

Supplementary

Table S1. Anisotropic atom displacement parameters for dmisteinbergite (\AA^2).

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca1	0.0103 (6)	$= U^{11}$	0.009 (1)	0	0	0.0051 (3)
Ca2	0.0162 (7)	$= U^{11}$	0.014 (1)	0	0	0.0081 (3)
T1	0.0053 (9)	$= U^{11}$	0.007 (1)	0	0	0.0027 (5)
T2	0.010 (1)	$= U^{11}$	0.014 (2)	0	0	0.0050 (7)
T3	0.014 (1)	$= U^{11}$	0.017 (2)	0	0	0.0071 (6)
T4	0.007 (1)	$= U^{11}$	0.006 (1)	0	0	0.0035 (5)
O1	0.019 (4)	$= U^{11}$	0.001 (4)	0	0	0.009 (2)
O2	0.015 (4)	$= U^{11}$	0.034 (7)	0	0	0.007 (2)
O3	0.005 (1)	0.007 (2)	0.006 (1)	0.004 (1)	0.002 (2)	0.003 (2)
O4	0.021 (4)	0.013 (4)	0.019 (3)	-0.005 (3)	0.004 (3)	0.010 (3)