

(b)

1) Definition of variables for the barycentric formula (cation)

$$y^* = x_{Al}^{*M2} = \frac{\frac{2}{17}p_{ged}^* + \frac{1}{18}p_{ompa}^* + \frac{2}{17}p_{omgl}^*}{\left(\frac{2}{17} - \frac{2}{17 \cdot 18}p_{ompa}^*\right)}$$

$$x^* = \frac{\left(\frac{2}{17} - \frac{2p_{ompa}^*}{17 \cdot 18}\right)x_{Fe}^{*M4} + \left(\frac{3}{17} - \frac{3p_{ompa}^*}{17 \cdot 18}\right)x_{Fe}^{*M13} + \left(\frac{2}{17} - \frac{2p_{ompa}^*}{17 \cdot 18}\right)x_{Fe}^{*M2}}{\left(\frac{2}{17} - \frac{2p_{omgl}^*}{17} - \frac{2p_{otr}^*}{17} - \frac{2p_{ompa}^*}{17 \cdot 18}\right) + \left(\frac{3}{17} - \frac{3p_{ompa}^*}{17 \cdot 18}\right) + \left(\frac{2}{17} - \frac{2p_{ged}^*}{17} - \frac{p_{ompa}^*}{18} - \frac{2p_{omgl}^*}{17} - \frac{2p_{ompa}^*}{17 \cdot 18}\right)}$$

$$Q_1^* = x^* - \frac{x_{Fe}^{*M13}}{x_{Fe}^{*M13} + x_{Mg}^{*M13}} = x^* - x_{Fe}^{*M13}$$

$$Q_2^* = x^* - \frac{x_{Fe}^{*M2}}{x_{Fe}^{*M2} + x_{Mg}^{*M2}} = x^* - \frac{x_{Fe}^{*M2}}{1 - y^*}$$

$$a^* = p_{ompa}^*$$

$$z^* = p_{omgl}^*$$

$$c^* = p_{otr}^*$$

2) Calculation formulas of phase component proportions for the barycentric formula (cation)

$$p_{anth}^* = \left(1 - \frac{1}{2}a^* - c^* - Q_2^* - x^* - y^* - \frac{3}{2}Q_1^*\right) + c^*x^* + Q_2^*y^* + x^*z^* + \frac{a^*}{18}\left(-\frac{1}{2} + y^* + x^* + Q_2^* + \frac{3}{2}Q_1^*\right) - \frac{a^*}{18}Q_2^*y^*$$

$$p_{ged}^* = \left(y^* - \frac{1}{2}a^* - z^*\right) + \frac{a^*}{18}\left(\frac{1}{2} - y^*\right)$$

$$p_{ompa}^* = a^*$$

$$p_{omgl}^* = z^*$$

$$p_{otr}^* = c^*$$

$$p_{fanth}^* = \left(x^* - 2Q_2^* - \frac{5}{2}Q_1^*\right) + c^*x^* + 2Q_2^*y^* - x^*y^* + x^*z^* + \frac{a^*}{18}\left(-x^* + 2Q_2^* + \frac{5}{2}Q_1^*\right) + \frac{a^*}{18}x^*y^* - \frac{a^*}{18}2Q_2^*y^*$$

$$p_a^* = \left(Q_2^* + \frac{5}{2}Q_1^*\right) - c^*x^* - Q_2^*y^* - x^*z^* - \frac{a^*}{18}\left(Q_2^* + \frac{5}{2}Q_1^*\right) + \frac{a^*}{18}Q_2^*y^*$$

$$p_b^* = \left(2Q_2^* + \frac{3}{2}Q_1^*\right) - c^*x^* - 2Q_2^*y^* + x^*y^* - x^*z^* - \frac{a^*}{18}\left(2Q_2^* + \frac{3}{2}Q_1^*\right) + \frac{a^*}{18}2Q_2^*y^* - \frac{a^*}{18}x^*y^*$$

3) Calculation formulas of variables expressed using phase component proportions for the Cartesian formula

$$a = p_{ompa}$$

$$z = p_{omgl}$$

$$c = p_{otr}$$

$$y = p_{ged} + \frac{1}{2}p_{ompa} + p_{omgl}$$

$$Q_1 = (2p_a - p_b) / \left(\frac{7}{2} - p_{ged} - \frac{1}{2}p_{ompa} - p_{otr} - 2p_{omgl}\right)$$

$$+ (p_{fanth} \cdot p_{otr} + p_{fanth} \cdot p_{omgl} + p_b \cdot p_{otr} + p_b \cdot p_{omgl}) / \left(\frac{7}{2} - p_{ged} - \frac{1}{2}p_{ompa} - p_{otr} - 2p_{omgl}\right)$$

$$+ (p_{ged} \cdot p_{fanth} + p_{ged} \cdot p_b + \frac{1}{2}p_{ompa} \cdot p_{fanth} + \frac{1}{2}p_{ompa} \cdot p_b) / \left(\frac{7}{2} - p_{ged} - \frac{1}{2}p_{ompa} - p_{otr} - 2p_{omgl}\right)$$

$$+ (p_{omgl} \cdot p_{fanth} + p_{omgl} \cdot p_b) / \left(\frac{7}{2} - p_{ged} - \frac{1}{2}p_{ompa} - p_{otr} - 2p_{omgl}\right)$$

$$Q_2 = Q_1 + (-p_a + p_b) / \left(1 - p_{ged} - \frac{1}{2}p_{ompa} - p_{omgl}\right)$$

$$+ (-p_{fanth} \cdot p_{ged} - \frac{1}{2}p_{fanth} \cdot p_{ompa} - p_{fanth} \cdot p_{omgl}) / \left(1 - p_{ged} - \frac{1}{2}p_{ompa} - p_{omgl}\right)$$

$$+ (-p_b \cdot p_{ged} - \frac{1}{2}p_b \cdot p_{ompa} - p_b \cdot p_{omgl}) / \left(1 - p_{ged} - \frac{1}{2}p_{ompa} - p_{omgl}\right)$$

$$x = Q_1 + p_{fanth} + p_b$$

(c)

(b) Code for calculation formulas of phase component proportions for the barycentric formula (cation)

p(anth*)	6	1	1	6	-1/2	a*	-1	c*	-1	Q2*	-1	x*	-1	y*	-3/2	Q1*
	2	0	1	1		c*	0	1	1	x*						
	2	0	1	1		Q2*	0	1	1	y*						
	2	0	1	1		x*	0	1	1	z*						
	2	0	1	1/18 a*	-1/2	4	1	y*	1	x*	1	Q2*	3/2	Q1*		
	3	0	1	-1/18 a*		0	1	1	Q2*	0	1	1	y*			
p(ged*)	2	1	0	3	1	y*	-1/2	a*	-1	z*						
	2	0	1	1/18 a*	1/2	1	-1	y*								
p(ompa*)	1	1	0	1	1	a*										
p(omgl*)	1	1	0	1	1	z*										
p(otr*)	1	1	0	1	1	c*										
p(fanth*)	8	1	0	3	1	x*	-2	Q2*	-5/2	Q1*						
	2	0	1	1		c*	0	1	1	x*						
	2	0	1	2		Q2*	0	1	1	y*						
	2	0	1	-1		x*	0	1	1	y*						
	2	0	1	1		x*	0	1	1	z*						
	2	0	1	1/18 a*	0	3	-1	x*	2	Q2*	5/2	Q1*				
	3	0	1	1/18 a*	0	1	1	x*	0	1	1	y*				
	3	0	1	-1/18 a*	0	1	2	Q2*	0	1	1	y*				
p(a*)	6	1	0	2	1	Q2*	5/2	Q1*								
	2	0	1	-1		c*	0	1	1	x*						
	2	0	1	-1		Q2*	0	1	1	y*						
	2	0	1	-1		x*	0	1	1	z*						
	2	0	1	-1/18 a*	0	2	1	Q2*	5/2	Q1*						
	3	0	1	1/18 a*	0	1	1	Q2*	0	1	1	y*				
p(b*)	8	1	0	2	2	Q2*	3/2	Q1*								
	2	0	1	-1		c*	0	1	1	x*						
	2	0	1	-2		Q2*	0	1	1	y*						
	2	0	1	1		x*	0	1	1	y*						
	2	0	1	-1		x*	0	1	1	z*						
	2	0	1	-1/18 a*	0	2	2	Q2*	3/2	Q1*						
	3	0	1	1/18 a*	0	1	2	Q2*	0	1	1	y*				
	3	0	1	-1/18 a*	0	1	1	x*	0	1	1	y*				
