TABLE 5. Detailed refinement results and Ca γ-tensor elements ($\times 10^6$) for malayaite (for deposit)

Refined	R (%)	R_w (%)	S	n	m	c_{222}	c_{112}	c_{233}	c_{123}
No γ-tensor	1.66	2.80	1.861	1342	41				
γ-tensor for Ca	1.51	2.29	1.251	1344	45	3(2)	-64(2)	1(2)	5(5)
Only c_{112} for γ-tensor of C	1.51	2.31	1.270	1343	42	0	-67(2)	0	0

$$R = \Sigma \left| |F_o| - k \cdot |F_c| \right| / \Sigma_h |F_o|$$

$$R_w = \{\Sigma_h w_h [|F_o| - k \cdot |F_c||^2 / \Sigma_h w_h |F_o|^2\}^{1/2}$$

$$S = \{\Sigma_h w_h [|F_o| - k \cdot |F_c||^2 / (n-m)\}^{1/2}$$

n: number of observations; *m:* number of refined parameters. The anharmonic correction to the temperature factor has the form

$$\exp[-i(h^3 c_{111} + l^3 c_{333} + ... + hllc_{133} + kklc_{223})].$$