.1} + v^0_{8.2}}{2}$$

$$v^0_{(6.2)\xi} = v^0_{6.2}\left(-18 + 3v^0_{1.1} + 14v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.1} + 2v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} - \frac{v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.2} + v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}} - \frac{v^0_{5.1}}{v^0_{3.1}}\right) - v^0_{8.2}$$

$$v^0_{(6.3)\xi} = v^0_{6.3}\left(-18 + 3v^0_{1.1} + 14v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.1} + v^0_{2.2} + 2v^0_{2.3} + 2v^0_{2.4} - 2\frac{v^0_{3.1} + v^0_{4.2} + v^0_{4.4}}{v^0_{1.2}} - \frac{v^0_{4.6}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.2}}\right) - v^0_{8.3}$$

$$v^0_{(6.4)\xi} = \frac{v^0_{6.4}}{2}\left(-36 + 4v^0_{1.1} + 26v^0_{1.2} + 10v^0_{1.3} + 3v^0_{2.1} + v^0_{2.2} + 3v^0_{2.3} + 7v^0_{2.4} - 2\frac{v^0_{3.2}}{v^0_{1.3}} - \frac{2v^0_{3.1} + 3v^0_{4.2} + 3v^0_{4.4}}{v^0_{1.2}} - 4\frac{v^0_{4.6}}{v^0_{1.3}} - 2\frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{8.3} + v^0_{8.4}}{2}$$

$$v^0_{(7.1)\xi} = v^0_{7.1}\left(-17 + 8v^0_{1.1} + 12v^0_{1.2} + 6v^0_{2.1} - 4\frac{v^0_{3.1} + v^0_{4.1}}{v^0_{1.1}}\right) - v^0_{8.1}$$

$$v^0_{(7.2)\xi} = v^0_{7.2}\left(-17 + 2v^0_{1.1} + 14v^0_{1.2} + 4v^0_{1.3} + v^0_{2.1} + 2v^0_{2.2} + v^0_{2.3} + 2v^0_{2.4} - 2\frac{2v^0_{3.2} + v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}}\right) - v^0_{8.2}$$

$$v^0_{(7.3)\xi} = v^0_{7.3}\left(-17 + 4v^0_{1.1} + 14v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.1} + v^0_{2.2} + 2v^0_{2.3} + v^0_{2.4} - 2\frac{2v^0_{3.1} + v^0_{4.2} + v^0_{4.4}}{v^0_{1.2}}\right) - v^0_{8.3}$$

$$v^0_{(7.4)\xi} = v^0_{7.4}\left(-17 + 12v^0_{1.2} + 8v^0_{1.3} + 6v^0_{2.4} - 4\frac{v^0_{3.2} + v^0_{4.6}}{v^0_{1.3}}\right) - v^0_{8.4}$$

$$v^0_{(8.1)\xi} = 2v^0_{8.1}\left(-13 + 4v^0_{1.1} + 9v^0_{1.2} + v^0_{1.3} + 3v^0_{2.1} + v^0_{2.2} + \frac{v^0_{2.3}}{4} + v^0_{2.4} - \frac{v^0_{3.1} + 2v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}} - \frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{9.1}}{2}$$

$$v^0_{(8.2)\xi} = v^0_{8.2}\left(-26 + 5v^0_{1.1} + 19v^0_{1.2} + 4v^0_{1.3} + \frac{7}{2}v^0_{2.1} + 3v^0_{2.2} + v^0_{2.3} + 3v^0_{2.4} - 2\frac{v^0_{4.1}}{v^0_{1.1}} - \frac{2v^0_{3.2} + 3v^0_{4.3} + 3v^0_{4.5}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{9.1}}{2}$$

$$v^0_{(8.3)\xi} = v^0_{8.3}\left(-26 + 4v^0_{1.1} + 19v^0_{1.2} + 5v^0_{1.3} + 3v^0_{2.1} + v^0_{2.2} + 3v^0_{2.3} + \frac{7}{2}v^0_{2.4} - \frac{2v^0_{3.1} + 3v^0_{4.2} + 3v^0_{4.4}}{v^0_{1.2}} - 2\frac{v^0_{4.6}}{v^0_{1.3}} - 2\frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{9.2}}{2}$$

$$v^0_{(8.4)\xi} = 2v^0_{8.4}\left(-13 + v^0_{1.1} + 9v^0_{1.2} + 4v^0_{1.3} + v^0_{2.1} + \frac{v^0_{2.2}}{4} + v^0_{2.3} + 3v^0_{2.4} - \frac{v^0_{3.2}}{v^0_{1.3}} - \frac{v^0_{4.2} + v^0_{4.4}}{v^0_{1.2}} - 2\frac{v^0_{4.6}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{9.2}}{2}$$

$$v^0_{(9.1)\xi} = 4v^0_{9.1}\left(-\frac{35}{4} + 2v^0_{1.1} + 6v^0_{1.2} + v^0_{1.3} + \frac{3}{2}v^0_{2.1} + v^0_{2.2} + \frac{v^0_{2.3}}{4} + v^0_{2.4} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.3} + v^0_{4.5}}{v^0_{1.2}} - \frac{v^0_{5.1}}{v^0_{3.1}}\right)$$
$$v^0_{(9.2)\xi} = 4v^0_{9.2}\left(-\frac{35}{4} + v^0_{1.1} + 6v^0_{1.2} + 2v^0_{1.3} + v^0_{2.1} + \frac{v^0_{2.2}}{4} + v^0_{2.3} + \frac{3}{2}v^0_{2.4} - \frac{v^0_{4.2} + v^0_{4.4}}{v^0_{1.2}} - \frac{v^0_{4.6}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = 1$; $u^0_{1.2} = -1$; $u^0_{1.3} = 1$; $u^0_{2.1} = 1$
$u^0_{2.2} = 1$; $u^0_{2.3} = 1$; $u^0_{2.4} = 1$; $u^0_{3.1} = 1$
$u^0_{3.2} = -1$; $u^0_{4.1} = -1$; $u^0_{4.2} = 1$; $u^0_{4.3} = 1$
$u^0_{4.4} = -1$; $u^0_{4.5} = -1$; $u^0_{4.6} = 1$; $u^0_{5.1} = 1$
$u^0_{6.1} = -1$; $u^0_{6.2} = 1$; $u^0_{6.3} = 1$; $u^0_{6.4} = -1$
$u^0_{7.1} = 1$; $u^0_{7.2} = 1$; $u^0_{7.3} = 1$; $u^0_{7.4} = 1$
$u^0_{8.1} = 1$; $u^0_{8.2} = -1$; $u^0_{8.3} = 1$; $u^0_{8.4} = -1$
$u^0_{9.1} = 1$; $u^0_{9.2} = 1$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = -2$; $u^0_{(1.2)0} = 0$; $u^0_{(1.3)0} = 2$; $u^0_{(2.1)0} = -2$
$u^0_{(2.2)0} = -2$; $u^0_{(2.3)0} = 2$; $u^0_{(2.4)0} = 2$; $u^0_{(3.1)0} = -1$
$u^0_{(3.2)0} = -1$; $u^0_{(4.1)0} = 3$; $u^0_{(4.2)0} = -1$; $u^0_{(4.3)0} = -1$
$u^0_{(4.4)0} = -1$; $u^0_{(4.5)0} = -1$; $u^0_{(4.6)0} = 3$; $u^0_{(5.1)0} = 0$
$u^0_{(6.1)0} = 2$; $u^0_{(6.2)0} = 0$; $u^0_{(6.3)0} = 0$; $u^0_{(6.4)0} = -2$
$u^0_{(7.1)0} = -4$; $u^0_{(7.2)0} = 0$; $u^0_{(7.3)0} = 0$; $u^0_{(7.4)0} = 4$
$u^0_{(8.1)0} = -3$; $u^0_{(8.2)0} = 1$; $u^0_{(8.3)0} = 1$; $u^0_{(8.4)0} = -3$
$u^0_{(9.1)0} = -2$; $u^0_{(9.2)0} = 2$

and

$u^0_{(1.1)\xi} = 2$; $u^0_{(1.2)\xi} = -2$; $u^0_{(1.3)\xi} = 2$; $u^0_{(2.1)\xi} = 2$
$u^0_{(2.2)\xi} = 2$; $u^0_{(2.3)\xi} = 2$; $u^0_{(2.4)\xi} = 2$; $u^0_{(3.1)\xi} = 3$
$u^0_{(3.2)\xi} = -3$; $u^0_{(4.1)\xi} = -3$; $u^0_{(4.2)\xi} = 3$; $u^0_{(4.3)\xi} = 3$
$u^0_{(4.4)\xi} = -3$; $u^0_{(4.5)\xi} = -3$; $u^0_{(4.6)\xi} = 3$; $u^0_{(5.1)\xi} = 4$
$u^0_{(6.1)\xi} = -4$; $u^0_{(6.2)\xi} = 4$; $u^0_{(6.3)\xi} = 4$; $u^0_{(6.4)\xi} = -4$
$u^0_{(7.1)\xi} = 4$; $u^0_{(7.2)\xi} = 4$; $u^0_{(7.3)\xi} = 4$; $u^0_{(7.4)\xi} = 4$
$u^0_{(8.1)\xi} = 5$; $u^0_{(8.2)\xi} = -5$; $u^0_{(8.3)\xi} = 5$; $u^0_{(8.4)\xi} = -5$
$u^0_{(9.1)\xi} = 6$; $u^0_{(9.2)\xi} = 6$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi 0}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1}$; $u^0_{(1.2)00} = 2v^0_{1.2}$; $u^0_{(1.3)00} = 2v^0_{1.3}$
$u^0_{(2.1)00} = 2v^0_{2.1}$; $u^0_{(2.2)00} = 2v^0_{2.2}$; $u^0_{(2.3)00} = 2v^0_{2.3}$
$u^0_{(2.4)00} = 2v^0_{2.4}$; $u^0_{(3.1)00} = 2v^0_{1.1} - 4v^0_{1.2}$; $u^0_{(3.2)00} = 4v^0_{1.2} - 2v^0_{1.3}$
$u^0_{(4.1)00} = -4v^0_{1.1} - 2v^0_{2.1}$; $u^0_{(4.2)00} = -4v^0_{1.2} + 2v^0_{2.1}$; $u^0_{(4.3)00} = -4v^0_{1.2} + 2v^0_{2.2}$
$u^0_{(4.4)00} = 4v^0_{1.2} - 2v^0_{2.3}$; $u^0_{(4.5)00} = 4v^0_{1.2} - 2v^0_{2.4}$; $u^0_{(4.6)00} = 4v^0_{1.3} + 2v^0_{2.4}$

$u^0_{(5.1)00} = 2v^0_{1.1} - 8v^0_{1.2} + 2v^0_{1.3}$; $u^0_{(6.1)00} = -4v^0_{1.1} + 6v^0_{1.2} - 2v^0_{2.1}$
$u^0_{(6.2)00} = 2v^0_{1.1} - 8v^0_{1.2} + 2v^0_{2.3}$; $u^0_{(6.3)00} = -8v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.2}$
$u^0_{(6.4)00} = 6v^0_{1.2} - 4v^0_{1.3} - 2v^0_{2.4}$; $u^0_{(7.1)00} = 8v^0_{1.1} + 4v^0_{2.1}$
$u^0_{(7.2)00} = -8v^0_{1.2} + 2v^0_{2.1} + 2v^0_{2.3}$; $u^0_{(7.3)00} = -8v^0_{1.2} + 2v^0_{2.2} + 2v^0_{2.4}$
$u^0_{(7.4)00} = 8v^0_{1.3} + 4v^0_{2.4}$; $u^0_{(8.1)00} = 8v^0_{1.1} - 8v^0_{1.2} + 4v^0_{2.1}$
$u^0_{(8.2)00} = -4v^0_{1.1} + 12v^0_{1.2} - 2v^0_{2.1} - 2v^0_{2.3}$; $u^0_{(8.3)00} = -12v^0_{1.2} + 4v^0_{1.3} + 2v^0_{2.2} + 2v^0_{2.4}$
$u^0_{(8.4)00} = 8v^0_{1.2} - 8v^0_{1.3} - 4v^0_{2.4}$; $u^0_{(9.1)00} = 8v^0_{1.1} - 16v^0_{1.2} + 4v^0_{2.1} + 2v^0_{2.3}$
$u^0_{(9.2)00} = -16v^0_{1.2} + 8v^0_{1.3} + 2v^0_{2.2} + 4v^0_{2.4}$

$u^0_{(1.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(1.2)\xi 0} = 0$; $u^0_{(1.3)\xi 0} = 2v^0_{1.3}$
$u^0_{(2.1)\xi 0} = -2v^0_{2.1}$; $u^0_{(2.2)\xi 0} = -2v^0_{2.2}$; $u^0_{(2.3)\xi 0} = 2v^0_{2.3}$
$u^0_{(2.4)\xi 0} = 2v^0_{2.4}$; $u^0_{(3.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(3.2)\xi 0} = -2v^0_{1.3}$
$u^0_{(4.1)\xi 0} = 4v^0_{1.1} + 2v^0_{2.1}$; $u^0_{(4.2)\xi 0} = -2v^0_{2.1}$; $u^0_{(4.3)\xi 0} = -2v^0_{2.2}$
$u^0_{(4.4)\xi 0} = -2v^0_{2.3}$; $u^0_{(4.5)\xi 0} = -2v^0_{2.4}$; $u^0_{(4.6)\xi 0} = 4v^0_{1.3} + 2v^0_{2.4}$
$u^0_{(5.1)\xi 0} = 2v^0_{1.3} - 2v^0_{1.1}$; $u^0_{(6.1)\xi 0} = 4v^0_{1.1} + 2v^0_{2.1}$; $u^0_{(6.2)\xi 0} = 2v^0_{2.3} - 2v^0_{1.1}$
$u^0_{(6.3)\xi 0} = 2v^0_{1.3} - 2v^0_{2.2}$; $u^0_{(6.4)\xi 0} = -4v^0_{1.3} - 2v^0_{2.4}$; $u^0_{(7.1)\xi 0} = -8v^0_{1.1} - 4v^0_{2.1}$
$u^0_{(7.2)\xi 0} = 2v^0_{2.3} - 2v^0_{2.1}$; $u^0_{(7.3)\xi 0} = 2v^0_{2.4} - 2v^0_{2.2}$; $u^0_{(7.4)\xi 0} = 8v^0_{1.3} + 4v^0_{2.4}$
$u^0_{(8.1)\xi 0} = -8v^0_{1.1} - 4v^0_{2.1}$; $u^0_{(8.2)\xi 0} = 4v^0_{1.1} + 2v^0_{2.1} - 2v^0_{2.3}$; $u^0_{(8.3)\xi 0} = 4v^0_{1.3} - 2v^0_{2.2} + 2v^0_{2.4}$
$u^0_{(8.4)\xi 0} = -8v^0_{1.3} - 4v^0_{2.4}$; $u^0_{(9.1)\xi 0} = -8v^0_{1.1} - 4v^0_{2.1} + 2v^0_{2.3}$; $u^0_{(9.2)\xi 0} = 8v^0_{1.3} - 2v^0_{2.2} + 4v^0_{2.4}$

and

$u^0_{(1.1)\xi\xi} = 2v^0_{1.1}$; $u^0_{(1.2)\xi\xi} = -2v^0_{1.2}$; $u^0_{(1.3)\xi\xi} = 2v^0_{1.3}$
$u^0_{(2.1)\xi\xi} = 2v^0_{2.1}$; $u^0_{(2.2)\xi\xi} = 2v^0_{2.2}$; $u^0_{(2.3)\xi\xi} = 2v^0_{2.3}$
$u^0_{(2.4)\xi\xi} = 2v^0_{2.4}$; $u^0_{(3.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2}$; $u^0_{(3.2)\xi\xi} = -4v^0_{1.2} - 2v^0_{1.3}$
$u^0_{(4.1)\xi\xi} = -4v^0_{1.1} - 2v^0_{2.1}$; $u^0_{(4.2)\xi\xi} = 4v^0_{1.2} + 2v^0_{2.1}$; $u^0_{(4.3)\xi\xi} = 4v^0_{1.2} + 2v^0_{2.2}$
$u^0_{(4.4)\xi\xi} = -4v^0_{1.2} - 2v^0_{2.3}$; $u^0_{(4.5)\xi\xi} = -4v^0_{1.2} - 2v^0_{2.4}$; $u^0_{(4.6)\xi\xi} = 4v^0_{1.3} + 2v^0_{2.4}$
$u^0_{(5.1)\xi\xi} = 2v^0_{1.1} + 8v^0_{1.2} + 2v^0_{1.3}$

$u^0_{(6.1)\xi\xi} = -4v^0_{1.1} - 6v^0_{1.2} - 2v^0_{2.1};$ $\quad u^0_{(6.2)\xi\xi} = 2v^0_{1.1} + 8v^0_{1.2} + 2v^0_{2.3}$

$u^0_{(6.3)\xi\xi} = 8v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.2};$ $\quad u^0_{(6.4)\xi\xi} = -6v^0_{1.2} - 4v^0_{1.3} - 2v^0_{2.4}$

$u^0_{(7.1)\xi\xi} = 8v^0_{1.1} + 4v^0_{2.1};$ $\quad u^0_{(7.2)\xi\xi} = 8v^0_{1.2} + 2v^0_{2.1} + 2v^0_{2.3}$

$u^0_{(7.3)\xi\xi} = 8v^0_{1.2} + 2v^0_{2.2} + 2v^0_{2.4};$ $\quad u^0_{(7.4)\xi\xi} = 8v^0_{1.3} + 4v^0_{2.4}$

$u^0_{(8.1)\xi\xi} = 8v^0_{1.1} + 8v^0_{1.2} + 4v^0_{2.1};$ $\quad u^0_{(8.2)\xi\xi} = -4v^0_{1.1} - 12v^0_{1.2} - 2v^0_{2.1} - 2v^0_{2.3}$

$u^0_{(8.3)\xi\xi} = 12v^0_{1.2} + 4v^0_{1.3} + 2v^0_{2.2} + 2v^0_{2.4};$ $\quad u^0_{(8.4)\xi\xi} = -8v^0_{1.2} - 8v^0_{1.3} - 4v^0_{2.4}$

$u^0_{(9.1)\xi\xi} = 8v^0_{1.1} + 16v^0_{1.2} + 4v^0_{2.1} + 2v^0_{2.3};$ $\quad u^0_{(9.2)\xi\xi} = 16v^0_{1.2} + 8v^0_{1.3} + 2v^0_{2.2} + 4v^0_{2.4}$

A.2.2 Thermodynamics of $L1_2$ phase using tetrahedron approximation

The tetrahedron cluster considered for $L1_2$ phase is shown in Figure A.4 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.4.

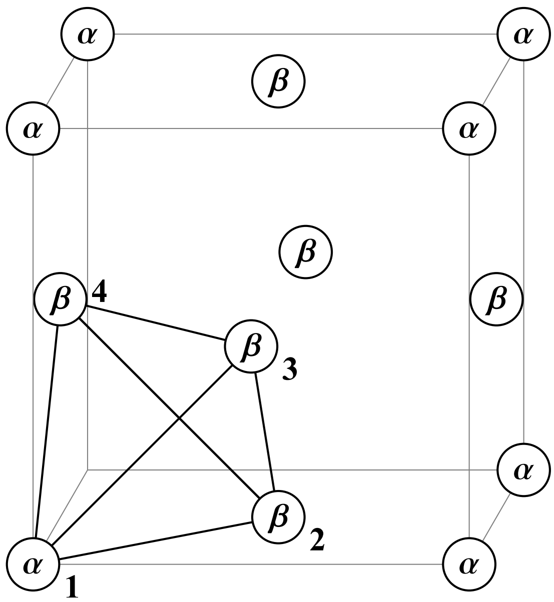

Figure A.4: The tetrahedron basic cluster in $L1_2$ phase along with the sublattice sites designated α and β.

Table A.4: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $L1_2$ phase using tetrahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Regular tetrahedron	$\alpha\beta\beta\beta$ (1,2,3,4)	3.1	2	1
Equilateral triangle	$\beta\beta\beta$ (2,3,4)	2.2	2	0
	$\alpha\beta\beta$ (1,2,3)	2.1	6	
I-n pair	$\beta\beta$ (2,3)	1.2	3	-1
	$\alpha\beta$ (1,2)	1.1	3	
Point	β (2)	0.1	3/4	5
	α (1)	0.1	1/4	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + 3u_{0.2})/4 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{1}{\eta_1\eta_2^2\sqrt{\eta_3}}; \qquad v^0_{1.2} = \frac{\eta_1}{\sqrt{\eta_3}}; \qquad v^0_{2.1} = \frac{1}{\eta_1\eta_2^3\eta_3}; \qquad v^0_{2.2} = \frac{\eta_1^3}{\eta_2\eta_3}; \qquad v^0_{3.1} = \frac{1}{\eta_2^4\eta_3^2}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = 2v^0_{1.1}\left(-1 + v^0_{1.1} + v^0_{1.2}\right) - 2v^0_{2.1}$$
$$v^0_{(1.2)0} = v^0_{1.2}\left(-1 - 2v^0_{1.1} + 3v^0_{1.2}\right) + v^0_{2.1} - v^0_{2.2}$$
$$v^0_{(2.1)0} = v^0_{2.1}\left(-4 + \frac{3}{2}v^0_{1.1} + 5v^0_{1.2} - 2\frac{v^0_{2.1}}{v^0_{1.1}} + \frac{v^0_{2.1} - v^0_{2.2}}{2v^0_{1.2}}\right) - \frac{v^0_{3.1}}{2}$$
$$v^0_{(2.2)0} = v^0_{2.2}\left(-2 - \frac{9}{2}v^0_{1.1} + 6v^0_{1.2} + 3\frac{v^0_{2.1} - v^0_{2.2}}{2v^0_{1.2}}\right) + \frac{v^0_{3.1}}{2}$$
$$v^0_{(3.1)0} = 3v^0_{3.1}\left(-2 + 3v^0_{1.2} - \frac{v^0_{2.1}}{v^0_{1.1}} + \frac{v^0_{2.1} - v^0_{2.2}}{2v^0_{1.2}}\right)$$

and

$$v^0_{(1.1)\xi} = v^0_{1.1}\left(-2 + 2v^0_{1.1} + v^0_{1.2}\right) - v^0_{2.1}$$
$$v^0_{(1.2)\xi} = \frac{v^0_{1.2}}{2}\left(-5 + 6v^0_{1.1} + 3v^0_{1.2}\right) - \frac{3v^0_{2.1} + v^0_{2.2}}{2}$$
$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-5 + \frac{19}{4}v^0_{1.1} + \frac{5}{2}v^0_{1.2} - \frac{v^0_{2.1}}{v^0_{1.1}} - \frac{3v^0_{2.1} + v^0_{2.2}}{4v^0_{1.2}}\right) - \frac{v^0_{3.1}}{4}$$
$$v^0_{(2.2)\xi} = \frac{3}{4}v^0_{2.2}\left(-8 + 9v^0_{1.1} + 4v^0_{1.2} - \frac{3v^0_{2.1} + v^0_{2.2}}{v^0_{1.2}}\right) - \frac{3}{4}v^0_{3.1}$$
$$v^0_{(3.1)\xi} = 9v^0_{3.1}\left(-1 + v^0_{1.1} + \frac{v^0_{1.2}}{2} - \frac{v^0_{2.1}}{6v^0_{1.1}} - \frac{3v^0_{2.1} + v^0_{2.2}}{12v^0_{1.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$$u^0_{1.1} = -1; \qquad u^0_{1.2} = 1; \qquad u^0_{2.1} = -1; \qquad u^0_{2.2} = 1; \qquad u^0_{3.1} = -1$$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$$u^0_{(1.1)0} = 0; \qquad u^0_{(1.2)0} = 2; \qquad u^0_{(2.1)0} = -1; \qquad u^0_{(2.2)0} = 3; \qquad u^0_{(3.1)0} = -2$$

$$u^0_{(1.1)\xi} = -2; \qquad u^0_{(1.2)\xi} = 1; \qquad u^0_{(2.1)\xi} = -\frac{5}{2}; \qquad u^0_{(2.2)\xi} = \frac{3}{2}; \qquad u^0_{(3.1)\xi} = -3$$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi 0}$ and $u^0_{(i.j)\xi\xi}$, are:

$$u^0_{(1.1)00} = 2v^0_{1.1}; \qquad u^0_{(1.2)00} = 2v^0_{1.2}; \qquad u^0_{(2.1)00} = 4v^0_{1.1} - 2v^0_{1.2}$$

$$u^0_{(2.2)00} = 6v^0_{1.2}; \qquad u^0_{(3.1)00} = 6v^0_{1.1} - 6v^0_{1.2}$$

$$u^0_{(1.1)\xi 0} = -v^0_{1.1}; \qquad u^0_{(1.2)\xi 0} = v^0_{1.2}; \qquad u^0_{(2.1)\xi 0} = -2v^0_{1.1} - v^0_{1.2}$$

$$u^0_{(2.2)\xi 0} = 3v^0_{1.2}; \qquad u^0_{(3.1)\xi 0} = -3v^0_{1.1} - 3v^0_{1.2}$$

$$u^0_{(1.1)\xi\xi} = -\frac{3}{2}v^0_{1.1}; \qquad u^0_{(1.2)\xi\xi} = \frac{v^0_{1.2}}{2}; \qquad u^0_{(2.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.2}}{2}$$

$$u^0_{(2.2)\xi\xi} = \frac{3}{2}v^0_{1.2}; \qquad u^0_{(3.1)\xi\xi} = -\frac{9v^0_{1.1} + 3v^0_{1.2}}{2}$$

A.2.3 Thermodynamics of $L1_2$ phase using tetrahedron – octahedron approximation

The tetrahedron–octahedron clusters considered for $L1_2$ phase is shown in Figure A.5 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.5.

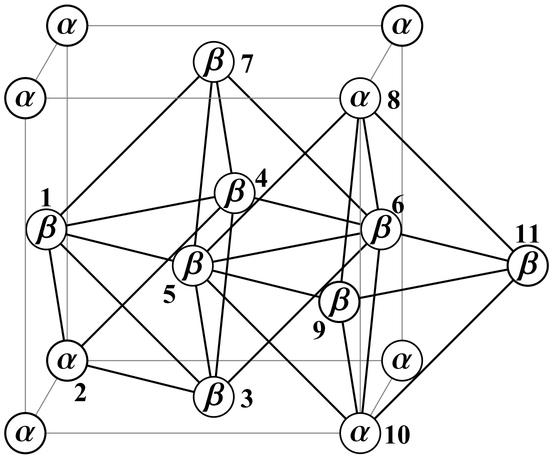

Figure A.5: The tetrahedron–octahedron basic clusters in $L1_2$ phase along with the sublattice sites designated α and β.

Table A.5: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $L1_2$ phase using tetrahedron–octahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Octahedron	$\beta\beta\beta\beta\beta\beta$(O2) (1,3,4,5,6,7)	9.2	1/4	1
	$\alpha\alpha\beta\beta\beta\beta$(O1) (8,10,5,6,9,11)	9.1	3/4	
Square pyramid	$\beta\beta\beta\beta\beta$ (1,3,4,5,6)	8.3	3/2	0
	$\alpha\beta\beta\beta\beta$ (8,5,6,9,11)	8.2	3/2	
	$\alpha\alpha\beta\beta\beta$ (8,10,5,6,9)	8.1	3	
Square	$\beta\beta\beta\beta$(O2) (1,4,5,6)	7.3	3/4	0
	$\beta\beta\beta\beta$(O1) (5,6,9,11)	7.2	3/4	
	$\alpha\alpha\beta\beta$ (8,10,5,11)	7.1	3/2	

cont ...

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Irregular tetrahedron	$\beta\beta\beta\beta$ (1,3,4,5)	6.3	3	0
	$\alpha\beta\beta\beta$ (8,5,6,9)	6.2	6	
	$\alpha\alpha\beta\beta$ (8,10,5,6)	6.1	3	
Regular tetrahedron	$\alpha\beta\beta\beta$ (1,2,3,4)	5.1	2	1
Isosceles triangle	$\beta\beta\beta$(O2) (1,3,6)	4.4	3	0
	$\beta\beta\beta$(O1) (5,6,9)	4.3	3	
	$\alpha\beta\beta$ (8,5,11)	4.2	3	
	$\alpha\alpha\beta$ (8,10,5)	4.1	3	
Equilateral triangle	$\beta\beta\beta$ (1,3,4)	3.2	2	-1
	$\alpha\beta\beta$ (2,1,3)	3.1	6	
II-n pair	$\beta\beta$(O2) (1,6)	2.3	3/4	0
	$\beta\beta$(O1) (5,11)	2.2	3/2	
	$\alpha\alpha$ (8,10)	2.1	3/4	
I-n pair	$\beta\beta$ (1,3)	1.2	3	1
	$\alpha\beta$ (2,1)	1.1	3	
Point	β (1)	0.2	3/4	-1
	α (2)	0.1	1/4	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + 3u_{0.2})/4 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{\eta_9^{1/8}}{\eta_1\eta_3^2}\sqrt{\frac{\eta_7\eta_8}{\eta_5\eta_6}}; \qquad v^0_{1.2} = \eta_1\eta_4^2\eta_9^{1/8}\sqrt{\frac{\eta_6\eta_7\eta_8}{\eta_5}}; \qquad v^0_{2.1} = \eta_2\eta_4^2\eta_6\sqrt{\eta_7\eta_8}\eta_9^{1/16}$$

$$v_{2.2}^0 = \frac{\eta_2\eta_9^{1/16}}{\eta_6}\sqrt{\eta_7}; \qquad v_{2.3}^0 = \eta_2\eta_4^2\eta_6\sqrt{\eta_7\eta_8}\eta_9^{1/16}; \qquad v_{3.1}^0 = \frac{\eta_4^2\eta_7^{3/2}\eta_8^{5/4}\eta_9^{1/4}}{\eta_1\eta_3^3\eta_5}$$

$$v_{3.2}^0 = \frac{\eta_1^3\eta_4^6\eta_7^{3/2}\eta_8^{3/4}\eta_9^{1/4}}{\eta_3\eta_5}; \qquad v_{4.1}^0 = \frac{\eta_2\eta_4\eta_7\eta_8^{3/4}\eta_9^{3/16}}{\eta_1^2\eta_3^4\eta_5\eta_6}; \qquad v_{4.2}^0 = \frac{\eta_2\eta_4\eta_7\eta_8^{3/4}\eta_9^{3/16}}{\eta_1^2\eta_3^4\eta_5\eta_6}$$

$$v_{4.3}^0 = \frac{\eta_1^2\eta_2\eta_4^3\eta_6\eta_7\eta_8^{5/4}\eta_9^{3/16}}{\eta_5}; \qquad v_{4.4}^0 = \frac{\eta_1^2\eta_2\eta_4^5\eta_6\eta_7\eta_8^{3/4}\eta_9^{3/16}}{\eta_5}; \qquad v_{5.1}^0 = \frac{\eta_4^6\eta_7^3\eta_8^{3/2}\eta_9^{1/4}}{\eta_3^4\eta_5^2}$$

$$v_{6.1}^0 = \frac{\eta_2\eta_4^2\eta_7^2\eta_8^2\eta_9^{7/16}}{\eta_1^3\eta_3^6\eta_5^{3/2}\sqrt{\eta_6}}; \qquad v_{6.2}^0 = \frac{\eta_2\eta_4^4\eta_7^2\eta_8^2\eta_9^{7/16}}{\eta_1\eta_3^4\eta_5^{3/2}}\sqrt{\eta_6}; \qquad v_{6.3}^0 = \frac{\eta_1^5\eta_2\eta_4^{10}\eta_7^2\eta_8\eta_9^{7/16}}{\eta_3^2\eta_5^{3/2}\sqrt{\eta_6}}$$

$$v_{7.1}^0 = \frac{\eta_2^2\eta_4^2\eta_7^2\eta_8^{3/2}\eta_9^{3/8}}{\eta_1^4\eta_3^8\eta_5^2\eta_6^2}; \qquad v_{7.2}^0 = \frac{\eta_1^4\eta_2^2\eta_4^4\eta_6^4\eta_7^2\eta_8^2\eta_9^{3/8}}{\eta_5^2}; \qquad v_{7.3}^0 = \frac{\eta_1^4\eta_2^2\eta_4^8\eta_7^2\eta_8\eta_9^{3/8}}{\eta_5^2}$$

$$v_{8.1}^0 = \frac{\eta_2^2\eta_4^4\eta_7^3\eta_8^3\eta_9^{5/8}}{\eta_1^4\eta_3^8\eta_5^2}; \qquad v_{8.2}^0 = \frac{\eta_2^2\eta_4^6\eta_6^2\eta_7^3\eta_8^{7/2}\eta_9^{5/8}}{\eta_3^4\eta_5^2}; \qquad v_{8.3}^0 = \frac{\eta_1^8\eta_2^2\eta_4^{14}\eta_7^3\eta_8^{3/2}\eta_9^{5/8}}{\eta_3^4\eta_5^2\eta_6^2}$$

$$v_{9.1}^0 = \frac{\eta_2^3\eta_4^6\eta_6\eta_7^{9/2}\eta_8^{9/2}\eta_9^{15/16}}{\eta_1^4\eta_3^8\eta_5^2}; \qquad v_{9.2}^0 = \frac{\eta_1^{12}\eta_2^3\eta_4^{18}\eta_7^{9/2}\eta_8^{3/2}\eta_9^{15/16}}{\eta_3^8\eta_5^2\eta_6^3}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v_{(i.j)0}^0$ and $v_{(i.j)\xi}^0$, are:

$$v_{(1.1)0}^0 = v_{1.1}^0\left(-2 + 2v_{1.1}^0 + 2v_{1.2}^0 - v_{2.1}^0 + v_{2.2}^0\right) - 2v_{3.1}^0 + v_{4.1}^0 - v_{4.2}^0$$

$$v_{(1.2)0}^0 = v_{1.2}^0\left(-3 - 2v_{1.1}^0 + 5v_{1.2}^0 + v_{2.2}^0 + v_{2.3}^0\right) + v_{3.1}^0 - v_{3.2}^0 - v_{4.3}^0 - v_{4.4}^0$$

$$v_{(2.1)0}^0 = v_{2.1}^0\left(-1 + 4v_{1.1}^0 - v_{2.1}^0\right) - 2v_{4.1}^0$$

$$v_{(2.2)0}^0 = v_{2.2}^0\left(-1 - 2v_{1.1}^0 + 2v_{1.2}^0 + v_{2.2}^0\right) + v_{4.2}^0 - v_{4.3}^0$$

$$v_{(2.3)0}^0 = v_{2.3}^0\left(-3 + 4v_{1.2}^0 + v_{2.3}^0\right) - 2v_{4.4}^0$$

$$v_{(3.1)0}^0 = \frac{v_{3.1}^0}{2}\left(-11 + 3v_{1.1}^0 + 12v_{1.2}^0 - 3v_{2.1}^0 + 4v_{2.2}^0 + 2v_{2.3}^0 - 2\frac{v_{3.1}^0 - v_{4.1}^0 + v_{4.2}^0}{v_{1.1}^0} - \frac{v_{3.2}^0 + 2v_{4.4}^0}{v_{1.2}^0}\right) - \frac{v_{5.1}^0 - v_{6.1}^0}{2} - v_{6.2}^0$$

$$v_{(3.2)0}^0 = \frac{v_{3.2}^0}{2}\left(-13 - 9v_{1.1}^0 + 18v_{1.2}^0 + 6v_{2.2}^0 + 3v_{2.3}^0 + \frac{3v_{3.1}^0 - 6v_{4.3}^0}{v_{1.2}^0}\right) + \frac{v_{5.1}^0 - 3v_{6.3}^0}{2}$$

$$v_{(4.1)0}^0 = v_{4.1}^0\left(-4 + 5v_{1.1}^0 + 3v_{1.2}^0 - 2v_{2.1}^0 + \frac{3}{2}v_{2.2}^0 - \frac{2v_{3.1}^0 - v_{4.1}^0 + v_{4.2}^0}{v_{1.1}^0}\right) - v_{6.1}^0 - \frac{v_{7.1}^0}{2}$$

$$v_{(4.2)0}^0 = v_{4.2}^0\left(-4 + 2v_{1.1}^0 + 4v_{1.2}^0 - \frac{3}{2}v_{2.1}^0 + 2v_{2.2}^0 - \frac{2v_{3.1}^0 - v_{4.1}^0 + v_{4.2}^0}{v_{1.1}^0}\right) - v_{6.2}^0 + \frac{v_{7.1}^0}{2}$$

$$v_{(4.3)0}^0 = v_{4.3}^0\left(-6 - 3v_{1.1}^0 + 9v_{1.2}^0 + \frac{3}{2}v_{2.2}^0 + 2v_{2.3}^0 - 2\frac{v_{3.2}^0 + v_{4.4}^0}{v_{1.2}^0}\right) + v_{6.2}^0 - \frac{v_{7.2}^0}{2}$$

$$v_{(4.4)0}^0 = v_{4.4}^0\left(-6 - 4v_{1.1}^0 + 8v_{1.2}^0 + 2v_{2.2}^0 + \frac{3}{2}v_{2.3}^0 + 2\frac{v_{3.1}^0 - v_{4.3}^0}{v_{1.2}^0}\right) - v_{6.3}^0 - \frac{v_{7.3}^0}{2}$$

$$v_{(5.1)0}^0 = \frac{3}{2}v_{5.1}^0\left(-6 + 6v_{1.2}^0 - v_{2.1}^0 + 2v_{2.2}^0 + v_{2.3}^0 + \frac{v_{6.1}^0 - 2v_{6.2}^0}{v_{3.1}^0} - \frac{v_{6.3}^0}{v_{3.2}^0}\right)$$

$$v_{(6.1)0}^0 = v_{6.1}^0\left(-8 + 5v_{1.1}^0 + 7v_{1.2}^0 - 3v_{2.1}^0 + 3v_{2.2}^0 + v_{2.3}^0 - 2\frac{v_{3.1}^0 - v_{4.1}^0 + v_{4.2}^0}{v_{1.1}^0} - \frac{v_{4.4}^0}{v_{1.2}^0} - \frac{v_{5.1}^0}{v_{3.1}^0}\right) - v_{8.1}^0$$

$$v^0_{(6.2)0} = v^0_{6.2}\left(-9 + v^0_{1.1} + 10v^0_{1.2} - 2v^0_{2.1} + 3v^0_{2.2} + 2v^0_{2.3} - \frac{2v^0_{3.1} - 3v^0_{4.1} + 3v^0_{4.2}}{2v^0_{1.1}} - \frac{v^0_{3.2} + 2v^0_{4.4}}{v^0_{1.2}} - \frac{v^0_{5.1}}{v^0_{3.1}}\right) + \frac{v^0_{8.1} - v^0_{8.2}}{2}$$

$$v^0_{(6.3)0} = v^0_{6.3}\left(-10 - 7v^0_{1.1} + 13v^0_{1.2} + 5v^0_{2.2} + 2v^0_{2.3} + \frac{2v^0_{3.1} - 5v^0_{4.3}}{v^0_{1.2}} + \frac{v^0_{5.1}}{v^0_{3.2}}\right) - v^0_{8.3}$$

$$v^0_{(7.1)0} = v^0_{7.1}\left(-7 + 6v^0_{1.1} + 6v^0_{1.2} - 3v^0_{2.1} + 3v^0_{2.2} - 2\frac{2v^0_{3.1} - v^0_{4.1} + v^0_{4.2}}{v^0_{1.1}}\right) - v^0_{8.1}$$

$$v^0_{(7.2)0} = v^0_{7.2}\left(-11 - 4v^0_{1.1} + 16v^0_{1.2} + 2v^0_{2.2} + 4v^0_{2.3} - 4\frac{v^0_{3.2} + v^0_{4.4}}{v^0_{1.2}}\right) + v^0_{8.2}$$

$$v^0_{(7.3)0} = v^0_{7.3}\left(-9 - 8v^0_{1.1} + 12v^0_{1.2} + 4v^0_{2.2} + 2v^0_{2.3} + 4\frac{v^0_{3.1} - v^0_{4.3}}{v^0_{1.2}}\right) - v^0_{8.3}$$

$$v^0_{(8.1)0} = v^0_{8.1}\left(-12 + 5v^0_{1.1} + 11v^0_{1.2} - 4v^0_{2.1} + \frac{9}{2}v^0_{2.2} + 2v^0_{2.3} - \frac{2v^0_{3.1} - 3v^0_{4.1} + 3v^0_{4.2}}{v^0_{1.1}} - 2\frac{v^0_{4.4}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{9.1}}{2}$$

$$v^0_{(8.2)0} = v^0_{8.2}\left(-14 + 16v^0_{1.2} - \frac{5}{2}v^0_{2.1} + 4v^0_{2.2} + 4v^0_{2.3} + 2\frac{v^0_{4.1} - v^0_{4.2}}{v^0_{1.1}} - \frac{2v^0_{3.2} + 4v^0_{4.4}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) + \frac{v^0_{9.1}}{2}$$

$$v^0_{(8.3)0} = v^0_{8.3}\left(-14 - 10v^0_{1.1} + 18v^0_{1.2} + 8v^0_{2.2} + \frac{5}{2}v^0_{2.3} + \frac{2v^0_{3.1} - 8v^0_{4.3}}{v^0_{1.2}} + 2\frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{9.2}}{2}$$

$$v^0_{(9.1)0} = v^0_{9.1}\left(-17 + 4v^0_{1.1} + 16v^0_{1.2} - 5v^0_{2.1} + 6v^0_{2.2} + 4v^0_{2.3} + 4\frac{v^0_{4.1} - v^0_{4.2}}{v^0_{1.1}} - 4\frac{v^0_{4.4}}{v^0_{1.2}} - 4\frac{v^0_{5.1}}{v^0_{3.1}}\right)$$

$$v^0_{(9.2)0} = v^0_{9.2}\left(-19 - 12v^0_{1.1} + 24v^0_{1.2} + 12v^0_{2.2} + 3v^0_{2.3} - 12\frac{v^0_{4.3}}{v^0_{1.2}} + 4\frac{v^0_{5.1}}{v^0_{3.2}}\right)$$

and

$$v^0_{(1.1)\xi} = \frac{v^0_{1.1}}{2}\left(-8 + 8v^0_{1.1} + 2v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2}\right) - v^0_{3.1} - \frac{3v^0_{4.1} + v^0_{4.2}}{2}$$

$$v^0_{(1.2)\xi} = \frac{v^0_{1.2}}{2}\left(-7 + 6v^0_{1.1} + 5v^0_{1.2} + v^0_{2.2} + v^0_{2.3}\right) - \frac{1}{2}\left(3v^0_{3.1} + v^0_{3.2} + v^0_{4.3} + v^0_{4.4}\right)$$

$$v^0_{(2.1)\xi} = \frac{v^0_{2.1}}{2}\left(-5 + 4v^0_{1.1} + 3v^0_{2.1}\right) - v^0_{4.1}$$

$$v^0_{(2.2)\xi} = \frac{v^0_{2.2}}{2}\left(-5 + 6v^0_{1.1} + 2v^0_{1.2} + v^0_{2.2}\right) - \frac{3v^0_{4.2} + v^0_{4.3}}{2}$$

$$v^0_{(2.3)\xi} = \frac{v^0_{2.3}}{2}\left(-3 + 4v^0_{1.2} + v^0_{2.3}\right) - v^0_{4.4}$$

$$v^0_{(3.1)\xi} = \frac{v^0_{3.1}}{4}\left(-35 + 27v^0_{1.1} + 12v^0_{1.2} + 9v^0_{2.1} + 4v^0_{2.2} + 2v^0_{2.3} - 2\frac{v^0_{3.1} + 3v^0_{4.1} + v^0_{4.2}}{v^0_{1.1}} - \frac{v^0_{3.2} + 2v^0_{4.4}}{v^0_{1.2}}\right) - \frac{1}{4}\left(v^0_{5.1} + 3v^0_{6.1} + 2v^0_{6.2}\right)$$

$$v^0_{(3.2)\xi} = \frac{3}{4}v^0_{3.2}\left(-11 + 9v^0_{1.1} + 6v^0_{1.2} + 2v^0_{2.2} + v^0_{2.3} - \frac{3v^0_{3.1} + 2v^0_{4.3}}{v^0_{1.2}}\right) - \frac{3}{4}\left(v^0_{5.1} + v^0_{6.3}\right)$$

$$v^0_{(4.1)\xi} = \frac{v^0_{4.1}}{2}\left(-16 + 13v^0_{1.1} + 3v^0_{1.2} + 6v^0_{2.1} + \frac{3}{2}v^0_{2.2} - \frac{2v^0_{3.1} + 3v^0_{4.1} + v^0_{4.2}}{v^0_{1.1}}\right) - \frac{2v^0_{6.1} + v^0_{7.1}}{4}$$

$$v^0_{(4.2)\xi} = v^0_{4.2}\left(-8 + 7v^0_{1.1} + 2v^0_{1.2} + \frac{9}{4}v^0_{2.1} + v^0_{2.2} - \frac{2v^0_{3.1} + 3v^0_{4.1} + v^0_{4.2}}{2v^0_{1.1}}\right) - \frac{2v^0_{6.2} + 3v^0_{7.1}}{4}$$

$$v^0_{(4.3)\xi} = v^0_{4.3}\left(-7 + \frac{9}{2}v^0_{1.1} + \frac{9}{2}v^0_{1.2} + \frac{3}{4}v^0_{2.2} + v^0_{2.3} - \frac{v^0_{3.2} + v^0_{4.4}}{v^0_{1.2}}\right) - \frac{6v^0_{6.2} + v^0_{7.2}}{4}$$

$$v^0_{(4.4)\xi} = v^0_{4.4}\left(-7 + 6v^0_{1.1} + 4v^0_{1.2} + v^0_{2.2} + \frac{3}{4}v^0_{2.3} - \frac{3v^0_{3.1} + v^0_{4.3}}{v^0_{1.2}}\right) - \frac{2v^0_{6.3} + v^0_{7.3}}{4}$$

$$v^0_{(5.1)\xi} = \frac{3}{4}v^0_{5.1}\left(-18 + 12v^0_{1.1} + 6v^0_{1.2} + 3v^0_{2.1} + 2v^0_{2.2} + v^0_{2.3} - \frac{3v^0_{6.1} + 2v^0_{6.2}}{v^0_{3.1}} - \frac{v^0_{6.3}}{v^0_{3.2}}\right)$$

$$v^0_{(6.1)\xi} = \frac{v^0_{6.1}}{2}\left(-28 + 21v^0_{1.1} + 7v^0_{1.2} + 9v^0_{2.1} + 3v^0_{2.2} + v^0_{2.3} - 2\frac{v^0_{3.1} + 3v^0_{4.1} + v^0_{4.2}}{v^0_{1.1}} - \frac{v^0_{4.4}}{v^0_{1.2}} - \frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{8.1}}{2}$$

$$v^0_{(6.2)\xi} = \frac{v^0_{6.2}}{4}\left(-54 + 38v^0_{1.1} + 20v^0_{1.2} + 12v^0_{2.1} + 6v^0_{2.2} + 4v^0_{2.3} - \frac{2v^0_{3.1} + 9v^0_{4.1} + 3v^0_{4.2}}{v^0_{1.1}} - \frac{2v^0_{3.2} + 4v^0_{4.4}}{v^0_{1.2}}\right.$$
$$\left. - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{3v^0_{8.1} + v^0_{8.2}}{4}$$

$$v^0_{(6.3)\xi} = \frac{v^0_{6.3}}{2}\left(-26 + 21v^0_{1.1} + 13v^0_{1.2} + 5v^0_{2.2} + 2v^0_{2.3} - \frac{6v^0_{3.1} + 5v^0_{4.3}}{v^0_{1.2}} - 3\frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{8.3}}{2}$$

$$v^0_{(7.1)\xi} = \frac{v^0_{7.1}}{2}\left(-27 + 22v^0_{1.1} + 6v^0_{1.2} + 9v^0_{2.1} + 3v^0_{2.2} - \frac{4v^0_{3.1} + 6v^0_{4.1} + 2v^0_{4.2}}{v^0_{1.1}}\right) - \frac{v^0_{8.1}}{2}$$

$$v^0_{(7.2)\xi} = v^0_{7.2}\left(-\frac{23}{2} + 6v^0_{1.1} + 8v^0_{1.2} + v^0_{2.2} + 2v^0_{2.3} - 2\frac{v^0_{3.2} + v^0_{4.4}}{v^0_{1.2}}\right) - \frac{3}{2}v^0_{8.2}$$

$$v^0_{(7.3)\xi} = v^0_{7.3}\left(-\frac{25}{2} + 12v^0_{1.1} + 6v^0_{1.2} + 2v^0_{2.2} + v^0_{2.3} - \frac{6v^0_{3.1} + 2v^0_{4.3}}{v^0_{1.2}}\right) - \frac{v^0_{8.3}}{2}$$

$$v^0_{(8.1)\xi} = \frac{v^0_{8.1}}{4}\left(-80 + 58v^0_{1.1} + 22v^0_{1.2} + 24v^0_{2.1} + 9v^0_{2.2} + 4v^0_{2.3} - \frac{4v^0_{3.1} + 18v^0_{4.1} + 6v^0_{4.2}}{v^0_{1.1}} - 4\frac{v^0_{4.4}}{v^0_{1.2}}\right.$$
$$\left. - 4\frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{v^0_{9.1}}{4}$$

$$v^0_{(8.2)\xi} = v^0_{8.2}\left(-19 + 12v^0_{1.1} + 8v^0_{1.2} + \frac{15}{4}v^0_{2.1} + 2v^0_{2.2} + 2v^0_{2.3} - \frac{3v^0_{4.1} + v^0_{4.2}}{v^0_{1.1}} - \frac{v^0_{3.2} + 2v^0_{4.4}}{v^0_{1.2}}\right.$$
$$\left. - \frac{v^0_{5.1}}{v^0_{3.1}}\right) - \frac{3}{4}v^0_{9.1}$$

$$v^0_{(8.3)\xi} = v^0_{8.3}\left(-19 + 15v^0_{1.1} + 9v^0_{1.2} + 4v^0_{2.2} + \frac{5}{4}v^0_{2.3} - \frac{3v^0_{3.1} + 4v^0_{4.3}}{v^0_{1.2}} - 3\frac{v^0_{5.1}}{v^0_{3.2}}\right) - \frac{v^0_{9.2}}{4}$$

$$v^0_{(9.1)\xi} = v^0_{9.1}\left(-\frac{53}{2} + 18v^0_{1.1} + 8v^0_{1.2} + \frac{15}{2}v^0_{2.1} + 3v^0_{2.2} + 2v^0_{2.3} - \frac{6v^0_{4.1} + 2v^0_{4.2}}{v^0_{1.1}} - 2\frac{v^0_{4.4}}{v^0_{1.2}} - 2\frac{v^0_{5.1}}{v^0_{3.1}}\right)$$

$$v^0_{(9.2)\xi} = \frac{3}{2}v^0_{9.2}\left(-17 + 12v^0_{1.1} + 8v^0_{1.2} + 4v^0_{2.2} + v^0_{2.3} - 4\frac{v^0_{4.3}}{v^0_{1.2}} - 4\frac{v^0_{5.1}}{v^0_{3.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$$\begin{array}{llll}
u^0_{1.1} = -1; & u^0_{1.2} = 1; & u^0_{2.1} = 1; & u^0_{2.2} = 1 \\
u^0_{2.3} = 1; & u^0_{3.1} = -1; & u^0_{3.2} = 1; & u^0_{4.1} = 1 \\
u^0_{4.2} = -1; & u^0_{4.3} = 1; & u^0_{4.4} = 1; & u^0_{5.1} = -1 \\
u^0_{6.1} = 1; & u^0_{6.2} = -1; & u^0_{6.3} = 1; & u^0_{7.1} = 1 \\
u^0_{7.2} = 1; & u^0_{7.3} = 1; & u^0_{8.1} = 1; & u^0_{8.2} = -1 \\
u^0_{8.3} = 1; & u^0_{9.1} = 1; & u^0_{9.2} = 1 &
\end{array}$$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$$\begin{array}{llll}
u^0_{(1.1)0} = 0; & u^0_{(1.2)0} = 2; & u^0_{(2.1)0} = -2; & u^0_{(2.2)0} = 2 \\
u^0_{(2.3)0} = 2; & u^0_{(3.1)0} = -1; & u^0_{(3.2)0} = 3; & u^0_{(4.1)0} = -1 \\
u^0_{(4.2)0} = -1; & u^0_{(4.3)0} = 3; & u^0_{(4.4)0} = 3; & u^0_{(5.1)0} = -2 \\
u^0_{(6.1)0} = 0; & u^0_{(6.2)0} = -2; & u^0_{(6.3)0} = 4; & u^0_{(7.1)0} = 0 \\
u^0_{(7.2)0} = 4; & u^0_{(7.3)0} = 4; & u^0_{(8.1)0} = 1; & u^0_{(8.2)0} = -3 \\
u^0_{(8.3)0} = 5; & u^0_{(9.1)0} = 2; & u^0_{(9.2)0} = 6 &
\end{array}$$

and

$$\begin{array}{llll}
u^0_{(1.1)\xi} = -2; & u^0_{(1.2)\xi} = 1; & u^0_{(2.1)\xi} = 3; & u^0_{(2.2)\xi} = 1 \\
u^0_{(2.3)\xi} = 1; & u^0_{(3.1)\xi} = -\frac{5}{2}; & u^0_{(3.2)\xi} = \frac{3}{2}; & u^0_{(4.1)\xi} = \frac{7}{2} \\
u^0_{(4.2)\xi} = -\frac{5}{2}; & u^0_{(4.3)\xi} = \frac{3}{2}; & u^0_{(4.4)\xi} = \frac{3}{2}; & u^0_{(5.1)\xi} = -3 \\
u^0_{(6.1)\xi} = 4; & u^0_{(6.2)\xi} = -3; & u^0_{(6.3)\xi} = 2; & u^0_{(7.1)\xi} = 4 \\
u^0_{(7.2)\xi} = 2; & u^0_{(7.3)\xi} = 2; & u^0_{(8.1)\xi} = \frac{9}{2}; & u^0_{(8.2)\xi} = -\frac{7}{2} \\
u^0_{(8.3)\xi} = \frac{5}{2}; & u^0_{(9.1)\xi} = 5; & u^0_{(9.2)\xi} = 3 &
\end{array}$$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}, u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$$\begin{array}{lll}
u^0_{(1.1)00} = 2v^0_{1.1}; & u^0_{(1.2)00} = 2v^0_{1.2}; & u^0_{(2.1)00} = 2v^0_{2.1} \\
u^0_{(2.2)00} = 2v^0_{2.2}; & u^0_{(2.3)00} = 2v^0_{2.3}; & u^0_{(3.1)00} = 4v^0_{1.1} - 2v^0_{1.2} \\
u^0_{(3.2)00} = 6v^0_{1.2}; & u^0_{(4.1)00} = -4v^0_{1.1} - 2v^0_{2.1}; & u^0_{(4.2)00} = 4v^0_{1.1} - 2v^0_{2.2} \\
u^0_{(4.3)00} = 4v^0_{1.2} + 2v^0_{2.2}; & u^0_{(4.4)00} = 4v^0_{1.2} + 2v^0_{2.3}; & u^0_{(5.1)00} = 6v^0_{1.1} - 6v^0_{1.2} \\
u^0_{(6.1)00} = -8v^0_{1.1} + 2v^0_{1.2} + 2v^0_{2.1}; & u^0_{(6.2)00} = 6v^0_{1.1} - 4v^0_{1.2} - 2v^0_{2.2}; & u^0_{(6.3)00} = 10v^0_{1.2} + 2v^0_{2.3} \\
u^0_{(7.1)00} = -8v^0_{1.1} + 2v^0_{2.1} + 2v^0_{2.2}; & u^0_{(7.2)00} = 8v^0_{1.2} + 4v^0_{2.2}; & u^0_{(7.3)00} = 8v^0_{1.2} + 4v^0_{2.3} \\
u^0_{(8.1)00} = -12v^0_{1.1} + 4v^0_{1.2} + 2v^0_{2.1} + 2v^0_{2.2}; & u^0_{(8.2)00} = 8v^0_{1.1} - 8v^0_{1.2} - 4v^0_{2.2}; & u^0_{(8.3)00} = 16v^0_{1.2} + 4v^0_{2.3}
\end{array}$$

$$u^0_{(9.1)00} = -16v^0_{1.1} + 8v^0_{1.2} + 2v^0_{2.1} + 4v^0_{2.2}; \quad u^0_{(9.2)00} = 24v^0_{1.2} + 6v^0_{2.3}$$

$$u^0_{(1.1)\xi 0} = -v^0_{1.1}; \quad u^0_{(1.2)\xi 0} = v^0_{1.2}; \quad u^0_{(2.1)\xi 0} = -3v^0_{2.1}$$
$$u^0_{(2.2)\xi} = v^0_{2.2}; \quad u^0_{(2.3)\xi 0} = v^0_{2.3}; \quad u^0_{(3.1)\xi 0} = -2v^0_{1.1} - v^0_{1.2}$$
$$u^0_{(3.2)\xi 0} = 3v^0_{1.2}; \quad u^0_{(4.1)\xi} = 2v^0_{1.1} - 3v^0_{2.1}; \quad u^0_{(4.2)\xi 0} = -2v^0_{1.1} - v^0_{2.2}$$
$$u^0_{(4.3)\xi 0} = 2v^0_{1.2} + v^0_{2.2}; \quad u^0_{(4.4)\xi 0} = 2v^0_{1.2} + v^0_{2.3}; \quad u^0_{(5.1)\xi} = -3v^0_{1.1} - 3v^0_{1.2}$$
$$u^0_{(6.1)\xi 0} = 4v^0_{1.1} + v^0_{1.2} - 3v^0_{2.1}; \quad u^0_{(6.2)\xi 0} = -3v^0_{1.1} - 2v^0_{1.2} - v^0_{2.2}; \quad u^0_{(6.3)\xi 0} = 5v^0_{1.2} + v^0_{2.3}$$
$$u^0_{(7.1)\xi 0} = 4v^0_{1.1} - 3v^0_{2.1} + v^0_{2.2}; \quad u^0_{(7.2)\xi 0} = 4v^0_{1.2} + 2v^0_{2.2}; \quad u^0_{(7.3)\xi 0} = 4v^0_{1.2} + 4v^0_{2.3}$$
$$u^0_{(8.1)\xi 0} = 6v^0_{1.1} + 2v^0_{1.2} - 3v^0_{2.1} + v^0_{2.2}; \quad u^0_{(8.2)\xi 0} = -4v^0_{1.1} - 4v^0_{1.2} - 2v^0_{2.2}; \quad u^0_{(8.3)\xi 0} = 8v^0_{1.2} + 2v^0_{2.3}$$
$$u^0_{(9.1)\xi 0} = 8v^0_{1.1} + 4v^0_{1.2} - 3v^0_{2.1} + 2v^0_{2.2}; \quad u^0_{(9.2)\xi 0} = 12v^0_{1.2} + 3v^0_{2.3}$$

and

$$u^0_{(1.1)\xi\xi} = -\frac{3}{2}v^0_{1.1}; \quad u^0_{(1.2)\xi\xi} = \frac{v^0_{1.2}}{2}; \quad u^0_{(2.1)\xi\xi} = \frac{9}{2}v^0_{2.1}$$
$$u^0_{(2.2)\xi\xi} = \frac{v^0_{2.2}}{2}; \quad u^0_{(2.3)\xi\xi} = \frac{v^0_{2.3}}{2}; \quad u^0_{(3.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.2}}{2}$$
$$u^0_{(3.2)\xi\xi} = \frac{3}{2}v^0_{1.2}; \quad u^0_{(4.1)\xi\xi} = 3v^0_{1.1} + \frac{9}{2}v^0_{2.1}; \quad u^0_{(4.2)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{2.2}}{2}$$
$$u^0_{(4.3)\xi\xi} = v^0_{1.2} + \frac{v^0_{2.2}}{2}; \quad u^0_{(4.4)\xi\xi} = v^0_{1.2} + \frac{v^0_{2.3}}{2}; \quad u^0_{(5.1)\xi\xi} = -\frac{9v^0_{1.1} + 3v^0_{1.2}}{2}$$
$$u^0_{(6.1)\xi\xi} = 6v^0_{1.1} + \frac{v^0_{1.2} + 9v^0_{2.1}}{2}; \quad u^0_{(6.2)\xi\xi} = -\frac{9v^0_{1.1} + v^0_{2.2}}{2} - v^0_{1.2}; \quad u^0_{(6.3)\xi\xi} = \frac{5v^0_{1.2} + v^0_{2.3}}{2}$$
$$u^0_{(7.1)\xi\xi} = 6v^0_{1.1} + \frac{9v^0_{2.1} + v^0_{2.2}}{2}; \quad u^0_{(7.2)\xi\xi} = 2v^0_{1.2} + v^0_{2.2}; \quad u^0_{(7.3)\xi\xi} = 2v^0_{1.2} + v^0_{2.3}$$
$$u^0_{(8.1)\xi\xi} = 9v^0_{1.1} + v^0_{1.2} + \frac{9v^0_{2.1} + v^0_{2.2}}{2}; \quad u^0_{(8.2)\xi\xi} = -6v^0_{1.1} - 2v^0_{1.2} - v^0_{2.2}; \quad u^0_{(8.3)\xi\xi} = 4v^0_{1.2} + v^0_{2.3}$$
$$u^0_{(9.1)\xi\xi} = 12v^0_{1.1} + 2v^0_{1.2} + \frac{9}{2}v^0_{2.1} + v^0_{2.2}; \quad u^0_{(9.2)\xi\xi} = 6v^0_{1.2} + \frac{3}{2}v^0_{2.3}$$

A.2.4 Thermodynamics of $L1_1$ phase using tetrahedron – octahedron approximation

The tetrahedron–octahedron clusters considered for $L1_1$ phase is shown in Figure A.6 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.6.

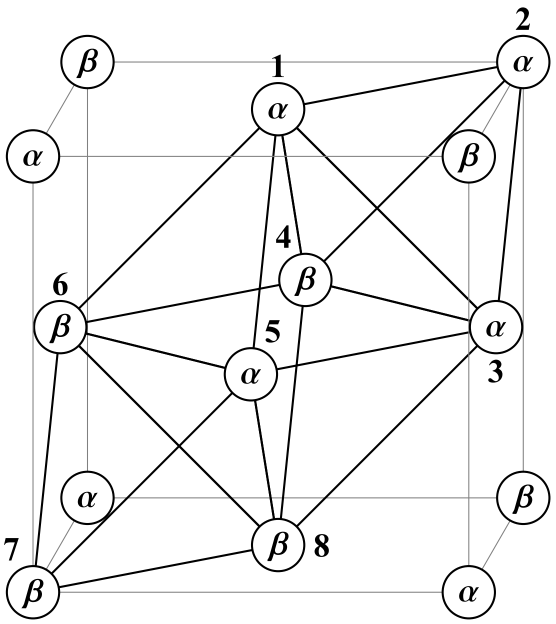

Figure A.6: The tetrahedron–octahedron basic clusters in the $L1_1$ phase along with the sublattice sites designated α and β.

Table A.6: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $L1_1$ phase using tetrahedron–octahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Octahedron	$\alpha\alpha\alpha\beta\beta\beta$ (1,3,5,6,8)	9.1	1	1
Square pyramid	$\alpha\alpha\beta\beta\beta$ (1,5,4,6,8)	8.2	3	0
	$\alpha\alpha\alpha\beta\beta$ (1,3,5,4,6)	8.1	3	
Square	$\alpha\alpha\beta\beta$ (1,3,6,8)	7.1	3	0
Irregular tetrahedron	$\alpha\beta\beta\beta$ (1,4,6,8)	6.3	3	0
	$\alpha\alpha\beta\beta$ (1,3,4,6)	6.2	6	
	$\alpha\alpha\alpha\beta$ (1,3,5,6)	6.1	3	

cont ...

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Regular tetrahedron	$\alpha\beta\beta\beta$ (5,6,7,8)	5.2	1	2
	$\alpha\alpha\alpha\beta$ (1,2,3,4)	5.1	1	
Isosceles triangle	$\alpha\beta\beta$ (1,4,8)	4.2	6	0
	$\alpha\alpha\beta$ (1,3,6)	4.1	6	
Equilateral triangle	$\beta\beta\beta$ (4,6,8)	3.4	1	-1
	$\alpha\beta\beta$ (1,4,6)	3.3	3	
	$\alpha\alpha\beta$ (1,3,4)	3.2	3	
	$\alpha\alpha\alpha$ (1,2,3)	3.1	1	
II-n pair	$\alpha\beta$ (1,8)	2.1	3	0
I-n pair	$\beta\beta$ (3,4)	1.3	3/2	1
	$\alpha\beta$ (1,4)	1.2	3	
	$\alpha\alpha$ (1,5)	1.1	3/2	
Point	β (4)	0.2	1/2	-1
	α (1)	0.1	1/2	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2})/2 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{\eta_1\eta_4^2}{\sqrt[8]{\eta_9}}\sqrt{\frac{\eta_7}{\eta_5\eta_6\eta_8}}; \quad v^0_{1.2} = \frac{1}{\eta_1\eta_9^{1/8}}\sqrt{\frac{\eta_6\eta_7}{\eta_5}}; \quad v^0_{1.3} = \frac{\eta_1}{\eta_4^2\eta_9^{1/8}}\sqrt{\frac{\eta_7\eta_8}{\eta_5\eta_6}}$$

$$v^0_{2.1} = \frac{\sqrt{\eta_7}}{\eta_2\eta_9^{1/16}}; \quad v^0_{3.1} = \frac{\eta_1^3\eta_3\eta_4^6\eta_7^{3/2}}{\eta_5\eta_8^{3/4}\eta_9^{1/4}}; \quad v^0_{3.2} = \frac{\eta_4^2\eta_7^{3/2}}{\eta_1\eta_3\eta_5\eta_8^{1/4}\eta_9^{1/4}}$$

$$v^0_{3.3} = \frac{\eta_3\eta_7^{3/2}\eta_8^{1/4}}{\eta_1\eta_4^2\eta_5\eta_9^{1/4}}; \quad v^0_{3.4} = \frac{\eta_1^3\eta_7^{3/2}\eta_8^{3/4}}{\eta_3\eta_4^6\eta_5\eta_9^{1/4}}; \quad v^0_{4.1} = \frac{\eta_4\eta_7}{\eta_2\eta_5\sqrt[4]{\eta_8}\eta_9^{3/16}}$$

$$v^0_{4.2} = \frac{\eta_7 \eta_8^{1/4}}{\eta_2 \eta_4 \eta_5 \eta_9^{3/16}}; \qquad v^0_{5.1} = \frac{\eta_4^6 \eta_7^3}{\eta_3^2 \eta_5^2 \eta_9^{1/4}}; \qquad v^0_{5.2} = \frac{\eta_3^2 \eta_7^3}{\eta_4^6 \eta_5^2 \eta_9^{1/4}}$$

$$v^0_{6.1} = \frac{\eta_1 \eta_4^4 \eta_7^2}{\eta_5^{3/2} \eta_2 \sqrt{\eta_6} \eta_8 \eta_9^{7/16}}; \qquad v^0_{6.2} = \frac{\eta_7^2 \sqrt{\eta_6}}{\eta_1 \eta_2 \eta_5^{3/2} \eta_9^{7/16}}; \qquad v^0_{6.3} = \frac{\eta_1 \eta_7^2 \eta_8}{\eta_2 \eta_4^4 \eta_5^{3/2} \sqrt{\eta_6} \eta_9^{7/16}}$$

$$v^0_{7.1} = \frac{\eta_7^2}{\eta_2^2 \eta_5^2 \eta_9^{3/8}}; \qquad v^0_{8.1} = \frac{\eta_4^2 \eta_7^3}{\eta_2^2 \eta_5^2 \sqrt{\eta_8} \eta_9^{5/8}}; \qquad v^0_{8.2} = \frac{\eta_7^3 \sqrt{\eta_8}}{\eta_2^2 \eta_4^2 \eta_5^2 \eta_9^{5/8}}$$

$$v^0_{9.1} = \frac{\eta_7^{9/2}}{\eta_2^3 \eta_5^2 \eta_9^{15/16}}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(-1 - 3v^0_{1.1} + 4v^0_{1.2} + 2v^0_{2.1}\right) + v^0_{3.1} - v^0_{3.2} - 2v^0_{4.1}$$

$$v^0_{(1.2)0} = 2v^0_{1.2}\left(-v^0_{1.1} + v^0_{1.3}\right) + v^0_{3.2} - v^0_{3.3} + v^0_{4.1} - v^0_{4.2}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(1 - 4v^0_{1.2} + 3v^0_{1.3} - 2v^0_{2.1}\right) + v^0_{3.3} - v^0_{3.4} + 2v^0_{4.2}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(-v^0_{1.1} + v^0_{1.3}\right) + v^0_{4.1} - v^0_{4.2}$$

$$v^0_{(3.1)0} = \frac{v^0_{3.1}}{2}\left(-5 - 12v^0_{1.1} + 15v^0_{1.2} + 9v^0_{2.1} + 3\frac{v^0_{3.1} - 2v^0_{4.1}}{v^0_{1.1}}\right) - \frac{v^0_{5.1} + 3v^0_{6.1}}{2}$$

$$v^0_{(3.2)0} = \frac{v^0_{3.2}}{2}\left(-3 - 8v^0_{1.1} + 7v^0_{1.2} + 6v^0_{1.3} + 3v^0_{2.1} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.3} - v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}}\right) + \frac{v^0_{5.1} + v^0_{6.1}}{2} - v^0_{6.2}$$

$$v^0_{(3.3)0} = \frac{v^0_{3.3}}{2}\left(3 - 6v^0_{1.1} - 7v^0_{1.2} + 8v^0_{1.3} - 3v^0_{2.1} + 2\frac{v^0_{3.2} + v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}} + \frac{v^0_{3.3} + 2v^0_{4.2}}{v^0_{1.3}}\right) - \frac{v^0_{5.2} + v^0_{6.3}}{2} + v^0_{6.2}$$

$$v^0_{(3.4)0} = \frac{v^0_{3.4}}{2}\left(5 - 15v^0_{1.2} + 12v^0_{1.3} - 9v^0_{2.1} - 3\frac{v^0_{3.4} - v^0_{4.2}}{v^0_{1.3}}\right) + \frac{v^0_{5.2} + 3v^0_{6.3}}{2}$$

$$v^0_{(4.1)0} = \frac{v^0_{4.1}}{2}\left(-2 - 8v^0_{1.1} + 6v^0_{1.2} + 4v^0_{1.3} + 3v^0_{2.1} + \frac{v^0_{3.1} - v^0_{3.2} - 2v^0_{4.1}}{v^0_{1.1}} + \frac{v^0_{3.2} - v^0_{3.3} + v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}}\right) + \frac{1}{2}\left(v^0_{6.1} - v^0_{6.2} - v^0_{7.1}\right)$$

$$v^0_{(4.2)0} = \frac{v^0_{4.2}}{2}\left(2 - 4v^0_{1.1} - 6v^0_{1.2} + 8v^0_{1.3} - 3v^0_{2.1} + \frac{v^0_{3.2} - v^0_{3.3} + v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}} + \frac{v^0_{3.3} - v^0_{3.4} + 2v^0_{4.2}}{v^0_{1.3}}\right) + \frac{1}{2}\left(v^0_{6.2} - v^0_{6.3} + v^0_{7.1}\right)$$

$$v^0_{(5.1)0} = 3v^0_{5.1}\left(-1 - 2v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + v^0_{2.1} - \frac{v^0_{6.1}}{2v^0_{3.1}} + \frac{v^0_{6.1} - 2v^0_{6.2}}{2v^0_{3.2}}\right)$$

$$v^0_{(5.2)0} = 3v^0_{5.2}\left(1 - v^0_{1.1} - 2v^0_{1.2} + 2v^0_{1.3} - v^0_{2.1} + \frac{v^0_{6.3}}{2v^0_{3.4}} + \frac{2v^0_{6.2} - v^0_{6.3}}{2v^0_{3.3}}\right)$$

$$v^0_{(6.1)0} = v^0_{6.1}\left(-3 - 7v^0_{1.1} + 7v^0_{1.2} + 3v^0_{1.3} + 4v^0_{2.1} + \frac{v^0_{3.1} - 3v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{3.3} - v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{5.1}}{2v^0_{3.1}}\right.$$

$$+ \frac{v^0_{5.1}}{2v^0_{3.2}}\Bigg) - v^0_{8.1}$$

$$v^0_{(6.2)0} = \frac{v^0_{6.1}}{2}\Bigg(-10v^0_{1.1} + 10v^0_{1.3} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} + \frac{v^0_{3.2} - v^0_{3.3} + 3v^0_{4.1} - 3v^0_{4.2}}{v^0_{1.2}} + \frac{v^0_{3.3} + 2v^0_{4.2}}{v^0_{1.3}}$$

$$+ \frac{v^0_{5.1}}{v^0_{3.2}} - \frac{v^0_{5.2}}{v^0_{3.3}}\Bigg) + \frac{v^0_{8.1} - v^0_{8.2}}{2}$$

$$v^0_{(6.3)0} = v^0_{6.3}\Bigg(3 - 3v^0_{1.1} - 7v^0_{1.2} + 7v^0_{1.3} - 4v^0_{2.1} + \frac{v^0_{3.2} + v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.4} - 3v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.2}}{2v^0_{3.3}}$$

$$+ \frac{v^0_{5.2}}{2v^0_{3.4}}\Bigg) + v^0_{8.2}$$

$$v^0_{(7.1)0} = \frac{v^0_{7.1}}{2}\Bigg(-10v^0_{1.1} + 10v^0_{1.3} + \frac{v^0_{3.1} - v^0_{3.2} - 2v^0_{4.1}}{v^0_{1.1}} + 2\frac{v^0_{3.2} - v^0_{3.3} + v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}}$$

$$+ \frac{v^0_{3.3} - v^0_{3.4} + 2v^0_{4.2}}{v^0_{1.3}}\Bigg) + \frac{v^0_{8.1} - v^0_{8.2}}{2}$$

$$v^0_{(8.1)0} = \frac{v^0_{8.1}}{2}\Bigg(-4 - 16v^0_{1.1} + 8v^0_{1.2} + 12v^0_{1.3} + 5v^0_{2.1} + \frac{v^0_{3.1} - 6v^0_{4.1}}{v^0_{1.1}} - \frac{2v^0_{3.3} - 4v^0_{4.1} + 4v^0_{4.2}}{v^0_{1.2}}$$

$$+ \frac{v^0_{3.3} + 2v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.1}} + 2\frac{v^0_{5.1}}{v^0_{3.2}} - \frac{v^0_{5.2}}{v^0_{3.3}}\Bigg) - \frac{v^0_{9.1}}{2}$$

$$v^0_{(8.2)0} = \frac{v^0_{8.2}}{2}\Bigg(4 - 12v^0_{1.1} - 8v^0_{1.2} + 16v^0_{1.3} - 5v^0_{2.1} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{3.4} - 6v^0_{4.2}}{v^0_{1.3}}$$

$$+ \frac{2v^0_{3.2} + 4v^0_{4.1} - 4v^0_{4.2}}{v^0_{1.2}} + \frac{v^0_{5.1}}{v^0_{3.2}} - 2\frac{v^0_{5.2}}{v^0_{3.3}} + \frac{v^0_{5.2}}{v^0_{3.4}}\Bigg) + \frac{v^0_{9.1}}{2}$$

$$v^0_{(9.1)0} = 3v^0_{9.1}\Bigg(-3v^0_{1.1} + 3v^0_{1.3} - \frac{v^0_{4.1}}{v^0_{1.1}} + \frac{v^0_{4.1} - v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.1}}{6v^0_{3.1}} + \frac{v^0_{5.1}}{2v^0_{3.2}} - \frac{v^0_{5.2}}{2v^0_{3.3}} + \frac{v^0_{5.2}}{6v^0_{3.4}}\Bigg)$$

and

$$v^0_{(1.1)\xi} = v^0_{1.1}\left(-5 + 3v^0_{1.1} + 4v^0_{1.2} + 2v^0_{2.1}\right) - v^0_{3.1} - v^0_{3.2} - 2v^0_{4.1}$$

$$v^0_{(1.2)\xi} = v^0_{1.2}\left(-5 + 2v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.1}\right) - v^0_{3.2} - v^0_{3.3} - v^0_{4.1} - v^0_{4.2}$$

$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-5 + 4v^0_{1.2} + 3v^0_{1.3} + 2v^0_{2.1}\right) - v^0_{3.3} - v^0_{3.4} - 2v^0_{4.2}$$

$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-3 + v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + v^0_{2.1}\right) - v^0_{4.1} - v^0_{4.2}$$

$$v^0_{(3.1)\xi} = \frac{v^0_{3.1}}{2}\Bigg(-23 + 12v^0_{1.1} + 15v^0_{1.2} + 9v^0_{2.1} - 3\frac{v^0_{3.1} + 2v^0_{4.1}}{v^0_{1.1}}\Bigg) - \frac{v^0_{5.1} + 3v^0_{6.1}}{2}$$

$$v^0_{(3.2)\xi} = \frac{v^0_{3.2}}{2}\Bigg(-23 + 8v^0_{1.1} + 13v^0_{1.2} + 6v^0_{1.3} + 9v^0_{2.1} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.3} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}}\Bigg)$$

$$- v^0_{6.2} - \frac{v^0_{5.1} + v^0_{6.1}}{2}$$

$$v^0_{(3.3)\xi} = \frac{v^0_{3.3}}{2}\Bigg(-23 + 6v^0_{1.1} + 13v^0_{1.2} + 8v^0_{1.3} + 9v^0_{2.1} - 2\frac{v^0_{3.2} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.3} + 2v^0_{4.2}}{v^0_{1.3}} - 23\Bigg)$$

$$- v^0_{6.2} - \frac{v^0_{5.2} + v^0_{6.3}}{2}$$

$$v^0_{(3.4)\xi} = \frac{v^0_{3.4}}{2}\left(-23 + 15v^0_{1.2} + 12v^0_{1.3} + 9v^0_{2.1} - 3\frac{v^0_{3.4} + 2v^0_{4.2}}{v^0_{1.3}}\right) - \frac{v^0_{5.2} + 3v^0_{6.3}}{2}$$

$$v^0_{(4.1)\xi} = \frac{v^0_{4.1}}{2}\left(-20 + 8v^0_{1.1} + 12v^0_{1.2} + 4v^0_{1.3} + 7v^0_{2.1} - \frac{v^0_{3.1} + v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{3.2} + v^0_{3.3} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}}\right) - \frac{1}{2}\left(v^0_{6.1} + v^0_{6.2} + v^0_{7.1}\right)$$

$$v^0_{(4.2)\xi} = \frac{v^0_{4.2}}{2}\left(-20 + 4v^0_{1.1} + 12v^0_{1.2} + 8v^0_{1.3} + 7v^0_{2.1} - \frac{v^0_{3.2} + v^0_{3.3} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.3} + v^0_{3.4} + 2v^0_{4.2}}{v^0_{1.3}}\right) - \frac{1}{2}\left(v^0_{6.2} + v^0_{6.3} + v^0_{7.1}\right)$$

$$v^0_{(5.1)\xi} = 3v^0_{5.1}\left(-6 + 2v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + 2v^0_{2.1} - \frac{v^0_{6.1}}{2v^0_{3.1}} - \frac{v^0_{6.1} + 2v^0_{6.2}}{2v^0_{3.2}}\right)$$

$$v^0_{(5.2)\xi} = 3v^0_{5.2}\left(-6 + v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.1} - \frac{2v^0_{6.2} + v^0_{6.3}}{2v^0_{3.3}} - \frac{v^0_{6.3}}{2v^0_{3.4}}\right)$$

$$v^0_{(6.1)\xi} = v^0_{6.1}\left(-18 + 7v^0_{1.1} + 10v^0_{1.2} + 3v^0_{1.3} + 7v^0_{2.1} - \frac{v^0_{3.1} + 3v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{3.3} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{5.1}}{2v^0_{3.1}} - \frac{v^0_{5.1}}{2v^0_{3.2}}\right) - v^0_{8.1}$$

$$v^0_{(6.2)\xi} = \frac{v^0_{6.2}}{2}\left(-36 + 10v^0_{1.1} + 20v^0_{1.2} + 10v^0_{1.3} + 14v^0_{2.1} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{3.2} + v^0_{3.3} + 3v^0_{4.1} + 3v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.3} + 2v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.2}} - \frac{v^0_{5.2}}{v^0_{3.3}}\right) - \frac{v^0_{8.1} + v^0_{8.2}}{2}$$

$$v^0_{(6.3)\xi} = v^0_{6.3}\left(-18 + 3v^0_{1.1} + 10v^0_{1.2} + 7v^0_{1.3} + 7v^0_{2.1} - \frac{v^0_{3.2} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.4} + 3v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.2}}{2v^0_{3.3}} - \frac{v^0_{5.2}}{2v^0_{3.4}}\right) - v^0_{8.2}$$

$$v^0_{(7.1)\xi} = \frac{v^0_{7.1}}{2}\left(-17 + 10v^0_{1.1} + 20v^0_{1.2} + 10v^0_{1.3} + 6v^0_{2.1} - \frac{v^0_{3.1} + v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{3.2} + v^0_{3.3} + v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.3} + v^0_{3.4} + 2v^0_{4.2}}{v^0_{1.3}}\right) - \frac{v^0_{8.1} + v^0_{8.2}}{2}$$

$$v^0_{(8.2)\xi} = \frac{v^0_{8.2}}{2}\left(-52 + 12v^0_{1.1} + 28v^0_{1.2} + 16v^0_{1.3} + 21v^0_{2.1} - \frac{v^0_{3.2} + 2v^0_{4.1}}{v^0_{1.1}} - \frac{2v^0_{3.2} + 4v^0_{4.1} + 4v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{3.4} + 6v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.2}} - 2\frac{v^0_{5.2}}{v^0_{3.3}} - \frac{v^0_{5.2}}{v^0_{3.4}}\right) - \frac{v^0_{9.1}}{2}$$

$$v^0_{(9.1)\xi} = \frac{v^0_{9.1}}{2}\left(-10 + 18v^0_{1.1} + 36v^0_{1.2} + 18v^0_{1.3} + 30v^0_{2.1} - 6\frac{v^0_{4.1}}{v^0_{1.1}} - 6\frac{v^0_{4.1} + v^0_{4.2}}{v^0_{1.2}} - 6\frac{v^0_{4.2}}{v^0_{1.3}} - \frac{v^0_{5.1}}{v^0_{3.1}} - \frac{3v^0_{5.1}}{v^0_{3.2}} - \frac{3v^0_{5.2}}{v^0_{3.3}} - \frac{v^0_{5.2}}{v^0_{3.4}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = 1$; $u^0_{1.2} = -1$; $u^0_{1.3} = 1$; $u^0_{2.1} = -1$
$u^0_{3.1} = -1$; $u^0_{3.2} = 1$; $u^0_{3.3} = -1$; $u^0_{3.4} = 1$
$u^0_{4.1} = 1$; $u^0_{4.2} = -1$; $u^0_{5.1} = -1$; $u^0_{5.2} = -1$
$u^0_{6.1} = -1$; $u^0_{6.2} = 1$; $u^0_{6.3} = -1$; $u^0_{7.1} = 1$
$u^0_{8.1} = -1$; $u^0_{8.2} = 1$; $u^0_{9.1} = -1$

The limiting first derivatives of the CFs with respect to u_0 and ξ in the orthogonal basis in the limit of perfect ordering,$u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{1.10} = -2$; $u^0_{1.20} = 0$; $u^0_{1.30} = 2$; $u^0_{2.10} = 0$
$u^0_{3.10} = 3$; $u^0_{3.20} = -1$; $u^0_{3.30} = -1$; $u^0_{3.40} = 3$
$u^0_{4.10} = -1$; $u^0_{4.20} = -1$; $u^0_{5.10} = 2$; $u^0_{5.20} = -2$
$u^0_{6.10} = 2$; $u^0_{6.20} = 0$; $u^0_{6.30} = -2$; $u^0_{7.10} = 0$
$u^0_{8.10} = 1$; $u^0_{8.20} = 1$; $u^0_{9.10} = 0$

and

$u^0_{1.1\xi} = 2$; $u^0_{1.2\xi} = -2$; $u^0_{1.3\xi} = 2$; $u^0_{2.1\xi} = -2$
$u^0_{3.1\xi} = -3$; $u^0_{3.2\xi} = 3$; $u^0_{3.3\xi} = -3$; $u^0_{3.4\xi} = 3$
$u^0_{4.1\xi} = 3$; $u^0_{4.2\xi} = -3$; $u^0_{5.1\xi} = -4$; $u^0_{5.2\xi} = -4$
$u^0_{6.1\xi} = -4$; $u^0_{6.2\xi} = 4$; $u^0_{6.3\xi} = -4$; $u^0_{7.1\xi} = 4$
$u^0_{8.1\xi} = -5$; $u^0_{8.2\xi} = 5$; $u^0_{9.1\xi} = -6$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}, u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1}$; $u^0_{(1.2)00} = 2v^0_{1.2}$; $u^0_{(1.3)00} = 2v^0_{1.3}$; $u^0_{(2.1)00} = 2v^0_{2.1}$
$u^0_{(3.1)00} = -6v^0_{1.1}$; $u^0_{(3.2)00} = 2v^0_{1.1} - 4v^0_{1.2}$; $u^0_{(3.3)00} = 4v^0_{1.2} - 2v^0_{1.3}$; $u^0_{(3.4)00} = 6v^0_{1.3}$
$u^0_{(4.1)00} = 2v^0_{1.1} - 2v^0_{1.2} - 2v^0_{2.1}$; $u^0_{(4.2)00} = 2v^0_{1.2} - 2v^0_{1.3} + 2v^0_{2.1}$
$u^0_{(5.1)00} = 6v^0_{1.2} - 6v^0_{1.1}$; $u^0_{(5.2)00} = 6v^0_{1.2} - 6v^0_{1.3}$
$u^0_{(6.1)00} = -6v^0_{1.1} + 4v^0_{1.2} + 2v^0_{2.1}$; $u^0_{(6.2)00} = 2v^0_{1.1} - 6v^0_{1.2} + 2v^0_{1.3} - 2v^0_{2.1}$
$u^0_{(6.3)00} = 4v^0_{1.2} - 6v^0_{1.3} + 2v^0_{2.1}$; $u^0_{(7.1)00} = 2v^0_{1.1} - 4v^0_{1.2} + 2v^0_{1.3} - 4v^0_{2.1}$
$u^0_{(8.1)00} = -6v^0_{1.1} + 8v^0_{1.2} - 2v^0_{1.3} + 4v^0_{2.1}$; $u^0_{(8.2)00} = 2v^0_{1.1} - 8v^0_{1.2} + 6v^0_{1.3} - 4v^0_{2.1}$
$u^0_{(9.1)00} = -6v^0_{1.1} + 12v^0_{1.2} - 6v^0_{1.3} + 6v^0_{2.1}$

$u^0_{(1.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(1.2)\xi 0} = 0$; $u^0_{(1.3)\xi 0} = 2v^0_{1.3}$; $u^0_{(2.1)\xi 0} = 0$
$u^0_{(3.1)\xi 0} = 6v^0_{1.1}$; $u^0_{(3.2)\xi 0} = -2v^0_{1.1}$; $u^0_{(3.3)\xi 0} = -2v^0_{1.3}$; $u^0_{(3.4)\xi 0} = 6v^0_{1.3}$
$u^0_{(4.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(4.2)\xi 0} = -2v^0_{1.3}$; $u^0_{(5.1)\xi 0} = 6v^0_{1.1}$; $u^0_{(5.2)\xi 0} = -6v^0_{1.3}$

$$u^0_{(6.1)\xi 0} = 6v^0_{1.1}; \quad u^0_{(6.2)\xi 0} = 2v^0_{1.3} - 2v^0_{1.1}; \quad u^0_{(6.3)\xi 0} = -6v^0_{1.3}; \quad u^0_{(7.1)\xi 0} = 2v^0_{1.3} - 2v^0_{1.1}$$
$$u^0_{(8.1)\xi 0} = 6v^0_{1.1} - 2v^0_{1.3}; \quad u^0_{(8.2)\xi 0} = 6v^0_{1.3} - 2v^0_{1.1}; \quad u^0_{(9.1)\xi 0} = 6v^0_{1.1} - 6v^0_{1.3}$$

and

$$u^0_{1.1\xi\xi} = 2v^0_{1.1}; \quad u^0_{1.2\xi\xi} = -2v^0_{1.2}; \quad u^0_{1.3\xi\xi} = 2v^0_{1.3}; \quad u^0_{2.1\xi\xi} = -2v^0_{2.1}$$
$$u^0_{3.1\xi\xi} = -6v^0_{1.1}; \quad u^0_{3.2\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2}; \quad u^0_{3.3\xi\xi} = -4v^0_{1.2} - 2v^0_{1.3}; \quad u^0_{3.4\xi\xi} = 6v^0_{1.3}$$

$$u^0_{4.1\xi\xi} = 2v^0_{1.1} + 2v^0_{1.2} + 2v^0_{2.1}; \quad u^0_{4.2\xi\xi} = -2v^0_{1.2} - 2v^0_{1.3} - 2v^0_{2.1}$$
$$u^0_{5.1\xi\xi} = -6v^0_{1.1} - 6v^0_{1.2}; \quad u^0_{5.2\xi\xi} = -6v^0_{1.2} - 6v^0_{1.3}$$
$$u^0_{6.1\xi\xi} = -6v^0_{1.1} - 4v^0_{1.2} - 2v^0_{2.1}; \quad u^0_{6.2\xi\xi} = 2v^0_{1.1} + 6v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.1}$$
$$u^0_{6.3\xi\xi} = -4v^0_{1.2} - 6v^0_{1.3} - 2v^0_{2.1}; \quad u^0_{7.1\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 4v^0_{2.1}$$
$$u^0_{8.1\xi\xi} = -6v^0_{1.1} - 8v^0_{1.2} - 2v^0_{1.3} - 4v^0_{2.1}; \quad u^0_{8.2\xi\xi} = 2v^0_{1.1} + 8v^0_{1.2} + 6v^0_{1.3} + 4v^0_{2.1}$$
$$u^0_{9.1\xi\xi} = -6v^0_{1.1} - 12v^0_{1.2} - 6v^0_{1.3} - 6v^0_{2.1}$$

A.3 CPH based ordered phases

A.3.1 Thermodynamics of $B19$ phase using triangle–tetrahedron approximation

The triangle–tetrahedron clusters considered for $B19$ phase is shown in Figure A.7 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.7.

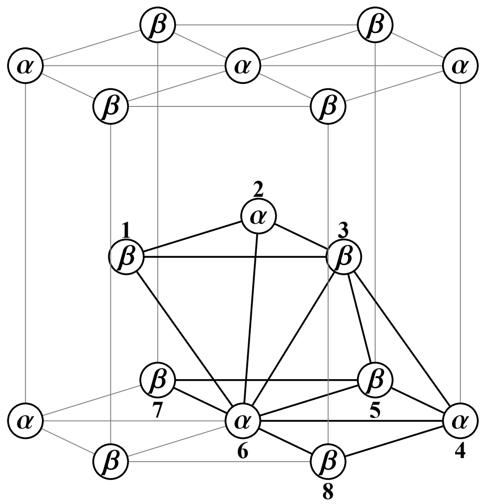

Figure A.7: The triangle–tetrahedron basic clusters in $B19$ phase along with the sublattice sites designated α and β.

Table A.7: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $B19$ phase using triangle–tetrahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Regular tetrahedron	$\alpha\alpha\beta\beta$(T2, $\alpha\alpha$OP) (2,6,1,3)	6.2	1	1
	$\alpha\alpha\beta\beta$(T1, $\alpha\alpha$IP) (4,6,3,5)	6.1	1	
Equilateral triangle (OP)	$\alpha\beta\beta$(T2) (6,1,3)	5.4	1	0
	$\alpha\beta\beta$(T1) (6,3,5)	5.3	2	
	$\alpha\alpha\beta$(T2) (2,6,1)	5.2	2	
	$\alpha\alpha\beta$(T1) (4,6,3)	5.1	1	
Equilateral triangle (OB)	$\alpha\beta\beta$ (6,5,7)	4.2	1/2	1
	$\alpha\alpha\beta$ (4,6,8)	4.1	1/2	

cont . . .

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Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Equilateral triangle (TB)	$\alpha\beta\beta$ (2,1,3)	3.2	1/2	-1
	$\alpha\alpha\beta$ (4,6,5)	3.1	1/2	
I-n pair (OP)	$\beta\beta$ (3,5)	2.3	1/2	-1
	$\alpha\beta$ (4,3)	2.2	2	
	$\alpha\alpha$ (2,6)	2.1	1/2	
I-n pair (IP)	$\beta\beta$ (1,3)	1.4	1/2	-1
	$\alpha\beta$(T2) (2,1)	1.3	1	
	$\alpha\beta$(T1) (4,5)	1.2	1	
	$\alpha\alpha$ (4,6)	1.1	1/2	
Point	β (1)	0.2	1/2	5
	α (2)	0.1	1/2	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2})/2 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \eta_1\eta_5\sqrt{\eta_3\eta_4\eta_6}; \quad v^0_{1.2} = \frac{1}{\eta_1\eta_5}\sqrt{\frac{\eta_3\eta_6}{\eta_4}}; \quad v^0_{1.3} = \frac{\eta_5}{\eta_1}\sqrt{\frac{\eta_4\eta_6}{\eta_3}}$$

$$v^0_{1.4} = \frac{\eta_1}{\eta_5}\sqrt{\frac{\eta_6}{\eta_3\eta_4}}; \quad v^0_{2.1} = \eta_2\eta_5^2\sqrt{\eta_6}; \quad v^0_{2.2} = \frac{\sqrt{\eta_6}}{\eta_2}$$

$$v^0_{2.3} = \frac{\eta_2}{\eta_5^2}\sqrt{\eta_6}; \quad v^0_{3.1} = \frac{1}{\eta_1\eta_5}\sqrt{\frac{\eta_3\eta_6}{\eta_4}}; \quad v^0_{3.2} = \frac{\eta_5}{\eta_1}\sqrt{\frac{\eta_4\eta_6}{\eta_3}}$$

$$v^0_{4.1} = \frac{\eta_5^3\eta_6^{3/2}}{\eta_1}\sqrt{\frac{\eta_4}{\eta_3}}; \quad v^0_{4.2} = \frac{\eta_6^{3/2}}{\eta_1\eta_5^3}\sqrt{\frac{\eta_3}{\eta_4}}; \quad v^0_{5.1} = \frac{\eta_1\eta_6}{\eta_2^2}\sqrt{\eta_3\eta_4}$$

$$v^0_{5.2} = \frac{\eta_5^2\eta_6}{\eta_1}\sqrt{\frac{\eta_4}{\eta_3}}; \quad v^0_{5.3} = \frac{\eta_6}{\eta_1\eta_5^2}\sqrt{\frac{\eta_3}{\eta_4}}; \quad v^0_{5.4} = \frac{\eta_1\eta_6}{\eta_2^2\sqrt{\eta_3\eta_4}}$$

$$v^0_{6.1} = \frac{\eta_6^{3/2}}{\eta_1\eta_2\eta_5^2}\sqrt{\frac{\eta_3}{\eta_4}}; \quad v^0_{6.2} = \frac{\eta_5^2\eta_6^{3/2}}{\eta_1\eta_2}\sqrt{\frac{\eta_4}{\eta_3}}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(-1 - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + 2v^0_{2.2}\right) - \frac{v^0_{3.1} + v^0_{4.1}}{2} - v^0_{5.1}$$

$$v^0_{(1.2)0} = v^0_{1.2}\left(-1 - \frac{v^0_{1.1}}{2} + \frac{v^0_{1.4}}{2} + v^0_{2.2} + v^0_{2.3}\right) + \frac{v^0_{3.1} - v^0_{4.2}}{2} - v^0_{5.3}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(1 - \frac{v^0_{1.1}}{2} + \frac{v^0_{1.4}}{2} - v^0_{2.1} - v^0_{2.2}\right) - \frac{v^0_{3.2} - v^0_{4.1}}{2} + v^0_{5.2}$$

$$v^0_{(1.4)0} = v^0_{1.4}\left(1 - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} - 2v^0_{2.2}\right) + \frac{v^0_{3.2} + v^0_{4.2}}{2} + v^0_{5.4}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(-1 + 2v^0_{1.3} - v^0_{2.1} + 2v^0_{2.2}\right) - 2v^0_{5.2}$$

$$v^0_{(2.2)0} = \frac{v^0_{2.2}}{2}\left(-v^0_{1.1} + v^0_{1.2} - v^0_{1.3} + v^0_{1.4} - v^0_{2.1} + v^0_{2.3}\right) + \frac{1}{2}\left(v^0_{5.1} + v^0_{5.2} - v^0_{5.3} - v^0_{5.4}\right)$$

$$v^0_{(2.3)0} = v^0_{2.3}\left(1 - 2v^0_{1.2} - 2v^0_{2.2} + v^0_{2.3}\right) + 2v^0_{5.3}$$

$$v^0_{(3.1)0} = v^0_{3.1}\left(-\frac{5}{2} - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 2v^0_{2.2} + v^0_{2.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}}\right) - v^0_{6.1}$$

$$v^0_{(3.2)0} = v^0_{3.2}\left(\frac{5}{2} - v^0_{1.1} - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} - v^0_{2.1} - 2v^0_{2.2} + \frac{v^0_{4.1}}{v^0_{1.3}} + \frac{v^0_{4.2}}{2v^0_{1.4}}\right) + v^0_{6.2}$$

$$v^0_{(4.1)0} = v^0_{4.1}\left(\frac{1}{2} - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - 2v^0_{2.1} - \frac{v^0_{3.1} + 2v^0_{5.1}}{2v^0_{1.1}} - \frac{v^0_{3.2} - 2v^0_{5.2}}{v^0_{1.3}}\right)$$

$$v^0_{(4.2)0} = v^0_{4.2}\left(-\frac{1}{2} - v^0_{1.1} - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} + 2v^0_{2.3} + \frac{v^0_{3.1} - 2v^0_{5.3}}{v^0_{1.2}} + \frac{v^0_{3.2} + 2v^0_{5.4}}{2v^0_{1.4}}\right)$$

$$v^0_{(5.1)0} = v^0_{5.1}\left(-1 - v^0_{1.1} + v^0_{1.2} + v^0_{1.4} - v^0_{2.1} + 2v^0_{2.2} + \frac{v^0_{2.3}}{2} - \frac{v^0_{4.1} + v^0_{5.1}}{2v^0_{1.1}} + \frac{v^0_{5.2} - v^0_{5.4}}{v^0_{2.2}}\right) - \frac{v^0_{6.1}}{2}$$

$$v^0_{(5.2)0} = \frac{v^0_{5.2}}{2}\left(-2v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} + v^0_{1.4} - 3v^0_{2.1} + v^0_{2.2} + v^0_{2.3} + \frac{v^0_{4.1} + v^0_{5.2}}{v^0_{1.3}} + \frac{v^0_{5.1} - v^0_{5.3}}{v^0_{2.2}} - 2\frac{v^0_{5.2}}{v^0_{2.1}}\right) - \frac{v^0_{6.2}}{2}$$

$$v^0_{(5.3)0} = \frac{v^0_{5.3}}{2}\left(-v^0_{1.1} - 2v^0_{1.2} - v^0_{1.3} + 2v^0_{1.4} - v^0_{2.1} - v^0_{2.2} + 3v^0_{2.3} - \frac{v^0_{4.2} + v^0_{5.3}}{v^0_{1.2}} + \frac{v^0_{5.2} - v^0_{5.4}}{v^0_{2.2}} + 2\frac{v^0_{5.3}}{v^0_{2.3}}\right) + \frac{v^0_{6.1}}{2}$$

$$v^0_{(5.4)0} = v^0_{5.4}\left(1 - v^0_{1.1} - v^0_{1.3} + v^0_{1.4} - \frac{v^0_{2.1}}{2} - 2v^0_{2.2} + v^0_{2.3} + \frac{v^0_{4.2} + v^0_{5.4}}{2v^0_{1.4}} + \frac{v^0_{5.1} - v^0_{5.3}}{v^0_{2.2}}\right) + \frac{v^0_{6.2}}{2}$$

$$v^0_{(6.1)0} = v^0_{6.1}\left(-\frac{3}{2} - v^0_{1.1} + 2v^0_{1.4} - v^0_{2.1} + v^0_{2.2} + \frac{3}{2}v^0_{2.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} + \frac{v^0_{5.2} - v^0_{5.4}}{v^0_{2.2}} + \frac{v^0_{5.3}}{v^0_{2.3}} - \frac{v^0_{6.1}}{2v^0_{3.1}}\right)$$

$$v^0_{(6.2)0} = v^0_{6.2}\left(\frac{3}{2} - 2v^0_{1.1} + v^0_{1.4} - \frac{3}{2}v^0_{2.1} - v^0_{2.2} + v^0_{2.3} + \frac{v^0_{4.1}}{v^0_{1.3}} + \frac{v^0_{4.2}}{2v^0_{1.4}} + \frac{v^0_{5.1} - v^0_{5.3}}{v^0_{2.2}} - \frac{v^0_{5.2}}{v^0_{2.1}} + \frac{v^0_{6.2}}{2v^0_{3.2}}\right)$$

and

$$v^0_{(1.1)\xi} = v^0_{1.1}\left(-3 + v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + 2v^0_{2.2}\right) - \frac{v^0_{3.1} + v^0_{4.1}}{2} - v^0_{5.1}$$
$$v^0_{(1.2)\xi} = \frac{v^0_{1.2}}{2}\left(-6 + v^0_{1.1} + 4v^0_{1.2} + v^0_{1.4} + 2v^0_{2.2} + 2v^0_{2.3}\right) - \frac{v^0_{3.1} + v^0_{4.2}}{2} - v^0_{5.3}$$
$$v^0_{(1.3)\xi} = \frac{v^0_{1.3}}{2}\left(-6 + v^0_{1.1} + 4v^0_{1.3} + v^0_{1.4} + 2v^0_{2.1} + 2v^0_{2.2}\right) - \frac{v^0_{3.2} + v^0_{4.1}}{2} - v^0_{5.2}$$
$$v^0_{(1.4)\xi} = v^0_{1.4}\left(-3 + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 2v^0_{2.2}\right) - \frac{v^0_{3.2} + v^0_{4.2}}{2} - v^0_{5.4}$$
$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-3 + 2v^0_{1.3} + v^0_{2.1} + 2v^0_{2.2}\right) - 2v^0_{5.2}$$
$$v^0_{(2.2)\xi} = \frac{v^0_{2.2}}{2}\left(-6 + v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 4v^0_{2.2} + v^0_{2.3}\right) - \frac{1}{2}\left(v^0_{5.1} + v^0_{5.2} + v^0_{5.3} + v^0_{5.4}\right)$$
$$v^0_{(2.3)\xi} = v^0_{2.3}\left(-3 + 2v^0_{1.2} + 2v^0_{2.2} + v^0_{2.3}\right) - 2v^0_{5.3}$$
$$v^0_{(3.1)\xi} = v^0_{3.1}\left(-\frac{13}{2} + v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 2v^0_{2.2} + v^0_{2.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}}\right) - v^0_{6.1}$$
$$v^0_{(3.2)\xi} = v^0_{3.2}\left(-\frac{13}{2} + v^0_{1.1} + v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 2v^0_{2.2} - \frac{v^0_{4.1}}{v^0_{1.3}} - \frac{v^0_{4.2}}{2v^0_{1.4}}\right) - v^0_{6.2}$$
$$v^0_{(4.1)\xi} = v^0_{4.1}\left(-\frac{15}{2} + v^0_{1.1} + v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 2v^0_{2.1} + 4v^0_{2.2} - \frac{v^0_{3.1} + 2v^0_{5.1}}{2v^0_{1.1}} - \frac{v^0_{3.2} + 2v^0_{5.2}}{v^0_{1.3}}\right)$$
$$v^0_{(4.2)\xi} = v^0_{4.2}\left(-\frac{15}{2} + v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 4v^0_{2.2} + 2v^0_{2.3} - \frac{v^0_{3.1} + 2v^0_{5.3}}{v^0_{1.2}} - \frac{v^0_{3.2} + 2v^0_{5.4}}{2v^0_{1.4}}\right)$$
$$v^0_{(5.1)\xi} = v^0_{5.1}\left(-7 + v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 4v^0_{2.2} + \frac{v^0_{2.3}}{2} - \frac{v^0_{4.1} + v^0_{5.1}}{2v^0_{1.1}} - \frac{v^0_{5.2} + v^0_{5.4}}{v^0_{2.2}}\right) - \frac{v^0_{6.1}}{2}$$
$$v^0_{(5.2)\xi} = \frac{v^0_{5.2}}{2}\left(-14 + 2v^0_{1.1} + v^0_{1.2} + 6v^0_{1.3} + v^0_{1.4} + 3v^0_{2.1} + 7v^0_{2.2} + v^0_{2.3} - \frac{v^0_{4.1} + v^0_{5.2}}{v^0_{1.3}} - 2\frac{v^0_{5.2}}{v^0_{2.1}} - \frac{v^0_{5.1} + v^0_{5.3}}{v^0_{2.2}}\right) - \frac{v^0_{6.2}}{2}$$
$$v^0_{(5.3)\xi} = \frac{v^0_{5.3}}{2}\left(-14 + v^0_{1.1} + 6v^0_{1.2} + v^0_{1.3} + 2v^0_{1.4} + v^0_{2.1} + 7v^0_{2.2} + 3v^0_{2.3} - \frac{v^0_{4.2} + v^0_{5.3}}{v^0_{1.2}} - \frac{v^0_{5.2} + v^0_{5.4}}{v^0_{2.2}} - 2\frac{v^0_{5.3}}{v^0_{2.3}}\right) - \frac{v^0_{6.1}}{2}$$
$$v^0_{(5.4)\xi} = v^0_{5.4}\left(-7 + v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + \frac{v^0_{2.1}}{2} + 4v^0_{2.2} + v^0_{2.3} - \frac{v^0_{4.2} + v^0_{5.4}}{2v^0_{1.4}} - \frac{v^0_{5.1} + v^0_{5.3}}{v^0_{2.2}}\right) - \frac{v^0_{6.2}}{2}$$
$$v^0_{(6.1)\xi} = v^0_{6.1}\left(-\frac{23}{2} + v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 2v^0_{1.4} + v^0_{2.1} + 5v^0_{2.2} + \frac{3}{2}v^0_{2.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{5.2} + v^0_{5.4}}{v^0_{2.2}} - \frac{v^0_{5.3}}{v^0_{2.3}} - \frac{v^0_{6.1}}{2v^0_{3.1}}\right)$$
$$v^0_{(6.2)\xi} = v^0_{6.2}\left(-\frac{23}{2} + 2v^0_{1.1} + 2v^0_{1.2} + 4v^0_{1.3} + v^0_{1.4} + \frac{3}{2}v^0_{2.1} + 5v^0_{2.2} + v^0_{2.3} - \frac{v^0_{4.1}}{v^0_{1.3}} - \frac{v^0_{4.2}}{2v^0_{1.4}} - \frac{v^0_{5.1} + v^0_{5.3}}{v^0_{2.2}} - \frac{v^0_{5.2}}{v^0_{2.1}} - \frac{v^0_{6.2}}{2v^0_{3.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$$u^0_{1.1} = 1; \quad u^0_{1.2} = -1; \quad u^0_{1.3} = -1; \quad u^0_{1.4} = 1$$
$$u^0_{2.1} = 1; \quad u^0_{2.2} = -1; \quad u^0_{2.3} = 1; \quad u^0_{3.1} = 1$$
$$u^0_{3.2} = -1; \quad u^0_{4.1} = 1; \quad u^0_{4.2} = -1; \quad u^0_{5.1} = 1$$
$$u^0_{5.2} = 1; \quad u^0_{5.3} = -1 \quad u^0_{5.4} = -1; \quad u^0_{6.1} = 1$$
$$u^0_{6.2} = 1$$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$$u^0_{(1.1)0} = -2; \quad u^0_{(1.2)0} = 0; \quad u^0_{(1.3)0} = 0; \quad u^0_{(1.4)0} = 2$$
$$u^0_{(2.1)0} = -2; \quad u^0_{(2.2)0} = 0; \quad u^0_{(2.3)0} = 2; \quad u^0_{(3.1)0} = -1$$
$$u^0_{(3.2)0} = -1; \quad u^0_{(4.1)0} = -1; \quad u^0_{(4.2)0} = -1; \quad u^0_{(5.1)0} = -1$$
$$u^0_{(5.2)0} = -1; \quad u^0_{(5.3)0} = -1; \quad u^0_{(5.4)0} = -1; \quad u^0_{(6.1)0} = 0$$
$$u^0_{(6.2)0} = 0$$

and

$$u^0_{(1.1)\xi} = 2; \quad u^0_{(1.2)\xi} = -2; \quad u^0_{(1.3)\xi} = -2; \quad u^0_{(1.4)\xi} = 2$$
$$u^0_{(2.1)\xi} = 2; \quad u^0_{(2.2)\xi} = -2; \quad u^0_{(2.3)\xi} = 2; \quad u^0_{(3.1)\xi} = 3$$
$$u^0_{(3.2)\xi} = -3; \quad u^0_{(4.1)\xi} = 3; \quad u^0_{(4.2)\xi} = -3; \quad u^0_{(5.1)\xi} = 3$$
$$u^0_{(5.2)\xi} = 3; \quad u^0_{(5.3)\xi} = -3 \quad u^0_{(5.4)\xi} = -3; \quad u^0_{(6.1)\xi} = 4$$
$$u^0_{(6.2)\xi} = 4$$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$$u^0_{(1.1)00} = 2v^0_{1.1}; \quad u^0_{(1.2)00} = 2v^0_{1.2}; \quad u^0_{(1.3)00} = 2v^0_{1.3}$$
$$u^0_{(1.4)00} = 2v^0_{1.4}; \quad u^0_{(2.1)00} = 2v^0_{2.1}; \quad u^0_{(2.2)00} = 2v^0_{2.2}$$
$$u^0_{(2.3)00} = 2v^0_{2.3}; \quad u^0_{(3.1)00} = 2v^0_{1.1} - 4v^0_{1.2}; \quad u^0_{(3.2)00} = 4v^0_{1.3} - 2v^0_{1.4}$$
$$u^0_{(4.1)00} = 2v^0_{1.1} - 4v^0_{1.3}; \quad u^0_{(4.2)00} = 4v^0_{1.2} - 2v^0_{1.4}; \quad u^0_{(5.1)00} = 2v^0_{1.1} - 4v^0_{2.2}$$
$$u^0_{(5.2)00} = -2v^0_{1.3} + 2v^0_{2.1} - 2v^0_{2.2}; \quad u^0_{(5.3)00} = 2v^0_{1.2} + 2v^0_{2.2} - 2v^0_{2.3}; \quad u^0_{(5.4)00} = -2v^0_{1.4} + 4v^0_{2.2}$$
$$u^0_{(6.1)00} = 2v^0_{1.1} - 4v^0_{1.2} - 4v^0_{2.2} + 2v^0_{2.3}; \quad u^0_{(6.2)00} = -4v^0_{1.3} + 2v^0_{1.4} + 2v^0_{2.1} - 4v^0_{2.2}$$

$$u^0_{(1.1)\xi 0} = -2v^0_{1.1}; \quad u^0_{(1.2)\xi 0} = 0; \quad u^0_{(1.3)\xi 0} = 0; \quad u^0_{(1.4)\xi 0} = 2v^0_{1.4}$$
$$u^0_{(2.1)\xi 0} = -2v^0_{2.1}; \quad u^0_{(2.2)\xi 0} = 0; \quad u^0_{(2.3)\xi 0} = 2v^0_{2.3}; \quad u^0_{(3.1)\xi 0} = -2v^0_{1.1}$$
$$u^0_{(3.2)\xi 0} = -2v^0_{1.4}; \quad u^0_{(4.1)\xi 0} = -2v^0_{1.1}; \quad u^0_{(4.2)\xi 0} = -2v^0_{1.4}; \quad u^0_{(5.1)\xi 0} = -2v^0_{1.1}$$
$$u^0_{(5.2)\xi 0} = -2v^0_{2.1}; \quad u^0_{(5.3)\xi 0} = -2v^0_{2.3}; \quad u^0_{(5.4)\xi 0} = -2v^0_{1.4} \quad u^0_{(6.1)\xi 0} = 2v^0_{2.3} - 2v^0_{1.1}$$
$$u^0_{(6.2)\xi 0} = 2v^0_{1.4} - 2v^0_{2.1}$$

and

$$
\begin{aligned}
&u^0_{(1.1)\xi\xi} = 2v^0_{1.1}; && u^0_{(1.2)\xi\xi} = -2v^0_{1.2}; && u^0_{(1.3)\xi\xi} = -2v^0_{1.3} \\
&u^0_{(1.4)\xi\xi} = 2v^0_{1.4}; && u^0_{(2.1)\xi\xi} = 2v^0_{2.1}; && u^0_{(2.2)\xi\xi} = -2v^0_{2.2} \\
&u^0_{(2.3)\xi\xi} = 2v^0_{2.3}; && u^0_{(3.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2}; && u^0_{(3.2)\xi\xi} = -4v^0_{1.3} - 2v^0_{1.4} \\
&u^0_{(4.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.3}; && u^0_{(4.2)\xi\xi} = -4v^0_{1.2} - 2v^0_{1.4}; && u^0_{(5.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{2.2} \\
&u^0_{(5.2)\xi\xi} = 2v^0_{1.3} + 2v^0_{2.1} + 2v^0_{2.2}; && u^0_{(5.3)\xi\xi} = -2v^0_{1.2} - 2v^0_{2.2} - 2v^0_{2.3}; && u^0_{(5.4)\xi\xi} = -2v^0_{1.4} - 4v^0_{2.2}
\end{aligned}
$$

$$
u^0_{(6.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2} + 4v^0_{2.2} + 2v^0_{2.3}; \qquad u^0_{(6.2)\xi\xi} = 4v^0_{1.3} + 2v^0_{1.4} + 2v^0_{2.1} + 4v^0_{2.2}
$$

A.3.2 Thermodynamics of $B19$ phase using tetrahedron – octahedron approximation

The tetrahedron–octahedron clusters considered for $B19$ phase is shown in Figure A.8 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.8.

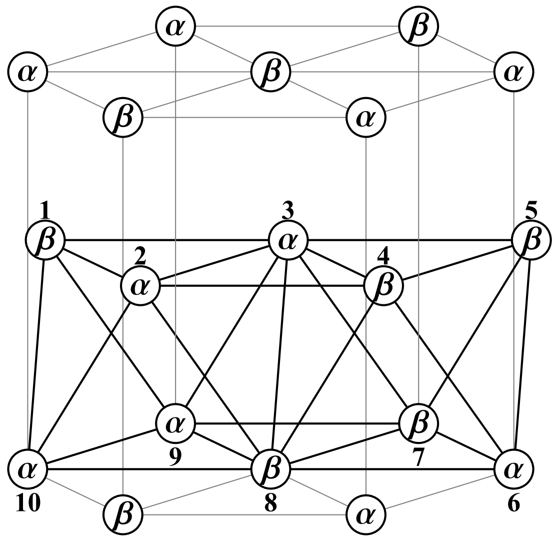

Figure A.8: The tetrahedron–octahedron basic clusters in $B19$ phase along with the sublattice sites designated α and β

Table A.8: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $B19$ phase using tetrahedron–octahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Octahedron	$\alpha\alpha\beta\beta\beta\beta$(O2) (3,6,4,5,7,8)	13.2	1/2	1
	$\alpha\alpha\alpha\alpha\beta\beta$(O1) (2,3,9,10,1,8)	13.1	1/2	
Square pyramid	$\alpha\beta\beta\beta\beta$ (3,4,5,7,8)	12.4	1	0
	$\alpha\alpha\beta\beta\beta$ (3,6,4,5,7)	12.3	2	
	$\alpha\alpha\alpha\beta\beta$ (2,3,9,1,8)	12.2	2	
	$\alpha\alpha\alpha\alpha\beta$ (2,3,9,10,1)	12.1	1	

cont ...

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Square	$\beta\beta\beta\beta$ (4,5,7,8)	11.4	1/2	0
	$\alpha\alpha\beta\beta$(O2) (3,6,4,7)	11.3	1	
	$\alpha\alpha\beta\beta$(O1) (2,9,1,8)	11.2	1	
	$\alpha\alpha\alpha\alpha$ (2,3,9,10)	11.1	1/2	
Irregular tetrahedron-2	$\alpha\beta\beta\beta$ (3,4,5,8)	10.4	2	0
	$\alpha\alpha\beta\beta$(O2) (3,6,4,8)	10.3	1	
	$\alpha\alpha\beta\beta$(O1) (2,10,1,8)	10.2	1	
	$\alpha\alpha\alpha\beta$ (2,3,10,8)	10.1	2	
Irregular tetrahedron-1	$\alpha\beta\beta\beta$ (3,4,5,7)	9.4	2	0
	$\alpha\alpha\beta\beta$(O2) (3,6,4,5)	9.3	1	
	$\alpha\alpha\beta\beta$(O1) (2,3,1,8)	9.2	1	
	$\alpha\alpha\alpha\beta$ (2,9,10,8)	9.1	2	
Regular tetrahedron	$\alpha\alpha\beta\beta$(T2, $\alpha\alpha$OP) (7,9,3,8)	8.2	1	1
	$\alpha\alpha\beta\beta$(T1, $\alpha\alpha$IP) (2,3,4,8)	8.1	1	
Isosceles triangle	$\beta\beta\beta$ (4,5,7)	7.6	2	0
	$\alpha\beta\beta$(O2) (3,4,7)	7.5	2	
	$\alpha\beta\beta$(O1) (2,1,8)	7.4	2	
	$\alpha\alpha\beta$(O2) (3,6,4)	7.3	2	
	$\alpha\alpha\beta$(O1) (2,9,1)	7.2	2	
	$\alpha\alpha\alpha$ (2,3,9)	7.1	2	

cont ...

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Equilateral triangle (OP)	$\alpha\beta\beta$(O2, $\beta\beta$OP) (4,8,3)	6.4	2	-1
	$\alpha\beta\beta$(O2, $\beta\beta$IP) (3,7,8)	6.3	1	
	$\alpha\alpha\beta$(O1, $\alpha\alpha$OP) (2,10,1)	6.2	2	
	$\alpha\alpha\beta$(O1, $\alpha\alpha$IP) (9,10,1)	6.1	1	
Equilateral triangle (OB)	$\alpha\beta\beta$ (3,4,5)	5.2	1/2	-1
	$\alpha\alpha\beta$ (2,3,1)	5.1	1/2	
Equilateral triangle (TB)	$\alpha\beta\beta$ (7,8,9)	4.2	1/2	-1
	$\alpha\alpha\beta$ (2,3,4)	4.1	1/2	
II-n pair	$\beta\beta$(O2) (4,7)	3.4	1	0
	$\beta\beta$(O1) (1,8)	3.3	1/2	
	$\alpha\alpha$(O2) (3,6)	3.2	1/2	
	$\alpha\alpha$(O1) (2,9)	3.1	1	
I-n pair (OP)	$\beta\beta$ (4,8)	2.3	1/2	1
	$\alpha\beta$ (9,10)	2.2	2	
	$\alpha\alpha$ (3,9)	2.1	1/2	
I-n pair (IP)	$\beta\beta$ (4,5)	1.4	1/2	1
	$\alpha\beta$(O2) (3,4)	1.3	1	
	$\alpha\beta$(O1) (2,1)	1.2	1	
	$\alpha\alpha$ (9,10)	1.1	1/2	
Point	β (1)	0.2	1/2	-1
	α (2)	0.1	1/2	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + u_{0.2})/2 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{\eta_1\eta_6\sqrt{\eta_4\eta_5\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_7^2\eta_{10}\sqrt{\eta_9}}; \qquad v^0_{1.2} = \frac{\eta_6\sqrt{\eta_5\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_1\sqrt{\eta_4\eta_9\eta_{12}}}$$

$$v^0_{1.3} = \frac{\sqrt{\eta_4\eta_8\eta_{11}\eta_{12}}\sqrt[8]{\eta_{13}}}{\eta_1\eta_6\sqrt{\eta_5\eta_9}}; \qquad v^0_{1.4} = \frac{\eta_1\eta_7^2\sqrt{\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_6\sqrt{\eta_4\eta_5\eta_9}\eta_{10}}$$

$$v^0_{2.1} = \frac{\eta_2\eta_6^2\sqrt{\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_7^2\eta_9\sqrt{\eta_{10}}}; \qquad v^0_{2.2} = \frac{\sqrt{\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_2\sqrt{\eta_{10}}}$$

$$v^0_{2.3} = \frac{\eta_2\eta_7^2\sqrt{\eta_8\eta_{11}}\sqrt[8]{\eta_{13}}}{\eta_6^2\eta_9\sqrt{\eta_{10}}}; \qquad v^0_{3.1} = \frac{\sqrt{\eta_{11}}\eta_3\sqrt[16]{\eta_{13}}}{\sqrt{\eta_9\eta_{10}}}$$

$$v^0_{3.2} = \eta_3\eta_7^2\sqrt{\eta_9\eta_{10}\eta_{11}\eta_{12}}\sqrt[16]{\eta_{13}}; \qquad v^0_{3.3} = \frac{\eta_3\sqrt{\eta_9\eta_{10}\eta_{11}}\sqrt[16]{\eta_{13}}}{\eta_7^2\sqrt{\eta_{12}}}$$

$$v^0_{3.4} = \frac{\eta_3\sqrt[16]{\eta_{13}}\sqrt{\eta_{11}}}{\sqrt{\eta_9\eta_{10}}}; \qquad v^0_{4.1} = \frac{\sqrt{\eta_4\eta_8\eta_{11}^3}\eta_{12}\eta_{13}^{3/8}}{\eta_1\eta_6\eta_7^2\eta_{10}\sqrt{\eta_5\eta_9^3}}$$

$$v^0_{4.2} = \frac{\eta_6\eta_7^2\sqrt{\eta_5\eta_8\eta_{11}^3}\eta_{13}^{3/8}}{\eta_1\eta_{10}\eta_{12}\sqrt{\eta_4\eta_9^3}}; \qquad v^0_{5.1} = \frac{\eta_6^3\sqrt{\eta_5\eta_8^3\eta_{11}^3}\sqrt[8]{\eta_{13}}}{\eta_1\eta_7^2\eta_{10}\sqrt{\eta_4\eta_9\eta_{12}}}$$

$$v^0_{5.2} = \frac{\eta_7^2\sqrt{\eta_4\eta_8^3\eta_{11}^3\eta_{12}}\sqrt[8]{\eta_{13}}}{\eta_1\eta_6^3\eta_{10}\sqrt{\eta_5\eta_9}}; \qquad v^0_{6.1} = \frac{\eta_1\eta_8\sqrt{\eta_4\eta_5\eta_{11}^3}\sqrt[4]{\eta_{12}\eta_{13}}}{\eta_2^2\eta_7^2\eta_9\eta_{10}}$$

$$v^0_{6.2} = \frac{\eta_6^2\eta_8\sqrt{\eta_5\eta_{11}^3}}{\eta_1\eta_7^2\eta_9\eta_{10}\eta_4}\sqrt[4]{\frac{\eta_{13}}{\eta_{12}}}; \qquad v^0_{6.3} = \frac{\eta_1\eta_7^2\eta_8\eta_{11}^{3/2}}{\eta_2^2\sqrt{\eta_4\eta_5}\eta_9\eta_{10}}\sqrt[4]{\frac{\eta_{13}}{\eta_{12}}}$$

$$v^0_{6.4} = \frac{\eta_7^2\eta_8\sqrt{\eta_4\eta_{11}^3}\sqrt[4]{\eta_{12}\eta_{13}}}{\eta_1\eta_6^2\eta_9\eta_{10}\sqrt{\eta_5}}; \qquad v^0_{7.1} = \frac{\eta_1\eta_2\eta_3\eta_6^3\eta_8\sqrt{\eta_4\eta_5}\eta_{11}\eta_{13}^{3/16}}{\eta_7^3\sqrt[4]{\eta_{12}}\sqrt{\eta_9^3\eta_{10}^3}}$$

$$v^0_{7.2} = \frac{\eta_3\eta_6\eta_8\eta_{11}\eta_{13}^{3/16}\sqrt{\eta_5}}{\eta_1\eta_2\eta_7\sqrt{\eta_4\eta_9\eta_{10}}\sqrt[4]{\eta_{12}}} \qquad v^0_{7.3} = \frac{\eta_3\eta_7\eta_8\eta_{11}\sqrt[4]{\eta_{12}}\eta_{13}^{3/16}\sqrt{\eta_4}}{\eta_1\eta_2\eta_6\sqrt{\eta_5\eta_9\eta_{10}}}$$

$$v^0_{7.4} = \frac{\eta_3\eta_6\eta_8\eta_{11}\eta_{13}^{3/16}\sqrt{\eta_5}}{\eta_1\eta_2\eta_7\sqrt{\eta_4\eta_9\eta_{10}}\sqrt[4]{\eta_{12}}}; \qquad v^0_{7.5} = \frac{\eta_3\eta_7\eta_8\eta_{11}\sqrt[4]{\eta_{12}}\eta_{13}^{3/16}\sqrt{\eta_4}}{\eta_1\eta_2\eta_6\sqrt{\eta_5\eta_9\eta_{10}}}$$

$$v^0_{7.6} = \frac{\eta_1\eta_2\eta_3\eta_7^3\eta_8\eta_{11}\sqrt[4]{\eta_{12}}\eta_{13}^{3/16}}{\eta_6^3\sqrt{\eta_4\eta_5\eta_9^3\eta_{10}^3}}; \qquad v^0_{8.1} = \frac{\sqrt{\eta_4\eta_8^3}\eta_{11}^3\eta_{12}^{3/4}\eta_{13}^{3/8}}{\eta_1\eta_2\eta_6^2\eta_9^2\sqrt{\eta_5\eta_{10}^3}}$$

$$v^0_{8.2} = \frac{\eta_6^2\sqrt{\eta_5\eta_8^3}\eta_{11}^3\eta_{13}^{3/8}}{\eta_1\eta_2\eta_9^2\eta_{12}^{3/4}\sqrt{\eta_4\eta_{10}^3}}; \qquad v^0_{9.1} = \frac{\eta_3\eta_6^4\eta_8^2\sqrt{\eta_5}\eta_{11}^2\eta_{13}^{5/16}}{\eta_1\eta_7^4\sqrt[4]{\eta_{12}}\sqrt{\eta_4\eta_9^3\eta_{10}^3}}$$

$$v^0_{9.2} = \frac{\eta_3\eta_6^2\eta_8^2\eta_{11}^2\eta_{13}^{5/16}\sqrt{\eta_5}}{\eta_1\eta_2^2\eta_7^2\sqrt{\eta_4\eta_9\eta_{10}^3}\sqrt[4]{\eta_{12}}}; \qquad v^0_{9.3} = \frac{\eta_3\eta_7^2\eta_8^2\eta_{11}^2\sqrt[4]{\eta_{12}}\eta_{13}^{5/16}\sqrt{\eta_4}}{\eta_1\eta_2^2\eta_6^2\sqrt{\eta_5\eta_9\eta_{10}^3}}$$

$$v^0_{9.4} = \frac{\eta_3\eta_7^4\eta_8^2\sqrt{\eta_4}\eta_{11}^2\sqrt[4]{\eta_{12}}\eta_{13}^{5/16}}{\eta_1\eta_6^4\sqrt{\eta_5\eta_9^3\eta_{10}^3}}; \qquad v^0_{10.1} = \frac{\eta_3\eta_5\eta_6^2\eta_{11}^2\eta_{13}^{7/16}}{\eta_2\eta_7^4\eta_{10}^2}\left(\frac{\eta_8}{\eta_9}\right)^{3/2}$$

$$v^0_{10.2} = \frac{\eta_3\eta_5\eta_6^2\eta_{11}^2\sqrt{\eta_8^3}\eta_{13}^{7/16}}{\eta_1^2\eta_2\eta_4\eta_7^2\eta_{10}\sqrt{\eta_9^3\eta_{12}}}; \qquad v^0_{10.3} = \frac{\eta_3\eta_4\eta_7^2\eta_{11}^2\sqrt{\eta_8^3\eta_{12}}\eta_{13}^{7/16}}{\eta_1^2\eta_2\eta_5\eta_6^2\eta_{10}\sqrt{\eta_9^3}}$$

$$v^0_{10.4} = \frac{\eta_3\eta_7^4\eta_{11}^2\eta_{13}^{7/16}}{\eta_2\eta_5\eta_6^2\eta_{10}^2}\left(\frac{\eta_8}{\eta_9}\right)^{3/2}; \qquad v^0_{11.1} = \frac{\eta_1^2\eta_2^2\eta_3^2\eta_4\eta_5\eta_6^6\eta_8^2\eta_{11}^2\eta_{13}^{3/8}}{\eta_7^4\eta_9^2\eta_{10}^2}$$

$$v^0_{11.2} = \frac{\eta_3^2\eta_5\eta_6^2\eta_8^2\eta_{11}^2\eta_{13}^{3/8}}{\eta_1^2\eta_2^2\eta_4\eta_7^2\eta_9\eta_{10}\sqrt{\eta_{12}}}; \qquad v^0_{11.3} = \frac{\eta_3^2\eta_4\eta_7^2\eta_8^2\eta_{11}^2\sqrt{\eta_{12}}\eta_{13}^{3/8}}{\eta_1^2\eta_2^2\eta_5\eta_6^2\eta_9\eta_{10}}$$

$$v^0_{11.4} = \frac{\eta_1^2\eta_2^2\eta_3^2\eta_7^4\eta_8^2\eta_{11}^2\eta_{13}^{3/8}}{\eta_4\eta_5\eta_6^6\eta_9^2\eta_{10}^2}; \qquad v^0_{12.1} = \frac{\eta_3^2\eta_5\eta_6^5\eta_{11}^3\sqrt{\eta_8^5\eta_{13}}}{\eta_7^6\eta_{10}^3\sqrt[4]{\eta_{12}}\sqrt{\eta_9^5}}$$

$$v^0_{12.2} = \frac{\eta_3^2\eta_5\eta_6^3\eta_{11}^3\sqrt{\eta_8^5\eta_{13}}}{\eta_1^2\eta_2^2\eta_4\eta_7^4\eta_{10}^2\sqrt[4]{\eta_{12}}\sqrt{\eta_9^3}}; \qquad v^0_{12.3} = \frac{\eta_3^2\eta_4\eta_7^4\eta_{11}^3\sqrt[4]{\eta_{12}}\sqrt{\eta_8^5\eta_{13}}}{\eta_1^2\eta_2^2\eta_5\eta_6^3\eta_{10}^2\sqrt{\eta_9^3}}$$

$$v^0_{12.4} = \frac{\eta_3^2\eta_7^6\eta_{11}^3\sqrt[4]{\eta_{12}}\sqrt{\eta_8^5\eta_{13}}}{\eta_5\eta_6^5\eta_{10}^3\sqrt{\eta_9^5}}; \qquad v^0_{13.1} = \frac{\eta_3^3\eta_5\eta_6^4\eta_8^3\sqrt{\eta_{11}^9}\eta_{13}^{11/16}}{\eta_1^2\eta_2^2\eta_4\eta_7^6\sqrt{\eta_9^5\eta_{10}^7}}$$

$$v^0_{13.2} = \frac{\eta_3^3\eta_4\eta_7^6\eta_8^3\sqrt{\eta_{11}^9}\eta_{13}^{11/16}}{\eta_1^2\eta_2^2\eta_5\eta_6^4\sqrt{\eta_9^5\eta_{10}^7}}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(1 - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} - 2v^0_{2.1} + 2v^0_{2.2} - 2v^0_{3.1}\right) - \frac{v^0_{4.1} + v^0_{5.1}}{2} - v^0_{6.1} + 2v^0_{7.1}$$

$$v^0_{(1.2)0} = v^0_{1.2}\left(1 - \frac{v^0_{1.1}}{2} + \frac{v^0_{1.4}}{2} - v^0_{2.1} - v^0_{2.2} - v^0_{3.1} + v^0_{3.3}\right) - \frac{v^0_{4.2} - v^0_{5.1}}{2} + v^0_{6.2} + v^0_{7.2} - v^0_{7.4}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(-1 - \frac{v^0_{1.1}}{2} + \frac{v^0_{1.4}}{2} + v^0_{2.2} + v^0_{2.3} - v^0_{3.2} + v^0_{3.4}\right) + \frac{v^0_{4.1} - v^0_{5.2}}{2} - v^0_{6.4} + v^0_{7.3} - v^0_{7.5}$$

$$v^0_{(1.4)0} = v^0_{1.4}\left(-1 - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} - 2v^0_{2.2} + 2v^0_{2.3} + 2v^0_{3.4}\right) + \frac{v^0_{4.2} + v^0_{5.2}}{2} + v^0_{6.3} - 2v^0_{7.6}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(1 - 2\left(v^0_{1.1} - v^0_{1.2} - v^0_{2.2} + v^0_{3.1}\right) - v^0_{2.1}\right) - 2v^0_{6.2} + 2v^0_{7.1}$$

$$v^0_{(2.2)0} = \frac{v^0_{2.2}}{2}\left(-v^0_{1.1} - v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - v^0_{2.1} + v^0_{2.3} - v^0_{3.1} - v^0_{3.2} + v^0_{3.3} + v^0_{3.4}\right)$$
$$+ \frac{1}{2}\left(v^0_{6.1} + v^0_{6.2} - v^0_{6.3} - v^0_{6.4} + v^0_{7.2} + v^0_{7.3} - v^0_{7.4} - v^0_{7.5}\right)$$

$$v^0_{(2.3)0} = v^0_{2.3}\left(-1 - 2\left(v^0_{1.3} - v^0_{1.4} + v^0_{2.2} - v^0_{3.4}\right) + v^0_{2.3}\right) + 2v^0_{6.4} - 2v^0_{7.6}$$

$$v^0_{(3.1)0} = v^0_{3.1}\left(1 - v^0_{1.1} + v^0_{1.2} - v^0_{2.1} + v^0_{2.2} - v^0_{3.1}\right) + v^0_{7.1} - v^0_{7.2}$$

$$v^0_{(3.2)0} = v^0_{3.2}\left(-1 + 2v^0_{1.3} + 2v^0_{2.2} - v^0_{3.2}\right) - 2v^0_{7.3}$$

$$v^0_{(3.3)0} = v^0_{3.3}\left(1 - 2v^0_{1.2} - 2v^0_{2.2} + v^0_{3.3}\right) + 2v^0_{7.4}$$

$$v^0_{(3.4)0} = v^0_{3.4}\left(-1 - v^0_{1.3} + v^0_{1.4} - v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right) + v^0_{7.5} - v^0_{7.6}$$

$$v^0_{(4.1)0} = v^0_{4.1}\left(-\frac{1}{2} - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - 2\left(v^0_{2.1} - v^0_{2.2} + v^0_{3.1} + v^0_{3.2} - v^0_{3.4}\right) + v^0_{2.3}\right.$$

$$- \frac{v^0_{5.1} - 4v^0_{7.1}}{2v^0_{1.1}} - \frac{v^0_{5.2} - 2v^0_{7.3} + 2v^0_{7.5}}{v^0_{1.3}}\Bigg) - v^0_{8.1}$$

$$v^0_{(4.2)0} = v^0_{4.2}\Bigg(\frac{1}{2} - v^0_{1.1} - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} - v^0_{2.1} - 2\left(v^0_{2.2} - v^0_{2.3} + v^0_{3.1} - v^0_{3.3} - v^0_{3.4}\right)$$

$$+ \frac{v^0_{5.1} + 2v^0_{7.2} - 2v^0_{7.4}}{v^0_{1.2}} + \frac{v^0_{5.2} - 4v^0_{7.6}}{2v^0_{1.4}}\Bigg) + v^0_{8.2}$$

$$v^0_{(5.1)0} = v^0_{5.1}\left(\frac{3}{2} - v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - 2v^0_{2.1} - 2v^0_{3.1} + v^0_{3.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}}\right) + 2v^0_{9.1} - v^0_{9.2}$$

$$v^0_{(5.2)0} = v^0_{5.2}\left(-\frac{3}{2} - v^0_{1.1} - v^0_{1.2} - v^0_{1.3} + v^0_{1.4} + 2v^0_{2.3} - v^0_{3.2} + 2v^0_{3.4} + \frac{v^0_{4.1}}{v^0_{1.3}} + \frac{v^0_{4.2}}{2v^0_{1.4}}\right) + v^0_{9.3} - 2v^0_{9.4}$$

$$v^0_{(6.1)0} = v^0_{6.1}\Bigg(\frac{1}{2} - v^0_{1.1} + v^0_{1.3} + v^0_{1.4} - 2v^0_{2.1} + 2v^0_{2.2} + \frac{v^0_{2.3}}{2} - 2v^0_{3.1} - v^0_{3.2} + \frac{v^0_{3.3}}{2} + v^0_{3.4} - \frac{v^0_{6.1} - 2v^0_{7.1}}{2v^0_{1.1}}$$

$$- \frac{v^0_{6.3} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\Bigg) - \frac{v^0_{8.1} + v^0_{9.2}}{2} + v^0_{10.1}$$

$$v^0_{(6.2)0} = \frac{v^0_{6.2}}{2}\Bigg(3 - 4v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - 3v^0_{2.1} + v^0_{2.2} + v^0_{2.3} - 5v^0_{3.1} - v^0_{3.2} + 2v^0_{3.3} + v^0_{3.4} + \frac{v^0_{6.2}}{v^0_{1.2}}$$

$$- \frac{v^0_{6.2} - 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} + \frac{v^0_{7.2} - v^0_{7.4}}{v^0_{1.2}}\Bigg) - \frac{1}{2}\left(v^0_{8.2} - v^0_{9.1} - v^0_{10.1} + v^0_{10.2}\right)$$

$$v^0_{(6.3)0} = v^0_{6.3}\Bigg(-\frac{1}{2} - v^0_{1.1} - v^0_{1.2} + v^0_{1.4} - \frac{v^0_{2.1}}{2} - 2v^0_{2.2} + 2v^0_{2.3} - v^0_{3.1} - \frac{v^0_{3.2}}{2} + v^0_{3.3} + 2v^0_{3.4}$$

$$+ \frac{v^0_{6.1} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{6.3} - 2v^0_{7.6}}{2v^0_{1.4}}\Bigg) + \frac{v^0_{8.2} + v^0_{9.3}}{2} - v^0_{10.4}$$

$$v^0_{(6.4)0} = \frac{v^0_{6.4}}{2}\Bigg(-3 - v^0_{1.1} - v^0_{1.2} - 2v^0_{1.3} + 4v^0_{1.4} - v^0_{2.1} - v^0_{2.2} + 3v^0_{2.3} - v^0_{3.1} - 2v^0_{3.2} + v^0_{3.3} + 5v^0_{3.4}$$

$$+ \frac{v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} + \frac{v^0_{6.4} - 2v^0_{7.6}}{v^0_{2.3}}\Bigg) + \frac{1}{2}\left(v^0_{8.1} - v^0_{9.4} + v^0_{10.3} - v^0_{10.4}\right)$$

$$v^0_{(7.1)0} = \frac{v^0_{7.1}}{2}\left(4 - 5v^0_{1.1} + 5v^0_{1.2} + 2v^0_{1.3} - 5v^0_{2.1} + 7v^0_{2.2} - 7v^0_{3.1} - \frac{v^0_{4.1} + v^0_{6.1} - 2v^0_{7.1}}{v^0_{1.1}} - 2\frac{v^0_{6.2} - v^0_{7.1}}{v^0_{2.1}}\right)$$

$$- \frac{1}{2}\left(v^0_{9.1} + v^0_{10.1} - v^0_{11.1}\right)$$

$$v^0_{(7.2)0} = \frac{v^0_{7.2}}{2}\Bigg(2\left(1 - v^0_{1.1} + v^0_{1.4} + v^0_{3.3}\right) + v^0_{1.2} + v^0_{1.3} - 3v^0_{2.1} + v^0_{2.3} - 3v^0_{3.1} - v^0_{3.2} + v^0_{3.4}$$

$$- \frac{v^0_{4.2} - v^0_{6.2} - v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\Bigg) + \frac{1}{2}\left(v^0_{9.1} + v^0_{10.1} - v^0_{11.2}\right)$$

$$v^0_{(7.3)0} = \frac{v^0_{7.3}}{2}\Bigg(2\left(-1 - v^0_{1.1} + v^0_{1.3} + v^0_{2.3} + v^0_{3.4}\right) - v^0_{1.2} + v^0_{1.4} - v^0_{2.1} + 3v^0_{2.2} - v^0_{3.1} - 3v^0_{3.2} + v^0_{3.3}$$

$$+ \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{4.1} - v^0_{6.4} + v^0_{7.3} - v^0_{7.5}}{v^0_{1.3}}\Bigg) - \frac{1}{2}\left(v^0_{9.3} + v^0_{10.3} + v^0_{11.3}\right)$$

$$v^0_{(7.4)0} = \frac{v^0_{7.4}}{2}\Bigg(2\left(1 - v^0_{1.2} + v^0_{1.4} - v^0_{2.1} - v^0_{3.1}\right) - v^0_{1.1} + v^0_{1.3} - 3v^0_{2.2} + v^0_{2.3} - v^0_{3.2} + 3v^0_{3.3} + v^0_{3.4}$$

$$- \frac{v^0_{4.2} - v^0_{6.2} - v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} \Bigg) + \frac{1}{2}\left(v^0_{9.2} + v^0_{10.2} + v^0_{11.2}\right)$$

$$v^0_{(7.5)0} = \frac{v^0_{7.5}}{2}\Bigg(2\left(-1 - v^0_{1.1} + v^0_{1.4} - v^0_{3.2}\right) - v^0_{1.2} - v^0_{1.3} - v^0_{2.1} + 3v^0_{2.3} - v^0_{3.1} + v^0_{3.3} + 3v^0_{3.4}$$
$$+ \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{4.1} - v^0_{6.4} + v^0_{7.3} - v^0_{7.5}}{v^0_{1.3}} \Bigg) - \frac{1}{2}\left(v^0_{9.4} + v^0_{10.4} - v^0_{11.3}\right)$$

$$v^0_{(7.6)0} = \frac{v^0_{7.6}}{2}\left(-4 - 2v^0_{1.2} - 5v^0_{1.3} + 5v^0_{1.4} - 7v^0_{2.2} + 5v^0_{2.3} + 7v^0_{3.4} + \frac{v^0_{4.2} + v^0_{6.3} - 2v^0_{7.6}}{v^0_{1.4}} + 2\frac{v^0_{6.4} - v^0_{7.6}}{v^0_{2.3}}\right)$$
$$+ \frac{1}{2}\left(v^0_{9.4} + v^0_{10.4} - v^0_{11.4}\right)$$

$$v^0_{(8.1)0} = v^0_{8.1}\Bigg(-1 - v^0_{1.1} + 2\left(v^0_{1.4} - v^0_{2.1} - v^0_{3.1} - v^0_{3.2}\right) + v^0_{2.2} + \frac{3}{2}v^0_{2.3} + \frac{v^0_{3.3}}{2} + 3v^0_{3.4} + \frac{v^0_{7.1}}{v^0_{1.1}}$$
$$+ \frac{v^0_{7.3} - v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{8.1}}{2v^0_{4.1}} - \frac{v^0_{9.2} - 2v^0_{10.1}}{2v^0_{6.1}} - \frac{v^0_{9.4} - v^0_{10.3} + v^0_{10.4}}{v^0_{6.4}} \Bigg)$$

$$v^0_{(8.2)0} = v^0_{8.2}\Bigg(1 - 2\left(v^0_{1.1} - v^0_{2.3} - v^0_{3.3} - v^0_{3.4}\right) + v^0_{1.4} - \frac{3}{2}v^0_{2.1} - v^0_{2.2} - 3v^0_{3.1} - \frac{v^0_{3.2}}{2} + \frac{v^0_{7.2} - v^0_{7.4}}{v^0_{1.2}}$$
$$- \frac{v^0_{7.6}}{v^0_{1.4}} + \frac{v^0_{8.2}}{2v^0_{4.2}} + \frac{v^0_{9.1} + v^0_{10.1} - v^0_{10.2}}{v^0_{6.2}} + \frac{v^0_{9.3} - 2v^0_{10.4}}{2v^0_{6.3}} \Bigg)$$

$$v^0_{(9.1)0} = \frac{v^0_{9.1}}{2}\Bigg(4 - 5v^0_{1.1} + 4v^0_{1.2} + 3v^0_{1.3} + 2v^0_{1.4} - 5v^0_{2.1} + 3v^0_{2.2} + v^0_{2.3} - 7v^0_{3.1} - v^0_{3.2} + 2v^0_{3.3}$$
$$+ v^0_{3.4} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{6.2} - 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}} + \frac{2v^0_{9.1} - v^0_{9.2}}{v^0_{5.1}} \Bigg)$$
$$+ \frac{v^0_{12.1} - v^0_{12.2}}{2}$$

$$v^0_{(9.2)0} = v^0_{9.2}\Bigg(1 - v^0_{1.1} + v^0_{1.3} + 2v^0_{1.4} - 2v^0_{2.1} + \frac{v^0_{2.3}}{2} - 2v^0_{3.1} - v^0_{3.2} + \frac{3}{2}v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.2}}{v^0_{1.2}}$$
$$- \frac{v^0_{6.3} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} + \frac{2v^0_{9.1} - v^0_{9.2}}{2v^0_{5.1}} \Bigg) + v^0_{12.2}$$

$$v^0_{(9.3)0} = v^0_{9.3}\Bigg(-1 - 2v^0_{1.1} - v^0_{1.2} + v^0_{1.4} - \frac{v^0_{2.1}}{2} + 2v^0_{2.3} - v^0_{3.1} - \frac{3}{2}v^0_{3.2} + v^0_{3.3} + 2v^0_{3.4} + \frac{v^0_{4.1}}{v^0_{1.3}}$$
$$+ \frac{v^0_{6.1} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{8.2}}{2v^0_{6.3}} + \frac{v^0_{9.3} - 2v^0_{9.4}}{2v^0_{5.2}} \Bigg) - v^0_{12.3}$$

$$v^0_{(9.4)0} = \frac{v^0_{9.4}}{2}\Bigg(-4 - 2v^0_{1.1} - 3v^0_{1.2} - 4v^0_{1.3} + 5v^0_{1.4} - v^0_{2.1} - 3v^0_{2.2} + 5v^0_{2.3} - v^0_{3.1} - 2v^0_{3.2} + v^0_{3.3}$$
$$+ 7v^0_{3.4} + \frac{v^0_{4.1}}{v^0_{1.3}} + \frac{v^0_{4.2}}{v^0_{1.4}} + \frac{v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{6.4} - 2v^0_{7.6}}{v^0_{2.3}} + \frac{v^0_{8.1}}{v^0_{6.4}} + \frac{v^0_{9.3} - 2v^0_{9.4}}{v^0_{5.2}} \Bigg)$$
$$+ \frac{v^0_{12.3} - v^0_{12.4}}{2}$$

$$v^0_{(10.1)0} = \frac{v^0_{10.1}}{2}\Bigg(4 - 5v^0_{1.1} + 3v^0_{1.2} + 2\left(v^0_{1.3} + v^0_{1.4} - v^0_{3.2} + v^0_{3.3} + v^0_{3.4}\right) - 6v^0_{2.1} + 5v^0_{2.2} + v^0_{2.3}$$

$$- 8v^0_{3.1} - \frac{v^0_{6.1} - 2v^0_{7.1}}{v^0_{1.1}} - \frac{v^0_{6.2} - 2v^0_{7.1}}{v^0_{2.1}} + \frac{v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} - 2v^0_{7.3} + 2v^0_{7.5}}{v^0_{2.2}}$$

$$- \frac{v^0_{8.1}}{v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) + \frac{v^0_{12.1} - v^0_{12.2}}{2}$$

$$v^0_{(10.2)0} = v^0_{10.2}\Bigg(2\left(1 - v^0_{1.1} - v^0_{2.1} + v^0_{3.3}\right) + v^0_{1.3} + v^0_{1.4} - v^0_{2.2} + v^0_{2.3} - 3v^0_{3.1} - v^0_{3.2} + v^0_{3.4}$$

$$+ \frac{v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} + \frac{v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) + v^0_{12.2}$$

$$v^0_{(10.3)0} = v^0_{10.3}\Bigg(2\left(-1 + v^0_{1.4} + v^0_{2.3} - v^0_{3.2}\right) - v^0_{1.1} - v^0_{1.2} - v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.3} + 3v^0_{3.4}$$

$$+ \frac{v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{7.6}}{v^0_{2.3}} + \frac{v^0_{8.1}}{v^0_{6.4}}\Bigg) - v^0_{12.3}$$

$$v^0_{(10.4)0} = \frac{v^0_{10.4}}{2}\Bigg(-4 - 2\left(v^0_{1.1} + v^0_{1.2} + v^0_{3.1} + v^0_{3.2} - v^0_{3.3}\right) - 3v^0_{1.3} + 5v^0_{1.4} - v^0_{2.1} - 5v^0_{2.2} + 6v^0_{2.3}$$

$$+ 8v^0_{3.4} + \frac{v^0_{6.1} + 2v^0_{7.2} - 2v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{6.3} - 2v^0_{7.6}}{v^0_{1.4}} - \frac{v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} + \frac{v^0_{6.4} - 2v^0_{7.6}}{v^0_{2.3}}$$

$$+ \frac{v^0_{8.1}}{v^0_{6.4}} + \frac{v^0_{8.2}}{v^0_{6.3}}\Bigg) + \frac{v^0_{12.3} - v^0_{12.4}}{2}$$

$$v^0_{(11.1)0} = v^0_{11.1}\left(3 - 4v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} - 4v^0_{2.1} + 6v^0_{2.2} - 6v^0_{3.1} - \frac{v^0_{4.1} + v^0_{6.1} - 2v^0_{7.1}}{v^0_{1.1}} - 2\frac{v^0_{6.2} - v^0_{7.1}}{v^0_{2.1}}\right)$$

$$- v^0_{12.1}$$

$$v^0_{(11.2)0} = v^0_{11.2}\Bigg(1 - v^0_{1.1} + v^0_{1.3} + 2\left(v^0_{1.4} - v^0_{2.1} - v^0_{3.1} + v^0_{3.3}\right) - v^0_{2.2} + v^0_{2.3} - v^0_{3.2} + v^0_{3.4}$$

$$- \frac{v^0_{4.2} - v^0_{6.2} - v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} - v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\Bigg) + v^0_{12.2}$$

$$v^0_{(11.3)0} = v^0_{11.3}\Bigg(-1 - 2\left(v^0_{1.1} - v^0_{2.3} + v^0_{3.2} - v^0_{3.4}\right) - v^0_{1.2} + v^0_{1.4} - v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.3}$$

$$+ \frac{v^0_{4.1} - v^0_{6.4} + v^0_{7.3} - v^0_{7.5}}{v^0_{1.3}} + \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}}\Bigg) - v^0_{12.3}$$

$$v^0_{(11.4)0} = v^0_{11.4}\Bigg(-3 - 2v^0_{1.2} - 4v^0_{1.3} + 4v^0_{1.4} - 6v^0_{2.2} + 4v^0_{2.3} + 6v^0_{3.4} + \frac{v^0_{4.2} + v^0_{6.3} - 2v^0_{7.6}}{v^0_{1.4}}$$

$$+ 2\frac{v^0_{6.4} - v^0_{7.6}}{v^0_{2.3}}\Bigg) + v^0_{12.4}$$

$$v^0_{(12.1)0} = v^0_{12.1}\Bigg(3 - 4v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + v^0_{1.4} - 4v^0_{2.1} + 4v^0_{2.2} + \frac{v^0_{2.3}}{2} - 6v^0_{3.1} - v^0_{3.2} + v^0_{3.3}$$

$$+ v^0_{3.4} - \frac{v^0_{4.1} + v^0_{6.1} - 2v^0_{7.1}}{2v^0_{1.1}} - \frac{v^0_{6.2} - 2v^0_{7.1}}{v^0_{2.1}} + \frac{v^0_{7.3} - v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}$$

$$+ \frac{2v^0_{9.1} - v^0_{9.2}}{2v^0_{5.1}}\Bigg) - \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.2)0} = \frac{v^0_{12.2}}{2}\Bigg(4 - 5v^0_{1.1} + 2v^0_{1.2} + 3v^0_{1.3} + 4v^0_{1.4} - 6v^0_{2.1} + v^0_{2.2} + 2v^0_{2.3} - 8v^0_{3.1} - 3v^0_{3.2} + 4v^0_{3.3}$$

$$+ 3v^0_{3.4} - \frac{v^0_{4.2} - v^0_{6.2} - v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} - 3v^0_{7.3} + 3v^0_{7.5}}{v^0_{2.2}} + 2\frac{v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{8.1}}{v^0_{6.1}}$$

$$- 2\frac{v^0_{8.2}}{v^0_{6.2}} + \frac{2v^0_{9.1} - v^0_{9.2}}{v^0_{5.1}}\Bigg) + \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.3)0} = \frac{v^0_{12.3}}{2}\Bigg(-4 - 4v^0_{1.1} - 3v^0_{1.2} - 2v^0_{1.3} + 5v^0_{1.4} - 2v^0_{2.1} - v^0_{2.2} + 6v^0_{2.3} - 3v^0_{3.1} - 4v^0_{3.2} + 3v^0_{3.3}$$

$$+ 8v^0_{3.4} + \frac{v^0_{4.1} - v^0_{6.4} + v^0_{7.3} - v^0_{7.5}}{v^0_{1.3}} + \frac{v^0_{6.1} + v^0_{6.2} + 3v^0_{7.2} - 3v^0_{7.4}}{v^0_{2.2}} - 2\frac{v^0_{7.6}}{v^0_{2.3}} + 2\frac{v^0_{8.1}}{v^0_{6.4}}$$

$$+ \frac{v^0_{8.2}}{v^0_{6.3}} + \frac{v^0_{9.3} - 2v^0_{9.4}}{v^0_{5.2}}\Bigg) - \frac{v^0_{13.2}}{2}$$

$$v^0_{(12.4)0} = v^0_{12.4}\Bigg(-3 - v^0_{1.1} - 2v^0_{1.2} - 3v^0_{1.3} + 4v^0_{1.4} - \frac{v^0_{2.1}}{2} - 4v^0_{2.2} + 4v^0_{2.3} - v^0_{3.1} - v^0_{3.2} + v^0_{3.3} + 6v^0_{3.4}$$

$$+ \frac{v^0_{4.2} + v^0_{6.3} - 2v^0_{7.6}}{2v^0_{1.4}} + \frac{v^0_{6.4} - 2v^0_{7.6}}{v^0_{2.3}} + \frac{v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{8.1}}{v^0_{6.4}} + \frac{v^0_{8.2}}{2v^0_{6.3}} + \frac{v^0_{9.3} - 2v^0_{9.4}}{2v^0_{5.2}}\Bigg)$$

$$+ \frac{v^0_{13.2}}{2}$$

$$v^0_{(13.1)0} = 2v^0_{13.1}\Bigg(\frac{3}{2} - 2v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} - 2v^0_{2.1} + v^0_{2.2} + \frac{v^0_{2.3}}{2} - 3v^0_{3.1} - v^0_{3.2} + v^0_{3.3} + v^0_{3.4}$$

$$+ \frac{v^0_{7.1}}{v^0_{2.1}} + \frac{v^0_{7.3} - v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}} + \frac{2v^0_{9.1} - v^0_{9.2}}{2v^0_{5.1}}\Bigg)$$

$$v^0_{(13.2)0} = 2v^0_{13.2}\Bigg(-\frac{3}{2} - v^0_{1.1} - v^0_{1.2} - v^0_{1.3} + 2v^0_{1.4} - \frac{v^0_{2.1}}{2} - v^0_{2.2} + 2v^0_{2.3} - v^0_{3.1} - v^0_{3.2} + v^0_{3.3} + 3v^0_{3.4}$$

$$+ \frac{v^0_{7.2} - v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{7.6}}{v^0_{2.3}} + \frac{v^0_{8.1}}{v^0_{6.4}} + \frac{v^0_{8.2}}{2v^0_{6.3}} + \frac{v^0_{9.3} - 2v^0_{9.4}}{2v^0_{5.2}}\Bigg)$$

and

$$v^0_{(1.1)\xi} = v^0_{1.1}\left(-5 + v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + 2v^0_{2.1} + 2v^0_{2.2} + 2v^0_{3.1}\right) - \frac{v^0_{4.1} + v^0_{5.1}}{2} - v^0_{6.1} - 2v^0_{7.1}$$

$$v^0_{(1.2)\xi} = v^0_{1.2}\left(-5 + \frac{v^0_{1.1}}{2} + 2v^0_{1.2} + \frac{v^0_{1.4}}{2} + v^0_{2.1} + 3v^0_{2.2} + v^0_{3.1} + v^0_{3.3}\right) - \frac{v^0_{4.2} + v^0_{5.1}}{2} - v^0_{6.2} - v^0_{7.2} - v^0_{7.4}$$

$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-5 + \frac{v^0_{1.1}}{2} + 2v^0_{1.3} + \frac{v^0_{1.4}}{2} + 3v^0_{2.2} + v^0_{2.3} + v^0_{3.2} + v^0_{3.4}\right) - \frac{v^0_{4.1} + v^0_{5.2}}{2} - v^0_{6.4} - v^0_{7.3} - v^0_{7.5}$$

$$v^0_{(1.4)\xi} = v^0_{1.4}\left(-5 + v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 2v^0_{2.2} + 2v^0_{2.3} + 2v^0_{3.4}\right) - \frac{v^0_{4.2} + v^0_{5.2}}{2} - v^0_{6.3} - 2v^0_{7.6}$$

$$v^0_{(2.1)\xi} = v^0_{2.1}\left(-5 + 2\left(v^0_{1.1} + v^0_{1.2} + v^0_{2.2} + v^0_{3.1}\right) + v^0_{2.1}\right) - 2v^0_{6.2} - 2v^0_{7.1}$$

$$v^0_{(2.2)\xi} = \frac{v^0_{2.2}}{2}\left(-10 + v^0_{1.1} + 3v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 4v^0_{2.2} + v^0_{2.3} + v^0_{3.1} + v^0_{3.2} + v^0_{3.3} + v^0_{3.4}\right)$$

$$- \frac{1}{2}\left(v^0_{6.1} + v^0_{6.2} + v^0_{6.3} + v^0_{6.4} + v^0_{7.2} + v^0_{7.3} + v^0_{7.4} + v^0_{7.5}\right)$$

$$v^0_{(2.3)\xi} = 2v^0_{2.3}\left(-\frac{5}{2} + v^0_{1.3} + v^0_{1.4} + v^0_{2.2} + \frac{v^0_{2.3}}{2} + v^0_{3.4}\right) - 2v^0_{6.4} - 2v^0_{7.6}$$

$$v^0_{(3.1)\xi} = v^0_{3.1}\left(-3 + v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2} + v^0_{3.1}\right) - v^0_{7.1} - v^0_{7.2}$$

$$v^0_{(3.2)\xi} = v^0_{3.2}\left(-3 + 2v^0_{1.3} + 2v^0_{2.2} + v^0_{3.2}\right) - 2v^0_{7.3}$$

$$v^0_{(3.3)\xi} = v^0_{3.3}\left(-3 + 2v^0_{1.2} + 2v^0_{2.2} + v^0_{3.3}\right) - 2v^0_{7.4}$$

$$v^0_{(3.4)\xi} = v^0_{3.4}\left(-3 + v^0_{1.3} + v^0_{1.4} + v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right) - v^0_{7.5} - v^0_{7.6}$$

$$v^0_{(4.1)\xi} = v^0_{4.1}\left(-\frac{25}{2} + v^0_{1.1} + v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 2\left(v^0_{2.1} + v^0_{3.1} + v^0_{3.2} + v^0_{3.4}\right) + 6v^0_{2.2} + v^0_{2.3} - \frac{v^0_{5.1} + 4v^0_{7.1}}{2v^0_{1.1}} - \frac{v^0_{5.2} + 2v^0_{7.3} + 2v^0_{7.5}}{v^0_{1.3}}\right) - v^0_{8.1}$$

$$v^0_{(4.2)\xi} = v^0_{4.2}\left(-\frac{25}{2} + v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 6v^0_{2.2} + 2\left(v^0_{2.3} + v^0_{3.1} + v^0_{3.3} + v^0_{3.4}\right) - \frac{v^0_{5.1} + 2v^0_{7.2} + 2v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{5.2} + 4v^0_{7.6}}{2v^0_{1.4}}\right) - v^0_{8.2}$$

$$v^0_{(5.1)\xi} = v^0_{5.1}\left(-\frac{21}{2} + v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + v^0_{1.4} + 2v^0_{2.1} + 4v^0_{2.2} + 2v^0_{3.1} + v^0_{3.3} - \frac{v^0_{4.1}}{2v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}}\right) - 2v^0_{9.1} - v^0_{9.2}$$

$$v^0_{(5.2)\xi} = v^0_{5.2}\left(-\frac{21}{2} + v^0_{1.1} + v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 4v^0_{2.2} + 2v^0_{2.3} + v^0_{3.2} + 2v^0_{3.4} - \frac{v^0_{4.1}}{v^0_{1.3}} - \frac{v^0_{4.2}}{2v^0_{1.4}}\right) - v^0_{9.3} - 2v^0_{9.4}$$

$$v^0_{(6.1)\xi} = v^0_{6.1}\left(-\frac{23}{2} + v^0_{1.1} + 2v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 2v^0_{2.1} + 4v^0_{2.2} + \frac{v^0_{2.3}}{2} + 2v^0_{3.1} + v^0_{3.2} + \frac{v^0_{3.3}}{2} + v^0_{3.4} - \frac{v^0_{6.1} + 2v^0_{7.1}}{2v^0_{1.1}} - \frac{v^0_{6.3} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\right) - \frac{v^0_{8.1} + v^0_{9.2}}{2} - v^0_{10.1}$$

$$v^0_{(6.2)\xi} = \frac{v^0_{6.2}}{2}\left(-23 + 4v^0_{1.1} + 6v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 3v^0_{2.1} + 9v^0_{2.2} + v^0_{2.3} + 5v^0_{3.1} + v^0_{3.2} + 2v^0_{3.3} + v^0_{3.4} - \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.2} + 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{8.2} + v^0_{9.1} + v^0_{10.1} + v^0_{10.2}\right)$$

$$v^0_{(6.3)\xi} = v^0_{6.3}\left(-\frac{23}{2} + v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + v^0_{1.4} + \frac{v^0_{2.1}}{2} + 4v^0_{2.2} + 2v^0_{2.3} + v^0_{3.1} + \frac{v^0_{3.2}}{2} + v^0_{3.3} + 2v^0_{3.4} - \frac{v^0_{6.1} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.3} + 2v^0_{7.6}}{2v^0_{1.4}}\right) - \frac{v^0_{8.2} + v^0_{9.3}}{2} - v^0_{10.4}$$

$$v^0_{(6.4)\xi} = \frac{v^0_{6.4}}{2}\left(-23 + v^0_{1.1} + 3v^0_{1.2} + 6v^0_{1.3} + 4v^0_{1.4} + v^0_{2.1} + 9v^0_{2.2} + 3v^0_{2.3} + v^0_{3.1} + 2v^0_{3.2} + v^0_{3.3} + 5v^0_{3.4} - \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.4} + 2v^0_{7.6}}{v^0_{2.3}}\right) - \frac{1}{2}\left(v^0_{8.1} + v^0_{9.4} + v^0_{10.3} + v^0_{10.4}\right)$$

$$v^0_{(7.1)\xi} = \frac{v^0_{7.1}}{2}\left(-20 + 5v^0_{1.1} + 5v^0_{1.2} + 2v^0_{1.3} + 5v^0_{2.1} + 7v^0_{2.2} + 7v^0_{3.1} - \frac{v^0_{4.1} + v^0_{6.1} + 2v^0_{7.1}}{v^0_{1.1}} - 2\frac{v^0_{6.2} + v^0_{7.1}}{v^0_{2.1}}\right) - \frac{1}{2}\left(v^0_{9.1} + v^0_{10.1} + v^0_{11.1}\right)$$

$$v^0_{(7.2)\xi} = \frac{v^0_{7.2}}{2}\left(-20 + 2v^0_{1.1} + 5v^0_{1.2} + 3v^0_{1.3} + 2v^0_{1.4} + 3v^0_{2.1} + 8v^0_{2.2} + v^0_{2.3} + 3v^0_{3.1} + v^0_{3.2} + 2v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.2} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{9.1} + v^0_{10.1} + v^0_{11.2}\right)$$

$$v^0_{(7.3)\xi} = \frac{v^0_{7.3}}{2}\left(-20 + 2v^0_{1.1} + 3v^0_{1.2} + 6v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 9v^0_{2.2} + 2v^0_{2.3} + v^0_{3.1} + 3v^0_{3.2} + v^0_{3.3} + 2v^0_{3.4} - \frac{v^0_{4.1} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{9.3} + v^0_{10.3} + v^0_{11.3}\right)$$

$$v^0_{(7.4)\xi} = \frac{v^0_{7.4}}{2}\left(-20 + v^0_{1.1} + 6v^0_{1.2} + 3v^0_{1.3} + 2v^0_{1.4} + 2v^0_{2.1} + 9v^0_{2.2} + v^0_{2.3} + 2v^0_{3.1} + v^0_{3.2} + 3v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.2} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{9.2} + v^0_{10.2} + v^0_{11.2}\right)$$

$$v^0_{(7.5)\xi} = \frac{v^0_{7.5}}{2}\left(20 + 2v^0_{1.1} + 3v^0_{1.2} + 5v^0_{1.3} + 2v^0_{1.4} + v^0_{2.1} + 8v^0_{2.2} + 3v^0_{2.3} + v^0_{3.1} + 2v^0_{3.2} + v^0_{3.3} + 3v^0_{3.4} - \frac{v^0_{4.1} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{9.4} + v^0_{10.4} + v^0_{11.3}\right)$$

$$v^0_{(7.6)\xi} = \frac{v^0_{7.6}}{2}\left(-20 + 2v^0_{1.2} + 5v^0_{1.3} + 5v^0_{1.4} + 7v^0_{2.2} + 5v^0_{2.3} + 7v^0_{3.4} - \frac{v^0_{4.2} + v^0_{6.3} - 2v^0_{7.6}}{v^0_{1.4}} - 2\frac{v^0_{6.4} + v^0_{7.6}}{v^0_{2.3}}\right) - \frac{1}{2}\left(v^0_{9.4} + v^0_{10.4} + v^0_{11.4}\right)$$

$$v^0_{(8.1)\xi} = v^0_{8.1}\left(-19 + v^0_{1.1} + 2\left(v^0_{1.2} + v^0_{1.4} + v^0_{2.1} + v^0_{3.1} + v^0_{3.2}\right) + 4v^0_{1.3} + 7v^0_{2.2} + \frac{3}{2}v^0_{2.3} + \frac{v^0_{3.3}}{2} + 3v^0_{3.4} - \frac{v^0_{7.1}}{v^0_{1.1}} - \frac{v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{8.1}}{2v^0_{4.1}} - \frac{v^0_{9.2} + 2v^0_{10.1}}{2v^0_{6.1}} - \frac{v^0_{9.4} + v^0_{10.3} + v^0_{10.4}}{v^0_{6.4}}\right)$$

$$v^0_{(8.2)\xi} = v^0_{8.2}\left(-19 + 2\left(v^0_{1.1} + v^0_{1.3} + v^0_{2.3} + v^0_{3.3} + v^0_{3.4}\right) + 4v^0_{1.2} + v^0_{1.4} + \frac{3}{2}v^0_{2.1} + 7v^0_{2.2} + 3v^0_{3.1} + \frac{v^0_{3.2}}{2} - \frac{v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{7.6}}{v^0_{1.4}} - \frac{v^0_{8.2}}{2v^0_{4.2}} - \frac{v^0_{9.1} + v^0_{10.1} + v^0_{10.2}}{v^0_{6.2}} - \frac{v^0_{9.3} + 2v^0_{10.4}}{2v^0_{6.3}}\right)$$

$$v^0_{(9.1)\xi} = \frac{v^0_{9.1}}{2}\left(-34 + 5v^0_{1.1} + 8v^0_{1.2} + 5v^0_{1.3} + 2v^0_{1.4} + 5v^0_{2.1} + 11v^0_{2.2} + v^0_{2.3} + 7v^0_{3.1} + v^0_{3.2} + 2v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{6.2} + 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}} - \frac{2v^0_{9.1} + v^0_{9.2}}{v^0_{5.1}}\right) - \frac{v^0_{12.1} + v^0_{12.2}}{2}$$

$$v^0_{(9.2)\xi} = v^0_{9.2}\left(-17 + v^0_{1.1} + 4v^0_{1.2} + 3v^0_{1.3} + 2v^0_{1.4} + 2v^0_{2.1} + 6v^0_{2.2} + \frac{v^0_{2.3}}{2} + 2v^0_{3.1} + v^0_{3.2} + \frac{3}{2}v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{2v^0_{9.1} + v^0_{9.2}}{2v^0_{5.1}}\right) - v^0_{12.2}$$

$$v^0_{(9.3)\xi} = v^0_{9.3}\left(-17 + 2v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} + v^0_{1.4} + \frac{v^0_{2.1}}{2} + 6v^0_{2.2} + 2v^0_{2.3} + v^0_{3.1} + \frac{3}{2}v^0_{3.2} + v^0_{3.3} + 2v^0_{3.4}\right.$$

$$- \frac{v^0_{4.1}}{v^0_{1.3}} - \frac{v^0_{6.1} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.2}}{2v^0_{6.3}} - \frac{v^0_{9.3} + 2v^0_{9.4}}{2v^0_{5.2}}\Bigg) - v^0_{12.3}$$

$$v^0_{(9.4)\xi} = \frac{v^0_{9.4}}{2}\Bigg(-34 + 2v^0_{1.1} + 5v^0_{1.2} + 8v^0_{1.3} + 5v^0_{1.4} + v^0_{2.1} + 11v^0_{2.2} + 5v^0_{2.3} + v^0_{3.1} + 2v^0_{3.2}$$
$$+ v^0_{3.3} + 7v^0_{3.4} - \frac{v^0_{4.1}}{v^0_{1.3}} - \frac{v^0_{4.2}}{v^0_{1.4}} - \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.4} + 2v^0_{7.6}}{v^0_{2.3}}$$
$$- \frac{v^0_{8.1}}{v^0_{6.4}} - \frac{v^0_{9.3} + 2v^0_{9.4}}{v^0_{5.2}}\Bigg) - \frac{v^0_{12.3} + v^0_{12.4}}{2}$$

$$v^0_{(10.1)\xi} = \frac{v^0_{10.1}}{2}\Bigg(-36 + 5v^0_{1.1} + 7v^0_{1.2} + 6v^0_{1.3} + 2\left(v^0_{1.4} + v^0_{3.2} + v^0_{3.3} + v^0_{3.4}\right) + 6v^0_{2.1} + 13v^0_{2.2} + v^0_{2.3}$$
$$+ 8v^0_{3.1} - \frac{v^0_{6.1} + 2v^0_{7.1}}{v^0_{1.1}} - \frac{v^0_{6.2} + 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + 2v^0_{7.3} + 2v^0_{7.5}}{v^0_{2.2}}$$
$$- \frac{v^0_{8.1}}{v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) - \frac{v^0_{12.1} + v^0_{12.2}}{2}$$

$$v^0_{(10.2)\xi} = v^0_{10.2}\Bigg(-18 + 2v^0_{1.1} + 4v^0_{1.2} + 3v^0_{1.3} + v^0_{1.4} + 2v^0_{2.1} + 7v^0_{2.2} + v^0_{2.3} + 3v^0_{3.1} + v^0_{3.2} + 2v^0_{3.3} + v^0_{3.4}$$
$$- \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) - v^0_{12.2}$$

$$v^0_{(10.3)\xi} = v^0_{10.3}\Bigg(-18 + v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} + 2v^0_{1.4} + v^0_{2.1} + 7v^0_{2.2} + 2v^0_{2.3} + v^0_{3.1} + 2v^0_{3.2} + v^0_{3.3} + 3v^0_{3.4}$$
$$- \frac{v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{7.6}}{v^0_{2.3}} - \frac{v^0_{8.1}}{v^0_{6.4}}\Bigg) - v^0_{12.3}$$

$$v^0_{(10.4)\xi} = \frac{v^0_{10.4}}{2}\Bigg(-36 + 2\left(v^0_{1.1} + v^0_{3.1} + v^0_{3.2} + v^0_{3.3}\right) + 6v^0_{1.2} + 7v^0_{1.3} + 5v^0_{1.4} + v^0_{2.1} + 13v^0_{2.2} + 6v^0_{2.3}$$
$$+ 8v^0_{3.4} - \frac{v^0_{6.1} + 2v^0_{7.2} + 2v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{6.3} + 2v^0_{7.6}}{v^0_{1.4}} - \frac{v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.4} + 2v^0_{7.6}}{v^0_{2.3}}$$
$$- \frac{v^0_{8.1}}{v^0_{6.4}} - \frac{v^0_{8.2}}{v^0_{6.3}}\Bigg) - \frac{v^0_{12.3} + v^0_{12.4}}{2}$$

$$v^0_{(11.1)\xi} = v^0_{11.1}\Bigg(-17 + 4v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 4v^0_{2.1} + 6v^0_{2.2} + 6v^0_{3.1} - \frac{v^0_{4.1} + v^0_{6.1} + 2v^0_{7.1}}{v^0_{1.1}}$$
$$- 2\frac{v^0_{6.2} + v^0_{7.1}}{v^0_{2.1}}\Bigg) - v^0_{12.1}$$

$$v^0_{(11.2)\xi} = v^0_{11.2}\Bigg(-17 + v^0_{1.1} + 4v^0_{1.2} + 3v^0_{1.3} + 2\left(v^0_{1.4} + v^0_{2.1} + v^0_{3.1} + v^0_{3.3}\right) + 7v^0_{2.2} + v^0_{2.3} + v^0_{3.2} + v^0_{3.4}$$
$$- \frac{v^0_{4.2} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}}\Bigg) - v^0_{12.2}$$

$$v^0_{(11.3)\xi} = v^0_{11.3}\Bigg(-17 + 2\left(v^0_{1.1} + v^0_{2.3} + v^0_{3.2} + v^0_{3.4}\right) + 3v^0_{1.2} + 4v^0_{1.3} + v^0_{1.4} + v^0_{2.1} + 7v^0_{2.2} + v^0_{3.1} + v^0_{3.3}$$
$$- \frac{v^0_{4.1} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.1} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}}\Bigg) - v^0_{12.3}$$

$$v^0_{(11.4)\xi} = v^0_{11.4}\left(-17 + 2v^0_{1.2} + 4v^0_{1.3} + 4v^0_{1.4} + 6v^0_{2.2} + 4v^0_{2.3} + 6v^0_{3.4} - 2\frac{v^0_{6.4} + v^0_{7.6}}{v^0_{2.3}} - \frac{v^0_{4.2} + v^0_{6.3} + 2v^0_{7.6}}{v^0_{1.4}}\right) - v^0_{12.4}$$

$$v^0_{(12.1)\xi} = v^0_{12.1}\left(-25 + 4v^0_{1.1} + 5v^0_{1.2} + 4v^0_{1.3} + v^0_{1.4} + 4v^0_{2.1} + 8v^0_{2.2} + \frac{v^0_{2.3}}{2} + 6v^0_{3.1} + v^0_{3.2} + v^0_{3.3} + v^0_{3.4} - \frac{v^0_{4.1} + v^0_{6.1} + 2v^0_{7.1}}{2v^0_{1.1}} - \frac{v^0_{6.2} + 2v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}} - \frac{2v^0_{9.1} + v^0_{9.2}}{2v^0_{5.1}}\right) - \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.2)\xi} = \frac{v^0_{12.2}}{2}\left(-50 + 5v^0_{1.1} + 10v^0_{1.2} + 9v^0_{1.3} + 4v^0_{1.4} + 6v^0_{2.1} + 17v^0_{2.2} + 2v^0_{2.3} + 8v^0_{3.1} + 3v^0_{3.2} + 4v^0_{3.3} + 3v^0_{3.4} - 2\frac{v^0_{7.1}}{v^0_{2.1}} - \frac{v^0_{4.2} + v^0_{6.2} + v^0_{7.2} + v^0_{7.4}}{v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{6.4} + 3v^0_{7.3} + 3v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} - \frac{2v^0_{9.1} + v^0_{9.2}}{v^0_{5.1}}\right) - \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.3)\xi} = \frac{v^0_{12.3}}{2}\left(-50 + 4v^0_{1.1} + 9v^0_{1.2} + 10v^0_{1.3} + 5v^0_{1.4} + 2v^0_{2.1} + 17v^0_{2.2} + 6v^0_{2.3} + 3v^0_{3.1} + 4v^0_{3.2} + 3v^0_{3.3} + 8v^0_{3.4} - \frac{v^0_{4.1} + v^0_{6.4} + v^0_{7.3} + v^0_{7.5}}{v^0_{1.3}} - \frac{v^0_{6.1} + v^0_{6.2} + 3v^0_{7.2} + 3v^0_{7.4}}{v^0_{2.2}} - 2\frac{v^0_{7.6}}{v^0_{2.3}} - 2\frac{v^0_{8.1}}{v^0_{6.4}} - \frac{v^0_{8.2}}{v^0_{6.3}} - \frac{v^0_{9.3} + 2v^0_{9.4}}{v^0_{5.2}}\right) - \frac{v^0_{13.2}}{2}$$

$$v^0_{(12.4)\xi} = v^0_{12.4}\left(-25 + v^0_{1.1} + 4v^0_{1.2} + 5v^0_{1.3} + 4v^0_{1.4} + \frac{v^0_{2.1}}{2} + 8v^0_{2.2} + 4v^0_{2.3} + v^0_{3.1} + v^0_{3.2} + v^0_{3.3} + 6v^0_{3.4} - \frac{v^0_{4.2} + v^0_{6.3} + 2v^0_{7.6}}{2v^0_{1.4}} - \frac{v^0_{6.4} + 2v^0_{7.6}}{v^0_{2.3}} - \frac{v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.4}} - \frac{v^0_{8.2}}{2v^0_{6.3}} - \frac{v^0_{9.3} + 2v^0_{9.4}}{2v^0_{5.2}}\right) - \frac{v^0_{13.2}}{2}$$

$$v^0_{(13.1)\xi} = v^0_{13.1}\left(-33 + 4v^0_{1.1} + 6v^0_{1.2} + 6v^0_{1.3} + 2\left(v^0_{1.4} + v^0_{3.2} + v^0_{3.3} + v^0_{3.4}\right) + 4v^0_{2.1} + 10v^0_{2.2} + v^0_{2.3} + 6v^0_{3.1} - 2\frac{v^0_{7.1}}{v^0_{2.1}} - 2\frac{v^0_{7.3} + v^0_{7.5}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} - \frac{2v^0_{9.1} + v^0_{9.2}}{v^0_{5.1}}\right)$$

$$v^0_{(13.2)\xi} = v^0_{13.2}\left(-33 + 2\left(v^0_{1.1} + v^0_{3.1} + v^0_{3.2} + v^0_{3.3}\right) + 6v^0_{1.2} + 6v^0_{1.3} + 4v^0_{1.4} + v^0_{2.1} + 10v^0_{2.2} + 4v^0_{2.3} + 6v^0_{3.4} - 2\frac{v^0_{7.2} + v^0_{7.4}}{v^0_{2.2}} - 2\frac{v^0_{7.6}}{v^0_{2.3}} - 2\frac{v^0_{8.1}}{v^0_{6.4}} - \frac{v^0_{8.2}}{v^0_{6.3}} - \frac{v^0_{9.3} + 2v^0_{9.4}}{v^0_{5.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = 1;$	$u^0_{1.2} = -1;$	$u^0_{1.3} = -1;$	$u^0_{1.4} = 1$
$u^0_{2.1} = 1;$	$u^0_{2.2} = -1;$	$u^0_{2.3} = 1;$	$u^0_{3.1} = 1$
$u^0_{3.2} = 1;$	$u^0_{3.3} = 1;$	$u^0_{3.4} = 1;$	$u^0_{4.1} = 1$
$u^0_{4.2} = -1;$	$u^0_{5.1} = 1;$	$u^0_{5.2} = -1;$	$u^0_{6.1} = 1$
$u^0_{6.2} = 1;$	$u^0_{6.3} = -1;$	$u^0_{6.4} = -1;$	$u^0_{7.1} = -1$
$u^0_{7.2} = 1;$	$u^0_{7.3} = 1;$	$u^0_{7.4} = -1;$	$u^0_{7.5} = -1$
$u^0_{7.6} = 1;$	$u^0_{8.1} = 1;$	$u^0_{8.2} = 1;$	$u^0_{9.1} = -1$
$u^0_{9.2} = 1;$	$u^0_{9.3} = 1;$	$u^0_{9.4} = -1;$	$u^0_{10.1} = -1$
$u^0_{10.2} = 1;$	$u^0_{10.3} = 1;$	$u^0_{10.4} = -1;$	$u^0_{11.1} = 1$
$u^0_{11.2} = 1;$	$u^0_{11.3} = 1;$	$u^0_{11.4} = 1;$	$u^0_{12.1} = 1$
$u^0_{12.2} = -1;$	$u^0_{12.3} = 1;$	$u^0_{12.4} = -1;$	$u^0_{13.1} = 1$
$u^0_{13.2} = 1$			

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = -2;$	$u^0_{(1.2)0} = 0;$	$u^0_{(1.3)0} = 0;$	$u^0_{(1.4)0} = 2$
$u^0_{(2.1)0} = -2;$	$u^0_{(2.2)0} = 0;$	$u^0_{(2.3)0} = 2;$	$u^0_{(3.1)0} = -2$
$u^0_{(3.2)0} = -2;$	$u^0_{(3.3)0} = 2;$	$u^0_{(3.4)0} = 2;$	$u^0_{(4.1)0} = -1$
$u^0_{(4.2)0} = -1;$	$u^0_{(5.1)0} = -1;$	$u^0_{(5.2)0} = -1;$	$u^0_{(6.1)0} = -1$
$u^0_{(6.2)0} = -1;$	$u^0_{(6.3)0} = -1;$	$u^0_{(6.4)0} = -1;$	$u^0_{(7.1)0} = 3$
$u^0_{(7.2)0} = -1;$	$u^0_{(7.3)0} = -1;$	$u^0_{(7.4)0} = -1;$	$u^0_{(7.5)0} = -1$
$u^0_{(7.6)0} = 3;$	$u^0_{(8.1)0} = 0;$	$u^0_{(8.2)0} = 0;$	$u^0_{(9.1)0} = 2$
$u^0_{(9.2)0} = 0;$	$u^0_{(9.3)0} = 0;$	$u^0_{(9.4)0} = -2;$	$u^0_{(10.1)0} = 2$
$u^0_{(10.2)0} = 0;$	$u^0_{(10.3)0} = 0;$	$u^0_{(10.4)0} = -2;$	$u^0_{(11.1)0} = -4$
$u^0_{(11.2)0} = 0;$	$u^0_{(11.3)0} = 0;$	$u^0_{(11.4)0} = 4;$	$u^0_{(12.1)0} = -3$
$u^0_{(12.2)0} = 1;$	$u^0_{(12.3)0} = 1;$	$u^0_{(12.4)0} = -3;$	$u^0_{(13.1)0} = -2$
$u^0_{(13.2)0} = 2$			

and

$u^0_{(1.1)\xi} = 2;$	$u^0_{(1.2)\xi} = -2;$	$u^0_{(1.3)\xi} = -2;$	$u^0_{(1.4)\xi} = 2$
$u^0_{(2.1)\xi} = 2;$	$u^0_{(2.2)\xi} = -2;$	$u^0_{(2.3)\xi} = 2;$	$u^0_{(3.1)\xi} = 2$
$u^0_{(3.2)\xi} = 2;$	$u^0_{(3.3)\xi} = 2;$	$u^0_{(3.4)\xi} = 2;$	$u^0_{(4.1)\xi} = 3$
$u^0_{(4.2)\xi} = -3;$	$u^0_{(5.1)\xi} = 3;$	$u^0_{(5.2)\xi} = -3;$	$u^0_{(6.1)\xi} = 3$
$u^0_{(6.2)\xi} = 3;$	$u^0_{(6.3)\xi} = -3;$	$u^0_{(6.4)\xi} = -3;$	$u^0_{(7.1)\xi} = -3$
$u^0_{(7.2)\xi} = 3;$	$u^0_{(7.3)\xi} = 3;$	$u^0_{(7.4)\xi} = -3;$	$u^0_{(7.5)\xi} = -3$

$u^0_{(7.6)\xi} = 3$; $u^0_{(8.1)\xi} = 4$; $u^0_{(8.2)\xi} = 4$; $u^0_{(9.1)\xi} = -4$
$u^0_{(9.2)\xi} = 4$; $u^0_{(9.3)\xi} = 4$; $u^0_{(9.4)\xi} = -4$; $u^0_{(10.1)\xi} = -4$
$u^0_{(10.2)\xi} = 4$; $u^0_{(10.3)\xi} = 4$; $u^0_{(10.4)\xi} = -4$; $u^0_{(11.1)\xi} = 4$
$u^0_{(11.2)\xi} = 4$; $u^0_{(11.3)\xi} = 4$; $u^0_{(11.4)\xi} = 4$; $u^0_{(12.1)\xi} = 5$
$u^0_{(12.2)\xi} = -5$; $u^0_{(12.3)\xi} = 5$; $u^0_{(12.4)\xi} = -5$; $u^0_{(13.1)\xi} = 6$
$u^0_{(13.2)\xi} = 6$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1}$; $u^0_{(1.2)00} = 2v^0_{1.2}$; $u^0_{(1.3)00} = 2v^0_{1.3}$
$u^0_{(1.4)00} = 2v^0_{1.4}$; $u^0_{(2.1)00} = 2v^0_{2.1}$; $u^0_{(2.2)00} = 2v^0_{2.2}$
$u^0_{(2.3)00} = 2v^0_{2.3}$; $u^0_{(3.1)00} = 2v^0_{3.1}$; $u^0_{(3.2)00} = 2v^0_{3.2}$
$u^0_{(3.3)00} = 2v^0_{3.3}$; $u^0_{(3.4)00} = 2v^0_{3.4}$; $u^0_{(4.1)00} = 2v^0_{1.1} - 4v^0_{1.3}$
$u^0_{(4.2)00} = 4v^0_{1.2} - 2v^0_{1.4}$; $u^0_{(5.1)00} = 2v^0_{1.1} - 4v^0_{1.2}$; $u^0_{(5.2)00} = 4v^0_{1.3} - 2v^0_{1.4}$
$u^0_{(6.1)00} = 2v^0_{1.1} - 4v^0_{2.2}$; $u^0_{(6.2)00} = -2v^0_{1.2} + 2v^0_{2.1} - 2v^0_{2.2}$; $u^0_{(6.3)00} = -2v^0_{1.4} + 4v^0_{2.2}$
$u^0_{(6.4)00} = 2v^0_{1.3} + 2v^0_{2.2} - 2v^0_{2.3}$; $u^0_{(7.1)00} = -2v^0_{1.1} - 2v^0_{2.1} - 2v^0_{3.1}$; $u^0_{(7.2)00} = -2v^0_{1.2} - 2v^0_{2.2} + 2v^0_{3.1}$
$u^0_{(7.3)00} = -2v^0_{1.3} - 2v^0_{2.2} + 2v^0_{3.2}$; $u^0_{(7.4)00} = 2v^0_{1.2} + 2v^0_{2.2} - 2v^0_{3.3}$; $u^0_{(7.5)00} = 2v^0_{1.3} + 2v^0_{2.2} - 2v^0_{3.4}$

$u^0_{(7.6)00} = 2v^0_{1.4} + 2v^0_{2.3} + 2v^0_{3.4}$; $u^0_{(8.1)00} = 2v^0_{1.1} - 4v^0_{1.3} - 4v^0_{2.2} + 2v^0_{2.3}$
$u^0_{(8.2)00} = -4v^0_{1.2} + 2v^0_{1.4} + 2v^0_{2.1} - 4v^0_{2.2}$; $u^0_{(9.1)00} = -2\left(v^0_{1.1} + v^0_{2.1} - v^0_{2.2} + v^0_{3.1}\right) + 4v^0_{1.2}$
$u^0_{(9.2)00} = 2v^0_{1.1} - 4v^0_{1.2} - 4v^0_{2.2} + 2v^0_{3.3}$; $u^0_{(9.3)00} = -4v^0_{1.3} + 2v^0_{1.4} - 4v^0_{2.2} + 2v^0_{3.2}$
$u^0_{(9.4)00} = 4v^0_{1.3} - 2\left(v^0_{1.4} - v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right)$; $u^0_{(10.1)00} = -2\left(v^0_{1.1} - v^0_{1.2} + v^0_{2.1} + v^0_{3.1}\right) + 4v^0_{2.2}$
$u^0_{(10.2)00} = -4v^0_{1.2} - 4v^0_{2.2} + 2v^0_{2.1} + 2v^0_{3.3}$; $u^0_{(10.3)00} = -4v^0_{1.3} - 4v^0_{2.2} + 2v^0_{2.3} + 2v^0_{3.2}$
$u^0_{(10.4)00} = -2\left(-v^0_{1.3} + v^0_{1.4} + v^0_{2.3} + v^0_{3.4}\right) + 4v^0_{2.2}$; $u^0_{(11.1)00} = 4v^0_{1.1} + 4v^0_{2.1} + 4v^0_{3.1}$
$u^0_{(11.2)00} = -4v^0_{1.2} - 4v^0_{2.2} + 2v^0_{3.1} + 2v^0_{3.3}$; $u^0_{(11.3)00} = -4v^0_{1.3} - 4v^0_{2.2} + 2v^0_{3.2} + 2v^0_{3.4}$
$u^0_{(11.4)00} = 4v^0_{1.4} + 4v^0_{2.3} + 4v^0_{3.4}$; $u^0_{(12.1)00} = 4\left(v^0_{1.1} - v^0_{1.2} + v^0_{2.1} - v^0_{2.2} + v^0_{3.1}\right)$

$$u^0_{(12.2)00} = -2\left(v^0_{1.1} + v^0_{2.1} + v^0_{3.1} + v^0_{3.3}\right) + 6v^0_{1.2} + 6v^0_{2.2}$$
$$u^0_{(12.3)00} = 2\left(v^0_{1.4} + v^0_{2.3} + v^0_{3.2} + v^0_{3.4}\right) - 6v^0_{1.3} - 6v^0_{2.2}$$
$$u^0_{(12.4)00} = -4\left(-v^0_{1.3} + v^0_{1.4} - v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right)$$
$$u^0_{(13.1)00} = 4v^0_{1.1} - 8v^0_{1.2} + 4v^0_{2.1} - 8v^0_{2.2} + 4v^0_{3.1} + 2v^0_{3.3}$$
$$u^0_{(13.2)00} = -8v^0_{1.3} + 4v^0_{1.4} - 8v^0_{2.2} + 4v^0_{2.3} + 2v^0_{3.2} + 4v^0_{3.4}$$

$u^0_{(1.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(1.2)\xi 0} = 0$; $u^0_{(1.3)\xi 0} = 0$; $u^0_{(1.4)\xi 0} = 2v^0_{1.4}$
$u^0_{(2.1)\xi 0} = -2v^0_{2.1}$; $u^0_{(2.2)\xi 0} = 0$; $u^0_{(2.3)\xi 0} = 2v^0_{2.3}$; $u^0_{(3.1)\xi 0} = -2v^0_{3.1}$
$u^0_{(3.2)\xi 0} = -2v^0_{3.2}$; $u^0_{(3.3)\xi 0} = 2v^0_{3.3}$; $u^0_{(3.4)\xi 0} = 2v^0_{3.4}$; $u^0_{(4.1)\xi 0} = -2v^0_{1.1}$
$u^0_{(4.2)\xi 0} = -2v^0_{1.4}$; $u^0_{(5.1)\xi 0} = -2v^0_{1.1}$; $u^0_{(5.2)\xi 0} = -2v^0_{1.4}$; $u^0_{(6.1)\xi 0} = -2v^0_{1.1}$
$u^0_{(6.2)\xi 0} = -2v^0_{2.1}$; $u^0_{(6.3)\xi 0} = -2v^0_{1.4}$; $u^0_{(6.4)\xi 0} = -2v^0_{2.3}$; $u^0_{(7.1)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} + 2v^0_{3.1}$

$$u^0_{(7.2)\xi 0} = -2v^0_{3.1};\quad u^0_{(7.3)\xi 0} = -2v^0_{3.2};\quad u^0_{(7.4)\xi 0} = -2v^0_{3.3};\quad u^0_{(7.5)\xi 0} = -2v^0_{3.4}$$

$$u^0_{(7.6)\xi 0} = 2v^0_{1.4} + 2v^0_{2.3} + 2v^0_{3.4};\quad u^0_{(8.1)\xi 0} = 2v^0_{2.3} - 2v^0_{1.1};\quad u^0_{(8.2)\xi 0} = 2v^0_{1.4} - 2v^0_{2.1}$$

$$u^0_{(9.1)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} + 2v^0_{3.1};\quad u^0_{(9.2)\xi 0} = 2v^0_{3.3} - 2v^0_{1.1};\quad u^0_{(9.3)\xi 0} = 2v^0_{1.4} - 2v^0_{3.2}$$

$$u^0_{(9.4)\xi 0} = -2v^0_{1.4} - 2v^0_{2.3} - 2v^0_{3.4};\quad u^0_{(10.1)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} + 2v^0_{3.1};\quad u^0_{(10.2)\xi 0} = 2v^0_{3.3} - 2v^0_{2.1}$$

$$u^0_{(10.3)\xi 0} = 2v^0_{2.3} - 2v^0_{3.2};\quad u^0_{(10.4)\xi 0} = -2v^0_{1.4} - 2v^0_{2.3} - 2v^0_{3.4};\quad u^0_{(11.1)\xi 0} = -4v^0_{1.1} - 4v^0_{2.1} - 4v^0_{3.1}$$

$$u^0_{(11.2)\xi 0} = 2v^0_{3.3} - 2v^0_{3.1};\quad u^0_{(11.3)\xi 0} = 2v^0_{3.4} - 2v^0_{3.2};\quad u^0_{(11.4)\xi 0} = 4v^0_{1.4} + 4v^0_{2.3} + 4v^0_{3.4}$$

$$u^0_{(12.1)\xi 0} = -4v^0_{1.1} - 4v^0_{2.1} - 4v^0_{3.1}$$
$$u^0_{(12.2)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} + 2v^0_{3.1} - 2v^0_{3.3}$$
$$u^0_{(12.3)\xi 0} = 2v^0_{1.4} + 2v^0_{2.3} - 2v^0_{3.2} + 2v^0_{3.4}$$
$$u^0_{(12.4)\xi 0} = -4v^0_{1.4} - 4v^0_{2.3} - 4v^0_{3.4}$$
$$u^0_{(13.1)\xi 0} = -4v^0_{1.1} - 4v^0_{2.1} - 4v^0_{3.1} + 2v^0_{3.3}$$
$$u^0_{(13.2)\xi 0} = 4v^0_{1.4} + 4v^0_{2.3} - 2v^0_{3.2} + 4v^0_{3.4}$$

and

$$u^0_{(1.1)\xi\xi} = 2v^0_{1.1};\quad u^0_{(1.2)\xi\xi} = -2v^0_{1.2};\quad u^0_{(1.3)\xi\xi} = -2v^0_{1.3}$$
$$u^0_{(1.4)\xi\xi} = 2v^0_{1.4};\quad u^0_{(2.1)\xi\xi} = 2v^0_{2.1};\quad u^0_{(2.2)\xi\xi} = -2v^0_{2.2}$$
$$u^0_{(2.3)\xi\xi} = 2v^0_{2.3};\quad u^0_{(3.1)\xi\xi} = 2v^0_{3.1};\quad u^0_{(3.2)\xi\xi} = 2v^0_{3.2}$$
$$u^0_{(3.3)\xi\xi} = 2v^0_{3.3};\quad u^0_{(3.4)\xi\xi} = 2v^0_{3.4};\quad u^0_{(4.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.3}$$
$$u^0_{(4.2)\xi\xi} = -4v^0_{1.2} - 2v^0_{1.4};\quad u^0_{(5.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2};\quad u^0_{(5.2)\xi\xi} = -4v^0_{1.3} - 2v^0_{1.4}$$
$$u^0_{(6.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{2.2};\quad u^0_{(6.2)\xi\xi} = 2v^0_{1.2} + 2v^0_{2.1} + 2v^0_{2.2};\quad u^0_{(6.3)\xi\xi} = -2v^0_{1.4} - 4v^0_{2.2}$$
$$u^0_{(6.4)\xi\xi} = -2v^0_{1.3} - 2v^0_{2.2} - 2v^0_{2.3};\quad u^0_{(7.1)\xi\xi} = -2v^0_{1.1} - 2v^0_{2.1} - 2v^0_{3.1};\quad u^0_{(7.2)\xi\xi} = 2v^0_{1.2} + 2v^0_{2.2} + 2v^0_{3.1}$$
$$u^0_{(7.3)\xi\xi} = 2v^0_{1.3} + 2v^0_{2.2} + 2v^0_{3.2};\quad u^0_{(7.4)\xi\xi} = -2v^0_{1.2} - 2v^0_{2.2} - 2v^0_{3.3};\quad u^0_{(7.5)\xi\xi} = -2v^0_{1.3} - 2v^0_{2.2} - 2v^0_{3.4}$$
$$u^0_{(7.6)\xi\xi} = 2v^0_{1.4} + 2v^0_{2.3} + 2v^0_{3.4};\quad u^0_{(8.1)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.3} + 4v^0_{2.2} + 2v^0_{2.3}$$
$$u^0_{(8.2)\xi\xi} = 4v^0_{1.2} + 2v^0_{1.4} + 2v^0_{2.1} + 4v^0_{2.2};\quad u^0_{(9.1)\xi\xi} = -2\left(v^0_{1.1} + v^0_{2.1} + v^0_{2.2} + v^0_{3.1}\right) - 4v^0_{1.2}$$
$$u^0_{(9.2)\xi\xi} = 2v^0_{1.1} + 4v^0_{1.2} + 4v^0_{2.2} + 2v^0_{3.3};\quad u^0_{(9.3)\xi\xi} = 4v^0_{1.3} + 2v^0_{1.4} + 4v^0_{2.2} + 2v^0_{3.2}$$
$$u^0_{(9.4)\xi\xi} = -4v^0_{1.3} - 2\left(v^0_{1.4} + v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right);\quad u^0_{(10.1)\xi\xi} = -2\left(v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{3.1}\right) - 4v^0_{2.2}$$
$$u^0_{(10.2)\xi\xi} = 4v^0_{1.2} + 2v^0_{2.1} + 4v^0_{2.2} + 2v^0_{3.3};\quad u^0_{(10.3)\xi\xi} = 4v^0_{1.3} + 4v^0_{2.2} + 2v^0_{2.3} + 2v^0_{3.2}$$
$$u^0_{(10.4)\xi\xi} = -2\left(v^0_{1.3} + v^0_{1.4} + v^0_{2.3} + v^0_{3.4}\right) - 4v^0_{2.2};\quad u^0_{(11.1)\xi\xi} = 4v^0_{1.1} + 4v^0_{2.1} + 4v^0_{3.1}$$
$$u^0_{(11.2)\xi\xi} = 4v^0_{1.2} + 4v^0_{2.2} + 2v^0_{3.1} + 2v^0_{3.3};\quad u^0_{(11.3)\xi\xi} = 4v^0_{1.3} + 4v^0_{2.2} + 2v^0_{3.2} + 2v^0_{3.4}$$
$$u^0_{(11.4)\xi\xi} = 4v^0_{1.4} + 4v^0_{2.3} + 4v^0_{3.4};\quad u^0_{(12.1)\xi\xi} = 4\left(v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2} + v^0_{3.1}\right)$$

$$u^0_{(12.2)\xi\xi} = -2\left(v^0_{1.1} + v^0_{2.1} + v^0_{3.1} + v^0_{3.3}\right) - 6v^0_{1.2} - 6v^0_{2.2}$$
$$u^0_{(12.3)\xi\xi} = 6v^0_{1.3} + 2\left(v^0_{1.4} + v^0_{2.3} + v^0_{3.2} + v^0_{3.4}\right) + 6v^0_{2.2}$$
$$u^0_{(12.4)\xi\xi} = -4\left(v^0_{1.3} + v^0_{1.4} + v^0_{2.2} + v^0_{2.3} + v^0_{3.4}\right)$$
$$u^0_{(13.1)\xi\xi} = 4v^0_{1.1} + 8v^0_{1.2} + 4v^0_{2.1} + 8v^0_{2.2} + 4v^0_{3.1} + 2v^0_{3.3}$$
$$u^0_{(13.2)\xi\xi} = 8v^0_{1.3} + 4v^0_{1.4} + 8v^0_{2.2} + 4v^0_{2.3} + 2v^0_{3.2} + 4v^0_{3.4}$$

A.3.3 Thermodynamics of $D0_{19}$ phase using triangle–tetrahedron approximation

The triangle–tetrahedron clusters considered for $D0_{19}$ phase is shown in Figure A.9 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.9.

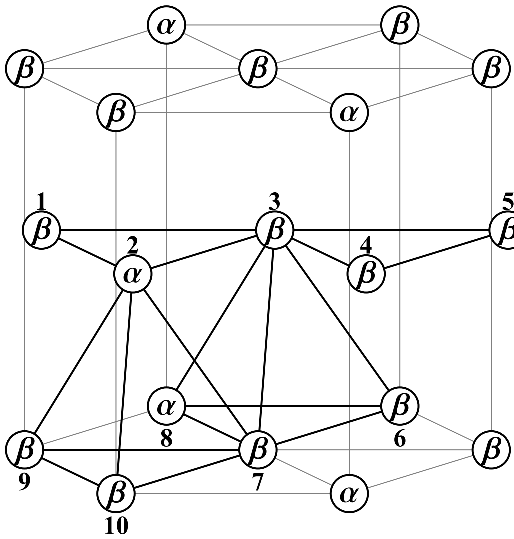

Figure A.9: The triangle–tetrahedron basic clusters in $D0_{19}$ phase along with the sublattice sites designated α and β.

Table A.9: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $D0_{19}$ phase using triangle–tetrahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Regular tetrahedron	$\alpha\beta\beta\beta$(T2, $\beta\beta\beta$OP) (8,3,6,7)	6.2	3/2	1
	$\alpha\beta\beta\beta$(T1, $\beta\beta\beta$IP) (2,7,9,10)	6.1	1/2	
Equilateral triangle (OP)	$\beta\beta\beta$ (3,6,7)	5.3	3/2	0
	$\alpha\beta\beta$(T2) (8,3,7)	5.2	3	
	$\alpha\beta\beta$(T1) (2,7,9)	5.1	3/2	
Equilateral triangle (OB)	$\beta\beta\beta$ (3,4,5)	4.2	1/4	1
	$\alpha\beta\beta$ (2,1,3)	4.1	3/4	
Equilateral triangle (TB)	$\beta\beta\beta$ (7,9,10)	3.2	1/4	-1
	$\alpha\beta\beta$ (8,6,7)	3.1	3/4	

cont . . .

cont ...

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
I-n pair (OP)	$\beta\beta$ (3,6)	2.2	3/2	-1
	$\alpha\beta$ (2,7)	2.1	3/2	
I-n pair (IP)	$\beta\beta$(T2) (6,7)	1.3	3/4	-1
	$\beta\beta$(T1) (7,9)	1.2	3/4	
	$\alpha\beta$ (8,6)	1.1	3/2	
Point	β (1)	0.2	3/4	5
	α (2)	0.1	1/4	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + 3u_{0.2})/4 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{1}{\eta_1\eta_5\sqrt{\eta_3\eta_4\eta_6}}; \quad v^0_{1.2} = \frac{\eta_1}{\eta_5}\sqrt{\frac{\eta_3}{\eta_4\eta_6}}; \quad v^0_{1.3} = \eta_1\eta_5\sqrt{\frac{\eta_4}{\eta_3\eta_6}}; \quad v^0_{2.1} = \frac{1}{\eta_2\eta_5^2\sqrt{\eta_6}}$$

$$v^0_{2.2} = \frac{\eta_2}{\sqrt{\eta_6}}; \quad v^0_{3.1} = \frac{1}{\eta_1\eta_5\sqrt{\eta_3\eta_4\eta_6}}; \quad v^0_{3.2} = \frac{\eta_1^3}{\eta_4^{3/2}\eta_5^3}\sqrt{\frac{\eta_3}{\eta_6}}; \quad v^0_{4.1} = \frac{1}{\eta_1\eta_5^3\eta_6^{3/2}\sqrt{\eta_3\eta_4}}$$

$$v^0_{4.2} = \frac{\eta_1^3\eta_5^3\sqrt{\eta_4}}{\eta_3^{3/2}\eta_6^{3/2}}; \quad v^0_{5.1} = \frac{\eta_1}{\eta_2^2\eta_5^4\eta_6}\sqrt{\frac{\eta_3}{\eta_4}}; \quad v^0_{5.2} = \frac{1}{\eta_1\eta_5^2\eta_6\sqrt{\eta_3\eta_4}}; \quad v^0_{5.3} = \frac{\eta_1\eta_2^2}{\eta_6}\sqrt{\frac{\eta_4}{\eta_3}}$$

$$v^0_{6.1} = \frac{\eta_1^3\sqrt{\eta_3}}{\eta_2^3\eta_4^{3/2}\eta_5^6\eta_6^{3/2}}; \quad v^0_{6.2} = \frac{\eta_2}{\eta_1\eta_5^2\eta_6^{3/2}\sqrt{\eta_3\eta_4}}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(-2 + v^0_{1.1} + \frac{v^0_{1.2}}{2} + \frac{v^0_{1.3}}{2} + v^0_{2.1} + v^0_{2.2}\right) - \frac{v^0_{3.1} + v^0_{4.1}}{2} - v^0_{5.2}$$

$$v^0_{(1.2)0} = v^0_{1.2}\left(-v^0_{1.1} + 2v^0_{1.2} - 2v^0_{2.1}\right) - \frac{v^0_{3.2} - v^0_{4.1}}{2} + v^0_{5.1}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(-2 - v^0_{1.1} + 2v^0_{1.3} + 2v^0_{2.2}\right) + \frac{v^0_{3.1} - v^0_{4.2}}{2} - v^0_{5.3}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(-2 + v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2}\right) - v^0_{5.1} - v^0_{5.2}$$
$$v^0_{(2.2)0} = v^0_{2.2}\left(-1 - v^0_{1.1} + v^0_{1.3} - v^0_{2.1} + 2v^0_{2.2}\right) + v^0_{5.2} - v^0_{5.3}$$
$$v^0_{(3.1)0} = v^0_{3.1}\left(-\frac{9}{2} + v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} + v^0_{2.1} + 2v^0_{2.2} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{2v^0_{1.3}}\right) - v^0_{6.2}$$
$$v^0_{(3.2)0} = v^0_{3.2}\left(\frac{1}{2} - 3v^0_{1.1} + 3v^0_{1.2} - 3v^0_{2.1} + \frac{3v^0_{4.1}}{2v^0_{1.2}}\right) + v^0_{6.1}$$
$$v^0_{(4.1)0} = v^0_{4.1}\left(-\frac{7}{2} + v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 2v^0_{2.2} - \frac{v^0_{3.2} - 2v^0_{5.1}}{2v^0_{1.2}} - \frac{v^0_{3.1} + 2v^0_{5.2}}{v^0_{1.1}}\right)$$
$$v^0_{(4.2)0} = \frac{3v^0_{4.2}}{2}\left(-3 - 2v^0_{1.1} + 2v^0_{1.3} + 4v^0_{2.2} + \frac{v^0_{3.1} - 2v^0_{5.3}}{v^0_{1.3}}\right)$$
$$v^0_{(5.1)0} = v^0_{5.1}\left(-3 + v^0_{1.1} + 2v^0_{1.2} - \frac{v^0_{2.1}}{2} + 2v^0_{2.2} + \frac{v^0_{4.1} + v^0_{5.1}}{2v^0_{1.2}} - 2\frac{v^0_{5.2}}{v^0_{2.1}}\right) - \frac{v^0_{6.1}}{2}$$
$$v^0_{(5.2)0} = \frac{v^0_{5.2}}{2}\left(-8 + v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + 2v^0_{2.1} + 5v^0_{2.2} - \frac{v^0_{4.1} + v^0_{5.2}}{v^0_{1.1}} - 2\frac{v^0_{5.1}}{v^0_{2.1}} + \frac{v^0_{5.2} - v^0_{5.3}}{v^0_{2.2}}\right) - \frac{v^0_{6.2}}{2}$$
$$v^0_{(5.3)0} = \frac{v^0_{5.3}}{2}\left(-6 - 4v^0_{1.1} + 6v^0_{1.3} - 3v^0_{2.1} + 8v^0_{2.2} + 2\frac{v^0_{5.2} - v^0_{5.3}}{v^0_{2.2}} - \frac{v^0_{4.2} + v^0_{5.3}}{v^0_{1.3}}\right) + \frac{v^0_{6.2}}{2}$$
$$v^0_{(6.1)0} = \frac{v^0_{6.1}}{2}\left(-7 + 6v^0_{1.2} - 3v^0_{2.1} + 6v^0_{2.2} + \frac{3v^0_{4.1}}{v^0_{1.2}} - \frac{6v^0_{5.2}}{v^0_{2.1}} + \frac{v^0_{6.1}}{v^0_{3.2}}\right)$$
$$v^0_{(6.2)0} = \frac{v^0_{6.2}}{2}\left(-1.3 + 4v^0_{1.2} + 6v^0_{1.3} + v^0_{2.1} + 8v^0_{2.2} - 2\frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.3}} - 2\frac{v^0_{5.1}}{v^0_{2.1}} + 2\frac{v^0_{5.2} - v^0_{5.3}}{v^0_{2.2}} - \frac{v^0_{6.2}}{v^0_{3.1}}\right)$$

and

$$v^0_{(1.1)\xi} = \frac{v^0_{1.1}}{4}\left(-8 + 6v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + 2v^0_{2.1} + 2v^0_{2.2}\right) - \frac{1}{4}\left(v^0_{3.1} + v^0_{4.1} + 2v^0_{5.2}\right)$$
$$v^0_{(1.2)\xi} = v^0_{1.2}\left(-3 + \frac{3}{2}v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1}\right) - \frac{1}{4}\left(v^0_{3.2} + 3v^0_{4.1} + 6v^0_{5.1}\right)$$
$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-2 + \frac{3}{2}v^0_{1.1} + v^0_{1.3} + v^0_{2.2}\right) - \frac{1}{4}\left(3v^0_{3.1} + v^0_{4.2} + 2v^0_{5.3}\right)$$
$$v^0_{(2.1)\xi} = \frac{v^0_{2.1}}{2}\left(-4 + v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2}\right) - \frac{v^0_{5.1} + v^0_{5.2}}{2}$$
$$v^0_{(2.2)\xi} = \frac{v^0_{2.2}}{2}\left(-5 + 3v^0_{1.1} + v^0_{1.3} + 3v^0_{2.1} + 2v^0_{2.2}\right) - \frac{3v^0_{5.2} + v^0_{5.3}}{2}$$
$$v^0_{(3.1)\xi} = \frac{v^0_{3.1}}{4}\left(-17 + 10v^0_{1.1} + 2v^0_{1.2} + 4v^0_{1.3} + 2v^0_{2.1} + 4v^0_{2.2} - 2\frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.3}}\right) - \frac{v^0_{6.2}}{2}$$
$$v^0_{(3.2)\xi} = \frac{3}{4}v^0_{3.2}\left(-9 + 6v^0_{1.1} + 2v^0_{1.2} + 6v^0_{2.1} - 3\frac{v^0_{4.1}}{v^0_{1.2}}\right) - \frac{3v^0_{6.1}}{2}$$
$$v^0_{(4.1)\xi} = \frac{v^0_{4.1}}{4}\left(-23 + 10v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 16v^0_{2.1} + 4v^0_{2.2} - \frac{v^0_{3.2} + 6v^0_{5.1}}{v^0_{1.2}} - \frac{2v^0_{3.1} + 4v^0_{5.2}}{v^0_{1.1}}\right)$$
$$v^0_{(4.2)\xi} = \frac{3}{4}v^0_{4.2}\left(-7 + 6v^0_{1.1} + 2v^0_{1.3} + 4v^0_{2.2} - \frac{3v^0_{3.1} + 2v^0_{5.3}}{v^0_{1.3}}\right)$$
$$v^0_{(5.1)\xi} = v^0_{5.1}\left(-\frac{11}{2} + \frac{5}{2}v^0_{1.1} + v^0_{1.2} + \frac{15}{4}v^0_{2.1} + v^0_{2.2} - 3\frac{v^0_{4.1} + v^0_{5.1}}{4v^0_{1.2}} - \frac{v^0_{5.2}}{v^0_{2.1}}\right) - \frac{v^0_{6.1}}{4}$$

$$v^0_{(5.2)\xi} = \frac{v^0_{5.2}}{4}\left(-20 + 9v^0_{1.1} + 3v^0_{1.2} + 2v^0_{1.3} + 10v^0_{2.1} + 5v^0_{2.2} - \frac{v^0_{4.1} + v^0_{5.2}}{v^0_{1.1}} - 2\frac{v^0_{5.1}}{v^0_{2.1}} - \frac{3v^0_{5.2} + v^0_{5.3}}{v^0_{2.2}}\right) - \frac{v^0_{6.2}}{4}$$

$$v^0_{(5.3)\xi} = \frac{v^0_{5.3}}{4}\left(-22 + 12v^0_{1.1} + 6v^0_{1.3} + 9v^0_{2.1} + 8v^0_{2.2} - \frac{v^0_{4.2} + v^0_{5.3}}{v^0_{1.3}} - \frac{6v^0_{5.2} + 2v^0_{5.3}}{v^0_{2.2}}\right) - \frac{3v^0_{6.2}}{4}$$

$$v^0_{(6.1)\xi} = \frac{3v^0_{6.1}}{4}\left(-13 + 8v^0_{1.1} + 2v^0_{1.2} + 7v^0_{2.1} + 2v^0_{2.2} - 3\frac{v^0_{4.1}}{v^0_{1.2}} - 2\frac{v^0_{5.2}}{v^0_{2.1}} - \frac{v^0_{6.1}}{v^0_{3.2}}\right)$$

$$v^0_{(6.2)\xi} = \frac{v^0_{6.2}}{4}\left(-33 + 16v^0_{1.1} + 4v^0_{1.2} + 6v^0_{1.3} + 13v^0_{2.1} + 8v^0_{2.2} - 2\frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.3}} - 2\frac{v^0_{5.1}}{v^0_{2.1}} - \frac{6v^0_{5.2} + 2v^0_{5.3}}{v^0_{2.2}} - \frac{v^0_{6.2}}{v^0_{3.1}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = -1$; $u^0_{1.2} = 1$; $u^0_{1.3} = 1$; $u^0_{2.1} = -1$
$u^0_{2.2} = 1$; $u^0_{3.1} = -1$; $u^0_{3.2} = 1$; $u^0_{4.1} = -1$
$u^0_{4.2} = 1$; $u^0_{5.1} = -1$; $u^0_{5.2} = -1$; $u^0_{5.3} = 1$
$u^0_{6.1} = -1$; $u^0_{6.2} = -1$

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = 0$; $u^0_{(1.2)0} = 2$; $u^0_{(1.3)0} = 2$; $u^0_{(2.1)0} = 0$
$u^0_{(2.2)0} = 2$; $u^0_{(3.1)0} = -1$; $u^0_{(3.2)0} = 3$; $u^0_{(4.1)0} = -1$
$u^0_{(4.2)0} = 3$; $u^0_{(5.1)0} = -1$; $u^0_{(5.2)0} = -1$; $u^0_{(5.3)0} = 3$
$u^0_{(6.1)0} = -2$; $u^0_{(6.2)0} = -2$
$u^0_{(1.1)\xi} = -2$; $u^0_{(1.2)\xi} = 1$; $u^0_{(1.3)\xi} = 1$; $u^0_{(2.1)\xi} = -2$
$u^0_{(2.2)\xi} = 1$; $u^0_{(3.1)\xi} = -\frac{5}{2}$; $u^0_{(3.2)\xi} = \frac{3}{2}$; $u^0_{(4.1)\xi} = -\frac{5}{2}$
$u^0_{(4.2)\xi} = \frac{3}{2}$; $u^0_{(5.1)\xi} = -\frac{5}{2}$; $u^0_{(5.2)\xi} = -\frac{5}{2}$; $u^0_{(5.3)\xi} = \frac{3}{2}$
$u^0_{(6.1)\xi} = -3$; $u^0_{(6.2)\xi} = -3$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1}$; $u^0_{(1.2)00} = 2v^0_{1.2}$; $u^0_{(1.3)00} = 2v^0_{1.3}$
$u^0_{(2.1)00} = 2v^0_{2.1}$; $u^0_{(2.2)00} = 2v^0_{2.2}$; $u^0_{(3.1)00} = 4v^0_{1.1} - 2v^0_{1.3}$
$u^0_{(3.2)00} = 6v^0_{1.2}$; $u^0_{(4.1)00} = 4v^0_{1.1} - 2v^0_{1.2}$; $u^0_{(4.2)00} = 6v^0_{1.3}$
$u^0_{(5.1)00} = -2v^0_{1.2} + 4v^0_{2.1}$; $u^0_{(5.2)00} = 2v^0_{1.1} + 2v^0_{2.1} - 2v^0_{2.2}$; $u^0_{(5.3)00} = 2v^0_{1.3} + 4v^0_{2.2}$
$u^0_{(6.1)00} = -6v^0_{1.2} + 6v^0_{2.1}$; $u^0_{(6.2)00} = 4v^0_{1.1} - 2v^0_{1.3} + 2v^0_{2.1} - 4v^0_{2.2}$

$$u^0_{(1.1)\xi 0} = -\, v^0_{1.1}; \qquad u^0_{(1.2)\xi 0} = v^0_{1.2}; \qquad u^0_{(1.3)\xi 0} = v^0_{1.3};$$
$$u^0_{(2.1)\xi 0} = -\, v^0_{2.1}; \qquad u^0_{(2.2)\xi 0} = v^0_{2.2}; \qquad u^0_{(3.1)\xi 0} = -\, 2v^0_{1.1} - v^0_{1.3}$$
$$u^0_{(3.2)\xi 0} = 3v^0_{1.2}; \qquad u^0_{(4.1)\xi 0} = -\, 2v^0_{1.1} - v^0_{1.2}; \qquad u^0_{(4.2)\xi 0} = 3v^0_{1.3}$$
$$u^0_{(5.1)\xi 0} = -\, v^0_{1.2} - 2v^0_{2.1}; \qquad u^0_{(5.2)\xi 0} = -\, v^0_{1.1} - v^0_{2.1} - v^0_{2.2}; \qquad u^0_{(5.3)\xi 0} = v^0_{1.3} + 2v^0_{2.2}$$
$$u^0_{(6.1)\xi 0} = -\, 3v^0_{1.2} - 3v^0_{2.1}; \qquad u^0_{(6.2)\xi 0} = -\, 2v^0_{1.1} - v^0_{1.3} - v^0_{2.1} - 2v^0_{2.2}$$

and

$$u^0_{(1.1)\xi\xi} = -\frac{3v^0_{1.1}}{2}; \qquad u^0_{(1.2)\xi\xi} = \frac{v^0_{1.2}}{2}; \qquad u^0_{(1.3)\xi\xi} = \frac{v^0_{1.3}}{2}$$
$$u^0_{(2.1)\xi\xi} = -\frac{3v^0_{2.1}}{2}; \qquad u^0_{(2.2)\xi\xi} = \frac{v^0_{2.2}}{2}; \qquad u^0_{(3.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.3}}{2}$$
$$u^0_{(3.2)\xi\xi} = \frac{3v^0_{1.2}}{2}; \qquad u^0_{(4.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.2}}{2}; \qquad u^0_{(4.2)\xi\xi} = \frac{3v^0_{1.3}}{2}$$
$$u^0_{(5.1)\xi\xi} = -\frac{v^0_{1.2}}{2} - 3v^0_{2.1}; \qquad u^0_{(5.2)\xi\xi} = -\frac{1}{2}\left(3v^0_{1.1} + 3v^0_{2.1} + v^0_{2.2}\right); \qquad u^0_{(5.3)\xi\xi} = \frac{v^0_{1.3}}{2} + v^0_{2.2}$$
$$u^0_{(6.1)\xi\xi} = -\frac{3v^0_{1.2} + 9v^0_{2.1}}{2}; \qquad u^0_{(6.2)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.3} + 3v^0_{2.1}}{2} - v^0_{2.2}$$

A.3.4 Thermodynamics of $D0_{19}$ phase using tetrahedron – octahedron approximation

The tetrahedron–octahedron clusters considered for $D0_{19}$ phase is shown in Figure A.10 and the details of the (sub-)clusters, their designations, multiplicities and K-B coefficients are given in Table A.10.

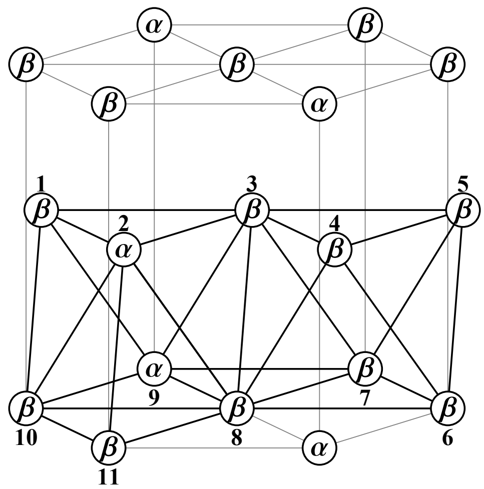

Figure A.10: The tetrahedron–octahedron basic clusters in $D0_{19}$ phase along with the sublattice sites designated α and β.

Table A.10: The clusters, their designations, multiplicities and the corresponding K-B coefficients ($\gamma_{i.j}$) for $D0_{19}$ phase using tetrahedron–octahedron approximation.

Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Octahedron	$\beta\beta\beta\beta\beta\beta$(O2) (3,4,5,6,7,8)	13.2	1/4	1
	$\alpha\alpha\beta\beta\beta\beta$(O1) (2,9,1,3,8,10)	13.1	3/4	
Square pyramid	$\beta\beta\beta\beta\beta$ (3,4,5,6,7)	12.3	3/2	0
	$\alpha\beta\beta\beta\beta$ (2,1,3,8,10)	12.2	3/2	
	$\alpha\alpha\beta\beta\beta$ (2,9,1,3,10)	12.1	3	
Square	$\beta\beta\beta\beta$(O2) (3,4,6,7)	11.3	3/4	0
	$\beta\beta\beta\beta$(O1) (1,3,8,10)	11.2	3/4	
	$\alpha\alpha\beta\beta$ (2,9,1,8)	11.1	3/2	

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Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
Irregular tetrahedron-2	$\beta\beta\beta\beta$ (3,6,4,8)	10.3	3/2	0
	$\alpha\beta\beta\beta$ (2,1,8,10)	10.2	3	
	$\alpha\alpha\beta\beta$ (2,9,3,8)	10.1	3/2	
Irregular tetrahedron-1	$\beta\beta\beta\beta$ (3,6,7,8)	9.3	3/2	0
	$\alpha\beta\beta\beta$ (2,1,8,10)	9.2	3	
	$\alpha\alpha\beta\beta$ (2,9,1,3)	9.1	3/2	
Regular tetrahedron	$\alpha\beta\beta\beta$($\beta\beta\beta$OP, T2) (9,3,7,8)	8.2	3/2	1
	$\alpha\beta\beta\beta$($\beta\beta\beta$IP, T1) (2,8,10,11)	8.1	1/2	
Isosceles triangle	$\beta\beta\beta$(O2) (3,4,6)	7.4	3	0
	$\beta\beta\beta$(O1) (1,3,8)	7.3	3	
	$\alpha\beta\beta$ (2,1,8)	7.2	3	
	$\alpha\alpha\beta$ (2,9,1)	7.1	3	
Equilateral triangle (OP)	$\beta\beta\beta$ (3,7,8)	6.3	3/2	-1
	$\alpha\beta\beta$($\beta\beta$OP) (2,1,10)	6.2	3	
	$\alpha\beta\beta$($\beta\beta$IP) (2,1,3)	6.1	3/2	
Equilateral triangle (OB)	$\beta\beta\beta$ (6,7,8)	5.2	1/4	-1
	$\alpha\beta\beta$ (9,8,10)	5.1	3/4	
Equilateral triangle (TB)	$\beta\beta\beta$ (8,10,11)	4.2	1/4	-1
	$\alpha\beta\beta$ (9,7,8)	4.1	3/4	
II-n pair	$\beta\beta$(O2) (3,6)	3.3	3/4	0
	$\beta\beta$(O1) (1,8)	3.2	3/2	
	$\alpha\alpha$ (2, 9)	3.1	3/4	

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Clusters	Ordered cluster	Designation	Multiplicity	$\gamma_{i.j}$
I-n pair (OP)	$\beta\beta$ (1,10)	2.2	3/2	1
	$\alpha\beta$ (9,1)	2.1	3/2	
I-n pair (IP)	$\beta\beta$(T2) (7,8)	1.3	3/4	1
	$\beta\beta$(T1) (8,10)	1.2	3/4	
	$\alpha\beta$ (2,1)	1.1	3/2	
Point	β (1)	0.2	3/4	-1
	α (2)	0.1	1/4	

The average composition of the system and the LRO parameters are related to the sublattice point CFs as

$$u_0 = (u_{0.1} + 3u_{0.2})/4 \quad \text{and} \quad \xi = (u_{0.2} - u_{0.1})/2$$

Correlation functions in the sublattice solvent bases

The limiting values of the transformed CFs in the sublattice solvent bases in the limit of perfect ordering, $v^0_{i.j}$, are:

$$v^0_{1.1} = \frac{\sqrt{\eta_{11}\eta_{12}}\,\eta_{13}^{1/8}}{\eta_1\eta_6\sqrt{\eta_4\eta_5\eta_8\eta_9}};$$

$$v^0_{1.2} = \frac{\eta_1\eta_7^2\sqrt{\eta_4\eta_{11}}\,\eta_{13}^{1/8}}{\eta_6\sqrt{\eta_5\eta_8\eta_9}\,\eta_{10}}$$

$$v^0_{1.3} = \eta_1\eta_6\eta_7^2\eta_{10}\sqrt{\frac{\eta_5\eta_9^3\eta_{11}}{\eta_4\eta_8}}\,\eta_{12}\eta_{13}^{1/8};$$

$$v^0_{2.1} = \frac{\sqrt{\eta_{11}\eta_{12}}\,\eta_{13}^{1/8}}{\eta_2\eta_6^2\sqrt{\eta_8\eta_{10}}};$$

$$v^0_{2.2} = \eta_2\eta_7^2\sqrt{\frac{\eta_{10}\eta_{11}\eta_{12}}{\eta_8}}\,\eta_{13}^{1/8};$$

$$v^0_{3.1} = \eta_3\eta_7^2\sqrt{\eta_9\eta_{10}\eta_{11}\eta_{12}}\,\eta_{13}^{1/16}$$

$$v^0_{3.2} = \frac{\eta_3\eta_{13}^{1/16}\sqrt{\eta_{11}}}{\sqrt{\eta_9\eta_{10}}};$$

$$v^0_{3.3} = \eta_3\eta_7^2\sqrt{\eta_9\eta_{10}\eta_{11}\eta_{12}}\,\eta_{13}^{1/16}$$

$$v^0_{4.1} = \frac{\eta_7^2\eta_{10}\eta_{12}^2\eta_{13}^{3/8}\sqrt{\eta_9\eta_{11}^3}}{\eta_1\eta_6\sqrt{\eta_4\eta_5\eta_8}};$$

$$v^0_{4.2} = \frac{\eta_1^3\eta_7^6\sqrt{\eta_4\eta_{11}^3}\,\eta_{13}^{3/8}}{\eta_6^3\eta_{10}^3\sqrt{\eta_5^3\eta_8\eta_9^3}}$$

$$v^0_{5.1} = \frac{\eta_7^2\eta_{13}^{1/8}\sqrt{\eta_{11}^3\eta_{12}}}{\eta_1\eta_6^3\eta_{10}\sqrt{\eta_4\eta_5\eta_8^3\eta_9}};$$

$$v^0_{5.2} = \eta_1^3\sqrt{\eta_5}\,\eta_6^3\eta_7^6\eta_{10}^3\left(\frac{\eta_9\eta_{11}\eta_{12}}{\eta_4\eta_8}\right)^{3/2}\eta_{13}^{1/8}$$

$$v^0_{6.1} = \frac{\eta_1\eta_7^2\sqrt{\eta_4\eta_{11}^3}\,(\eta_{12}^3\eta_{13})^{1/4}}{\eta_2^2\eta_6^4\eta_8\eta_9\eta_{10}\sqrt{\eta_5}};$$

$$v^0_{6.2} = \frac{\eta_7^2\eta_{11}^{3/2}\sqrt[4]{\eta_{12}^5\eta_{13}}}{\eta_1\sqrt{\eta_4\eta_5}\,\eta_6^2\eta_8}$$

$$v^0_{6.3} = \frac{\eta_1\eta_2^2\eta_7^6\eta_9\eta_{10}\sqrt{\eta_5\eta_{11}^3}\,(\eta_{12}^5\eta_{13})^{1/4}}{\eta_8\sqrt{\eta_4}};$$

$$v^0_{7.1} = \frac{\eta_3\eta_7\eta_{11}\eta_{12}^{3/4}\eta_{13}^{3/16}}{\eta_1\eta_2\eta_6^3\eta_8\sqrt{\eta_4\eta_5\eta_9\eta_{10}}}$$

$$v^0_{7.2} = \frac{\eta_3\eta_7\eta_{11}\eta_{12}^{3/4}\eta_{13}^{3/16}}{\eta_1\eta_2\eta_6^3\eta_8\sqrt{\eta_4\eta_5\eta_9\eta_{10}}}; \qquad v^0_{7.3} = \frac{\eta_1\eta_2\eta_3\eta_7^3\eta_{11}\eta_{12}^{3/4}\eta_{13}^{3/16}\sqrt{\eta_4}}{\eta_6\eta_8\sqrt{\eta_5\eta_9\eta_{10}}}$$

$$v^0_{7.4} = \frac{\eta_1\eta_2\eta_3\eta_6\eta_7^5\sqrt{\eta_5\eta_9^3\eta_{10}^3}\eta_{11}\eta_{12}^{5/4}\eta_{13}^{3/16}}{\eta_8\sqrt{\eta_4}}; \qquad v^0_{8.1} = \frac{\eta_1^3\sqrt{\eta_4}\eta_7^6\eta_{11}^3\eta_{12}^{3/4}\eta_{13}^{3/8}}{\eta_2^3\eta_6^6\eta_9^3(\eta_5\eta_8\eta_{10})^{3/2}}$$

$$v^0_{8.2} = \frac{\eta_2\eta_7^6\eta_9\eta_{11}^3\eta_{12}^{9/4}\eta_{13}^{3/8}\sqrt{\eta_{10}}}{\eta_1\eta_6^2\sqrt{\eta_4\eta_5\eta_8^3}}; \qquad v^0_{9.1} = \frac{\eta_3\eta_7^2\eta_{11}^2\eta_{12}^{5/4}\eta_{13}^{5/16}}{\eta_1\eta_2^2\eta_6^6\eta_8^2\sqrt{\eta_4\eta_5\eta_9\eta_{10}^3}}$$

$$v^0_{9.2} = \frac{\eta_3\eta_7^4\eta_{11}^2\eta_{12}^{5/4}\eta_{13}^{5/16}}{\eta_1\eta_6^4\eta_8^2\sqrt{\eta_4\eta_5\eta_9\eta_{10}}}; \qquad v^0_{9.3} = \frac{\eta_1^3\eta_2^2\eta_3\eta_6^2\eta_7^{10}\sqrt{\eta_5\eta_9^3\eta_{10}^5}\eta_{11}^2\eta_{12}^{7/4}\eta_{13}^{5/16}}{\eta_8^2\sqrt{\eta_4^3}}$$

$$v^0_{10.1} = \frac{\eta_3\eta_7^2\eta_{11}^2\eta_{12}^2\eta_{13}^{7/16}}{\eta_1^2\eta_2\eta_4\eta_5\eta_6^4\sqrt{\eta_8^3\eta_9}}; \qquad v^0_{10.2} = \frac{\eta_3\eta_7^4\eta_{11}^2\sqrt{\eta_{12}^3}\eta_{13}^{7/16}}{\eta_2\eta_5\eta_6^4\eta_{10}\sqrt{\eta_8^3\eta_9}}$$

$$v^0_{10.3} = \frac{\eta_1^2\eta_2^3\eta_3\eta_5\eta_7^{10}\eta_{10}^2\eta_{11}^2\eta_{12}^2\eta_{13}^{7/16}}{\eta_4}\left(\frac{\eta_9}{\eta_8}\right)^{3/2}; \qquad v^0_{11.1} = \frac{\eta_3^2\eta_7^2\eta_{11}^2\eta_{12}^{3/2}\eta_{13}^{3/8}}{\eta_1^2\eta_2^2\eta_4\eta_5\eta_6^6\eta_8^2\eta_9\eta_{10}}$$

$$v^0_{11.2} = \frac{\eta_1^2\eta_2^2\eta_3^2\eta_4\eta_7^4\eta_{11}^2\eta_{12}\eta_{13}^{3/8}}{\eta_5\eta_6^2\eta_8^2}; \qquad v^0_{11.3} = \frac{\eta_1^2\eta_2^2\eta_3^2\eta_5\eta_6^2\eta_7^8\eta_9^2\eta_{10}^2\eta_{11}^2\eta_{12}^2\eta_{13}^{3/8}}{\eta_4\eta_8^2}$$

$$v^0_{12.1} = \frac{\eta_3^2\eta_7^4\eta_{11}^3\eta_{12}^{9/4}\sqrt{\eta_{13}}}{\eta_1^2\eta_2^2\eta_4\eta_5\eta_6^7\eta_{10}\sqrt{\eta_8^5\eta_9}}; \qquad v^0_{12.2} = \frac{\eta_3^2\eta_7^6\eta_{11}^3\eta_{12}^{9/4}\sqrt{\eta_{13}}}{\eta_5\eta_6^5\eta_{10}\sqrt{\eta_8^5\eta_9}}$$

$$v^0_{12.3} = \frac{\eta_1^4\eta_2^4\eta_3^2\eta_5\eta_6\eta_7^{14}\eta_{10}^3\eta_{11}^3\eta_{12}^{11/4}\sqrt{\eta_9^3\eta_{13}}}{\eta_4^2\sqrt{\eta_8^5}}; \qquad v^0_{13.1} = \frac{\eta_3^3\eta_7^6\eta_{11}^{9/2}\eta_{12}^3\eta_{13}^{11/16}}{\eta_1^2\eta_2^2\eta_4\eta_5\eta_6^8\eta_8^3\sqrt{\eta_9\eta_{10}^3}}$$

$$v^0_{13.2} = \frac{\eta_1^6\eta_2^6\eta_3^3\eta_5\eta_7^{18}\eta_9^{3/2}(\eta_{10}\eta_{11})^{9/2}\eta_{12}^3\eta_{13}^{11/16}}{\eta_4^3\eta_8^3}$$

The limiting first derivatives of the transformed CFs with respect to u_0 and ξ, in the sublattice solvent bases in the limit of perfect ordering, $v^0_{(i.j)0}$ and $v^0_{(i.j)\xi}$, are:

$$v^0_{(1.1)0} = v^0_{1.1}\left(-2 + v^0_{1.1} + \frac{v^0_{1.2}}{2} + \frac{v^0_{1.3}}{2} + v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.2}\right) - \frac{v^0_{4.1} + v^0_{5.1}}{2} - v^0_{6.2} + v^0_{7.1} - v^0_{7.2}$$

$$v^0_{(1.2)0} = v^0_{1.2}\left(2\left(-1 + v^0_{1.2} - v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right) - v^0_{1.1}\right) - \frac{v^0_{4.2} - v^0_{5.1}}{2} + v^0_{6.1} - 2v^0_{7.3}$$

$$v^0_{(1.3)0} = v^0_{1.3}\left(-4 - v^0_{1.1} + 2v^0_{1.3} + 4v^0_{2.2} + 2v^0_{3.3}\right) + \frac{v^0_{4.1} - v^0_{5.2}}{2} - v^0_{6.3} - 2v^0_{7.4}$$

$$v^0_{(2.1)0} = v^0_{2.1}\left(-2 + v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.2}\right) - v^0_{6.1} - v^0_{6.2} + v^0_{7.1} - v^0_{7.2}$$

$$v^0_{(2.2)0} = v^0_{2.2}\left(-3 - v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} - v^0_{2.1} + 2v^0_{2.2} + v^0_{3.2} + v^0_{3.3}\right) + v^0_{6.2} - v^0_{6.3} - v^0_{7.3} - v^0_{7.4}$$

$$v^0_{(3.1)0} = v^0_{3.1}\left(-1 + 2v^0_{1.1} + 2v^0_{2.1} - v^0_{3.1}\right) - 2v^0_{7.1}$$

$$v^0_{(3.2)0} = v^0_{3.2}\left(-1 - v^0_{1.1} + v^0_{1.2} - v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right) + v^0_{7.2} - v^0_{7.3}$$

$$v^0_{(3.3)0} = v^0_{3.3}\left(-3 + 2v^0_{1.3} + 2v^0_{2.2} + v^0_{3.3}\right) - 2v^0_{7.4}$$

$$v^0_{(4.1)0} = v^0_{4.1}\left(-\frac{13}{2} + v^0_{1.1} + v^0_{1.2} + 2\left(v^0_{1.3} - v^0_{3.1} + v^0_{3.2} + v^0_{3.3}\right) + v^0_{2.1} + 4v^0_{2.2} - \frac{v^0_{5.1} - 2v^0_{7.1} + 2v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{5.2} + 4v^0_{7.4}}{2v^0_{1.3}}\right) - v^0_{8.2}$$

$$v^0_{(4.2)0} = v^0_{4.2}\left(-\frac{11}{2} - 3v^0_{1.1} + 3v^0_{1.2} - 3v^0_{2.1} + 6v^0_{2.2} + 6v^0_{3.2} + 3\frac{v^0_{5.1} - 4v^0_{7.3}}{2v^0_{1.2}}\right) + v^0_{8.1}$$

$$v^0_{(5.1)0} = v^0_{5.1}\left(-\frac{9}{2} + v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 2v^0_{2.2} - v^0_{3.1} + 2v^0_{3.2} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{2v^0_{1.2}}\right) + v^0_{9.1} - 2v^0_{9.2}$$

$$v^0_{(5.2)0} = \frac{3}{2}v^0_{5.2}\left(-5 - 2v^0_{1.1} + 2v^0_{1.3} + 4v^0_{2.2} + 2v^0_{3.3} + \frac{v^0_{4.1}}{v^0_{1.3}}\right) - 3v^0_{9.3}$$

$$v^0_{(6.1)0} = \frac{v^0_{6.1}}{2}\left(-9 + 2v^0_{1.1} + 4v^0_{1.2} - v^0_{2.1} + 6v^0_{2.2} - 3v^0_{3.1} + 6v^0_{3.2} + \frac{v^0_{6.1} - 2v^0_{7.3}}{v^0_{1.2}} - 2\frac{v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right)$$
$$- \frac{v^0_{8.1} - v^0_{9.1}}{2} - v^0_{10.2}$$

$$v^0_{(6.2)0} = \frac{v^0_{6.2}}{2}\left(-11 + v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} + 2v^0_{2.1} + 5v^0_{2.2} - 3v^0_{3.1} + 4v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{6.1} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right.$$
$$\left. - \frac{v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{8.2} + v^0_{9.2} - v^0_{10.1} + v^0_{10.2}\right)$$

$$v^0_{(6.3)0} = \frac{v^0_{6.3}}{2}\left(-15 - 4v^0_{1.1} + 4v^0_{1.2} + 6v^0_{1.3} - 3v^0_{2.1} + 10v^0_{2.2} + 4v^0_{3.2} + 5v^0_{3.3} + \frac{2v^0_{6.2} - 4v^0_{7.3}}{v^0_{2.2}}\right.$$
$$\left. - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{1.3}}\right) + \frac{v^0_{8.2} - v^0_{9.3}}{2} - v^0_{10.3}$$

$$v^0_{(7.1)0} = \frac{v^0_{7.1}}{2}\left(-8 + 5v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 5v^0_{2.1} + 3v^0_{2.2} - 4v^0_{3.1} + 3v^0_{3.2} - \frac{v^0_{4.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}}\right.$$
$$\left. - \frac{v^0_{6.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - \frac{1}{2}\left(v^0_{9.1} + v^0_{10.1} + v^0_{11.1}\right)$$

$$v^0_{(7.2)0} = \frac{v^0_{7.2}}{2}\left(-8 + 2v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + 2v^0_{2.1} + 4v^0_{2.2} - 3v^0_{3.1} + 4v^0_{3.2} - \frac{v^0_{4.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}}\right.$$
$$\left. - \frac{v^0_{6.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - \frac{1}{2}\left(v^0_{9.2} + v^0_{10.2} - v^0_{11.1}\right)$$

$$v^0_{(7.3)0} = \frac{v^0_{7.3}}{2}\left(-10 - 3v^0_{1.1} + 5v^0_{1.2} + 4v^0_{1.3} - 5v^0_{2.1} + 7v^0_{2.2} + 5v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.2} - v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}}\right.$$
$$\left. - 2\frac{v^0_{6.3} + v^0_{7.4}}{v^0_{2.2}}\right) + \frac{1}{2}\left(v^0_{9.2} + v^0_{10.2} - v^0_{11.2}\right)$$

$$v^0_{(7.4)0} = v^0_{7.4}\left(-7 - 2v^0_{1.1} + v^0_{1.2} + 3v^0_{1.3} - v^0_{2.1} + 5v^0_{2.2} + v^0_{3.2} + \frac{5}{2}v^0_{3.3} + \frac{v^0_{4.1} - v^0_{6.3} - 2v^0_{7.4}}{2v^0_{1.3}}\right.$$
$$\left. + \frac{v^0_{6.2} - v^0_{7.3}}{v^0_{2.2}}\right) - \frac{1}{2}\left(v^0_{9.3} + v^0_{10.3} + v^0_{11.3}\right)$$

$$v^0_{(8.1)0} = \frac{v^0_{8.1}}{2}\left(-16 + 6v^0_{1.2} - 3v^0_{2.1} + 12v^0_{2.2} - 3v^0_{3.1} + 12v^0_{3.2} - 6\frac{v^0_{7.3}}{v^0_{1.2}} + \frac{v^0_{8.1}}{v^0_{4.2}} + \frac{3v^0_{9.1} - 6v^0_{10.2}}{v^0_{6.1}}\right)$$

$$v^0_{(8.2)0} = v^0_{8.2}\left(-10 + 2v^0_{1.2} + 3v^0_{1.3} + \frac{v^0_{2.1}}{2} + 5v^0_{2.2} - 2v^0_{3.1} + 3v^0_{3.2} + \frac{5}{2}v^0_{3.3} + \frac{v^0_{7.1} - v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{7.4}}{v^0_{1.3}}\right.$$
$$\left. - \frac{v^0_{8.2}}{2v^0_{4.1}} - \frac{v^0_{9.2} - v^0_{10.1} + v^0_{10.2}}{v^0_{6.2}} - \frac{v^0_{9.3} + 2v^0_{10.3}}{2v^0_{6.3}}\right)$$

$$v^0_{(9.1)0} = v^0_{9.1}\left(-7 + 3v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + \frac{3}{2}v^0_{2.1} + 3v^0_{2.2} - \frac{5}{2}v^0_{3.1} + 3v^0_{3.2} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{8.1}}{2v^0_{6.1}} + \frac{v^0_{9.1} - 2v^0_{9.2}}{2v^0_{5.1}}\right) - v^0_{12.1}$$

$$v^0_{(9.2)0} = \frac{v^0_{9.2}}{2}\left(-16 + v^0_{1.1} + 6v^0_{1.2} + 5v^0_{1.3} + 7v^0_{2.2} - 3v^0_{3.1} + 6v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{6.1} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}} + \frac{v^0_{9.1} - 2v^0_{9.2}}{v^0_{5.1}}\right) + \frac{v^0_{12.1} - v^0_{12.2}}{2}$$

$$v^0_{(9.3)0} = v^0_{9.3}\left(-11 - 4v^0_{1.1} + 2v^0_{1.2} + 4v^0_{1.3} - \frac{3}{2}v^0_{2.1} + 7v^0_{2.2} + 2v^0_{3.2} + \frac{7}{2}v^0_{3.3} + \frac{v^0_{4.1}}{v^0_{1.3}} + \frac{v^0_{6.2} - 2v^0_{7.3}}{v^0_{2.2}} + \frac{v^0_{8.2}}{2v^0_{6.3}} - \frac{3}{2}\frac{v^0_{9.3}}{v^0_{5.2}}\right) - v^0_{12.3}$$

$$v^0_{(10.1)0} = v^0_{10.1}\left(-8 + 2v^0_{1.1} + 2v^0_{1.2} + 2v^0_{1.3} + 3\left(v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.2}\right) + v^0_{3.3} - \frac{v^0_{6.1} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}}\right) - v^0_{12.1}$$

$$v^0_{(10.2)0} = \frac{v^0_{10.2}}{2}\left(-16 + v^0_{1.1} + 5v^0_{1.2} + 4v^0_{1.3} - v^0_{2.1} + 9v^0_{2.2} - 4v^0_{3.1} + 8v^0_{3.2} + 2v^0_{3.3} + \frac{v^0_{6.1} - 2v^0_{7.3}}{v^0_{1.2}} - \frac{v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.2} - 2v^0_{7.1} + 2v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\right) + \frac{v^0_{12.1} - v^0_{12.2}}{2}$$

$$v^0_{(10.3)0} = v^0_{10.3}\left(-12 - 3v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} - 2v^0_{2.1} + 8v^0_{2.2} + 3v^0_{3.2} + 4v^0_{3.3} + \frac{v^0_{6.2} - 3v^0_{7.3}}{v^0_{2.2}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{1.3}} + \frac{v^0_{8.2}}{v^0_{6.3}}\right) - v^0_{12.3}$$

$$v^0_{(11.1)0} = v^0_{11.1}\left(-7 + 3\left(v^0_{1.1} + v^0_{2.1} + v^0_{2.2} - v^0_{3.1} + v^0_{3.2}\right) + 2v^0_{1.2} + v^0_{1.3} - \frac{v^0_{4.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - v^0_{12.1}$$

$$v^0_{(11.2)0} = v^0_{11.2}\left(-9 - 2v^0_{1.1} + 4\left(v^0_{1.2} + v^0_{1.3} - v^0_{2.1} + v^0_{3.2}\right) + 6v^0_{2.2} + 2v^0_{3.3} - \frac{v^0_{4.2} - v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}} - 2\frac{v^0_{6.3} + v^0_{7.4}}{v^0_{2.2}}\right) + v^0_{12.2}$$

$$v^0_{(11.3)0} = v^0_{11.3}\left(-11 - 4v^0_{1.1} + 2v^0_{1.2} + 4v^0_{1.3} - 2v^0_{2.1} + 8v^0_{2.2} + 2v^0_{3.2} + 4v^0_{3.3} + \frac{v^0_{4.1} - v^0_{6.3} - 2v^0_{7.4}}{v^0_{1.3}} + 2\frac{v^0_{6.2} - v^0_{7.3}}{v^0_{2.2}}\right) - v^0_{12.3}$$

$$v^0_{(12.1)0} = \frac{v^0_{12.1}}{2}\left(-22 + 5v^0_{1.1} + 6v^0_{1.2} + 5v^0_{1.3} + 4v^0_{2.1} + 9v^0_{2.2} - 7v^0_{3.1} + 9v^0_{3.2} + 2v^0_{3.3}\right.$$

$$- \frac{v^0_{4.1} + v^0_{6.2} - v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} - 3v^0_{7.1} + 3v^0_{7.2}}{v^0_{2.1}} - 2\frac{v^0_{7.4}}{v^0_{2.2}}$$

$$- \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} + \frac{v^0_{9.1} - 2v^0_{9.2}}{v^0_{5.1}} \Bigg) - \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.2)0} = v^0_{12.2} \Bigg(-12 + 4v^0_{1.2} + 4v^0_{1.3} - \frac{3}{2}v^0_{2.1} + 6v^0_{2.2} - 2v^0_{3.1} + 5v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.2} - v^0_{6.1} + 2v^0_{7.3}}{2v^0_{1.2}}$$

$$- \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}} + \frac{v^0_{7.1} - v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}} + \frac{v^0_{9.1} - 2v^0_{9.2}}{2v^0_{5.1}} \Bigg) + \frac{v^0_{13.1}}{2}$$

$$v^0_{(12.3)0} = \frac{v^0_{12.3}}{2} \Bigg(-32 - 10v^0_{1.1} + 8v^0_{1.2} + 10v^0_{1.3} - 5v^0_{2.1} + 20v^0_{2.2} + 8v^0_{3.2} + 10v^0_{3.3} + \frac{2v^0_{6.2} - 8v^0_{7.3}}{v^0_{2.2}}$$

$$+ \frac{v^0_{4.1} - v^0_{6.3} - 2v^0_{7.4}}{v^0_{1.3}} + 3\frac{v^0_{8.2}}{v^0_{6.3}} - 3\frac{v^0_{9.3}}{v^0_{5.2}} \Bigg) - \frac{v^0_{13.2}}{2}$$

$$v^0_{(13.1)0} = v^0_{13.1} \Bigg(-15 + 2v^0_{1.1} + 4v^0_{1.2} + 4v^0_{1.3} + v^0_{2.1} + 6v^0_{2.2} - 4v^0_{3.1} + 6v^0_{3.2} + 2v^0_{3.3} + 2\frac{v^0_{7.1} - v^0_{7.2}}{v^0_{2.1}}$$

$$- 2\frac{v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} + \frac{v^0_{9.1} - 2v^0_{9.2}}{v^0_{5.1}} \Bigg)$$

$$v^0_{(13.2)0} = 3v^0_{13.2} \Bigg(-7 - 2\left(v^0_{1.1} - v^0_{1.2} - v^0_{1.3} - v^0_{3.2} - v^0_{3.3}\right) - v^0_{2.1} + 4v^0_{2.2} - 2\frac{v^0_{7.3}}{v^0_{2.2}} + \frac{v^0_{8.2}}{v^0_{6.3}} - \frac{v^0_{9.3}}{v^0_{5.2}} \Bigg)$$

and

$$v^0_{(1.1)\xi} = \frac{v^0_{1.1}}{4}\left(-16 + 6v^0_{1.1} + v^0_{1.2} + v^0_{1.3} + 10v^0_{2.1} + 2v^0_{2.2} + 6v^0_{3.2} + 2v^0_{3.2}\right)$$

$$- \frac{1}{4}\left(v^0_{4.1} + v^0_{5.1} + 2v^0_{6.2} + 6v^0_{7.1} + 2v^0_{7.2}\right)$$

$$v^0_{(1.2)\xi} = v^0_{1.2}\left(-4 + \frac{3}{2}v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right) - \frac{1}{4}\left(v^0_{4.2} + 3v^0_{5.1} + 6v^0_{6.1}\right) - v^0_{7.3}$$

$$v^0_{(1.3)\xi} = v^0_{1.3}\left(-3 + \frac{3}{2}v^0_{1.1} + v^0_{1.3} + 2v^0_{2.2} + v^0_{3.3}\right) - \frac{1}{4}\left(3v^0_{4.1} + v^0_{5.2} + 2v^0_{6.3}\right) - v^0_{7.4}$$

$$v^0_{(2.1)\xi} = \frac{v^0_{2.1}}{2}\left(-8 + 5v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2} + 3v^0_{3.1} + v^0_{3.2}\right) - \frac{1}{2}\left(v^0_{6.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}\right)$$

$$v^0_{(2.2)\xi} = \frac{v^0_{2.2}}{2}\left(-7 + 3v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} + 3v^0_{2.1} + 2v^0_{2.2} + v^0_{3.2} + v^0_{3.3}\right) - \frac{1}{2}\left(3v^0_{6.2} + v^0_{6.3} + v^0_{7.3} + v^0_{7.4}\right)$$

$$v^0_{(3.1)\xi} = v^0_{3.1}\left(-\frac{5}{2} + v^0_{1.1} + v^0_{2.1} + \frac{3}{2}v^0_{3.1}\right) - v^0_{7.1}$$

$$v^0_{(3.2)\xi} = \frac{v^0_{3.2}}{2}\left(-5 + 3v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right) - \frac{3v^0_{7.2} + v^0_{7.3}}{2}$$

$$v^0_{(3.3)\xi} = v^0_{3.3}\left(-\frac{3}{2} + v^0_{1.3} + v^0_{2.2} + \frac{v^0_{3.3}}{2}\right) - v^0_{7.4}$$

$$v^0_{(4.1)\xi} = v^0_{4.1}\Bigg(-\frac{37}{4} + \frac{5}{2}v^0_{1.1} + \frac{v^0_{1.2}}{2} + v^0_{1.3} + \frac{9}{2}v^0_{2.1} + 2v^0_{2.2} + 3v^0_{3.1} + v^0_{3.2} + v^0_{3.3}$$

$$- \frac{v^0_{5.1} + 6v^0_{7.1} + 2v^0_{7.2}}{2v^0_{1.1}} - \frac{v^0_{5.2}}{4v^0_{1.3}} - \frac{v^0_{7.4}}{v^0_{1.3}}\Bigg) - \frac{v^0_{8.2}}{2}$$

$$v^0_{(4.2)\xi} = \frac{v^0_{4.2}}{2}\left(-\frac{39}{2} + 9v^0_{1.1} + 3v^0_{1.2} + 9v^0_{2.1} + 6v^0_{2.2} + 6v^0_{3.2} - \frac{9v^0_{5.1} + 12v^0_{7.3}}{2v^0_{1.2}}\right) - \frac{3}{2}v^0_{8.1}$$

$$v^0_{(5.1)\xi} = \frac{v^0_{5.1}}{2}\left(-\frac{33}{2} + 5v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 8v^0_{2.1} + 2v^0_{2.2} + 3v^0_{3.1} + 2v^0_{3.2} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{2v^0_{1.2}}\right) - \frac{3}{2}v^0_{9.1} - v^0_{9.2}$$

$$v^0_{(5.2)\xi} = \frac{3}{4}v^0_{5.2}\left(-9 + 6v^0_{1.1} + 2v^0_{1.3} + 4v^0_{2.2} + 2v^0_{3.3} - 3\frac{v^0_{4.1}}{v^0_{1.3}}\right) - \frac{3}{2}v^0_{9.3}$$

$$v^0_{(6.1)\xi} = \frac{v^0_{6.1}}{4}\left(-37 + 18v^0_{1.1} + 4v^0_{1.2} + 15v^0_{2.1} + 6v^0_{2.2} + 9v^0_{3.1} + 6v^0_{3.2} - \frac{3v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}} - 2\frac{v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - \frac{1}{4}\left(v^0_{8.1} + 3v^0_{9.1} + 2v^0_{10.2}\right)$$

$$v^0_{(6.2)\xi} = \frac{v^0_{6.2}}{4}\left(-35 + 13v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} + 14v^0_{2.1} + 5v^0_{2.2} + 9v^0_{3.1} + 4v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{6.1} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}}\right) - \frac{1}{4}\left(v^0_{8.2} + v^0_{9.2} + 3v^0_{10.1} + v^0_{10.2}\right)$$

$$v^0_{(6.3)\xi} = \frac{v^0_{6.3}}{4}\left(-31 + 12v^0_{1.1} + 4v^0_{1.2} + 6v^0_{1.3} + 9v^0_{2.1} + 10v^0_{2.2} + 4v^0_{3.2} + 5v^0_{3.3} - \frac{v^0_{6.3}}{v^0_{1.3}} - \frac{6v^0_{6.2} + 4v^0_{7.3}}{v^0_{2.2}} - 2\frac{v^0_{7.4}}{v^0_{1.3}}\right) - \frac{1}{4}\left(3v^0_{8.2} + v^0_{9.3} + 2v^0_{10.3}\right)$$

$$v^0_{(7.1)\xi} = \frac{v^0_{7.1}}{4}\left(-32 + 13v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 13v^0_{2.1} + 3v^0_{2.2} + 12v^0_{3.1} + 3v^0_{3.2} - \frac{v^0_{4.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - \frac{1}{4}\left(v^0_{9.1} + v^0_{10.1} + v^0_{11.1}\right)$$

$$v^0_{(7.2)\xi} = \frac{v^0_{7.2}}{4}\left(-32 + 14v^0_{1.1} + 3v^0_{1.2} + v^0_{1.3} + 14v^0_{2.1} + 4v^0_{2.2} + 9v^0_{3.1} + 4v^0_{3.2} - \frac{v^0_{4.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\right) - \frac{1}{4}\left(v^0_{9.2} + v^0_{10.2} + 3v^0_{11.1}\right)$$

$$v^0_{(7.3)\xi} = \frac{v^0_{7.3}}{4}\left(-30 + 9v^0_{1.1} + 5v^0_{1.2} + 4v^0_{1.3} + 15v^0_{2.1} + 7v^0_{2.2} + 5v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.2} + 3v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}} - 2\frac{v^0_{6.3} + v^0_{7.4}}{v^0_{2.2}}\right) - \frac{1}{4}\left(3v^0_{9.2} + 3v^0_{10.2} + v^0_{11.2}\right)$$

$$v^0_{(7.4)\xi} = \frac{v^0_{7.4}}{4}\left(-26 + 12v^0_{1.1} + 2v^0_{1.2} + 6v^0_{1.3} + 6v^0_{2.1} + 10v^0_{2.2} + 2v^0_{3.2} + 5v^0_{3.3} - \frac{3v^0_{4.1} + v^0_{6.3} + 2v^0_{7.4}}{v^0_{1.3}} - \frac{6v^0_{6.2} + 2v^0_{7.3}}{v^0_{2.2}}\right) - \frac{1}{4}\left(v^0_{9.3} + v^0_{10.3} + v^0_{11.3}\right)$$

$$v^0_{(8.1)\xi} = \frac{3}{4}v^0_{8.1}\left(-20 + 8v^0_{1.1} + 2v^0_{1.2} + 7v^0_{2.1} + 4v^0_{2.2} + 3v^0_{3.1} + 4v^0_{3.2} - 2\frac{v^0_{7.3}}{v^0_{1.2}} - \frac{v^0_{8.1}}{v^0_{4.2}} - \frac{3v^0_{9.1} + 2v^0_{10.2}}{v^0_{6.1}}\right)$$

$$v^0_{(8.2)\xi} = \frac{v^0_{8.2}}{4}\left(-56 + 16v^0_{1.1} + 4v^0_{1.2} + 6v^0_{1.3} + 21v^0_{2.1} + 10v^0_{2.2} + 12v^0_{3.1} + 6v^0_{3.2} + 5v^0_{3.3}\right.$$

$$- \frac{6v^0_{7.1} + 2v^0_{7.2}}{v^0_{1.1}} - 2\frac{v^0_{7.4}}{v^0_{1.3}} - \frac{v^0_{8.2}}{v^0_{4.1}} - 2\frac{v^0_{9.2} + 3v^0_{10.1} + v^0_{10.2}}{v^0_{6.2}} - \frac{v^0_{9.3} + 2v^0_{10.3}}{v^0_{6.3}}\Bigg)$$

$$v^0_{(9.1)\xi} = \frac{v^0_{9.1}}{4}\Bigg(-54 + 22v^0_{1.1} + 4v^0_{1.2} + 2v^0_{1.3} + 19v^0_{2.1} + 6v^0_{2.2} + 15v^0_{3.1} + 6v^0_{3.2} - 2\frac{v^0_{4.1}}{v^0_{1.1}} - 2\frac{v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{8.1}}{v^0_{6.1}} - \frac{3v^0_{9.1} + 2v^0_{9.2}}{v^0_{5.1}}\Bigg) - \frac{v^0_{12.1}}{2}$$

$$v^0_{(9.2)\xi} = \frac{v^0_{9.2}}{4}\Bigg(-52 + 17v^0_{1.1} + 6v^0_{1.2} + 5v^0_{1.3} + 20v^0_{2.1} + 7v^0_{2.2} + 9v^0_{3.1} + 6v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.1}}{v^0_{1.1}} - \frac{v^0_{4.2}}{v^0_{1.2}} - \frac{v^0_{6.1} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}} - 3\frac{v^0_{9.1}}{v^0_{5.1}} - 2\frac{v^0_{9.2}}{v^0_{5.1}}\Bigg) - \frac{1}{4}\left(3v^0_{12.1} + v^0_{12.2}\right)$$

$$v^0_{(9.3)\xi} = \frac{v^0_{9.3}}{4}\Bigg(-46 + 24v^0_{1.1} + 4v^0_{1.2} + 8v^0_{1.3} + 9v^0_{2.1} + 14v^0_{2.2} + 4v^0_{3.2} + 7v^0_{3.3} - 6\frac{v^0_{4.1}}{v^0_{1.3}} - \frac{6v^0_{6.2} + 4v^0_{7.3}}{v^0_{2.2}} - 3\frac{v^0_{8.2}}{v^0_{6.3}} - 3\frac{v^0_{9.3}}{v^0_{5.2}}\Bigg) - \frac{v^0_{12.3}}{2}$$

$$v^0_{(10.1)\xi} = \frac{v^0_{10.1}}{2}\Bigg(-28 + 10v^0_{1.1} + 2v^0_{1.2} + 2v^0_{1.3} + 11v^0_{2.1} + 3v^0_{2.2} + 9v^0_{3.1} + 3v^0_{3.2} + v^0_{3.3} - \frac{v^0_{6.1} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) - \frac{v^0_{12.1}}{2}$$

$$v^0_{(10.2)\xi} = \frac{v^0_{10.2}}{4}\Bigg(-56 + 21v^0_{1.1} + 5v^0_{1.2} + 4v^0_{1.3} + 23v^0_{2.1} + 9v^0_{2.2} + 12v^0_{3.1} + 8v^0_{3.2} + 2v^0_{3.3} - \frac{3v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}} - \frac{v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.2} + 6v^0_{7.1} + 2v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}}\Bigg) - \frac{3v^0_{12.1} + v^0_{12.2}}{4}$$

$$v^0_{(10.3)\xi} = \frac{v^0_{10.3}}{2}\Bigg(-24 + 9v^0_{1.1} + 3v^0_{1.2} + 4v^0_{1.3} + 6v^0_{2.1} + 8v^0_{2.2} + 3v^0_{3.2} + 4v^0_{3.3} - 3\frac{v^0_{6.2} + v^0_{7.3}}{v^0_{2.2}} - \frac{v^0_{6.3} + 2v^0_{7.4}}{v^0_{1.3}} - 3\frac{v^0_{8.2}}{v^0_{6.3}}\Bigg) - \frac{v^0_{12.3}}{2}$$

$$v^0_{(11.1)\xi} = \frac{v^0_{11.1}}{2}\Bigg(-27 + 11v^0_{1.1} + 2v^0_{1.2} + v^0_{1.3} + 11v^0_{2.1} + 3v^0_{2.2} + 9v^0_{3.1} + 3v^0_{3.2} - \frac{v^0_{4.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}}\Bigg) - \frac{v^0_{12.1}}{2}$$

$$v^0_{(11.2)\xi} = v^0_{11.2}\Bigg(-\frac{25}{2} + 3v^0_{1.1} + 2v^0_{1.2} + 2v^0_{1.3} + 6v^0_{2.1} + 3v^0_{2.2} + 2v^0_{3.2} + v^0_{3.3} - \frac{v^0_{4.2} + 3v^0_{6.1} + 2v^0_{7.3}}{2v^0_{1.2}} - \frac{v^0_{6.3} + v^0_{7.4}}{v^0_{2.2}}\Bigg) - \frac{3}{2}v^0_{12.2}$$

$$v^0_{(11.3)\xi} = v^0_{11.3}\Bigg(-\frac{23}{2} + 6v^0_{1.1} + v^0_{1.2} + 2v^0_{1.3} + 3v^0_{2.1} + 4v^0_{2.2} + v^0_{3.2} + 2v^0_{3.3} - \frac{3v^0_{4.1} + v^0_{6.3} + 2v^0_{7.4}}{2v^0_{1.3}} - \frac{3v^0_{6.2} + v^0_{7.3}}{v^0_{2.2}}\Bigg) - \frac{v^0_{12.3}}{2}$$

$$v^0_{(12.1)\xi} = \frac{v^0_{12.1}}{4}\left(-78 + 29v^0_{1.1} + 6v^0_{1.2} + 5v^0_{1.3} + 28v^0_{2.1} + 9v^0_{2.2} + 21v^0_{3.1} + 9v^0_{3.2} + 2v^0_{3.3} - \frac{v^0_{4.1} + v^0_{6.2} + 3v^0_{7.1} + v^0_{7.2}}{v^0_{1.1}} - \frac{v^0_{6.1} + v^0_{6.2} + 9v^0_{7.1} + 3v^0_{7.2}}{v^0_{2.1}} - 2\frac{v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} - \frac{3v^0_{9.1} + 2v^0_{9.2}}{v^0_{5.1}}\right) - \frac{v^0_{13.1}}{4}$$

$$v^0_{(12.2)\xi} = \frac{v^0_{12.2}}{4}\left(-76 + 24v^0_{1.1} + 8v^0_{1.2} + 8v^0_{1.3} + 29v^0_{2.1} + 12v^0_{2.2} + 12v^0_{3.1} + 10v^0_{3.2} + 4v^0_{3.3} - \frac{v^0_{4.2} + 3v^0_{6.1} + 2v^0_{7.3}}{v^0_{1.2}} - \frac{2v^0_{6.3} + 4v^0_{7.4}}{v^0_{2.2}} - \frac{6v^0_{7.1} + 2v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{8.1}}{v^0_{6.1}} - 2\frac{v^0_{8.2}}{v^0_{6.2}} - \frac{3v^0_{9.1} + 2v^0_{9.2}}{v^0_{5.1}}\right) - \frac{3}{4}v^0_{13.1}$$

$$v^0_{(12.3)\xi} = \frac{v^0_{12.3}}{4}\left(-68 + 30v^0_{1.1} + 8v^0_{1.2} + 10v^0_{1.3} + 15v^0_{2.1} + 20v^0_{2.2} + 8v^0_{3.2} + 10v^0_{3.3} - \frac{3v^0_{4.1} + v^0_{6.3} + 2v^0_{7.4}}{v^0_{1.3}} - \frac{6v^0_{6.2} + 8v^0_{7.3}}{v^0_{2.2}} - 9\frac{v^0_{8.2}}{v^0_{6.3}} - 3\frac{v^0_{9.3}}{v^0_{5.2}}\right) - \frac{v^0_{13.2}}{4}$$

$$v^0_{(13.1)\xi} = v^0_{13.1}\left(-\frac{51}{2} + 9v^0_{1.1} + 2v^0_{1.2} + 2v^0_{1.3} + \frac{17}{2}v^0_{2.1} + 3v^0_{2.2} + 6v^0_{3.1} + 3v^0_{3.2} + v^0_{3.3} - \frac{3v^0_{7.1} + v^0_{7.2}}{v^0_{2.1}} - \frac{v^0_{7.4}}{v^0_{2.2}} - \frac{v^0_{8.1}}{2v^0_{6.1}} - \frac{v^0_{8.2}}{v^0_{6.2}} - \frac{3v^0_{9.1} + 2v^0_{9.2}}{2v^0_{5.1}}\right)$$

$$v^0_{(13.2)\xi} = \frac{3}{2}v^0_{13.2}\left(-15 + 6v^0_{1.1} + 2\left(v^0_{1.2} + v^0_{1.3} + v^0_{3.2} + v^0_{3.3}\right) + 3v^0_{2.1} + 4v^0_{2.2} - 2\frac{v^0_{7.3}}{v^0_{2.2}} - 3\frac{v^0_{8.2}}{v^0_{6.3}} - \frac{v^0_{9.3}}{v^0_{5.2}}\right)$$

Correlation functions in the orthogonal basis

The limiting values of the CFs in the orthogonal basis in the limit of perfect ordering, $u^0_{i.j}$, are:

$u^0_{1.1} = -1$;	$u^0_{1.2} = 1$;	$u^0_{1.3} = 1$;	$u^0_{2.1} = -1$
$u^0_{2.2} = 1$;	$u^0_{3.1} = 1$;	$u^0_{3.2} = 1$;	$u^0_{3.3} = 1$
$u^0_{4.1} = -1$;	$u^0_{4.2} = 1$;	$u^0_{5.1} = -1$;	$u^0_{5.2} = 1$
$u^0_{6.1} = -1$;	$u^0_{6.2} = -1$;	$u^0_{6.3} = 1$;	$u^0_{7.1} = 1$
$u^0_{7.2} = -1$;	$u^0_{7.3} = 1$;	$u^0_{7.4} = 1$;	$u^0_{8.1} = -1$
$u^0_{8.2} = -1$;	$u^0_{9.1} = 1$;	$u^0_{9.2} = -1$;	$u^0_{9.3} = 1$
$u^0_{10.1} = 1$;	$u^0_{10.2} = -1$;	$u^0_{10.3} = 1$;	$u^0_{11.1} = 1$
$u^0_{11.2} = 1$;	$u^0_{11.3} = 1$;	$u^0_{12.1} = 1$;	$u^0_{12.2} = -1$
$u^0_{12.3} = 1$;	$u^0_{13.1} = 1$;	$u^0_{13.2} = 1$	

The limiting first derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)0}$ and $u^0_{(i.j)\xi}$, are:

$u^0_{(1.1)0} = 0$;	$u^0_{(1.2)0} = 2$;	$u^0_{(1.3)0} = 2$;	$u^0_{(2.1)0} = 0$
$u^0_{(2.2)0} = 2$;	$u^0_{(3.1)0} = -2$;	$u^0_{(3.2)0} = 2$;	$u^0_{(3.3)0} = 2$

$u^0_{(4.1)0} = -1;$ $u^0_{(4.2)0} = 3;$ $u^0_{(5.1)0} = -1;$ $u^0_{(5.2)0} = 3$

$u^0_{(6.1)0} = -1;$ $u^0_{(6.2)0} = -1;$ $u^0_{(6.3)0} = 3;$ $u^0_{(7.1)0} = -1$

$u^0_{(7.2)0} = -1;$ $u^0_{(7.3)0} = 3;$ $u^0_{(7.4)0} = 3;$ $u^0_{(8.1)0} = -2$

$u^0_{(8.2)0} = -2;$ $u^0_{(9.1)0} = 0;$ $u^0_{(9.2)0} = -2;$ $u^0_{(9.3)0} = 4$

$u^0_{(10.1)0} = 0;$ $u^0_{(10.2)0} = -2;$ $u^0_{(10.3)0} = 4;$ $u^0_{(11.1)0} = 0$

$u^0_{(11.2)0} = 4;$ $u^0_{(11.3)0} = 4;$ $u^0_{(12.1)0} = 1;$ $u^0_{(12.2)0} = -3$

$u^0_{(12.3)0} = 5;$ $u^0_{(13.1)0} = 2;$ $u^0_{(13.2)0} = 6$

and

$u^0_{(1.1)\xi} = -2;$ $u^0_{(1.2)\xi} = 1;$ $u^0_{(1.3)\xi} = 1;$ $u^0_{(2.1)\xi} = -2$

$u^0_{(2.2)\xi} = 1;$ $u^0_{(3.1)\xi} = 3;$ $u^0_{(3.2)\xi} = 1;$ $u^0_{(3.3)\xi} = 1$

$u^0_{(4.1)\xi} = -\frac{5}{2};$ $u^0_{(4.2)\xi} = \frac{3}{2};$ $u^0_{(5.1)\xi} = -\frac{5}{2};$ $u^0_{(5.2)\xi} = \frac{3}{2}$

$u^0_{(6.1)\xi} = -\frac{5}{2};$ $u^0_{(6.2)\xi} = -\frac{5}{2};$ $u^0_{(6.3)\xi} = \frac{3}{2};$ $u^0_{(7.1)\xi} = \frac{7}{2}$

$u^0_{(7.2)\xi} = -\frac{5}{2};$ $u^0_{(7.3)\xi} = \frac{3}{2};$ $u^0_{(7.4)\xi} = \frac{3}{2};$ $u^0_{(8.1)\xi} = -3$

$u^0_{(8.2)\xi} = -3;$ $u^0_{(9.1)\xi} = 4;$ $u^0_{(9.2)\xi} = -3;$ $u^0_{(9.3)\xi} = 2$

$u^0_{(10.1)\xi} = 4;$ $u^0_{(10.2)\xi} = -3;$ $u^0_{10.3\xi} = 2;$ $u^0_{(11.1)\xi} = 4$

$u^0_{(11.2)\xi} = 2;$ $u^0_{(11.3)\xi} = 2;$ $u^0_{(12.1)\xi} = \frac{9}{2};$ $u^0_{(12.2)\xi} = -\frac{7}{2}$

$u^0_{(12.3)\xi} = \frac{5}{2};$ $u^0_{13.1\xi} = 5;$ $u^0_{(13.2)\xi} = 3$

The limiting second derivatives of the CFs with respect to u_0 and ξ, in the orthogonal basis in the limit of perfect ordering, $u^0_{(i.j)00}$, $u^0_{(i.j)\xi}$ and $u^0_{(i.j)\xi\xi}$, are:

$u^0_{(1.1)00} = 2v^0_{1.1};$ $u^0_{(1.2)00} = 2v^0_{1.2};$ $u^0_{(1.3)00} = 2v^0_{1.3}$

$u^0_{(2.1)00} = 2v^0_{2.1};$ $u^0_{(2.2)00} = 2v^0_{2.2};$ $u^0_{(3.1)00} = 2v^0_{3.1}$

$u^0_{(3.2)00} = 2v^0_{3.2};$ $u^0_{(3.3)00} = 2v^0_{3.3};$ $u^0_{(4.1)00} = 4v^0_{1.1} - 2v^0_{1.3}$

$u^0_{(4.2)00} = 6v^0_{1.2};$ $u^0_{(5.1)00} = 4v^0_{1.1} - 2v^0_{1.2};$ $u^0_{(5.2)00} = 6v^0_{1.3}$

$u^0_{(6.1)00} = -2v^0_{1.2} + 4v^0_{2.1};$ $u^0_{(6.2)00} = 2v^0_{1.1} + 2v^0_{2.1} - 2v^0_{2.2};$ $u^0_{(6.3)00} = 2v^0_{1.3} + 4v^0_{2.2}$

$u^0_{(7.1)00} = -2v^0_{1.1} - 2v^0_{2.1} + 2v^0_{3.1};$ $u^0_{(7.2)00} = 2v^0_{1.1} + 2v^0_{2.1} - 2v^0_{3.2};$ $u^0_{(7.3)00} = 2v^0_{1.2} + 2v^0_{2.2} + 2v^0_{3.2}$

$u^0_{(7.4)00} = 2v^0_{1.3} + 2v^0_{2.2} + 2v^0_{3.3};$ $u^0_{(8.1)00} = -6v^0_{1.2} + 6v^0_{2.1}$

$u^0_{(8.2)00} = 4v^0_{1.1} - 2v^0_{1.3} + 2v^0_{2.1} - 4v^0_{2.2};$ $u^0_{(9.1)00} = -4v^0_{1.1} + 2v^0_{1.2} - 4v^0_{2.1} + 2v^0_{3.1}$

$u^0_{(9.2)00} = 4v^0_{1.1} - 2\left(v^0_{1.2} - v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right);$ $u^0_{(9.3)00} = 6v^0_{1.3} + 4v^0_{2.2} + 2v^0_{3.3}$

$u^0_{(10.1)00} = -4v^0_{1.1} - 4v^0_{2.1} + 2v^0_{2.2} + 2v^0_{3.1};$ $u^0_{(10.2)00} = 2\left(v^0_{1.1} - v^0_{1.2} - v^0_{2.2} - v^0_{3.2}\right) + 4v^0_{2.1}$

$u^0_{(10.3)00} = 4v^0_{1.3} + 6v^0_{2.2} + 2v^0_{3.3};$ $u^0_{(11.1)00} = -4v^0_{1.1} - 4v^0_{2.1} + 2v^0_{3.1} + 2v^0_{3.2}$

$u^0_{(11.2)00} = 4v^0_{1.2} + 4v^0_{2.2} + 4v^0_{3.2};$ $u^0_{(11.3)00} = 4v^0_{1.3} + 4v^0_{2.2} + 4v^0_{3.3}$

$$u^0_{(12.1)00} = -6v^0_{1.1} - 6v^0_{2.1} + 2\left(v^0_{1.2} + v^0_{2.2} + v^0_{3.1} + v^0_{3.2}\right)$$

$$u^0_{(12.2)00} = 4\left(v^0_{1.1} - v^0_{1.2} + v^0_{2.1} - v^0_{2.2} - v^0_{3.2}\right)$$
$$u^0_{(12.3)00} = 8v^0_{1.3} + 8v^0_{2.2} + 4v^0_{3.3}$$
$$u^0_{(13.1)00} = -8v^0_{1.1} + 4v^0_{1.2} - 8v^0_{2.1} + 4v^0_{2.2} + 2v^0_{3.1} + 4v^0_{3.2}$$
$$u^0_{(13.2)00} = 12v^0_{1.3} + 12v^0_{2.2} + 6v^0_{3.3}$$

$$u^0_{(1.1)\xi 0} = -v^0_{1.1}; \quad u^0_{(1.2)\xi 0} = v^0_{1.2}; \quad u^0_{(1.3)\xi 0} = v^0_{1.3}; \quad u^0_{(2.1)\xi 0} = -v^0_{2.1}$$
$$u^0_{(2.2)\xi 0} = v^0_{2.2}; \quad u^0_{(3.1)\xi 0} = -3v^0_{3.1}; \quad u^0_{(3.2)\xi 0} = v^0_{3.2}; \quad u^0_{(3.3)\xi 0} = v^0_{3.3}$$
$$u^0_{(4.1)\xi 0} = -2v^0_{1.1} - v^0_{1.3}; \quad u^0_{(4.2)\xi 0} = 3v^0_{1.2}; \quad u^0_{(5.1)\xi 0} = -2v^0_{1.1} - v^0_{1.2}; \quad u^0_{(5.2)\xi 0} = 3v^0_{1.3}$$

$$u^0_{(6.1)\xi 0} = -v^0_{1.2} - 2v^0_{2.1}; \quad u^0_{(6.2)\xi 0} = -v^0_{1.1} - v^0_{2.1} - v^0_{2.2}$$
$$u^0_{(6.3)\xi 0} = v^0_{1.3} + 2v^0_{2.2}; \quad u^0_{(7.1)\xi 0} = v^0_{1.1} + v^0_{2.1} - 3v^0_{3.1}$$
$$u^0_{(7.2)\xi 0} = -v^0_{1.1} - v^0_{2.1} - v^0_{3.2}; \quad u^0_{(7.3)\xi 0} = v^0_{1.2} + v^0_{2.2} + v^0_{3.2}$$
$$u^0_{(7.4)\xi 0} = v^0_{1.3} + v^0_{2.2} + v^0_{3.3}; \quad u^0_{(8.1)\xi 0} = -3v^0_{1.2} - 3v^0_{2.1}$$
$$u^0_{(8.2)\xi 0} = -2v^0_{1.1} - v^0_{1.3} - v^0_{2.1} - 2v^0_{2.2}; \quad u^0_{(9.1)\xi 0} = 2v^0_{1.1} + v^0_{1.2} + 2v^0_{2.1} - 3v^0_{3.1}$$
$$u^0_{(9.2)\xi 0} = -2v^0_{1.1} - v^0_{1.2} - v^0_{2.1} - v^0_{2.2} - v^0_{3.2}; \quad u^0_{(9.3)\xi 0} = 3v^0_{1.3} + 2v^0_{2.2} + v^0_{3.3}$$
$$u^0_{(10.1)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} + v^0_{2.2} - 3v^0_{3.1}; \quad u^0_{(10.2)\xi 0} = -v^0_{1.1} - v^0_{1.2} - 2v^0_{2.1} - v^0_{2.2} - v^0_{3.2}$$
$$u^0_{(10.3)\xi 0} = 2v^0_{1.3} + 3v^0_{2.2} + v^0_{3.3}; \quad u^0_{(11.1)\xi 0} = 2v^0_{1.1} + 2v^0_{2.1} - 3v^0_{3.1} + v^0_{3.2}$$
$$u^0_{(11.2)\xi 0} = 2v^0_{1.2} + 2v^0_{2.2} + 2v^0_{3.2}; \quad u^0_{(11.3)\xi 0} = 2v^0_{1.3} + 2v^0_{2.2} + 2v^0_{3.3}$$
$$u^0_{(12.1)\xi 0} = 3v^0_{1.1} + v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2} - 3v^0_{3.1} + v^0_{3.2}$$
$$u^0_{(12.2)\xi 0} = -2\left(v^0_{1.1} + v^0_{1.2} + v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right)$$
$$u^0_{(12.3)\xi 0} = 2v^0_{1.3} + 2v^0_{2.2} + 4v^0_{3.3}$$
$$u^0_{(13.1)\xi 0} = 4v^0_{1.1} + 2v^0_{1.2} + 4v^0_{2.1} + 2v^0_{2.2} - 3v^0_{3.1} + 2v^0_{3.2}$$
$$u^0_{(13.2)\xi 0} = 6v^0_{1.3} + 6v^0_{2.2} + 3v^0_{3.3}$$

and

$$u^0_{(1.1)\xi\xi} = -\frac{3}{2}v^0_{1.1}; \quad u^0_{(1.2)\xi\xi} = \frac{v^0_{1.2}}{2}; \quad u^0_{(1.3)\xi\xi} = \frac{v^0_{1.3}}{2}; \quad u^0_{(2.1)\xi\xi} = -\frac{3}{2}v^0_{2.1}$$
$$u^0_{(2.2)\xi\xi} = \frac{v^0_{2.2}}{2}; \quad u^0_{(3.1)\xi\xi} = \frac{9}{2}v^0_{3.1}; \quad u^0_{(3.2)\xi\xi} = \frac{v^0_{3.2}}{2}; \quad u^0_{(3.3)\xi\xi} = \frac{v^0_{3.3}}{2}$$
$$u^0_{(4.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.3}}{2}; \quad u^0_{(4.2)\xi\xi} = \frac{3}{2}v^0_{1.2}; \quad u^0_{(5.1)\xi\xi} = -3v^0_{1.1} - \frac{v^0_{1.2}}{2}; \quad u^0_{(5.2)\xi\xi} = \frac{3}{2}v^0_{1.3}$$

$$u^0_{(6.1)\xi\xi} = -\frac{v^0_{1.2}}{2} - 3v^0_{2.1}; \quad u^0_{(6.2)\xi\xi} = -\frac{3v^0_{1.1} + 3v^0_{2.1} + v^0_{2.2}}{2}$$
$$u^0_{(6.3)\xi\xi} = \frac{v^0_{1.3}}{2} + v^0_{2.2}; \quad u^0_{(7.1)\xi\xi} = \frac{3}{2}\left(v^0_{1.1} + v^0_{2.1} + 3v^0_{3.1}\right)$$
$$u^0_{(7.2)\xi\xi} = -\frac{1}{2}\left(3v^0_{1.1} + 3v^0_{2.1} + v^0_{3.2}\right); \quad u^0_{(7.3)\xi\xi} = \frac{1}{2}\left(v^0_{1.2} + v^0_{2.2} + v^0_{3.2}\right)$$
$$u^0_{(7.4)\xi\xi} = \frac{1}{2}\left(v^0_{1.3} + v^0_{2.2} + v^0_{3.3}\right); \quad u^0_{(8.1)\xi\xi} = -\frac{3}{2}\left(v^0_{1.2} + 3v^0_{2.1}\right)$$
$$u^0_{(8.2)\xi\xi} = -3v^0_{1.1} - v^0_{2.2} - \frac{v^0_{1.3} + 3v^0_{2.1}}{2}; \quad u^0_{(9.1)\xi\xi} = 3v^0_{1.1} + 3v^0_{2.1} + \frac{v^0_{1.2} + 9v^0_{3.1}}{2}$$

$$u^0_{(9.2)\xi\xi} = -3v^0_{1.1} - \frac{1}{2}\left(v^0_{1.2} + 3v^0_{2.1} + v^0_{2.2} + v^0_{3.2}\right); \quad u^0_{(9.3)\xi\xi} = \frac{1}{2}\left(3v^0_{1.3} + 2v^0_{2.2} + v^0_{3.3}\right)$$

$$u^0_{(10.1)\xi\xi} = 3v^0_{1.1} + 3v^0_{2.1} + \frac{v^0_{2.2} + 9v^0_{3.1}}{2}; \quad u^0_{(10.2)\xi\xi} = 3v^0_{2.1} - \frac{1}{2}\left(3v^0_{1.1} + v^0_{1.2} + v^0_{2.2} + v^0_{3.2}\right)$$

$$u^0_{(10.3)\xi\xi} = v^0_{1.3} + \frac{3v^0_{2.2} + v^0_{3.3}}{2}; \quad u^0_{(11.1)\xi\xi} = 3v^0_{1.1} + 3v^0_{2.1} + \frac{9v^0_{3.1} + v^0_{3.2}}{2}$$

$$u^0_{(11.2)\xi\xi} = v^0_{1.2} + v^0_{2.2} + v^0_{3.2}; \quad u^0_{(11.3)\xi\xi} = v^0_{1.3} + v^0_{2.2} + v^0_{3.3}$$

$$u^0_{(12.1)\xi\xi} = \frac{1}{2}\left(9v^0_{1.1} + v^0_{1.2} + 9v^0_{2.1} + v^0_{2.2} + 9v^0_{3.1} + v^0_{3.2}\right)$$

$$u^0_{(12.2)\xi\xi} = -3v^0_{1.1} - v^0_{1.2} - 3v^0_{2.1} - v^0_{2.2} - v^0_{3.2}$$

$$u^0_{(12.3)\xi\xi} = 2v^0_{1.3} + 2v^0_{2.2} + v^0_{3.3}$$

$$u^0_{(13.1)\xi\xi} = 6v^0_{1.1} + v^0_{1.2} + 6v^0_{2.1} + v^0_{2.2} + \frac{9}{2}v^0_{3.1} + v^0_{3.2}$$

$$u^0_{(13.2)\xi\xi} = 3v^0_{1.3} + 3v^0_{2.2} + \frac{3}{2}v^0_{3.3}$$

Appendix B

Derivation of $\Delta\psi$

At the phase boundary (ref. Eq. (3.28)),

$$\begin{aligned}\Delta\psi &= -x_\mathrm{A}x_\mathrm{B}\left(\frac{\partial}{\partial\xi}\left(\frac{\partial G^{mix}_{B32}}{\partial x_\mathrm{B}}\right)_\xi\right)_{x_\mathrm{B}}\frac{d\xi}{dx_\mathrm{B}}\\ &= -\frac{x_\mathrm{A}x_\mathrm{B}}{2\xi}\left(\frac{\partial}{\partial\xi}\left(\frac{\partial G^{mix}_{B32}}{\partial x_\mathrm{B}}\right)_\xi\right)_{x_\mathrm{B}}\frac{d\xi^2}{dx_\mathrm{B}}\end{aligned} \tag{B.1}$$

At the phase boundary, the differential terms in the numerator as well as the denominator in Eq. 3.43 vanish, making their ratio indeterminate. It can be evaluated by considering

$$\frac{d\xi^2}{dx_\mathrm{B}} = 2\xi\frac{d\xi}{dx_\mathrm{B}} = -2\xi\left(\frac{\partial}{\partial x_\mathrm{B}}\left(\frac{\partial G^{mix}_{B32}}{\partial\xi}\right)_{x_\mathrm{B}}\right)_\xi \Bigg/ \left(\frac{\partial^2 G^{mix}_{B32}}{\partial\xi^2}\right)_{x_\mathrm{B}} \tag{B.2}$$

The derivatives in Eq. (B.2) are evaluated from Eq. (3.17) and substituted in Eq. (B.2) which after simplification becomes

$$\frac{d\xi^2}{dx_\mathrm{B}} = -\frac{4u_0\xi^2\left(1+\left(u_0^2-\xi^2\right)\left(1-\eta_2\right)+\eta_2-4\mathrm{X}/3\right)}{\left(1-u_0^2\right)\left(\eta_2+u_0^2\left(1-\eta_2\right)-2\mathrm{X}/3\right)+\xi^2\left(u_0^2\left(1-\eta_2\right)-\eta_2+2\mathrm{X}/3\right)} \tag{B.3}$$

where

$$\mathrm{X} = \sqrt{\eta_2+\left(1-\eta_2\right)\left(u_0^2-\eta_2\xi^2\right)} \tag{B.4}$$

The terms which are independent of ξ^2 in the denominator of RHS in Eq. (B.3) together are expanded around u_0 corresponding to its value at the phase boundary, viz., $u_0 = u_{0b}$ (given in Eq. (3.28)) which yields

$$\begin{aligned}&\left(1-u_{0b}^2\right)\left(\eta_2+u_{0b}^2\left(1-\eta_2\right)+2\mathrm{Xb}/3\right)-2u_{0b}\left(u_0-u_{0b}\right)\Bigg(u_{0b}^2-\left(1-u_{0b}^2\right)\left(1-2\eta_2\right)\\ &\quad+\frac{1-\left(3u_{0b}^2-2\eta_2\xi^2\right)\left(1-\eta_2\right)-3\eta_2}{3\mathrm{Xb}}\Bigg)+\mathrm{O}\left(\left(u_0-u_{0b}\right)^2\right)\end{aligned}$$

Xb in the above expression corresponds to the value of X at u_0=u_{0b}. Expanding the terms which are independent of $(u_0 - u_{0b})$ in the above expression together around ξ =0 and with substitution of boundary condition corresponding to u_0 from Eq. (3.28) yields

$$\frac{5}{18}\xi^2\eta_2 + \mathrm{O}\left(\xi^4\right) + \frac{5}{9}u_{0b}\left(u_0 - u_{0b}\right) + \mathrm{O}\left(\left(u_0 - u_{0b}\right)^2\right)$$

Substituting the above expression in Eq. (B.3) and cancelling ξ^2 from the numerator and denominator

$$\frac{d\xi^2}{dx_{\mathrm{B}}} = -\frac{4u_0\left(1 + \left(u_0^2 - \xi^2\right)\left(1 - \eta_2\right) + \eta_2 - 4\mathrm{X}/3\right)}{-\frac{13}{18}\eta_2 + u_0^2\left(1 - \eta_2\right) - 2\mathrm{X}/3 + \mathrm{O}\left(\xi^2\right) + \frac{5}{9}u_{0b}\frac{\left(u_0 - u_{0b}\right)}{\xi^2} + \frac{\left(u_0 - u_{0b}\right)}{\xi^2}\mathrm{O}\left(\left(u_0 - u_{0b}\right)\right)} \tag{B.5}$$

In the limit of $u_0 \to u_{0b}$ and $\xi \to 0$ corresponding to the phase boundary,

$$\left.\frac{\left(u_0 - u_{0b}\right)}{\xi^2}\right|_{u_0 \to u_{0b}, \xi \to 0} = \frac{du_0}{d\xi^2} = \frac{1}{\left(\frac{d\xi^2}{du_0}\right)} = \frac{1}{\left(\frac{d\xi^2}{2dx_{\mathrm{B}}}\right)} \tag{B.6}$$

Substituting from Eq. (B.6) in Eq. (B.5), we obtain

$$\frac{d\xi^2}{dx_{\mathrm{B}}} = -\frac{4u_{0b}}{\frac{4+27u_{0b}^2}{18\left(1-u_{0b}^2\right)} + \frac{u_{0b}}{\left(\frac{d\xi^2}{2dx_{\mathrm{B}}}\right)}} \tag{B.7}$$

The above equation can be solved for $d\xi^2/dx_{\mathrm{B}}$ in terms of u_{0b} to yield

$$\frac{d\xi^2}{dx_{\mathrm{B}}} = \frac{54u_{0b}\left(-1 + u_{0b}^2\right)}{4 + 27u_{0b}^2} \tag{B.8}$$

Substituting from Eq. (B.8) in (3.43) and utilizing the boundary equation, Eq. (3.28), we get

$$\Delta\psi = \frac{135u_0^2}{8 + 54u_0^2} = \frac{60 - 135\eta_2}{32 - 62\eta_2} \tag{B.9}$$

Appendix C

Determination of coefficients of the polynomials

The coefficients of the polynomials, P_i, are chosen as rational functions of η_2. In order to determine the functional dependence of these coefficients on η_2, a set of η_2 values is chosen for which the equilibrium values of the CFs are numerically determined. Based on these values, the constraints mentioned in Section 4.4 are determined. The procedure for selection of coefficients of polynomials for pair and tetrahedron CFs is illustrated below.

At $\eta_2 = 4$, the permissible domain for the coefficients of P_2 is shown in Figure C.1. The surface represents the region where the constraints are just satisfied and the white region represents the permissible domain. The point shown in red in the figure represents the approximate midpoint of the permissible domain at $u_0 = 0$ for which the constraints are satisfied for the entire range of compositions.

The midpoint of the permissible domain is determined for each selected value of η_2 in a similar manner. The data are then fit to an appropriate rational function in η_2 and the fitted functions thus obtained are given below

$$\begin{aligned} u_2\big|_{u_0=0} &= \frac{a_{20}}{4} = \frac{-2.4675\left(1-\sqrt{\eta_2}\right)}{4\left(1+0.1945\sqrt{\eta_2}\right)} \\ u_2\big|_{u_0=0.5} &= \frac{1}{4} + \frac{9}{1024}\left(16a_{20}+4a_{22}+a_{24}\right) \\ &= \frac{-0.0398+0.2992\sqrt{\eta_2}}{1+0.0374\sqrt{\eta_2}} \equiv g \end{aligned} \tag{C.1}$$

The rational function fits are shown in Figure C.2 for a_{20} and g. From the figure it can be observed that the deviations of the rational function fits are only marginal from

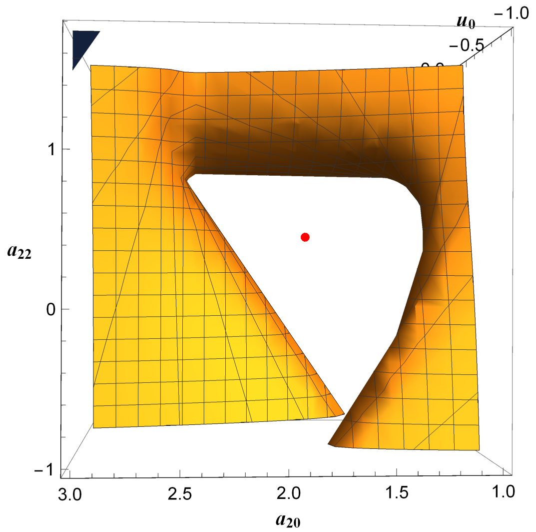

Figure C.1: The permissible domain (white region) for the coefficients of P_2.

the data. Since the data point is selected from the middle of the permissible domain, these marginal deviations do not lead to a violation of the constraints.

Determination of the polynomial coefficient a_{40} corresponding to the tetrahedron CF at $\eta_2 = 1/3$, where both $A2$ and $B32$ phases are in equilibrium is discussed below. The permissible domain (white region) for a_{40} satisfying all the constraints is shown in Figure C.3. In the present case, all the constraints are satisfied for the entire range of compositions for $0.33 < a_{40} < 1.87$. The mid value in this range should be chosen as initial value for fitting.

Next consider determination of the coefficients of the polynomials for the $B32$ phase. At the selected value of η_2, the coefficients a_{20}, a_{22} and a_{24} of $A2$ phase determined earlier are substituted into the polynomials for the CFs of the $B32$ phase and the permissible domain for the remaining coefficients of the polynomial is

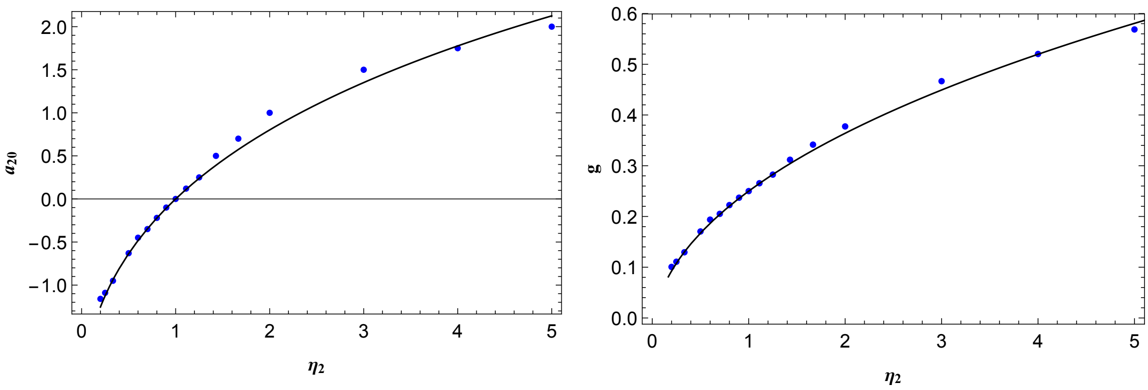

Figure C.2: Rational functions fits to a_{20} and g.

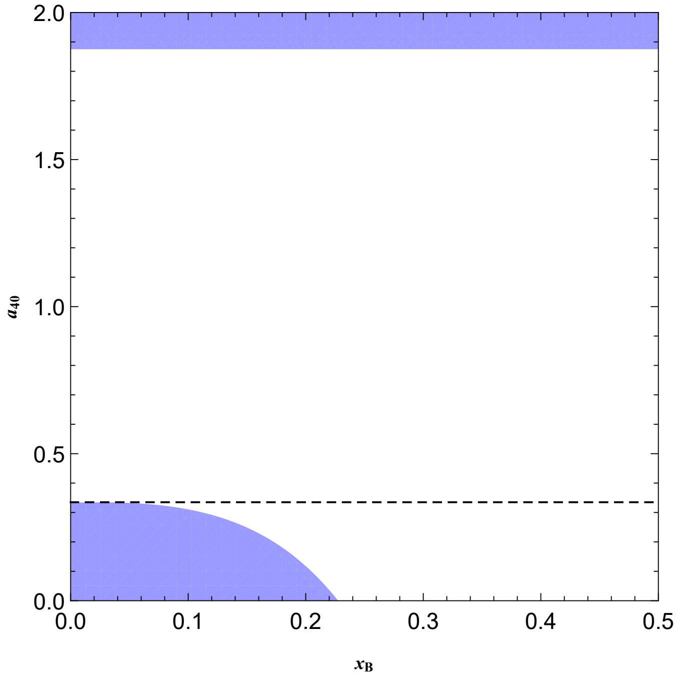

Figure C.3: The permissible domain for a_{40} for the $A2$ phase.

determined in each case. As the ordered phase has 2 point CFs, namely, $u_{0.1}$ and $u_{0.2}$, the CV constraints are chosen along the edges of the configuration square shown in Figure 2.2.

Even though the same coefficient a_{40} appears in the polynomials for tetrahedron CF in both the $A2$ and $B32$ phases (ref. Eq. (4.47)), the permissible domain in the ordered case is $0.347 < a_{40} < 1.875$, which is different from that of the disordered phase, as the constraints operating on these coefficients are different. The approximate midpoint of the intersection of the permissible domains for both phases, namely, 1.11 is chosen to be the value of a_{40} corresponding to $\eta_2 = 1/3$.

The values of the polynomial coefficients are determined at all other selected values of η_2 in a similar manner. These data are fitted to the rational functions of η_2 given in Eq. (4.52) by least squares method. It was ensured that the fitted rational function lies within the permissible domains of a_{40} for the entire range of η_2 values selected, as shown in Figure C.4.

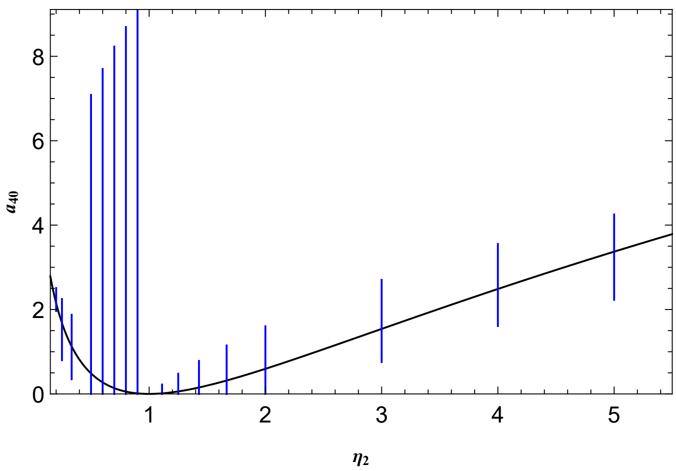

Figure C.4: Rational function fit to a_{40}. The vertical lines represent the permissible range of values for a_{40} corresponding to the selected values of η_2.