

Table 5b: Refined isotropic displacement parameters of zoisite [100*Uiso]

sample	Au32	Au40	Au45	Pt4	Au31	Au34	Au30	Au42	Pt3	Pt36	Pt2	Au23	Au22	Au33	Au44	Au21
A1	0.43(68)	0.86(27)	0.34(64)	1.16(16)	0.22(72)	-0.03(51)	0.36(32)	0.25(80)	0.94(16)	0.92(15)	0.13(14)	0.58(16)	0.06(20)	1.27(21)	-0.17(12)	0.86(4)
A2	0.35(68)	1.00(24)	0.63(48)	1.46(12)	0.63(52)	0.71(39)	0.98(22)	0.80(96)	0.94(10)	1.04(8)	0.18(10)	0.55(12)	0.14(17)	2.54(21)	-0.02(12)	1.31(5)
M1	-0.39(76)	-0.34(15)	-0.35(40)	0.79(11)	-0.43(44)	0.37(39)	0.16(22)	-0.61(52)	0.65(13)	0.51(12)	0.46(16)	0.35(17)	-0.02(24)	1.00(30)	-0.05(16)	0.54(8)
M2	0.32(76)	0.28(28)	0.90(80)	1.08(20)	1.18(98)	0.46(63)	0.38(40)	-0.74(88)	0.97(22)	1.28(23)	0.52(26)	0.63(29)	0.62(44)	1.09(39)	0.29(27)	0.55(13)
T1	-0.07(68)	0.12(28)	1.00(80)	0.47(17)	0.37(88)	0.03(57)	0.14(38)	-0.97(80)	0.38(18)	0.79(20)	-0.13(22)	-0.22(24)	-0.04(37)	0.65(45)	0.30(26)	0.67(12)
T2	0.83(76)	-0.31(26)	-0.18(60)	0.74(17)	-0.51(72)	-0.03(54)	0.76(38)	-0.21(88)	0.82(20)	0.67(19)	0.38(24)	0.34(25)	-0.50(34)	1.17(45)	-0.06(22)	0.51(11)
T3	-0.75(64)	-0.17(26)	-0.14(64)	0.58(17)	-0.80(68)	-0.07(54)	0.91(40)	-0.19(98)	0.62(20)	0.41(20)	0.36(24)	0.02(26)	0.36(42)	0.46(45)	-0.27(24)	0.39(11)
O1	-0.36(96)	-0.17(40)	-0.53(92)	0.91(25)	-0.97(100)	-0.44(75)	-0.05(52)	-1.76(108)	0.71(30)	0.68(28)	-0.09(32)	-0.44(32)	-0.76(48)	1.36(63)	0.18(36)	1.44(19)
O2	0.20(88)	0.40(40)	0.20(88)	1.12(25)	0.58(112)	0.57(75)	0.47(51)	2.03(148)	0.94(28)	1.02(27)	-0.15(30)	0.82(35)	-0.59(46)	1.70(62)	0.18(32)	0.92(16)
O3	-0.50(92)	0.30(44)	-0.19(24)	1.11(28)	-1.15(112)	-0.24(87)	0.23(60)	-0.79(128)	1.21(35)	0.96(34)	0.88(40)	0.80(42)	-0.84(52)	0.40(63)	-0.01(36)	0.96(19)
O4	-0.59(144)	-0.44(60)	-0.22(144)	1.04(40)	-0.30(160)	0.08(115)	1.04(84)	-0.51(180)	0.48(40)	1.96(47)	-0.04(47)	1.71(63)	-0.45(74)	0.54(84)	0.65(52)	0.18(24)
O5	-0.94(120)	0.71(60)	-0.16(120)	1.14(32)	-1.00(128)	0.35(105)	0.73(74)	-1.04(160)	0.97(40)	0.66(40)	0.11(47)	1.94(59)	0.59(76)	1.13(84)	0.27(48)	0.52(25)
O6	0.19(144)	0.91(56)	1.03(132)	1.39(35)	-0.40(132)	0.96(111)	-0.03(66)	-0.97(159)	0.70(37)	1.14(40)	0.23(42)	1.82(51)	-0.10(62)	0.44(72)	0.19(42)	0.42(21)
O7	0.68(164)	0.06(64)	-0.23(144)	1.15(40)	-0.37(168)	0.59(129)	-0.09(80)	-2.52(152)	2.36(54)	0.92(46)	0.51(55)	-0.64(49)	0.67(88)	1.57(101)	1.27(61)	1.07(28)
O8	1.20(176)	0.66(66)	2.2(16)	1.12(40)	2.28(212)	1.35(129)	0.91(84)	-0.74(180)	1.16(45)	1.92(48)	1.33(58)	1.62(65)	0.12(84)	1.02(96)	1.44(60)	0.56(27)
O9	0.14(150)	1.01(62)	0.27(140)	2.6(4)	0.25(168)	0.67(120)	1.03(84)	-2.5(13)	2.29(50)	2.84(51)	1.54(56)	2.89(69)	1.03(84)	2.15(98)	1.37(56)	0.57(25)
O10	-0.59(124)	-0.26(54)	0.02(128)	0.97(34)	0.37(148)	0.48(115)	2.5(8)	0.56(178)	2.08(45)	0.65(39)	-0.26(44)	-0.57(45)	-0.99(66)	0.19(75)	0.23(47)	0.15(22)

Note: In general, isotropic displacement parameters obtained from Powder-XRD-data are afflicted with errors, especially when more than one phase is present in the powder-pattern. The values given in this table were obtained from the Rietveld-analysis with structure-refinement. Negative values are physically implausible; these values are caused by peak-overlap with other phases and are influenced strongly by peak shape parameters in the structure refinement.

Table 6b: Refined isotropic displacement parameters of clinozoisite [100*Uiso]

sample	Au32	Au45	Au31	Au35	Au34	Pt8	Au42	Pt35	Au43
A1	1.49(88)	1.05(40)	-0.06(51)	0.18(40)	-0.21(54)	1.77(37)	0.36(38)	-0.05(22)	0.03(19)
A2	1.28(84)	1.19(40)	1.07(40)	-0.30(26)	-0.10(35)	0.53(16)	-0.12(20)	0.24(12)	0.32(11)
M1	0.46(72)	0.13(42)	-1.58(40)	-0.45(38)	0.45(56)	0.77(28)	0.17(40)	-1.05(20)	0.23(22)
M2	0.97(84)	2.24(60)	1.74(64)	1.09(48)	0.96(61)	1.57(32)	0.34(41)	1.21(30)	1.62(28)
M3	1.56(100)	0.63(54)	-1.88(43)	-0.10(44)	0.50(64)	2.34(38)	-0.15(40)	0.14(50)	0.99(52)
T1	0.58(84)	-0.13(45)	-0.95(48)	-0.13(42)	-0.29(54)	0.59(27)	-0.02(38)	-0.26(44)	0.38(23)
T2	0.30(80)	-0.36(40)	-0.94(46)	-0.48(38)	-0.69(50)	0.33(26)	-0.52(34)	-1.30(40)	-0.41(29)
T3	0.61(88)	0.76(54)	2.39(73)	0.24(44)	0.70(61)	0.55(29)	0.01(39)	-1.06(44)	0.63(25)
O1	2.62(136)	1.49(74)	2.32(94)	0.46(60)	0.52(78)	1.09(42)	0.29(56)	-0.67(64)	1.42(33)
O2	-0.92(96)	-0.65(64)	-2.85(56)	-1.36(54)	-1.36(70)	-0.04(40)	-0.04(58)	-0.94(60)	-0.15(30)
O3	0.54(112)	-0.62(60)	-0.37(70)	0.51(64)	0.66(86)	1.10(42)	0.19(58)	-0.40(62)	1.38(38)
O4	0.22(160)	-0.21(90)	2.33(152)	0.07(86)	0.37(116)	0.54(55)	-0.20(80)	-1.54(82)	-1.76(37)
O5	0.94(160)	2.6(12)	-0.18(106)	1.4(11)	-1.20(101)	2.30(72)	0.57(90)	2.5(12)	0.36(48)
O6	13(4)	10(2)	25(5)	7(2)	5(2)	2.39(85)	-1.9(7)	1.6(8)	0.68(52)
O7	2(2)	2.6(13)	4(2)	2(1)	2.2(14)	1.25(64)	1.26(92)	3.3(14)	2.17(55)
O8	0.97(42)	0.36(94)	-0.26(110)	2(1)	4.4(16)	2.05(68)	2.4(10)	1.2(12)	3.9(7)
O9	6(2)	5.9(16)	8.5(22)	4.5(14)	4.6(18)	3.46(82)	2.9(11)	1.1(12)	2.9(6)
O10	5(3)	10(2)	7.3(22)	3.4(12)	4.8(18)	2.31(74)	0.4(8)	0.64(121)	0.68(5)

Note: In general, isotropic displacement parameters obtained from Powder-XRD-data are afflicted with errors, especially when more than one phase is present in the powder-pattern. The values given in this table were obtained from the Rietveld-analysis with structure-refinement. Negative values are physically implausible; these negative values are caused by peak-overlap with other phases and are influenced strongly by peak shape parameters in the structure refinement.

Table A1: Interatomic distances in zoisite [Å]

Run no.		Au32	Au40	Au45	Pt4	Au31	Au34	Au30	Pt3
X _{Sr} ^{zo}		0.06	0.13	0.16	0.22	0.25	0.24	0.32	0.42
Distances A1									
-O1	x 2	2.526(8)	2.541(7)	2.548(8)	2.528(5)	2.542(8)	2.551(4)	2.541(1)	2.539(5)
-O3	x 2	2.443(9)	2.432(8)	2.455(9)	2.440(5)	2.451(9)	2.417(3)	2.461(1)	2.441(6)
-O5		2.570(12)	2.547(12)	2.552(12)	2.577(7)	2.518(13)	2.552(4)	2.588(1)	2.595(7)
-O6		2.595(12)	2.581(10)	2.607(12)	2.562(6)	2.611(12)	2.610(4)	2.585(1)	2.564(6)
-O7		2.314(14)	2.258(11)	2.305(13)	2.270(7)	2.299(14)	2.296(3)	2.299(1)	2.273(8)
	Mean (7)	2.49	2.48	2.50	2.48	2.49	2.49	2.50	2.48
-O9	x2	2.917(4)	2.912(3)	2.912(4)	2.903(2)	2.912(4)	2.908(4)	2.912(1)	2.898(2)
Distances A2									
-O2	x2	2.548(9)	2.543(7)	2.574(8)	2.584(5)	2.605(10)	2.620(3)	2.631(1)	2.620(5)
-O2	x2	2.810(7)	2.787(6)	2.779(7)	2.763(4)	2.782(9)	2.766(4)	2.763(2)	2.745(4)
-O3	x2	2.492(8)	2.472(7)	2.494(8)	2.519(5)	2.490(9)	2.469(2)	2.484(1)	2.551(5)
-O7		2.357(13)	2.357(10)	2.329(12)	2.384(7)	2.372(13)	2.383(4)	2.367(2)	2.470(8)
	Mean (7)	2.58	2.57	2.57	2.59	2.59	2.59	2.59	2.61
-O8	x2	3.047(7)	3.032(5)	3.049(7)	3.022(3)	3.041(7)	3.041(4)	3.046(2)	3.028(3)
-O10		3.054(12)	3.042(10)	3.057(12)	3.066(6)	3.128(14)	3.086(5)	3.079(2)	3.110(7)
Distances M1,2									
Al1-O1		1.965(7)	1.991(6)	1.972(7)	2.000(4)	1.973(8)	1.969(3)	1.996(1)	1.990(5)
Al1-O3		1.885(7)	1.874(7)	1.885(8)	1.874(4)	1.884(8)	1.908(3)	1.882(1)	1.867(5)
Al1-O4		1.822(7)	1.820(7)	1.836(8)	1.817(5)	1.867(9)	1.816(2)	1.796(1)	1.824(5)
Al1-O5		1.947(8)	1.924(7)	1.957(9)	1.927(5)	1.976(9)	1.954(2)	1.946(1)	1.924(5)
Al1-O6		1.898(8)	1.931(8)	1.879(9)	1.928(5)	1.854(9)	1.875(2)	1.891(1)	1.953(6)
Al1-O10		1.812(7)	1.814(6)	1.797(8)	1.825(4)	1.786(9)	1.814(2)	1.806(1)	1.835(5)
	Mean (6)	1.89	1.89	1.89	1.90	1.89	1.89	1.89	1.90
Distances M3									
Al2-O1	x2	2.070(9)	2.067(8)	2.070(9)	2.112(5)	2.093(10)	2.089(2)	2.091(1)	2.097(6)
Al2-O2	x2	1.962(9)	1.963(7)	1.970(8)	1.953(5)	1.989(10)	1.987(2)	1.989(1)	1.974(6)
Al2-O4		1.825(13)	1.815(12)	1.824(13)	1.825(7)	1.893(16)	1.884(3)	1.860(1)	1.837(7)
Al2-O8		1.638(15)	1.743(12)	1.659(16)	1.749(7)	1.669(18)	1.718(3)	1.737(1)	1.771(8)
	Mean (6)	1.92	1.94	1.93	1.95	1.95	1.96	1.96	1.96
Distances T1									
Si1-O1	x2	1.654(8)	1.637(7)	1.645(8)	1.634(4)	1.641(9)	1.653(2)	1.639(1)	1.643(4)
Si1-O7		1.561(12)	1.594(10)	1.577(12)	1.555(6)	1.575(13)	1.544(2)	1.551(1)	1.526(7)
Si1-O9		1.644(13)	1.584(11)	1.552(13)	1.613(8)	1.537(15)	1.610(3)	1.566(1)	1.651(9)
	Mean (4)	1.63	1.61	1.60	1.61	1.60	1.62	1.60	1.62
Distances T2									
Si2-O3	x2	1.602(9)	1.613(7)	1.599(9)	1.592(4)	1.635(9)	1.608(2)	1.600(1)	1.594(5)
Si2-O8		1.679(14)	1.618(12)	1.638(15)	1.611(7)	1.641(17)	1.626(2)	1.604(1)	1.611(8)
Si2-O9		1.584(12)	1.660(11)	1.698(13)	1.638(8)	1.675(15)	1.654(3)	1.691(1)	1.615(8)
	Mean (4)	1.62	1.63	1.63	1.61	1.65	1.62	1.62	1.60
Distances T3									
Si3-O2	x2	1.577(8)	1.604(7)	1.591(8)	1.604(4)	1.544(10)	1.562(2)	1.555(1)	1.604(4)
Si3-O5		1.589(12)	1.632(11)	1.597(13)	1.619(7)	1.624(14)	1.638(2)	1.618(1)	1.613(8)
Si3-O6		1.735(13)	1.682(11)	1.725(14)	1.679(7)	1.773(14)	1.721(2)	1.744(1)	1.668(7)
	Mean (4)	1.62	1.63	1.63	1.63	1.62	1.62	1.62	1.62

(Continued)

(Table A1, continued)

Run no.		Au42	Pt36	Pt2	Au23	Au22	Au33	Au44	Au21
X _{Sr} ^{zo}		0.37	0.52	0.63	0.66	0.77	0.86	0.87	1
Distances A1									
-O1	x 2	2.541(10)	2.536(4)	2.530(6)	2.567(11)	2.565(8)	2.551(6)	2.558(5)	2.562(6)
-O3	x 2	2.453(12)	2.475(5)	2.478(6)	2.487(13)	2.518(8)	2.528(6)	2.529(6)	2.562(6)
-O5		2.578(15)	2.545(6)	2.594(8)	2.605(19)	2.622(13)	2.579(9)	2.621(8)	2.617(8)
-O6		2.618(15)	2.562(6)	2.577(8)	2.611(17)	2.563(11)	2.637(8)	2.624(8)	2.651(8)
-O7		2.233(15)	2.253(7)	2.312(8)	2.271(18)	2.300(15)	2.334(10)	2.314(10)	2.416(9)
	Mean (7)	2.49	2.48	2.50	2.51	2.52	2.53	2.53	2.56
-O9	x2	2.899(4)	2.905(2)	2.895(2)	2.898(5)	2.895(3)	2.902(2)	2.902(2)	2.900(2)
Distances A2									
-O2	x2	2.657(13)	2.649(4)	2.650(6)	2.698(13)	2.670(8)	2.682(6)	2.668(6)	2.690(6)
-O2	x2	2.753(12)	2.765(4)	2.771(5)	2.782(12)	2.794(8)	2.784(6)	2.796(5)	2.790(6)
-O3	x2	2.482(12)	2.533(5)	2.539(6)	2.561(13)	2.561(8)	2.550(6)	2.535(6)	2.539(6)
-O7		2.451(13)	2.458(6)	2.446(8)	2.440(16)	2.477(13)	2.494(9)	2.477(8)	2.474(9)
	Mean (7)	2.61	2.62	2.62	2.65	2.65	2.65	2.64	2.65
-O8	x2	3.044(7)	3.0539(29)	3.065(4)	3.073(8)	3.084(6)	3.085(4)	3.099(4)	3.105(4)
-O10		3.113(16)	3.060(6)	3.067(7)	3.062(16)	3.012(11)	3.012(8)	3.038(8)	3.005(7)
Distances M1,2									
Al1-O1		1.987(11)	1.996(5)	1.987(6)	1.978(13)	1.955(9)	1.969(7)	1.974(6)	1.965(7)
Al1-O3		1.934(12)	1.869(5)	1.872(7)	1.877(14)	1.869(10)	1.859(7)	1.863(7)	1.869(7)
Al1-O4		1.833(10)	1.811(4)	1.832(5)	1.833(12)	1.803(8)	1.826(6)	1.849(6)	1.806(6)
Al1-O5		1.956(11)	1.922(4)	1.950(6)	1.929(13)	1.954(9)	1.930(6)	1.921(6)	1.937(6)
Al1-O6		1.831(11)	1.934(5)	1.948(6)	1.901(14)	1.926(10)	1.963(7)	1.952(7)	1.964(7)
Al1-O10		1.817(10)	1.839(4)	1.854(5)	1.803(11)	1.836(8)	1.874(6)	1.836(6)	1.856(6)
	Mean (6)	1.89	1.90	1.91	1.89	1.89	1.90	1.90	
Distances M3									
Al2-O1	x2	2.063(12)	2.111(5)	2.128(7)	2.105(14)	2.097(10)	2.096(7)	2.115(6)	2.124(7)
Al2-O2	x2	1.994(13)	1.979(5)	1.962(6)	1.958(13)	2.010(10)	1.978(7)	1.966(6)	1.954(6)
Al2-O4		1.914(17)	1.846(8)	1.831(9)	1.816(21)	1.847(15)	1.848(10)	1.876(10)	1.840(9)
Al2-O8		1.715(18)	1.701(8)	1.756(9)	1.684(23)	1.706(16)	1.747(11)	1.706(11)	1.717(10)
	Mean (6)	1.96	1.95	1.96	1.94	1.96	1.96	1.96	
Distances T1									
Si1-O1	x2	1.657(10)	1.642(4)	1.649(5)	1.670(11)	1.652(8)	1.661(6)	1.670(5)	1.652(6)
Si1-O7		1.569(14)	1.575(7)	1.538(8)	1.599(17)	1.567(14)	1.538(10)	1.553(9)	1.507(9)
Si1-O9		1.678(15)	1.592(7)	1.607(9)	1.506(20)	1.567(13)	1.638(9)	1.600(9)	1.595(9)
	Mean (4)	1.64	1.61	1.61	1.61	1.61	1.62	1.62	
Distances T2									
Si2-O3	x2	1.562(12)	1.594(5)	1.598(6)	1.572(13)	1.590(9)	1.600(7)	1.597(6)	1.574(6)
Si2-O8		1.625(18)	1.661(8)	1.606(9)	1.698(22)	1.661(16)	1.649(10)	1.668(11)	1.669(10)
Si2-O9		1.592(15)	1.667(7)	1.675(9)	1.742(20)	1.710(13)	1.663(9)	1.676(9)	1.724(9)
	Mean (4)	1.59	1.63	1.62	1.65	1.64	1.63	1.63	
Distances T3									
Si3-O2	x2	1.539(13)	1.577(5)	1.583(5)	1.547(11)	1.558(8)	1.573(6)	1.592(5)	1.592(5)
Si3-O5		1.618(17)	1.638(6)	1.604(8)	1.620(20)	1.571(13)	1.652(9)	1.640(8)	1.632(9)
Si3-O6		1.820(17)	1.700(7)	1.684(8)	1.742(18)	1.728(13)	1.662(9)	1.660(9)	1.641(9)
	Mean (4)	1.63	1.62	1.61	1.61	1.60	1.62	1.62	

Table A2: Interatomic angles in zoisite [°]

Run no. X _{Sr} ^{zO}	Au32 0.06	Au40 0.13	Au45 0.16	Pt4 0.22	Au31 0.25	Au34 0.24	Au30 0.32	Pt3 0.42
Angles M1,2								
O1-AI1-O4	83.2(4)	83.2(4)	82.2(4)	82.48(24)	85.4(5)	84.3(1)	83.8(0)	82.96(27)
O1-AI1-O5	87.1(5)	87.4(4)	87.0(5)	86.95(24)	87.6(5)	86.2(1)	85.7(0)	86.57(25)
O1-AI1-O6	94.6(5)	94.3(4)	95.2(5)	92.66(24)	95.5(5)	95.1(1)	93.9(0)	92.44(25)
O1-AI1-O10	91.2(5)	91.0(4)	91.8(5)	90.73(26)	89.6(6)	90.3(2)	90.0(0)	89.94(27)
O3-AI1-O4	92.1(5)	93.1(4)	92.5(5)	93.12(27)	90.0(6)	92.0(1)	92.7(1)	92.59(29)
O3-AI1-O5	90.4(5)	89.3(5)	89.5(5)	90.35(26)	87.8(5)	88.0(1)	90.1(1)	90.31(28)
O3-AI1-O6	87.9(4)	89.1(4)	88.2(5)	90.18(24)	88.8(5)	90.5(1)	90.4(1)	90.92(25)
O3-AI1-O10	93.4(5)	92.6(4)	93.5(5)	93.60(25)	94.6(6)	93.2(1)	93.2(0)	94.42(26)
O4-AI1-O5	95.2(4)	96.0(4)	94.6(4)	96.20(27)	92.9(5)	95.4(2)	96.3(1)	96.21(27)
O4-AI1-O6	84.7(4)	85.85(33)	84.4(4)	85.62(21)	85.0(4)	84.1(1)	84.1(1)	86.52(23)
O5-AI1-O10	83.2(4)	82.26(31)	83.0(4)	82.28(20)	82.6(4)	82.7(2)	81.8(1)	82.16(25)
O6-AI1-O10	97.1(4)	96.0(4)	98.3(5)	95.84(26)	99.8(5)	98.1(1)	97.8(1)	94.97(29)
Mean(12)	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
Angles M3								
O1-AI2-O1	84.2(5)	85.2(4)	85.2(5)	82.79(26)	85.1(5)	85.6(2)	85.8(1)	83.74(31)
O1-AI2-O2	x2 89.37(32)	89.26(26)	88.34(31)	89.11(16)	88.11(35)	87.6(2)	87.6(1)	88.76(17)
O1-AI2-O4	x2 80.3(4)	81.22(33)	79.8(4)	79.24(22)	81.5(4)	79.4(3)	79.7(0)	79.72(25)
O1-AI2-O8	x2 99.6(5)	98.9(4)	99.6(5)	99.00(25)	100.5(6)	100.1(4)	99.0(0)	99.94(28)
O2-AI2-O2	95.8(5)	95.5(5)	96.7(5)	97.90(31)	97.2(6)	97.8(2)	98.0(1)	97.5(4)
O2-AI2-O4	x2 90.8(4)	91.85(34)	90.9(4)	92.04(23)	89.0(5)	91.0(1)	91.7(0)	91.29(25)
O2-AI2-O8	x2 89.3(5)	88.0(4)	89.7(5)	89.52(23)	89.2(5)	89.5(1)	89.4(0)	89.01(25)
Mean(12)	89.9	89.9	89.9	89.9	89.9	89.9	89.9	89.9
Angles T1								
O1-Si1-O1	114.0(7)	114.4(6)	113.4(7)	115.6(4)	112.4(7)	110.9(1)	111.7(1)	114.8(4)
O1-Si1-O7	x2 107.5(4)	108.49(33)	107.6(4)	110.20(22)	107.9(5)	109.8(1)	109.3(1)	111.22(26)
O1-Si1-O9	x2 108.37(34)	107.41(31)	107.9(4)	104.96(21)	107.8(4)	106.8(1)	106.8(0)	104.86(26)
O7-Si1-O9	111.1(7)	110.6(6)	112.4(7)	110.6(4)	113.2(8)	112.6(3)	112.8(1)	109.3(5)
Mean (6)	109.5	109.5	109.5	109.4	109.5	109.5	109.5	109.4
Angles T2								
O3-Si2-O3	109.0(7)	111.0(6)	109.1(7)	109.5(4)	108.4(7)	115.1(3)	111.6(1)	110.3(4)
O3-Si2-O8	x2 112.8(4)	111.1(4)	112.8(4)	110.67(24)	111.8(5)	110.9(4)	111.4(1)	111.00(27)
O3-Si2-O9	x2 105.3(4)	105.9(4)	105.4(4)	105.81(24)	105.4(5)	104.4(4)	105.8(0)	105.07(29)
O8-Si2-O9	111.0(8)	111.6(7)	111.0(9)	114.1(4)	113.6(10)	110.7(3)	110.5(1)	114.1(5)
Mean (6)	109.4	109.4	109.4	109.4	109.4	109.4	109.4	109.4
Angles T3								
O2-Si3-O2	113.6(6)	111.0(5)	110.2(6)	109.01(31)	112.8(7)	110.4(1)	110.7(1)	108.2(4)
O2-Si3-O5	x2 111.0(4)	111.5(4)	111.3(5)	110.96(26)	111.7(5)	110.6(1)	111.15(1)	111.13(31)
O2-Si3-O6	x2 111.9(4)	113.1(4)	113.2(4)	114.19(25)	112.1(5)	113.7(1)	113.23(1)	114.07(28)
O5-Si3-O6	96.3(6)	95.8(5)	97.2(6)	97.07(35)	95.2(6)	97.2(1)	96.64(1)	97.9(4)
Mean (6)	109.3	109.3	109.4	109.4	109.3	109.4	109.4	109.4

(continued)

Table A2, continued

Run no. X _{Sr} ^{zo}	Au42 0.37	Pt36 0.52	Pt2 0.63	Au23 0.66	Au22 0.77	Au33 0.86	Au44 0.87	Au21 1
Angles M1,2								
O1-AI1-O4	84.6(6)	82.89(28)	82.85(32)	81.6(8)	83.2(5)	83.1(4)	83.33(33)	82.97(33)
O1-AI1-O5	86.3(6)	88.11(25)	86.78(29)	86.1(7)	86.0(5)	87.9(4)	86.27(32)	86.07(32)
O1-AI1-O6	94.5(6)	91.88(24)	92.09(29)	93.3(6)	91.6(4)	92.86(33)	92.33(30)	93.10(31)
O1-AI1-O10	90.1(7)	91.11(25)	90.59(30)	91.8(6)	93.0(5)	92.60(34)	91.60(32)	91.50(32)
O3-AI1-O4	90.2(7)	93.46(30)	93.48(35)	93.1(8)	91.9(5)	92.7(4)	92.15(34)	94.11(34)
O3-AI1-O5	89.3(6)	89.56(27)	90.16(33)	90.5(8)	91.4(5)	89.9(4)	91.56(35)	92.46(35)
O3-AI1-O6	89.7(6)	90.61(26)	91.12(32)	90.2(7)	91.1(5)	89.50(34)	90.02(32)	88.55(32)
O3-AI1-O10	94.9(7)	92.52(25)	93.02(31)	93.4(7)	91.8(5)	91.66(34)	92.85(33)	91.40(33)
O4-AI1-O5	94.7(6)	97.03(22)	95.42(28)	96.2(7)	96.4(5)	96.66(33)	95.95(30)	97.15(32)
O4-AI1-O6	83.0(5)	85.18(22)	86.55(26)	84.7(6)	85.0(4)	86.45(30)	86.21(27)	86.17(29)
O5-AI1-O10	82.9(5)	82.34(22)	83.24(28)	81.0(6)	82.2(4)	83.07(32)	82.23(28)	81.97(30)
O6-AI1-O10	99.5(6)	95.43(22)	94.64(29)	98.0(6)	96.3(5)	93.86(33)	95.47(31)	94.60(33)
Mean(12)	90.0	90.0	90.0	90.0	90.0	90.0	90.0	
Angles M3								
O1-AI2-O1	85.7(6)	83.62(28)	82.88(35)	84.2(7)	84.3(5)	83.8(4)	83.57(35)	84.0(4)
O1-AI2-O2	x2	86.7(4)	88.16(15)	88.23(20)	85.8(4)	87.53(27)	87.46(22)	86.77(21)
O1-AI2-O4	x2	80.6(5)	78.96(23)	79.02(28)	78.5(6)	78.3(4)	79.10(32)	77.86(29)
O1-AI2-O8	x2	100.2(6)	99.92(26)	98.13(32)	99.1(7)	99.0(5)	98.34(34)	97.99(32)
O2-AI2-O2		99.6(8)	98.49(31)	99.2(4)	102.5(9)	99.0(6)	99.9(5)	99.7(4)
O2-AI2-O4	x2	90.0(6)	90.79(24)	91.11(28)	90.7(6)	91.2(4)	91.28(30)	90.51(27)
O2-AI2-O8	x2	89.3(6)	90.20(25)	91.37(30)	91.3(7)	91.2(5)	90.96(34)	91.56(30)
Mean(12)	89.9	89.8	89.8	89.8	89.8	89.8	89.8	
Angles T1								
O1-Si1-O1	112.6(9)	114.2(4)	113.7(5)	111.5(10)	114.2(7)	114.6(6)	112.3(5)	113.0(5)
O1-Si1-O7	x2	109.9(5)	110.80(24)	110.91(29)	108.9(6)	110.1(4)	110.70(32)	110.74(29)
O1-Si1-O9	x2	107.0(5)	105.42(23)	104.62(28)	107.4(6)	106.6(4)	106.57(30)	106.77(29)
O7-Si1-O9		110.4(8)	109.9(4)	111.7(5)	112.6(11)	108.9(9)	107.3(6)	109.3(5)
Mean (6)	109.5	109.4	109.4	109.5	109.4	109.4	109.4	
Angles T2								
O3-Si2-O3	115.1(11)	110.1(4)	110.8(5)	110.6(12)	106.7(8)	108.8(6)	109.4(5)	109.3(5)
O3-Si2-O8	x2	110.9(6)	110.73(23)	111.52(30)	111.6(6)	112.2(4)	111.02(32)	110.73(29)
O3-Si2-O9	x2	104.0(6)	106.24(24)	104.78(32)	104.8(7)	105.4(5)	106.25(35)	106.70(31)
O8-Si2-O9		111.6(11)	112.6(4)	113.1(5)	112.9(12)	114.3(8)	113.2(6)	112.4(5)
Mean (6)	109.4	109.4	109.4	109.4	109.4	109.4	109.4	
Angles T3								
O2-Si3-O2	109.8(10)	109.3(4)	109.8(5)	109.5(11)	108.5(7)	109.3(5)	108.8(4)	108.5(5)
O2-Si3-O5	x2	110.9(7)	111.46(26)	111.01(33)	109.8(7)	112.0(5)	111.1(4)	109.98(32)
O2-Si3-O6	x2	113.6(7)	113.63(24)	113.64(30)	113.9(7)	112.8(5)	113.25(34)	113.57(30)
O5-Si3-O6		97.6(8)	96.9(4)	97.2(4)	99.5(10)	98.6(7)	98.4(5)	100.6(4)
Mean (6)	109.4	109.4	109.4	109.4	109.5	109.4	109.4	

Table A3: Conventional valence bond calculations for positions A1 and A2 in zoisite, based on bond valence data of Brown & Altermatt (1985)

Run no.		Au32	Au40	Au45	Pt4	Au31	Au34	Au30	Pt3	Au42	Pt36	Pt2	Au23	Au22	Au33	Au44	Au21
X_{Sr}^{zo}		0.06	0.13	0.16	0.22	0.25	0.24	0.32	0.42	0.37	0.52	0.63	0.66	0.77	0.86	0.87	1
X_{Sr} A1		0.02	0.04	0.03	0.03	0.06	0.00	0.04	0.13	0.09	0.20	0.38	0.41	0.61	0.76	0.82	1
X_{Sr} A2		0.09	0.22	0.29	0.40	0.44	0.48	0.59	0.72	0.67	0.84	0.89	0.92	0.93	0.96	0.92	1
Valence bond parameters*																	
Ro_{\dagger} (A1)		1.970	1.973	1.972	1.972	1.976	1.967	1.973	1.987	1.981	1.997	2.024	2.029	2.059	2.082	2.091	2.118
Ro_{\dagger} (A2)		1.981	2.000	2.011	2.027	2.033	2.039	2.056	2.076	2.068	2.094	2.101	2.106	2.107	2.112	2.106	2.118
B		0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37	0.37
Valence bond strength for A1																	
A1-O1	2x	0.223	0.215	0.211	0.222	0.217	0.206	0.215	0.225	0.220	0.233	0.255	0.234	0.255	0.281	0.283	0.301
A1-O3	2x	0.279	0.289	0.271	0.282	0.277	0.296	0.267	0.293	0.279	0.275	0.293	0.290	0.289	0.299	0.306	0.301
A1-O5		0.198	0.212	0.208	0.195	0.231	0.206	0.190	0.193	0.199	0.228	0.214	0.211	0.218	0.261	0.239	0.260
A1-O6		0.185	0.193	0.180	0.203	0.180	0.176	0.191	0.210	0.179	0.217	0.225	0.207	0.256	0.223	0.237	0.237
A1-O7		0.395	0.463	0.406	0.446	0.418	0.411	0.414	0.461	0.506	0.501	0.460	0.520	0.521	0.506	0.547	0.447
A1-O9	2x	0.077	0.079	0.079	0.081	0.080	0.079	0.079	0.085	0.084	0.086	0.095	0.095	0.104	0.109	0.112	0.121
Total bond strength A1		1.934	2.036	1.914	2.014	1.975	1.955	1.919	2.070	2.048	2.134	2.186	2.176	2.293	2.369	2.423	2.39
Reference value		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
Valence bond strength for A2																	
A2-O2	2x	0.216	0.231	0.218	0.222	0.213	0.208	0.211	0.230	0.204	0.223	0.227	0.202	0.219	0.214	0.219	0.213
A2-O2	2x	0.106	0.119	0.125	0.137	0.132	0.140	0.148	0.164	0.157	0.163	0.164	0.161	0.156	0.163	0.155	0.163
A2-O3	2x	0.251	0.279	0.271	0.265	0.291	0.313	0.314	0.277	0.327	0.305	0.306	0.292	0.294	0.306	0.314	0.321
A2-O7		0.362	0.381	0.423	0.381	0.401	0.395	0.431	0.345	0.355	0.374	0.394	0.405	0.368	0.356	0.367	0.382
A2-O8	2x	0.056	0.062	0.060	0.068	0.066	0.067	0.069	0.076	0.072	0.075	0.074	0.073	0.071	0.072	0.068	0.069
A2-O10		0.055	0.060	0.059	0.060	0.052	0.059	0.063	0.061	0.059	0.073	0.074	0.075	0.087	0.088	0.081	0.091
Total bond strength A2		1.675	1.823	1.832	1.826	1.857	1.911	1.979	1.899	1.933	1.979	2.010	1.937	1.935	1.954	1.959	2.004
Reference value		2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2

*Bond length from table A1

†Ro = $Ro_{Ca} + ((Ro_{Sr} - Ro_{Ca}) * X_{Sr}(A1, A2))$; $Ro_{Ca} = 1.967$, $Ro_{Sr} = 2.118$

Table A4: Calculated polyhedra volume [\AA^3] for A1, A2, M1,2, M3, T1, T2, T3 with quadratic elongation and variance for zoisite

Run no.	Au32	Au40	Au45	Pt4	Au31	Au34	Au30	Au42	Pt3
VA1[7]	19.81	19.49	19.96	19.67	19.83	19.57	19.91	19.71	19.86
VA2[7]	23.46	23.06	23.30	23.66	23.54	23.36	23.54	23.84	24.32
VM1,2	8.87	8.93	8.85	8.97	8.90	8.88	8.83	8.93	9.03
quad	1.00818	1.00821	1.00959	1.00844	1.00872	1.00896	1.01026	1.00991	1.00777
variance	22.5696	21.71959	26.72909	22.50972	24.52246	24.58820	26.77836	27.1855	21.03378
VM3	9.23	9.49	9.30	9.65	9.66	9.77	9.80	9.71	9.77
quad	1.02266	1.01708	1.02254	1.02173	1.02218	1.02109	1.01998	1.02027	1.02016
variance	40.5455	34.74556	42.42622	47.12962	41.23824	47.39537	43.36998	47.17551	46.66571
VT1	2.21	2.14	2.11	2.12	2.08	2.16	2.09	2.26	2.15
quad	1.00299	1.0025	1.00306	1.0049	1.00291	1.00219	1.00252	1.00203	1.00521
variance	6.72736	7.29725	7.23252	16.17863	6.62983	5.22204	6.16956	4.73104	15.44221
VT2	2.15	2.20	2.23	2.13	2.16	2.18	2.15	1.98	2.10
quad	1.00477	1.00195	1.00354	1.00281	1.00454	1.00445	1.00254	1.00536	1.00341
variance	11.90902	7.63337	11.63823	10.24526	15.700081	17.51716	7.95131	20.48916	13.05005
VT3	2.14	2.18	2.17	2.17	2.14	2.15	2.13	2.18	2.15
quad	1.01247	1.01193	1.01123	1.01101	1.0155	1.01141	1.01285	1.01613	1.00979
variance	41.1068	44.98664	36.95821	40.64444	47.73619	37.78345	39.98624	35.87196	36.48328
Run no.	Pt36	Au43	Pt2	Au23	Au22	Au33	Au44	Au21	
VA1[7]	19.80	19.96	20.04	20.30	20.52	20.69	20.65	21.41	
VA2[7]	24.40	24.44	24.49	24.92	25.06	25.08	24.90	25.12	
VM1,2	8.98	8.76	9.17	8.83	8.91	9.11	9.04	9.04	
variance	21.69545	34.23686	17.9355	30.35174	22.73402	17.91309	20.15701	23.2133	
VM3	9.68	9.57	9.80	9.39	9.77	9.74	9.74	9.63	
quad	1.0244	1.01963	1.02216	1.02787	1.02435	1.02121	1.02259	1.0256	
variance	51.05659	51.23664	47.44314	59.85964	51.41402	48.36439	48.19829	55.75985	
VT1	2.14	2.17	2.13	2.13	2.12	2.19	2.18	2.09	
quad	1.00394	1.00303	1.00495	1.00408	1.00383	1.00442	1.00309	1.00394	
variance	11.79461	8.57276	14.89172	4.54559	7.94464	10.14814	5.21533	6.46747	
VT2	2.21	2.15	2.16	2.12	2.23	2.20	2.23	2.23	
quad	1.00269	1.00505	1.00364	1.00728	1.00594	1.00269	1.00245	1.00458	
variance	6.8798	14.12947	13.40125	16.70919	15.74913	7.94769	5.40128	7.11989	
VT3	2.16	2.25	2.12	2.13	2.09	2.13	2.16	2.14	
quad	1.01119	1.01912	1.0106	1.01045	1.0105	1.00834	1.00597	1.00636	
variance	40.26778	62.63542	37.89872	27.61253	30.63564	31.38462	22.50358	24.47464	

Table A5: Interatomic distances in clinozoisite [Å]

Run no.		Au32	Au45	Au35	Au34	Pt8	Au42	Au43
X _{Sr} ^{CZ}		0.078	0.150	0.248	0.248	0.292	0.349	0.513
Distances A1								
A1-O1	X 2	2.502(11)	2.533(14)	2.528(12)	2.554(15)	2.541(8)	2.523(11)	2.559(11)
-O3	X 2	2.339(10)	2.313(13)	2.355(12)	2.375(14)	2.376(8)	2.406(10)	2.415(11)
-O5		2.532(15)	2.546(20)	2.401(15)	2.432(16)	2.456(11)	2.457(13)	2.511(14)
-O6		2.640(28)	2.649(29)	2.731(21)	2.755(25)	2.718(12)	2.717(12)	2.700(16)
-O7		2.164(15)	2.137(21)	2.120(18)	2.054(21)	2.241(11)	2.199(16)	2.211(19)
Mean (7)		2.43	2.43	2.43	2.44	2.46	2.46	2.48
-O9	X 2	2.933(6)	2.933(7)	2.922(6)	2.904(7)	2.915(4)	2.908(5)	2.911(5)
Distances A2								
A2-O2	X 2	2.807(9)	2.772(11)	2.770(9)	2.781(12)	2.783(7)	2.778(10)	2.810(11)
-O2	X 2	2.493(9)	2.600(11)	2.589(9)	2.608(11)	2.602(7)	2.615(9)	2.647(9)
-O3	X 2	2.493(10)	2.493(12)	2.517(9)	2.521(12)	2.584(7)	2.605(9)	2.619(11)
-O7		2.449(17)	2.394(22)	2.414(19)	2.421(23)	2.381(13)	2.396(16)	2.417(17)
-O10		2.638(16)	2.579(26)	2.676(18)	2.637(24)	2.698(12)	2.643(15)	2.664(18)
Mean (8)		2.58	2.59	2.61	2.61	2.63	2.63	2.65
-O8	X 2	3.024(6)	2.957(6)	3.015(7)	3.041(10)	3.024(5)	3.037(7)	3.068(7)
Distances M1								
Al1-O1	X 2	1.896(10)	1.955(12)	1.924(10)	1.887(13)	1.949(6)	1.878(9)	1.917(11)
Al1-O4	X 2	1.776(9)	1.808(11)	1.839(10)	1.847(13)	1.834(7)	1.827(9)	1.827(8)
Al1-O5	X 2	1.922(11)	1.900(14)	1.959(12)	1.958(12)	1.981(9)	1.940(10)	1.969(10)
Mean (6)		1.86	1.89	1.91	1.90	1.92	1.88	1.90
Distances M2								
Al2-O3	X 2	1.895(9)	1.898(11)	1.906(10)	1.932(13)	1.855(8)	1.926(10)	1.912(13)
Al2-O6	X 2	1.980(22)	1.917(26)	1.953(17)	1.988(20)	1.973(8)	1.977(9)	1.986(11)
Al2-O10	X 2	1.927(15)	1.867(20)	1.804(13)	1.786(17)	1.824(8)	1.826(10)	1.841(11)
Mean (6)		1.93	1.89	1.89	1.90	1.88	1.91	1.91
Distances M3								
Al3-O1	X 2	2.175(12)	2.156(15)	2.127(13)	2.067(16)	2.152(9)	2.129(12)	2.111(13)
Al3-O2	X 2	1.969(11)	1.924(13)	1.966(10)	1.993(13)	1.942(8)	1.959(10)	1.949(10)
Al3-O4		1.931(17)	1.921(19)	1.893(14)	1.963(18)	1.827(11)	1.908(13)	1.954(15)
Al3-O8		1.806(19)	1.934(23)	1.774(20)	1.696(26)	1.755(13)	1.762(20)	1.685(22)
Mean (6)		2.00	2.00	1.98	1.96	1.96	1.97	1.96
Distances T1								
Si1-O1	X 2	1.664(12)	1.683(15)	1.690(13)	1.750(16)	1.638(8)	1.727(11)	1.686(12)
Si1-O7		1.549(17)	1.585(22)	1.610(19)	1.642(23)	1.539(13)	1.585(17)	1.584(18)
Si1-O9		1.652(21)	1.655(27)	1.653(21)	1.651(25)	1.681(13)	1.642(17)	1.544(18)
Mean (4)		1.63	1.65	1.66	1.70	1.62	1.67	1.63
Distances T2								
Si2-O3	X 2	1.613(9)	1.614(11)	1.600(10)	1.566(12)	1.616(7)	1.521(9)	1.545(11)
Si2-O8		1.596(18)	1.576(21)	1.653(18)	1.657(25)	1.657(12)	1.630(18)	1.653(20)
Si2-O9		1.594(21)	1.562(24)	1.592(19)	1.548(22)	1.563(13)	1.568(16)	1.660(17)
Mean (4)		1.60	1.59	1.61	1.58	1.61	1.56	1.60
Distances T3								
Si3-O2	X 2	1.621(8)	1.629(10)	1.611(9)	1.608(10)	1.617(6)	1.605(9)	1.596(9)
Si3-O5		1.681(16)	1.698(20)	1.693(16)	1.658(18)	1.628(13)	1.649(14)	1.598(16)
Si3-O6		1.599(28)	1.66(4)	1.621(24)	1.587(27)	1.599(12)	1.635(14)	1.651(16)
Mean (4)		1.63	1.65	1.63	1.62	1.62	1.62	1.61

Table A6. Selected interatomic angles in clinozoisite [°]

Run no.		Au32	Au45	Au35	Au34	Pt8	Au42	Au43
X _{Sr} ^{CZ}		0.078	0.150	0.248	0.248	0.292	0.349	0.513
Angles M1								
O1-Al1-O4	X 2	86.1(6)	86.1(7)	85.3(5)	85.7(7)	83.3(4)	85.0(5)	85.5(6)
O1-Al1-O4	X 2	93.9(6)	93.9(7)	94.7(5)	94.3(7)	96.7(4)	95.0(5)	94.5(6)
O1-Al1-O5	X 2	89.8(5)	89.7(7)	93.2(5)	92.7(6)	90.0(4)	91.7(5)	89.7(5)
O1-Al1-O5	X 2	90.2(5)	90.3(7)	86.8(5)	87.3(6)	90.0(4)	88.3(5)	90.3(5)
O4-Al1-O5	X 2	81.7(5)	82.3(6)	84.9(5)	85.3(6)	85.2(4)	83.9(4)	84.8(4)
O4-Al1-O5	X 2	98.3(5)	97.7(6)	95.1(5)	94.7(6)	94.8(4)	96.1(4)	95.2(4)
Mean (12)		90	90	90	90	90	90	90
Angles M2								
O3-Al2-O6	X 2	86.8(8)	86.5(9)	89.9(7)	91.4(8)	89.7(4)	90.1(4)	89.2(5)
O3-Al2-O6	X 2	93.2(8)	93.5(9)	90.1(7)	88.6(8)	90.3(4)	89.9(4)	90.8(5)
O3-Al2-O10	X 2	89.0(6)	85.9(9)	86.9(7)	85.2(8)	89.0(4)	88.0(5)	87.8(6)
O3-Al2-O10	X 2	91.0(6)	94.1(9)	93.1(7)	94.8(8)	91.0(4)	92.0(5)	92.2(6)
O6-Al2-O10	X 2	88.6(7)	84.4(9)	83.6(6)	83.6(8)	84.95(34)	84.7(4)	85.3(4)
O6-Al2-O10	X 2	91.4(7)	95.6(9)	96.4(6)	96.4(8)	95.05(34)	95.3(4)	94.7(4)
Mean (12)		90	90	90	90	90	90	90
Angles M3								
O1-Al3-O1		79.7(7)	79.9(9)	81.1(7)	82.3(10)	82.4(5)	80.9(6)	83.1(7)
O2-Al3-O2		97.2(6)	102.8(8)	98.8(7)	96.9(8)	98.5(5)	99.1(7)	98.0(7)
O1-Al3-O2	X 2	91.11(32)	88.5(4)	89.65(34)	89.5(4)	89.09(24)	89.19(33)	88.2(4)
O1-Al3-O4	X 2	75.0(5)	78.0(6)	78.5(5)	78.1(6)	77.9(4)	76.4(4)	77.3(5)
O1-Al3-O8	X 2	99.4(5)	100.3(7)	101.4(6)	102.9(8)	100.3(4)	101.7(5)	101.3(7)
O2-Al3-O4	X 2	96.3(5)	96.3(6)	93.8(5)	91.1(7)	93.8(4)	92.9(5)	90.1(5)
O2-Al3-O8	X 2	88.6(5)	85.1(6)	86.3(5)	88.0(8)	87.8(4)	88.8(5)	91.1(7)
Mean (12)		89.8	89.9	89.9	89.9	89.9	89.8	89.8
Angles T1								
O7-Si1-O9		101.8(10)	107.1(12)	107.2(10)	109.1(13)	110.5(7)	112.3(9)	111.4(11)
O1-Si1-O1		113.8(9)	113.0(11)	112.5(9)	109.5(11)	113.5(6)	109.2(8)	111.2(10)
O1-Si1-O7	X 2	113.3(6)	109.8(7)	111.9(6)	111.7(7)	111.5(4)	111.1(5)	109.1(6)
O1-Si1-O9	X 2	106.8(5)	108.5(6)	106.4(6)	107.4(7)	104.7(4)	106.4(5)	108.0(6)
Mean (6)		109.3	109.5	109.4	109.5	109.4	109.4	109.5
Angles T2								
O8-Si2-O9		113.1(10)	117.8(13)	114.8(11)	114.5(14)	116.1(7)	114.0(10)	112.5(10)
O3-Si2-O3		114.0(8)	115.0(9)	113.9(9)	112.8(11)	108.4(6)	111.1(9)	109.3(11)
O3-Si2-O8	X 2	109.2(5)	107.5(6)	109.5(5)	110.6(7)	110.8(4)	111.6(5)	112.3(6)
O3-Si2-O9	X 2	105.6(6)	104.7(8)	104.6(6)	104.1(8)	105.1(4)	104.1(6)	105.0(7)
Mean (6)		109.5	109.5	109.5	109.5	109.4	109.4	109.4
Angles T3								
O5-Si3-O6		96.2(11)	99.8(13)	96.6(9)	97.8(11)	97.9(6)	97.8(7)	97.0(9)
O2-Si3-O2		107.9(7)	104.0(9)	107.0(8)	107.6(10)	109.2(5)	108.1(8)	111.8(10)
O2-Si3-O5	X 2	113.0(5)	110.5(7)	114.0(5)	114.8(6)	112.0(4)	114.0(5)	112.3(6)
O2-Si3-O6	X 2	113.3(6)	116.1(7)	112.6(6)	110.9(7)	112.7(4)	111.3(5)	111.4(6)
Mean (6)		109.5	109.5	109.5	109.5	109.4	109.4	109.4
Other Angles								
Si1-O9-Si2		164.58	165.66	169.7	173.99	172.93	172.65	171.64
Si2-O8-Al3		150.41	141.22	146.97	150.215	147.62	150.8	153.023
O5-O6-O10		156.19	154.24	148.46	146.15	150.4	149.61	152.06
O7-O9-O8		124.32	127.53	121.13	116.37	121.22	120.45	119.88

Table A7: Conventional valence bond calculations for positions A1 and A2 in clinozoisite, based on bond valence data of Brown & Altermatt (1985)

Run no		Au32	Au45	Au35	Au34	Pt8	Au42	Au43
X_{Sr}^{cz}		0.078	0.15	0.248	0.248	0.292	0.349	0.513
XSr A1		0.029	0	0.034	0	0.058	0	0.148
XSr A2		0.128	0.3	0.462	0.496	0.526	0.698	0.878
Valence bond parameters*								
Ro† A1		1.971	1.967	1.972	1.967	1.976	1.967	1.989
Ro† A2		1.986	2.012	2.037	2.042	2.046	2.072	2.100
B		0.37	0.37	0.37	0.37	0.37	0.37	0.37
Valence bond strength for A1								
Ca1-O1	2x	0.238	0.217	0.223	0.205	0.217	0.223	0.214
Ca1-O3	2x	0.370	0.393	0.355	0.332	0.339	0.305	0.317
Ca1-O5		0.220	0.209	0.314	0.285	0.273	0.266	0.244
Ca1-O6		0.164	0.158	0.129	0.119	0.135	0.132	0.147
Ca1-O7		0.594	0.632	0.671	0.790	0.488	0.534	0.549
Ca1-O9	2x	0.074	0.073	0.077	0.079	0.079	0.079	0.083
Total bond strength A1		2.34	2.36	2.42	2.43	2.17	2.14	2.17
Reference value		2	2	2	2	2	2	2
Valence bond strength for A2								
Ca2-O2	2x	0.109	0.128	0.138	0.136	0.137	0.149	0.147
Ca2-O2	2x	0.254	0.204	0.225	0.217	0.223	0.231	0.228
Ca2-O3	2x	0.254	0.273	0.273	0.274	0.234	0.237	0.246
Ca2-O7		0.286	0.356	0.361	0.359	0.405	0.417	0.424
Ca2-O8	2x	0.061	0.078	0.071	0.067	0.071	0.074	0.073
Ca2-O10		0.172	0.216	0.178	0.200	0.172	0.214	0.218
Total bond strength A2		1.814	1.939	1.952	1.946	1.906	2.011	2.028
Reference value		2	2	2	2	2	2	2

*Bond length from table 9

†Ro = $Ro_{Ca} + ((Ro_{Sr} - Ro_{Ca}) * X_{Sr}(A1, A2))$; $Ro_{Ca} = 1.967$, $Ro_{Sr} = 2.118$

Table A8: Calculated polyhedra volume[Å³] for A1, A2, M1, M2, M3, T1, T2, T3 with quadratic elongation and variance for clinozoisite

Run no.	Au32	Au45	Au35	Au34	Pt8	Au42	Au43
Volume A1[7]	18.15	18.14	18.24	18.39	19.13	18.91	19.41
Volume A2[8]	28.13	28.25	28.62	28.82	29.36	29.64	30.26
Volume M1	8.52	8.85	9.16	9.04	9.34	8.79	9.13
quad	1.01104	1.00979	1.00717	1.00583	1.0092	1.00776	1.00678
variance	30.6728	27.15581	21.37043	17.27255	24.83691	23.89955	17.27171
Volume M2	9.62	8.98	8.89	9.05	8.86	9.23	9.28
quad	1.00196	1.0062	1.0074	1.10096	1.00501	1.00542	1.0047
variance	4.64458	22.18364	18.55096	23.82497	9.62043	11.57355	9.98549
Volume M3	10.05	9.94	9.61	9.45	9.50	9.57	9.48
quad	1.02955	1.02718	1.02506	1.02426	1.02637	1.02769	1.02537
variance	77.89204	75.1301	63.49569	64.06396	57.51065	71.49942	59.8722
Volume T1	2.21	2.31	2.34	2.51	2.19	2.21	2.20
quad	1.00812	1.00234	1.00314	1.00258	1.00436	1.00812	1.00308
variance	24.31766	3.94579	8.92979	3.82534	14.13191	24.31766	2.2352
Volume T2	2.11	2.04	2.13	2.02	2.14	1.93	2.09
quad	1.00344	1.00833	1.00571	1.00717	1.00557	1.00679	1.00558
variance	12.77299	30.69957	18.8788	19.30594	17.67768	17.98549	12.86811
Volume T3	2.18	2.29	2.20	2.13	2.13	2.16	2.11
quad	1.0124	1.01063	1.0124	1.01113	1.00885	1.00952	1.00967
variance	46.39472	42.7078	46.64687	40.08846	33.43891	37.16529	36.88566