Table S2. Atom coordinates and displacement parameters (Å^2) for protocaseyite.

	x/*a*	*y*/*b*	*z*/*c*	U_{eq}
V1	0.33162(4)	0.44567(4)	0.55593(3)	0.01406(9)
V2	0.52667(4)	0.43936(4)	0.74133(4)	0.01598(9)
V3	0.39000(4)	0.70038(4)	0.61917(4)	0.01677(9)
V4	0.47362(4)	0.18897(4)	0.67493(4)	0.01815(10)
V5	0.79104(4)	0.28754(4)	0.57242(4)	0.01874(10)
Al1	0.91017(8)	0.52198(7)	0.91335(7)	0.01731(15)
Al2	0.76964(8)	0.76711(7)	0.82192(7)	0.01791(15)
O1	0.49704(19)	0.49385(18)	0.86850(16)	0.0237(4)
O2	0.3627(2)	0.74896(17)	0.75162(17)	0.0246(4)
O3	0.3946(2)	0.06094(17)	0.75838(17)	0.0266(4)
O4	0.9547(2)	0.23124(19)	0.57856(18)	0.0295(4)
O5	0.28344(18)	0.29977(16)	0.64677(15)	0.0184(3)
O6	0.17011(17)	0.53160(16)	0.53678(15)	0.0179(3)
O7	0.44536(18)	0.28333(16)	0.80289(15)	0.0185(3)
O8	0.72176(18)	0.37043(16)	0.71043(15)	0.0191(3)
O9	0.21364(18)	0.74391(16)	0.58654(15)	0.0195(3)
O10	0.49040(18)	0.82963(16)	0.49370(16)	0.0192(3)
O11	0.67494(18)	0.15042(16)	0.66401(16)	0.0206(3)
O12	0.40565(17)	0.40061(15)	0.39008(14)	0.0155(3)
O13	0.34018(17)	0.51829(15)	0.69455(14)	0.0153(3)
O14	0.55534(17)	0.38574(15)	0.55351(14)	0.0152(3)
OH1	0.09995(18)	0.45459(16)	0.92282(15)	0.0188(3)
H1	0.190(2)	0.472(4)	0.848(2)	0.071(3)
OH2	0.96105(18)	0.69246(16)	0.81960(16)	0.0194(3)
H2	1.048(3)	0.717(4)	0.744(2)	0.071(3)
OH3	0.72583(18)	0.60314(16)	0.90930(16)	0.0195(3)
H3	0.6273(18)	0.568(3)	0.942(4)	0.071(3)
OW1	0.94292(19)	0.45909(19)	0.75779(16)	0.0241(4)
H4	0.859(2)	0.427(3)	0.744(3)	0.071(3)
H5	1.014(3)	0.494(4)	0.6742(17)	0.071(3)
OW2	0.8178(2)	0.35666(18)	0.99198(18)	0.0270(4)
H6	0.745(3)	0.334(4)	1.0777(15)	0.071(3)
H7	0.874(4)	0.2754(18)	0.975(4)	0.071(3)
OW3	0.7434(2)	0.82596(17)	0.98004(16)	0.0231(4)
H8	0.835(2)	0.826(4)	1.003(3)	0.071(3)
H9	0.663(3)	0.782(3)	1.052(2)	0.071(3)
OW4	0.5657(2)	0.83138(19)	0.84384(19)	0.0284(4)
H10	0.505(3)	0.810(3)	0.796(2)	0.071(3)
H11	0.488(3)	0.858(3)	0.917(2)	0.071(3)
OW5	0.8416(2)	0.93013(17)	0.72825(18)	0.0252(4)
H12	0.780(3)	1.0088(19)	0.705(4)	0.071(3)
H13	0.934(2)	0.958(3)	0.731(3)	0.071(3)
OW6	0.7754(2)	0.73624(18)	0.66011(17)	0.0263(4)
H14	0.711(3)	0.679(2)	0.649(3)	0.071(3)

H15	0.794(4)	0.808(2)	0.584(2)	0.071(3)
OW7	0.7349(2)	0.9506(2)	0.4781(2)	0.0358(5)
H16	0.640(2)	0.925(4)	0.478(4)	0.106(4)
H17	0.708(5)	1.0336(18)	0.504(4)	0.106(4)
OW8	0.0433(3)	0.1825(2)	0.8970(2)	0.0466(6)
H18	0.034(5)	0.104(2)	0.872(4)	0.106(4)
H19	0.096(5)	0.242(3)	0.818(2)	0.106(4)
OW9	0.0860(3)	0.9813(2)	0.7678(2)	0.0450(6)
H20	0.141(5)	1.018(4)	0.6780(15)	0.106(4)
H21	0.148(4)	0.913(3)	0.808(4)	0.106(4)
OW10	0.3486(3)	0.8898(3)	0.0420(2)	0.0545(7)
H22	0.323(6)	0.840(4)	0.1315(15)	0.106(4)
H23	0.323(6)	0.9831(8)	0.022(5)	0.106(4)

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
V1	0.01191(18)	0.01683(19)	0.01187(18)	-0.00229(14)	-0.00147(14)	-0.00246(14)
V2	0.01581(19)	0.0201(2)	0.01117(18)	-0.00213(15)	-0.00315(14)	-0.00286(15)
V3	0.01741(19)	0.0176(2)	0.01389(19)	-0.00439(15)	-0.00247(15)	-0.00049(15)
V4	0.0178(2)	0.0167(2)	0.0169(2)	-0.00016(15)	-0.00331(15)	-0.00223(15)
V5	0.01433(19)	0.0203(2)	0.0185(2)	-0.00107(15)	-0.00369(15)	0.00009(15)
Al1	0.0148(3)	0.0201(4)	0.0156(3)	-0.0031(3)	-0.0032(3)	-0.0010(3)
Al2	0.0162(3)	0.0189(4)	0.0174(3)	-0.0018(3)	-0.0049(3)	-0.0013(3)
O1	0.0229(9)	0.0334(10)	0.0151(8)	-0.0060(7)	-0.0033(7)	-0.0071(8)
O2	0.0267(9)	0.0279(10)	0.0200(9)	-0.0095(7)	-0.0051(7)	-0.0011(8)
O3	0.0261(9)	0.0215(9)	0.0276(9)	0.0020(7)	-0.0060(8)	-0.0051(7)
O4	0.0182(9)	0.0362(11)	0.0301(10)	-0.0037(8)	-0.0067(7)	0.0030(8)
O5	0.0161(8)	0.0196(8)	0.0171(8)	-0.0013(6)	-0.0027(6)	-0.0037(6)
O6	0.0141(7)	0.0213(8)	0.0161(8)	-0.0025(6)	-0.0023(6)	-0.0022(6)
O7	0.0175(8)	0.0216(8)	0.0137(7)	-0.0005(6)	-0.0028(6)	-0.0034(7)
O8	0.0161(8)	0.0251(9)	0.0154(8)	-0.0022(7)	-0.0047(6)	-0.0024(7)
O9	0.0173(8)	0.0208(8)	0.0182(8)	-0.0047(7)	-0.0024(6)	0.0003(7)
O10	0.0190(8)	0.0175(8)	0.0192(8)	-0.0043(6)	-0.0030(7)	-0.0012(7)
O11	0.0194(8)	0.0186(8)	0.0202(8)	0.0007(7)	-0.0055(7)	0.0002(7)
O12	0.0139(7)	0.0185(8)	0.0133(7)	-0.0032(6)	-0.0024(6)	-0.0025(6)
O13	0.0138(7)	0.0184(8)	0.0118(7)	-0.0027(6)	-0.0013(6)	-0.0019(6)
O14	0.0146(7)	0.0174(8)	0.0124(7)	-0.0023(6)	-0.0024(6)	-0.0024(6)
OH1	0.0135(8)	0.0256(9)	0.0159(8)	-0.0054(7)	-0.0029(6)	0.0007(7)
OH2	0.0157(8)	0.0221(9)	0.0170(8)	-0.0013(7)	-0.0029(6)	-0.0012(7)
OH3	0.0154(8)	0.0211(9)	0.0196(8)	-0.0011(7)	-0.0036(6)	-0.0038(7)
OW1	0.0201(8)	0.0364(10)	0.0170(8)	-0.0096(7)	-0.0026(7)	-0.0063(8)
OW2	0.0278(10)	0.0242(9)	0.0240(9)	-0.0027(8)	-0.0011(7)	-0.0057(8)
OW3	0.0233(9)	0.0262(9)	0.0183(8)	-0.0053(7)	-0.0028(7)	-0.0043(7)
OW4	0.0188(9)	0.0336(11)	0.0340(10)	-0.0105(8)	-0.0105(8)	0.0050(8)
OW5	0.0261(9)	0.0196(9)	0.0287(9)	0.0012(7)	-0.0104(8)	-0.0039(7)
OW6	0.0306(10)	0.0306(10)	0.0183(8)	-0.0010(7)	-0.0083(7)	-0.0094(8)
OW7	0.0387(12)	0.0304(11)	0.0423(12)	-0.0108(9)	-0.0175(10)	0.0023(9)

OW8	0.0453(13)	0.0424(13)	0.0555(15)	-0.0193(11)	-0.0145(11)	0.0002(11)
OW9	0.0364(12)	0.0504(14)	0.0515(14)	-0.0110(11)	-0.0148(11)	-0.0096(11)
OW10	0.0655(17)	0.0523(15)	0.0330(12)	-0.0078(11)	-0.0092(12)	0.0189(13)