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Crystal structure of hillebrandite: A natural analogue of calcium silicate hydrate (CSH) phases in Portland cement

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For deposit: Tables 4 and 5

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For Deposit

Table 4. Anisotropic temperature factors for hillebrandite structure

Atom	$U_{(1,1)}$	$U_{(2,2)}$	$U_{(3,3)}$	$U_{(1,2)}$	$U_{(1,3)}$	$U_{(2,3)}$
Ca1	0.014(1)	0.012(1)	0.014(1)	0	0	0.004(1)
Ca2	0.014(1)	0.011(1)	0.009(1)	0	0	-0.003(1)
Ca3	0.015(1)	0.014(1)	0.007(1)	0	0	0.004(1)
Si1	0.023(5)	0.004(2)	0.008(2)	-0.000(2)	0.005(2)	-0.002(2)
Si2	0.009(3)	0.007(3)	0.005(3)	0	0	0.001(3)

The form of the anisotropic displacement parameter is: $\exp[-2\pi^2\{h^2a^2U_{(1,1)} + k^2b^2U_{(2,2)} + l^2c^2U_{(3,3)} + 2hkabU_{(1,2)} + 2hlacU_{(1,3)} + 2klbcU_{(2,3)}\}]$ where a, b, and c are reciprocal lattice constants.